

This file contains the initial conditions for each forward and reverse trajectory including:

- The random seed numbers were generated using the excel RANDBETWEEN() command.
- Center of mass coordinates are in bohrs.
- The starting potential and kinetic energy.
- Center of mass initial velocity in bohrs/second.

RHODIUM:

Seed: 10048645518

CM Start Point Coordinates: bohr

I= 0 X= -2.436674622593D+00 Y= 2.285391887253D+00 Z= -5.334945907688D-01
I= 1 X= -2.683869404368D+00 Y= 1.561336712596D-01 Z= -2.044736459192D+00
I= 2 X= -1.895818941440D+00 Y= 1.634953735019D+00 Z= 2.032348161483D+00
I= 3 X= -2.530585256813D+00 Y= -2.015521844380D+00 Z= -2.971037700704D-01
I= 4 X= -2.163304883172D+00 Y= -1.046444939975D+00 Z= 2.310232854210D+00
I= 5 X= 4.016971555738D+00 Y= 2.757758853794D+00 Z= -1.279427013440D+00
I= 6 X= 2.216949296247D+00 Y= 8.321595498469D-01 Z= -3.329367282920D+00
I= 7 X= 5.465230443992D+00 Y= 2.275657277113D+00 Z= -2.461547936718D+00
I= 8 X= 3.494290265670D+00 Y= 4.487882245010D+00 Z= -2.318462407540D+00
I= 9 X= -1.882809277328D+00 Y= -2.487134968976D+00 Z= 4.633962207189D+00
I= 10 X= -3.621780515278D+00 Y= -3.148412819824D+00 Z= 5.689164304947D+00
I= 11 X= -9.531460960365D-01 Y= -4.350084643369D+00 Z= 4.451657609088D+00
I= 12 X= -2.462747711635D-01 Y= -1.191022532199D+00 Z= 5.909789613093D+00
I= 13 X= -1.564613205431D+00 Y= 3.380559293203D+00 Z= 4.222396990226D+00
I= 14 X= -3.732531310841D+00 Y= 3.850531977370D+00 Z= 4.626646682797D+00
I= 15 X= -7.535918692418D-01 Y= 2.414759565688D+00 Z= 5.855126499095D+00
I= 16 X= -8.112959092912D-01 Y= 5.164657691649D+00 Z= 3.729051742297D+00
I= 17 X= -1.969628971561D+00 Y= 4.803695101148D+00 Z= -1.711032983992D+00
I= 18 X= -3.377271300370D+00 Y= 6.156194084180D+00 Z= -1.189348293935D+00
I= 19 X= 1.471080577885D-02 Y= 5.884840751114D+00 Z= -1.375476372815D+00
I= 20 X= -2.040236687454D+00 Y= 4.747565906301D+00 Z= -3.821664594202D+00

I= 21 X= -3.427266061594D+00 Y= -3.934388347635D-01 Z= -4.749014028758D+00
I= 22 X= -5.525567165892D+00 Y= -9.268467667052D-01 Z= -5.110973048462D+00
I= 23 X= -2.896321785480D+00 Y= 1.498163480991D+00 Z= -5.519694737253D+00
I= 24 X= -2.452011224569D+00 Y= -1.697133547675D+00 Z= -5.619691701171D+00
I= 25 X= -3.517830916182D+00 Y= -4.748188080324D+00 Z= -6.768293308313D-01
I= 26 X= -3.922905902667D+00 Y= -5.521422113738D+00 Z= -2.702464246007D+00
I= 27 X= -2.577278834261D+00 Y= -6.167155272304D+00 Z= 7.135258583117D-01
I= 28 X= -5.599329956611D+00 Y= -4.719013195434D+00 Z= 5.263895030044D-01
I= 29 X= 3.259139131388D+00 Y= -3.621845338683D+00 Z= -1.538455821308D+00
I= 30 X= 3.398302518677D+00 Y= -3.088084120748D+00 Z= 1.071514061227D+00
I= 31 X= 1.868707315322D+00 Y= -5.386613445739D+00 Z= -1.986018016468D+00
I= 32 X= 4.444624078831D+00 Y= -2.976292618106D+00 Z= -2.835524251920D+00
I= 33 X= 5.392088363283D+00 Y= -2.804862421013D+00 Z= 2.081870614878D+00
I= 34 X= 2.035123882323D+00 Y= -4.230613901574D+00 Z= 2.385256228358D+00
I= 35 X= 1.169081269635D+00 Y= -3.589629693998D-02 Z= -3.607666430026D-01
I= 36 X= 3.839117457381D+00 Y= 2.690967472398D+00 Z= 1.448350431866D+00
I= 37 X= 5.382046061251D+00 Y= 1.850023724354D+00 Z= 2.318490620547D+00
I= 38 X= 2.641610633037D+00 Y= 3.945406654785D+00 Z= 2.424253527353D+00

Forward Direction:

Total Energy: -656.4356723 Hartrees

Potential Energy: -656.6078026 Hartress

Kinetic Energy: 0.1721303 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.588471098139D+12 Y= 2.989463176008D+13 Z= -2.140785323606D+13
I= 1 X= 1.022523288950D+13 Y= -1.392171967041D+13 Z= 1.220242701976D+13
I= 2 X= -1.583469617772D+11 Y= 2.067413319200D+13 Z= -7.759762425147D+12
I= 3 X= 3.054266975055D+12 Y= 1.836988140981D+13 Z= 2.487182593240D+13
I= 4 X= 7.556548936095D+12 Y= -6.047720882632D+12 Z= -7.418715581524D+12
I= 5 X= 7.255877708951D+12 Y= 8.276872852609D+12 Z= 2.149019703559D+13
I= 6 X= 2.743336007446D+13 Y= -3.257243399490D+13 Z= -1.753425378062D+13

I= 7 X= 2.715342733453D+13 Y= -1.015445903115D+13 Z= -8.361287521211D+13
I= 8 X= -2.554510215153D+13 Y= -7.412629135116D+13 Z= 1.728938328031D+13
I= 9 X= 7.483510530501D+12 Y= 7.815994873823D+12 Z= -1.456460922299D+13
I= 10 X= -1.795041470218D+14 Y= -2.759905765037D+13 Z= 3.929760287488D+13
I= 11 X= 6.093095181123D+13 Y= -2.727605739551D+13 Z= 6.071986232133D+13
I= 12 X= 1.506481334139D+13 Y= -5.692087985571D+13 Z= -6.612804774856D+13
I= 13 X= -6.274148181867D+12 Y= -8.651026220056D+12 Z= -2.101725659596D+13
I= 14 X= 2.269201395740D+13 Y= -6.721574957640D+13 Z= 4.530545830767D+13
I= 15 X= -8.443492771461D+12 Y= 4.823523208029D+13 Z= 2.961784674723D+13
I= 16 X= -1.380030813684D+12 Y= -1.169103272455D+14 Z= 9.728953935926D+13
I= 17 X= 7.293929326037D+12 Y= -1.727682072845D+13 Z= 2.963929434593D+13
I= 18 X= -1.073777308333D+14 Y= 5.942484689641D+13 Z= 2.907540627866D+13
I= 19 X= -8.144242331005D+13 Y= 5.861866195054D+13 Z= -3.861730211375D+13
I= 20 X= 4.608420762245D+13 Y= -2.297447953703D+13 Z= -9.816071987435D+12
I= 21 X= -3.826182050895D+12 Y= -4.861397241354D+12 Z= -1.033282082174D+13
I= 22 X= -7.722168997828D+13 Y= 9.799747000547D+12 Z= 2.208428358492D+13
I= 23 X= 9.147577368722D+13 Y= 9.309086020601D+13 Z= 6.824067700946D+12
I= 24 X= 9.670073663535D+12 Y= 2.521046374096D+13 Z= 4.926974409700D+13
I= 25 X= -1.600507058163D+13 Y= -1.101613870614D+13 Z= 1.446226015108D+13
I= 26 X= 6.444824820544D+13 Y= -3.864602121822D+12 Z= -9.902487501972D+13
I= 27 X= -1.065332921524D+13 Y= 3.180329811078D+13 Z= -1.249024295296D+13
I= 28 X= 6.935316209617D+13 Y= -4.630530129758D+13 Z= -4.081646131136D+13
I= 29 X= 1.428055771202D+13 Y= 1.086926757491D+13 Z= 1.066055753473D+13
I= 30 X= 6.856690308605D+12 Y= -7.196372389496D+12 Z= -2.411226272914D+13
I= 31 X= -5.152244571597D+13 Y= 3.886120975736D+12 Z= -1.262974114443D+13
I= 32 X= 9.684521654457D+12 Y= -5.390508939269D+13 Z= -3.835564718072D+13
I= 33 X= 2.006365740780D+13 Y= -3.878214353972D+13 Z= -6.538230673188D+13
I= 34 X= -8.963385639081D+13 Y= -2.267962037613D+13 Z= 7.160688866806D+13
I= 35 X= -2.799877049935D+12 Y= -2.954691203518D+12 Z= 6.609290310048D+11
I= 36 X= 8.596553968854D+12 Y= 1.359873705235D+13 Z= -9.030971298663D+12

I= 37 X= -6.895550841556D+13 Y= 7.624158322617D+13 Z= -1.074438818962D+13

I= 38 X= 1.448105374034D+13 Y= 1.410304605212D+13 Z= -1.311623297887D+13

Backward Direction:

Total Energy: -656.4356664 Hartrees

Potential Energy: -656.6078026 Hartress

Kinetic Energy: 0.1721362 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.899943912129D+12 Y= 2.948789343312D+13 Z= -2.124868573981D+13

I= 1 X= 9.744824232556D+12 Y= -1.496764544184D+13 Z= 1.157455485548D+13

I= 2 X= -6.054780995098D+11 Y= 2.108514565739D+13 Z= -8.421509892888D+12

I= 3 X= 2.138118379859D+12 Y= 1.839130356672D+13 Z= 2.354442079376D+13

I= 4 X= 9.123519520117D+12 Y= -6.187523138068D+12 Z= -8.459992733160D+12

I= 5 X= 4.669744803036D+12 Y= 4.599109157144D+12 Z= 1.414748628631D+13

I= 6 X= 8.536230432589D+13 Y= 3.356041186496D+13 Z= 8.529988012204D+12

I= 7 X= 3.773415081905D+13 Y= -1.367645633601D+11 Z= -8.296554887593D+13

I= 8 X= -1.218208504397D+13 Y= -6.332470924000D+13 Z= 1.853258185291D+13

I= 9 X= 7.981539641701D+12 Y= 8.049878704489D+12 Z= -1.512754602154D+13

I= 10 X= -1.794130614854D+14 Y= -2.644157564782D+13 Z= 3.795584133659D+13

I= 11 X= 6.078711114643D+13 Y= -2.728871048846D+13 Z= 6.069189185446D+13

I= 12 X= 1.535669339975D+13 Y= -5.684270326167D+13 Z= -6.640521755126D+13

I= 13 X= -6.175421176927D+12 Y= -8.699063003254D+12 Z= -2.122504667920D+13

I= 14 X= 2.285985688438D+13 Y= -6.751168688101D+13 Z= 4.534938528447D+13

I= 15 X= -8.134828629414D+12 Y= 4.795213373299D+13 Z= 2.910672159502D+13

I= 16 X= -1.401532259550D+12 Y= -1.168193391744D+14 Z= 9.736150075102D+13

I= 17 X= 7.445118603139D+12 Y= -1.761047296171D+13 Z= 2.960625307849D+13

I= 18 X= -1.073458533365D+14 Y= 5.889291672104D+13 Z= 2.863904249030D+13

I= 19 X= -8.176203440748D+13 Y= 5.851219159785D+13 Z= -3.828773321752D+13

I= 20 X= 4.630615511837D+13 Y= -2.327260928563D+13 Z= -9.854143658645D+12

I= 21 X= -4.016426259609D+12 Y= -4.980912901018D+12 Z= -1.079723591307D+13

I= 22 X= -7.725568816348D+13 Y= 1.033534915956D+13 Z= 2.022307583580D+13

I= 23 X= 9.216729122165D+13 Y= 9.278985003540D+13 Z= 6.608251649578D+12
I= 24 X= 9.336703721556D+12 Y= 2.502322943155D+13 Z= 4.872062614475D+13
I= 25 X= -1.621182785938D+13 Y= -1.122500678993D+13 Z= 1.435556773287D+13
I= 26 X= 6.393684685357D+13 Y= -4.424035688281D+12 Z= -9.908727275306D+13
I= 27 X= -1.022711472036D+13 Y= 3.216213610206D+13 Z= -1.261393874682D+13
I= 28 X= 6.937428215844D+13 Y= -4.693833209767D+13 Z= -4.036837533033D+13
I= 29 X= 1.332303963191D+13 Y= 1.113822694389D+13 Z= 1.032472127504D+13
I= 30 X= 6.913077687715D+12 Y= -7.381676314126D+12 Z= -2.452817142149D+13
I= 31 X= -5.218444427119D+13 Y= 3.690272045624D+12 Z= -1.260905602750D+13
I= 32 X= 7.747140119688D+12 Y= -5.229621180435D+13 Z= -3.950910540362D+13
I= 33 X= 2.012340659301D+13 Y= -3.901632075055D+13 Z= -6.571357951710D+13
I= 34 X= -8.900966608958D+13 Y= -2.311419795293D+13 Z= 7.148742387800D+13
I= 35 X= -2.810293778084D+12 Y= -2.711388687223D+12 Z= 2.204533607351D+12
I= 36 X= 5.230193363631D+12 Y= 9.346746225490D+12 Z= -1.058263018145D+13
I= 37 X= -6.595240318040D+13 Y= 7.776615365964D+13 Z= -1.448974102654D+13
I= 38 X= 1.612567066661D+13 Y= 1.393167396527D+13 Z= -1.591335389223D+13

Seed: 10237587652

CM Start Point Coordinates: bohr

I= 0 X= -2.319852615712D+00 Y= 2.300001111386D+00 Z= -6.248632713730D-01
I= 1 X= -2.786885803084D+00 Y= -2.710483490405D-02 Z= -1.920708902410D+00
I= 2 X= -2.076586144651D+00 Y= 1.675816532869D+00 Z= 2.042852968564D+00
I= 3 X= -2.586412219068D+00 Y= -2.109499013481D+00 Z= -1.690626651684D-01
I= 4 X= -1.989593898014D+00 Y= -9.959840500036D-01 Z= 2.295645060253D+00
I= 5 X= 4.320709197137D+00 Y= 2.881390036602D+00 Z= -1.304220593045D+00
I= 6 X= 2.237654991385D+00 Y= 6.523638227996D-01 Z= -3.276334258788D+00
I= 7 X= 5.860227246059D+00 Y= 2.246930856358D+00 Z= -2.748203627158D+00
I= 8 X= 3.580674499016D+00 Y= 4.551797682318D+00 Z= -1.845810074978D+00
I= 9 X= -2.357935111966D+00 Y= -2.428321313753D+00 Z= 4.771458276230D+00
I= 10 X= -3.955724178954D+00 Y= -1.198255734936D+00 Z= 5.662219799987D+00

I= 11 X= -2.756465114623D+00 Y= -4.625332902099D+00 Z= 4.356260559489D+00
I= 12 X= -8.264666989777D-01 Y= -2.224955734453D+00 Z= 6.393858607554D+00
I= 13 X= -1.693990698542D+00 Y= 3.549494865478D+00 Z= 4.469813574714D+00
I= 14 X= -3.450755918284D+00 Y= 3.649834350743D+00 Z= 5.411531624992D+00
I= 15 X= -3.894579452996D-01 Y= 2.164401436551D+00 Z= 5.614186069255D+00
I= 16 X= -1.217338422969D+00 Y= 5.295310580761D+00 Z= 3.796604174674D+00
I= 17 X= -2.101623269945D+00 Y= 4.893356488636D+00 Z= -1.721785293199D+00
I= 18 X= -4.036204725887D+00 Y= 6.044547549932D+00 Z= -9.417793718396D-01
I= 19 X= -4.198082077682D-01 Y= 6.012102214366D+00 Z= -1.392024963947D+00
I= 20 X= -2.265282756255D+00 Y= 4.383919691897D+00 Z= -4.129674357331D+00
I= 21 X= -3.722114480439D+00 Y= -3.982277380406D-01 Z= -4.674781868899D+00
I= 22 X= -5.821363023543D+00 Y= 4.593432830644D-01 Z= -4.848051369809D+00
I= 23 X= -2.398580717784D+00 Y= 8.907571953092D-01 Z= -6.248046635367D+00
I= 24 X= -3.210300689333D+00 Y= -2.501893306184D+00 Z= -5.028185684409D+00
I= 25 X= -2.866676605058D+00 Y= -4.886258188528D+00 Z= -5.408187670034D-01
I= 26 X= -3.200044059852D+00 Y= -5.243772202942D+00 Z= -2.588118712920D+00
I= 27 X= -1.549223762119D+00 Y= -6.029538692754D+00 Z= 2.561794728592D-01
I= 28 X= -4.688523480191D+00 Y= -5.322085251640D+00 Z= 4.068272432952D-01
I= 29 X= 3.272312010571D+00 Y= -3.327509797367D+00 Z= -1.628179981857D+00
I= 30 X= 3.082419780482D+00 Y= -3.419302412253D+00 Z= 1.146757160137D+00
I= 31 X= 2.021207106363D+00 Y= -4.353180969998D+00 Z= -3.019703792309D+00
I= 32 X= 4.888803551295D+00 Y= -2.762947804354D+00 Z= -2.827001980861D+00
I= 33 X= 4.623060158068D+00 Y= -2.986618448795D+00 Z= 2.384795496010D+00
I= 34 X= 1.512340540904D+00 Y= -4.046705868664D+00 Z= 2.319649549489D+00
I= 35 X= 1.219871873261D+00 Y= 1.386366395872D-02 Z= -4.243180697637D-01
I= 36 X= 3.961528912965D+00 Y= 2.191231024232D+00 Z= 1.266491165445D+00
I= 37 X= 5.534691076352D+00 Y= 1.150825992087D+00 Z= 2.556008283929D+00
I= 38 X= 2.828168417623D+00 Y= 3.579196375934D+00 Z= 2.474578942492D+00

Forward Direction:

Total Energy: -656.4195699 Hartrees

Potential Energy: -656.6060630 Hartress

Kinetic Energy: 0.1864931 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.127457697732D+13 Y= 6.212295685223D+11 Z= -7.300162508565D+12
I= 1 X= -1.763704246740D+13 Y= 4.572441952265D+12 Z= -1.848466565242D+13
I= 2 X= -6.338818520132D+11 Y= 2.133428198761D+13 Z= 3.803487055834D+13
I= 3 X= 6.575101355071D+12 Y= 1.313946734621D+13 Z= 1.136745186997D+13
I= 4 X= 7.098555085259D+12 Y= -1.438253104745D+13 Z= 1.005006198240D+13
I= 5 X= 2.082844109468D+13 Y= -3.709178679594D+12 Z= -2.332446060727D+13
I= 6 X= -5.365633089709D+13 Y= -1.039312137289D+14 Z= 5.334158954908D+13
I= 7 X= -2.324680292747D+13 Y= 2.812760606201D+13 Z= 3.751046067310D+13
I= 8 X= 3.770125914795D+13 Y= 7.245731299988D+13 Z= -3.853937080443D+13
I= 9 X= -8.524427656833D+12 Y= -1.582404223085D+13 Z= -1.703812569497D+13
I= 10 X= 7.887115266317D+12 Y= -4.969673382974D+13 Z= -3.033211289478D+13
I= 11 X= 4.980141559499D+13 Y= 9.972045873904D+13 Z= -6.243836178433D+13
I= 12 X= 2.745349625709D+13 Y= 3.546262904856D+13 Z= 2.009353438310D+13
I= 13 X= -8.692421311763D+12 Y= -1.603384822531D+13 Z= 7.634878810021D+12
I= 14 X= 1.288051817623D+13 Y= -1.450433727606D+13 Z= 8.540157974547D+12
I= 15 X= 6.182319227351D+13 Y= -5.573303616982D+12 Z= 3.435965523295D+13
I= 16 X= -4.763784124807D+13 Y= 1.596084625436D+14 Z= -2.756322785399D+13
I= 17 X= -8.516851187147D+12 Y= 1.532837285780D+13 Z= -1.230094297382D+13
I= 18 X= 5.696509751605D+13 Y= -1.240436632608D+14 Z= 6.178372549493D+12
I= 19 X= -2.007974576387D+12 Y= 1.121657017164D+13 Z= 2.897074796447D+13
I= 20 X= 5.280564284913D+13 Y= 1.051669309821D+13 Z= 7.638471070216D+13
I= 21 X= 1.954452275845D+13 Y= -6.548691241122D+12 Z= 1.527402271716D+13
I= 22 X= -7.438281544828D+13 Y= -1.819785467089D+13 Z= -7.286110774785D+13
I= 23 X= -1.288115849503D+13 Y= -5.357733248097D+13 Z= -4.987151694005D+12
I= 24 X= -7.376393837588D+13 Y= 9.150889516695D+12 Z= -1.018729276737D+13
I= 25 X= 8.713493483675D+12 Y= -1.200265112512D+13 Z= 3.041623649134D+13
I= 26 X= -3.195584995048D+13 Y= 9.525118479564D+13 Z= -9.771669987910D+13

I= 27 X= -5.221467191051D+13 Y= -8.634255053467D+13 Z= 1.499286213167D+13
I= 28 X= 6.643160869097D+13 Y= 5.736497524170D+12 Z= -7.102419926338D+13
I= 29 X= 1.431220098450D+13 Y= -3.296777759615D+12 Z= 4.359742440898D+12
I= 30 X= -1.909143540408D+13 Y= -2.176713584766D+12 Z= -4.179608741999D+12
I= 31 X= -1.434361624044D+14 Y= -1.281301224136D+14 Z= -8.027499246720D+13
I= 32 X= 2.027212884890D+13 Y= 3.262739976995D+13 Z= 5.793997776354D+13
I= 33 X= -7.720409924808D+13 Y= 4.950836065413D+13 Z= 4.793508655813D+12
I= 34 X= 5.635080116586D+13 Y= 1.144764708460D+12 Z= 4.968553939075D+13
I= 35 X= 7.291128930731D+11 Y= -7.773741091897D+11 Z= -2.766550220722D+12
I= 36 X= 3.084768739513D+12 Y= 2.736470708539D+13 Z= -1.884021896657D+12
I= 37 X= 4.061635722309D+12 Y= -9.510547859864D+12 Z= -3.648164639604D+13
I= 38 X= -5.391163078718D+12 Y= -3.749821196453D+13 Z= 3.363234079606D+13

Backward Direction:

Total Energy: -656.4196296 Hartrees

Potential Energy: -656.6060630 Hartress

Kinetic Energy: 0.1864334 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.174273626943D+13 Y= 9.881424086503D+09 Z= -7.060925763525D+12
I= 1 X= -1.835912081794D+13 Y= 3.000362958211D+12 Z= -1.942838906921D+13
I= 2 X= -1.305942423357D+12 Y= 2.195205437974D+13 Z= 3.704023085916D+13
I= 3 X= 5.198083977693D+12 Y= 1.317166592556D+13 Z= 9.372295240975D+12
I= 4 X= 9.453790614622D+12 Y= -1.459266086222D+13 Z= 8.484970095236D+12
I= 5 X= 1.694135337598D+13 Y= -9.237042333967D+12 Z= -3.436092385918D+13
I= 6 X= 3.341378343086D+13 Y= -4.530223013783D+12 Z= 9.251745477675D+13
I= 7 X= -7.343443813241D+12 Y= 4.318470426906D+13 Z= 3.848342468769D+13
I= 8 X= 5.778654538957D+13 Y= 8.869263372601D+13 Z= -3.667078087205D+13
I= 9 X= -7.775864873929D+12 Y= -1.547250307827D+13 Z= -1.788424799258D+13
I= 10 X= 8.024021391995D+12 Y= -4.795698019008D+13 Z= -3.234884791818D+13
I= 11 X= 4.958521582409D+13 Y= 9.970144049002D+13 Z= -6.248040279059D+13
I= 12 X= 2.789220664205D+13 Y= 3.558013238484D+13 Z= 1.967693423667D+13

I= 13 X= -8.544029658818D+12 Y= -1.610604992521D+13 Z= 7.322559873995D+12
I= 14 X= 1.313279452025D+13 Y= -1.494914593814D+13 Z= 8.606182420951D+12
I= 15 X= 6.228712998603D+13 Y= -5.998814657873D+12 Z= 3.359140844862D+13
I= 16 X= -4.767015901934D+13 Y= 1.597452221909D+14 Z= -2.745506625283D+13
I= 17 X= -8.289606110977D+12 Y= 1.482687678306D+13 Z= -1.235060566580D+13
I= 18 X= 5.701301098946D+13 Y= -1.248431810437D+14 Z= 5.522495846603D+12
I= 19 X= -2.488366103580D+12 Y= 1.105653990186D+13 Z= 2.946610659127D+13
I= 20 X= 5.313924107091D+13 Y= 1.006858910516D+13 Z= 7.632748710635D+13
I= 21 X= 1.925857615040D+13 Y= -6.728329283212D+12 Z= 1.457598349752D+13
I= 22 X= -7.443391643107D+13 Y= -1.739281771353D+13 Z= -7.565859652474D+13
I= 23 X= -1.184177288876D+13 Y= -5.402976589535D+13 Z= -5.311534071595D+12
I= 24 X= -7.426501015833D+13 Y= 8.869466941804D+12 Z= -1.101264464082D+13
I= 25 X= 8.402726907525D+12 Y= -1.231659035274D+13 Z= 3.025587242668D+13
I= 26 X= -3.272451187832D+13 Y= 9.441032803057D+13 Z= -9.781048681801D+13
I= 27 X= -5.157405011538D+13 Y= -8.580319900091D+13 Z= 1.480694113378D+13
I= 28 X= 6.646335320465D+13 Y= 4.785020431474D+12 Z= -7.035070351396D+13
I= 29 X= 1.287300319101D+13 Y= -2.892518310085D+12 Z= 3.854963664824D+12
I= 30 X= -1.900668233873D+13 Y= -2.455234694761D+12 Z= -4.804740408904D+12
I= 31 X= -1.444311794995D+14 Y= -1.284244931963D+14 Z= -8.024390169770D+13
I= 32 X= 1.736014704018D+13 Y= 3.504562363658D+13 Z= 5.620627208799D+13
I= 33 X= -7.711429321619D+13 Y= 4.915638053907D+13 Z= 4.295589009705D+12
I= 34 X= 5.728899055683D+13 Y= 4.915727708919D+11 Z= 4.950597780985D+13
I= 35 X= 7.134560280469D+11 Y= -4.116782012598D+11 Z= -4.464349710026D+11
I= 36 X= -1.975040418727D+12 Y= 2.097375119538D+13 Z= -4.216243173402D+12
I= 37 X= 8.575453809346D+12 Y= -7.219041882897D+12 Z= -4.211109992652D+13
I= 38 X= -2.919221183816D+12 Y= -3.775579282492D+13 Z= 2.942812750276D+13

Seed: 11811650333

CM Start Point Coordinates: bohr

I= 0 X= -2.457439256028D+00 Y= 2.468440907583D+00 Z= -4.565086461609D-01

I= 1 X= -2.689591323268D+00 Y= 8.780393281655D-02 Z= -2.123928196363D+00
I= 2 X= -2.262742661335D+00 Y= 1.577966264747D+00 Z= 2.157590819335D+00
I= 3 X= -2.510767946867D+00 Y= -1.932412884104D+00 Z= -2.608186945306D-01
I= 4 X= -2.260348880059D+00 Y= -9.576412832713D-01 Z= 2.290877416252D+00
I= 5 X= 4.707072094487D+00 Y= 2.209269655429D+00 Z= -1.599394684680D+00
I= 6 X= 2.060793862448D+00 Y= 4.733044964149D-01 Z= -3.028444009733D+00
I= 7 X= 6.198949984968D+00 Y= 7.672716155391D-01 Z= -2.112928078003D+00
I= 8 X= 4.324846071012D+00 Y= 3.755156299928D+00 Z= -2.707147731129D+00
I= 9 X= -2.349590703676D+00 Y= -2.595808975656D+00 Z= 4.606002040023D+00
I= 10 X= -4.208727305626D+00 Y= -3.105057010768D+00 Z= 5.069616500902D+00
I= 11 X= -9.758616722945D-01 Y= -4.262995896028D+00 Z= 4.176085244883D+00
I= 12 X= -1.512570294670D+00 Y= -1.398423521151D+00 Z= 6.250427320430D+00
I= 13 X= -1.701956637601D+00 Y= 3.255686864713D+00 Z= 4.415136680194D+00
I= 14 X= -3.676564715840D+00 Y= 4.137289127083D+00 Z= 4.872313114948D+00
I= 15 X= -8.123517246673D-01 Y= 2.404588453644D+00 Z= 6.149283495232D+00
I= 16 X= -3.274907923713D-03 Y= 4.662035495616D+00 Z= 3.760334935079D+00
I= 17 X= -2.410855919397D+00 Y= 5.091238167791D+00 Z= -1.501887157204D+00
I= 18 X= -4.806939976691D+00 Y= 5.512460185568D+00 Z= -2.187708119976D+00
I= 19 X= -1.975855208017D+00 Y= 6.516122772562D+00 Z= 2.639132832639D-01
I= 20 X= -7.918739076801D-01 Y= 5.211839800036D+00 Z= -3.349667172442D+00
I= 21 X= -3.598382381241D+00 Y= -3.155072228462D-02 Z= -4.679246066420D+00
I= 22 X= -5.715003626808D+00 Y= 2.341196794356D-01 Z= -4.649067649830D+00
I= 23 X= -2.585657009663D+00 Y= 1.429565801629D+00 Z= -5.775498020562D+00
I= 24 X= -3.084501499038D+00 Y= -2.122244922051D+00 Z= -5.521922428534D+00
I= 25 X= -3.037679865141D+00 Y= -4.663590317642D+00 Z= -6.606844087984D-01
I= 26 X= -2.671734062786D+00 Y= -5.400865138921D+00 Z= -2.593844774556D+00
I= 27 X= -1.796680147034D+00 Y= -6.066674839301D+00 Z= 4.544657466182D-01
I= 28 X= -4.789950163280D+00 Y= -5.238216255537D+00 Z= -1.656936851303D-01
I= 29 X= 3.062625944213D+00 Y= -3.742855355103D+00 Z= -1.196557497891D+00
I= 30 X= 3.999403218449D+00 Y= -2.923051067124D+00 Z= 1.171623457630D+00

I= 31 X= 1.617354227499D+00 Y= -5.492602593388D+00 Z= -1.178925444769D+00
I= 32 X= 4.504973791827D+00 Y= -3.524735129945D+00 Z= -2.929393521844D+00
I= 33 X= 6.080792300815D+00 Y= -2.058363776849D+00 Z= 9.523100571824D-01
I= 34 X= 3.128764006453D+00 Y= -3.326546641200D+00 Z= 2.981892088426D+00
I= 35 X= 1.160340886455D+00 Y= -6.098350865695D-02 Z= -3.850733177712D-01
I= 36 X= 3.852599861086D+00 Y= 2.707004729625D+00 Z= 9.124986008333D-01
I= 37 X= 4.930671042495D+00 Y= 1.866297226581D+00 Z= 2.686508633620D+00
I= 38 X= 3.074881874221D+00 Y= 4.698737642685D+00 Z= 1.291346811789D+00

Forward Direction:

Total Energy: -656.4357636 Hartrees

Potential Energy: -656.6132585 Hartress

Kinetic Energy: 0.1774950 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.245241792671D+10 Y= -4.330848586852D+12 Z= -1.344017415811D+13
I= 1 X= -5.080324987538D+12 Y= -9.302726261322D+12 Z= 7.009242626630D+12
I= 2 X= -3.671176326332D+12 Y= -8.155874149035D+12 Z= 1.418550595299D+12
I= 3 X= 9.624983929838D+12 Y= 2.824751705784D+13 Z= 2.749941127320D+13
I= 4 X= -1.185668436655D+13 Y= -1.623718051735D+13 Z= -2.621490988491D+13
I= 5 X= 2.398919035012D+13 Y= 1.056080803263D+13 Z= 1.023704903532D+13
I= 6 X= -7.481071058499D+13 Y= 1.815454791158D+13 Z= 1.283647962249D+13
I= 7 X= 1.324714598261D+13 Y= 2.017411633461D+13 Z= -6.108398121368D+13
I= 8 X= -9.815038353540D+13 Y= 2.717766771343D+13 Z= -1.184404560079D+14
I= 9 X= 2.628564383392D+12 Y= -5.797011223313D+12 Z= 7.144511801539D+12
I= 10 X= -7.508115460115D+13 Y= -1.577305684247D+13 Z= -3.477899320601D+13
I= 11 X= -1.525450790307D+13 Y= -1.028124886918D+14 Z= 2.788586173025D+13
I= 12 X= -8.495900807948D+13 Y= 3.608317447568D+13 Z= -5.146118761110D+12
I= 13 X= -6.220456524498D+12 Y= -9.646412530670D+12 Z= -3.244459090513D+13
I= 14 X= -6.421876480633D+12 Y= -6.061045644384D+12 Z= 8.490874741422D+12
I= 15 X= 1.330283574109D+14 Y= 2.955527270678D+13 Z= 1.363233229709D+14
I= 16 X= 4.263688551001D+13 Y= 5.801864380203D+13 Z= 1.110245077608D+13

I= 17 X= 5.073172711988D+12 Y= 1.301921967012D+13 Z= 6.595233777776D+12
I= 18 X= -3.694411303672D+13 Y= -6.971243930534D+13 Z= 2.808509678314D+13
I= 19 X= -7.800944245632D+13 Y= -3.378748964530D+13 Z= -9.145481740394D+13
I= 20 X= 2.310287522396D+13 Y= -8.944477575760D+13 Z= -5.012622863098D+13
I= 21 X= -1.270369100838D+12 Y= -3.088699501622D+12 Z= 1.551585009558D+13
I= 22 X= 4.222016897301D+13 Y= 2.343775784419D+13 Z= -4.814125112005D+13
I= 23 X= 8.375115151029D+12 Y= 1.593876094286D+13 Z= 3.007281792393D+11
I= 24 X= 1.183164008622D+14 Y= -4.489189501268D+13 Z= -1.660619121168D+13
I= 25 X= -7.796310767855D+11 Y= -1.357242861472D+13 Z= -8.959849370758D+12
I= 26 X= -1.114206642299D+13 Y= 1.708925889709D+13 Z= 5.260985268842D+13
I= 27 X= 3.862885138688D+13 Y= -3.723462845082D+13 Z= 9.867488364902D+13
I= 28 X= -7.122830281833D+13 Y= -1.342556694082D+12 Z= 4.122490709227D+13
I= 29 X= -4.202426019723D+12 Y= 5.669478698652D+12 Z= 3.699222003957D+12
I= 30 X= 1.415823145950D+13 Y= 2.278563958921D+12 Z= -1.175920140154D+12
I= 31 X= -3.432466364956D+13 Y= -5.555021428854D+13 Z= 3.698840810429D+13
I= 32 X= 6.594430598947D+12 Y= 3.153459533673D+13 Z= -4.977783249082D+13
I= 33 X= -2.909032123821D+13 Y= -9.749775970000D+12 Z= -3.125801941105D+13
I= 34 X= -1.206156939832D+14 Y= -8.735819522256D+13 Z= 1.147161668692D+14
I= 35 X= -4.921045988912D+11 Y= 4.609409811705D+12 Z= -1.272157243513D+12
I= 36 X= -5.352283231464D+11 Y= -6.199126940884D+12 Z= 6.609120726904D+12
I= 37 X= -1.678745982332D+13 Y= 6.885925615429D+13 Z= 2.245160120838D+13
I= 38 X= 1.174021987118D+14 Y= -6.583782602342D+13 Z= 3.430365620836D+12

Backward Direction:

Total Energy: -656.4357955 Hartrees

Potential Energy: -656.6132585 Hartress

Kinetic Energy: 0.1774631 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.889102269268D+11 Y= -4.757155143838D+12 Z= -1.327334909452D+13

I= 1 X= -5.583846161764D+12 Y= -1.039897164767D+13 Z= 6.351163455859D+12

I= 2 X= -4.139818997001D+12 Y= -7.725087823458D+12 Z= 7.249663765194D+11

I= 3 X= 8.664759311745D+12 Y= 2.826996983752D+13 Z= 2.610814451296D+13
I= 4 X= -1.021432663839D+13 Y= -1.638370867645D+13 Z= -2.730628300716D+13
I= 5 X= 2.127863827417D+13 Y= 6.706106680330D+12 Z= 2.541079579564D+12
I= 6 X= -1.409479778106D+13 Y= 8.746905302739D+13 Z= 4.015467525754D+13
I= 7 X= 2.433690936040D+13 Y= 3.067376330511D+13 Z= -6.040551192957D+13
I= 8 X= -8.414447005498D+13 Y= 3.849891525466D+13 Z= -1.171374469985D+14
I= 9 X= 3.150553737967D+12 Y= -5.551875215091D+12 Z= 6.554492044270D+12
I= 10 X= -7.498568693311D+13 Y= -1.455988824291D+13 Z= -3.618530706533D+13
I= 11 X= -1.540526876125D+13 Y= -1.028257505138D+14 Z= 2.785654560638D+13
I= 12 X= -8.465308563541D+13 Y= 3.616511216291D+13 Z= -5.436623219392D+12
I= 13 X= -6.116979750642D+12 Y= -9.696760368613D+12 Z= -3.266237779399D+13
I= 14 X= -6.245958615288D+12 Y= -6.371220528314D+12 Z= 8.536915043359D+12
I= 15 X= 1.333518714184D+14 Y= 2.925855446326D+13 Z= 1.357876075318D+14
I= 16 X= 4.261434962468D+13 Y= 5.811400931596D+13 Z= 1.117787424339D+13
I= 17 X= 5.231635724459D+12 Y= 1.266951538564D+13 Z= 6.560602886565D+12
I= 18 X= -3.691070191037D+13 Y= -7.026996070999D+13 Z= 2.762773947670D+13
I= 19 X= -7.834443007740D+13 Y= -3.389908228870D+13 Z= -9.110939289883D+13
I= 20 X= 2.333550063974D+13 Y= -8.975724856363D+13 Z= -5.016613191678D+13
I= 21 X= -1.469765982442D+12 Y= -3.213965073736D+12 Z= 1.502909193859D+13
I= 22 X= 4.218453512922D+13 Y= 2.399912788534D+13 Z= -5.009200179312D+13
I= 23 X= 9.099901674433D+12 Y= 1.562326913551D+13 Z= 7.452918472095D+10
I= 24 X= 1.179669924468D+14 Y= -4.508813718728D+13 Z= -1.718172729338D+13
I= 25 X= -9.963354698926D+11 Y= -1.379134536731D+13 Z= -9.071674776206D+12
I= 26 X= -1.167807136835D+13 Y= 1.650291091626D+13 Z= 5.254445300261D+13
I= 27 X= 3.907557109914D+13 Y= -3.685852673237D+13 Z= 9.854523683744D+13
I= 28 X= -7.120616667582D+13 Y= -2.006042663454D+12 Z= 4.169455055105D+13
I= 29 X= -5.206010410647D+12 Y= 5.951377736482D+12 Z= 3.347228620700D+12
I= 30 X= 1.421733164269D+13 Y= 2.084345040943D+12 Z= -1.611838249729D+12
I= 31 X= -3.501851103648D+13 Y= -5.575548553660D+13 Z= 3.701008838542D+13
I= 32 X= 4.563841406975D+12 Y= 3.322087622374D+13 Z= -5.098678372893D+13

I= 33 X= -2.902769751839D+13 Y= -9.995219476735D+12 Z= -3.160522977117D+13
I= 34 X= -1.199614738056D+14 Y= -8.781368037463D+13 Z= 1.145909546098D+14
I= 35 X= -5.030224768205D+11 Y= 4.864417640970D+12 Z= 3.457103365115D+11
I= 36 X= -4.063544946937D+12 Y= -1.065568156376D+13 Z= 4.982811347755D+12
I= 37 X= -1.363987482866D+13 Y= 7.045717385642D+13 Z= 1.852605899104D+13
I= 38 X= 1.191259383595D+14 Y= -6.601744284488D+13 Z= 4.986748829389D+11

Seed: 12095833256

CM Start Point Coordinates: bohr

I= 0 X= -2.187880575902D+00 Y= 2.348462979543D+00 Z= -6.469689402547D-01
I= 1 X= -2.775625865566D+00 Y= 1.411676514817D-01 Z= -1.976114111357D+00
I= 2 X= -2.044783075979D+00 Y= 1.723926171384D+00 Z= 2.136288971514D+00
I= 3 X= -2.758359307936D+00 Y= -1.898593206588D+00 Z= -2.000027794225D-01
I= 4 X= -2.185673234747D+00 Y= -9.430905657951D-01 Z= 2.307046849850D+00
I= 5 X= 4.280321665708D+00 Y= 2.737762113847D+00 Z= -1.333585563992D+00
I= 6 X= 2.647339472243D+00 Y= 4.118770178291D-01 Z= -3.142209133892D+00
I= 7 X= 5.930013004097D+00 Y= 1.554622287991D+00 Z= -2.105910436610D+00
I= 8 X= 3.606382403981D+00 Y= 4.061997748687D+00 Z= -2.673574903976D+00
I= 9 X= -1.992532033114D+00 Y= -2.522112829141D+00 Z= 4.591663755082D+00
I= 10 X= -3.912206183730D+00 Y= -2.487820620019D+00 Z= 5.480392295942D+00
I= 11 X= -1.263663992156D+00 Y= -4.208747518622D+00 Z= 4.226184430103D+00
I= 12 X= -8.506712507305D-01 Y= -1.561885069972D+00 Z= 6.073541397565D+00
I= 13 X= -1.756930124743D+00 Y= 3.454561597865D+00 Z= 4.302202856844D+00
I= 14 X= -3.455416362306D+00 Y= 3.234909566478D+00 Z= 5.601533336204D+00
I= 15 X= 4.359022447388D-01 Y= 3.554730189758D+00 Z= 5.487869612505D+00
I= 16 X= -1.980672058028D+00 Y= 5.658221374819D+00 Z= 3.537987836448D+00
I= 17 X= -2.269139946388D+00 Y= 4.955102604006D+00 Z= -1.865336404287D+00
I= 18 X= -4.398907623089D+00 Y= 5.357729193263D+00 Z= -2.957909928031D+00
I= 19 X= -1.765397673598D+00 Y= 6.521542546240D+00 Z= -1.179084287046D-01
I= 20 X= -6.306689688542D-01 Y= 4.875662196481D+00 Z= -3.640255539294D+00

I= 21 X= -3.585559100523D+00 Y= -2.099568082217D-01 Z= -4.654447520973D+00
I= 22 X= -5.669972581130D+00 Y= -3.440806610112D-01 Z= -4.802310303553D+00
I= 23 X= -2.790199421922D+00 Y= 1.258435304494D+00 Z= -5.769573808666D+00
I= 24 X= -3.045418902054D+00 Y= -1.914139627483D+00 Z= -5.291348630152D+00
I= 25 X= -3.370486705987D+00 Y= -4.726962972980D+00 Z= -6.032301405402D-01
I= 26 X= -3.011804120819D+00 Y= -5.083705202600D+00 Z= -2.536722837528D+00
I= 27 X= -2.131521283910D+00 Y= -6.096276734662D+00 Z= 4.360717005472D-01
I= 28 X= -5.320289231176D+00 Y= -4.708745609172D+00 Z= -3.694575935925D-01
I= 29 X= 3.449910196135D+00 Y= -3.478524119537D+00 Z= -1.644435365231D+00
I= 30 X= 3.642877775395D+00 Y= -3.236971525302D+00 Z= 9.552562443863D-01
I= 31 X= 1.617987277614D+00 Y= -4.454235584942D+00 Z= -2.574174596196D+00
I= 32 X= 5.400148387491D+00 Y= -3.345403787106D+00 Z= -2.799001514669D+00
I= 33 X= 5.430312433541D+00 Y= -2.570159214247D+00 Z= 1.186336887985D+00
I= 34 X= 2.450817383942D+00 Y= -4.348599276414D+00 Z= 2.343177834226D+00
I= 35 X= 1.173781864016D+00 Y= -1.240776030945D-01 Z= -3.178059929623D-01
I= 36 X= 3.872639072516D+00 Y= 2.626953329232D+00 Z= 1.364446099332D+00
I= 37 X= 5.287431663515D+00 Y= 1.584726667831D+00 Z= 2.357001910077D+00
I= 38 X= 2.843160216273D+00 Y= 4.148233858310D+00 Z= 1.961311177500D+00

Forward Direction:

Total Energy: -656.4238018 Hartrees

Potential Energy: -656.6121711 Hartress

Kinetic Energy: 0.1883693 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.884010037324D+12 Y= 1.320648868288D+13 Z= -2.985599894082D+12
I= 1 X= 7.567534223383D+12 Y= -1.235365936952D+13 Z= 4.552062852135D+12
I= 2 X= -1.594453898198D+13 Y= -1.229734007533D+13 Z= 1.710884499681D+13
I= 3 X= -1.367459484920D+13 Y= -8.416973719771D+12 Z= -1.455556270591D+13
I= 4 X= 6.457227933998D+12 Y= 2.055217515873D+12 Z= 5.828821309413D+12
I= 5 X= -5.386882653456D+12 Y= 2.080126732837D+13 Z= -2.129399181158D+13
I= 6 X= -4.994951155700D+13 Y= -2.336976624500D+13 Z= -1.806127241049D+13

I= 7 X= -2.715357393488D+12 Y= 5.151731280461D+12 Z= 1.208727490332D+13
I= 8 X= 9.300488368605D+13 Y= -1.145653363611D+14 Z= 2.723098706837D+13
I= 9 X= 1.642595335594D+12 Y= 7.062742367490D+12 Z= 1.819331876082D+12
I= 10 X= 8.556294838876D+12 Y= 1.398979775633D+14 Z= -9.973919166785D+12
I= 11 X= 9.102369164282D+13 Y= 8.516376490600D+13 Z= 1.332610340326D+13
I= 12 X= 5.234077652054D+13 Y= -6.578240125408D+13 Z= -1.430123965445D+14
I= 13 X= 1.047114876882D+13 Y= 1.452352017861D+13 Z= 2.246666548075D+12
I= 14 X= 4.784197708985D+13 Y= 3.399489058101D+13 Z= -2.937057533276D+13
I= 15 X= -4.106719602613D+13 Y= -6.828060698393D+13 Z= -9.112120623954D+13
I= 16 X= -1.788894424984D+13 Y= -1.589497861272D+14 Z= 1.214963364590D+14
I= 17 X= -1.938003327261D+13 Y= 8.636204571132D+12 Z= -1.757670941090D+12
I= 18 X= 1.097601667581D+14 Y= -4.880034551675D+13 Z= -1.422516265583D+13
I= 19 X= 8.922428922604D+12 Y= -4.788017527230D+13 Z= -2.866351880632D+13
I= 20 X= 4.578508126383D+13 Y= 4.078144535797D+13 Z= -5.844206063699D+13
I= 21 X= -9.359322604922D+12 Y= -1.149861377121D+13 Z= 2.579444523795D+13
I= 22 X= -1.034360681464D+14 Y= 6.144698905935D+13 Z= 3.518693007448D+13
I= 23 X= 5.047450093028D+13 Y= 6.318730343335D+13 Z= -2.279941449913D+13
I= 24 X= 1.033333605764D+14 Y= 7.685299246724D+13 Z= 7.059044336358D+13
I= 25 X= 1.181531489413D+13 Y= -9.838603617341D+12 Z= 9.280128668293D+12
I= 26 X= -5.112857975313D+13 Y= 1.023624466829D+13 Z= -9.523433410203D+13
I= 27 X= -7.218941676192D+13 Y= 4.536197502640D+13 Z= -7.497536681723D+13
I= 28 X= 1.525418750185D+13 Y= 5.480380084448D+13 Z= -4.167883369206D+12
I= 29 X= -3.390130939064D+12 Y= -6.222853058622D+12 Z= -4.325225312234D+12
I= 30 X= -1.684122231305D+13 Y= 2.067458014179D+11 Z= 9.980411036555D+12
I= 31 X= -1.366961889537D+13 Y= -4.513265820299D+13 Z= -2.011053493956D+12
I= 32 X= -3.836371432906D+13 Y= 4.655355474240D+13 Z= -3.194785026274D+13
I= 33 X= 6.240483547095D+12 Y= -3.126972910790D+13 Z= -2.840067326192D+13
I= 34 X= -1.705384511461D+13 Y= 7.508715789383D+13 Z= -8.981800286150D+13
I= 35 X= 2.218080873972D+12 Y= 4.873269746179D+11 Z= -1.638988425119D+10
I= 36 X= 8.533934403041D+12 Y= -6.094549112235D+12 Z= 4.644993264053D+12

I= 37 X= -1.231816107040D+13 Y= -8.925737230860D+13 Z= 3.485236047145D+13

I= 38 X= 4.147777262190D+13 Y= -9.224716184660D+13 Z= -3.538474958851D+12

Backward Direction:

Total Energy: -656.4238429 Hartrees

Potential Energy: -656.6121711 Hartress

Kinetic Energy: 0.1883281 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.088981874120D+12 Y= 1.293882518801D+13 Z= -2.880856069176D+12

I= 1 X= 7.251390277895D+12 Y= -1.304195483829D+13 Z= 4.138877157134D+12

I= 2 X= -1.623878389511D+13 Y= -1.202686388482D+13 Z= 1.667336688170D+13

I= 3 X= -1.427748746975D+13 Y= -8.402876377044D+12 Z= -1.542909213535D+13

I= 4 X= 7.488408902296D+12 Y= 1.963217431246D+12 Z= 5.143584971301D+12

I= 5 X= -7.088746795370D+12 Y= 1.838103048531D+13 Z= -2.612603121517D+13

I= 6 X= -1.182803969165D+13 Y= 2.015047144546D+13 Z= -9.090996388881D+11

I= 7 X= 4.247530636339D+12 Y= 1.174410514780D+13 Z= 1.251326285646D+13

I= 8 X= 1.017987239184D+14 Y= -1.074571072397D+14 Z= 2.804910243124D+13

I= 9 X= 1.970334834067D+12 Y= 7.216654993401D+12 Z= 1.448878391544D+12

I= 10 X= 8.616235769956D+12 Y= 1.406596851846D+14 Z= -1.085689615957D+13

I= 11 X= 9.092903398076D+13 Y= 8.515543824034D+13 Z= 1.330769680109D+13

I= 12 X= 5.253285490018D+13 Y= -6.573095535606D+13 Z= -1.431947944950D+14

I= 13 X= 1.053611834504D+13 Y= 1.449190846944D+13 Z= 2.109925512616D+12

I= 14 X= 4.795242997982D+13 Y= 3.380014222658D+13 Z= -2.934166818182D+13

I= 15 X= -4.086407249664D+13 Y= -6.846690634734D+13 Z= -9.145756387684D+13

I= 16 X= -1.790309377972D+13 Y= -1.588899093335D+14 Z= 1.215436923100D+14

I= 17 X= -1.928053969526D+13 Y= 8.416637058114D+12 Z= -1.779414509448D+12

I= 18 X= 1.097811444758D+14 Y= -4.915039438931D+13 Z= -1.451232187578D+13

I= 19 X= 8.712101500743D+12 Y= -4.795024051979D+13 Z= -2.844663841808D+13

I= 20 X= 4.593113891556D+13 Y= 4.058525423271D+13 Z= -5.846711455864D+13

I= 21 X= -9.484517172696D+12 Y= -1.157726379561D+13 Z= 2.548882622346D+13

I= 22 X= -1.034584414305D+14 Y= 6.179945435880D+13 Z= 3.396211957829D+13

I= 23 X= 5.092956992644D+13 Y= 6.298921677729D+13 Z= -2.294143721011D+13
I= 24 X= 1.031139788302D+14 Y= 7.672977863008D+13 Z= 7.022908368773D+13
I= 25 X= 1.167925352138D+13 Y= -9.976054056314D+12 Z= 9.209917270789D+12
I= 26 X= -5.146511914744D+13 Y= 9.868096562099D+12 Z= -9.527539636402D+13
I= 27 X= -7.190893654843D+13 Y= 4.559811660635D+13 Z= -7.505676766862D+13
I= 28 X= 1.526808603405D+13 Y= 5.438722040498D+13 Z= -3.873010113228D+12
I= 29 X= -4.020247697784D+12 Y= -6.045858170111D+12 Z= -4.546230074861D+12
I= 30 X= -1.680411530274D+13 Y= 8.480229925920D+10 Z= 9.706712771307D+12
I= 31 X= -1.410526224519D+13 Y= -4.526154108870D+13 Z= -1.997441176315D+12
I= 32 X= -3.963865273252D+13 Y= 4.761231358012D+13 Z= -3.270690993055D+13
I= 33 X= 6.279802872954D+12 Y= -3.142383479552D+13 Z= -2.861867492621D+13
I= 34 X= -1.664308235313D+13 Y= 7.480117413856D+13 Z= -8.989661940727D+13
I= 35 X= 2.211225906344D+12 Y= 6.474377814666D+11 Z= 9.994145504429D+11
I= 36 X= 6.318623510674D+12 Y= -8.892669304940D+12 Z= 3.623888509256D+12
I= 37 X= -1.034189871446D+13 Y= -8.825409373247D+13 Z= 3.238764503427D+13
I= 38 X= 4.256005054999D+13 Y= -9.235993718360D+13 Z= -5.379184601558D+12

Seed: 12121088233

CM Start Point Coordinates: bohr

I= 0 X= -2.290237446629D+00 Y= 2.437042731123D+00 Z= -4.921188630353D-01
I= 1 X= -2.668228166166D+00 Y= 3.998910072567D-03 Z= -1.968767255763D+00
I= 2 X= -2.009354758612D+00 Y= 1.798226993175D+00 Z= 2.150239407233D+00
I= 3 X= -2.712868396627D+00 Y= -1.871248276626D+00 Z= -6.107884019356D-02
I= 4 X= -2.117933392442D+00 Y= -9.448248682358D-01 Z= 2.351232782094D+00
I= 5 X= 4.103662609353D+00 Y= 2.543308734542D+00 Z= -1.733777105818D+00
I= 6 X= 2.273807105685D+00 Y= 3.671916336439D-01 Z= -3.056639657516D+00
I= 7 X= 5.727051178633D+00 Y= 1.836903190292D+00 Z= -2.894119290150D+00
I= 8 X= 3.193248467505D+00 Y= 4.356396747542D+00 Z= -2.684082756860D+00
I= 9 X= -2.063239592771D+00 Y= -2.352542003968D+00 Z= 4.736602343259D+00
I= 10 X= -3.844643040981D+00 Y= -3.528377104167D+00 Z= 5.501430348895D+00

I= 11 X= -8.027959346531D-01 Y= -4.269753323527D+00 Z= 4.149697026905D+00
I= 12 X= -1.462642994644D+00 Y= -1.196979145158D+00 Z= 6.523712259472D+00
I= 13 X= -1.999317075266D+00 Y= 3.554752449421D+00 Z= 4.217765523833D+00
I= 14 X= -3.894124159885D+00 Y= 4.324276522719D+00 Z= 4.644626633482D+00
I= 15 X= -1.238354890495D+00 Y= 2.609687140823D+00 Z= 5.718976908446D+00
I= 16 X= -1.036209470348D+00 Y= 5.431069758758D+00 Z= 3.864902920658D+00
I= 17 X= -2.350645581771D+00 Y= 5.081488773994D+00 Z= -1.541757149225D+00
I= 18 X= -4.381827734241D+00 Y= 5.808954143664D+00 Z= -1.346240697413D+00
I= 19 X= -1.161584442444D+00 Y= 6.268131613422D+00 Z= -6.790763905213D-01
I= 20 X= -1.961106259343D+00 Y= 4.942956847713D+00 Z= -3.554493560296D+00
I= 21 X= -3.281250779515D+00 Y= -1.919473696764D-01 Z= -4.555897685599D+00
I= 22 X= -5.428520708897D+00 Y= 2.414957717086D-01 Z= -4.930339545579D+00
I= 23 X= -1.843466136750D+00 Y= 1.156440059385D+00 Z= -5.526904832619D+00
I= 24 X= -2.798239765452D+00 Y= -2.154533489975D+00 Z= -5.299097576364D+00
I= 25 X= -2.870676444865D+00 Y= -4.529534342999D+00 Z= -7.380914063400D-01
I= 26 X= -2.399459316586D+00 Y= -4.936715868593D+00 Z= -2.798737586867D+00
I= 27 X= -1.330290909370D+00 Y= -6.120366993846D+00 Z= -1.029358066460D-01
I= 28 X= -4.848812433389D+00 Y= -5.259741817907D+00 Z= -2.457565987063D-01
I= 29 X= 3.582446579724D+00 Y= -3.337573242629D+00 Z= -1.594275605369D+00
I= 30 X= 3.072240485736D+00 Y= -3.549771059821D+00 Z= 1.083978135687D+00
I= 31 X= 2.526530761058D+00 Y= -4.707983180380D+00 Z= -3.045343771405D+00
I= 32 X= 5.391686634368D+00 Y= -2.373011488848D+00 Z= -2.388279839010D+00
I= 33 X= 4.583322925955D+00 Y= -2.644706785438D+00 Z= 2.347218943614D+00
I= 34 X= 1.783519084196D+00 Y= -4.634254140777D+00 Z= 1.882359265970D+00
I= 35 X= 1.132626783241D+00 Y= -1.565136153708D-01 Z= -3.430917474541D-01
I= 36 X= 4.268042141561D+00 Y= 2.648929042309D+00 Z= 1.076075411572D+00
I= 37 X= 5.483457090526D+00 Y= 1.149401615334D+00 Z= 1.904119268651D+00
I= 38 X= 3.000013708096D+00 Y= 3.951011028924D+00 Z= 2.158115826512D+00

Forward Direction:

Total Energy: -656.4330064 Hartrees

Potential Energy: -656.6383440 Hartress

Kinetic Energy: 0.2053376 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.832687069638D+12 Y= 1.737899505188D+13 Z= 2.388971383102D+12
I= 1 X= -1.477856053297D+13 Y= 2.306498042824D+13 Z= -1.679732826066D+13
I= 2 X= -1.584208043650D+12 Y= -1.702189403603D+13 Z= -1.275609296691D+13
I= 3 X= -1.426905152908D+12 Y= 2.088334784059D+12 Z= 3.654130894813D+12
I= 4 X= 3.354441287321D+12 Y= -3.485814626511D+12 Z= -2.259683670469D+12
I= 5 X= 8.701269943828D+12 Y= -5.380988535310D+12 Z= 1.085882587282D+13
I= 6 X= -1.687600493075D+13 Y= -1.166752636460D+13 Z= -9.860570300763D+13
I= 7 X= 7.019241458283D+13 Y= -7.181241531640D+13 Z= -1.131793760045D+14
I= 8 X= -4.769402966520D+13 Y= 1.774463722356D+13 Z= 2.878369789563D+13
I= 9 X= -5.535482964972D+12 Y= -1.427253742666D+13 Z= 1.046796470944D+13
I= 10 X= 6.051362308913D+13 Y= 5.820937396536D+13 Z= -2.553268283385D+13
I= 11 X= 1.174411157780D+13 Y= -1.116015151772D+14 Z= -3.494623685380D+13
I= 12 X= 8.705604450596D+13 Y= 9.263138582725D+13 Z= 2.758872077022D+13
I= 13 X= -1.115612278808D+13 Y= -1.608224366116D+13 Z= -4.327538248790D+12
I= 14 X= -5.415445703941D+13 Y= -3.625463511549D+13 Z= 1.184957019553D+14
I= 15 X= -4.899706078021D+13 Y= -1.865515679247D+13 Z= -3.537007085659D+13
I= 16 X= 1.457093887981D+14 Y= 1.576574489003D+13 Z= -8.237077476993D+13
I= 17 X= 5.857538134762D+12 Y= 1.476584981070D+13 Z= 1.247212710454D+13
I= 18 X= 3.620080501147D+13 Y= -3.407111785582D+13 Z= -1.152518892623D+13
I= 19 X= -5.476221104261D+13 Y= -1.395534016689D+14 Z= -1.158309535130D+14
I= 20 X= 2.514672430340D+13 Y= -1.434412106327D+14 Z= -1.644853204406D+12
I= 21 X= -6.519839126393D+12 Y= -1.231811077919D+13 Z= 8.128763552909D+12
I= 22 X= 1.361845822183D+14 Y= -6.008183304173D+13 Z= -9.795632114630D+11
I= 23 X= 7.417076449211D+13 Y= 4.391393043328D+13 Z= -1.673251689839D+13
I= 24 X= -9.308781984928D+12 Y= 2.609144564069D+13 Z= -4.639438871934D+11
I= 25 X= 6.624577153384D+12 Y= -1.566808075199D+13 Z= -8.244463437451D+12
I= 26 X= -1.505781317576D+13 Y= -1.149600008441D+13 Z= 1.279035588282D+14

I= 27 X= 2.115498194116D+12 Y= 3.334656227087D+13 Z= -5.312052224012D+13
I= 28 X= -9.379174796473D+12 Y= -6.482076946357D+12 Z= -4.472984106211D+13
I= 29 X= -8.115173930140D+12 Y= 7.560906092439D+12 Z= 2.318765168633D+12
I= 30 X= -1.191602596051D+13 Y= 1.656516170926D+13 Z= -6.425874831677D+12
I= 31 X= 9.253225660882D+13 Y= 4.909015467534D+13 Z= -1.066267515038D+14
I= 32 X= -4.369408005302D+13 Y= -5.938600776838D+13 Z= 5.686343312186D+13
I= 33 X= 6.367351640493D+12 Y= -2.831797604436D+12 Z= -2.589894499542D+13
I= 34 X= 3.734641439753D+13 Y= 5.701616750046D+13 Z= -5.013929103940D+13
I= 35 X= 4.362822150664D+11 Y= 3.365443009425D+12 Z= 4.063530382485D+12
I= 36 X= 6.412618061885D+10 Y= -9.688202203366D+12 Z= -2.675161758498D+11
I= 37 X= -8.102194377095D+13 Y= -4.238843217996D+13 Z= -3.163847857927D+13
I= 38 X= -7.265322911278D+13 Y= 1.610420917828D+14 Z= 8.418436576582D+13

Backward Direction:

Total Energy: -656.4330241 Hartrees

Potential Energy: -656.6383440 Hartress

Kinetic Energy: 0.2053199 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.528814065149D+12 Y= 1.698218097539D+13 Z= 2.544255256760D+12
I= 1 X= -1.524724741178D+13 Y= 2.204457482166D+13 Z= -1.740988059957D+13
I= 2 X= -2.020429363988D+12 Y= -1.662091010746D+13 Z= -1.340169406513D+13
I= 3 X= -2.320700094581D+12 Y= 2.109234249127D+12 Z= 2.359113902892D+12
I= 4 X= 4.883178423867D+12 Y= -3.622205763493D+12 Z= -3.275554082679D+12
I= 5 X= 6.178237629438D+12 Y= -8.969016291030D+12 Z= 3.695274281484D+12
I= 6 X= 3.963949661943D+13 Y= 5.285170492877D+13 Z= -7.317741812346D+13
I= 7 X= 8.051497271326D+13 Y= -6.203914852374D+13 Z= -1.125478441670D+14
I= 8 X= -3.465706474917D+13 Y= 2.828266512037D+13 Z= 2.999656293002D+13
I= 9 X= -5.049605559654D+12 Y= -1.404436026608D+13 Z= 9.918763340340D+12
I= 10 X= 6.060248617406D+13 Y= 5.933861387684D+13 Z= -2.684170593670D+13
I= 11 X= 1.160378056618D+13 Y= -1.116138595399D+14 Z= -3.497352484955D+13
I= 12 X= 8.734080280500D+13 Y= 9.270765494521D+13 Z= 2.731831379771D+13

I= 13 X= -1.105980468121D+13 Y= -1.612910836587D+13 Z= -4.530258337747D+12
I= 14 X= -5.399070941444D+13 Y= -3.654335166972D+13 Z= 1.185385571287D+14
I= 15 X= -4.869592792096D+13 Y= -1.893134765633D+13 Z= -3.586872475938D+13
I= 16 X= 1.456884119769D+14 Y= 1.585451288683D+13 Z= -8.230056920350D+13
I= 17 X= 6.005038455361D+12 Y= 1.444033855557D+13 Z= 1.243989202767D+13
I= 18 X= 3.623190470809D+13 Y= -3.459006915383D+13 Z= -1.195090562031D+13
I= 19 X= -5.507402375153D+13 Y= -1.396572741746D+14 Z= -1.155094259487D+14
I= 20 X= 2.536325636721D+13 Y= -1.437320661326D+14 Z= -1.681995915894D+12
I= 21 X= -6.705441452515D+12 Y= -1.243471030677D+13 Z= 7.675680001675D+12
I= 22 X= 1.361514135753D+14 Y= -5.955929936644D+13 Z= -2.795358244068D+12
I= 23 X= 7.484540927713D+13 Y= 4.362026478860D+13 Z= -1.694306713014D+13
I= 24 X= -9.634017831028D+12 Y= 2.590877977341D+13 Z= -9.996635822883D+11
I= 25 X= 6.422864670638D+12 Y= -1.587185254008D+13 Z= -8.348552604423D+12
I= 26 X= -1.555673654485D+13 Y= -1.204178369669D+13 Z= 1.278426835736D+14
I= 27 X= 2.531313220646D+12 Y= 3.369664476209D+13 Z= -5.324119991251D+13
I= 28 X= -9.358570061423D+12 Y= -7.099662047756D+12 Z= -4.429268819711D+13
I= 29 X= -9.049328958548D+12 Y= 7.823302962213D+12 Z= 1.991123176329D+12
I= 30 X= -1.186101441063D+13 Y= 1.638437912527D+13 Z= -6.831635521373D+12
I= 31 X= 9.188641054962D+13 Y= 4.889908437885D+13 Z= -1.066065710956D+14
I= 32 X= -4.558419026615D+13 Y= -5.781638614022D+13 Z= 5.573811881098D+13
I= 33 X= 6.425642970568D+12 Y= -3.060260986167D+12 Z= -2.622213486142D+13
I= 34 X= 3.795537470760D+13 Y= 5.659219343939D+13 Z= -5.025584093749D+13
I= 35 X= 4.261196506601D+11 Y= 3.602809043095D+12 Z= 5.569471634426D+12
I= 36 X= -3.220096593393D+12 Y= -1.383644618223D+13 Z= -1.781315212523D+12
I= 37 X= -7.809211308319D+13 Y= -4.090106064500D+13 Z= -3.529244632850D+13
I= 38 X= -7.104874016925D+13 Y= 1.608749011032D+14 Z= 8.145549346825D+13

Seed: 12310538170

CM Start Point Coordinates: bohr

I= 0 X= -2.082752440241D+00 Y= 2.335133067798D+00 Z= -7.513919510917D-01

I= 1 X= -2.805227021770D+00 Y= 5.417854831083D-02 Z= -1.939963552233D+00
I= 2 X= -1.934119979002D+00 Y= 1.737273609041D+00 Z= 1.958595314573D+00
I= 3 X= -2.583325352804D+00 Y= -2.096544768690D+00 Z= -3.034989067191D-01
I= 4 X= -2.228198228696D+00 Y= -9.991408699259D-01 Z= 2.208971001228D+00
I= 5 X= 4.339943750982D+00 Y= 2.551603631664D+00 Z= -1.369564571264D+00
I= 6 X= 2.255427291066D+00 Y= 3.471802181624D-01 Z= -3.060851589585D+00
I= 7 X= 5.917678127314D+00 Y= 1.465480840841D+00 Z= -2.046695164855D+00
I= 8 X= 3.867687084214D+00 Y= 3.953076534451D+00 Z= -2.649857670439D+00
I= 9 X= -2.251095723982D+00 Y= -2.168654736361D+00 Z= 4.682623049243D+00
I= 10 X= -3.960683245158D+00 Y= -1.766789788221D+00 Z= 5.711271808844D+00
I= 11 X= -2.191838553583D+00 Y= -4.605210842854D+00 Z= 4.467400242133D+00
I= 12 X= -6.374422616531D-01 Y= -1.913583894807D+00 Z= 5.862669212656D+00
I= 13 X= -1.822703404254D+00 Y= 3.454191381893D+00 Z= 4.226158303169D+00
I= 14 X= -3.454706085078D+00 Y= 2.985643378840D+00 Z= 5.865492530400D+00
I= 15 X= 5.956618287848D-01 Y= 3.103404672847D+00 Z= 5.081563587273D+00
I= 16 X= -2.349543499914D+00 Y= 5.774776462355D+00 Z= 3.272089265765D+00
I= 17 X= -2.315846979868D+00 Y= 5.069865107101D+00 Z= -1.480603986938D+00
I= 18 X= -4.155148169635D+00 Y= 5.724083737168D+00 Z= -1.230617534471D+00
I= 19 X= -1.159023255820D+00 Y= 6.156747588094D+00 Z= -3.323233234913D-01
I= 20 X= -1.502304884407D+00 Y= 5.298603424415D+00 Z= -3.325718635191D+00
I= 21 X= -3.647774994508D+00 Y= -1.774397762073D-01 Z= -4.663315410920D+00
I= 22 X= -5.915295651922D+00 Y= 7.882052610093D-01 Z= -4.620321492173D+00
I= 23 X= -2.440162820344D+00 Y= 1.199890147992D+00 Z= -5.660510629200D+00
I= 24 X= -3.383111432019D+00 Y= -2.017292053748D+00 Z= -5.781262239898D+00
I= 25 X= -2.979959907466D+00 Y= -4.806592215965D+00 Z= -6.615994743856D-01
I= 26 X= -3.109141288455D+00 Y= -5.107819680219D+00 Z= -2.774528760153D+00
I= 27 X= -1.340649745981D+00 Y= -5.778907293077D+00 Z= 2.197766017448D-01
I= 28 X= -4.985464078380D+00 Y= -5.331824028350D+00 Z= 1.039608575937D-01
I= 29 X= 3.258949189264D+00 Y= -3.648641164097D+00 Z= -1.546335803442D+00
I= 30 X= 3.756053550300D+00 Y= -3.145475927692D+00 Z= 9.192686606888D-01

I= 31 X= 1.631514956436D+00 Y= -5.037844255518D+00 Z= -1.818303167749D+00
I= 32 X= 4.426150617880D+00 Y= -2.921069406037D+00 Z= -2.916273949646D+00
I= 33 X= 5.645933075119D+00 Y= -2.510990471265D+00 Z= 1.351731338187D+00
I= 34 X= 3.022587477899D+00 Y= -4.081425049323D+00 Z= 2.444294973575D+00
I= 35 X= 1.161145955301D+00 Y= -9.881395600369D-02 Z= -3.265889399849D-01
I= 36 X= 3.788192957329D+00 Y= 2.519254591709D+00 Z= 1.272921244386D+00
I= 37 X= 5.238541329221D+00 Y= 2.244457189485D+00 Z= 2.650856537509D+00
I= 38 X= 2.632089579134D+00 Y= 4.035825731256D+00 Z= 2.143419073422D+00

Forward Direction:

Total Energy: -656.4390619 Hartrees

Potential Energy: -656.6058433 Hartress

Kinetic Energy: 0.1667815 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.471844738237D+12 Y= 3.307709300002D+12 Z= -3.801676550997D+11
I= 1 X= -5.616154989913D+12 Y= -4.389546024334D+12 Z= -1.720000755606D+13
I= 2 X= 3.635674330765D+12 Y= 2.572121399066D+13 Z= 1.558328755666D+13
I= 3 X= 1.493849656231D+13 Y= -2.438251332704D+13 Z= 7.993444305629D+12
I= 4 X= 8.576396972081D+12 Y= 3.687357530952D+12 Z= 3.747627973881D+11
I= 5 X= 1.680701664793D+13 Y= 1.376382002692D+13 Z= -1.388200320561D+13
I= 6 X= -1.424836461936D+13 Y= -1.203479761904D+14 Z= 7.386386789513D+13
I= 7 X= -3.079145084316D+13 Y= -4.012097290027D+13 Z= 1.396999397152D+13
I= 8 X= -1.156079800946D+13 Y= -1.073663673887D+14 Z= 9.261824412523D+13
I= 9 X= -1.245467900498D+13 Y= -3.776778912759D+12 Z= -6.553930430734D+12
I= 10 X= -3.647853649685D+13 Y= 3.917487470785D+13 Z= -3.024986164175D+13
I= 11 X= 8.958982774618D+13 Y= -1.106119482242D+14 Z= -5.397218813512D+13
I= 12 X= 1.180905410543D+14 Y= 7.767918812712D+13 Z= 4.313844271898D+13
I= 13 X= 1.908528839385D+12 Y= -1.825978854447D+13 Z= 3.303541615356D+12
I= 14 X= -3.914876520533D+13 Y= -2.570159948422D+13 Z= -9.377864651891D+12
I= 15 X= -1.009221328595D+14 Y= -2.109737101048D+12 Z= -6.003929277551D+13
I= 16 X= 2.578908611327D+13 Y= 2.747107300996D+13 Z= -1.305543478650D+13

I= 17 X= 5.913262071935D+12 Y= -1.885870222059D+13 Z= 7.558837342556D+12
I= 18 X= -4.681473502690D+13 Y= 6.003315234290D+13 Z= 8.023932188228D+13
I= 19 X= -5.756924218073D+13 Y= -2.861080965426D+13 Z= -8.392525227972D+13
I= 20 X= -1.327835372178D+13 Y= 3.994514169797D+13 Z= 2.163144479541D+11
I= 21 X= 3.082870009720D+11 Y= -2.677356509090D+13 Z= 6.268998893029D+12
I= 22 X= -9.740869291384D+12 Y= 1.878801399798D+13 Z= -8.240749371665D+13
I= 23 X= 2.079811885614D+13 Y= 1.670047287701D+13 Z= 2.273814062251D+13
I= 24 X= -4.558584355616D+13 Y= 9.966743470856D+13 Z= 5.953758827018D+13
I= 25 X= 3.914884349230D+12 Y= 2.252760658380D+13 Z= -1.394849440598D+13
I= 26 X= -3.928556394060D+13 Y= 8.423376118313D+12 Z= -7.658289183787D+13
I= 27 X= 3.217537621474D+13 Y= 8.167722589277D+13 Z= 6.855978277836D+13
I= 28 X= -1.945415856084D+13 Y= -5.220568100306D+13 Z= 2.302338357998D+13
I= 29 X= -7.785950204757D+12 Y= -9.986930309553D+12 Z= 1.985473803338D+13
I= 30 X= -8.319271197532D+12 Y= -6.425553110580D+12 Z= -1.372551801655D+13
I= 31 X= 4.956725037932D+13 Y= -6.763677557309D+12 Z= 1.858890826166D+13
I= 32 X= 2.670635437640D+13 Y= -1.355880731738D+13 Z= -7.600631290209D+13
I= 33 X= 3.506971272962D+13 Y= 4.941208677141D+13 Z= 7.308118291827D+13
I= 34 X= 1.463884496539D+13 Y= 8.134811405603D+13 Z= -4.757557256895D+13
I= 35 X= -3.025419238365D+12 Y= 4.776193956139D+12 Z= -1.677172204949D+12
I= 36 X= -3.637769961639D+12 Y= -3.611339388893D+12 Z= 1.627613298009D+13
I= 37 X= 4.024217496647D+13 Y= 4.458814020140D+13 Z= -6.295363482576D+13
I= 38 X= 6.321578449937D+13 Y= -6.012543028198D+13 Z= 6.060987356586D+13

Backward Direction:

Total Energy: -656.4390612 Hartrees

Potential Energy: -656.6058433 Hartress

Kinetic Energy: 0.1667822 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.992177600627D+12 Y= 2.681333578110D+12 Z= -1.350502206448D+11
I= 1 X= -6.355982781288D+12 Y= -6.000268364149D+12 Z= -1.816692868023D+13
I= 2 X= 2.947093809029D+12 Y= 2.635417187280D+13 Z= 1.456419857475D+13

I= 3 X= 1.352763065939D+13 Y= -2.434952327277D+13 Z= 5.949244640558D+12
I= 4 X= 1.098952665370D+13 Y= 3.472062504050D+12 Z= -1.228800682592D+12
I= 5 X= 1.282438024911D+13 Y= 8.100075706332D+12 Z= -2.518975425973D+13
I= 6 X= 7.496202414103D+13 Y= -1.850360520902D+13 Z= 1.140027168442D+14
I= 7 X= -1.449717053781D+13 Y= -2.469375547895D+13 Z= 1.496687446130D+13
I= 8 X= 9.018205565526D+12 Y= -9.073196550438D+13 Z= 9.453276595431D+13
I= 9 X= -1.168771576431D+13 Y= -3.416598561017D+12 Z= -7.420851296734D+12
I= 10 X= -3.633826506859D+13 Y= 4.095739329104D+13 Z= -3.231617012486D+13
I= 11 X= 8.936831358481D+13 Y= -1.106314339639D+14 Z= -5.401526255743D+13
I= 12 X= 1.185400353933D+14 Y= 7.779957982411D+13 Z= 4.271160210760D+13
I= 13 X= 2.060568115527D+12 Y= -1.833376503571D+13 Z= 2.983545551403D+12
I= 14 X= -3.889028763854D+13 Y= -2.615734198787D+13 Z= -9.310217260036D+12
I= 15 X= -1.004467910697D+14 Y= -2.545707645876D+12 Z= -6.082642386787D+13
I= 16 X= 2.575597395672D+13 Y= 2.761119434891D+13 Z= -1.294461447024D+13
I= 17 X= 6.146093072734D+12 Y= -1.937252559517D+13 Z= 7.507953888765D+12
I= 18 X= -4.676564378734D+13 Y= 5.921398157551D+13 Z= 7.956732304427D+13
I= 19 X= -5.806144222670D+13 Y= -2.877477363685D+13 Z= -8.341771722115D+13
I= 20 X= -1.293655530753D+13 Y= 3.948602283809D+13 Z= 1.576842365383D+11
I= 21 X= 1.531152736727D+10 Y= -2.695761882456D+13 Z= 5.553801139437D+12
I= 22 X= -9.793226389042D+12 Y= 1.961283960649D+13 Z= -8.527374769255D+13
I= 23 X= 2.186305364280D+13 Y= 1.623691818020D+13 Z= 2.240578459126D+13
I= 24 X= -4.609923220243D+13 Y= 9.937909447301D+13 Z= 5.869194838434D+13
I= 25 X= 3.596478803282D+12 Y= 2.220595040275D+13 Z= -1.411280038859D+13
I= 26 X= -4.007312038120D+13 Y= 7.561850217043D+12 Z= -7.667898416394D+13
I= 27 X= 3.283174516081D+13 Y= 8.222983525926D+13 Z= 6.836929164031D+13
I= 28 X= -1.942163373796D+13 Y= -5.318054640535D+13 Z= 2.371343455350D+13
I= 29 X= -9.260524982921D+12 Y= -9.572733741948D+12 Z= 1.933755126762D+13
I= 30 X= -8.232434813104D+12 Y= -6.710920561256D+12 Z= -1.436601607303D+13
I= 31 X= 4.854777472638D+13 Y= -7.065284282661D+12 Z= 1.862076327731D+13
I= 32 X= 2.372279301323D+13 Y= -1.108114098275D+13 Z= -7.778263487162D+13

I= 33 X= 3.516172629091D+13 Y= 4.905145461847D+13 Z= 7.257102388998D+13
I= 34 X= 1.560009603086D+13 Y= 8.067886597482D+13 Z= -4.775954795806D+13
I= 35 X= -3.041460966837D+12 Y= 5.150879052501D+12 Z= 6.999739025976D+11
I= 36 X= -8.821954520252D+12 Y= -1.015939165604D+13 Z= 1.388658326792D+13
I= 37 X= 4.486694741730D+13 Y= 4.693597379119D+13 Z= -6.872146620579D+13
I= 38 X= 6.574848930577D+13 Y= -6.038934275100D+13 Z= 5.630231631653D+13

Seed: 12336245867

CM Start Point Coordinates: bohr

I= 0 X= -2.112629277882D+00 Y= 2.332342470568D+00 Z= -5.328445435992D-01
I= 1 X= -2.813426986282D+00 Y= 9.769548338396D-02 Z= -2.037223048764D+00
I= 2 X= -1.975387032028D+00 Y= 1.575606981116D+00 Z= 2.034165348935D+00
I= 3 X= -2.525209382235D+00 Y= -2.044379121814D+00 Z= -2.838211794494D-01
I= 4 X= -2.057520961088D+00 Y= -1.038528884403D+00 Z= 2.324368216847D+00
I= 5 X= 4.569121832980D+00 Y= 2.598816307785D+00 Z= -1.334066922026D+00
I= 6 X= 2.510679178052D+00 Y= 3.603168630329D-01 Z= -2.918082695908D+00
I= 7 X= 6.377757309354D+00 Y= 1.583327191762D+00 Z= -1.638472915718D+00
I= 8 X= 4.157260841669D+00 Y= 4.277166150121D+00 Z= -2.839978400180D+00
I= 9 X= -2.251142387213D+00 Y= -2.232530308184D+00 Z= 4.725559019163D+00
I= 10 X= -4.060259225539D+00 Y= -2.907852797411D+00 Z= 5.146133283868D+00
I= 11 X= -1.113579699586D+00 Y= -4.083407635774D+00 Z= 4.756053558254D+00
I= 12 X= -1.322806525337D+00 Y= -1.194418996714D+00 Z= 6.262840257157D+00
I= 13 X= -1.959506050392D+00 Y= 3.414727380187D+00 Z= 4.331039788502D+00
I= 14 X= -3.831170765679D+00 Y= 3.479763428008D+00 Z= 5.018867050199D+00
I= 15 X= -7.009300721280D-01 Y= 2.967069026996D+00 Z= 6.077241133632D+00
I= 16 X= -1.577346803816D+00 Y= 5.714480454726D+00 Z= 3.877174589813D+00
I= 17 X= -2.088582289217D+00 Y= 4.991111340208D+00 Z= -1.582147914554D+00
I= 18 X= -3.919013086526D+00 Y= 5.555714544632D+00 Z= -2.115501342814D+00
I= 19 X= -1.422038155759D+00 Y= 6.336968294830D+00 Z= 1.629677217861D-02
I= 20 X= -6.080710820145D-01 Y= 4.919620661783D+00 Z= -3.398263049106D+00

I= 21 X= -3.721868337951D+00 Y= -4.715261336132D-01 Z= -4.638710771681D+00
I= 22 X= -5.881162541220D+00 Y= -1.534328065453D+00 Z= -4.525946527785D+00
I= 23 X= -4.128083245866D+00 Y= 1.817219708261D+00 Z= -5.596595087685D+00
I= 24 X= -2.506347973282D+00 Y= -1.581766964784D+00 Z= -5.714829476694D+00
I= 25 X= -3.349992679004D+00 Y= -4.625858330283D+00 Z= -8.023591799727D-01
I= 26 X= -4.077465373091D+00 Y= -5.012325209346D+00 Z= -2.985153478721D+00
I= 27 X= -1.609698052098D+00 Y= -6.051912299030D+00 Z= -4.385813649129D-01
I= 28 X= -5.149061609255D+00 Y= -5.575775095912D+00 Z= 5.591744422561D-01
I= 29 X= 2.907767032042D+00 Y= -3.579883698518D+00 Z= -1.528653218249D+00
I= 30 X= 3.947556801926D+00 Y= -3.015010463581D+00 Z= 8.568795503700D-01
I= 31 X= 1.193652299172D+00 Y= -4.871769779353D+00 Z= -1.829465340247D+00
I= 32 X= 4.278260628860D+00 Y= -3.443449690085D+00 Z= -3.297052596030D+00
I= 33 X= 5.929465008438D+00 Y= -2.573033228444D+00 Z= 1.047497585598D+00
I= 34 X= 3.069378425632D+00 Y= -3.447581879815D+00 Z= 3.078885599302D+00
I= 35 X= 1.185570731889D+00 Y= -8.913075876790D-02 Z= -3.661470250071D-01
I= 36 X= 3.871468964455D+00 Y= 2.710247580426D+00 Z= 1.335753616309D+00
I= 37 X= 4.737604154299D+00 Y= 1.776666911560D+00 Z= 2.870792588195D+00
I= 38 X= 2.420857931851D+00 Y= 4.102525624516D+00 Z= 1.824651637844D+00

Forward Direction:

Total Energy: -656.4193797 Hartrees

Potential Energy: -656.5953838 Hartress

Kinetic Energy: 0.1760041 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.334601132288D+12 Y= 1.260754612291D+13 Z= 2.383763616986D+13
I= 1 X= 1.754096364886D+13 Y= 6.550141886188D+12 Z= 7.839107878110D+12
I= 2 X= -1.173775370148D+13 Y= -9.361714301597D+11 Z= -1.463705758361D+13
I= 3 X= 7.721999790841D+12 Y= -1.820455544626D+13 Z= -1.883948201365D+13
I= 4 X= -3.330413544257D+12 Y= 2.778189850893D+13 Z= 8.402722757559D+12
I= 5 X= 6.386863305974D+12 Y= 1.711027228245D+13 Z= -1.492503898694D+13
I= 6 X= 2.182009631598D+13 Y= -2.755145959460D+13 Z= -4.958867625321D+13

I= 7 X= -2.874050543854D+13 Y= -2.272562615823D+13 Z= 3.404340262226D+13
I= 8 X= -8.498549862760D+13 Y= -8.146359796887D+13 Z= 8.967041970283D+13
I= 9 X= 5.097767737893D+12 Y= 2.566365721279D+13 Z= 6.470706361054D+12
I= 10 X= 7.588865868897D+12 Y= -1.360309466380D+13 Z= -3.360126808709D+13
I= 11 X= -6.408539228334D+12 Y= -5.437239529010D+13 Z= -4.105042318764D+13
I= 12 X= -1.141726225960D+14 Y= 3.591151937574D+13 Z= -7.543824559019D+13
I= 13 X= -8.791623222500D+12 Y= 1.469279483422D+13 Z= -7.229061872609D+12
I= 14 X= 3.799554856823D+13 Y= -1.061663705956D+14 Z= 4.942647254033D+12
I= 15 X= 2.044582698453D+13 Y= -4.059049612207D+13 Z= 2.374050762994D+13
I= 16 X= 9.847339767786D+12 Y= -4.416337297291D+13 Z= -1.220548218838D+13
I= 17 X= 5.469451363342D+11 Y= 2.512717210817D+13 Z= -2.429441081422D+13
I= 18 X= 6.573624544048D+13 Y= -8.207527778025D+13 Z= 5.762041259308D+13
I= 19 X= 3.068552372404D+13 Y= 6.859472452744D+13 Z= 9.145226429168D+13
I= 20 X= 5.430335938124D+13 Y= -2.298879539856D+13 Z= 1.146558396292D+14
I= 21 X= 4.794883718953D+12 Y= -4.981421002023D+12 Z= -2.580508091058D+13
I= 22 X= 2.568024316625D+13 Y= 3.834917214692D+13 Z= 4.685740977373D+13
I= 23 X= -5.664767264083D+13 Y= -7.494322158761D+12 Z= -2.146930607271D+13
I= 24 X= 5.018695357968D+13 Y= 8.056314718542D+13 Z= -2.726468842825D+13
I= 25 X= -1.069444155821D+13 Y= -9.861802104230D+12 Z= -1.600264420902D+13
I= 26 X= -3.582009332999D+13 Y= 4.827596579063D+12 Z= 6.662280847922D+13
I= 27 X= -1.055965900955D+13 Y= 7.338270574734D+13 Z= -1.912788219177D+13
I= 28 X= 4.197368847578D+13 Y= -3.233994101255D+13 Z= 2.242290488788D+13
I= 29 X= -9.572111948748D+12 Y= 1.734555780672D+13 Z= -4.726877407370D+12
I= 30 X= -1.233375919979D+13 Y= -2.367886434981D+13 Z= 5.427036497651D+11
I= 31 X= -1.502037063438D+13 Y= 2.334944187264D+13 Z= 3.864183353216D+13
I= 32 X= 9.901256186208D+13 Y= -3.331181881753D+13 Z= -8.530289386166D+13
I= 33 X= -8.683703478221D+12 Y= 2.216336430678D+13 Z= -3.245100500448D+13
I= 34 X= 2.940822284498D+13 Y= -3.246787253006D+13 Z= -1.578971088976D+14
I= 35 X= 1.042923727190D+12 Y= -9.142178697844D+12 Z= 7.253913405034D+12
I= 36 X= 1.859999139869D+11 Y= 4.879376661236D+12 Z= 1.387161906287D+13

I= 37 X= -1.054211176842D+13 Y= 9.628402732031D+13 Z= 3.847322871954D+13

I= 38 X= 2.663411195049D+13 Y= -2.902184238678D+13 Z= -3.457384155122D+13

Backward Direction:

Total Energy: -656.4193922 Hartrees

Potential Energy: -656.5953838 Hartress

Kinetic Energy: 0.1759916 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.513185154416D+12 Y= 1.237434128644D+13 Z= 2.392889540806D+13

I= 1 X= 1.726551967376D+13 Y= 5.950456703220D+12 Z= 7.479115186290D+12

I= 2 X= -1.199411789580D+13 Y= -7.005160028027D+11 Z= -1.501647279823D+13

I= 3 X= 7.196722805267D+12 Y= -1.819227297851D+13 Z= -1.960055437023D+13

I= 4 X= -2.431985506094D+12 Y= 2.770174239847D+13 Z= 7.805702877547D+12

I= 5 X= 4.904095001730D+12 Y= 1.500161366712D+13 Z= -1.913500775544D+13

I= 6 X= 5.503385815576D+13 Y= 1.036603778852D+13 Z= -3.464465249097D+13

I= 7 X= -2.267401079642D+13 Y= -1.698194616214D+13 Z= 3.441454943216D+13

I= 8 X= -7.732376625543D+13 Y= -7.527047326298D+13 Z= 9.038321193402D+13

I= 9 X= 5.383314459936D+12 Y= 2.579775532145D+13 Z= 6.147944588735D+12

I= 10 X= 7.641090073942D+12 Y= -1.293944832771D+13 Z= -3.437057173535D+13

I= 11 X= -6.491010774135D+12 Y= -5.437964998211D+13 Z= -4.106646014587D+13

I= 12 X= -1.140052721553D+14 Y= 3.595634220388D+13 Z= -7.559716185926D+13

I= 13 X= -8.735017748609D+12 Y= 1.466525277802D+13 Z= -7.348199041611D+12

I= 14 X= 3.809178189540D+13 Y= -1.063360472819D+14 Z= 4.967832936715D+12

I= 15 X= 2.062280064648D+13 Y= -4.075281154521D+13 Z= 2.344745224359D+13

I= 16 X= 9.835011840133D+12 Y= -4.411120464820D+13 Z= -1.216422287069D+13

I= 17 X= 6.336300331181D+11 Y= 2.493587143714D+13 Z= -2.431335514110D+13

I= 18 X= 6.575452251128D+13 Y= -8.238026179991D+13 Z= 5.737022189521D+13

I= 19 X= 3.050227359316D+13 Y= 6.853367938812D+13 Z= 9.164122377259D+13

I= 20 X= 5.443061374573D+13 Y= -2.315972912917D+13 Z= 1.146340111208D+14

I= 21 X= 4.685806539662D+12 Y= -5.049945718845D+12 Z= -2.607135491978D+13

I= 22 X= 2.566075018900D+13 Y= 3.865626151923D+13 Z= 4.579027983053D+13

I= 23 X= -5.625118864807D+13 Y= -7.666907388351D+12 Z= -2.159304495779D+13
I= 24 X= 4.999581475081D+13 Y= 8.045579574170D+13 Z= -2.757952711715D+13
I= 25 X= -1.081298656520D+13 Y= -9.981557348439D+12 Z= -1.606381667694D+13
I= 26 X= -3.611330707596D+13 Y= 4.506843399173D+12 Z= 6.658703252337D+13
I= 27 X= -1.031528744925D+13 Y= 7.358844675805D+13 Z= -1.919880360654D+13
I= 28 X= 4.198579773325D+13 Y= -3.270289142862D+13 Z= 2.267981655106D+13
I= 29 X= -1.012110827106D+13 Y= 1.749976659741D+13 Z= -4.919430296532D+12
I= 30 X= -1.230142929885D+13 Y= -2.378510900082D+13 Z= 3.042409529256D+11
I= 31 X= -1.539992980890D+13 Y= 2.323715120687D+13 Z= 3.865369341478D+13
I= 32 X= 9.790175741851D+13 Y= -3.238936325086D+13 Z= -8.596423314800D+13
I= 33 X= -8.649446074876D+12 Y= 2.202909798681D+13 Z= -3.264094140809D+13
I= 34 X= 2.976610452796D+13 Y= -3.271703909715D+13 Z= -1.579656044515D+14
I= 35 X= 1.036951260128D+12 Y= -9.002680353261D+12 Z= 8.138944462064D+12
I= 36 X= -1.744114657311D+12 Y= 2.441482919994D+12 Z= 1.298197004120D+13
I= 37 X= -8.820270926897D+12 Y= 9.715814508743D+13 Z= 3.632581763377D+13
I= 38 X= 2.757705879128D+13 Y= -2.912009917129D+13 Z= -3.617758056144D+13

Seed: 12341092432

CM Start Point Coordinates: bohr

I= 0 X= -2.084818210621D+00 Y= 2.205886919071D+00 Z= -6.312169122025D-01
I= 1 X= -2.849771968370D+00 Y= 4.350812195442D-02 Z= -1.959014134451D+00
I= 2 X= -2.078178474485D+00 Y= 1.571597700196D+00 Z= 2.219469149728D+00
I= 3 X= -2.773049466441D+00 Y= -2.100436504002D+00 Z= -2.614933330819D-01
I= 4 X= -2.167264814511D+00 Y= -1.194902365693D+00 Z= 2.408248420828D+00
I= 5 X= 4.515377556909D+00 Y= 2.398917629714D+00 Z= -1.598431457283D+00
I= 6 X= 2.856555434513D+00 Y= 4.619550209555D-01 Z= -3.325580267763D+00
I= 7 X= 6.092015035720D+00 Y= 1.235146169916D+00 Z= -1.662484284105D+00
I= 8 X= 4.189572534304D+00 Y= 3.901269572000D+00 Z= -3.231459917837D+00
I= 9 X= -2.168895731112D+00 Y= -2.750592013296D+00 Z= 4.680124704044D+00
I= 10 X= -4.136855192339D+00 Y= -3.258108085486D+00 Z= 5.109817214111D+00

I= 11 X= -8.080572025820D-01 Y= -4.345365462929D+00 Z= 4.589282898468D+00
I= 12 X= -1.577370256820D+00 Y= -1.641068716611D+00 Z= 6.493452790192D+00
I= 13 X= -1.741750943129D+00 Y= 3.566798229367D+00 Z= 4.371936152123D+00
I= 14 X= -3.431928485498D+00 Y= 3.185810610411D+00 Z= 5.263659860348D+00
I= 15 X= -3.142120414594D-01 Y= 2.706942613944D+00 Z= 5.868448633737D+00
I= 16 X= -1.229739673309D+00 Y= 5.343723161068D+00 Z= 3.682477922741D+00
I= 17 X= -1.926574093740D+00 Y= 4.959111809689D+00 Z= -1.510752987037D+00
I= 18 X= -3.497079479877D+00 Y= 6.279100766257D+00 Z= -1.694557438354D+00
I= 19 X= -7.711256879540D-01 Y= 6.276656133323D+00 Z= -4.499338398230D-01
I= 20 X= -1.023619426490D+00 Y= 4.863373521050D+00 Z= -3.258192338253D+00
I= 21 X= -3.869925963668D+00 Y= 3.047648487886D-02 Z= -4.489792602207D+00
I= 22 X= -5.864125684245D+00 Y= -5.413179114980D-01 Z= -4.383323440127D+00
I= 23 X= -3.402343156676D+00 Y= 1.640104794788D+00 Z= -6.057988406628D+00
I= 24 X= -2.804154009299D+00 Y= -1.344233928331D+00 Z= -5.671325189276D+00
I= 25 X= -3.315222026611D+00 Y= -4.730545962888D+00 Z= -7.010304764472D-01
I= 26 X= -3.179977411834D+00 Y= -5.142415944246D+00 Z= -2.690525612983D+00
I= 27 X= -2.024888930260D+00 Y= -6.103900416395D+00 Z= 1.058205025551D-01
I= 28 X= -5.405256267252D+00 Y= -5.433740748941D+00 Z= -1.251466829336D-01
I= 29 X= 3.654874613279D+00 Y= -3.438217280961D+00 Z= -1.146594027436D+00
I= 30 X= 3.453690440720D+00 Y= -3.296807158057D+00 Z= 1.457351275660D+00
I= 31 X= 2.170571322697D+00 Y= -4.730609138191D+00 Z= -2.064896609254D+00
I= 32 X= 5.509904250688D+00 Y= -3.134658097266D+00 Z= -2.139079330994D+00
I= 33 X= 4.915563744118D+00 Y= -2.524152072453D+00 Z= 2.715241513647D+00
I= 34 X= 2.221773263034D+00 Y= -4.035669780253D+00 Z= 2.573022321542D+00
I= 35 X= 1.171934173255D+00 Y= -3.945162602755D-02 Z= -4.829946944263D-01
I= 36 X= 3.670014416341D+00 Y= 3.069460580291D+00 Z= 9.818661196226D-01
I= 37 X= 4.633271544109D+00 Y= 2.063411180762D+00 Z= 2.335083022772D+00
I= 38 X= 2.496105965821D+00 Y= 4.326056138307D+00 Z= 1.842693499525D+00

Forward Direction:

Total Energy: -656.4393488 Hartrees

Potential Energy: -656.6355684 Hartress

Kinetic Energy: 0.1962196 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.195802366676D+12 Y= 1.059226738464D+13 Z= -1.010208748636D+13
I= 1 X= -6.727507711448D+11 Y= 2.182245131009D+13 Z= -1.093912543508D+13
I= 2 X= 6.141421856220D+12 Y= 2.319600725964D+12 Z= 1.324748597590D+13
I= 3 X= 1.452535791471D+13 Y= -2.622754534215D+12 Z= -1.084994723506D+13
I= 4 X= -1.995026257846D+13 Y= -3.079929184958D+13 Z= 9.912792913635D+12
I= 5 X= 5.505112385142D+12 Y= -2.904336176827D+12 Z= -9.483592511438D+12
I= 6 X= 1.584637047428D+12 Y= -4.203714429543D+13 Z= 7.870579787939D+11
I= 7 X= 3.743135110254D+13 Y= -1.359332710571D+13 Z= -2.422365389756D+13
I= 8 X= -9.608084911716D+13 Y= 9.528662490381D+13 Z= -7.503950677803D+13
I= 9 X= 1.109550319047D+13 Y= -1.085634132608D+13 Z= -1.916635484223D+13
I= 10 X= -1.082006393855D+14 Y= -5.604483674700D+13 Z= 4.825778330106D+13
I= 11 X= 9.991195011968D+12 Y= 1.013044455520D+14 Z= 3.047457084387D+12
I= 12 X= -5.887721712148D+12 Y= 1.804570166616D+13 Z= 9.370925050132D+13
I= 13 X= 1.854858084795D+12 Y= 6.982496440517D+12 Z= 1.265114320913D+13
I= 14 X= -8.174157083451D+12 Y= -5.413529429733D+13 Z= 1.108593552008D+13
I= 15 X= -2.183972521901D+13 Y= 1.314857411447D+13 Z= -1.377511179025D+14
I= 16 X= -1.254482629895D+13 Y= -3.738044626406D+13 Z= 1.159300781491D+13
I= 17 X= -2.777635972540D+13 Y= -2.243177005640D+13 Z= -4.243537894455D+12
I= 18 X= 6.605892478422D+12 Y= -8.042740970537D+13 Z= 7.629603636535D+13
I= 19 X= 6.535427094998D+13 Y= -2.310449409982D+12 Z= -1.976270008332D+13
I= 20 X= 1.354797386992D+14 Y= -3.847653756730D+13 Z= -7.368576391189D+13
I= 21 X= -6.350071071769D+12 Y= 1.020511370218D+13 Z= 7.998019286261D+12
I= 22 X= -2.113271220295D+13 Y= -2.974383084333D+12 Z= 2.937632219408D+13
I= 23 X= -1.263273719830D+13 Y= -9.404720227752D+12 Z= -6.932520087552D+13
I= 24 X= 1.529217048748D+13 Y= -1.355157392832D+14 Z= -1.062544872745D+14
I= 25 X= -4.705949152485D+12 Y= 2.669705899997D+12 Z= 1.239171338311D+13
I= 26 X= -2.503708769317D+13 Y= -7.627060542092D+12 Z= -1.086953504825D+14

I= 27 X= 6.360259076919D+13 Y= 4.525800350605D+13 Z= 5.579357636214D+13
I= 28 X= -4.573920440300D+13 Y= -5.451169840282D+13 Z= -3.366374131326D+13
I= 29 X= -1.483445090254D+12 Y= -2.306073539586D+13 Z= -2.077581135414D+13
I= 30 X= 5.984179113270D+12 Y= -8.040964703804D+12 Z= 1.454109239754D+13
I= 31 X= 8.059461290119D+13 Y= 2.263212773420D+13 Z= 5.871244875056D+13
I= 32 X= 1.624127463688D+13 Y= 8.407172988953D+13 Z= -4.265037183720D+13
I= 33 X= -7.419064201112D+13 Y= -6.078759600041D+13 Z= -2.268237918397D+13
I= 34 X= 6.123025774585D+13 Y= 9.261797177050D+13 Z= 1.984418210245D+13
I= 35 X= -1.107056767103D+12 Y= 5.079214217129D+12 Z= 1.642035727152D+12
I= 36 X= 3.394013241156D+13 Y= 9.105758070918D+12 Z= 2.800937757326D+13
I= 37 X= -9.133445511275D+13 Y= 3.748322000463D+13 Z= -2.696328233516D+13
I= 38 X= -9.932693690077D+13 Y= 7.537433939197D+12 Z= 7.468119966208D+12

Backward Direction:

Total Energy: -656.4392944 Hartrees

Potential Energy: -656.6355684 Hartress

Kinetic Energy: 0.1962740 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.910028267379D+12 Y= 1.021908785398D+13 Z= -9.956052437916D+12
I= 1 X= -1.113522306551D+12 Y= 2.086282182994D+13 Z= -1.151519369552D+13
I= 2 X= 5.731182209358D+12 Y= 2.696701748571D+12 Z= 1.264033736376D+13
I= 3 X= 1.368479807241D+13 Y= -2.603099856905D+12 Z= -1.206783203964D+13
I= 4 X= -1.851257817599D+13 Y= -3.092755942891D+13 Z= 8.957428509268D+12
I= 5 X= 3.132353777048D+12 Y= -6.278658294580D+12 Z= -1.622047757106D+13
I= 6 X= 5.473403274480D+13 Y= 1.863927296799D+13 Z= 2.470081505592D+13
I= 7 X= 4.713908989388D+13 Y= -4.402163446257D+12 Z= -2.362973656953D+13
I= 8 X= -8.382037565370D+13 Y= 1.051969999214D+14 Z= -7.389888089610D+13
I= 9 X= 1.155244136853D+13 Y= -1.064175456929D+13 Z= -1.968284536333D+13
I= 10 X= -1.081170690528D+14 Y= -5.498285521334D+13 Z= 4.702672661012D+13
I= 11 X= 9.859222221900D+12 Y= 1.012928364192D+14 Z= 3.021794379419D+12
I= 12 X= -5.619923827836D+12 Y= 1.811742813422D+13 Z= 9.345494916419D+13

I= 13 X= 1.945439413081D+12 Y= 6.938423032147D+12 Z= 1.246049727945D+13
I= 14 X= -8.020162385265D+12 Y= -5.440681467234D+13 Z= 1.112623821339D+13
I= 15 X= -2.155652805599D+13 Y= 1.288883338370D+13 Z= -1.382200716097D+14
I= 16 X= -1.256455372061D+13 Y= -3.729696535741D+13 Z= 1.165903188099D+13
I= 17 X= -2.763764463789D+13 Y= -2.273789361489D+13 Z= -4.273853023456D+12
I= 18 X= 6.635139854152D+12 Y= -8.091545187299D+13 Z= 7.589567568575D+13
I= 19 X= 6.506103003573D+13 Y= -2.408135197348D+12 Z= -1.946032295190D+13
I= 20 X= 1.356833739411D+14 Y= -3.875006949677D+13 Z= -7.372069438587D+13
I= 21 X= -6.524618782904D+12 Y= 1.009545893045D+13 Z= 7.571921731523D+12
I= 22 X= -2.116390529564D+13 Y= -2.482971905219D+12 Z= 2.766867728042D+13
I= 23 X= -1.199827476073D+13 Y= -9.680894928656D+12 Z= -6.952321057745D+13
I= 24 X= 1.498630593225D+13 Y= -1.356875254353D+14 Z= -1.067582991026D+14
I= 25 X= -4.895647491034D+12 Y= 2.478070913372D+12 Z= 1.229382384825D+13
I= 26 X= -2.550629481594D+13 Y= -8.140336871880D+12 Z= -1.087525999693D+14
I= 27 X= 6.399363954106D+13 Y= 4.558723481854D+13 Z= 5.568008633990D+13
I= 28 X= -4.571982689683D+13 Y= -5.509249966951D+13 Z= -3.325262559765D+13
I= 29 X= -2.361961141627D+12 Y= -2.281396708193D+13 Z= -2.108393874123D+13
I= 30 X= 6.035914135112D+12 Y= -8.210979741255D+12 Z= 1.415949912060D+13
I= 31 X= 7.998723391772D+13 Y= 2.245243773044D+13 Z= 5.873142720169D+13
I= 32 X= 1.446374081154D+13 Y= 8.554786367038D+13 Z= -4.370866157865D+13
I= 33 X= -7.413582255260D+13 Y= -6.100245193023D+13 Z= -2.298631961605D+13
I= 34 X= 6.180294792305D+13 Y= 9.221924992319D+13 Z= 1.973457400890D+13
I= 35 X= -1.116614041361D+12 Y= 5.302442551329D+12 Z= 3.058281982971D+12
I= 36 X= 3.085152042076D+13 Y= 5.204586629099D+12 Z= 2.658574154905D+13
I= 37 X= -8.857912734908D+13 Y= 3.888200257030D+13 Z= -3.039961700915D+13
I= 38 X= -9.781801252930D+13 Y= 7.380201260914D+12 Z= 4.901781361782D+12

Seed: 13240811936

CM Start Point Coordinates: bohr

I= 0 X= -2.197069500830D+00 Y= 2.343846123339D+00 Z= -5.506482787344D-01

I= 1 X= -2.775815433694D+00 Y= 1.615660523827D-01 Z= -1.992074324096D+00
I= 2 X= -1.977586470468D+00 Y= 1.605932742368D+00 Z= 2.105049881958D+00
I= 3 X= -2.728515062619D+00 Y= -2.004013635777D+00 Z= -3.461737705833D-01
I= 4 X= -2.029437600941D+00 Y= -1.113779874470D+00 Z= 2.123799944929D+00
I= 5 X= 3.849116412587D+00 Y= 2.601783881924D+00 Z= -2.124741070552D+00
I= 6 X= 2.368222227834D+00 Y= -3.309300393712D-01 Z= -3.091870564498D+00
I= 7 X= 5.579073280154D+00 Y= 1.712455796533D+00 Z= -2.945225609479D+00
I= 8 X= 2.175318940208D+00 Y= 3.958035299128D+00 Z= -3.342287015517D+00
I= 9 X= -2.108106656132D+00 Y= -2.992340385459D+00 Z= 4.448443590570D+00
I= 10 X= -4.349773399022D+00 Y= -3.173239980776D+00 Z= 4.887181075176D+00
I= 11 X= -1.902494647038D+00 Y= -4.889905794775D+00 Z= 3.852625059904D+00
I= 12 X= -9.224008897120D-01 Y= -2.071191997532D+00 Z= 5.969888402217D+00
I= 13 X= -1.540574217423D+00 Y= 3.280754257472D+00 Z= 4.312254945525D+00
I= 14 X= -3.428131510979D+00 Y= 3.674113309553D+00 Z= 5.459263388833D+00
I= 15 X= -1.799027093812D-01 Y= 2.204175629552D+00 Z= 5.608472513206D+00
I= 16 X= -5.602775528880D-01 Y= 5.301955014333D+00 Z= 4.307441664954D+00
I= 17 X= -1.995340392877D+00 Y= 4.989603533305D+00 Z= -1.423307071469D+00
I= 18 X= -3.576644618905D+00 Y= 6.059244013402D+00 Z= -1.084190729037D+00
I= 19 X= -3.064742481490D-01 Y= 5.792247956656D+00 Z= -4.880129229885D-01
I= 20 X= -1.886457086404D+00 Y= 5.004603340134D+00 Z= -3.614836960333D+00
I= 21 X= -3.463105762647D+00 Y= 2.526622570067D-01 Z= -4.804706549960D+00
I= 22 X= -5.420796407303D+00 Y= 1.171088552238D+00 Z= -5.256364376390D+00
I= 23 X= -1.820278933283D+00 Y= 1.855862532177D+00 Z= -5.379243763895D+00
I= 24 X= -3.356951377398D+00 Y= -1.795351302099D+00 Z= -5.631598306057D+00
I= 25 X= -3.232420200858D+00 Y= -4.804026679666D+00 Z= -7.299899619914D-01
I= 26 X= -4.081861781518D+00 Y= -5.152141471885D+00 Z= -3.047442625749D+00
I= 27 X= -1.238765117577D+00 Y= -5.902345007585D+00 Z= -1.522357618191D-01
I= 28 X= -4.879742106510D+00 Y= -5.363770861271D+00 Z= 6.604265599624D-01
I= 29 X= 3.428915025576D+00 Y= -3.653995541644D+00 Z= -7.827506214367D-01
I= 30 X= 3.335642986503D+00 Y= -3.023854470217D+00 Z= 1.810861469299D+00

I= 31 X= 2.326449626385D+00 Y= -4.928512306323D+00 Z= -1.975435317363D+00
I= 32 X= 5.155715303500D+00 Y= -3.108222846618D+00 Z= -1.735262879890D+00
I= 33 X= 4.762176087621D+00 Y= -2.072685695312D+00 Z= 2.795442785951D+00
I= 34 X= 1.855104516132D+00 Y= -3.902300255754D+00 Z= 3.256703133496D+00
I= 35 X= 1.170449677675D+00 Y= -9.528321403703D-02 Z= -3.211050114624D-01
I= 36 X= 3.819391198206D+00 Y= 3.078291809829D+00 Z= 5.194640439594D-01
I= 37 X= 5.713078753142D+00 Y= 2.352260209961D+00 Z= 1.604997011107D+00
I= 38 X= 2.949125785866D+00 Y= 4.731675393065D+00 Z= 1.581497936487D+00

Forward Direction:

Total Energy: -656.4333339 Hartrees

Potential Energy: -656.6094370 Hartress

Kinetic Energy: 0.1761031 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.718978389507D+12 Y= -1.855235060580D+12 Z= 7.538876019127D+12
I= 1 X= -6.975713014937D+12 Y= -2.953768602091D+12 Z= 1.553748368518D+13
I= 2 X= 3.526813199037D+12 Y= -1.072621627691D+13 Z= -6.228495975733D+12
I= 3 X= -6.293539173342D+12 Y= 1.921274351433D+13 Z= 7.098211686657D+12
I= 4 X= -8.362886127721D+12 Y= 1.933459786919D+12 Z= 1.352728782665D+12
I= 5 X= -9.514535845661D+11 Y= 3.999685199991D+12 Z= 2.334382357310D+13
I= 6 X= 3.163802909356D+13 Y= -1.769202498594D+13 Z= -7.921679531839D+13
I= 7 X= 1.336241307566D+13 Y= -2.182351506585D+13 Z= 4.442249226310D+13
I= 8 X= 3.801504381024D+13 Y= -6.175946462630D+13 Z= 6.273977166146D+13
I= 9 X= 1.884665000145D+13 Y= 1.619987235839D+13 Z= -1.030604503731D+13
I= 10 X= -5.480276146397D+13 Y= -2.445825088395D+13 Z= 4.301444760111D+12
I= 11 X= -4.260153406007D+13 Y= -2.413768188082D+13 Z= -3.004019850423D+13
I= 12 X= -8.203142898818D+13 Y= -1.069262882965D+14 Z= -1.320161590146D+14
I= 13 X= -8.398231368851D+11 Y= -6.270142295324D+12 Z= -1.423393244584D+13
I= 14 X= 1.177165940704D+14 Y= 4.269112234761D+12 Z= 3.743894846678D+12
I= 15 X= 6.333183336958D+13 Y= -2.162372144364D+13 Z= 1.281396364308D+13
I= 16 X= -1.425378484863D+13 Y= -2.945456625151D+13 Z= 1.057046706814D+14

I= 17 X= 1.429240999396D+13 Y= 1.755967451133D+13 Z= -1.339482217187D+12
I= 18 X= 9.576980130269D+12 Y= -6.078957622400D+13 Z= 7.869776315067D+13
I= 19 X= -7.298978991858D+13 Y= -3.605118554102D+13 Z= -3.352352024009D+13
I= 20 X= 2.027690817797D+13 Y= -2.736199799366D+12 Z= 4.704253202867D+13
I= 21 X= -1.044785402866D+12 Y= -1.318913363116D+10 Z= 4.999540219113D+12
I= 22 X= -3.062688370063D+13 Y= 4.804237623869D+13 Z= 1.339697228780D+13
I= 23 X= -2.328826292724D+13 Y= 1.597799979464D+13 Z= 1.226209156650D+13
I= 24 X= 1.470692894398D+14 Y= -1.658572761381D+14 Z= -1.678987959444D+13
I= 25 X= -1.305049095896D+13 Y= 2.092627943560D+12 Z= -4.597093601895D+12
I= 26 X= 5.648704172226D+13 Y= -8.954337597333D+13 Z= -1.131787847066D+14
I= 27 X= -2.750340829737D+13 Y= 5.336926462344D+13 Z= -3.575739521084D+12
I= 28 X= -6.615930806004D+13 Y= -1.325372625873D+14 Z= 6.114153821645D+13
I= 29 X= 1.283948176525D+13 Y= -6.148025977416D+12 Z= -1.561470604423D+13
I= 30 X= 8.955864068518D+12 Y= -1.643221006338D+13 Z= 8.529714490458D+12
I= 31 X= 3.666556510497D+13 Y= 6.884521114230D+13 Z= 6.039718298142D+13
I= 32 X= 8.007806748946D+13 Y= 9.098432639455D+13 Z= 2.879430410250D+13
I= 33 X= 2.333110102356D+13 Y= -3.689853550276D+13 Z= -4.197038645080D+13
I= 34 X= 1.692410144304D+12 Y= 9.811626464216D+13 Z= -7.502924814980D+13
I= 35 X= -3.956030349041D+12 Y= 1.625669642405D+12 Z= -7.607748609832D+11
I= 36 X= -4.925247334637D+12 Y= 1.008931939138D+13 Z= -1.437038300889D+13
I= 37 X= 5.945642397144D+13 Y= 1.525478030901D+13 Z= 2.879733105654D+13
I= 38 X= -3.126938680384D+12 Y= -4.633726958158D+13 Z= 1.840076181695D+13

Backward Direction:

Total Energy: -656.4333899 Hartrees

Potential Energy: -656.6094370 Hartress

Kinetic Energy: 0.1760471 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.940006491132D+12 Y= -2.143865709621D+12 Z= 7.651824848387D+12

I= 1 X= -7.316621782767D+12 Y= -3.695981011731D+12 Z= 1.509193149973D+13

I= 2 X= 3.209518904467D+12 Y= -1.043455260469D+13 Z= -6.698086836349D+12

I= 3 X= -6.943658785008D+12 Y= 1.922794515842D+13 Z= 6.156255198966D+12
I= 4 X= -7.250928623045D+12 Y= 1.834252966735D+12 Z= 6.138151380918D+11
I= 5 X= -2.786631557014D+12 Y= 1.389861513259D+12 Z= 1.813327117247D+13
I= 6 X= 7.274570851258D+13 Y= 2.923732720195D+13 Z= -6.072102416703D+13
I= 7 X= 2.087073201013D+13 Y= -1.471473416175D+13 Z= 4.488184956693D+13
I= 8 X= 4.749774075890D+13 Y= -5.409441945013D+13 Z= 6.362197328316D+13
I= 9 X= 1.920006264208D+13 Y= 1.636584157616D+13 Z= -1.070551762667D+13
I= 10 X= -5.473812512637D+13 Y= -2.363687565573D+13 Z= 3.349300649734D+12
I= 11 X= -4.270360663900D+13 Y= -2.414666080527D+13 Z= -3.006004696565D+13
I= 12 X= -8.182430434542D+13 Y= -1.068708124332D+14 Z= -1.322128449273D+14
I= 13 X= -7.697642360397D+11 Y= -6.304230274680D+12 Z= -1.438138495570D+13
I= 14 X= 1.178356991732D+14 Y= 4.059108473157D+12 Z= 3.775066403479D+12
I= 15 X= 6.355086837044D+13 Y= -2.182461438681D+13 Z= 1.245125776440D+13
I= 16 X= -1.426904276011D+13 Y= -2.938999907384D+13 Z= 1.057557361041D+14
I= 17 X= 1.439969729914D+13 Y= 1.732290739522D+13 Z= -1.362929044441D+12
I= 18 X= 9.599601115976D+12 Y= -6.116704581850D+13 Z= 7.838810960692D+13
I= 19 X= -7.321659312413D+13 Y= -3.612673927952D+13 Z= -3.328965074407D+13
I= 20 X= 2.043440709678D+13 Y= -2.947759361004D+12 Z= 4.701551553604D+13
I= 21 X= -1.179786964611D+12 Y= -9.800012887042D+10 Z= 4.669980844575D+12
I= 22 X= -3.065100957602D+13 Y= 4.842245155781D+13 Z= 1.207621748589D+13
I= 23 X= -2.279754655576D+13 Y= 1.576439621787D+13 Z= 1.210894364977D+13
I= 24 X= 1.468327226387D+14 Y= -1.659901418095D+14 Z= -1.717954601866D+13
I= 25 X= -1.319721056809D+13 Y= 1.944410462117D+12 Z= -4.672804937953D+12
I= 26 X= 5.612413983966D+13 Y= -8.994036259142D+13 Z= -1.132230635465D+14
I= 27 X= -2.720095692560D+13 Y= 5.362390411832D+13 Z= -3.663516839668D+12
I= 28 X= -6.614432079161D+13 Y= -1.329864754506D+14 Z= 6.145951009232D+13
I= 29 X= 1.216000543898D+13 Y= -5.957166371066D+12 Z= -1.585302299384D+13
I= 30 X= 8.995877821058D+12 Y= -1.656370588850D+13 Z= 8.234576344791D+12
I= 31 X= 3.619579606815D+13 Y= 6.870623234222D+13 Z= 6.041186160455D+13
I= 32 X= 7.870325805587D+13 Y= 9.212602204986D+13 Z= 2.797578424859D+13

I= 33 X= 2.337350038951D+13 Y= -3.706471290696D+13 Z= -4.220546506125D+13
I= 34 X= 2.135349597953D+12 Y= 9.780787863578D+13 Z= -7.511402304786D+13
I= 35 X= -3.963422292903D+12 Y= 1.798322570104D+12 Z= 3.346016020558D+11
I= 36 X= -7.314092399576D+12 Y= 7.072011238636D+12 Z= -1.547147498812D+13
I= 37 X= 6.158749486928D+13 Y= 1.633664971875D+13 Z= 2.613954459736D+13
I= 38 X= -1.959881584119D+12 Y= -4.645887906340D+13 Z= 1.641586202249D+13

Seed: 13731475592

CM Start Point Coordinates: bohr

I= 0 X= -2.115865129518D+00 Y= 2.343455662319D+00 Z= -6.342930982641D-01
I= 1 X= -2.790897447188D+00 Y= -5.983369338575D-02 Z= -1.908573943046D+00
I= 2 X= -1.994388487891D+00 Y= 1.663093516225D+00 Z= 2.060809814733D+00
I= 3 X= -2.588671641492D+00 Y= -2.092418531039D+00 Z= -1.293893061425D-01
I= 4 X= -2.220264213656D+00 Y= -9.502916210831D-01 Z= 2.371896063452D+00
I= 5 X= 4.012654422097D+00 Y= 3.158896603111D+00 Z= -1.587001369279D+00
I= 6 X= 2.431761117216D+00 Y= 6.064143870435D-01 Z= -3.246648287056D+00
I= 7 X= 5.508749685752D+00 Y= 2.820758422654D+00 Z= -3.369410225339D+00
I= 8 X= 2.380211732294D+00 Y= 4.828290578129D+00 Z= -1.893119160745D+00
I= 9 X= -2.273165214464D+00 Y= -2.483747013072D+00 Z= 4.764705367818D+00
I= 10 X= -4.220063052882D+00 Y= -2.779183794171D+00 Z= 5.664888668137D+00
I= 11 X= -1.425630867285D+00 Y= -4.636850555085D+00 Z= 4.557884245745D+00
I= 12 X= -8.528591151094D-01 Y= -1.724771432973D+00 Z= 6.010692172649D+00
I= 13 X= -1.741027238233D+00 Y= 3.397398865977D+00 Z= 4.112294388452D+00
I= 14 X= -3.518031206123D+00 Y= 3.811103002242D+00 Z= 4.906274315164D+00
I= 15 X= -4.945808886709D-01 Y= 2.998995649486D+00 Z= 5.842953437202D+00
I= 16 X= -1.161023525626D+00 Y= 5.284591873917D+00 Z= 3.571188603952D+00
I= 17 X= -1.900475890826D+00 Y= 4.855733977519D+00 Z= -1.792426741790D+00
I= 18 X= -3.883804733829D+00 Y= 5.856802497359D+00 Z= -1.545200332923D+00
I= 19 X= -3.169734545373D-01 Y= 6.018608615975D+00 Z= -9.725189392052D-01
I= 20 X= -1.675407886091D+00 Y= 4.817615286687D+00 Z= -3.993233278332D+00

I= 21 X= -3.670749770727D+00 Y= -2.325580023814D-01 Z= -4.592023841344D+00
I= 22 X= -5.684335694888D+00 Y= 1.744037954815D-01 Z= -4.760204838160D+00
I= 23 X= -2.967154450355D+00 Y= 1.634862869852D+00 Z= -5.514056458040D+00
I= 24 X= -2.659912744231D+00 Y= -1.903921058517D+00 Z= -5.649333971577D+00
I= 25 X= -3.054548840179D+00 Y= -4.759138511248D+00 Z= -7.494708990519D-01
I= 26 X= -3.063751845005D+00 Y= -4.992197818145D+00 Z= -2.777338485355D+00
I= 27 X= -1.462517237672D+00 Y= -5.957117684362D+00 Z= 8.523038532324D-02
I= 28 X= -4.853661843725D+00 Y= -4.948588351338D+00 Z= -1.670147982807D-01
I= 29 X= 3.331401383502D+00 Y= -3.395886207736D+00 Z= -1.472976868567D+00
I= 30 X= 3.342187586724D+00 Y= -3.279961430893D+00 Z= 1.192687706802D+00
I= 31 X= 1.727803520860D+00 Y= -4.327821891378D+00 Z= -2.674182746678D+00
I= 32 X= 5.077116744882D+00 Y= -3.020524970580D+00 Z= -2.403573091917D+00
I= 33 X= 5.040212596275D+00 Y= -2.627576974530D+00 Z= 2.371442059312D+00
I= 34 X= 2.251781993471D+00 Y= -4.274806356837D+00 Z= 2.660832306166D+00
I= 35 X= 1.133059470320D+00 Y= -7.722305768855D-02 Z= -3.557424028310D-01
I= 36 X= 4.309428230331D+00 Y= 2.312889759413D+00 Z= 1.284864929340D+00
I= 37 X= 6.375150104590D+00 Y= 1.093833520213D+00 Z= 1.942673677812D+00
I= 38 X= 3.135983136195D+00 Y= 3.444905150904D+00 Z= 2.894080519854D+00

Forward Direction:

Total Energy: -656.4317839 Hartrees

Potential Energy: -656.6140748 Hartress

Kinetic Energy: 0.1822909 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.317226962241D+12 Y= 2.811777289699D+12 Z= -4.693212813089D+12
I= 1 X= 4.608623807449D+12 Y= -1.117339527942D+13 Z= 1.738280998960D+13
I= 2 X= -1.224739457640D+13 Y= -1.010787954597D+13 Z= -3.104760215025D+13
I= 3 X= -1.143388607875D+12 Y= 5.585925828613D+12 Z= -1.730720855671D+13
I= 4 X= -2.261107172173D+13 Y= 1.655342423849D+13 Z= -7.869705569521D+12
I= 5 X= 3.285814724049D+12 Y= 1.089994945062D+13 Z= -2.096231748991D+13
I= 6 X= -2.704739204110D+13 Y= -2.768687807038D+13 Z= -2.149203205369D+13

I= 7 X= 2.224867038579D+13 Y= -4.105888715414D+13 Z= -5.204982119519D+13
I= 8 X= -3.826861099039D+13 Y= -1.695690954531D+13 Z= 1.080283459793D+14
I= 9 X= 1.460028517883D+13 Y= 2.934765978056D+12 Z= 2.721946946003D+13
I= 10 X= -2.806304566850D+13 Y= 5.396108830471D+13 Z= -3.270846193231D+13
I= 11 X= -5.647100354662D+13 Y= 3.952105591532D+13 Z= 1.774891240170D+13
I= 12 X= -5.435895921033D+12 Y= -4.472059060359D+13 Z= -3.039356658079D+13
I= 13 X= 5.032060582852D+12 Y= -1.003855454318D+13 Z= 2.031576091211D+13
I= 14 X= 2.923276273791D+13 Y= -1.430769323632D+13 Z= 1.898331746219D+13
I= 15 X= -8.724712913429D+11 Y= 7.315785758237D+13 Z= 4.768619459886D+13
I= 16 X= 2.046948969063D+13 Y= 1.529969307466D+14 Z= -1.023457548896D+13
I= 17 X= -7.864719452176D+12 Y= 1.534475720795D+13 Z= 2.073715067075D+13
I= 18 X= 5.687170956461D+13 Y= -7.282354542510D+13 Z= -8.268918840173D+13
I= 19 X= 1.328253139070D+13 Y= -1.511292754932D+13 Z= 3.228365651838D+13
I= 20 X= -4.751421788326D+12 Y= 3.639288804980D+13 Z= -9.584808044616D+13
I= 21 X= -1.608628302518D+13 Y= 1.439088457493D+13 Z= -3.805128961710D+12
I= 22 X= 9.557412941283D+13 Y= -3.468714742985D+13 Z= 2.295844558872D+13
I= 23 X= 4.585920686423D+13 Y= 2.433341398498D+13 Z= -3.983178667836D+13
I= 24 X= 5.678016271051D+12 Y= 9.405682553882D+13 Z= 1.246430352518D+13
I= 25 X= 3.458658376466D+12 Y= -4.062457974186D+12 Z= -1.920898352674D+13
I= 26 X= -1.621273137075D+13 Y= -2.954128242868D+13 Z= 1.614673918131D+13
I= 27 X= -2.068585493169D+13 Y= 2.627443895072D+13 Z= 2.533307475738D+13
I= 28 X= -1.208488399272D+14 Y= -5.111784678352D+13 Z= 6.324406773943D+13
I= 29 X= 1.533820755056D+13 Y= 9.082886521383D+12 Z= -2.789785506763D+13
I= 30 X= 1.223741830327D+13 Y= -8.462190573717D+12 Z= 1.294336997833D+13
I= 31 X= -4.183915057709D+13 Y= -3.516931351224D+13 Z= -3.474802000511D+13
I= 32 X= -8.945041982622D+13 Y= 8.801615735300D+13 Z= 1.034500210794D+14
I= 33 X= -1.383457405172D+14 Y= 1.519956997051D+13 Z= 6.342423235803D+12
I= 34 X= 1.036450765907D+14 Y= 1.983671303284D+13 Z= -8.738871602585D+13
I= 35 X= 3.746383521880D+12 Y= -6.198675370967D+12 Z= 2.065359684133D+12
I= 36 X= -2.705119826146D+12 Y= -1.962433017622D+12 Z= 9.144337856947D+12

I= 37 X= -7.957622909106D+13 Y= 2.733056557548D+13 Z= 2.568870672717D+13

I= 38 X= -1.101436321507D+14 Y= -1.358057158865D+13 Z= 7.439632231142D+13

Backward Direction:

Total Energy: -656.4317901 Hartrees

Potential Energy: -656.6140748 Hartress

Kinetic Energy: 0.1822847 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.109293829315D+12 Y= 2.540246773361D+12 Z= -4.586955720662D+12

I= 1 X= 4.287912426467D+12 Y= -1.187163477679D+13 Z= 1.696365486677D+13

I= 2 X= -1.254589054047D+13 Y= -9.833495698291D+12 Z= -3.148937175987D+13

I= 3 X= -1.754991415234D+12 Y= 5.600226839394D+12 Z= -1.819335815043D+13

I= 4 X= -2.156499294419D+13 Y= 1.646009499897D+13 Z= -8.564841739961D+12

I= 5 X= 1.559363200773D+12 Y= 8.444746657218D+12 Z= -2.586416693709D+13

I= 6 X= 1.162483312430D+13 Y= 1.646211064232D+13 Z= -4.092056265458D+12

I= 7 X= 2.931215352559D+13 Y= -3.437127112440D+13 Z= -5.161767885057D+13

I= 8 X= -2.934772328710D+13 Y= -9.745985526606D+12 Z= 1.088582809241D+14

I= 9 X= 1.493275962979D+13 Y= 3.090902227561D+12 Z= 2.684366391180D+13

I= 10 X= -2.800223875532D+13 Y= 5.473380055501D+13 Z= -3.360419557795D+13

I= 11 X= -5.656702875252D+13 Y= 3.951260895946D+13 Z= 1.773023986855D+13

I= 12 X= -5.241042526131D+12 Y= -4.466840144831D+13 Z= -3.057859969178D+13

I= 13 X= 5.097968796519D+12 Y= -1.007062295585D+13 Z= 2.017704433318D+13

I= 14 X= 2.934481138214D+13 Y= -1.450525517210D+13 Z= 1.901264224785D+13

I= 15 X= -6.664131668444D+11 Y= 7.296886668900D+13 Z= 4.734497748946D+13

I= 16 X= 2.045513574519D+13 Y= 1.530576725938D+14 Z= -1.018653547799D+13

I= 17 X= -7.763788463114D+12 Y= 1.512201753097D+13 Z= 2.071509296680D+13

I= 18 X= 5.689299035230D+13 Y= -7.317865156177D+13 Z= -8.298049628976D+13

I= 19 X= 1.306916530996D+13 Y= -1.518400505464D+13 Z= 3.250367024509D+13

I= 20 X= -4.603254016640D+12 Y= 3.619386248964D+13 Z= -9.587349632605D+13

I= 21 X= -1.621328631972D+13 Y= 1.431109826772D+13 Z= -4.115163354259D+12

I= 22 X= 9.555143289390D+13 Y= -3.432958995064D+13 Z= 2.171593986005D+13

I= 23 X= 4.632085038768D+13 Y= 2.413246550607D+13 Z= -3.997586123972D+13
I= 24 X= 5.455465048140D+12 Y= 9.393183159138D+13 Z= 1.209772316901D+13
I= 25 X= 3.320631280614D+12 Y= -4.201894204176D+12 Z= -1.928020928965D+13
I= 26 X= -1.655413288340D+13 Y= -2.991474928492D+13 Z= 1.610508368325D+13
I= 27 X= -2.040132251175D+13 Y= 2.651399213869D+13 Z= 2.525049787275D+13
I= 28 X= -1.208347405923D+14 Y= -5.154044570075D+13 Z= 6.354320114639D+13
I= 29 X= 1.469898729122D+13 Y= 9.262438512839D+12 Z= -2.812205275742D+13
I= 30 X= 1.227506141148D+13 Y= -8.585895832401D+12 Z= 1.266571750561D+13
I= 31 X= -4.228108780784D+13 Y= -3.530005841096D+13 Z= -3.473421102465D+13
I= 32 X= -9.074377767716D+13 Y= 8.909021242619D+13 Z= 1.026799950306D+14
I= 33 X= -1.383058531358D+14 Y= 1.504323786541D+13 Z= 6.121272031793D+12
I= 34 X= 1.040617737786D+14 Y= 1.954659758328D+13 Z= -8.746846837261D+13
I= 35 X= 3.739429518626D+12 Y= -6.036251390684D+12 Z= 3.095839775424D+12
I= 36 X= -4.952436033567D+12 Y= -4.800978563871D+12 Z= 8.108480870645D+12
I= 37 X= -7.757141503059D+13 Y= 2.834833884515D+13 Z= 2.318838274988D+13
I= 38 X= -1.090457181970D+14 Y= -1.369497622781D+13 Z= 7.252901933992D+13

Seed: 13956542053

CM Start Point Coordinates: bohr

I= 0 X= -2.196599093780D+00 Y= 2.368034157338D+00 Z= -5.144600064169D-01
I= 1 X= -2.720373966655D+00 Y= 1.016639139841D-01 Z= -1.936192422370D+00
I= 2 X= -1.864326651829D+00 Y= 1.675270151504D+00 Z= 2.136276091989D+00
I= 3 X= -2.569999287900D+00 Y= -1.990229701791D+00 Z= -3.794017296440D-01
I= 4 X= -2.180277892811D+00 Y= -1.041016079752D+00 Z= 2.259172881333D+00
I= 5 X= 3.926560295881D+00 Y= 2.592815102765D+00 Z= -1.980266514387D+00
I= 6 X= 1.802685216726D+00 Y= 1.360206457275D-01 Z= -3.074333348050D+00
I= 7 X= 5.458528503783D+00 Y= 1.716922763396D+00 Z= -3.074701396228D+00
I= 8 X= 2.886354012598D+00 Y= 4.176498855429D+00 Z= -3.110118195259D+00
I= 9 X= -2.397871812773D+00 Y= -2.707659857932D+00 Z= 4.549141101942D+00
I= 10 X= -4.503312779188D+00 Y= -2.355041220862D+00 Z= 5.560223145206D+00

I= 11 X= -2.693560651624D+00 Y= -4.861418819436D+00 Z= 3.558989956932D+00
I= 12 X= -9.197050717320D-01 Y= -2.611430514568D+00 Z= 5.851596305107D+00
I= 13 X= -1.731410098473D+00 Y= 3.461357264327D+00 Z= 4.207979459918D+00
I= 14 X= -3.565807951660D+00 Y= 4.203628641657D+00 Z= 4.619224949663D+00
I= 15 X= -9.277780311231D-01 Y= 2.630785477975D+00 Z= 5.772864482931D+00
I= 16 X= -7.660007270202D-01 Y= 5.452482968258D+00 Z= 3.896663222814D+00
I= 17 X= -2.115162932378D+00 Y= 5.018206382481D+00 Z= -1.471820064746D+00
I= 18 X= -4.029572217269D+00 Y= 5.888521803226D+00 Z= -5.783734722171D-01
I= 19 X= -4.366041469734D-01 Y= 6.255636288283D+00 Z= -8.155042272326D-01
I= 20 X= -2.082408527244D+00 Y= 5.193352331041D+00 Z= -3.545910664807D+00
I= 21 X= -3.421636272562D+00 Y= 2.991892074359D-01 Z= -4.588147729822D+00
I= 22 X= -5.294602545649D+00 Y= 1.030970938710D+00 Z= -4.775853769627D+00
I= 23 X= -1.898288227186D+00 Y= 1.305860622651D+00 Z= -5.581655561827D+00
I= 24 X= -3.338042564696D+00 Y= -1.878427384459D+00 Z= -5.248833269542D+00
I= 25 X= -2.981659445598D+00 Y= -4.786639179584D+00 Z= -1.001849409177D+00
I= 26 X= -2.984497049726D+00 Y= -4.522694676273D+00 Z= -3.329045952190D+00
I= 27 X= -9.616289496509D-01 Y= -5.780249487843D+00 Z= -2.855302006156D-01
I= 28 X= -4.707550358097D+00 Y= -5.691505529116D+00 Z= 8.927183166730D-02
I= 29 X= 3.090510795869D+00 Y= -3.894648074514D+00 Z= -9.056406871192D-01
I= 30 X= 4.021102858769D+00 Y= -2.704259986422D+00 Z= 1.320712488913D+00
I= 31 X= 1.849708769528D+00 Y= -5.718575058676D+00 Z= -7.318288921007D-01
I= 32 X= 3.999825802202D+00 Y= -3.806148689304D+00 Z= -2.958947786322D+00
I= 33 X= 5.666656201306D+00 Y= -1.318625389073D+00 Z= 9.066891767510D-01
I= 34 X= 3.085010274505D+00 Y= -3.111543738655D+00 Z= 3.316053636367D+00
I= 35 X= 1.133046014708D+00 Y= -1.614184163743D-01 Z= -2.905509309924D-01
I= 36 X= 3.925773625500D+00 Y= 2.758027278865D+00 Z= 7.923488105019D-01
I= 37 X= 5.804796166012D+00 Y= 2.137186092299D+00 Z= 1.872648207198D+00
I= 38 X= 2.591034334516D+00 Y= 4.315382994246D+00 Z= 1.710921722361D+00

Forward Direction:

Total Energy: -656.4231938 Hartrees

Potential Energy: -656.6122078 Hartress

Kinetic Energy: 0.1890140 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.109151818840D+12 Y= -1.248467643863D+13 Z= 1.992390559535D+13
I= 1 X= 5.474751584973D+12 Y= 2.165797415572D+13 Z= 1.891337435703D+13
I= 2 X= -3.076437131020D+12 Y= -3.122700641646D+13 Z= -5.236277436914D+12
I= 3 X= -1.384457420318D+13 Y= -1.234560103648D+13 Z= 2.584029591870D+12
I= 4 X= -4.552379184497D+12 Y= 8.495781435864D+12 Z= -1.219309543780D+13
I= 5 X= 1.961862031985D+13 Y= 1.340582076080D+13 Z= 8.113344792299D+11
I= 6 X= 1.253466611369D+11 Y= 2.476617092048D+13 Z= -4.586588448281D+13
I= 7 X= -3.997697979448D+13 Y= -3.683463840870D+13 Z= -8.462892097064D+13
I= 8 X= -8.724053137758D+13 Y= 1.179889084058D+14 Z= -7.397378305715D+13
I= 9 X= 5.786977113058D+12 Y= 8.167929430522D+12 Z= 4.657015327836D+12
I= 10 X= 7.180639985142D+13 Y= -4.571623843786D+13 Z= 7.309578951898D+13
I= 11 X= -1.316166134244D+14 Y= 1.055419054548D+14 Z= -1.854948752901D+13
I= 12 X= -6.630888275513D+13 Y= 3.813704741415D+13 Z= 8.438934819409D+13
I= 13 X= -2.935719581397D+13 Y= -6.697519613061D+12 Z= 1.327480476213D+13
I= 14 X= 8.009190485605D+13 Y= 7.319924231819D+13 Z= -2.560313073028D+12
I= 15 X= -6.774358227859D+13 Y= -5.592226549125D+13 Z= -2.141263347024D+13
I= 16 X= -5.743402009209D+12 Y= -7.369602152649D+13 Z= -3.253039420517D+13
I= 17 X= 6.757711593925D+12 Y= 3.751840743510D+12 Z= -1.486946419038D+13
I= 18 X= -1.475011721399D+13 Y= -1.015398438962D+13 Z= 9.393967556947D+12
I= 19 X= -3.153023003605D+13 Y= -7.361697795997D+13 Z= -1.869080545084D+13
I= 20 X= -1.640196892270D+13 Y= 2.063408698819D+13 Z= 1.390209621377D+14
I= 21 X= 2.933956303887D+13 Y= 1.234516024119D+13 Z= -6.573131465741D+12
I= 22 X= -4.380448896415D+12 Y= -9.986407166390D+11 Z= -1.120374682486D+14
I= 23 X= -7.253818571369D+13 Y= -4.791122109668D+13 Z= 6.777881503689D+13
I= 24 X= -1.199249533103D+12 Y= 3.166390118234D+13 Z= 5.461924950497D+13
I= 25 X= -4.673393645794D+11 Y= 2.588620442186D+12 Z= -7.676299775945D+12
I= 26 X= 4.151377416016D+13 Y= 3.353373006658D+12 Z= -7.842059238250D+13

I= 27 X= 2.632042247401D+13 Y= 4.232819393166D+13 Z= -5.191197118813D+13
I= 28 X= -1.089940546137D+14 Y= 1.370833669575D+13 Z= 2.032941203657D+13
I= 29 X= 2.514229673619D+13 Y= -1.075517607507D+13 Z= -9.957658326361D+12
I= 30 X= -8.791393665277D+11 Y= 2.211607058158D+12 Z= 1.583354930945D+13
I= 31 X= 1.528066688804D+13 Y= -4.434740889970D+13 Z= -1.891263796855D+13
I= 32 X= 2.932123589586D+13 Y= -8.682883143725D+13 Z= 4.065102669490D+13
I= 33 X= -1.507263071847D+14 Y= -4.143783650495D+13 Z= -1.140766607937D+14
I= 34 X= -3.366216604546D+13 Y= -7.347056666124D+12 Z= 2.646999602734D+13
I= 35 X= -1.497160714423D+11 Y= 1.714106903306D+12 Z= -8.624084292055D+10
I= 36 X= 6.004842600934D+12 Y= -9.745049140403D+12 Z= 2.349061489519D+12
I= 37 X= 1.612695649174D+12 Y= -4.068038567657D+13 Z= -3.514812943574D+13
I= 38 X= 2.172930979276D+13 Y= 4.572314733852D+13 Z= -5.828200216851D+13

Backward Direction:

Total Energy: -656.4232075 Hartrees

Potential Energy: -656.6122078 Hartress

Kinetic Energy: 0.1890003 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.855996613783D+11 Y= -1.264601763950D+13 Z= 1.998704268608D+13
I= 1 X= 5.284187521657D+12 Y= 2.124308598782D+13 Z= 1.866431582980D+13
I= 2 X= -3.253800977851D+12 Y= -3.106396979150D+13 Z= -5.498773305686D+12
I= 3 X= -1.420798355818D+13 Y= -1.233710349441D+13 Z= 2.057486791299D+12
I= 4 X= -3.930807778756D+12 Y= 8.440325968841D+12 Z= -1.260613963307D+13
I= 5 X= 1.859277702412D+13 Y= 1.194695945424D+13 Z= -2.101304147427D+12
I= 6 X= 2.310406480010D+13 Y= 5.099913691855D+13 Z= -3.552696197267D+13
I= 7 X= -3.577991620514D+13 Y= -3.286091196526D+13 Z= -8.437214554439D+13
I= 8 X= -8.193981327051D+13 Y= 1.222735801525D+14 Z= -7.348064253978D+13
I= 9 X= 5.984530699681D+12 Y= 8.260704306760D+12 Z= 4.433714763483D+12
I= 10 X= 7.184253082407D+13 Y= -4.525709917004D+13 Z= 7.256355195698D+13
I= 11 X= -1.316736708120D+14 Y= 1.055368863463D+14 Z= -1.856058258741D+13
I= 12 X= -6.619310246507D+13 Y= 3.816805778774D+13 Z= 8.427940304180D+13

I= 13 X= -2.931803369511D+13 Y= -6.716574400417D+12 Z= 1.319238051055D+13
I= 14 X= 8.015848324207D+13 Y= 7.308185263516D+13 Z= -2.542888522971D+12
I= 15 X= -6.762114423122D+13 Y= -5.603456232390D+13 Z= -2.161538187647D+13
I= 16 X= -5.751931009551D+12 Y= -7.365992921795D+13 Z= -3.250184922837D+13
I= 17 X= 6.817683958453D+12 Y= 3.619490659397D+12 Z= -1.488257069371D+13
I= 18 X= -1.473747234418D+13 Y= -1.036498553635D+13 Z= 9.220874802823D+12
I= 19 X= -3.165701041504D+13 Y= -7.365921163704D+13 Z= -1.856007510226D+13
I= 20 X= -1.631392883677D+13 Y= 2.051582763779D+13 Z= 1.390058602205D+14
I= 21 X= 2.926409872906D+13 Y= 1.229775187362D+13 Z= -6.757351352418D+12
I= 22 X= -4.393934977327D+12 Y= -7.861830071828D+11 Z= -1.127757549399D+14
I= 23 X= -7.226388092462D+13 Y= -4.803062302810D+13 Z= 6.769320712189D+13
I= 24 X= -1.331487632187D+12 Y= 3.158963080866D+13 Z= 5.440143046939D+13
I= 25 X= -5.493539330767D+11 Y= 2.505768580386D+12 Z= -7.718621537952D+12
I= 26 X= 4.131091620664D+13 Y= 3.131462073440D+12 Z= -7.844534372980D+13
I= 27 X= 2.648948930370D+13 Y= 4.247053447365D+13 Z= -5.196103769137D+13
I= 28 X= -1.089856769065D+14 Y= 1.345723187775D+13 Z= 2.050715463700D+13
I= 29 X= 2.476247731135D+13 Y= -1.064848775690D+13 Z= -1.009087475143D+13
I= 30 X= -8.567721448044D+11 Y= 2.138102410565D+12 Z= 1.566857049269D+13
I= 31 X= 1.501807141467D+13 Y= -4.442509644177D+13 Z= -1.890443278791D+13
I= 32 X= 2.855273329458D+13 Y= -8.619063674643D+13 Z= 4.019348354802D+13
I= 33 X= -1.507026064358D+14 Y= -4.153072775878D+13 Z= -1.142080670216D+14
I= 34 X= -3.341456800627D+13 Y= -7.519440880410D+12 Z= 2.642260783642D+13
I= 35 X= -1.538480834824D+11 Y= 1.810617896720D+12 Z= 5.260619523905D+11
I= 36 X= 4.669505793248D+12 Y= -1.143168955731D+13 Z= 1.733563787292D+12
I= 37 X= 2.803939675819D+12 Y= -4.007563317141D+13 Z= -3.663380137747D+13
I= 38 X= 2.238168123299D+13 Y= 4.565516904227D+13 Z= -5.939153823921D+13

Seed: 14005120571

CM Start Point Coordinates: bohr

I= 0 X= -2.287474504689D+00 Y= 2.331946752424D+00 Z= -6.474356901701D-01

I= 1 X= -2.760246983548D+00 Y= 1.415068705241D-02 Z= -2.071689423507D+00
I= 2 X= -1.842281911785D+00 Y= 1.720854180496D+00 Z= 1.959167424051D+00
I= 3 X= -2.685792856503D+00 Y= -2.049352429492D+00 Z= -2.884129456476D-01
I= 4 X= -2.051458588417D+00 Y= -1.051811717822D+00 Z= 2.350983351929D+00
I= 5 X= 4.272487613840D+00 Y= 2.813804257477D+00 Z= -1.469982270273D+00
I= 6 X= 2.358003522566D+00 Y= 5.680833259989D-01 Z= -3.202400597668D+00
I= 7 X= 5.888554232262D+00 Y= 1.875546384494D+00 Z= -2.241772764549D+00
I= 8 X= 3.427773665854D+00 Y= 4.120090486004D+00 Z= -2.546730623945D+00
I= 9 X= -2.120934179375D+00 Y= -2.342823898719D+00 Z= 4.739306497847D+00
I= 10 X= -3.745207661479D+00 Y= -1.190002002944D+00 Z= 6.229905002185D+00
I= 11 X= -2.847504691114D+00 Y= -4.578411096893D+00 Z= 4.053546528172D+00
I= 12 X= 2.042797263425D-01 Y= -2.088172538817D+00 Z= 5.779982292850D+00
I= 13 X= -1.835544736150D+00 Y= 3.429111589452D+00 Z= 4.200041903179D+00
I= 14 X= -3.684713877103D+00 Y= 4.016556992190D+00 Z= 4.987629252459D+00
I= 15 X= -6.911153289161D-01 Y= 2.280219591690D+00 Z= 5.589857185565D+00
I= 16 X= -1.026064601486D+00 Y= 4.994636095962D+00 Z= 3.684816835045D+00
I= 17 X= -2.269553395215D+00 Y= 5.027004712149D+00 Z= -1.652069326771D+00
I= 18 X= -4.187655363086D+00 Y= 6.098952976626D+00 Z= -1.280997231746D+00
I= 19 X= -1.068623737331D+00 Y= 6.104344258021D+00 Z= -2.670370632346D-01
I= 20 X= -1.592525516695D+00 Y= 5.367262405151D+00 Z= -3.517102908131D+00
I= 21 X= -3.701794890072D+00 Y= -2.161443469940D-01 Z= -4.658661909742D+00
I= 22 X= -5.834685360028D+00 Y= -5.643218435066D-01 Z= -4.686686002396D+00
I= 23 X= -3.359992433142D+00 Y= 1.909075133346D+00 Z= -5.658435031339D+00
I= 24 X= -2.524637592032D+00 Y= -1.741965890716D+00 Z= -5.752087063019D+00
I= 25 X= -3.190338005240D+00 Y= -4.834359320078D+00 Z= -8.422802414200D-01
I= 26 X= -3.536401609932D+00 Y= -5.228415039117D+00 Z= -2.875480938730D+00
I= 27 X= -1.578936120578D+00 Y= -5.932981293280D+00 Z= -3.190284185496D-01
I= 28 X= -5.043726561672D+00 Y= -5.401686783753D+00 Z= 1.344717381244D-01
I= 29 X= 3.148523906974D+00 Y= -3.634369287855D+00 Z= -1.478047332749D+00
I= 30 X= 3.520972121101D+00 Y= -3.186165452717D+00 Z= 1.136301450652D+00

I= 31 X= 1.788083970595D+00 Y= -5.026479751628D+00 Z= -2.246670685948D+00
I= 32 X= 4.968609466767D+00 Y= -3.369876702836D+00 Z= -2.669830931991D+00
I= 33 X= 5.438874631568D+00 Y= -2.418995265877D+00 Z= 1.820343404349D+00
I= 34 X= 2.529330008625D+00 Y= -4.098815310438D+00 Z= 2.647879572217D+00
I= 35 X= 1.199113193005D+00 Y= -9.553851507409D-02 Z= -3.164464920810D-01
I= 36 X= 4.027824181479D+00 Y= 2.683961417346D+00 Z= 1.208879296714D+00
I= 37 X= 5.133904780678D+00 Y= 1.748370457772D+00 Z= 2.568528230711D+00
I= 38 X= 2.944482272395D+00 Y= 3.908098972330D+00 Z= 2.476752226552D+00

Forward Direction:

Total Energy: -656.4387853 Hartrees

Potential Energy: -656.6226719 Hartress

Kinetic Energy: 0.1838866 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.510757366099D+11 Y= -2.012273595887D+13 Z= 1.226375156528D+13
I= 1 X= -1.233402849099D+13 Y= -2.260671762739D+12 Z= -1.779708941599D+13
I= 2 X= -1.232635881935D+13 Y= -6.404233702247D+12 Z= -1.818268777664D+13
I= 3 X= -2.982597804277D+12 Y= -2.509415455192D+13 Z= -2.193334139017D+13
I= 4 X= 5.173666248852D+12 Y= -5.519464672758D+12 Z= 1.050546318705D+13
I= 5 X= -1.211456484162D+13 Y= -7.808539507722D+11 Z= -2.322378187412D+12
I= 6 X= -1.059231526193D+14 Y= -7.419257010130D+12 Z= 3.845649559963D+13
I= 7 X= -4.168780465378D+13 Y= 9.436872005308D+12 Z= -3.285719149595D+13
I= 8 X= -2.154314429124D+13 Y= -7.484585254571D+13 Z= 6.207375847549D+13
I= 9 X= 8.079855681003D+11 Y= 4.462514957010D+12 Z= 2.733985216838D+12
I= 10 X= 2.194433658604D+13 Y= 7.025806843324D+13 Z= -2.701984290622D+13
I= 11 X= 2.908098560140D+13 Y= -1.083194956464D+13 Z= 3.872300252928D+13
I= 12 X= -6.622938053538D+13 Y= -8.108162488915D+13 Z= -1.498952441081D+14
I= 13 X= 8.277632539501D+12 Y= 1.912286364272D+13 Z= 6.134308477452D+12
I= 14 X= -3.833595310641D+13 Y= 3.517069265443D+13 Z= 8.512754001608D+13
I= 15 X= -7.075405187492D+13 Y= -4.353577984894D+12 Z= -4.327512145942D+13
I= 16 X= -8.256794478601D+13 Y= 4.985243323656D+13 Z= 3.300700027497D+13

I= 17 X= -1.542726698947D+12 Y= 2.812819589148D+13 Z= -1.853581842186D+13
I= 18 X= 4.357399629416D+13 Y= 3.209742573742D+13 Z= -2.902116625030D+12
I= 19 X= 8.646051741996D+12 Y= -3.968169478998D+12 Z= -1.125660583274D+14
I= 20 X= 2.751898231558D+12 Y= 2.757008138736D+13 Z= 1.242148343945D+14
I= 21 X= -1.208020438802D+13 Y= 1.111620598331D+13 Z= -1.027884251120D+13
I= 22 X= 4.593198599601D+13 Y= -3.400562213686D+13 Z= -7.311936818401D+12
I= 23 X= -1.728739246640D+13 Y= 2.556869534371D+13 Z= 1.103939294047D+14
I= 24 X= 7.265500297007D+13 Y= -1.198997146193D+14 Z= 4.728615004844D+13
I= 25 X= 9.577209862219D+12 Y= 8.858944341021D+12 Z= 8.979060918533D+12
I= 26 X= 3.670918648803D+13 Y= -2.821032279214D+13 Z= -6.114548091999D+13
I= 27 X= -6.539502347269D+12 Y= -3.820664394440D+13 Z= -4.236757042506D+13
I= 28 X= -8.734605168012D+13 Y= 1.099814995690D+12 Z= 5.426333096195D+13
I= 29 X= 1.499455626015D+13 Y= -6.581083662327D+11 Z= -1.559996622727D+13
I= 30 X= 3.054851893710D+12 Y= 9.347327942172D+12 Z= 1.133433828781D+13
I= 31 X= -1.205672444471D+14 Y= -4.230955512948D+13 Z= -4.929485375955D+13
I= 32 X= 6.857503037001D+12 Y= -3.070972808286D+13 Z= 1.514733812361D+14
I= 33 X= -3.802939166608D+13 Y= -5.813585098342D+13 Z= -5.159456074482D+12
I= 34 X= 3.833847536534D+13 Y= -1.537921889605D+13 Z= -6.422657232245D+13
I= 35 X= 2.397799473155D+12 Y= 1.572699979960D+12 Z= 3.869445182243D+12
I= 36 X= 2.177761228118D+13 Y= -1.651558425091D+13 Z= 1.914810667711D+13
I= 37 X= -2.220564771185D+13 Y= 6.624543010711D+13 Z= -7.894139023297D+13
I= 38 X= 3.869807949527D+13 Y= 2.765570296903D+13 Z= -6.366214155193D+13

Backward Direction:

Total Energy: -656.4387731 Hartrees

Potential Energy: -656.6226719 Hartress

Kinetic Energy: 0.1838988 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.510015733794D+11 Y= -2.051458930064D+13 Z= 1.241709417166D+13

I= 1 X= -1.279685612370D+13 Y= -3.268320860976D+12 Z= -1.840198398803D+13

I= 2 X= -1.275712675792D+13 Y= -6.008262638271D+12 Z= -1.882021795188D+13

I= 3 X= -3.865219046777D+12 Y= -2.507351635858D+13 Z= -2.321216884400D+13
I= 4 X= 6.683292016087D+12 Y= -5.654150728906D+12 Z= 9.502292586604D+12
I= 5 X= -1.460605569392D+13 Y= -4.324026301552D+12 Z= -9.396375284605D+12
I= 6 X= -5.011417450937D+13 Y= 5.629339293700D+13 Z= 6.356689107565D+13
I= 7 X= -3.149429305068D+13 Y= 1.908795918443D+13 Z= -3.223355469559D+13
I= 8 X= -8.669159813336D+12 Y= -6.443956485361D+13 Z= 6.327146098770D+13
I= 9 X= 1.287788819960D+12 Y= 4.687839581040D+12 Z= 2.191649638788D+12
I= 10 X= 2.203208875423D+13 Y= 7.137319125223D+13 Z= -2.831250137833D+13
I= 11 X= 2.894240892287D+13 Y= -1.084413960726D+13 Z= 3.869605567402D+13
I= 12 X= -6.594818211415D+13 Y= -8.100630924313D+13 Z= -1.501622706089D+14
I= 13 X= 8.372746535070D+12 Y= 1.907658481303D+13 Z= 5.934122674418D+12
I= 14 X= -3.817425255919D+13 Y= 3.488558546094D+13 Z= 8.516985943525D+13
I= 15 X= -7.045668360003D+13 Y= -4.626316071585D+12 Z= -4.376754148457D+13
I= 16 X= -8.258865936637D+13 Y= 4.994009150807D+13 Z= 3.307632817476D+13
I= 17 X= -1.397070343988D+12 Y= 2.780675398581D+13 Z= -1.856765051496D+13
I= 18 X= 4.360470719837D+13 Y= 3.158496206565D+13 Z= -3.322511249251D+12
I= 19 X= 8.338137139793D+12 Y= -4.070743429237D+12 Z= -1.122485503142D+14
I= 20 X= 2.965723327448D+12 Y= 2.728286198923D+13 Z= 1.241781560268D+14
I= 21 X= -1.226348642417D+13 Y= 1.100106411414D+13 Z= -1.072626187929D+13
I= 22 X= 4.589923200834D+13 Y= -3.348962086478D+13 Z= -9.105031859471D+12
I= 23 X= -1.662118168773D+13 Y= 2.527870093331D+13 Z= 1.101860113510D+14
I= 24 X= 7.233383302230D+13 Y= -1.200800969085D+14 Z= 4.675712760563D+13
I= 25 X= 9.378019066261D+12 Y= 8.657719987753D+12 Z= 8.876273013427D+12
I= 26 X= 3.621650037113D+13 Y= -2.874928334067D+13 Z= -6.120559514928D+13
I= 27 X= -6.128885589534D+12 Y= -3.786093797500D+13 Z= -4.248673945465D+13
I= 28 X= -8.732570453341D+13 Y= 4.899505744554D+11 Z= 5.469501880105D+13
I= 29 X= 1.407207948616D+13 Y= -3.989918271926D+11 Z= -1.592351223212D+13
I= 30 X= 3.109175721221D+12 Y= 9.168805395717D+12 Z= 1.093365017896D+13
I= 31 X= -1.212050165198D+14 Y= -4.249823677783D+13 Z= -4.927492563441D+13
I= 32 X= 4.991021866027D+12 Y= -2.915972893882D+13 Z= 1.503621349412D+14

I= 33 X= -3.797182906015D+13 Y= -5.836145825121D+13 Z= -5.478605610650D+12
I= 34 X= 3.893982281462D+13 Y= -1.579789268285D+13 Z= -6.434166518265D+13
I= 35 X= 2.387763955585D+12 Y= 1.807098603650D+12 Z= 5.356560045520D+12
I= 36 X= 1.853444692245D+13 Y= -2.061196933167D+13 Z= 1.765323226267D+13
I= 37 X= -1.931244403782D+13 Y= 6.771420740116D+13 Z= -8.254967823370D+13
I= 38 X= 4.028251006603D+13 Y= 2.749060240824D+13 Z= -6.635689909887D+13

Seed: 16826952480

CM Start Point Coordinates: bohr

I= 0 X= -2.050155802435D+00 Y= 2.320758540897D+00 Z= -5.876528719828D-01
I= 1 X= -2.891727202028D+00 Y= 7.547869898131D-02 Z= -1.883519800974D+00
I= 2 X= -1.863717104498D+00 Y= 1.563025333897D+00 Z= 2.189341648538D+00
I= 3 X= -2.698687307767D+00 Y= -2.107145372424D+00 Z= -2.585563101108D-01
I= 4 X= -2.229837707127D+00 Y= -1.047115301119D+00 Z= 2.248782709503D+00
I= 5 X= 3.740788090498D+00 Y= 2.994032485656D+00 Z= -1.965159155235D+00
I= 6 X= 2.291495028310D+00 Y= 1.682486622034D-03 Z= -2.979230940398D+00
I= 7 X= 5.387317557724D+00 Y= 2.924522971735D+00 Z= -3.334697538427D+00
I= 8 X= 2.526417610181D+00 Y= 4.521426484553D+00 Z= -2.916072076868D+00
I= 9 X= -2.267185438853D+00 Y= -2.457890103593D+00 Z= 4.652061286615D+00
I= 10 X= -3.893982748383D+00 Y= -1.759877166972D+00 Z= 6.178490873153D+00
I= 11 X= -2.860628650644D+00 Y= -4.423497061997D+00 Z= 4.151827758044D+00
I= 12 X= -7.111424835618D-01 Y= -1.930935493640D+00 Z= 5.958682802525D+00
I= 13 X= -1.545244928173D+00 Y= 3.411883128305D+00 Z= 4.372673947750D+00
I= 14 X= -3.545022925429D+00 Y= 4.524597827032D+00 Z= 5.254762045509D+00
I= 15 X= -5.804501900774D-01 Y= 2.076514370702D+00 Z= 5.865612488630D+00
I= 16 X= -6.787074094712D-02 Y= 4.717099198509D+00 Z= 3.841009150150D+00
I= 17 X= -2.103770967776D+00 Y= 4.931446725050D+00 Z= -1.452690663523D+00
I= 18 X= -3.844270437303D+00 Y= 5.846310901856D+00 Z= -5.955548801345D-01
I= 19 X= -3.398532296847D-01 Y= 6.150952256643D+00 Z= -6.801208637437D-01
I= 20 X= -1.962183976181D+00 Y= 5.154620213390D+00 Z= -3.729624535399D+00

I= 21 X= -3.377958390187D+00 Y= -2.635844600091D-02 Z= -4.863078654316D+00
I= 22 X= -5.431883187648D+00 Y= -2.394470623399D-02 Z= -5.591914100275D+00
I= 23 X= -2.471886873957D+00 Y= 2.012527231315D+00 Z= -5.716313038316D+00
I= 24 X= -2.425794675286D+00 Y= -1.631473845141D+00 Z= -5.775585168796D+00
I= 25 X= -3.236156729848D+00 Y= -4.842291009111D+00 Z= -9.906694850931D-01
I= 26 X= -3.612340226513D+00 Y= -4.827670889671D+00 Z= -3.149429215925D+00
I= 27 X= -1.504487139876D+00 Y= -6.295624843637D+00 Z= -1.935990424226D-01
I= 28 X= -5.128186842146D+00 Y= -5.260645466304D+00 Z= 1.517340600910D-01
I= 29 X= 3.628608308427D+00 Y= -3.686188041827D+00 Z= -1.156477028458D+00
I= 30 X= 3.369839304327D+00 Y= -3.127155578658D+00 Z= 1.540639795431D+00
I= 31 X= 2.530417666475D+00 Y= -5.273867881523D+00 Z= -2.203509115674D+00
I= 32 X= 5.188921993177D+00 Y= -2.900141364707D+00 Z= -2.295729452255D+00
I= 33 X= 4.815150062770D+00 Y= -2.215515816777D+00 Z= 2.603952053228D+00
I= 34 X= 1.926778359546D+00 Y= -4.375868192081D+00 Z= 2.896147719270D+00
I= 35 X= 1.141809767377D+00 Y= -1.251686997799D-01 Z= -3.271959488046D-01
I= 36 X= 4.107564076901D+00 Y= 2.785680210852D+00 Z= 8.572351349787D-01
I= 37 X= 5.884106924148D+00 Y= 1.806433837284D+00 Z= 1.738096219983D+00
I= 38 X= 3.378205555678D+00 Y= 4.578326270557D+00 Z= 1.746343978211D+00

Forward Direction:

Total Energy: -656.4360327 Hartrees

Potential Energy: -656.6048169 Hartress

Kinetic Energy: 0.1687842 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.814356921011D+12 Y= 2.455255708899D+13 Z= -8.244331770184D+12
I= 1 X= -6.482403029100D+12 Y= -1.421849070119D+13 Z= -2.250025419751D+12
I= 2 X= -1.359228617947D+12 Y= 1.300078702003D+12 Z= 2.322871773793D+12
I= 3 X= 1.403764605707D+13 Y= -5.893528014123D+12 Z= 2.663976943695D+13
I= 4 X= -2.255606987782D+13 Y= 4.570421642814D+12 Z= -1.117427429663D+13
I= 5 X= -6.486542747854D+12 Y= -1.762585576284D+13 Z= 2.691532954452D+13
I= 6 X= -1.915125090957D+13 Y= -1.342690609529D+13 Z= -8.390431710634D+13

I= 7 X= 5.470312070928D+13 Y= 3.456586759985D+13 Z= -2.461006947194D+13
I= 8 X= 4.420719413771D+13 Y= -3.727631605063D+13 Z= 4.963553140405D+13
I= 9 X= -2.837464065947D+13 Y= 4.264314602075D+12 Z= -3.300933936748D+12
I= 10 X= -1.478740818259D+13 Y= -7.408044507812D+13 Z= 5.251125461973D+13
I= 11 X= -4.717027297620D+12 Y= -2.783466202449D+13 Z= 9.877606065032D+13
I= 12 X= 1.648583476900D+13 Y= -1.092629606489D+13 Z= -7.988765920838D+11
I= 13 X= 5.109729642690D+12 Y= -1.483125875341D+13 Z= 7.684651993428D+12
I= 14 X= -8.886360441382D+13 Y= 7.843756381825D+13 Z= 5.868657099305D+13
I= 15 X= 4.920611112076D+13 Y= 7.573386477235D+13 Z= -2.984286696389D+13
I= 16 X= -8.383397008040D+12 Y= 5.938500936394D+13 Z= 2.400682700691D+12
I= 17 X= 3.004686583300D+12 Y= -1.408338473276D+13 Z= -5.763022533795D+12
I= 18 X= 6.237025197818D+13 Y= -7.170425757481D+13 Z= 9.793839009280D+12
I= 19 X= 2.535636723087D+13 Y= 2.407577295984D+12 Z= 1.383557751912D+13
I= 20 X= -1.554235086874D+13 Y= 6.321348515587D+13 Z= 8.392135358102D+13
I= 21 X= -5.914715015533D+12 Y= 2.156842491227D+13 Z= 1.295033411971D+13
I= 22 X= 2.805532625092D+13 Y= -7.480361969805D+13 Z= -8.812195571223D+13
I= 23 X= 3.323884947184D+13 Y= 6.247812125915D+13 Z= -4.964713336263D+13
I= 24 X= -3.607358524125D+13 Y= -7.644150138168D+13 Z= -5.609944654568D+13
I= 25 X= -1.036720002843D+13 Y= 2.224234370441D+12 Z= -2.983023692348D+12
I= 26 X= -5.135207909489D+13 Y= 6.535636841471D+13 Z= 1.477192305483D+14
I= 27 X= -5.616490726838D+13 Y= 7.358744216428D+12 Z= 9.953407251505D+12
I= 28 X= 1.513597488492D+12 Y= -5.147836625687D+13 Z= -4.742472555116D+13
I= 29 X= -5.295480258902D+12 Y= -2.169971353911D+12 Z= -4.338054519598D+12
I= 30 X= 1.436377070420D+13 Y= -5.450516777781D+12 Z= -2.941569778156D+13
I= 31 X= 2.735171039585D+13 Y= 3.062874236901D+12 Z= -4.564190734498D+13
I= 32 X= 1.556826461605D+14 Y= -4.849882010254D+12 Z= -5.824782150231D+13
I= 33 X= 1.197812032518D+13 Y= -3.667049284363D+13 Z= 3.853887425260D+13
I= 34 X= 1.242460956661D+14 Y= -3.285006679704D+13 Z= 4.669943773872D+13
I= 35 X= 3.274976400651D+12 Y= 2.842354949480D+12 Z= -1.129227216065D+12
I= 36 X= -1.032305902863D+13 Y= 2.595800245371D+10 Z= -4.133866521125D+12

I= 37 X= 2.131955458572D+13 Y= 4.508813904158D+13 Z= -3.300622176137D+13

I= 38 X= 7.241541569238D+13 Y= -8.723061434147D+13 Z= -3.828508033263D+13

Backward Direction:

Total Energy: -656.4360850 Hartrees

Potential Energy: -656.6048169 Hartress

Kinetic Energy: 0.1687319 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.067579368481D+12 Y= 2.422188529393D+13 Z= -8.114931124888D+12

I= 1 X= -6.872967630787D+12 Y= -1.506881172846D+13 Z= -2.760475510876D+12

I= 2 X= -1.722739126526D+12 Y= 1.634225303907D+12 Z= 1.784881600642D+12

I= 3 X= 1.329283181337D+13 Y= -5.876112140010D+12 Z= 2.556061015953D+13

I= 4 X= -2.128214770153D+13 Y= 4.456764631930D+12 Z= -1.202081607001D+13

I= 5 X= -8.589027693129D+12 Y= -2.061581919025D+13 Z= 2.094582241715D+13

I= 6 X= 2.794405999434D+13 Y= 4.033804641720D+13 Z= -6.271450281606D+13

I= 7 X= 6.330508072406D+13 Y= 4.271009397056D+13 Z= -2.408380344733D+13

I= 8 X= 5.507111464072D+13 Y= -2.849480148332D+13 Z= 5.064623208770D+13

I= 9 X= -2.796975090806D+13 Y= 4.454458439162D+12 Z= -3.758592606069D+12

I= 10 X= -1.471335709795D+13 Y= -7.313943061087D+13 Z= 5.142042380390D+13

I= 11 X= -4.833967472889D+12 Y= -2.784494879655D+13 Z= 9.875332111010D+13

I= 12 X= 1.672312860080D+13 Y= -1.086273973837D+13 Z= -1.024211234900D+12

I= 13 X= 5.189993130172D+12 Y= -1.487031189363D+13 Z= 7.515721958120D+12

I= 14 X= -8.872715078482D+13 Y= 7.819697149146D+13 Z= 5.872228291910D+13

I= 15 X= 4.945705015940D+13 Y= 7.550371031855D+13 Z= -3.025840358573D+13

I= 16 X= -8.400877344042D+12 Y= 5.945898121980D+13 Z= 2.459186172552D+12

I= 17 X= 3.127601060391D+12 Y= -1.435463869586D+13 Z= -5.789884563808D+12

I= 18 X= 6.239616787444D+13 Y= -7.213670835216D+13 Z= 9.439082189726D+12

I= 19 X= 2.509652849788D+13 Y= 2.321018603647D+12 Z= 1.410351180300D+13

I= 20 X= -1.536191109024D+13 Y= 6.297111041201D+13 Z= 8.389040194211D+13

I= 21 X= -6.069380534204D+12 Y= 2.147126057936D+13 Z= 1.257277203291D+13

I= 22 X= 2.802768626557D+13 Y= -7.436818366748D+13 Z= -8.963508802971D+13

I= 23 X= 3.380104223128D+13 Y= 6.223340477586D+13 Z= -4.982258838426D+13
I= 24 X= -3.634460970769D+13 Y= -7.659371989985D+13 Z= -5.654587071099D+13
I= 25 X= -1.053529040765D+13 Y= 2.054427936720D+12 Z= -3.069762931262D+12
I= 26 X= -5.176784026253D+13 Y= 6.490155781879D+13 Z= 1.476685021767D+14
I= 27 X= -5.581840164974D+13 Y= 7.650473807123D+12 Z= 9.852844525312D+12
I= 28 X= 1.530767767770D+12 Y= -5.199301024016D+13 Z= -4.706043875584D+13
I= 29 X= -6.073927239924D+12 Y= -1.951311661251D+12 Z= -4.611084062327D+12
I= 30 X= 1.440961274642D+13 Y= -5.601165924367D+12 Z= -2.975382493880D+13
I= 31 X= 2.681351609257D+13 Y= 2.903652170640D+12 Z= -4.562509067732D+13
I= 32 X= 1.541075857656D+14 Y= -3.541890106519D+12 Z= -5.918556470513D+13
I= 33 X= 1.202669546425D+13 Y= -3.686087519421D+13 Z= 3.826955473953D+13
I= 34 X= 1.247535524553D+14 Y= -3.320337146209D+13 Z= 4.660231476161D+13
I= 35 X= 3.266507766381D+12 Y= 3.040156028524D+12 Z= 1.256987693318D+11
I= 36 X= -1.305985669034D+13 Y= -3.430842957078D+12 Z= -5.395340528334D+12
I= 37 X= 2.376103140986D+13 Y= 4.632759056841D+13 Z= -3.605113408480D+13
I= 38 X= 7.375246311745D+13 Y= -8.736993712777D+13 Z= -4.055909517035D+13

Seed: 17974054075

CM Start Point Coordinates: bohr

I= 0 X= -2.575263341923D+00 Y= 2.378096174478D+00 Z= -4.778545117778D-01
I= 1 X= -2.849251407961D+00 Y= 1.947232489127D-02 Z= -1.843484849499D+00
I= 2 X= -1.956701103722D+00 Y= 1.756698177720D+00 Z= 2.139681085495D+00
I= 3 X= -2.724208073417D+00 Y= -2.088986835490D+00 Z= -5.895914687970D-02
I= 4 X= -2.238615877323D+00 Y= -9.360036236720D-01 Z= 2.316485555132D+00
I= 5 X= 4.564882875576D+00 Y= 2.413161854144D+00 Z= -1.193657684903D+00
I= 6 X= 2.620479260137D+00 Y= 6.261002394740D-01 Z= -3.043944125186D+00
I= 7 X= 6.115155575825D+00 Y= 1.215420505629D+00 Z= -2.310639478142D+00
I= 8 X= 4.326785841534D+00 Y= 4.156924309582D+00 Z= -2.403632263568D+00
I= 9 X= -2.108385063779D+00 Y= -2.342301306313D+00 Z= 4.821113662591D+00
I= 10 X= -3.841806811176D+00 Y= -1.354109874151D+00 Z= 5.989312194957D+00

I= 11 X= -2.226589250488D+00 Y= -4.423352803782D+00 Z= 4.369592737758D+00
I= 12 X= 2.366730123621D-01 Y= -1.784461693385D+00 Z= 5.598007206427D+00
I= 13 X= -1.578465577078D+00 Y= 3.490285310523D+00 Z= 4.285753869784D+00
I= 14 X= -3.250748586305D+00 Y= 4.514400717749D+00 Z= 4.936373762088D+00
I= 15 X= -3.453720930229D-01 Y= 2.486568412950D+00 Z= 5.921994374530D+00
I= 16 X= -1.940953777815D-01 Y= 5.018254860066D+00 Z= 3.941624424256D+00
I= 17 X= -2.754418837250D+00 Y= 4.851800111905D+00 Z= -1.762373576175D+00
I= 18 X= -4.744016851787D+00 Y= 5.825022488846D+00 Z= -1.190950598911D+00
I= 19 X= -1.286578382345D+00 Y= 5.960023146333D+00 Z= -9.046919966655D-01
I= 20 X= -2.574958689826D+00 Y= 5.169335482114D+00 Z= -3.772595575877D+00
I= 21 X= -3.069336855485D+00 Y= -4.735833393952D-01 Z= -4.591399004793D+00
I= 22 X= -5.053270925728D+00 Y= -4.906665303673D-01 Z= -5.309421837964D+00
I= 23 X= -2.224488129144D+00 Y= 8.668719110670D-01 Z= -5.593850976802D+00
I= 24 X= -2.262792813756D+00 Y= -2.176638843534D+00 Z= -5.342067481361D+00
I= 25 X= -3.253952581622D+00 Y= -4.634337179938D+00 Z= -9.263974026341D-01
I= 26 X= -2.511623033030D+00 Y= -4.791282789891D+00 Z= -3.020224334061D+00
I= 27 X= -2.245037587493D+00 Y= -6.101558597941D+00 Z= 2.467491802371D-01
I= 28 X= -5.127560811248D+00 Y= -5.292074179560D+00 Z= -7.764297785686D-01
I= 29 X= 3.400782971624D+00 Y= -3.634585694626D+00 Z= -1.602481637983D+00
I= 30 X= 3.652964700868D+00 Y= -3.369496687738D+00 Z= 8.895196794307D-01
I= 31 X= 2.246162069708D+00 Y= -5.208298820491D+00 Z= -2.456724507715D+00
I= 32 X= 4.609827309092D+00 Y= -3.064219345114D+00 Z= -3.132570872614D+00
I= 33 X= 5.589887362403D+00 Y= -2.990532070072D+00 Z= 1.721874202796D+00
I= 34 X= 2.257602851608D+00 Y= -4.448573802482D+00 Z= 2.305324285304D+00
I= 35 X= 1.110292821813D+00 Y= 1.629421764835D-02 Z= -3.959406279789D-01
I= 36 X= 4.130088411807D+00 Y= 2.505317100173D+00 Z= 1.351829847755D+00
I= 37 X= 5.137590205701D+00 Y= 1.373453779036D+00 Z= 2.688770652189D+00
I= 38 X= 2.827903101221D+00 Y= 4.017216269692D+00 Z= 2.104568837619D+00

Forward Direction:

Total Energy: -656.4346582 Hartrees

Potential Energy: -656.6436230 Hartress

Kinetic Energy: 0.2089648 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.054972362741D+12 Y= 2.527461188503D+12 Z= 2.895804534851D+13
I= 1 X= -1.408170382422D+13 Y= 6.528116603467D+12 Z= -1.834528888222D+13
I= 2 X= -2.526921168440D+12 Y= 1.291501564212D+13 Z= -1.452629229348D+13
I= 3 X= 2.005248050077D+13 Y= 3.842979329202D+12 Z= 1.714968181561D+13
I= 4 X= 4.303199668089D+12 Y= -6.024571361528D+12 Z= 7.013768479227D+12
I= 5 X= 1.601139539088D+13 Y= 6.197046443510D+12 Z= -1.082367138560D+13
I= 6 X= -7.946890347390D+13 Y= -6.486415586363D+12 Z= 5.823282416262D+13
I= 7 X= -9.006711291200D+13 Y= -7.842757908109D+12 Z= 6.785726696761D+13
I= 8 X= -4.696456690207D+13 Y= 7.112664694211D+13 Z= 6.684939811126D+13
I= 9 X= -2.097510143505D+13 Y= 2.050840660738D+13 Z= -2.271491728237D+13
I= 10 X= -6.717515096972D+13 Y= -5.524713021306D+11 Z= 9.670129750948D+13
I= 11 X= 4.455154826256D+13 Y= -1.586869721408D+14 Z= -5.143573727327D+13
I= 12 X= 8.397852908598D+12 Y= 2.102870826826D+13 Z= -3.190215116855D+13
I= 13 X= 1.427279125441D+13 Y= -3.325470767724D+12 Z= 2.196248966062D+13
I= 14 X= -3.111026599921D+13 Y= 8.477956981386D+13 Z= -2.575720465889D+13
I= 15 X= -5.732214087366D+13 Y= 1.216685212338D+14 Z= -2.521954585028D+12
I= 16 X= 8.010713912290D+12 Y= -2.961815598634D+13 Z= -1.730257199498D+13
I= 17 X= 5.723242911373D+12 Y= -4.819540267233D+12 Z= -1.106322562036D+13
I= 18 X= -1.031385520855D+14 Y= 2.119641565443D+12 Z= -4.940230512637D+13
I= 19 X= -3.351085670405D+11 Y= 1.168019333897D+13 Z= 4.797043466603D+13
I= 20 X= 3.402199030950D+13 Y= -5.942414324926D+12 Z= -6.740880007323D+13
I= 21 X= 5.152306361470D+12 Y= 3.889457996503D+11 Z= 9.114090184311D+12
I= 22 X= 1.456340457441D+13 Y= 1.605308695547D+13 Z= -1.954592035527D+12
I= 23 X= -7.340883329440D+13 Y= 3.668702993602D+13 Z= -1.643721219843D+12
I= 24 X= -2.481878396145D+13 Y= -1.392272913891D+14 Z= -1.024732636778D+14
I= 25 X= 2.082052325376D+13 Y= -1.471138835331D+13 Z= -7.503384928592D+11
I= 26 X= -9.186328263259D+13 Y= -3.070066060709D+13 Z= -7.418534630910D+13

I= 27 X= -8.089870787648D+13 Y= -3.685203065300D+12 Z= 2.539052365869D+13
I= 28 X= -9.943957848665D+13 Y= -1.031108100066D+14 Z= 2.593973851753D+13
I= 29 X= -4.786470710719D+12 Y= -6.093893450289D+12 Z= -1.676218224434D+13
I= 30 X= 8.271782477581D+12 Y= -2.084683829661D+13 Z= 1.499303067122D+13
I= 31 X= 6.684951344210D+13 Y= 9.594117362124D+13 Z= -1.006342005680D+13
I= 32 X= -5.426541624863D+13 Y= -1.066172472404D+14 Z= 2.533805555858D+13
I= 33 X= 1.303025079705D+14 Y= 6.665308722601D+13 Z= 1.137261768629D+14
I= 34 X= 9.896023330560D+12 Y= -1.623363734689D+12 Z= -7.948227827917D+13
I= 35 X= -1.416138549984D+12 Y= 1.492545511856D+12 Z= 9.541943076329D+11
I= 36 X= 5.716126878434D+11 Y= -2.510429863122D+12 Z= -1.835166767827D+13
I= 37 X= 8.238020000828D+13 Y= -4.901292937108D+13 Z= 8.957008950818D+13
I= 38 X= -3.117257461218D+13 Y= 2.755600552023D+13 Z= -3.103156369608D+13

Backward Direction:

Total Energy: -656.4346763 Hartrees

Potential Energy: -656.6436230 Hartress

Kinetic Energy: 0.2089467 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.830402857327D+12 Y= 2.234205981212D+12 Z= 2.907280388882D+13
I= 1 X= -1.442807477127D+13 Y= 5.774012163398D+12 Z= -1.879797988730D+13
I= 2 X= -2.849299282346D+12 Y= 1.321135247110D+13 Z= -1.500340713050D+13
I= 3 X= 1.939194440694D+13 Y= 3.858424540142D+12 Z= 1.619263291489D+13
I= 4 X= 5.432973412738D+12 Y= -6.125367712913D+12 Z= 6.263015656977D+12
I= 5 X= 1.414681344481D+13 Y= 3.545407090246D+12 Z= -1.611770939312D+13
I= 6 X= -3.770257996881D+13 Y= 4.119485791419D+13 Z= 7.702494213947D+13
I= 7 X= -8.243849261376D+13 Y= -6.200772025750D+11 Z= 6.832398428076D+13
I= 8 X= -3.732993429309D+13 Y= 7.891450461261D+13 Z= 6.774573472824D+13
I= 9 X= -2.061602627117D+13 Y= 2.067703505131D+13 Z= -2.312079038755D+13
I= 10 X= -6.710947900279D+13 Y= 2.820643274100D+11 Z= 9.573389775534D+13
I= 11 X= 4.444784024609D+13 Y= -1.586960949289D+14 Z= -5.145590376216D+13
I= 12 X= 8.608296182091D+12 Y= 2.108507298845D+13 Z= -3.210198846900D+13

I= 13 X= 1.434397266873D+13 Y= -3.360104918702D+12 Z= 2.181267460803D+13
I= 14 X= -3.098925254386D+13 Y= 8.456620128707D+13 Z= -2.572553364889D+13
I= 15 X= -5.709959639974D+13 Y= 1.214644095016D+14 Z= -2.890471884594D+12
I= 16 X= 7.995211532088D+12 Y= -2.955255428830D+13 Z= -1.725068837994D+13
I= 17 X= 5.832249215955D+12 Y= -5.060100964779D+12 Z= -1.108704812588D+13
I= 18 X= -1.031155686602D+14 Y= 1.736124000749D+12 Z= -4.971692006389D+13
I= 19 X= -5.655456891015D+11 Y= 1.160342905996D+13 Z= 4.820805133071D+13
I= 20 X= 3.418201273254D+13 Y= -6.157363577530D+12 Z= -6.743624940237D+13
I= 21 X= 5.015141750649D+12 Y= 3.027759264832D+11 Z= 8.779250472329D+12
I= 22 X= 1.453889214539D+13 Y= 1.643925198282D+13 Z= -3.296508514844D+12
I= 23 X= -7.291025446915D+13 Y= 3.647000392047D+13 Z= -1.799322938137D+12
I= 24 X= -2.505914111894D+13 Y= -1.393622858827D+14 Z= -1.028691734989D+14
I= 25 X= 2.067145284813D+13 Y= -1.486198063617D+13 Z= -8.272629046475D+11
I= 26 X= -9.223199907514D+13 Y= -3.110400790957D+13 Z= -7.423033460632D+13
I= 27 X= -8.059141051013D+13 Y= -3.426483624774D+12 Z= 2.530133993757D+13
I= 28 X= -9.942435108160D+13 Y= -1.035672203431D+14 Z= 2.626280506536D+13
I= 29 X= -5.476833888522D+12 Y= -5.899975813349D+12 Z= -1.700431760608D+13
I= 30 X= 8.312437343297D+12 Y= -2.098044100234D+13 Z= 1.469316370079D+13
I= 31 X= 6.637221757157D+13 Y= 9.579996804790D+13 Z= -1.004850624373D+13
I= 32 X= -5.566225344516D+13 Y= -1.054572588689D+14 Z= 2.450642104904D+13
I= 33 X= 1.303455866756D+14 Y= 6.648424725655D+13 Z= 1.134873317320D+14
I= 34 X= 1.034605973688D+13 Y= -1.936690828092D+12 Z= -7.956841147075D+13
I= 35 X= -1.423648931112D+12 Y= 1.667964755849D+12 Z= 2.067121341667D+12
I= 36 X= -1.855507430937D+12 Y= -5.576082564520D+12 Z= -1.947040180529D+13
I= 37 X= 8.454541579830D+13 Y= -4.791372580684D+13 Z= 8.686971890368D+13
I= 38 X= -2.998681844666D+13 Y= 2.743244755990D+13 Z= -3.304826637192D+13

Seed: 18114500697

CM Start Point Coordinates: bohr

I= 0 X= -2.218033911456D+00 Y= 2.375985288799D+00 Z= -2.699575198847D-01

I= 1 X= -2.784123232076D+00 Y= 1.637246691762D-01 Z= -1.973624995289D+00
I= 2 X= -1.981174547307D+00 Y= 1.540692903137D+00 Z= 2.229758888666D+00
I= 3 X= -2.538766249843D+00 Y= -1.886565520129D+00 Z= -3.539442794298D-01
I= 4 X= -2.129581479650D+00 Y= -1.052248489488D+00 Z= 2.275615772014D+00
I= 5 X= 4.251809373957D+00 Y= 2.410508392579D+00 Z= -2.223159046602D+00
I= 6 X= 2.154487011824D+00 Y= 3.227852991754D-01 Z= -3.398387992962D+00
I= 7 X= 5.910371455133D+00 Y= 1.262948635230D+00 Z= -2.725550396583D+00
I= 8 X= 3.136338990088D+00 Y= 3.720872941450D+00 Z= -3.763747820821D+00
I= 9 X= -2.047556264377D+00 Y= -2.758125262628D+00 Z= 4.537207489340D+00
I= 10 X= -3.955439152438D+00 Y= -2.025464956856D+00 Z= 5.441260305206D+00
I= 11 X= -2.713426348869D+00 Y= -4.973177832093D+00 Z= 3.930822425646D+00
I= 12 X= -1.714333247650D-01 Y= -2.379646056408D+00 Z= 5.603064334207D+00
I= 13 X= -1.870140792507D+00 Y= 3.299781419891D+00 Z= 4.367046353945D+00
I= 14 X= -3.795796389215D+00 Y= 3.837101241028D+00 Z= 4.728731212555D+00
I= 15 X= -8.149887541632D-01 Y= 2.427493356898D+00 Z= 6.277183413470D+00
I= 16 X= -7.069796673533D-01 Y= 4.922742644103D+00 Z= 3.825953024652D+00
I= 17 X= -2.426707107480D+00 Y= 5.110363582367D+00 Z= -1.212798314634D+00
I= 18 X= -4.482964091589D+00 Y= 5.907987036350D+00 Z= -2.573866402306D-01
I= 19 X= -4.744151700580D-01 Y= 6.012891800756D+00 Z= -5.959840611663D-01
I= 20 X= -2.446894793861D+00 Y= 5.105459357737D+00 Z= -3.232233045820D+00
I= 21 X= -3.541365059001D+00 Y= 2.235645826168D-01 Z= -4.661214038588D+00
I= 22 X= -5.512762425169D+00 Y= 5.368972376306D-01 Z= -5.123344361083D+00
I= 23 X= -2.359182119718D+00 Y= 1.540536376362D+00 Z= -6.247466158521D+00
I= 24 X= -2.614440064053D+00 Y= -1.557214591585D+00 Z= -5.471836529783D+00
I= 25 X= -3.060136469840D+00 Y= -4.519572199428D+00 Z= -1.114545571875D+00
I= 26 X= -2.826226518235D+00 Y= -4.770119451887D+00 Z= -3.382212770963D+00
I= 27 X= -1.586668490739D+00 Y= -5.747138021380D+00 Z= -4.252801997735D-02
I= 28 X= -4.879344881346D+00 Y= -5.028591447931D+00 Z= -3.062933398074D-01
I= 29 X= 3.661470576246D+00 Y= -3.820622784920D+00 Z= -5.114239220590D-01
I= 30 X= 3.414149101626D+00 Y= -3.167981242668D+00 Z= 1.933414311289D+00

I= 31 X= 2.386850860816D+00 Y= -5.134541937279D+00 Z= -1.518277982692D+00
I= 32 X= 5.141708891682D+00 Y= -3.082003119547D+00 Z= -1.718703117502D+00
I= 33 X= 5.061951932294D+00 Y= -1.976244987492D+00 Z= 3.235071549047D+00
I= 34 X= 2.219293753282D+00 Y= -4.257049218661D+00 Z= 3.317186862914D+00
I= 35 X= 1.114049446015D+00 Y= -1.168882029166D-01 Z= -4.146985433583D-01
I= 36 X= 4.123329002840D+00 Y= 2.965884776099D+00 Z= 4.100695704391D-01
I= 37 X= 5.523099902667D+00 Y= 2.255851974302D+00 Z= 1.912720842490D+00
I= 38 X= 2.965631455697D+00 Y= 4.470400945417D+00 Z= 9.855615640016D-01

Forward Direction:

Total Energy: -656.4423067 Hartrees

Potential Energy: -656.6203109 Hartress

Kinetic Energy: 0.1780042 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.113197817190D+13 Y= -5.191411967132D+12 Z= -3.718228370246D+12
I= 1 X= 2.926666178506D+12 Y= -1.198183463466D+12 Z= 5.540819645489D+12
I= 2 X= 5.170455032421D+12 Y= 1.993475969417D+13 Z= 9.576643600529D+11
I= 3 X= -2.831783409226D+12 Y= -6.772294352433D+12 Z= 5.796993674771D+12
I= 4 X= 2.172965043804D+13 Y= -2.554859749943D+12 Z= 1.157526942640D+13
I= 5 X= 6.399208060861D+12 Y= 1.839844063672D+12 Z= 1.179762378871D+13
I= 6 X= -1.606180941739D+13 Y= -3.108417259757D+12 Z= 6.723971340784D+13
I= 7 X= 1.035723050052D+13 Y= -6.373089118851D+13 Z= 2.484278050128D+13
I= 8 X= -5.431104263313D+13 Y= 5.520783143132D+13 Z= -1.822352961801D+13
I= 9 X= -5.259203117867D+12 Y= -1.426646332058D+13 Z= -7.499524557327D+12
I= 10 X= 1.080604744931D+14 Y= 1.060231250267D+14 Z= -8.247066099485D+13
I= 11 X= -5.036078043200D+13 Y= -3.119686988152D+12 Z= 1.114022328978D+14
I= 12 X= 1.041943554144D+13 Y= 1.291311452720D+13 Z= -4.665908204146D+13
I= 13 X= -2.069951770629D+12 Y= -4.444235347239D+12 Z= -2.488246965307D+13
I= 14 X= -4.337235416364D+13 Y= 4.609618756565D+12 Z= 6.556471282643D+13
I= 15 X= 2.968663524380D+13 Y= -4.158306271623D+13 Z= 4.962594323534D+13
I= 16 X= 8.349716770495D+12 Y= -1.386189075355D+13 Z= 1.713902098009D+13

I= 17 X= 3.785609704062D+10 Y= -1.228104069606D+12 Z= -2.940638495614D+12
I= 18 X= -6.710658954525D+13 Y= -9.498666628842D+12 Z= -5.584961535103D+13
I= 19 X= 7.993906772400D+13 Y= 5.990913777985D+13 Z= -2.273556237448D+12
I= 20 X= -6.965964022561D+13 Y= 9.845603750051D+13 Z= 9.569424890336D+12
I= 21 X= -1.338974732175D+13 Y= -9.458351770828D+12 Z= -1.106074938184D+13
I= 22 X= 4.050390751558D+13 Y= 7.131066115434D+12 Z= 9.314190972979D+13
I= 23 X= 9.750636413700D+13 Y= 3.033566126957D+13 Z= 5.244849180931D+13
I= 24 X= -1.955568634820D+13 Y= 1.378895870432D+14 Z= 2.041293664174D+13
I= 25 X= -3.918116183188D+12 Y= 1.564307982113D+13 Z= 2.895349449417D+12
I= 26 X= 1.077165178347D+13 Y= -2.412792462867D+13 Z= 6.224912797687D+12
I= 27 X= 9.295678212633D+13 Y= -1.134509078904D+14 Z= 9.445607884188D+13
I= 28 X= -2.541595458393D+13 Y= 3.274107348102D+13 Z= 3.292557345043D+13
I= 29 X= -2.049202740414D+13 Y= -1.969601456209D+13 Z= 2.349195829845D+13
I= 30 X= -7.177505574645D+12 Y= -4.691532035638D+12 Z= -1.217273582931D+13
I= 31 X= -2.863021498857D+13 Y= 5.395254657378D+13 Z= 8.528846370922D+13
I= 32 X= 1.866639959127D+14 Y= -6.053824900889D+13 Z= -4.516136083073D+13
I= 33 X= -1.884340344054D+13 Y= 2.699395241135D+13 Z= 5.003524638385D+13
I= 34 X= 2.792882438995D+13 Y= -1.541147222113D+13 Z= -2.319980369980D+13
I= 35 X= -1.102884965423D+12 Y= 1.238565552251D+12 Z= -3.667986004616D+12
I= 36 X= 3.515389291335D+12 Y= 3.315687926822D+12 Z= -1.067139536299D+13
I= 37 X= 1.483801862086D+14 Y= -7.808864596034D+13 Z= -2.828190629789D+13
I= 38 X= -3.017098160659D+13 Y= 1.642890234948D+13 Z= 2.599089904194D+13

Backward Direction:

Total Energy: -656.4422977 Hartrees

Potential Energy: -656.6203109 Hartress

Kinetic Energy: 0.1780132 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.122285774170D+13 Y= -5.310087505109D+12 Z= -3.671787485100D+12

I= 1 X= 2.786495577397D+12 Y= -1.503357073408D+12 Z= 5.357623072351D+12

I= 2 X= 5.039993935876D+12 Y= 2.005468231317D+13 Z= 7.645838657630D+11

I= 3 X= -3.099091457474D+12 Y= -6.766043930369D+12 Z= 5.409691794212D+12
I= 4 X= 2.218685121094D+13 Y= -2.595650368860D+12 Z= 1.127145215969D+13
I= 5 X= 5.644642549239D+12 Y= 7.667694189660D+11 Z= 9.655214059914D+12
I= 6 X= 8.403317693346D+11 Y= 1.618740647910D+13 Z= 7.484457312649D+13
I= 7 X= 1.344440712010D+13 Y= -6.080799161840D+13 Z= 2.503165328824D+13
I= 8 X= -5.041206596688D+13 Y= 5.835944878184D+13 Z= -1.786079699696D+13
I= 9 X= -5.113891331170D+12 Y= -1.419822217535D+13 Z= -7.663774699428D+12
I= 10 X= 1.080870508549D+14 Y= 1.063608478005D+14 Z= -8.286215169701D+13
I= 11 X= -5.040274934570D+13 Y= -3.123378820641D+12 Z= 1.113940718504D+14
I= 12 X= 1.050459846101D+13 Y= 1.293592440258D+13 Z= -4.673995289345D+13
I= 13 X= -2.041145830101D+12 Y= -4.458251215875D+12 Z= -2.494309733072D+13
I= 14 X= -4.332338201649D+13 Y= 4.523272044009D+12 Z= 6.557752956662D+13
I= 15 X= 2.977669531977D+13 Y= -4.166566336116D+13 Z= 4.947681036621D+13
I= 16 X= 8.343443215400D+12 Y= -1.383534283075D+13 Z= 1.716001741792D+13
I= 17 X= 8.196914847795D+10 Y= -1.325455007642D+12 Z= -2.950279065560D+12
I= 18 X= -6.709728852735D+13 Y= -9.653869852277D+12 Z= -5.597693481238D+13
I= 19 X= 7.984581361716D+13 Y= 5.987807253055D+13 Z= -2.177396705652D+12
I= 20 X= -6.959488179189D+13 Y= 9.836905109233D+13 Z= 9.558316582132D+12
I= 21 X= -1.344525557390D+13 Y= -9.493223294658D+12 Z= -1.119625348279D+13
I= 22 X= 4.049398773973D+13 Y= 7.287340724864D+12 Z= 9.259885830128D+13
I= 23 X= 9.770813074756D+13 Y= 3.024783442555D+13 Z= 5.238552236121D+13
I= 24 X= -1.965295492340D+13 Y= 1.378349569999D+14 Z= 2.025271847470D+13
I= 25 X= -3.978442512367D+12 Y= 1.558213761026D+13 Z= 2.864219411016D+12
I= 26 X= 1.062243830711D+13 Y= -2.429115261993D+13 Z= 6.206706784576D+12
I= 27 X= 9.308114030019D+13 Y= -1.133462084185D+14 Z= 9.441998765979D+13
I= 28 X= -2.540979230252D+13 Y= 3.255637176551D+13 Z= 3.305631316620D+13
I= 29 X= -2.077140597772D+13 Y= -1.961753929735D+13 Z= 2.339397011778D+13
I= 30 X= -7.161053222368D+12 Y= -4.745598843028D+12 Z= -1.229408703766D+13
I= 31 X= -2.882336874402D+13 Y= 5.389540301063D+13 Z= 8.529449908296D+13
I= 32 X= 1.860987189754D+14 Y= -6.006882087514D+13 Z= -4.549790957783D+13

I= 33 X= -1.882597020486D+13 Y= 2.692562566391D+13 Z= 4.993858970661D+13
I= 34 X= 2.811094669072D+13 Y= -1.553827051670D+13 Z= -2.323466038116D+13
I= 35 X= -1.105924292427D+12 Y= 1.309554822467D+12 Z= -3.217602818440D+12
I= 36 X= 2.533173872720D+12 Y= 2.075068920644D+12 Z= -1.112412858340D+13
I= 37 X= 1.492564132718D+14 Y= -7.764381643703D+13 Z= -2.937470167304D+13
I= 38 X= -2.969112567543D+13 Y= 1.637890048508D+13 Z= 2.517477278044D+13

Seed: 18408551020

CM Start Point Coordinates: bohr

I= 0 X= -2.440049694636D+00 Y= 2.322775633310D+00 Z= -5.026908204860D-01
I= 1 X= -2.803049832164D+00 Y= 9.465742386469D-02 Z= -1.988230591074D+00
I= 2 X= -2.009711354529D+00 Y= 1.764663882374D+00 Z= 1.936443986572D+00
I= 3 X= -2.601443733965D+00 Y= -1.982833088960D+00 Z= -2.935236326657D-01
I= 4 X= -2.143290824145D+00 Y= -9.322731998318D-01 Z= 2.131047960463D+00
I= 5 X= 4.273793261068D+00 Y= 2.323600912924D+00 Z= -1.611876087843D+00
I= 6 X= 2.310364177304D+00 Y= 2.141109464897D-01 Z= -2.950029899974D+00
I= 7 X= 5.826577508426D+00 Y= 1.702970415157D+00 Z= -2.335256597183D+00
I= 8 X= 3.473170903924D+00 Y= 3.766378509561D+00 Z= -2.931723299278D+00
I= 9 X= -2.402181221195D+00 Y= -2.492026873866D+00 Z= 4.631981550083D+00
I= 10 X= -4.188409650551D+00 Y= -2.622881844374D+00 Z= 5.268339979652D+00
I= 11 X= -1.345324440283D+00 Y= -4.289686437992D+00 Z= 4.086135230710D+00
I= 12 X= -1.403870479239D+00 Y= -1.523544957126D+00 Z= 6.126363802109D+00
I= 13 X= -1.945129470062D+00 Y= 3.342924363323D+00 Z= 4.183287352483D+00
I= 14 X= -4.020406176435D+00 Y= 3.604202210907D+00 Z= 4.991836546288D+00
I= 15 X= -4.629011860539D-01 Y= 2.819489738572D+00 Z= 5.539310484606D+00
I= 16 X= -1.402094019823D+00 Y= 5.420546242245D+00 Z= 3.971552125912D+00
I= 17 X= -2.311116397418D+00 Y= 5.086766184368D+00 Z= -1.350915693546D+00
I= 18 X= -3.916601944712D+00 Y= 6.526761020925D+00 Z= -2.326353761746D-01
I= 19 X= -4.045527223897D-01 Y= 5.928331253423D+00 Z= -8.454004274390D-01
I= 20 X= -2.801248150752D+00 Y= 4.889636138657D+00 Z= -3.800350089859D+00

I= 21 X= -3.677035521301D+00 Y= 4.274149919200D-02 Z= -4.642165261930D+00
I= 22 X= -5.831361868216D+00 Y= 1.211342805017D-01 Z= -4.584584098235D+00
I= 23 X= -2.716881973786D+00 Y= 1.545625781695D+00 Z= -5.709834087610D+00
I= 24 X= -2.903103095204D+00 Y= -2.013615424750D+00 Z= -5.244351934952D+00
I= 25 X= -2.984034102483D+00 Y= -4.632722716795D+00 Z= -7.334915921345D-01
I= 26 X= -2.465825591980D+00 Y= -5.456810378177D+00 Z= -2.465024943468D+00
I= 27 X= -1.904534709331D+00 Y= -5.699376387614D+00 Z= 7.112492073182D-01
I= 28 X= -5.181606896636D+00 Y= -4.912346213534D+00 Z= -2.421129104901D-01
I= 29 X= 3.435648777931D+00 Y= -3.799944197932D+00 Z= -1.229087093149D+00
I= 30 X= 3.982454030576D+00 Y= -3.016784045119D+00 Z= 1.145501005740D+00
I= 31 X= 1.773800041125D+00 Y= -5.198383115091D+00 Z= -1.384115008870D+00
I= 32 X= 4.918284708631D+00 Y= -3.467541108916D+00 Z= -2.773272101875D+00
I= 33 X= 5.778027400958D+00 Y= -2.034262379752D+00 Z= 1.785188948334D+00
I= 34 X= 3.188589599450D+00 Y= -4.201196135934D+00 Z= 2.617227695210D+00
I= 35 X= 1.150967357424D+00 Y= -9.111452431947D-02 Z= -3.540984519417D-01
I= 36 X= 4.170422403745D+00 Y= 2.582448280793D+00 Z= 1.034346530691D+00
I= 37 X= 5.858187879076D+00 Y= 1.827759135712D+00 Z= 2.005331809771D+00
I= 38 X= 2.877031483097D+00 Y= 3.973685166787D+00 Z= 2.276688644651D+00

Forward Direction:

Total Energy: -656.4423645 Hartrees

Potential Energy: -656.6277447 Hartress

Kinetic Energy: 0.1853802 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.924481515222D+12 Y= 2.069182536847D+13 Z= 5.619784577854D+11
I= 1 X= -5.269406343547D+12 Y= 3.759141431437D+12 Z= 1.019705213867D+13
I= 2 X= 2.256662083288D+13 Y= 1.685851162130D+13 Z= 6.115465617085D+12
I= 3 X= 1.215101205863D+13 Y= 6.990893579938D+12 Z= 3.607570658663D+12
I= 4 X= 5.394733716566D+12 Y= -3.028869127786D+13 Z= 5.681814601860D+12
I= 5 X= -8.557022428465D+11 Y= -7.886957339985D+12 Z= -2.473729800440D+13
I= 6 X= -3.047415360539D+13 Y= -1.863152568115D+13 Z= 3.300510604779D+13

I= 7 X= -2.202483363291D+13 Y= 4.402570888787D+13 Z= 1.687166897406D+13
I= 8 X= -2.772158313637D+13 Y= 1.996416211835D+13 Z= -5.616883683978D+13
I= 9 X= 1.802130743565D+12 Y= 3.945719564244D+12 Z= 1.316315581722D+13
I= 10 X= 1.265013952071D+14 Y= 3.955522325184D+12 Z= -8.152083792004D+13
I= 11 X= -4.387904100617D+13 Y= -3.724660204175D+13 Z= 2.108353243628D+13
I= 12 X= 2.487318122670D+13 Y= 8.286340849786D+13 Z= -9.287808671241D+12
I= 13 X= 4.574913975908D+12 Y= -1.320440889720D+13 Z= 1.188536011209D+13
I= 14 X= 4.320480186881D+13 Y= -3.836997001113D+13 Z= -4.681498773947D+13
I= 15 X= -1.066808155342D+14 Y= 4.410021239456D+13 Z= -9.529022942703D+13
I= 16 X= 2.792818867021D+13 Y= -8.004473181194D+12 Z= -8.502455130192D+13
I= 17 X= -8.478825650451D+12 Y= -2.171417200129D+13 Z= 2.857780299247D+12
I= 18 X= 1.034998221986D+14 Y= -1.182910137975D+14 Z= 4.007792712716D+13
I= 19 X= -3.033659429318D+13 Y= 7.033567338140D+13 Z= 1.776700410586D+12
I= 20 X= -2.239195794374D+13 Y= 9.436336933056D+12 Z= 2.084090237566D+13
I= 21 X= -1.775852081747D+13 Y= 1.590995034051D+12 Z= -1.583826914719D+11
I= 22 X= 1.015903490870D+14 Y= 7.839686455556D+13 Z= -4.546640749895D+12
I= 23 X= -9.230552998273D+13 Y= -2.853781265248D+12 Z= -8.964349993154D+12
I= 24 X= 9.825985285852D+13 Y= -4.080788346995D+13 Z= -4.572181180604D+13
I= 25 X= -1.592692369483D+12 Y= -4.978897653477D+12 Z= -9.035977044616D+12
I= 26 X= -9.015313768418D+13 Y= 1.576070224618D+13 Z= 4.884466847360D+13
I= 27 X= -6.165695413737D+13 Y= -4.040243311014D+13 Z= 4.947088926129D+13
I= 28 X= 1.081397261598D+14 Y= 3.239701129690D+13 Z= 1.000903701596D+13
I= 29 X= -2.395420561387D+13 Y= -3.234868114561D+12 Z= 2.052655079839D+13
I= 30 X= 7.834032691614D+12 Y= 1.127455572159D+13 Z= 3.515154483096D+12
I= 31 X= 2.698386310579D+13 Y= -9.745400690303D+13 Z= -4.595692406012D+13
I= 32 X= 1.203249431207D+14 Y= -5.930872621525D+13 Z= -1.239744114805D+14
I= 33 X= -6.203657538514D+13 Y= -1.580489544465D+13 Z= -3.355780825213D+13
I= 34 X= 1.087195984819D+12 Y= -2.981552875047D+13 Z= -3.379810375918D+12
I= 35 X= -1.917508656727D+12 Y= 1.661878109725D+12 Z= -8.930511556263D+11
I= 36 X= 1.553333788946D+13 Y= 5.277545692961D+12 Z= -8.988251270264D+12

I= 37 X= -1.305962052911D+14 Y= 1.116020589972D+14 Z= 3.006745675545D+13

I= 38 X= 1.431133594838D+13 Y= -4.552587893319D+13 Z= 4.032203558235D+13

Backward Direction:

Total Energy: -656.4423627 Hartrees

Potential Energy: -656.6277447 Hartress

Kinetic Energy: 0.1853820 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.985038099636D+12 Y= 2.061274725087D+13 Z= 5.929238233215D+11

I= 1 X= -5.362807456126D+12 Y= 3.555792408235D+12 Z= 1.007498115157D+13

I= 2 X= 2.247968953987D+13 Y= 1.693842071726D+13 Z= 5.986808589064D+12

I= 3 X= 1.197289433140D+13 Y= 6.995058479416D+12 Z= 3.349496381821D+12

I= 4 X= 5.699384336920D+12 Y= -3.031587165066D+13 Z= 5.479369364451D+12

I= 5 X= -1.358498532973D+12 Y= -8.601988628287D+12 Z= -2.616486876801D+13

I= 6 X= -1.921160084614D+13 Y= -5.773969322318D+12 Z= 3.807251927441D+13

I= 7 X= -1.996772801804D+13 Y= 4.597335032875D+13 Z= 1.699752224396D+13

I= 8 X= -2.512354364005D+13 Y= 2.206420709392D+13 Z= -5.592713401490D+13

I= 9 X= 1.898957628018D+12 Y= 3.991191288980D+12 Z= 1.305370957329D+13

I= 10 X= 1.265191040659D+14 Y= 4.180560126398D+12 Z= -8.178170337124D+13

I= 11 X= -4.390700653535D+13 Y= -3.724906205931D+13 Z= 2.107809441760D+13

I= 12 X= 2.492992858614D+13 Y= 8.287860760050D+13 Z= -9.341696060998D+12

I= 13 X= 4.594108494665D+12 Y= -1.321374821470D+13 Z= 1.184496153662D+13

I= 14 X= 4.323743391056D+13 Y= -3.842750617926D+13 Z= -4.680644745589D+13

I= 15 X= -1.066208050164D+14 Y= 4.404517237520D+13 Z= -9.538960244327D+13

I= 16 X= 2.792400835525D+13 Y= -7.986783268104D+12 Z= -8.501056055710D+13

I= 17 X= -8.449431411585D+12 Y= -2.177904071057D+13 Z= 2.851356412813D+12

I= 18 X= 1.035060198258D+14 Y= -1.183944317283D+14 Z= 3.999308922833D+13

I= 19 X= -3.039873311844D+13 Y= 7.031497340487D+13 Z= 1.840775241437D+12

I= 20 X= -2.234880688511D+13 Y= 9.378374511412D+12 Z= 2.083350048422D+13

I= 21 X= -1.779550812211D+13 Y= 1.567758783757D+12 Z= -2.486743331117D+11

I= 22 X= 1.015837391547D+14 Y= 7.850099639478D+13 Z= -4.908497002682D+12

I= 23 X= -9.217108505435D+13 Y= -2.912303700962D+12 Z= -9.006308976539D+12
I= 24 X= 9.819503902970D+13 Y= -4.084428558894D+13 Z= -4.582857138806D+13
I= 25 X= -1.632890146361D+12 Y= -5.019505813618D+12 Z= -9.056720199092D+12
I= 26 X= -9.025256439899D+13 Y= 1.565193709652D+13 Z= 4.883253709895D+13
I= 27 X= -6.157408945483D+13 Y= -4.033266777894D+13 Z= 4.944684030715D+13
I= 28 X= 1.081438323262D+14 Y= 3.227393737055D+13 Z= 1.009615394779D+13
I= 29 X= -2.414036640100D+13 Y= -3.182577000872D+12 Z= 2.046125747133D+13
I= 30 X= 7.844995534517D+12 Y= 1.123852890891D+13 Z= 3.434293462048D+12
I= 31 X= 2.685515726370D+13 Y= -9.749208387828D+13 Z= -4.595290245620D+13
I= 32 X= 1.199482771534D+14 Y= -5.899592803240D+13 Z= -1.241986669773D+14
I= 33 X= -6.202495893689D+13 Y= -1.585042420690D+13 Z= -3.362221435081D+13
I= 34 X= 1.208551144887D+12 Y= -2.990001937963D+13 Z= -3.403036734044D+12
I= 35 X= -1.919533878540D+12 Y= 1.709181016117D+12 Z= -5.929433564850D+11
I= 36 X= 1.487884962882D+13 Y= 4.450873092936D+12 Z= -9.289924988840D+12
I= 37 X= -1.300123411884D+14 Y= 1.118984661770D+14 Z= 2.933928477822D+13
I= 38 X= 1.463108258146D+13 Y= -4.555919711514D+13 Z= 3.977821897554D+13

Seed: 18445319666

CM Start Point Coordinates: bohr

I= 0 X= -2.470985051694D+00 Y= 2.327657951253D+00 Z= -6.354932749596D-01
I= 1 X= -2.727129763202D+00 Y= 3.844334688527D-02 Z= -1.960793004144D+00
I= 2 X= -2.007541396539D+00 Y= 1.764317671658D+00 Z= 2.086600324201D+00
I= 3 X= -2.572621735242D+00 Y= -2.044222386929D+00 Z= -2.210926550552D-01
I= 4 X= -2.365298038350D+00 Y= -9.785517506617D-01 Z= 2.347557648825D+00
I= 5 X= 4.529652496794D+00 Y= 2.506323004361D+00 Z= -1.123683895615D+00
I= 6 X= 2.313787602805D+00 Y= 5.326969609555D-01 Z= -2.970276551575D+00
I= 7 X= 6.471313482685D+00 Y= 1.773521088581D+00 Z= -1.906069541707D+00
I= 8 X= 3.842832096471D+00 Y= 4.203783011354D+00 Z= -2.042683491121D+00
I= 9 X= -1.985746684097D+00 Y= -2.396554283703D+00 Z= 4.782576829296D+00
I= 10 X= -3.655581608789D+00 Y= -2.209137719726D+00 Z= 5.751659100014D+00

I= 11 X= -1.681192040778D+00 Y= -4.403838699767D+00 Z= 4.502801271680D+00
I= 12 X= -5.795234427374D-01 Y= -1.436066926177D+00 Z= 5.969277124014D+00
I= 13 X= -1.712496002102D+00 Y= 3.641598130839D+00 Z= 4.016822742205D+00
I= 14 X= -3.833325791550D+00 Y= 4.722308753660D+00 Z= 4.374913552991D+00
I= 15 X= -1.038637804677D+00 Y= 2.957221657289D+00 Z= 5.858762945671D+00
I= 16 X= -7.458229062581D-01 Y= 5.337203326052D+00 Z= 2.956516994080D+00
I= 17 X= -2.311726779594D+00 Y= 5.026503867527D+00 Z= -1.572177480437D+00
I= 18 X= -3.907033006269D+00 Y= 6.426983304522D+00 Z= -3.784782220560D-02
I= 19 X= 7.115444677015D-02 Y= 5.925342473290D+00 Z= -1.255924130436D+00
I= 20 X= -3.074570764598D+00 Y= 4.963290047286D+00 Z= -3.857581223474D+00
I= 21 X= -3.334901018330D+00 Y= -4.029689294025D-01 Z= -4.744212872030D+00
I= 22 X= -5.472031284022D+00 Y= -7.085310330048D-01 Z= -4.782460148433D+00
I= 23 X= -2.821973178897D+00 Y= 1.386293768628D+00 Z= -5.981413958062D+00
I= 24 X= -2.422905907066D+00 Y= -2.024781775511D+00 Z= -5.461847091329D+00
I= 25 X= -2.949808853066D+00 Y= -4.777398484915D+00 Z= -6.848967491930D-01
I= 26 X= -3.181844548137D+00 Y= -5.143314465371D+00 Z= -2.933419630734D+00
I= 27 X= -1.412318093707D+00 Y= -5.552918492675D+00 Z= 3.602547832891D-01
I= 28 X= -4.987641149336D+00 Y= -5.421578000245D+00 Z= -1.128206229850D-01
I= 29 X= 2.867111349011D+00 Y= -3.643277968321D+00 Z= -1.743436407659D+00
I= 30 X= 4.016552128168D+00 Y= -3.248887468254D+00 Z= 6.708923078273D-01
I= 31 X= 1.241431165558D+00 Y= -5.012357883700D+00 Z= -2.064798669334D+00
I= 32 X= 4.081969403629D+00 Y= -3.571214466610D+00 Z= -3.578667887027D+00
I= 33 X= 5.923871441729D+00 Y= -2.555559095669D+00 Z= 1.041435619068D+00
I= 34 X= 2.982714410878D+00 Y= -3.916126118476D+00 Z= 2.477331347624D+00
I= 35 X= 1.109591985370D+00 Y= -4.589709267118D-02 Z= -3.361883614330D-01
I= 36 X= 3.821960389525D+00 Y= 2.426221547038D+00 Z= 1.546285445449D+00
I= 37 X= 5.225950970599D+00 Y= 1.476728380187D+00 Z= 2.840973111640D+00
I= 38 X= 2.941872282305D+00 Y= 4.088248125100D+00 Z= 2.256899220507D+00

Forward Direction:

Total Energy: -656.4303815 Hartrees

Potential Energy: -656.6106911 Hartress

Kinetic Energy: 0.1803096 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.205417700612D+12 Y= 3.563444359132D+12 Z= 5.678105770497D+12
I= 1 X= -7.789830797979D+12 Y= -1.616950086748D+13 Z= -3.269793033338D+13
I= 2 X= -7.399726596875D+11 Y= 1.693839518014D+13 Z= 1.507102647862D+13
I= 3 X= -5.756863211249D+11 Y= 5.387825056065D+12 Z= 9.894403072031D+12
I= 4 X= 6.116874187788D+12 Y= 4.409076954412D+11 Z= -9.748114846826D+10
I= 5 X= -2.497468014864D+12 Y= -1.512671215318D+13 Z= -3.155242131277D+12
I= 6 X= -5.706095374726D+13 Y= -1.039335352852D+14 Z= 4.269588098724D+13
I= 7 X= 1.905346998339D+13 Y= 1.923072023180D+12 Z= 3.191455565748D+13
I= 8 X= -7.358313038363D+13 Y= 7.757314301143D+13 Z= -1.261306820262D+14
I= 9 X= 1.154527579599D+13 Y= -1.430005657163D+13 Z= -2.150559750495D+13
I= 10 X= -1.268250467828D+14 Y= 2.104366857639D+13 Z= -1.755709522792D+13
I= 11 X= -1.780226325191D+13 Y= 3.886409447791D+13 Z= 1.827134936637D+12
I= 12 X= 1.212717262493D+14 Y= 9.456662587438D+12 Z= -4.734810832983D+13
I= 13 X= 1.568899222327D+13 Y= -4.413725937665D+11 Z= 2.494141870451D+13
I= 14 X= -3.089165376132D+12 Y= 4.803651910643D+13 Z= 3.521845676782D+13
I= 15 X= -3.128353956578D+13 Y= 1.923459874135D+13 Z= -5.686180867351D+13
I= 16 X= -5.668096172019D+13 Y= -4.273593300414D+13 Z= 1.994052780086D+13
I= 17 X= -6.615552953651D+12 Y= 1.536902888153D+13 Z= -1.521990951923D+13
I= 18 X= 8.837383846478D+13 Y= -7.253615636087D+13 Z= -1.999517500031D+13
I= 19 X= 1.069764712676D+14 Y= -3.658937295478D+13 Z= 9.232303930678D+13
I= 20 X= -3.714056788687D+13 Y= 2.184164655020D+13 Z= 5.666747742394D+13
I= 21 X= -2.710772186299D+13 Y= 1.268222459518D+12 Z= 1.910560293348D+13
I= 22 X= 1.310854030381D+14 Y= -6.967413967729D+13 Z= 4.381453954314D+13
I= 23 X= 3.108876513385D+13 Y= -4.994516266084D+12 Z= 3.545905286327D+13
I= 24 X= 2.862680145886D+13 Y= -1.120031882693D+13 Z= 3.856999484930D+13
I= 25 X= 8.258834813433D+12 Y= 9.504693338317D+12 Z= 1.574512344528D+12
I= 26 X= 4.328599648311D+13 Y= -1.083412704091D+14 Z= -9.216466536330D+12

I= 27 X= -7.237327256521D+12 Y= -5.061920060254D+13 Z= 1.052119534169D+13
I= 28 X= -7.051159435955D+13 Y= 1.632497162837D+13 Z= -5.817245501196D+12
I= 29 X= 9.127157685216D+12 Y= 9.180231540869D+12 Z= -1.511871717624D+13
I= 30 X= -1.504558803851D+12 Y= 9.457433484267D+12 Z= -5.138910929936D+12
I= 31 X= 1.852271228832D+13 Y= -9.323738116705D+13 Z= 4.031175674448D+13
I= 32 X= -1.505160922073D+14 Y= -4.968549949521D+13 Z= 8.628196738706D+13
I= 33 X= 3.253507183455D+13 Y= -3.766085338274D+13 Z= 3.235857226893D+13
I= 34 X= 1.459320499188D+13 Y= -1.477260890696D+13 Z= 2.813795654067D+13
I= 35 X= -9.161710932931D+11 Y= 3.072175280430D+12 Z= -1.379823793803D+12
I= 36 X= 6.428060356304D+12 Y= -1.504852607151D+13 Z= 4.967381257340D+12
I= 37 X= -7.632517870171D+13 Y= 6.808968860258D+13 Z= -1.116944358905D+13
I= 38 X= 9.321197381126D+13 Y= -5.944846332634D+13 Z= -2.173221767696D+13

Backward Direction:

Total Energy: -656.4303349 Hartrees

Potential Energy: -656.6106911 Hartress

Kinetic Energy: 0.1803562 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.628853246912D+12 Y= 3.010498941225D+12 Z= 5.894487979746D+12
I= 1 X= -8.442928249388D+12 Y= -1.759139751340D+13 Z= -3.355149886564D+13
I= 2 X= -1.347830580779D+12 Y= 1.749715112912D+13 Z= 1.417140574957D+13
I= 3 X= -1.821155789585D+12 Y= 5.416947671097D+12 Z= 8.089845839786D+12
I= 4 X= 8.247111608932D+12 Y= 2.508518007238D+11 Z= -1.513058171585D+12
I= 5 X= -6.013218183387D+12 Y= -2.012649321837D+13 Z= -1.313738052144D+13
I= 6 X= 2.169126161342D+13 Y= -1.402842503513D+13 Z= 7.812923488997D+13
I= 7 X= 3.343756459050D+13 Y= 1.554174990816D+13 Z= 3.279457140651D+13
I= 8 X= -5.541661251340D+13 Y= 9.225748659271D+13 Z= -1.244406004418D+14
I= 9 X= 1.222232759294D+13 Y= -1.398210032370D+13 Z= -2.227088885512D+13
I= 10 X= -1.267012194371D+14 Y= 2.261722171041D+13 Z= -1.938116944591D+13
I= 11 X= -1.799780920938D+13 Y= 3.884689307488D+13 Z= 1.789110145958D+12
I= 12 X= 1.216685261781D+14 Y= 9.562940721415D+12 Z= -4.772491022162D+13

I= 13 X= 1.582320786418D+13 Y= -5.066767880611D+11 Z= 2.465893592278D+13
I= 14 X= -2.860989251566D+12 Y= 4.763420350348D+13 Z= 3.527817383042D+13
I= 15 X= -3.086392230861D+13 Y= 1.884973721206D+13 Z= -5.755666404060D+13
I= 16 X= -5.671019211952D+13 Y= -4.261223815732D+13 Z= 2.003835660503D+13
I= 17 X= -6.410016833861D+12 Y= 1.491544125029D+13 Z= -1.526482787907D+13
I= 18 X= 8.841717471535D+13 Y= -7.325929537648D+13 Z= -2.058839512279D+13
I= 19 X= 1.065419720412D+14 Y= -3.673411536792D+13 Z= 9.277107581237D+13
I= 20 X= -3.683883864260D+13 Y= 2.143635040328D+13 Z= 5.661572045444D+13
I= 21 X= -2.736635169015D+13 Y= 1.105745423944D+12 Z= 1.847424812843D+13
I= 22 X= 1.310391837877D+14 Y= -6.894600875215D+13 Z= 4.128429779306D+13
I= 23 X= 3.202885714165D+13 Y= -5.403728243231D+12 Z= 3.516565907540D+13
I= 24 X= 2.817359760018D+13 Y= -1.145485681131D+13 Z= 3.782348970205D+13
I= 25 X= 7.977756090415D+12 Y= 9.220745054407D+12 Z= 1.429468025220D+12
I= 26 X= 4.259076562942D+13 Y= -1.091017992438D+14 Z= -9.301293902513D+12
I= 27 X= -6.657904726858D+12 Y= -5.013137388421D+13 Z= 1.035303557229D+13
I= 28 X= -7.048288243386D+13 Y= 1.546439012973D+13 Z= -5.208089508423D+12
I= 29 X= 7.825447960997D+12 Y= 9.545871660874D+12 Z= -1.557527390831D+13
I= 30 X= -1.427902287463D+12 Y= 9.205519784121D+12 Z= -5.704323115033D+12
I= 31 X= 1.762275021490D+13 Y= -9.350363040411D+13 Z= 4.033987737928D+13
I= 32 X= -1.531498893494D+14 Y= -4.749829107995D+13 Z= 8.471388442649D+13
I= 33 X= 3.261629859858D+13 Y= -3.797920847441D+13 Z= 3.190821940796D+13
I= 34 X= 1.544176817066D+13 Y= -1.536340073586D+13 Z= 2.797554866137D+13
I= 35 X= -9.303322427244D+11 Y= 3.402935877453D+12 Z= 7.186484220987D+11
I= 36 X= 1.851620050781D+12 Y= -2.082894726972D+13 Z= 2.857959514627D+12
I= 37 X= -7.224257037430D+13 Y= 7.016228462072D+13 Z= -1.626110954112D+13
I= 38 X= 9.544776851183D+13 Y= -5.968143721982D+13 Z= -2.553479808251D+13

Seed: 18494611204

CM Start Point Coordinates: bohr

I= 0 X= -2.112160098458D+00 Y= 2.385892303857D+00 Z= -5.935249105590D-01

I= 1 X= -2.849478588103D+00 Y= 1.770631817640D-01 Z= -1.875428466913D+00
I= 2 X= -1.844310996213D+00 Y= 1.745890799247D+00 Z= 2.174216617763D+00
I= 3 X= -2.655260561180D+00 Y= -1.893010904829D+00 Z= -3.579732916471D-01
I= 4 X= -1.988892876606D+00 Y= -8.944224034992D-01 Z= 2.218766469278D+00
I= 5 X= 3.717197824894D+00 Y= 2.868041171795D+00 Z= -1.842979988816D+00
I= 6 X= 1.918087491148D+00 Y= 2.965613331241D-01 Z= -3.127891170459D+00
I= 7 X= 5.223880711481D+00 Y= 2.316187554179D+00 Z= -3.221236237806D+00
I= 8 X= 2.481105851980D+00 Y= 4.517296589915D+00 Z= -2.419313206504D+00
I= 9 X= -2.089355581816D+00 Y= -2.582723980197D+00 Z= 4.585503164715D+00
I= 10 X= -4.152173407255D+00 Y= -2.376104399232D+00 Z= 5.521492149026D+00
I= 11 X= -1.911289468698D+00 Y= -4.594006421991D+00 Z= 4.602142186832D+00
I= 12 X= -7.351286249269D-01 Y= -2.093199198707D+00 Z= 6.284426786808D+00
I= 13 X= -1.862090732035D+00 Y= 3.413562489879D+00 Z= 4.287312739186D+00
I= 14 X= -3.652481250547D+00 Y= 2.747052488176D+00 Z= 5.652244296957D+00
I= 15 X= -1.108119588623D-01 Y= 2.949516458859D+00 Z= 5.549435583488D+00
I= 16 X= -1.522532780441D+00 Y= 5.676763084446D+00 Z= 3.941291116067D+00
I= 17 X= -1.917681218413D+00 Y= 5.064115665414D+00 Z= -1.411765697598D+00
I= 18 X= -3.476536260416D+00 Y= 6.414358440215D+00 Z= -2.333204384999D-01
I= 19 X= 2.933877841194D-03 Y= 5.957894975167D+00 Z= -8.334386791610D-01
I= 20 X= -2.353325118991D+00 Y= 5.072601239761D+00 Z= -3.519411427512D+00
I= 21 X= -3.221058546428D+00 Y= -9.469228787206D-02 Z= -4.762275177144D+00
I= 22 X= -5.430716661986D+00 Y= 2.900193757989D-01 Z= -5.165590454001D+00
I= 23 X= -2.205502665196D+00 Y= 1.403428141392D+00 Z= -5.757989822353D+00
I= 24 X= -2.809774492309D+00 Y= -1.885874301441D+00 Z= -5.892239365749D+00
I= 25 X= -3.129319548904D+00 Y= -4.655517884540D+00 Z= -7.796465796496D-01
I= 26 X= -3.498199291977D+00 Y= -5.205171845741D+00 Z= -2.903086328455D+00
I= 27 X= -1.788009113064D+00 Y= -5.983679352592D+00 Z= 2.337909142205D-01
I= 28 X= -5.059954668683D+00 Y= -5.039400983402D+00 Z= 6.876146234493D-02
I= 29 X= 3.538999327834D+00 Y= -3.562117793445D+00 Z= -1.049239108276D+00
I= 30 X= 3.647143101554D+00 Y= -3.102682010673D+00 Z= 1.475425016187D+00

I= 31 X= 2.298847294669D+00 Y= -4.857437007681D+00 Z= -1.954845671365D+00
I= 32 X= 4.933697968734D+00 Y= -3.118696952440D+00 Z= -2.192959134202D+00
I= 33 X= 5.296187474340D+00 Y= -2.354193172436D+00 Z= 2.217059824919D+00
I= 34 X= 2.207874615336D+00 Y= -3.799617793468D+00 Z= 2.916482862344D+00
I= 35 X= 1.101596678207D+00 Y= -1.751911095714D-01 Z= -3.731124764737D-01
I= 36 X= 3.854105359213D+00 Y= 2.504450839132D+00 Z= 8.305724840335D-01
I= 37 X= 5.579654269337D+00 Y= 1.553615721303D+00 Z= 1.772324817810D+00
I= 38 X= 2.400335186047D+00 Y= 3.641930794712D+00 Z= 2.041365770211D+00

Forward Direction:

Total Energy: -656.4380051 Hartrees

Potential Energy: -656.6449760 Hartress

Kinetic Energy: 0.2069709 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.308751143305D+13 Y= -7.394283545137D+12 Z= 9.675603064665D+11
I= 1 X= 5.422686071984D+12 Y= 1.441816923784D+13 Z= -9.561842191846D+12
I= 2 X= -4.313733578873D+12 Y= 3.637135626927D+12 Z= 2.615058992732D+12
I= 3 X= 1.445761192204D+13 Y= 6.917257761741D+12 Z= -1.838145938652D+13
I= 4 X= 6.146039531659D+12 Y= -1.502344644401D+13 Z= 8.454645820403D+12
I= 5 X= 5.167500683652D+12 Y= 5.787938152460D+12 Z= 2.033895383730D+13
I= 6 X= 5.497870352005D+13 Y= -1.914908876731D+13 Z= -5.386847627959D+13
I= 7 X= -1.063544124857D+14 Y= 5.434079332243D+13 Z= 4.011129168265D+11
I= 8 X= 2.957146899488D+13 Y= -2.988604821374D+12 Z= -3.791150645609D+13
I= 9 X= 2.475610727667D+13 Y= 2.317680378503D+12 Z= -3.771250277023D+12
I= 10 X= -3.434863429154D+13 Y= 3.442941554716D+13 Z= 1.023066895770D+14
I= 11 X= 5.664877865260D+12 Y= -1.852485422195D+13 Z= -4.691536032887D+13
I= 12 X= -9.470199133417D+13 Y= 6.360181388174D+13 Z= -1.953166354546D+13
I= 13 X= 6.614057364675D+12 Y= 2.936422535588D+12 Z= -1.523849987493D+13
I= 14 X= -8.071032876012D+13 Y= -3.934133788277D+13 Z= -2.755085288667D+13
I= 15 X= 3.830612455094D+13 Y= 3.297844808679D+13 Z= 9.384371018515D+13
I= 16 X= 3.607224953912D+13 Y= 3.641022075511D+13 Z= 3.860407098620D+11

I= 17 X= 1.378644074623D+13 Y= 3.667153074777D+13 Z= -9.776697014393D+12
I= 18 X= 1.574908124457D+13 Y= -1.565085654551D+13 Z= -4.854908743146D+13
I= 19 X= -1.070288934242D+14 Y= -1.417634352297D+14 Z= -6.979175894976D+13
I= 20 X= -6.112001346224D+13 Y= -3.803713619783D+13 Z= -4.071774186645D+13
I= 21 X= -1.352847703583D+13 Y= 3.768024756483D+12 Z= 5.739156531693D+12
I= 22 X= -7.222492139183D+12 Y= -1.551015139378D+13 Z= 8.849428071484D+13
I= 23 X= 4.547140563081D+13 Y= -5.958922025095D+13 Z= 1.786635727630D+12
I= 24 X= 5.807820412906D+13 Y= -1.084843883600D+14 Z= -1.118898990916D+14
I= 25 X= 7.400756534022D+12 Y= 2.645520925887D+12 Z= 1.623567408900D+13
I= 26 X= -3.474424802594D+13 Y= 6.000507433422D+13 Z= 9.163891546324D+13
I= 27 X= -4.920925888549D+13 Y= -3.020226816297D+13 Z= -9.260732507648D+12
I= 28 X= -1.601320212839D+14 Y= -4.572546150959D+13 Z= 1.457852567972D+13
I= 29 X= -2.416076392198D+12 Y= 3.280383815465D+11 Z= 1.299336705394D+13
I= 30 X= -1.931545886921D+13 Y= -1.800681781472D+13 Z= 4.958668411406D+10
I= 31 X= 6.052382313292D+13 Y= 2.946477861990D+12 Z= 4.171901988278D+13
I= 32 X= 1.698127758207D+14 Y= 2.857012545391D+13 Z= -6.050674845294D+13
I= 33 X= -3.323720536224D+13 Y= -9.047209565022D+13 Z= -6.300490259214D+13
I= 34 X= 3.331132379316D+13 Y= 3.217515888318D+12 Z= 3.851910798083D+12
I= 35 X= 3.564716010301D+11 Y= -1.883381340199D+12 Z= 3.132060689594D+12
I= 36 X= 1.668989314238D+12 Y= 1.258806706791D+13 Z= -3.350802265104D+13
I= 37 X= 9.234991624263D+13 Y= -7.440043645518D+13 Z= 8.490335946716D+13
I= 38 X= -5.939669788308D+13 Y= -3.864438365709D+13 Z= 1.778374160918D+13

Backward Direction:

Total Energy: -656.4379762 Hartrees

Potential Energy: -656.6449760 Hartress

Kinetic Energy: 0.2069998 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.320831615078D+13 Y= -7.552036989294D+12 Z= 1.029293413367D+12

I= 1 X= 5.236359595004D+12 Y= 1.401250697239D+13 Z= -9.805362385264D+12

I= 2 X= -4.487153371550D+12 Y= 3.796546793412D+12 Z= 2.358400266679D+12

I= 3 X= 1.410228372981D+13 Y= 6.925566344892D+12 Z= -1.889629341326D+13
I= 4 X= 6.753789004010D+12 Y= -1.507766874226D+13 Z= 8.050786521474D+12
I= 5 X= 4.164469147142D+12 Y= 4.361517660262D+12 Z= 1.749108378834D+13
I= 6 X= 7.744644207073D+13 Y= 6.500532670416D+12 Z= -4.375946121469D+13
I= 7 X= -1.022506793343D+14 Y= 5.822615569442D+13 Z= 6.521784077427D+11
I= 8 X= 3.475431461074D+13 Y= 1.200788336747D+12 Z= -3.742933194416D+13
I= 9 X= 2.494926784706D+13 Y= 2.408392212166D+12 Z= -3.989585289281D+12
I= 10 X= -3.431330677475D+13 Y= 3.487834489169D+13 Z= 1.017862874188D+14
I= 11 X= 5.609089272141D+12 Y= -1.852976172341D+13 Z= -4.692620867060D+13
I= 12 X= -9.458878566973D+13 Y= 6.363213466973D+13 Z= -1.963916384004D+13
I= 13 X= 6.652348630382D+12 Y= 2.917791471360D+12 Z= -1.531909125047D+13
I= 14 X= -8.064523088933D+13 Y= -3.945611715487D+13 Z= -2.753381581333D+13
I= 15 X= 3.842583992791D+13 Y= 3.286864841003D+13 Z= 9.364547031787D+13
I= 16 X= 3.606391020740D+13 Y= 3.644551047085D+13 Z= 4.139509325405D+11
I= 17 X= 1.384507950057D+13 Y= 3.654212374189D+13 Z= -9.789512069296D+12
I= 18 X= 1.576144493066D+13 Y= -1.585716564146D+13 Z= -4.871833110225D+13
I= 19 X= -1.071528545667D+14 Y= -1.418047297502D+14 Z= -6.966393566447D+13
I= 20 X= -6.103393113975D+13 Y= -3.815276580528D+13 Z= -4.073250795233D+13
I= 21 X= -1.360226324457D+13 Y= 3.721670612946D+12 Z= 5.559033157156D+12
I= 22 X= -7.235678334407D+12 Y= -1.530241812519D+13 Z= 8.777241136610D+13
I= 23 X= 4.573961067339D+13 Y= -5.970596703093D+13 Z= 1.702931479356D+12
I= 24 X= 5.794890661125D+13 Y= -1.085570071793D+14 Z= -1.121028744646D+14
I= 25 X= 7.320565732432D+12 Y= 2.564511449392D+12 Z= 1.619429343998D+13
I= 26 X= -3.494259502318D+13 Y= 5.978809805313D+13 Z= 9.161471450405D+13
I= 27 X= -4.904395160956D+13 Y= -3.006309285977D+13 Z= -9.308707919135D+12
I= 28 X= -1.601238298663D+14 Y= -4.597098248134D+13 Z= 1.475231581533D+13
I= 29 X= -2.787449738169D+12 Y= 4.323542613017D+11 Z= 1.286311297480D+13
I= 30 X= -1.929358902663D+13 Y= -1.807868793465D+13 Z= -1.117234846985D+11
I= 31 X= 6.026706702074D+13 Y= 2.870517863448D+12 Z= 4.172704260522D+13
I= 32 X= 1.690613624762D+14 Y= 2.919412855761D+13 Z= -6.095411717401D+13

I= 33 X= -3.321403164436D+13 Y= -9.056292127105D+13 Z= -6.313338672630D+13
I= 34 X= 3.355341597488D+13 Y= 3.048964994363D+12 Z= 3.805576385737D+12
I= 35 X= 3.524314733881D+11 Y= -1.789016469400D+12 Z= 3.730747658328D+12
I= 36 X= 3.633464970834D+11 Y= 1.093893260773D+13 Z= -3.410983348155D+13
I= 37 X= 9.351467047837D+13 Y= -7.380913188058D+13 Z= 8.345072452989D+13
I= 38 X= -5.875883328035D+13 Y= -3.871085031494D+13 Z= 1.669887838099D+13

Seed: 18860130065

CM Start Point Coordinates: bohr

I= 0 X= -2.270368170449D+00 Y= 2.342256786553D+00 Z= -4.476269420076D-01
I= 1 X= -2.725829974924D+00 Y= 7.476116935841D-02 Z= -1.869918269666D+00
I= 2 X= -1.763628241183D+00 Y= 1.671744244187D+00 Z= 2.211877762054D+00
I= 3 X= -2.632635464662D+00 Y= -1.913593951883D+00 Z= -1.644233523254D-01
I= 4 X= -2.199436887466D+00 Y= -9.557509991996D-01 Z= 2.250703422099D+00
I= 5 X= 4.561543964094D+00 Y= 2.297480101659D+00 Z= -1.755590367398D+00
I= 6 X= 2.327668188678D+00 Y= 2.254734118405D-01 Z= -3.162785212725D+00
I= 7 X= 6.319551878520D+00 Y= 9.720483928298D-01 Z= -2.017134220086D+00
I= 8 X= 4.610209456978D+00 Y= 3.780501813915D+00 Z= -3.187499104204D+00
I= 9 X= -2.618368652942D+00 Y= -2.582160386308D+00 Z= 4.665188459800D+00
I= 10 X= -4.477358350157D+00 Y= -2.153470063414D+00 Z= 5.772921719718D+00
I= 11 X= -2.232243350891D+00 Y= -4.718532592826D+00 Z= 4.010829100204D+00
I= 12 X= -1.031813992640D+00 Y= -2.012662590395D+00 Z= 6.145024008818D+00
I= 13 X= -1.558504721729D+00 Y= 3.470397469540D+00 Z= 4.331468382082D+00
I= 14 X= -3.662679773125D+00 Y= 3.739463273710D+00 Z= 4.968110111003D+00
I= 15 X= -5.010647054059D-01 Y= 2.723996452483D+00 Z= 5.928433740909D+00
I= 16 X= -1.054569029289D+00 Y= 5.273628122186D+00 Z= 3.780251916150D+00
I= 17 X= -2.205734875078D+00 Y= 5.014600678126D+00 Z= -1.314294005442D+00
I= 18 X= -4.512345809219D+00 Y= 5.676300428756D+00 Z= -1.878895819038D+00
I= 19 X= -1.666010668685D+00 Y= 6.855654941343D+00 Z= 1.252740753354D-01
I= 20 X= -1.049602071668D+00 Y= 5.057714571575D+00 Z= -3.032028012926D+00

I= 21 X= -3.322990756740D+00 Y= -1.598649938127D-01 Z= -4.659699732308D+00
I= 22 X= -5.322459423157D+00 Y= -5.731625385593D-01 Z= -5.145792833215D+00
I= 23 X= -2.823199963539D+00 Y= 1.393878598634D+00 Z= -5.513626257177D+00
I= 24 X= -2.213559048365D+00 Y= -1.678981134141D+00 Z= -5.569131900870D+00
I= 25 X= -2.638488468740D+00 Y= -4.826123300116D+00 Z= -7.035064895424D-01
I= 26 X= -2.232740510051D+00 Y= -4.977759703462D+00 Z= -2.913558770020D+00
I= 27 X= -1.094573236125D+00 Y= -5.868038193874D+00 Z= 7.877502206927D-02
I= 28 X= -4.524436631645D+00 Y= -6.115746252434D+00 Z= 1.459835409183D-01
I= 29 X= 3.212206628377D+00 Y= -3.620169924933D+00 Z= -1.439528709153D+00
I= 30 X= 3.624219358370D+00 Y= -3.497388534603D+00 Z= 1.208414022561D+00
I= 31 X= 1.599018432210D+00 Y= -4.770140255809D+00 Z= -1.776469351904D+00
I= 32 X= 4.828699282417D+00 Y= -3.108617438849D+00 Z= -2.949530293742D+00
I= 33 X= 5.468258329086D+00 Y= -2.710638399369D+00 Z= 1.876965381380D+00
I= 34 X= 2.645316007440D+00 Y= -4.724818975275D+00 Z= 2.576211441694D+00
I= 35 X= 1.053411693430D+00 Y= -3.788419248473D-02 Z= -3.875381207928D-01
I= 36 X= 3.799072689857D+00 Y= 3.057922892065D+00 Z= 8.744137813689D-01
I= 37 X= 4.857628632091D+00 Y= 2.483161319109D+00 Z= 2.449318519343D+00
I= 38 X= 2.235946996753D+00 Y= 4.644464734198D+00 Z= 9.054962611247D-01

Forward Direction:

Total Energy: -656.4281811 Hartrees

Potential Energy: -656.6120116 Hartress

Kinetic Energy: 0.1838305 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.437865072202D+12 Y= -4.594212102711D+12 Z= -7.466071483976D+12
I= 1 X= -9.441568696435D+12 Y= 1.611693927080D+13 Z= -2.757201150767D+12
I= 2 X= 2.716505493546D+12 Y= 3.101948910621D+12 Z= 2.030615543523D+13
I= 3 X= -1.649357141288D+12 Y= -1.824364338915D+13 Z= -3.912853035489D+13
I= 4 X= -4.972264282274D+12 Y= 3.332051872584D+12 Z= -3.209683545851D+12
I= 5 X= 9.123316779260D+12 Y= -9.820733889973D+11 Z= -1.593639854766D+13
I= 6 X= -5.727289480127D+13 Y= -3.146968192530D+13 Z= 7.474198525696D+13

I= 7 X= 2.818425030539D+13 Y= -3.398169134989D+13 Z= -8.517322646479D+13
I= 8 X= -9.555137049589D+13 Y= 1.068176927268D+14 Z= -5.921961234070D+13
I= 9 X= -1.801441986738D+12 Y= -7.507521487240D+12 Z= 1.969917627894D+11
I= 10 X= 2.479569452487D+13 Y= -1.120293769195D+13 Z= -3.213487641492D+13
I= 11 X= 1.126244150848D+14 Y= -5.989693918410D+13 Z= 5.255801222012D+13
I= 12 X= 3.027006415907D+13 Y= -8.503910471162D+13 Z= 9.493285393455D+13
I= 13 X= -4.605925896548D+12 Y= 2.825171387539D+12 Z= -2.793886624187D+13
I= 14 X= -3.556802546287D+13 Y= -1.343180328332D+13 Z= 5.030281818031D+13
I= 15 X= 2.840431958252D+13 Y= -5.991770349951D+13 Z= 1.261509456903D+14
I= 16 X= -5.907216001338D+13 Y= 9.967040309374D+12 Z= -2.270976952467D+13
I= 17 X= -2.022525611531D+12 Y= -3.204714974448D+13 Z= -6.347620813459D+12
I= 18 X= 9.869120300677D+13 Y= 4.425094443646D+12 Z= 1.528704122193D+12
I= 19 X= -4.639809823539D+13 Y= 4.237433768689D+13 Z= 1.369497964051D+13
I= 20 X= -4.895371622702D+13 Y= -2.687397234617D+13 Z= 3.602099220937D+13
I= 21 X= 1.208197323457D+13 Y= -6.543577627271D+12 Z= -2.637420128202D+12
I= 22 X= -1.133335668771D+13 Y= -7.290612381891D+12 Z= 9.523157840825D+12
I= 23 X= -2.289563588821D+13 Y= -1.248271123344D+13 Z= 4.537202084435D+13
I= 24 X= -9.540877394269D+13 Y= 4.899326977909D+13 Z= 7.424550665281D+13
I= 25 X= -7.742840671830D+12 Y= 9.605737978055D+12 Z= -3.548015410778D+12
I= 26 X= 4.624162225700D+13 Y= 1.184844849363D+14 Z= 4.519577535364D+13
I= 27 X= 7.478598047652D+13 Y= -2.040572969500D+13 Z= 6.823015157531D+13
I= 28 X= 2.703247103928D+13 Y= -1.234352850871D+13 Z= 4.505702445294D+13
I= 29 X= 1.187701074180D+12 Y= -4.259955817331D+12 Z= 4.723283971425D+12
I= 30 X= 8.537692423979D+12 Y= 9.259067541498D+12 Z= 2.670766059195D+13
I= 31 X= -8.891377376697D+13 Y= -3.975126906495D+13 Z= -5.868571670250D+13
I= 32 X= 9.022578134335D+13 Y= 8.101884942986D+13 Z= -7.509232962772D+13
I= 33 X= -1.281086750627D+14 Y= 1.671496607489D+13 Z= -7.497765893423D+12
I= 34 X= -1.451189287368D+13 Y= -1.813119000183D+11 Z= 5.237248030245D+13
I= 35 X= -4.371887375910D+10 Y= -6.033071960503D+11 Z= 8.242807193731D+11
I= 36 X= 5.616482028253D+12 Y= 1.637747267052D+13 Z= 8.659191135949D+12

I= 37 X= 3.217332685798D+13 Y= 7.419452723463D+13 Z= 1.362644769582D+13

I= 38 X= -5.721636469930D+13 Y= 1.343334561565D+14 Z= 2.880657377428D+13

Backward Direction:

Total Energy: -656.4281583 Hartrees

Potential Energy: -656.6120116 Hartress

Kinetic Energy: 0.1838533 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.227070775900D+12 Y= -4.869478883498D+12 Z= -7.358352291487D+12

I= 1 X= -9.766693071870D+12 Y= 1.540909198639D+13 Z= -3.182123854743D+12

I= 2 X= 2.413902220636D+12 Y= 3.380108284590D+12 Z= 1.985830706782D+13

I= 3 X= -2.269375610527D+12 Y= -1.822914559588D+13 Z= -4.002687338282D+13

I= 4 X= -3.911791442830D+12 Y= 3.237438420711D+12 Z= -3.914384802130D+12

I= 5 X= 7.373109252709D+12 Y= -3.471059817524D+12 Z= -2.090569753217D+13

I= 6 X= -1.806853912664D+13 Y= 1.328679765924D+13 Z= 9.238138502246D+13

I= 7 X= 3.534492709984D+13 Y= -2.720205360745D+13 Z= -8.473513783029D+13

I= 8 X= -8.650773121998D+13 Y= 1.141278391889D+14 Z= -5.837825747533D+13

I= 9 X= -1.464392680637D+12 Y= -7.349236799177D+12 Z= -1.839848753783D+11

I= 10 X= 2.485733814202D+13 Y= -1.041959291355D+13 Z= -3.304293537072D+13

I= 11 X= 1.125270685766D+14 Y= -5.990550237410D+13 Z= 5.253908275315D+13

I= 12 X= 3.046759873077D+13 Y= -8.498619743003D+13 Z= 9.474527476222D+13

I= 13 X= -4.539110787586D+12 Y= 2.792661712592D+12 Z= -2.807949156270D+13

I= 14 X= -3.545443503146D+13 Y= -1.363208366785D+13 Z= 5.033254647225D+13

I= 15 X= 2.861321306437D+13 Y= -6.010929491171D+13 Z= 1.258050334268D+14

I= 16 X= -5.908671146672D+13 Y= 1.002861796385D+13 Z= -2.266106848105D+13

I= 17 X= -1.920205808643D+12 Y= -3.227295432263D+13 Z= -6.369982031192D+12

I= 18 X= 9.871277662083D+13 Y= 4.065102041221D+12 Z= 1.233387826997D+12

I= 19 X= -4.661440023828D+13 Y= 4.230228215070D+13 Z= 1.391802075906D+13

I= 20 X= -4.880350965539D+13 Y= -2.707573650165D+13 Z= 3.599522660246D+13

I= 21 X= 1.195322236896D+13 Y= -6.624461795587D+12 Z= -2.951720597603D+12

I= 22 X= -1.135636551422D+13 Y= -6.928134904087D+12 Z= 8.263555212297D+12

I= 23 X= -2.242764014573D+13 Y= -1.268642476498D+13 Z= 4.522596381620D+13
I= 24 X= -9.563438748072D+13 Y= 4.886655591305D+13 Z= 7.387388214635D+13
I= 25 X= -7.882767022759D+12 Y= 9.464383103921D+12 Z= -3.620221242060D+12
I= 26 X= 4.589552308491D+13 Y= 1.181058791659D+14 Z= 4.515354666891D+13
I= 27 X= 7.507442806037D+13 Y= -2.016288024128D+13 Z= 6.814643843863D+13
I= 28 X= 2.704676438173D+13 Y= -1.277194240246D+13 Z= 4.536027391842D+13
I= 29 X= 5.396851326573D+11 Y= -4.077933187522D+12 Z= 4.496001318126D+12
I= 30 X= 8.575853500872D+12 Y= 9.133660095543D+12 Z= 2.642618761696D+13
I= 31 X= -8.936179205943D+13 Y= -3.988381301555D+13 Z= -5.867171771357D+13
I= 32 X= 8.891462686309D+13 Y= 8.210768351690D+13 Z= -7.587295125042D+13
I= 33 X= -1.280682388281D+14 Y= 1.655648283737D+13 Z= -7.721960143035D+12
I= 34 X= -1.408946193055D+13 Y= -4.754193470694D+11 Z= 5.229163056123D+13
I= 35 X= -5.076856420052D+10 Y= -4.386482590225D+11 Z= 1.868940234982D+12
I= 36 X= 3.338242709649D+12 Y= 1.349986868769D+13 Z= 7.609080737313D+12
I= 37 X= 3.420572719297D+13 Y= 7.522630508582D+13 Z= 1.109171921897D+13
I= 38 X= -5.610334343065D+13 Y= 1.342174773069D+14 Z= 2.691357668136D+13

Seed: 19497515402

CM Start Point Coordinates: bohr

I= 0 X= -2.412324706681D+00 Y= 2.258879477003D+00 Z= -5.588492333910D-01
I= 1 X= -2.810728344449D+00 Y= 1.311012476064D-05 Z= -1.983076664740D+00
I= 2 X= -2.021271242968D+00 Y= 1.605729334601D+00 Z= 2.050540191253D+00
I= 3 X= -2.695275694903D+00 Y= -1.966408404511D+00 Z= -2.379224522393D-01
I= 4 X= -2.126505068000D+00 Y= -9.822767972569D-01 Z= 2.359243909560D+00
I= 5 X= 4.655527270268D+00 Y= 2.444136747385D+00 Z= -1.086734221975D+00
I= 6 X= 2.587411449815D+00 Y= 5.900899711081D-01 Z= -2.864366726202D+00
I= 7 X= 6.171401135272D+00 Y= 1.542391459359D+00 Z= -1.802124025120D+00
I= 8 X= 4.080206967352D+00 Y= 4.238959005589D+00 Z= -2.179130246850D+00
I= 9 X= -1.992974334056D+00 Y= -2.325889780348D+00 Z= 4.895574917073D+00
I= 10 X= -3.893854316734D+00 Y= -2.074561681969D+00 Z= 5.903313815920D+00

I= 11 X= -1.690576205491D+00 Y= -4.420904808501D+00 Z= 4.673552880898D+00
I= 12 X= -8.138013135020D-01 Y= -1.320541972460D+00 Z= 5.898615408899D+00
I= 13 X= -1.662665848335D+00 Y= 3.374967248569D+00 Z= 4.304391521760D+00
I= 14 X= -3.473335145472D+00 Y= 2.669888827572D+00 Z= 5.534238728916D+00
I= 15 X= 3.729939030655D-01 Y= 3.196392403295D+00 Z= 5.455027151530D+00
I= 16 X= -1.970574482913D+00 Y= 5.599728050085D+00 Z= 3.720488639454D+00
I= 17 X= -2.351496531130D+00 Y= 4.832609172668D+00 Z= -1.846721636238D+00
I= 18 X= -4.285110653796D+00 Y= 5.437719507594D+00 Z= -3.055361770779D+00
I= 19 X= -1.797901640357D+00 Y= 6.301059970529D+00 Z= -8.330286209237D-02
I= 20 X= -9.796730657669D-01 Y= 5.194122768856D+00 Z= -3.707935283920D+00
I= 21 X= -3.497911011776D+00 Y= -4.311282988298D-02 Z= -4.715482510118D+00
I= 22 X= -5.728547066265D+00 Y= -3.780920299332D-01 Z= -4.805146334014D+00
I= 23 X= -2.829522276055D+00 Y= 1.417592236290D+00 Z= -5.774454777963D+00
I= 24 X= -2.814253611120D+00 Y= -1.862428719704D+00 Z= -5.460698303352D+00
I= 25 X= -3.061357318067D+00 Y= -4.789278815607D+00 Z= -7.195164278262D-01
I= 26 X= -3.424070510462D+00 Y= -5.561367590857D+00 Z= -2.606590512201D+00
I= 27 X= -1.170814032958D+00 Y= -5.642174980714D+00 Z= 3.291468875027D-02
I= 28 X= -4.841428113630D+00 Y= -5.637040537727D+00 Z= 5.989054309712D-01
I= 29 X= 2.879844758395D+00 Y= -3.802758497766D+00 Z= -1.541550507819D+00
I= 30 X= 3.714802265722D+00 Y= -2.973823837779D+00 Z= 8.568790401996D-01
I= 31 X= 1.361816263859D+00 Y= -5.031732472136D+00 Z= -1.744240721031D+00
I= 32 X= 4.367811051636D+00 Y= -3.543858166951D+00 Z= -3.032950262060D+00
I= 33 X= 5.688130068084D+00 Y= -1.904596639764D+00 Z= 8.845319160535D-01
I= 34 X= 2.864800359698D+00 Y= -4.056349724918D+00 Z= 2.629231899258D+00
I= 35 X= 1.147749196487D+00 Y= -1.929326113461D-02 Z= -4.193722194240D-01
I= 36 X= 3.934241633431D+00 Y= 2.510556581848D+00 Z= 1.511534636501D+00
I= 37 X= 4.691365236996D+00 Y= 1.379134421043D+00 Z= 3.016573801914D+00
I= 38 X= 2.832493358760D+00 Y= 4.129767846771D+00 Z= 2.435900726453D+00

Forward Direction:

Total Energy: -656.4357916 Hartrees

Potential Energy: -656.6157799 Hartress

Kinetic Energy: 0.1799883 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.339457201467D+12 Y= -2.473113084544D+12 Z= 5.992749432918D+12
I= 1 X= -1.447680186649D+13 Y= -6.288442345303D+12 Z= -1.871113725561D+13
I= 2 X= 2.428909697234D+11 Y= 1.845007975336D+13 Z= -1.047192771405D+13
I= 3 X= 3.702929866713D+12 Y= -2.572925948434D+13 Z= 4.918885126470D+12
I= 4 X= 2.230183992503D+12 Y= -3.342383811409D+13 Z= 7.995375096484D+12
I= 5 X= 5.658814258813D+12 Y= -7.663759080030D+12 Z= -2.546902744457D+13
I= 6 X= -8.394805037057D+13 Y= -3.888300323151D+13 Z= 1.049141820833D+13
I= 7 X= -8.494137055240D+13 Y= 2.195096607663D+13 Z= 7.081682594937D+13
I= 8 X= 7.053746114551D+13 Y= 2.520768164627D+13 Z= 3.325046201278D+13
I= 9 X= -6.751929277827D+12 Y= 2.343371433797D+12 Z= -1.971958088904D+13
I= 10 X= 5.486027456046D+13 Y= -3.015931899017D+13 Z= 4.624490897740D+13
I= 11 X= -6.255134105730D+13 Y= -1.496647593825D+13 Z= 3.065563341684D+13
I= 12 X= -1.099367680234D+14 Y= -8.978002820416D+12 Z= 5.330561528357D+13
I= 13 X= -1.331141088278D+13 Y= 9.209725197939D+10 Z= 9.527509023577D+12
I= 14 X= 1.109735325714D+13 Y= -5.181100234017D+12 Z= 2.184484229027D+13
I= 15 X= -2.134115093294D+13 Y= 3.460041500746D+13 Z= -4.486672095955D+13
I= 16 X= -7.819538019838D+13 Y= -1.401559484522D+14 Z= 5.205515063082D+13
I= 17 X= -3.209804747534D+12 Y= -1.171844394600D+11 Z= 1.822104810102D+13
I= 18 X= -5.140853484027D+13 Y= 5.407658422941D+13 Z= -9.535681684726D+12
I= 19 X= 5.847069675420D+13 Y= -4.211468039308D+13 Z= -5.634918747565D+12
I= 20 X= 3.475486766686D+13 Y= -2.131872579983D+13 Z= -1.237577867618D+14
I= 21 X= 4.226135520261D+12 Y= 8.519069319776D+12 Z= -1.272999749569D+13
I= 22 X= -5.852191361055D+13 Y= 9.047833263390D+13 Z= 3.705264859540D+13
I= 23 X= 1.744582630200D+13 Y= -2.477369131097D+13 Z= -3.419374013768D+13
I= 24 X= 5.320612382411D+13 Y= -9.546287682891D+13 Z= -9.729020990155D+13
I= 25 X= -2.542303866197D+12 Y= 2.496087775109D+13 Z= 2.183336718936D+12
I= 26 X= 5.431437197098D+13 Y= 7.426191306486D+12 Z= -7.347175374490D+13

I= 27 X= 1.642456543440D+13 Y= -6.769650340559D+13 Z= 1.159187578657D+14
I= 28 X= -1.202607279070D+13 Y= -3.913919206207D+13 Z= 9.843222276196D+13
I= 29 X= 4.207720828263D+12 Y= 3.986655506941D+12 Z= -5.917552243481D+12
I= 30 X= 3.163008242511D+12 Y= 9.217785854838D+12 Z= 5.506216988022D+12
I= 31 X= 2.435765932099D+13 Y= 4.555227001002D+13 Z= -3.510251841918D+12
I= 32 X= 4.695577420104D+13 Y= 2.505376527160D+13 Z= 6.311533892555D+13
I= 33 X= -1.343445694388D+14 Y= -3.063604982757D+13 Z= -6.127101725733D+13
I= 34 X= 3.376965283279D+13 Y= -5.742356521531D+13 Z= -4.012642671108D+13
I= 35 X= 3.722116096477D+12 Y= 6.712428185042D+12 Z= 2.052956762278D+12
I= 36 X= 3.197236868809D+12 Y= -1.757732168285D+13 Z= 1.665412698904D+13
I= 37 X= -1.395348507738D+13 Y= 3.057336146053D+13 Z= 1.776777436181D+13
I= 38 X= 4.546674602334D+13 Y= -9.736741083653D+13 Z= -1.047238460616D+14

Backward Direction:

Total Energy: -656.4357908 Hartrees

Potential Energy: -656.6157799 Hartress

Kinetic Energy: 0.1799892 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.497125138837D+12 Y= -2.679004545576D+12 Z= 6.073320223343D+12
I= 1 X= -1.471998534292D+13 Y= -6.817891308791D+12 Z= -1.902896694905D+13
I= 2 X= 1.655261644846D+10 Y= 1.865813478920D+13 Z= -1.080690512954D+13
I= 3 X= 3.239174275052D+12 Y= -2.571841556097D+13 Z= 4.246950947233D+12
I= 4 X= 3.023386507549D+12 Y= -3.349460619504D+13 Z= 7.468279269930D+12
I= 5 X= 4.349710472938D+12 Y= -9.525447770909D+12 Z= -2.918591702373D+13
I= 6 X= -5.462434464832D+13 Y= -5.406472015841D+12 Z= 2.368517076286D+13
I= 7 X= -7.958539478097D+13 Y= 2.702193583534D+13 Z= 7.114450337232D+13
I= 8 X= 7.730183751047D+13 Y= 3.067545633417D+13 Z= 3.387977072028D+13
I= 9 X= -6.499826303733D+12 Y= 2.461763728647D+12 Z= -2.000454021590D+13
I= 10 X= 5.490638217626D+13 Y= -2.957340010928D+13 Z= 4.556570757698D+13
I= 11 X= -6.262415339441D+13 Y= -1.497288095214D+13 Z= 3.064147473073D+13
I= 12 X= -1.097890179596D+14 Y= -8.938429733623D+12 Z= 5.316531156887D+13

I= 13 X= -1.326143514796D+13 Y= 6.778097104558D+10 Z= 9.422325417484D+12
I= 14 X= 1.118231555650D+13 Y= -5.330904068972D+12 Z= 2.186707817721D+13
I= 15 X= -2.118490475617D+13 Y= 3.445711025891D+13 Z= -4.512545316187D+13
I= 16 X= -7.820626425563D+13 Y= -1.401098901769D+14 Z= 5.209157758049D+13
I= 17 X= -3.133272543575D+12 Y= -2.860796273659D+11 Z= 1.820432256886D+13
I= 18 X= -5.139239841260D+13 Y= 5.380732049521D+13 Z= -9.756569583261D+12
I= 19 X= 5.830890921523D+13 Y= -4.216857581480D+13 Z= -5.468090548828D+12
I= 20 X= 3.486721775893D+13 Y= -2.146963945707D+13 Z= -1.237770586799D+14
I= 21 X= 4.129833659318D+12 Y= 8.458570339028D+12 Z= -1.296508500956D+13
I= 22 X= -5.853912353487D+13 Y= 9.074945512682D+13 Z= 3.611050285399D+13
I= 23 X= 1.779587336290D+13 Y= -2.492606304479D+13 Z= -3.430298650203D+13
I= 24 X= 5.303737153391D+13 Y= -9.555765507564D+13 Z= -9.756817411111D+13
I= 25 X= -2.646964664690D+12 Y= 2.485514845978D+13 Z= 2.129328879818D+12
I= 26 X= 5.405549995251D+13 Y= 7.143005317957D+12 Z= -7.350333955970D+13
I= 27 X= 1.664031574336D+13 Y= -6.751485915978D+13 Z= 1.158561428965D+14
I= 28 X= -1.201538179469D+13 Y= -3.945963305152D+13 Z= 9.865904445282D+13
I= 29 X= 3.723023951133D+12 Y= 4.122803083798D+12 Z= -6.087552989012D+12
I= 30 X= 3.191551606536D+12 Y= 9.123984771174D+12 Z= 5.295683475020D+12
I= 31 X= 2.402255480756D+13 Y= 4.545313102999D+13 Z= -3.499781009119D+12
I= 32 X= 4.597506918838D+13 Y= 2.586818116607D+13 Z= 6.253145689743D+13
I= 33 X= -1.343143243233D+14 Y= -3.075459063104D+13 Z= -6.143870796675D+13
I= 34 X= 3.408561876181D+13 Y= -5.764354894188D+13 Z= -4.018689994130D+13
I= 35 X= 3.716843135539D+12 Y= 6.835588230002D+12 Z= 2.834331374458D+12
I= 36 X= 1.493180821558D+12 Y= -1.972968488042D+13 Z= 1.586867527633D+13
I= 37 X= -1.243330936540D+13 Y= 3.134510096722D+13 Z= 1.587187196288D+13
I= 38 X= 4.629925321660D+13 Y= -9.745415960458D+13 Z= -1.061397522497D+14

Seed: 20322869887

CM Start Point Coordinates: bohr

I= 0 X= -2.184793103714D+00 Y= 2.446239350493D+00 Z= -5.415926526146D-01

I= 1 X= -2.758477668238D+00 Y= 6.285582772431D-02 Z= -2.007088830056D+00
I= 2 X= -1.949041994859D+00 Y= 1.719077482936D+00 Z= 2.143530811859D+00
I= 3 X= -2.364696831682D+00 Y= -1.998025044196D+00 Z= -2.123488588676D-01
I= 4 X= -2.018463173642D+00 Y= -9.479763000867D-01 Z= 2.228217931918D+00
I= 5 X= 4.703911741914D+00 Y= 2.028002312293D+00 Z= -1.613940416651D+00
I= 6 X= 2.255876348595D+00 Y= 1.554369392456D-01 Z= -3.118169171056D+00
I= 7 X= 6.324269010388D+00 Y= 9.588372397045D-01 Z= -2.178828575109D+00
I= 8 X= 4.355048079306D+00 Y= 4.005895185551D+00 Z= -2.804080514890D+00
I= 9 X= -1.904112972441D+00 Y= -2.703901822708D+00 Z= 4.591780728644D+00
I= 10 X= -3.614119706814D+00 Y= -2.516441896633D+00 Z= 5.375744542968D+00
I= 11 X= -1.387651632533D+00 Y= -4.552733132652D+00 Z= 3.940091581655D+00
I= 12 X= -3.341150716878D-01 Y= -1.807848820578D+00 Z= 5.895652739608D+00
I= 13 X= -2.117675520104D+00 Y= 3.471363333637D+00 Z= 4.363165143695D+00
I= 14 X= -4.069762963532D+00 Y= 3.130188985250D+00 Z= 5.630296137442D+00
I= 15 X= -3.101756701516D-01 Y= 2.859426984025D+00 Z= 5.538482016292D+00
I= 16 X= -2.055465074441D+00 Y= 5.608471775302D+00 Z= 3.908740239078D+00
I= 17 X= -2.706408957582D+00 Y= 5.030411396619D+00 Z= -1.462715395804D+00
I= 18 X= -5.070610577631D+00 Y= 4.880390000896D+00 Z= -1.865974451860D+00
I= 19 X= -2.136905307720D+00 Y= 6.892436678947D+00 Z= 7.881424278479D-02
I= 20 X= -1.244893513698D+00 Y= 5.579939613764D+00 Z= -3.251274738185D+00
I= 21 X= -3.524482748137D+00 Y= -1.251821118108D-01 Z= -4.738871997282D+00
I= 22 X= -5.438426499102D+00 Y= -3.516494916726D-01 Z= -4.975964891608D+00
I= 23 X= -3.305742685557D+00 Y= 1.911448379864D+00 Z= -5.576426057366D+00
I= 24 X= -2.705451296884D+00 Y= -1.741661813108D+00 Z= -5.530769886821D+00
I= 25 X= -3.025767648254D+00 Y= -4.717658736548D+00 Z= -7.682620654330D-01
I= 26 X= -2.282764053323D+00 Y= -5.084090693347D+00 Z= -2.850338071362D+00
I= 27 X= -2.242077340833D+00 Y= -6.082321066354D+00 Z= 8.254269995121D-01
I= 28 X= -5.150479701887D+00 Y= -5.140506759767D+00 Z= -1.047975055339D+00
I= 29 X= 2.861790268641D+00 Y= -3.839597805926D+00 Z= -1.188884312281D+00
I= 30 X= 3.581275997980D+00 Y= -3.124513026472D+00 Z= 1.361738626292D+00

I= 31 X= 1.114965891901D+00 Y= -5.209821255804D+00 Z= -1.289455365769D+00
I= 32 X= 4.095236480467D+00 Y= -3.840187950369D+00 Z= -2.738446038247D+00
I= 33 X= 5.322673038405D+00 Y= -2.355876443321D+00 Z= 1.825381733645D+00
I= 34 X= 2.705252064343D+00 Y= -3.991519865024D+00 Z= 2.835457233954D+00
I= 35 X= 1.146026376181D+00 Y= 1.707035960798D-02 Z= -4.031573601354D-01
I= 36 X= 4.122620270640D+00 Y= 2.585954975469D+00 Z= 1.071403715110D+00
I= 37 X= 5.307713430408D+00 Y= 1.578027273639D+00 Z= 2.482794889467D+00
I= 38 X= 3.398480938892D+00 Y= 4.716055398250D+00 Z= 1.642526629544D+00

Forward Direction:

Total Energy: -656.4328949 Hartrees

Potential Energy: -656.5983302 Hartress

Kinetic Energy: 0.1654354 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.795073596153D+11 Y= -3.393777905072D+12 Z= -8.822232340500D+12
I= 1 X= 5.826794934983D+12 Y= -1.419672406152D+13 Z= 1.727122950794D+13
I= 2 X= 2.473885774989D+13 Y= -9.298928434088D+12 Z= 1.093642607760D+12
I= 3 X= -1.536238599910D+13 Y= -2.037036622047D+13 Z= -1.136300342803D+13
I= 4 X= -1.110114240016D+13 Y= 2.820611259035D+13 Z= -1.437821936977D+13
I= 5 X= 5.549076251629D+12 Y= 1.199583045055D+13 Z= 1.812182866045D+13
I= 6 X= 1.089273839455D+13 Y= -5.258740484559D+13 Z= -5.699308583315D+13
I= 7 X= 5.785455421481D+13 Y= 1.203964500357D+13 Z= -8.090032953282D+13
I= 8 X= 2.983681330844D+12 Y= 2.691365375063D+13 Z= -5.356639321978D+13
I= 9 X= -1.258650715517D+13 Y= -3.429988988655D+13 Z= 7.408474236389D+12
I= 10 X= 2.648266988349D+13 Y= 6.938722196642D+13 Z= 9.461633502155D+12
I= 11 X= -5.294236616651D+12 Y= 1.225216750727D+14 Z= 4.216651780922D+13
I= 12 X= 1.502666260901D+13 Y= 2.595365752613D+13 Z= 2.627165078483D+13
I= 13 X= 5.270768131471D+11 Y= -1.575096482983D+13 Z= -6.607108409647D+12
I= 14 X= -3.983602964659D+13 Y= 3.858508196836D+13 Z= 3.036240734686D+13
I= 15 X= -1.104224183312D+14 Y= 4.138676907339D+13 Z= -7.640737098132D+13
I= 16 X= 2.420288307443D+12 Y= -9.898598407999D+11 Z= -7.138458218928D+12

I= 17 X= 7.042659450040D+12 Y= 2.090383887254D+13 Z= 8.431786684595D+12
I= 18 X= -9.606091556286D+13 Y= 1.988314536092D+13 Z= -2.841395717879D+13
I= 19 X= -3.437959026244D+13 Y= -4.528573829353D+13 Z= -4.946654270599D+12
I= 20 X= -4.885944769837D+13 Y= -4.143470953942D+13 Z= -5.842030946284D+13
I= 21 X= 8.405445475489D+09 Y= -1.223210346015D+13 Z= 1.146877834157D+13
I= 22 X= -7.419454228965D+13 Y= -3.875531103662D+13 Z= -7.317534105572D+13
I= 23 X= 5.811790267180D+12 Y= -1.336592220964D+13 Z= -1.004310171702D+13
I= 24 X= -4.808173550652D+13 Y= 9.289171937060D+13 Z= 2.658710500791D+13
I= 25 X= 5.165202567320D+12 Y= 3.926753570513D+13 Z= -8.323055085959D+12
I= 26 X= -6.084395892023D+13 Y= -6.083510532905D+12 Z= -9.617545259512D+13
I= 27 X= 2.338191815814D+13 Y= -9.091130046842D+13 Z= 7.845952312018D+13
I= 28 X= -2.492367625991D+13 Y= 3.379131748392D+13 Z= -3.332039463316D+13
I= 29 X= 7.930755872761D+12 Y= 4.006149073066D+12 Z= 8.853968013510D+12
I= 30 X= 2.449170842729D+13 Y= 6.941525714415D+12 Z= -2.368723790135D+10
I= 31 X= 7.855910615317D+12 Y= -4.131405452343D+12 Z= -3.684432204208D+13
I= 32 X= -1.388303488883D+14 Y= -2.842069084906D+13 Z= 1.135381956343D+14
I= 33 X= -2.584075812197D+13 Y= 7.282950771768D+13 Z= -3.088580974228D+13
I= 34 X= -2.211070326559D+13 Y= 2.545830470818D+13 Z= 1.407255923160D+13
I= 35 X= 3.361033397067D+11 Y= -3.479909295391D+12 Z= 5.990892322529D+11
I= 36 X= 9.565374116329D+12 Y= 9.792826653019D+12 Z= -4.439141796044D+12
I= 37 X= -1.975584843332D+13 Y= 4.430752872025D+13 Z= 5.906064171929D+11
I= 38 X= -6.002814235508D+13 Y= -8.643906797957D+13 Z= 2.197283755115D+13

Backward Direction:

Total Energy: -656.4329349 Hartrees

Potential Energy: -656.5983302 Hartress

Kinetic Energy: 0.1653953 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.037652796784D+10 Y= -3.914984889126D+12 Z= -8.618270222352D+12

I= 1 X= 5.211184527800D+12 Y= -1.553700546909D+13 Z= 1.646665483017D+13

I= 2 X= 2.416589017660D+13 Y= -8.772244436131D+12 Z= 2.456590768786D+11

I= 3 X= -1.653636694787D+13 Y= -2.034291521019D+13 Z= -1.306398114360D+13
I= 4 X= -9.093178168038D+12 Y= 2.802696568594D+13 Z= -1.571254389485D+13
I= 5 X= 2.235126112595D+12 Y= 7.283031088701D+12 Z= 8.712653575657D+12
I= 6 X= 8.512466684037D+13 Y= 3.215725510200D+13 Z= -2.359356583852D+13
I= 7 X= 7.141301827334D+13 Y= 2.487662638622D+13 Z= -8.007082568232D+13
I= 8 X= 2.010746189335D+13 Y= 4.075513283514D+13 Z= -5.197332038378D+13
I= 9 X= -1.194831735282D+13 Y= -3.400018396126D+13 Z= 6.687109733247D+12
I= 10 X= 2.659938968392D+13 Y= 7.087045496353D+13 Z= 7.742259049242D+12
I= 11 X= -5.478558467771D+12 Y= 1.225054609974D+14 Z= 4.213067559684D+13
I= 12 X= 1.540068667539D+13 Y= 2.605383541153D+13 Z= 2.591647688531D+13
I= 13 X= 6.535886336849D+11 Y= -1.581252063884D+13 Z= -6.873377004624D+12
I= 14 X= -3.962095056710D+13 Y= 3.820585881428D+13 Z= 3.041869671400D+13
I= 15 X= -1.100268866203D+14 Y= 4.102399815697D+13 Z= -7.706234244285D+13
I= 16 X= 2.392735698942D+12 Y= -8.732649344792D+11 Z= -7.046244675104D+12
I= 17 X= 7.236398031984D+12 Y= 2.047628665192D+13 Z= 8.389446587289D+12
I= 18 X= -9.602006676132D+13 Y= 1.920151369506D+13 Z= -2.897312713558D+13
I= 19 X= -3.478914973008D+13 Y= -4.542217266109D+13 Z= -4.524334554234D+12
I= 20 X= -4.857503737342D+13 Y= -4.181674215155D+13 Z= -5.846909564660D+13
I= 21 X= -2.353793253371D+11 Y= -1.238525449874D+13 Z= 1.087366257782D+13
I= 22 X= -7.423810860681D+13 Y= -3.806897398519D+13 Z= -7.556034983585D+13
I= 23 X= 6.697922079133D+12 Y= -1.375164588932D+13 Z= -1.031965503899D+13
I= 24 X= -4.850892599110D+13 Y= 9.265179157380D+13 Z= 2.588344840016D+13
I= 25 X= 4.900257441971D+12 Y= 3.899988572704D+13 Z= -8.459774027084D+12
I= 26 X= -6.149928432135D+13 Y= -6.800385886483D+12 Z= -9.625541097655D+13
I= 27 X= 2.392808249895D+13 Y= -9.045147444009D+13 Z= 7.830101552413D+13
I= 28 X= -2.489661236442D+13 Y= 3.298013237349D+13 Z= -3.274620348873D+13
I= 29 X= 6.703762794582D+12 Y= 4.350801869911D+12 Z= 8.423617114000D+12
I= 30 X= 2.456396494786D+13 Y= 6.704071573866D+12 Z= -5.566454119344D+11
I= 31 X= 7.007605334918D+12 Y= -4.382372287509D+12 Z= -3.681781549584D+13
I= 32 X= -1.413129690935D+14 Y= -2.635902569093D+13 Z= 1.120601188407D+14

I= 33 X= -2.576419367727D+13 Y= 7.252942584848D+13 Z= -3.131031286471D+13
I= 34 X= -2.131084664104D+13 Y= 2.490142365189D+13 Z= 1.391947338352D+13
I= 35 X= 3.227550239813D+11 Y= -3.168133978259D+12 Z= 2.577111548427D+12
I= 36 X= 5.251616238366D+12 Y= 4.344195008360D+12 Z= -6.427485147183D+12
I= 37 X= -1.590757714438D+13 Y= 4.626116010143D+13 Z= -4.208803745637D+12
I= 38 X= -5.792067971008D+13 Y= -8.665866943675D+13 Z= 1.838852089957D+13

Seed: 20399373177

CM Start Point Coordinates: bohr

I= 0 X= -2.367595947111D+00 Y= 2.380223585189D+00 Z= -5.268981864298D-01
I= 1 X= -2.679271458453D+00 Y= 1.664484832725D-01 Z= -1.979691869696D+00
I= 2 X= -2.024147266797D+00 Y= 1.674178694507D+00 Z= 2.131241834342D+00
I= 3 X= -2.700995158157D+00 Y= -1.991803915200D+00 Z= -2.476659464822D-01
I= 4 X= -2.235355362848D+00 Y= -1.014386032493D+00 Z= 2.312163054340D+00
I= 5 X= 3.953614619187D+00 Y= 2.849324729723D+00 Z= -1.492488171501D+00
I= 6 X= 2.067730630889D+00 Y= 5.431762314445D-01 Z= -2.922572892861D+00
I= 7 X= 5.741280683712D+00 Y= 2.561397254554D+00 Z= -2.248244582120D+00
I= 8 X= 3.019006416203D+00 Y= 4.354476993072D+00 Z= -2.651179646632D+00
I= 9 X= -2.112913766427D+00 Y= -2.453611410557D+00 Z= 4.745390354780D+00
I= 10 X= -3.886608697632D+00 Y= -2.470208765097D+00 Z= 6.025766873570D+00
I= 11 X= -1.591091326616D+00 Y= -4.477673860796D+00 Z= 3.952366595770D+00
I= 12 X= -8.322374845080D-01 Y= -1.585778527051D+00 Z= 6.018803422275D+00
I= 13 X= -1.604348368539D+00 Y= 3.623971730560D+00 Z= 4.044057441220D+00
I= 14 X= -3.308211899884D+00 Y= 4.857151934959D+00 Z= 4.724512759104D+00
I= 15 X= -7.802925664381D-01 Y= 3.000422297060D+00 Z= 5.918363755868D+00
I= 16 X= -8.374816442005D-02 Y= 5.288932372395D+00 Z= 3.124016845032D+00
I= 17 X= -2.212854259183D+00 Y= 5.065130247022D+00 Z= -1.402754857958D+00
I= 18 X= -4.010388210114D+00 Y= 6.443654116337D+00 Z= -1.188477913180D-01
I= 19 X= -2.871315290761D-01 Y= 5.882227895781D+00 Z= -6.591680014892D-01
I= 20 X= -2.644952432386D+00 Y= 5.297720971439D+00 Z= -3.647975190462D+00

I= 21 X= -3.319427095594D+00 Y= -3.868455022979D-01 Z= -4.867817784211D+00
I= 22 X= -5.467640412282D+00 Y= -1.210192191301D+00 Z= -4.890374958888D+00
I= 23 X= -2.828196894087D+00 Y= 1.332600766796D+00 Z= -5.924318877442D+00
I= 24 X= -1.785443229166D+00 Y= -2.111010543349D+00 Z= -5.749486442181D+00
I= 25 X= -3.438603826965D+00 Y= -4.627482600688D+00 Z= -8.043870335060D-01
I= 26 X= -2.220665471851D+00 Y= -5.319992196509D+00 Z= -2.486414324027D+00
I= 27 X= -3.127762626099D+00 Y= -5.864477454330D+00 Z= 9.115164853089D-01
I= 28 X= -5.817007693712D+00 Y= -4.415092110447D+00 Z= -1.374478897134D+00
I= 29 X= 3.440409973352D+00 Y= -3.689537641138D+00 Z= -1.529085933885D+00
I= 30 X= 3.867127003956D+00 Y= -3.309643552566D+00 Z= 1.003529910916D+00
I= 31 X= 2.211538694417D+00 Y= -5.108570728988D+00 Z= -2.373706778411D+00
I= 32 X= 4.784224641997D+00 Y= -3.206882129465D+00 Z= -3.133626998946D+00
I= 33 X= 5.320811631893D+00 Y= -2.039069778845D+00 Z= 1.577054899628D+00
I= 34 X= 2.808044019514D+00 Y= -4.209963288451D+00 Z= 2.534502231184D+00
I= 35 X= 1.168984217655D+00 Y= -1.413363016816D-01 Z= -3.102183368871D-01
I= 36 X= 3.825654862023D+00 Y= 2.645405288664D+00 Z= 1.172045923669D+00
I= 37 X= 5.172839677117D+00 Y= 1.876569070335D+00 Z= 2.298175141257D+00
I= 38 X= 2.595028510410D+00 Y= 3.922152365419D+00 Z= 2.317047369193D+00

Forward Direction:

Total Energy: -656.4326769 Hartrees

Potential Energy: -656.6072447 Hartress

Kinetic Energy: 0.1745679 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.806236142771D+12 Y= -1.252774097105D+13 Z= -4.847852754905D+12
I= 1 X= -1.341982079665D+13 Y= -1.720020121932D+13 Z= 1.462282037892D+13
I= 2 X= 1.332956705654D+13 Y= -6.355907562685D+12 Z= 1.393318443317D+13
I= 3 X= 9.633574986956D+12 Y= -3.018651501018D+13 Z= -9.667912151457D+12
I= 4 X= -1.307591043831D+13 Y= 1.478886786804D+13 Z= -1.457858097582D+13
I= 5 X= 1.510330164600D+13 Y= 7.758026102495D+12 Z= 1.429697934047D+13
I= 6 X= -8.229041907155D+13 Y= -4.554025450231D+11 Z= -1.847937561622D+12

I= 7 X= 1.439860993005D+13 Y= 2.437413350217D+13 Z= 1.597179680103D+13
I= 8 X= -6.677763327823D+13 Y= 8.415524657788D+13 Z= 4.915867997168D+12
I= 9 X= -3.346797694552D+13 Y= -6.237397340401D+12 Z= -7.428393708017D+10
I= 10 X= -4.150377230229D+13 Y= 4.072717781686D+13 Z= -4.084388351087D+13
I= 11 X= -5.687391060867D+12 Y= -8.339001045396D+13 Z= -1.896778804429D+13
I= 12 X= 1.085382376878D+14 Y= 1.058590250647D+14 Z= 5.056124739943D+13
I= 13 X= 5.520150502535D+12 Y= 2.556046775251D+13 Z= -8.717929106159D+11
I= 14 X= 7.467316802176D+13 Y= -2.456545503359D+13 Z= 5.791967846814D+13
I= 15 X= -1.501592936070D+12 Y= -4.290780678697D+13 Z= -1.916441559588D+13
I= 16 X= -9.383970754854D+12 Y= -9.664425358235D+13 Z= 3.961407443622D+13
I= 17 X= 7.737751559059D+12 Y= 2.369460069724D+10 Z= 1.020287409375D+13
I= 18 X= 5.613002658857D+13 Y= -2.125969514472D+13 Z= 2.530065328870D+13
I= 19 X= -6.656087964102D+13 Y= -6.069678697581D+13 Z= -5.898332389162D+13
I= 20 X= -2.158078985637D+13 Y= 2.863547541340D+13 Z= -1.150872999500D+14
I= 21 X= -1.094861958823D+13 Y= 1.103579730792D+13 Z= 6.848359296251D+12
I= 22 X= 7.407039937037D+13 Y= -4.744275669086D+13 Z= 2.929856140843D+13
I= 23 X= -2.086530546520D+13 Y= 6.185359785323D+11 Z= -9.111345670751D+12
I= 24 X= -6.190199619558D+13 Y= -4.194343876320D+13 Z= -5.256643248715D+13
I= 25 X= -1.752021184764D+13 Y= 1.228151105496D+13 Z= 2.502959243458D+13
I= 26 X= 7.317305449234D+13 Y= -1.292781701313D+13 Z= 3.125139390826D+13
I= 27 X= 1.046137178859D+14 Y= 2.056362108410D+13 Z= -1.009292573090D+14
I= 28 X= 1.932898170468D+13 Y= 8.424119704041D+13 Z= 1.044215347299D+13
I= 29 X= -9.442201538410D+12 Y= -1.839492575104D+12 Z= -1.661717343441D+13
I= 30 X= 1.582614382511D+13 Y= 8.089285639573D+12 Z= -3.722263283142D+12
I= 31 X= 7.205821006008D+13 Y= 1.732306791193D+14 Z= 3.878701807576D+13
I= 32 X= 6.046067738825D+12 Y= -4.581028071507D+13 Z= -2.899362136252D+13
I= 33 X= -2.523477873224D+13 Y= 1.812611447144D+13 Z= 7.155278666019D+13
I= 34 X= 1.368812519533D+13 Y= -1.634423851877D+13 Z= -3.302850523672D+12
I= 35 X= 2.619475331210D+12 Y= -2.266519421509D+12 Z= -8.257671095384D+11
I= 36 X= -4.426517013497D+12 Y= -1.935392550535D+11 Z= -1.789777336065D+13

I= 37 X= -6.680386817271D+13 Y= 9.977034933050D+13 Z= -4.896257362190D+13

I= 38 X= 4.976450599574D+13 Y= -1.398550591879D+13 Z= 9.138876863340D+12

Backward Direction:

Total Energy: -656.4326883 Hartrees

Potential Energy: -656.6072447 Hartress

Kinetic Energy: 0.1745564 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.161965363868D+12 Y= -1.299227174868D+13 Z= -4.666069540289D+12

I= 1 X= -1.396848953806D+13 Y= -1.839474001813D+13 Z= 1.390573539869D+13

I= 2 X= 1.281890415024D+13 Y= -5.886495343198D+12 Z= 1.317741089063D+13

I= 3 X= 8.587253086832D+12 Y= -3.016204903141D+13 Z= -1.118392503043D+13

I= 4 X= -1.128629284971D+13 Y= 1.462920145364D+13 Z= -1.576781064373D+13

I= 5 X= 1.214971145674D+13 Y= 3.557697983471D+12 Z= 5.910960825025D+12

I= 6 X= -1.613049318411D+13 Y= 7.507409721175D+13 Z= 2.791970843291D+13

I= 7 X= 2.648272246910D+13 Y= 3.581521761344D+13 Z= 1.671110014978D+13

I= 8 X= -5.151589784400D+13 Y= 9.649159900488D+13 Z= 6.335709608654D+12

I= 9 X= -3.289918409480D+13 Y= -5.970281528251D+12 Z= -7.172070446336D+11

I= 10 X= -4.139974465083D+13 Y= 4.204912360596D+13 Z= -4.237629266967D+13

I= 11 X= -5.851669691083D+12 Y= -8.340446141499D+13 Z= -1.899973276113D+13

I= 12 X= 1.088715902457D+14 Y= 1.059483095742D+14 Z= 5.024469521672D+13

I= 13 X= 5.632905382405D+12 Y= 2.550560554010D+13 Z= -1.109107375489D+12

I= 14 X= 7.486485933147D+13 Y= -2.490344136421D+13 Z= 5.796984692073D+13

I= 15 X= -1.149071465353D+12 Y= -4.323112987829D+13 Z= -1.974816526573D+13

I= 16 X= -9.408527312111D+12 Y= -9.654033723062D+13 Z= 3.969626065141D+13

I= 17 X= 7.910422950464D+12 Y= -3.573654608779D+11 Z= 1.016513806967D+13

I= 18 X= 5.616643347918D+13 Y= -2.186720597266D+13 Z= 2.480228763093D+13

I= 19 X= -6.692590348808D+13 Y= -6.081838542713D+13 Z= -5.860692734469D+13

I= 20 X= -2.132730638321D+13 Y= 2.829498514248D+13 Z= -1.151307811070D+14

I= 21 X= -1.116589513232D+13 Y= 1.089929995997D+13 Z= 6.317956604874D+12

I= 22 X= 7.403157046338D+13 Y= -4.683105214777D+13 Z= 2.717289921706D+13

I= 23 X= -2.007553190729D+13 Y= 2.747560134124D+11 Z= -9.357826495120D+12
I= 24 X= -6.228273384703D+13 Y= -4.215727673154D+13 Z= -5.319357326312D+13
I= 25 X= -1.775634676298D+13 Y= 1.204296541770D+13 Z= 2.490774035443D+13
I= 26 X= 7.258898937580D+13 Y= -1.356673912060D+13 Z= 3.118013021996D+13
I= 27 X= 1.051004921416D+14 Y= 2.097344549681D+13 Z= -1.010705287460D+14
I= 28 X= 1.935310265773D+13 Y= 8.351822044381D+13 Z= 1.095390689375D+13
I= 29 X= -1.053577101595D+13 Y= -1.532317429768D+12 Z= -1.700072784619D+13
I= 30 X= 1.589054314848D+13 Y= 7.877652333558D+12 Z= -4.197267423165D+12
I= 31 X= 7.130214975365D+13 Y= 1.730070024963D+14 Z= 3.881064229270D+13
I= 32 X= 3.833408410828D+12 Y= -4.397280165930D+13 Z= -3.031097163328D+13
I= 33 X= -2.516653992422D+13 Y= 1.785866359638D+13 Z= 7.117444413696D+13
I= 34 X= 1.440100516280D+13 Y= -1.684056416252D+13 Z= -3.439289767016D+12
I= 35 X= 2.607578516635D+12 Y= -1.988646647576D+12 Z= 9.371644559522D+11
I= 36 X= -8.271195541306D+12 Y= -5.049685030985D+12 Z= -1.966990365001D+13
I= 37 X= -6.337405907637D+13 Y= 1.015115422411D+14 Z= -5.324009445983D+13
I= 38 X= 5.164280251116D+13 Y= -1.418122784606D+13 Z= 5.944319901414D+12

Seed: 2072860618

CM Start Point Coordinates: bohr

I= 0 X= -2.159241153972D+00 Y= 2.253543150710D+00 Z= -7.904082539582D-01
I= 1 X= -2.808183044367D+00 Y= -7.168751289311D-02 Z= -2.015835453979D+00
I= 2 X= -2.010464488712D+00 Y= 1.721708408119D+00 Z= 1.911490571869D+00
I= 3 X= -2.759109190604D+00 Y= -2.044668971965D+00 Z= -2.179767057321D-01
I= 4 X= -2.124718626737D+00 Y= -9.911688531718D-01 Z= 2.452995133422D+00
I= 5 X= 4.590789738654D+00 Y= 2.514013047045D+00 Z= -7.901690305004D-01
I= 6 X= 2.641436405470D+00 Y= 8.237746103537D-01 Z= -3.121674544806D+00
I= 7 X= 6.186798213003D+00 Y= 1.071197943528D+00 Z= -1.071818057113D+00
I= 8 X= 4.672630746615D+00 Y= 4.007421979500D+00 Z= -2.065818975429D+00
I= 9 X= -2.048529692652D+00 Y= -2.340230068528D+00 Z= 4.774467924269D+00
I= 10 X= -4.158580465543D+00 Y= -2.397417581403D+00 Z= 5.584101342995D+00

I= 11 X= -1.494310761140D+00 Y= -4.317673508317D+00 Z= 4.354844057275D+00
I= 12 X= -9.995050722017D-01 Y= -1.237411514839D+00 Z= 6.132341780679D+00
I= 13 X= -1.550054104045D+00 Y= 3.490298112029D+00 Z= 3.916932946898D+00
I= 14 X= -3.573204966984D+00 Y= 3.206608000553D+00 Z= 5.409810475665D+00
I= 15 X= 1.391315014165D-01 Y= 3.102449122319D+00 Z= 5.019721388911D+00
I= 16 X= -1.200881255300D+00 Y= 5.640415340543D+00 Z= 3.239434329789D+00
I= 17 X= -2.683247060184D+00 Y= 5.003336218277D+00 Z= -1.627504507824D+00
I= 18 X= -4.607316152000D+00 Y= 5.927704132206D+00 Z= -8.943101087337D-01
I= 19 X= -1.286624056140D+00 Y= 6.050416018606D+00 Z= -5.943454177923D-01
I= 20 X= -2.503210790467D+00 Y= 5.273288581691D+00 Z= -3.691560736990D+00
I= 21 X= -3.594202407394D+00 Y= -4.126369720754D-01 Z= -4.629577038010D+00
I= 22 X= -5.745785923920D+00 Y= -6.842140206599D-01 Z= -4.358379790343D+00
I= 23 X= -2.854853839850D+00 Y= 1.440306066886D+00 Z= -5.782500915427D+00
I= 24 X= -2.884576641269D+00 Y= -2.200821230093D+00 Z= -5.486791170820D+00
I= 25 X= -3.430555167833D+00 Y= -4.631486178087D+00 Z= -4.240279553976D-01
I= 26 X= -3.629370110782D+00 Y= -5.210514368476D+00 Z= -2.417180493613D+00
I= 27 X= -2.200461045188D+00 Y= -6.016546151850D+00 Z= 6.631974687763D-01
I= 28 X= -5.315889765911D+00 Y= -4.805979847959D+00 Z= 9.385250416413D-01
I= 29 X= 3.449695553703D+00 Y= -3.584333337961D+00 Z= -1.772653396848D+00
I= 30 X= 3.714093226819D+00 Y= -3.356631097974D+00 Z= 7.526027284639D-01
I= 31 X= 2.041111413348D+00 Y= -4.694388575512D+00 Z= -2.728786118210D+00
I= 32 X= 4.732114954292D+00 Y= -2.742393039627D+00 Z= -3.333646241197D+00
I= 33 X= 5.415122303863D+00 Y= -2.365274238537D+00 Z= 1.502172699863D+00
I= 34 X= 2.399931402281D+00 Y= -4.339799376317D+00 Z= 2.403666776558D+00
I= 35 X= 1.212371950647D+00 Y= 1.380230067581D-02 Z= -4.326575182080D-01
I= 36 X= 3.602250902530D+00 Y= 2.252896424892D+00 Z= 1.745605873235D+00
I= 37 X= 4.587401294191D+00 Y= 1.240854652642D+00 Z= 3.239786454350D+00
I= 38 X= 2.672220152555D+00 Y= 4.164914181619D+00 Z= 2.110902428512D+00

Forward Direction:

Total Energy: -656.4419772 Hartrees

Potential Energy: -656.6352476 Hartress

Kinetic Energy: 0.1932704 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.411647488149D+13 Y= -2.047789572458D+11 Z= 8.946149554349D+12
I= 1 X= -1.444055598961D+13 Y= -1.818043258604D+13 Z= -3.266530012405D+12
I= 2 X= -9.114213224250D+12 Y= 7.952096496418D+12 Z= -2.184202236264D+13
I= 3 X= 1.978645192962D+13 Y= 9.447453885276D+12 Z= 1.687961359778D+13
I= 4 X= 2.957505319437D+12 Y= -1.897477639253D+13 Z= -2.596726950343D+13
I= 5 X= 4.949057957785D+12 Y= -4.957555582078D+12 Z= -1.390989328587D+12
I= 6 X= -2.895229657048D+13 Y= -3.040907968962D+13 Z= -1.135985778164D+14
I= 7 X= -5.940618572478D+13 Y= 8.113457334742D+13 Z= 2.887026654265D+13
I= 8 X= 5.695034192205D+13 Y= -7.808026516106D+13 Z= -3.763306956481D+13
I= 9 X= -1.139370927772D+13 Y= -8.469051674568D+12 Z= -8.802446508284D+12
I= 10 X= -5.980298494732D+13 Y= -5.950961855081D+13 Z= 3.319391771177D+13
I= 11 X= -2.596883591866D+13 Y= 1.126542104155D+13 Z= 2.019963528562D+13
I= 12 X= 3.190418207785D+13 Y= -1.533066017460D+13 Z= 5.952387374404D+13
I= 13 X= 2.581904142978D+13 Y= 6.102547592608D+12 Z= 4.314117452161D+12
I= 14 X= -4.640186461986D+13 Y= 7.013813330910D+11 Z= 9.800262123842D+13
I= 15 X= -1.032785670672D+14 Y= 7.518198135578D+13 Z= 4.780840703404D+13
I= 16 X= -2.948039949947D+13 Y= 9.412342184254D+12 Z= -9.316552312153D+13
I= 17 X= -6.132920091203D+11 Y= 2.238250696237D+13 Z= 2.268902490853D+13
I= 18 X= 1.914870251563D+13 Y= -1.847925992776D+13 Z= 2.984085936415D+13
I= 19 X= -7.114348155248D+13 Y= -9.469747272310D+13 Z= -1.739868812918D+14
I= 20 X= 5.363581130165D+13 Y= -9.952050575225D+12 Z= -4.668194033858D+11
I= 21 X= 3.540079132649D+12 Y= -1.218313376630D+13 Z= 1.358512012594D+13
I= 22 X= -1.114124240555D+14 Y= -3.082438636144D+12 Z= -2.813672465197D+13
I= 23 X= 4.765734031673D+13 Y= 3.116104232021D+12 Z= -9.351939892292D+12
I= 24 X= -4.277738814610D+13 Y= 3.688521840769D+13 Z= 3.539502506203D+13
I= 25 X= -1.510736446432D+13 Y= 1.619885263132D+13 Z= 8.703897122493D+12
I= 26 X= 6.265519127301D+11 Y= -6.152122002142D+13 Z= -1.081063785196D+14

I= 27 X= 7.008712406064D+13 Y= 7.905904797801D+12 Z= 3.292537051053D+13
I= 28 X= 9.954379327734D+12 Y= -1.671929521336D+13 Z= -2.827664353002D+13
I= 29 X= -6.857237984521D+12 Y= -3.070194121751D+13 Z= -1.151906418796D+13
I= 30 X= -7.282595604862D+11 Y= 2.241154820757D+12 Z= 2.538742224435D+13
I= 31 X= 7.466965367666D+13 Y= 3.490679589378D+13 Z= 9.333287753258D+12
I= 32 X= 1.019923078994D+13 Y= -3.271517761448D+13 Z= -1.073333294441D+14
I= 33 X= 2.487555615593D+13 Y= -1.414449615567D+13 Z= -3.207870738089D+13
I= 34 X= 8.250022536874D+13 Y= -3.567190929857D+13 Z= -1.306110626155D+14
I= 35 X= -2.138347010042D+12 Y= 5.250279397903D+12 Z= 3.369633444218D+11
I= 36 X= -7.533426695566D+12 Y= 4.397144206944D+12 Z= 7.283818053259D+12
I= 37 X= 4.167845732316D+13 Y= 7.382379715093D+13 Z= 8.008923106839D+12
I= 38 X= 8.994095217421D+13 Y= -1.030303044523D+14 Z= 8.488534509155D+12

Backward Direction:

Total Energy: -656.4419899 Hartrees

Potential Energy: -656.6352476 Hartress

Kinetic Energy: 0.1932578 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.378019850762D+13 Y= -6.439071357107D+11 Z= 9.117992058441D+12
I= 1 X= -1.495922109783D+13 Y= -1.930964871653D+13 Z= -3.944401612289D+12
I= 2 X= -9.596950819545D+12 Y= 8.395839177448D+12 Z= -2.255646686379D+13
I= 3 X= 1.879734754038D+13 Y= 9.470581955956D+12 Z= 1.544650301186D+13
I= 4 X= 4.649258700987D+12 Y= -1.912571154133D+13 Z= -2.709146682932D+13
I= 5 X= 2.156983152195D+12 Y= -8.928191170648D+12 Z= -9.318423236409D+12
I= 6 X= 3.358971176238D+13 Y= 4.099013274225D+13 Z= -8.545875844915D+13
I= 7 X= -4.798288594059D+13 Y= 9.195000833724D+13 Z= 2.956914152224D+13
I= 8 X= 7.137749811497D+13 Y= -6.641851907954D+13 Z= -3.629087116883D+13
I= 9 X= -1.085602054194D+13 Y= -8.216542935906D+12 Z= -9.410211732887D+12
I= 10 X= -5.970464598708D+13 Y= -5.825996262065D+13 Z= 3.174530748966D+13
I= 11 X= -2.612413106310D+13 Y= 1.125176033066D+13 Z= 2.016943743816D+13
I= 12 X= 3.221930544935D+13 Y= -1.524625813695D+13 Z= 5.922463201971D+13

I= 13 X= 2.592563037756D+13 Y= 6.050685489264D+12 Z= 4.089780391224D+12
I= 14 X= -4.622065583247D+13 Y= 3.818776150529D+11 Z= 9.805004626182D+13
I= 15 X= -1.029453230273D+14 Y= 7.487633899814D+13 Z= 4.725657937496D+13
I= 16 X= -2.950361316453D+13 Y= 9.510575916209D+12 Z= -9.308783121944D+13
I= 17 X= -4.500630553042D+11 Y= 2.202228495115D+13 Z= 2.265335245789D+13
I= 18 X= 1.918311851586D+13 Y= -1.905354937523D+13 Z= 2.936974654543D+13
I= 19 X= -7.148854428100D+13 Y= -9.481242163436D+13 Z= -1.736310677755D+14
I= 20 X= 5.387543316623D+13 Y= -1.027392133122D+13 Z= -5.079228201584D+11
I= 21 X= 3.334685178384D+12 Y= -1.231216683487D+13 Z= 1.308372219933D+13
I= 22 X= -1.114491296247D+14 Y= -2.504184794303D+12 Z= -3.014614622393D+13
I= 23 X= 4.840392557003D+13 Y= 2.791123672944D+12 Z= -9.584942058482D+12
I= 24 X= -4.313730539170D+13 Y= 3.668307403957D+13 Z= 3.480217912081D+13
I= 25 X= -1.533058647440D+13 Y= 1.597335172406D+13 Z= 8.588708452915D+12
I= 26 X= 7.442607672502D+10 Y= -6.212520304742D+13 Z= -1.081737451958D+14
I= 27 X= 7.054727933983D+13 Y= 8.293318196578D+12 Z= 3.279182442613D+13
I= 28 X= 9.977181238687D+12 Y= -1.740273624660D+13 Z= -2.779287506701D+13
I= 29 X= -7.891006241018D+12 Y= -3.041156376661D+13 Z= -1.188164414624D+13
I= 30 X= -6.673818757363D+11 Y= 2.041094561657D+12 Z= 2.493839343318D+13
I= 31 X= 7.395493809989D+13 Y= 3.469535089961D+13 Z= 9.355620087654D+12
I= 32 X= 8.107569464696D+12 Y= -3.097818004449D+13 Z= -1.085786411748D+14
I= 33 X= 2.494006336597D+13 Y= -1.439732162987D+13 Z= -3.243636046237D+13
I= 34 X= 8.317412189973D+13 Y= -3.614109365973D+13 Z= -1.307400407601D+14
I= 35 X= -2.149593255371D+12 Y= 5.512956858743D+12 Z= 2.003490009594D+12
I= 36 X= -1.116786118666D+13 Y= -1.934460272022D+11 Z= 5.608595691871D+12
I= 37 X= 4.492070927429D+13 Y= 7.546977393179D+13 Z= 3.965316048502D+12
I= 38 X= 9.171653512482D+13 Y= -1.032153234421D+14 Z= 5.468670067402D+12

Seed: 20872618492

CM Start Point Coordinates: bohr

I= 0 X= -2.077868724576D+00 Y= 2.382707653302D+00 Z= -6.774552938908D-01

I= 1 X= -2.619967199103D+00 Y= 8.097160786033D-02 Z= -1.801783694688D+00
I= 2 X= -2.105830171938D+00 Y= 1.716179249469D+00 Z= 2.097629485538D+00
I= 3 X= -2.681748733091D+00 Y= -1.963205776286D+00 Z= -8.840495242856D-02
I= 4 X= -2.314259021200D+00 Y= -9.175005493012D-01 Z= 2.299086132174D+00
I= 5 X= 4.584066961742D+00 Y= 2.357480476698D+00 Z= -1.438533206646D+00
I= 6 X= 2.302013410854D+00 Y= 7.335767767683D-01 Z= -2.903377835260D+00
I= 7 X= 6.073752192365D+00 Y= 8.911711143531D-01 Z= -1.787127945996D+00
I= 8 X= 3.811966064707D+00 Y= 3.785487915613D+00 Z= -2.407104334653D+00
I= 9 X= -2.426800078304D+00 Y= -2.316746315109D+00 Z= 4.675207611696D+00
I= 10 X= -4.461602896798D+00 Y= -2.263046186228D+00 Z= 5.281755443186D+00
I= 11 X= -1.370165660232D+00 Y= -4.211664405147D+00 Z= 4.770723571182D+00
I= 12 X= -1.343480865692D+00 Y= -1.270710654115D+00 Z= 6.590598460337D+00
I= 13 X= -1.928911295499D+00 Y= 3.492569748814D+00 Z= 4.221054315410D+00
I= 14 X= -3.566391433856D+00 Y= 3.738849928079D+00 Z= 5.318397236667D+00
I= 15 X= -6.322164760230D-01 Y= 2.555618090231D+00 Z= 5.638760112205D+00
I= 16 X= -1.345390031064D+00 Y= 5.326187038222D+00 Z= 3.605531829758D+00
I= 17 X= -2.708227714111D+00 Y= 5.093565912838D+00 Z= -1.543890172102D+00
I= 18 X= -4.861439192749D+00 Y= 5.244640783201D+00 Z= -9.001840595702D-01
I= 19 X= -1.578803084364D+00 Y= 6.657870759236D+00 Z= -2.958744813197D-01
I= 20 X= -2.267917317724D+00 Y= 5.756077333814D+00 Z= -3.594651096698D+00
I= 21 X= -3.134660738330D+00 Y= -1.764821466713D-01 Z= -4.666896526074D+00
I= 22 X= -5.044843580277D+00 Y= 3.845520057407D-01 Z= -5.157220213124D+00
I= 23 X= -2.140369591276D+00 Y= 1.134434795567D+00 Z= -5.703782851786D+00
I= 24 X= -2.766190646631D+00 Y= -2.046960989424D+00 Z= -5.350647896890D+00
I= 25 X= -3.119258439808D+00 Y= -4.805127885515D+00 Z= -4.089601887044D-01
I= 26 X= -3.916817708869D+00 Y= -5.354249240165D+00 Z= -2.517290012126D+00
I= 27 X= -1.443637769900D+00 Y= -6.140873582700D+00 Z= -2.731911218069D-02
I= 28 X= -4.870531645034D+00 Y= -5.447956713584D+00 Z= 1.206295759300D+00
I= 29 X= 3.446355729398D+00 Y= -3.565900788524D+00 Z= -1.893747783308D+00
I= 30 X= 3.714319368535D+00 Y= -3.483704332860D+00 Z= 7.646015675659D-01

I= 31 X= 2.162515985749D+00 Y= -5.105197002768D+00 Z= -2.570453937438D+00
I= 32 X= 5.024374601630D+00 Y= -2.996189768554D+00 Z= -3.369584879535D+00
I= 33 X= 5.437653091764D+00 Y= -2.614626549794D+00 Z= 1.422902692555D+00
I= 34 X= 2.549305448731D+00 Y= -5.216495058497D+00 Z= 1.824603788827D+00
I= 35 X= 1.153852170995D+00 Y= -8.247100880160D-02 Z= -3.429377606817D-01
I= 36 X= 3.989104750968D+00 Y= 2.823609952043D+00 Z= 1.112892805528D+00
I= 37 X= 5.178644972537D+00 Y= 1.786498342298D+00 Z= 2.743946131323D+00
I= 38 X= 2.984484942518D+00 Y= 4.539709299199D+00 Z= 1.634421763622D+00

Forward Direction:

Total Energy: -656.4353260 Hartrees

Potential Energy: -656.6228802 Hartress

Kinetic Energy: 0.1875541 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.528106867449D+12 Y= -9.502243196140D+11 Z= 2.584232221973D+13
I= 1 X= 1.118594747355D+13 Y= -1.930056021458D+12 Z= -3.360983656301D+12
I= 2 X= 3.363151163816D+12 Y= 5.322188550517D+12 Z= -5.675269339187D+12
I= 3 X= -7.478512771823D+12 Y= 1.689690620566D+13 Z= -1.182657652321D+13
I= 4 X= -1.263986923390D+12 Y= 3.959597356109D+12 Z= -3.195964397883D+13
I= 5 X= -4.173010265468D+12 Y= 1.706447552587D+13 Z= 5.824255469520D+12
I= 6 X= -5.303180979975D+13 Y= -2.673911996759D+13 Z= 5.687248247165D+13
I= 7 X= 1.521708208827D+14 Y= -4.492327043014D+13 Z= 2.730126931978D+12
I= 8 X= 2.901639158121D+13 Y= -5.368684631903D+13 Z= -2.860394127650D+13
I= 9 X= 1.180110234673D+11 Y= -1.757098242351D+13 Z= 1.282060888149D+13
I= 10 X= 7.364430365502D+13 Y= -1.259484379222D+13 Z= 2.581905869127D+13
I= 11 X= -2.141678577873D+13 Y= 8.199980468399D+13 Z= -1.527551768269D+13
I= 12 X= 4.064453935137D+12 Y= 7.877599710251D+13 Z= 1.542313586862D+13
I= 13 X= -4.313293932944D+12 Y= 5.326110319759D+12 Z= 1.006481175119D+13
I= 14 X= 1.336156590403D+14 Y= -5.266239874579D+13 Z= -7.173560704657D+13
I= 15 X= -2.200065803674D+13 Y= -5.516048870039D+13 Z= -7.573436448226D+13
I= 16 X= 5.251556344254D+13 Y= 5.014153871541D+13 Z= -8.222920140822D+13

I= 17 X= -2.202621997521D+13 Y= -1.134272389431D+13 Z= 1.157592753777D+12
I= 18 X= 7.845463136729D+13 Y= -5.260276631461D+13 Z= -6.701957660937D+13
I= 19 X= 4.508269042596D+13 Y= -9.117653016983D+13 Z= -5.076510227462D+13
I= 20 X= 5.646892933862D+11 Y= 2.440773359458D+13 Z= -8.007668218529D+13
I= 21 X= -1.607916919467D+13 Y= 1.674640825436D+13 Z= 3.553593469257D+13
I= 22 X= 3.746825347809D+13 Y= 3.617006609344D+13 Z= -5.077465304242D+13
I= 23 X= 1.286551319871D+13 Y= -5.635419878202D+13 Z= -2.078550999386D+13
I= 24 X= 5.747259556015D+13 Y= -9.322473544619D+13 Z= -1.001359614009D+14
I= 25 X= -1.068385869700D+12 Y= -2.080445969569D+13 Z= -8.462770984659D+12
I= 26 X= 4.361517245167D+13 Y= 4.182063965605D+13 Z= -5.192238873689D+13
I= 27 X= -4.920444319539D+13 Y= 1.653958349286D+13 Z= -2.791760355350D+12
I= 28 X= 9.670569427332D+13 Y= 1.082329261599D+14 Z= -3.336115305187D+13
I= 29 X= 8.898646368903D+12 Y= -1.173176118989D+13 Z= -1.291899758766D+13
I= 30 X= 1.443262279816D+13 Y= 1.112508598658D+13 Z= 1.100670104042D+13
I= 31 X= -3.355848971142D+13 Y= -7.086985847595D+13 Z= 6.151226500376D+13
I= 32 X= -7.016851126119D+12 Y= 4.291126323307D+13 Z= -2.910539101488D+13
I= 33 X= -1.233657742567D+14 Y= -7.430208510319D+13 Z= -1.695013874766D+11
I= 34 X= -1.216474077245D+13 Y= 7.348912332399D+13 Z= 4.858958096136D+13
I= 35 X= -4.300700179838D+12 Y= 7.028329240955D+11 Z= 5.571050457061D+11
I= 36 X= 5.830541119881D+12 Y= -1.337282071200D+13 Z= 4.294053315443D+12
I= 37 X= 8.848971947785D+13 Y= 2.150448838245D+13 Z= 8.389948279325D+13
I= 38 X= -1.334259257142D+13 Y= 5.157011359935D+13 Z= 2.366540820477D+13

Backward Direction:

Total Energy: -656.4353304 Hartrees

Potential Energy: -656.6228802 Hartress

Kinetic Energy: 0.1875498 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.373126819549D+12 Y= -1.152605785287D+12 Z= 2.592151945552D+13

I= 1 X= 1.094690973905D+13 Y= -2.450479048423D+12 Z= -3.673395054911D+12

I= 2 X= 3.140671378231D+12 Y= 5.526696707593D+12 Z= -6.004536128556D+12

I= 3 X= -7.934362354182D+12 Y= 1.690756526410D+13 Z= -1.248705570842D+13
I= 4 X= -4.843067615461D+11 Y= 3.890035714803D+12 Z= -3.247775398536D+13
I= 5 X= -5.459796720107D+12 Y= 1.523452451728D+13 Z= 2.170730654488D+12
I= 6 X= -2.420800854264D+13 Y= 6.166710272546D+12 Z= 6.984131066365D+13
I= 7 X= 1.574354890879D+14 Y= -3.993874951501D+13 Z= 3.052218174439D+12
I= 8 X= 3.566545025816D+13 Y= -4.831228512453D+13 Z= -2.798536089369D+13
I= 9 X= 3.658162015834D+11 Y= -1.745460845665D+13 Z= 1.254050748142D+13
I= 10 X= 7.368962523485D+13 Y= -1.201891354588D+13 Z= 2.515143616021D+13
I= 11 X= -2.148835681551D+13 Y= 8.199350886128D+13 Z= -1.528943499094D+13
I= 12 X= 4.209685175144D+12 Y= 7.881489555851D+13 Z= 1.528522403466D+13
I= 13 X= -4.264170172047D+12 Y= 5.302208578270D+12 Z= 9.961421293002D+12
I= 14 X= 1.336991729206D+14 Y= -5.280964876702D+13 Z= -7.171375023277D+13
I= 15 X= -2.184707550763D+13 Y= -5.530135041221D+13 Z= -7.598868587159D+13
I= 16 X= 5.250486493038D+13 Y= 5.018681180098D+13 Z= -8.219339545785D+13
I= 17 X= -2.195099247594D+13 Y= -1.150873979114D+13 Z= 1.141152356071D+12
I= 18 X= 7.847049270697D+13 Y= -5.286743969489D+13 Z= -6.723669885284D+13
I= 19 X= 4.492366101286D+13 Y= -9.122950679559D+13 Z= -5.060111813243D+13
I= 20 X= 6.751240602323D+11 Y= 2.425939268317D+13 Z= -8.009562555798D+13
I= 21 X= -1.617382932216D+13 Y= 1.668694064705D+13 Z= 3.530485490220D+13
I= 22 X= 3.745133694437D+13 Y= 3.643656653740D+13 Z= -5.170073727975D+13
I= 23 X= 1.320959272222D+13 Y= -5.650397290940D+13 Z= -2.089289394551D+13
I= 24 X= 5.730672013135D+13 Y= -9.331789793071D+13 Z= -1.004091869352D+14
I= 25 X= -1.171262429232D+12 Y= -2.090838653557D+13 Z= -8.515858110457D+12
I= 26 X= 4.336071362648D+13 Y= 4.154228136489D+13 Z= -5.195343608647D+13
I= 27 X= -4.899237094441D+13 Y= 1.671813110828D+13 Z= -2.853307877641D+12
I= 28 X= 9.671620302035D+13 Y= 1.079179479765D+14 Z= -3.313819816428D+13
I= 29 X= 8.422212502338D+12 Y= -1.159793462822D+13 Z= -1.308610019387D+13
I= 30 X= 1.446067955790D+13 Y= 1.103288400458D+13 Z= 1.079975666124D+13
I= 31 X= -3.388788143522D+13 Y= -7.096730735235D+13 Z= 6.152255733392D+13
I= 32 X= -7.980837281649D+12 Y= 4.371179513302D+13 Z= -2.967931914010D+13

I= 33 X= -1.233360447578D+14 Y= -7.441860504748D+13 Z= -3.343333356757D+11
I= 34 X= -1.185416136657D+13 Y= 7.327288983666D+13 Z= 4.853013866863D+13
I= 35 X= -4.305883248913D+12 Y= 8.238933623464D+11 Z= 1.325158944966D+12
I= 36 X= 4.155535468515D+12 Y= -1.548849086905D+13 Z= 3.521991820918D+12
I= 37 X= 8.998397955218D+13 Y= 2.226307143042D+13 Z= 8.203590134559D+13
I= 38 X= -1.252427778484D+13 Y= 5.148484370483D+13 Z= 2.227364009140D+13

Seed: 21012156505

CM Start Point Coordinates: bohr

I= 0 X= -2.133571965608D+00 Y= 2.233038906086D+00 Z= -5.040286329597D-01
I= 1 X= -2.747854969949D+00 Y= 6.185429013941D-02 Z= -2.171144181291D+00
I= 2 X= -2.000729051529D+00 Y= 1.596674752328D+00 Z= 2.086558164842D+00
I= 3 X= -2.693199556350D+00 Y= -2.035489727979D+00 Z= -3.483173126530D-01
I= 4 X= -2.284897957674D+00 Y= -1.136836795231D+00 Z= 2.316937936512D+00
I= 5 X= 3.905633521264D+00 Y= 2.853831567670D+00 Z= -2.094183756474D+00
I= 6 X= 1.733428491199D+00 Y= 2.226173006526D-01 Z= -3.569430289276D+00
I= 7 X= 5.719849187324D+00 Y= 2.293977254836D+00 Z= -3.064200215465D+00
I= 8 X= 2.780245919428D+00 Y= 4.508067316519D+00 Z= -3.300845074024D+00
I= 9 X= -2.221610189282D+00 Y= -2.717641223835D+00 Z= 4.666201469278D+00
I= 10 X= -4.049467425702D+00 Y= -2.256820947922D+00 Z= 5.844631475822D+00
I= 11 X= -1.802017011300D+00 Y= -4.748244608447D+00 Z= 4.380344404162D+00
I= 12 X= -8.052390865521D-01 Y= -1.906141275223D+00 Z= 5.514532637519D+00
I= 13 X= -2.097039191404D+00 Y= 3.336679866368D+00 Z= 4.402257159806D+00
I= 14 X= -3.822052759932D+00 Y= 3.898462304895D+00 Z= 4.826300828941D+00
I= 15 X= -6.127698147265D-01 Y= 2.866171974741D+00 Z= 5.885770015616D+00
I= 16 X= -1.142643115221D+00 Y= 4.979891089360D+00 Z= 3.894732030820D+00
I= 17 X= -1.988685121821D+00 Y= 5.007788682522D+00 Z= -1.439092208472D+00
I= 18 X= -3.770072367339D+00 Y= 6.025672664222D+00 Z= -1.166707910019D+00
I= 19 X= -7.975956994107D-01 Y= 6.043364851458D+00 Z= -4.407404982633D-01
I= 20 X= -2.052900180975D+00 Y= 5.401790884882D+00 Z= -3.501427190499D+00

I= 21 X= -3.551978196146D+00 Y= -4.703991284656D-02 Z= -4.797011135065D+00
I= 22 X= -5.880696082020D+00 Y= 3.181715379542D-01 Z= -4.589079087157D+00
I= 23 X= -3.254336898637D+00 Y= 1.465599197773D+00 Z= -6.021962353744D+00
I= 24 X= -3.142115140531D+00 Y= -1.878332845565D+00 Z= -5.844653976662D+00
I= 25 X= -3.318952158381D+00 Y= -4.660551846605D+00 Z= -7.658874335970D-01
I= 26 X= -3.574870061714D+00 Y= -5.014895548736D+00 Z= -3.047147018745D+00
I= 27 X= -1.792094111640D+00 Y= -6.031077227819D+00 Z= -2.864872816493D-01
I= 28 X= -5.281683629444D+00 Y= -5.554174320869D+00 Z= 3.319414087167D-01
I= 29 X= 3.338872150753D+00 Y= -3.398441592923D+00 Z= -1.206855174901D+00
I= 30 X= 3.321114750832D+00 Y= -3.275394820070D+00 Z= 1.633645178959D+00
I= 31 X= 2.365404530835D+00 Y= -5.145726651701D+00 Z= -1.932525134901D+00
I= 32 X= 5.537993759971D+00 Y= -3.013462724747D+00 Z= -2.093133133250D+00
I= 33 X= 4.990516256792D+00 Y= -2.517124762213D+00 Z= 2.826535518782D+00
I= 34 X= 1.892702668584D+00 Y= -4.438115252432D+00 Z= 2.739601154135D+00
I= 35 X= 1.259797505942D+00 Y= -6.153365981795D-02 Z= -2.773084505256D-01
I= 36 X= 4.312305298870D+00 Y= 2.613704186237D+00 Z= 5.399615779984D-01
I= 37 X= 6.028989549008D+00 Y= 1.822467083513D+00 Z= 1.279843174850D+00
I= 38 X= 3.079203173103D+00 Y= 3.794957867663D+00 Z= 2.036481222077D+00

Forward Direction:

Total Energy: -656.4344657 Hartrees

Potential Energy: -656.5825778 Hartress

Kinetic Energy: 0.1481121 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.150586110431D+12 Y= 6.522588559135D+11 Z= 5.543196946943D+12
I= 1 X= 1.581776326075D+13 Y= 7.473034030519D+12 Z= 1.207717562463D+13
I= 2 X= 1.094016227121D+12 Y= 1.137867548138D+11 Z= 1.982350285116D+13
I= 3 X= 4.320695384498D+12 Y= -2.900402670917D+13 Z= -1.187021246640D+13
I= 4 X= 1.080368535375D+13 Y= 2.078265809880D+13 Z= 5.096993638032D+12
I= 5 X= -2.119696203692D+12 Y= 7.346207397970D+12 Z= -1.385316745902D+13
I= 6 X= -6.031569030837D+12 Y= -4.183490619474D+13 Z= 2.636999739648D+13

I= 7 X= 2.054994197243D+13 Y= 1.717048752256D+13 Z= -5.702064310801D+13
I= 8 X= 1.755945051826D+13 Y= -2.631787652716D+13 Z= 3.829749888175D+13
I= 9 X= -8.762474822740D+12 Y= 1.840429696179D+12 Z= 5.352752407625D+11
I= 10 X= -1.587262058519D+13 Y= -1.617240649211D+13 Z= 7.349280335362D+13
I= 11 X= -5.223103596608D+13 Y= -9.701221386117D+13 Z= 5.360100138708D+13
I= 12 X= -1.019828597774D+14 Y= -4.520795953460D+13 Z= -3.619757113887D+13
I= 13 X= -5.955705217274D+11 Y= -7.624568766190D+12 Z= 3.594382054510D+12
I= 14 X= 3.671693189655D+13 Y= 2.086549995817D+13 Z= -3.878036068955D+13
I= 15 X= 3.984807143596D+12 Y= 1.820674501836D+13 Z= -2.091057534782D+13
I= 16 X= -1.186651749987D+14 Y= -1.477664628023D+13 Z= 1.914996987804D+13
I= 17 X= -1.354295523972D+13 Y= -5.008230938858D+12 Z= -3.789480058239D+12
I= 18 X= 2.194631177589D+13 Y= -5.306446726280D+13 Z= -2.752355592731D+13
I= 19 X= 1.099040888182D+14 Y= 3.855478126300D+13 Z= -2.685122713507D+13
I= 20 X= 2.018384689969D+13 Y= 2.443423017890D+13 Z= -4.382320623548D+12
I= 21 X= -1.492187604877D+13 Y= -3.101162708578D+12 Z= -1.337168602135D+13
I= 22 X= -5.603776843007D+13 Y= 7.314599079089D+12 Z= 2.580139814026D+13
I= 23 X= 2.065748355853D+13 Y= 5.305409664117D+13 Z= -5.146168849780D+13
I= 24 X= -2.994222803070D+13 Y= -9.930389663790D+13 Z= 3.977621009141D+12
I= 25 X= 7.704507164098D+11 Y= 4.153959058116D+12 Z= 2.109566150318D+11
I= 26 X= -2.082976421227D+13 Y= -7.904797097121D+12 Z= 5.588632722141D+13
I= 27 X= -3.951143724332D+13 Y= 5.147162988593D+13 Z= 4.359518365615D+13
I= 28 X= -8.872463706851D+13 Y= -1.110013388326D+14 Z= 5.676312588496D+13
I= 29 X= 3.484502292073D+12 Y= 3.804308349520D+10 Z= 2.402210963100D+13
I= 30 X= 2.305497358143D+12 Y= 1.554629602288D+13 Z= -1.556403280945D+13
I= 31 X= -6.562522580966D+13 Y= 5.685936301407D+12 Z= -9.390708638863D+12
I= 32 X= 1.322310333468D+14 Y= -2.686643020545D+13 Z= -6.075745675334D+13
I= 33 X= -6.139094435197D+13 Y= -9.946577387652D+13 Z= 3.741427047698D+13
I= 34 X= -4.664168643263D+13 Y= -2.316530491739D+13 Z= 8.282653300290D+11
I= 35 X= 3.046568269072D+12 Y= 3.573720254898D+12 Z= -3.626790648650D+12
I= 36 X= 2.164046010599D+12 Y= -1.085468704217D+13 Z= -6.110489539736D+11

I= 37 X= -2.873069956579D+13 Y= -6.525215918025D+13 Z= -1.110772174717D+13

I= 38 X= -4.556334820084D+13 Y= 9.766190354200D+13 Z= 1.384987340727D+14

Backward Direction:

Total Energy: -656.4344642 Hartrees

Potential Energy: -656.5825778 Hartress

Kinetic Energy: 0.1481136 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.017627141920D+12 Y= 4.786337255635D+11 Z= 5.611141065831D+12

I= 1 X= 1.561269034406D+13 Y= 7.026557791667D+12 Z= 1.180915469046D+13

I= 2 X= 9.031485440793D+11 Y= 2.892363948087D+11 Z= 1.954102150336D+13

I= 3 X= 3.929617364451D+12 Y= -2.899488219328D+13 Z= -1.243684431510D+13

I= 4 X= 1.147258094029D+13 Y= 2.072298045490D+13 Z= 4.652501763243D+12

I= 5 X= -3.223643467448D+12 Y= 5.776273710858D+12 Z= -1.698756376883D+13

I= 6 X= 1.869666491006D+13 Y= -1.360465783657D+13 Z= 3.749608776177D+13

I= 7 X= 2.506655467806D+13 Y= 2.144675900757D+13 Z= -5.674431773614D+13

I= 8 X= 2.326374596963D+13 Y= -2.170698549836D+13 Z= 3.882818532148D+13

I= 9 X= -8.549880229226D+12 Y= 1.940268113581D+12 Z= 2.949733842207D+11

I= 10 X= -1.583373873376D+13 Y= -1.567831003403D+13 Z= 7.292004316685D+13

I= 11 X= -5.229243749986D+13 Y= -9.701761511271D+13 Z= 5.358906157991D+13

I= 12 X= -1.018582644004D+14 Y= -4.517458815281D+13 Z= -3.631588711925D+13

I= 13 X= -5.534267446587D+11 Y= -7.645074315007D+12 Z= 3.505682322661D+12

I= 14 X= 3.678857931264D+13 Y= 2.073917266979D+13 Z= -3.876160950654D+13

I= 15 X= 4.116567164066D+12 Y= 1.808589830846D+13 Z= -2.112876027043D+13

I= 16 X= -1.186743533521D+14 Y= -1.473780603921D+13 Z= 1.918068816846D+13

I= 17 X= -1.347841680131D+13 Y= -5.150657676163D+12 Z= -3.803584444412D+12

I= 18 X= 2.195991937927D+13 Y= -5.329153326329D+13 Z= -2.770982732182D+13

I= 19 X= 1.097676558529D+14 Y= 3.850933207345D+13 Z= -2.671054345985D+13

I= 20 X= 2.027859001682D+13 Y= 2.430696699064D+13 Z= -4.398572336887D+12

I= 21 X= -1.500308593999D+13 Y= -3.152180576875D+12 Z= -1.356993173769D+13

I= 22 X= -5.605228129670D+13 Y= 7.543232550391D+12 Z= 2.500690099921D+13

I= 23 X= 2.095267291126D+13 Y= 5.292560387778D+13 Z= -5.155381429001D+13
I= 24 X= -3.008453426635D+13 Y= -9.938382169185D+13 Z= 3.743218030648D+12
I= 25 X= 6.821918580824D+11 Y= 4.064799159656D+12 Z= 1.654126279995D+11
I= 26 X= -2.104806703736D+13 Y= -8.143603520567D+12 Z= 5.585969138683D+13
I= 27 X= -3.932949829347D+13 Y= 5.162480771497D+13 Z= 4.354238140711D+13
I= 28 X= -8.871562151477D+13 Y= -1.112715618424D+14 Z= 5.695440116101D+13
I= 29 X= 3.075764805946D+12 Y= 1.528542596650D+11 Z= 2.387875059511D+13
I= 30 X= 2.329567543311D+12 Y= 1.546719500034D+13 Z= -1.574157251102D+13
I= 31 X= -6.590781433821D+13 Y= 5.602333910910D+12 Z= -9.381878744708D+12
I= 32 X= 1.314040197623D+14 Y= -2.617964570067D+13 Z= -6.124983556653D+13
I= 33 X= -6.136543910779D+13 Y= -9.956573752877D+13 Z= 3.727285945783D+13
I= 34 X= -4.637523717874D+13 Y= -2.335081383671D+13 Z= 7.772691780934D+11
I= 35 X= 3.042121661800D+12 Y= 3.677579242849D+12 Z= -2.967869351815D+12
I= 36 X= 7.270415279761D+11 Y= -1.266974211115D+13 Z= -1.273408406099D+12
I= 37 X= -2.744875856323D+13 Y= -6.460136302338D+13 Z= -1.270650733350D+13
I= 38 X= -4.486130757904D+13 Y= 9.758874962578D+13 Z= 1.373047219744D+14

Seed: 21165468539

CM Start Point Coordinates: bohr

I= 0 X= -2.191323022495D+00 Y= 2.413398935893D+00 Z= -3.993397454254D-01
I= 1 X= -2.756773264846D+00 Y= -1.101767058880D-02 Z= -1.979200401498D+00
I= 2 X= -1.879691120165D+00 Y= 1.691283553520D+00 Z= 2.137131674965D+00
I= 3 X= -2.611370094668D+00 Y= -2.111186236732D+00 Z= -1.765079481856D-01
I= 4 X= -2.175287609594D+00 Y= -1.016368120820D+00 Z= 2.254694163199D+00
I= 5 X= 4.078014676715D+00 Y= 2.527954058108D+00 Z= -1.872342271862D+00
I= 6 X= 1.969243107780D+00 Y= 3.341742742250D-01 Z= -3.456986665245D+00
I= 7 X= 5.943130507588D+00 Y= 1.766142134417D+00 Z= -2.695967329848D+00
I= 8 X= 3.317641292611D+00 Y= 4.158497446998D+00 Z= -3.121373411085D+00
I= 9 X= -2.497665897243D+00 Y= -2.544056231935D+00 Z= 4.623063440364D+00
I= 10 X= -4.540810735087D+00 Y= -2.338925792242D+00 Z= 5.150730607319D+00

I= 11 X= -1.860249297359D+00 Y= -4.539776732993D+00 Z= 4.199156614044D+00
I= 12 X= -1.590598542071D+00 Y= -1.676497282966D+00 Z= 6.252419038469D+00
I= 13 X= -1.839344585388D+00 Y= 3.555296293273D+00 Z= 4.329469284802D+00
I= 14 X= -3.687652277824D+00 Y= 3.067522456290D+00 Z= 5.236595490004D+00
I= 15 X= -2.198893136923D-01 Y= 3.030791410195D+00 Z= 5.722500485419D+00
I= 16 X= -1.465255283726D+00 Y= 5.417776356130D+00 Z= 3.725873194953D+00
I= 17 X= -2.443551719270D+00 Y= 4.977519824314D+00 Z= -1.518435647755D+00
I= 18 X= -4.779070697199D+00 Y= 5.244057554910D+00 Z= -2.009110169200D+00
I= 19 X= -1.980515255171D+00 Y= 6.708201347809D+00 Z= 2.406690579150D-01
I= 20 X= -1.270292771221D+00 Y= 5.396345704921D+00 Z= -3.396331213316D+00
I= 21 X= -3.862718625764D+00 Y= 2.336887184686D-01 Z= -4.578125235973D+00
I= 22 X= -5.972563746538D+00 Y= 8.245695044212D-01 Z= -4.207732576765D+00
I= 23 X= -3.085547980389D+00 Y= 2.087902091129D+00 Z= -5.822200154634D+00
I= 24 X= -4.153725635911D+00 Y= -1.740934621887D+00 Z= -5.850107460243D+00
I= 25 X= -2.958189681119D+00 Y= -4.673765638686D+00 Z= -1.018961184537D+00
I= 26 X= -2.307228500597D+00 Y= -4.885841887909D+00 Z= -2.909492311312D+00
I= 27 X= -2.314471189151D+00 Y= -6.184890708811D+00 Z= 4.352369067772D-01
I= 28 X= -5.244435692335D+00 Y= -5.261303870014D+00 Z= -9.917592131100D-01
I= 29 X= 3.542100095181D+00 Y= -3.617277922191D+00 Z= -1.029651324471D+00
I= 30 X= 3.610858924779D+00 Y= -3.321625532268D+00 Z= 1.536636116327D+00
I= 31 X= 2.016291149555D+00 Y= -5.074272780088D+00 Z= -1.738538945599D+00
I= 32 X= 5.051502772807D+00 Y= -3.390701194775D+00 Z= -2.444369526613D+00
I= 33 X= 5.224662659746D+00 Y= -2.751932059883D+00 Z= 2.494972717864D+00
I= 34 X= 1.968361064967D+00 Y= -4.036411612773D+00 Z= 2.623619676300D+00
I= 35 X= 1.281954165293D+00 Y= -1.067514780826D-01 Z= -3.544488610837D-01
I= 36 X= 3.933569940382D+00 Y= 2.664773729272D+00 Z= 6.642021165524D-01
I= 37 X= 5.041119874231D+00 Y= 1.688844094721D+00 Z= 2.048759800156D+00
I= 38 X= 2.725339211776D+00 Y= 3.904811238913D+00 Z= 1.310094224864D+00

Forward Direction:

Total Energy: -656.4410985 Hartrees

Potential Energy: -656.6205758 Hartress

Kinetic Energy: 0.1794773 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.240681654421D+13 Y= -2.575765749410D+13 Z= 3.841757041949D+12
I= 1 X= -7.158777060005D+12 Y= -2.737931220569D+13 Z= -6.652187784931D+12
I= 2 X= 2.762238155563D+12 Y= 7.802619158202D+12 Z= -8.530867363519D+12
I= 3 X= 2.148432661849D+13 Y= 1.821325867940D+13 Z= -1.422294185819D+12
I= 4 X= -6.259388359947D+12 Y= 4.523525713822D+12 Z= -1.031322861301D+13
I= 5 X= 4.999655070691D+12 Y= 1.118622357365D+13 Z= 1.300182874356D+12
I= 6 X= -2.094009690112D+13 Y= -1.003292725412D+13 Z= 7.360264598456D+13
I= 7 X= -1.618935927126D+13 Y= -5.212362830135D+12 Z= -4.257845630847D+13
I= 8 X= -3.853070892781D+13 Y= -6.218916900780D+13 Z= 6.013180391823D+13
I= 9 X= -1.251105485120D+13 Y= 9.801871884608D+12 Z= -9.363529563700D+12
I= 10 X= 3.716616033093D+11 Y= 5.533833680372D+12 Z= 7.539793983629D+13
I= 11 X= 1.055096125898D+14 Y= -1.443657730720D+14 Z= 3.694256235282D+13
I= 12 X= 1.169035466331D+14 Y= -1.926438581866D+13 Z= 5.205963431111D+13
I= 13 X= 1.025149456957D+13 Y= 1.305456880620D+13 Z= 5.235235221984D+12
I= 14 X= -2.039467248099D+13 Y= -4.821659244497D+13 Z= 4.311507901165D+12
I= 15 X= -6.486917906273D+13 Y= -3.160656986163D+13 Z= -3.085208086611D+13
I= 16 X= -6.514896344787D+13 Y= -4.973673487478D+12 Z= 1.058506524287D+13
I= 17 X= -2.331833637413D+13 Y= -1.577624040062D+12 Z= 1.854046121683D+12
I= 18 X= -2.694325504182D+13 Y= -8.034674098765D+13 Z= 5.656977975800D+12
I= 19 X= 1.313564034522D+14 Y= 1.048906244685D+14 Z= 7.316773090467D+13
I= 20 X= 7.339141195362D+13 Y= -3.457915815698D+12 Z= 5.998642330670D+13
I= 21 X= -5.701552778483D+12 Y= -1.119561777656D+13 Z= 7.719859037733D+11
I= 22 X= -3.203884543644D+13 Y= -3.313359934892D+13 Z= 3.749311867327D+13
I= 23 X= -3.191728504186D+13 Y= 7.183770068838D+13 Z= -9.219437947875D+12
I= 24 X= 1.017360368549D+13 Y= -4.452494884786D+12 Z= 8.049466709963D+13
I= 25 X= -2.021140472398D+13 Y= 8.140003714384D+12 Z= -1.896790032805D+13
I= 26 X= 7.815326290073D+13 Y= -2.375813913152D+13 Z= -2.550426400743D+13

I= 27 X= 1.157566305589D+13 Y= -6.962220055657D+13 Z= 9.086539687216D+13
I= 28 X= 1.576392156747D+13 Y= -2.520285724287D+13 Z= 6.026878874989D+13
I= 29 X= 1.903929424480D+13 Y= 4.182506205809D+11 Z= -6.841377364215D+12
I= 30 X= -1.644392358370D+13 Y= -6.629930463001D+12 Z= 1.355058424759D+12
I= 31 X= -5.184808198855D+13 Y= -7.642989209858D+13 Z= 2.843342644273D+13
I= 32 X= 3.273371609596D+13 Y= -3.054291086009D+12 Z= 1.604170058669D+13
I= 33 X= 1.733120678172D+14 Y= 2.264442367375D+13 Z= -5.271495759700D+13
I= 34 X= -4.142679736181D+13 Y= -7.140968008415D+13 Z= -4.377421157911D+13
I= 35 X= -1.405967160958D+11 Y= 4.653949425628D+12 Z= 4.539137306289D+11
I= 36 X= 9.202932149946D+11 Y= -1.003825901052D+13 Z= -6.368831910344D+12
I= 37 X= -8.557839595713D+13 Y= 7.042290788814D+13 Z= -5.603185156074D+13
I= 38 X= -4.018888629759D+12 Y= 7.858204796436D+13 Z= 9.307130196421D+13

Backward Direction:

Total Energy: -656.4411068 Hartrees

Potential Energy: -656.6205758 Hartress

Kinetic Energy: 0.1794691 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.232045467680D+13 Y= -2.587043357001D+13 Z= 3.885889311539D+12
I= 1 X= -7.291979660227D+12 Y= -2.766931537444D+13 Z= -6.826277497879D+12
I= 2 X= 2.638262393260D+12 Y= 7.916580320070D+12 Z= -8.714349660331D+12
I= 3 X= 2.123030668421D+13 Y= 1.821919838715D+13 Z= -1.790342958109D+12
I= 4 X= -5.824915429992D+12 Y= 4.484762831987D+12 Z= -1.060194286148D+13
I= 5 X= 4.282599657107D+12 Y= 1.016649239044D+13 Z= -7.357258298018D+11
I= 6 X= -4.878175640300D+12 Y= 8.303684548629D+12 Z= 8.082946160840D+13
I= 7 X= -1.325564884820D+13 Y= -2.434763101816D+12 Z= -4.239897254839D+13
I= 8 X= -3.482555373403D+13 Y= -5.919422125494D+13 Z= 6.047650479177D+13
I= 9 X= -1.237296664043D+13 Y= 9.866720704967D+12 Z= -9.519614688689D+12
I= 10 X= 3.969168272780D+11 Y= 5.854767967760D+12 Z= 7.502591047421D+13
I= 11 X= 1.054697299850D+14 Y= -1.443692813879D+14 Z= 3.693480699797D+13
I= 12 X= 1.169844760230D+14 Y= -1.924270984526D+13 Z= 5.198278361290D+13

I= 13 X= 1.027886854498D+13 Y= 1.304124967831D+13 Z= 5.177621397559D+12
I= 14 X= -2.034813477703D+13 Y= -4.829864678806D+13 Z= 4.323687507467D+12
I= 15 X= -6.478359595208D+13 Y= -3.168506435878D+13 Z= -3.099380021406D+13
I= 16 X= -6.515492513457D+13 Y= -4.948445285999D+12 Z= 1.060501792991D+13
I= 17 X= -2.327641622152D+13 Y= -1.670135581894D+12 Z= 1.844884789911D+12
I= 18 X= -2.693441638945D+13 Y= -8.049422892591D+13 Z= 5.535987668101D+12
I= 19 X= 1.312677850908D+14 Y= 1.048611035025D+14 Z= 7.325911026272D+13
I= 20 X= 7.345295119171D+13 Y= -3.540578059825D+12 Z= 5.997586720444D+13
I= 21 X= -5.754301669933D+12 Y= -1.122875580717D+13 Z= 6.432178287358D+11
I= 22 X= -3.204827209348D+13 Y= -3.298509328418D+13 Z= 3.697706279451D+13
I= 23 X= -3.172554842202D+13 Y= 7.175423979374D+13 Z= -9.279277126156D+12
I= 24 X= 1.008117041303D+13 Y= -4.504409221289D+12 Z= 8.034241351744D+13
I= 25 X= -2.026873218306D+13 Y= 8.082090994838D+12 Z= -1.899748286642D+13
I= 26 X= 7.801146697458D+13 Y= -2.391325292221D+13 Z= -2.552156499070D+13
I= 27 X= 1.169383927490D+13 Y= -6.952270577586D+13 Z= 9.083109981601D+13
I= 28 X= 1.576977751346D+13 Y= -2.537837728734D+13 Z= 6.039302926263D+13
I= 29 X= 1.877380382071D+13 Y= 4.928248133192D+11 Z= -6.934494468651D+12
I= 30 X= -1.642828909049D+13 Y= -6.681309563256D+12 Z= 1.239739688440D+12
I= 31 X= -5.203163390347D+13 Y= -7.648419500330D+13 Z= 2.843916179263D+13
I= 32 X= 3.219653955850D+13 Y= -2.608198625675D+12 Z= 1.572188196564D+13
I= 33 X= 1.733286344372D+14 Y= 2.257949350922D+13 Z= -5.280680938864D+13
I= 34 X= -4.125372851717D+13 Y= -7.153017513085D+13 Z= -4.380733550353D+13
I= 35 X= -1.434849555878D+11 Y= 4.721409758524D+12 Z= 8.819079824838D+11
I= 36 X= -1.309543339699D+10 Y= -1.121720578299D+13 Z= -6.799059373632D+12
I= 37 X= -8.474572689259D+13 Y= 7.084562455544D+13 Z= -5.707032314168D+13
I= 38 X= -3.562886748218D+12 Y= 7.853453173538D+13 Z= 9.229574604069D+13

Seed: 2121407000

CM Start Point Coordinates: bohr

I= 0 X= -2.228356171100D+00 Y= 2.336416288720D+00 Z= -5.545945363594D-01

I= 1 X= -2.898403093886D+00 Y= 1.045348460208D-01 Z= -1.848787824602D+00
I= 2 X= -1.896452349255D+00 Y= 1.719243665344D+00 Z= 2.086780682513D+00
I= 3 X= -2.709746841409D+00 Y= -2.001312355486D+00 Z= -2.160864808457D-01
I= 4 X= -2.097476514259D+00 Y= -9.958358008324D-01 Z= 2.319364898187D+00
I= 5 X= 4.606521733119D+00 Y= 2.119067223505D+00 Z= -1.437021885810D+00
I= 6 X= 2.457946124009D+00 Y= 2.518642516389D-01 Z= -3.074094119827D+00
I= 7 X= 6.550426392336D+00 Y= 1.149568068554D+00 Z= -1.616062370068D+00
I= 8 X= 4.535078321276D+00 Y= 3.432558031022D+00 Z= -2.934157073224D+00
I= 9 X= -1.886954215687D+00 Y= -2.627395543132D+00 Z= 4.471204916349D+00
I= 10 X= -3.734411297714D+00 Y= -2.750922080506D+00 Z= 5.347201079729D+00
I= 11 X= -1.634879872740D+00 Y= -4.726643775508D+00 Z= 3.545706487998D+00
I= 12 X= -4.833566100516D-01 Y= -2.039304565273D+00 Z= 6.036247045462D+00
I= 13 X= -1.656323637068D+00 Y= 3.454357328766D+00 Z= 4.297201381583D+00
I= 14 X= -3.317619045072D+00 Y= 3.448589932296D+00 Z= 5.658843198186D+00
I= 15 X= -1.937947936355D-01 Y= 3.189981591332D+00 Z= 5.849807944883D+00
I= 16 X= -1.403003261191D+00 Y= 5.295201661248D+00 Z= 3.683927219159D+00
I= 17 X= -2.474225230386D+00 Y= 5.025173775813D+00 Z= -1.616090770360D+00
I= 18 X= -4.682595318236D+00 Y= 5.540026545184D+00 Z= -1.606774646257D+00
I= 19 X= -1.345244398652D+00 Y= 6.406761231964D+00 Z= -8.472690220423D-01
I= 20 X= -2.138121165270D+00 Y= 4.921816074504D+00 Z= -3.810409985062D+00
I= 21 X= -3.651119333714D+00 Y= -1.174531090144D-01 Z= -4.598823439154D+00
I= 22 X= -5.757469444241D+00 Y= -1.894763266352D-01 Z= -4.363947158393D+00
I= 23 X= -2.871314115843D+00 Y= 1.490784196024D+00 Z= -5.605950484574D+00
I= 24 X= -3.248768163501D+00 Y= -1.494310521033D+00 Z= -5.702922189463D+00
I= 25 X= -3.214321852413D+00 Y= -4.811877242102D+00 Z= -9.336839855130D-01
I= 26 X= -1.837624631432D+00 Y= -5.254666043613D+00 Z= -2.787657960644D+00
I= 27 X= -2.827095126983D+00 Y= -6.064703068100D+00 Z= 9.634507137966D-01
I= 28 X= -5.678439080282D+00 Y= -4.698569474891D+00 Z= -1.490335462137D+00
I= 29 X= 3.384654321078D+00 Y= -3.701568867020D+00 Z= -1.121928716132D+00
I= 30 X= 3.741775534404D+00 Y= -3.159163247762D+00 Z= 1.317140231477D+00

I= 31 X= 2.072701499565D+00 Y= -5.057708057602D+00 Z= -1.804950031964D+00
I= 32 X= 4.944836858301D+00 Y= -3.392557655088D+00 Z= -2.506831240920D+00
I= 33 X= 5.456880161665D+00 Y= -2.108448026809D+00 Z= 1.812080283017D+00
I= 34 X= 2.414540207644D+00 Y= -3.830977623513D+00 Z= 3.094959715030D+00
I= 35 X= 1.126659894942D+00 Y= 1.830568827583D-03 Z= -4.058835802610D-01
I= 36 X= 3.796551861032D+00 Y= 2.657837886831D+00 Z= 1.106588770500D+00
I= 37 X= 4.478065022285D+00 Y= 2.044851322855D+00 Z= 3.108739283925D+00
I= 38 X= 2.555566481055D+00 Y= 4.225263046269D+00 Z= 1.543103018479D+00

Forward Direction:

Total Energy: -656.4389757 Hartrees

Potential Energy: -656.6250633 Hartress

Kinetic Energy: 0.1860876 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.094078882479D+12 Y= -9.282988227791D+12 Z= -8.687144791715D+12
I= 1 X= 1.772379371550D+13 Y= 3.661566118290D+12 Z= -1.268021023389D+13
I= 2 X= 1.253453219687D+13 Y= -2.178634651786D+13 Z= -1.562838578223D+13
I= 3 X= -1.026962278113D+13 Y= -2.861465444130D+12 Z= 2.106761502868D+13
I= 4 X= -8.383319369900D+12 Y= -1.291919554747D+13 Z= 8.992844520115D+12
I= 5 X= -1.078106558445D+13 Y= 2.916486819390D+12 Z= 1.347541893326D+13
I= 6 X= -3.475551028219D+13 Y= -4.138594542800D+13 Z= 7.088376645738D+13
I= 7 X= 1.191434712446D+14 Y= -1.177332914284D+12 Z= -1.063253196384D+14
I= 8 X= 4.550841963292D+13 Y= 6.137160694277D+12 Z= 2.871049979732D+13
I= 9 X= 3.658549061806D+12 Y= 1.126143835509D+13 Z= -2.783405089180D+13
I= 10 X= -1.245525683686D+14 Y= 1.467923501003D+13 Z= 9.795289358563D+13
I= 11 X= 3.488695019083D+13 Y= -4.265730272253D+13 Z= 7.324779803339D+13
I= 12 X= -8.877157484799D+12 Y= 4.204979007759D+13 Z= -1.560143532467D+13
I= 13 X= 7.563982827496D+08 Y= 1.198322806862D+13 Z= -8.064763621876D+12
I= 14 X= -2.413286025015D+13 Y= 3.597896716858D+12 Z= 7.018695245183D+13
I= 15 X= 6.421263646339D+12 Y= 4.248432272729D+13 Z= -5.669859641043D+13
I= 16 X= 1.350319532922D+13 Y= -1.413712557071D+14 Z= 2.500796232208D+12

I= 17 X= -1.201526525336D+13 Y= 3.324430425348D+12 Z= -4.401037133296D+12
I= 18 X= 9.368777574414D+13 Y= -2.362462188374D+13 Z= -8.431079841831D+12
I= 19 X= 6.998250825682D+12 Y= -1.643612984863D+13 Z= -6.160295626367D+11
I= 20 X= 2.185298830629D+12 Y= 3.924306546670D+13 Z= 3.168668034513D+13
I= 21 X= -7.416616658817D+12 Y= 2.931462417395D+12 Z= 2.379024028140D+13
I= 22 X= -1.969282635276D+13 Y= 1.941754423190D+13 Z= -3.711053291511D+13
I= 23 X= -7.791714206883D+13 Y= 7.378091414876D+12 Z= -1.084647003020D+14
I= 24 X= 2.305398694451D+13 Y= -8.725479316412D+12 Z= 1.480511527473D+13
I= 25 X= -2.104291969875D+13 Y= 2.435414869233D+13 Z= 2.332137305912D+13
I= 26 X= 7.344840308956D+13 Y= -1.258392077556D+14 Z= -8.269781187535D+13
I= 27 X= -2.889876940267D+13 Y= -5.022905590588D+12 Z= -3.495535308484D+13
I= 28 X= -3.907519346535D+13 Y= 3.307084636924D+13 Z= 7.798499111038D+13
I= 29 X= 1.321458917856D+12 Y= 5.609130853561D+12 Z= 2.723145091978D+13
I= 30 X= 1.779675705614D+13 Y= 3.238053571875D+12 Z= -8.315414050785D+12
I= 31 X= -1.311471372228D+13 Y= 1.697227340298D+13 Z= -6.230675963867D+13
I= 32 X= -3.418676546679D+13 Y= 4.945976786291D+13 Z= 1.234921459065D+13
I= 33 X= 4.827503538601D+13 Y= 8.581290902037D+13 Z= -2.253498656410D+13
I= 34 X= -1.246835913403D+14 Y= -7.868731446590D+13 Z= 3.669184110405D+13
I= 35 X= -5.097256814819D+11 Y= -1.502535470464D+12 Z= -4.403505006723D+12
I= 36 X= 1.392268984552D+13 Y= 1.000460098177D+13 Z= 1.257095612551D+13
I= 37 X= 3.259108245397D+13 Y= 2.180059028837D+13 Z= 3.376086153694D+13
I= 38 X= 6.861081195765D+13 Y= -1.299510192103D+14 Z= -9.928433083839D+13

Backward Direction:

Total Energy: -656.4390100 Hartrees

Potential Energy: -656.6250633 Hartress

Kinetic Energy: 0.1860533 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.855092730139D+12 Y= -9.595069487385D+12 Z= -8.565019117119D+12

I= 1 X= 1.735518685466D+13 Y= 2.859050570518D+12 Z= -1.316196256180D+13

I= 2 X= 1.219145843385D+13 Y= -2.147098580779D+13 Z= -1.613612987407D+13

I= 3 X= -1.097256319232D+13 Y= -2.845028699666D+12 Z= 2.004912663106D+13
I= 4 X= -7.181017742875D+12 Y= -1.302646270393D+13 Z= 8.193895754513D+12
I= 5 X= -1.276534776282D+13 Y= 9.462065162977D+10 Z= 7.841520520597D+12
I= 6 X= 9.692078387927D+12 Y= 9.356314219545D+12 Z= 9.088227865464D+13
I= 7 X= 1.272618247099D+14 Y= 6.509020928928D+12 Z= -1.058286405589D+14
I= 8 X= 5.576156502353D+13 Y= 1.442497406426D+13 Z= 2.966437837341D+13
I= 9 X= 4.040675708793D+12 Y= 1.144089220916D+13 Z= -2.826597975813D+13
I= 10 X= -1.244826804661D+14 Y= 1.556734517255D+13 Z= 9.692338984100D+13
I= 11 X= 3.477658445162D+13 Y= -4.266701116254D+13 Z= 7.322633691990D+13
I= 12 X= -8.653204417526D+12 Y= 4.210977323634D+13 Z= -1.581410153973D+13
I= 13 X= 7.650743234010D+10 Y= 1.194637051468D+13 Z= -8.224196324269D+12
I= 14 X= -2.400407811210D+13 Y= 3.370830613616D+12 Z= 7.022065663867D+13
I= 15 X= 6.658094767460D+12 Y= 4.226710767170D+13 Z= -5.709077135166D+13
I= 16 X= 1.348669775020D+13 Y= -1.413014425901D+14 Z= 2.556010607081D+12
I= 17 X= -1.189926108955D+13 Y= 3.068426497024D+12 Z= -4.426388963713D+12
I= 18 X= 9.371223463587D+13 Y= -2.403276005974D+13 Z= -8.765892054880D+12
I= 19 X= 6.753020358289D+12 Y= -1.651782217142D+13 Z= -3.631586849363D+11
I= 20 X= 2.355594193315D+12 Y= 3.901431715233D+13 Z= 3.165746881624D+13
I= 21 X= -7.562586801363D+12 Y= 2.839760714311D+12 Z= 2.343390492544D+13
I= 22 X= -1.971891240142D+13 Y= 1.982849983743D+13 Z= -3.853859616835D+13
I= 23 X= -7.738655606480D+13 Y= 7.147133016938D+12 Z= -1.086302911517D+14
I= 24 X= 2.279819961561D+13 Y= -8.869140030253D+12 Z= 1.438378930077D+13
I= 25 X= -2.120155995421D+13 Y= 2.419388886358D+13 Z= 2.323951034347D+13
I= 26 X= 7.305601622871D+13 Y= -1.262684486709D+14 Z= -8.274568827120D+13
I= 27 X= -2.857174452135D+13 Y= -4.747577187081D+12 Z= -3.505026211195D+13
I= 28 X= -3.905898851456D+13 Y= 3.258513593582D+13 Z= 7.832879749856D+13
I= 29 X= 5.867766211897D+11 Y= 5.815497385644D+12 Z= 2.697377123877D+13
I= 30 X= 1.784002183653D+13 Y= 3.095873997978D+12 Z= -8.634531526311D+12
I= 31 X= -1.362265046961D+13 Y= 1.682200288048D+13 Z= -6.229088840442D+13
I= 32 X= -3.567327516438D+13 Y= 5.069422380107D+13 Z= 1.146419178664D+13

I= 33 X= 4.832087960527D+13 Y= 8.563323006425D+13 Z= -2.278916479242D+13
I= 34 X= -1.242046640213D+14 Y= -7.902075615674D+13 Z= 3.660017843200D+13
I= 35 X= -5.177182052851D+11 Y= -1.315854868977D+12 Z= -3.219131596599D+12
I= 36 X= 1.133975633007D+13 Y= 6.742143125206D+12 Z= 1.138040282552D+13
I= 37 X= 3.489529821367D+13 Y= 2.297035922636D+13 Z= 3.088713572588D+13
I= 38 X= 6.987268989562D+13 Y= -1.300825091953D+14 Z= -1.014304994158D+14

Seed: 21461384799

CM Start Point Coordinates: bohr

I= 0 X= -2.138268947404D+00 Y= 2.135010939029D+00 Z= -6.204390241233D-01
I= 1 X= -2.968072670415D+00 Y= 3.361488368323D-02 Z= -1.927926515123D+00
I= 2 X= -1.972927829454D+00 Y= 1.599592452010D+00 Z= 2.045049372165D+00
I= 3 X= -2.579601404425D+00 Y= -2.059955054664D+00 Z= -3.141813043896D-01
I= 4 X= -2.138575940834D+00 Y= -1.002941330726D+00 Z= 2.248925936678D+00
I= 5 X= 4.480097315057D+00 Y= 2.457710726630D+00 Z= -1.514696290166D+00
I= 6 X= 1.949141072024D+00 Y= 7.638778921822D-01 Z= -3.049003462950D+00
I= 7 X= 5.987877310970D+00 Y= 1.471070316349D+00 Z= -2.700893044636D+00
I= 8 X= 3.635302682310D+00 Y= 4.159239971811D+00 Z= -2.721505266979D+00
I= 9 X= -2.293124093979D+00 Y= -2.441368895837D+00 Z= 4.846338863474D+00
I= 10 X= -4.584059408079D+00 Y= -2.873505233252D+00 Z= 4.871673359320D+00
I= 11 X= -6.573265272950D-01 Y= -3.922348072477D+00 Z= 4.803006757474D+00
I= 12 X= -2.216992408162D+00 Y= -1.400125357580D+00 Z= 6.872924496698D+00
I= 13 X= -1.872544255537D+00 Y= 3.377471852044D+00 Z= 4.071285366540D+00
I= 14 X= -3.705322608914D+00 Y= 3.893355827802D+00 Z= 4.974623509803D+00
I= 15 X= -4.879919717336D-01 Y= 2.480128587635D+00 Z= 5.620416333436D+00
I= 16 X= -8.765470123496D-01 Y= 5.218589639829D+00 Z= 3.905928113873D+00
I= 17 X= -2.511799639945D+00 Y= 4.926909634841D+00 Z= -1.339223037622D+00
I= 18 X= -4.505627319244D+00 Y= 5.327564824902D+00 Z= -1.554705806986D+00
I= 19 X= -1.709928320812D+00 Y= 6.089612782987D+00 Z= 7.544988152036D-02
I= 20 X= -1.548709642601D+00 Y= 4.903795838896D+00 Z= -3.389134487668D+00

I= 21 X= -3.719041495653D+00 Y= -1.806760847212D-01 Z= -4.716140123044D+00
I= 22 X= -5.602570919177D+00 Y= 7.474184272163D-01 Z= -4.690752680564D+00
I= 23 X= -2.518969962532D+00 Y= 9.903749339573D-01 Z= -5.812333896962D+00
I= 24 X= -3.619460865091D+00 Y= -2.174254259256D+00 Z= -5.481532575245D+00
I= 25 X= -3.128271105204D+00 Y= -4.645601700906D+00 Z= -8.597594287123D-01
I= 26 X= -2.767784252031D+00 Y= -4.983309990957D+00 Z= -2.934001715878D+00
I= 27 X= -2.272482064247D+00 Y= -6.440579219767D+00 Z= 4.046367706492D-01
I= 28 X= -5.330721076959D+00 Y= -5.072360802485D+00 Z= -8.085975225472D-01
I= 29 X= 3.432945346773D+00 Y= -3.767451854453D+00 Z= -1.240603007586D+00
I= 30 X= 3.719036133623D+00 Y= -2.937194709369D+00 Z= 1.237089212591D+00
I= 31 X= 1.659170596329D+00 Y= -5.226306345312D+00 Z= -1.417002059493D+00
I= 32 X= 4.805540109693D+00 Y= -3.427617770990D+00 Z= -2.746155814046D+00
I= 33 X= 5.755762045083D+00 Y= -2.437448228173D+00 Z= 1.315805955582D+00
I= 34 X= 2.720448155885D+00 Y= -3.927178800972D+00 Z= 2.638690171301D+00
I= 35 X= 1.139809718580D+00 Y= 3.318187603432D-02 Z= -3.786586069400D-01
I= 36 X= 4.432975316350D+00 Y= 2.315577368963D+00 Z= 1.102002035110D+00
I= 37 X= 6.054503032704D+00 Y= 1.159960452054D+00 Z= 2.194112908434D+00
I= 38 X= 3.679121146826D+00 Y= 3.545965759150D+00 Z= 2.360097596379D+00

Forward Direction:

Total Energy: -656.4360215 Hartrees

Potential Energy: -656.6202912 Hartress

Kinetic Energy: 0.1842697 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.840354822512D+13 Y= 3.364426787470D+13 Z= -6.845526915141D+12
I= 1 X= 1.728491152888D+12 Y= -1.023422508591D+13 Z= 1.810223477883D+13
I= 2 X= 1.140649986266D+11 Y= -1.027212210296D+13 Z= 5.106440213234D+12
I= 3 X= 2.255817955928D+12 Y= 3.489368353606D+12 Z= -4.368854231277D+12
I= 4 X= -2.303969479363D+12 Y= 6.035983388264D+11 Z= 2.602513454885D+13
I= 5 X= 8.062994014717D+12 Y= 1.444516165934D+13 Z= 1.437614847055D+13
I= 6 X= -1.735548396368D+13 Y= -1.726424024218D+13 Z= 7.921669785192D+13

I= 7 X= 3.666443675884D+13 Y= -5.334696062313D+13 Z= 1.330434939967D+13
I= 8 X= -6.768888299938D+13 Y= -5.287362679191D+13 Z= -6.542085632977D+13
I= 9 X= 1.735467635446D+13 Y= 2.391861847269D+13 Z= -4.810175643009D+12
I= 10 X= -1.140517610684D+14 Y= 5.422626492045D+13 Z= -5.699662166224D+13
I= 11 X= 8.217143890624D+13 Y= 1.646585215073D+13 Z= -6.217716408616D+13
I= 12 X= 2.797211174979D+13 Y= 3.123596971022D+12 Z= -4.370995034625D+13
I= 13 X= 1.779881587637D+13 Y= 7.419903648799D+12 Z= -1.610833572736D+13
I= 14 X= -3.744415082242D+13 Y= -3.345005383225D+13 Z= 8.453589511793D+12
I= 15 X= -1.208019012381D+14 Y= -3.142415888281D+13 Z= 1.738813944681D+12
I= 16 X= -6.195878070333D+13 Y= -2.682012495235D+13 Z= 7.143953528944D+12
I= 17 X= 7.653159325884D+12 Y= -1.755875490505D+13 Z= 3.493028311336D+12
I= 18 X= -1.524896561814D+14 Y= 3.092337991833D+13 Z= -6.078113497589D+12
I= 19 X= -5.615502875386D+12 Y= -3.064914650624D+13 Z= -8.933876019656D+13
I= 20 X= 3.778382595799D+13 Y= -3.829682476076D+13 Z= -5.250107680535D+13
I= 21 X= -2.456782347097D+13 Y= -1.281180603320D+13 Z= 4.721095224005D+12
I= 22 X= 7.809934964697D+13 Y= -3.428051903359D+13 Z= 4.807510449347D+13
I= 23 X= 4.495175995809D+13 Y= 6.550039011102D+13 Z= -2.965381940522D+13
I= 24 X= 5.428299096099D+13 Y= 2.536672843059D+13 Z= -3.317039637974D+12
I= 25 X= -6.328227648268D+12 Y= -1.153757348902D+13 Z= -3.488941242106D+12
I= 26 X= 7.149349349439D+13 Y= -4.212959243040D+13 Z= -1.698647248917D+14
I= 27 X= -8.314069962775D+11 Y= 3.988080510134D+13 Z= -2.714782179663D+13
I= 28 X= -1.220467834663D+12 Y= 6.871277490318D+13 Z= -5.422817147179D+13
I= 29 X= -2.225104327583D+12 Y= -2.356489667634D+11 Z= -3.376131735513D+12
I= 30 X= -1.605755212460D+13 Y= 7.297533361056D+12 Z= 2.699834308791D+13
I= 31 X= 1.084425407001D+13 Y= 1.064271730385D+13 Z= -1.061267031511D+13
I= 32 X= -2.231371215494D+13 Y= -1.324796905586D+13 Z= 8.540545007528D+13
I= 33 X= 6.702168830983D+12 Y= 3.802563253014D+13 Z= -6.702390382545D+13
I= 34 X= 1.006437648028D+14 Y= 2.176746006468D+13 Z= -1.080837668278D+14
I= 35 X= 1.613885498915D+12 Y= -2.628340769886D+12 Z= 2.107873972896D+12
I= 36 X= 2.491266337790D+12 Y= -1.420308837680D+13 Z= -1.434968528751D+13

I= 37 X= -3.305269502361D+13 Y= 1.128254414024D+14 Z= -8.891151116985D+13

I= 38 X= 6.639314348399D+13 Y= -1.159057495301D+13 Z= -6.495852224058D+13

Backward Direction:

Total Energy: -656.4360566 Hartrees

Potential Energy: -656.6202912 Hartress

Kinetic Energy: 0.1842346 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.853817778081D+13 Y= 3.346846119808D+13 Z= -6.776729099614D+12

I= 1 X= 1.520841557076D+12 Y= -1.068631116035D+13 Z= 1.783084624388D+13

I= 2 X= -7.920087753447D+10 Y= -1.009446799275D+13 Z= 4.820409574702D+12

I= 3 X= 1.859826163147D+12 Y= 3.498627767244D+12 Z= -4.942605634498D+12

I= 4 X= -1.626669426161D+12 Y= 5.431708636170D+11 Z= 2.557505777136D+13

I= 5 X= 6.945175996560D+12 Y= 1.285550224187D+13 Z= 1.120236944188D+13

I= 6 X= 7.683452575069D+12 Y= 1.132071243982D+13 Z= 9.048258409523D+13

I= 7 X= 4.123779930396D+13 Y= -4.901695911519D+13 Z= 1.358414671729D+13

I= 8 X= -6.191291484516D+13 Y= -4.820480134633D+13 Z= -6.488350197745D+13

I= 9 X= 1.756994213449D+13 Y= 2.401971132901D+13 Z= -5.053496817855D+12

I= 10 X= -1.140123906805D+14 Y= 5.472656953912D+13 Z= -5.757657840876D+13

I= 11 X= 8.210926588710D+13 Y= 1.646038302898D+13 Z= -6.218925391255D+13

I= 12 X= 2.809827262142D+13 Y= 3.157387659304D+12 Z= -4.382975293302D+13

I= 13 X= 1.784148917681D+13 Y= 7.399140453833D+12 Z= -1.619814994401D+13

I= 14 X= -3.737160318192D+13 Y= -3.357796839209D+13 Z= 8.472576298658D+12

I= 15 X= -1.206684856932D+14 Y= -3.154652399081D+13 Z= 1.517887598603D+12

I= 16 X= -6.196807438906D+13 Y= -2.678079669299D+13 Z= 7.175057785998D+12

I= 17 X= 7.718508671092D+12 Y= -1.770297118971D+13 Z= 3.478746705507D+12

I= 18 X= -1.524758776021D+14 Y= 3.069346090631D+13 Z= -6.266725328731D+12

I= 19 X= -5.753650062681D+12 Y= -3.069516674505D+13 Z= -8.919630887451D+13

I= 20 X= 3.787975948588D+13 Y= -3.842568697151D+13 Z= -5.251753270410D+13

I= 21 X= -2.465005374208D+13 Y= -1.286346492325D+13 Z= 4.520358612131D+12

I= 22 X= 7.808465442784D+13 Y= -3.404901285440D+13 Z= 4.727062474290D+13

I= 23 X= 4.525065827313D+13 Y= 6.537028287783D+13 Z= -2.974710273067D+13
I= 24 X= 5.413889668751D+13 Y= 2.528579914746D+13 Z= -3.554387819791D+12
I= 25 X= -6.417595449979D+12 Y= -1.162785365517D+13 Z= -3.535057473224D+12
I= 26 X= 7.127244776333D+13 Y= -4.237139938573D+13 Z= -1.698916954027D+14
I= 27 X= -6.471820339651D+11 Y= 4.003590756385D+13 Z= -2.720128749098D+13
I= 28 X= -1.211338994950D+12 Y= 6.843915662075D+13 Z= -5.403449287819D+13
I= 29 X= -2.638977473242D+12 Y= -1.193952241684D+11 Z= -3.521292032357D+12
I= 30 X= -1.603317950781D+13 Y= 7.217438457426D+12 Z= 2.681857265665D+13
I= 31 X= 1.055811490543D+13 Y= 1.055806447671D+13 Z= -1.060372947726D+13
I= 32 X= -2.315111690665D+13 Y= -1.255255531553D+13 Z= 8.490688467738D+13
I= 33 X= 6.727994539752D+12 Y= 3.792441286554D+13 Z= -6.716709162638D+13
I= 34 X= 1.009135619035D+14 Y= 2.157962028047D+13 Z= -1.081354037307D+14
I= 35 X= 1.609383021155D+12 Y= -2.523176825723D+12 Z= 2.775074411494D+12
I= 36 X= 1.036206339218D+12 Y= -1.604094905022D+13 Z= -1.502036708153D+13
I= 37 X= -3.175464683130D+13 Y= 1.134844146127D+14 Z= -9.053038499963D+13
I= 38 X= 6.710400503099D+13 Y= -1.166464802596D+13 Z= -6.616753672879D+13

Seed: 21530788848

CM Start Point Coordinates: bohr

I= 0 X= -2.416076603663D+00 Y= 2.411309043792D+00 Z= -5.873525189516D-01
I= 1 X= -2.862638902267D+00 Y= 3.967556659545D-02 Z= -1.992771449508D+00
I= 2 X= -1.974348388936D+00 Y= 1.751714554304D+00 Z= 2.002897938736D+00
I= 3 X= -2.430222649268D+00 Y= -1.986274000035D+00 Z= -1.144907351926D-01
I= 4 X= -1.982801211759D+00 Y= -9.077933721136D-01 Z= 2.331189984865D+00
I= 5 X= 4.394757973279D+00 Y= 2.312610672733D+00 Z= -1.160156173285D+00
I= 6 X= 2.474256532186D+00 Y= 1.028769997321D+00 Z= -3.230916672723D+00
I= 7 X= 5.951491925038D+00 Y= 8.404612210899D-01 Z= -2.107860024837D+00
I= 8 X= 3.811826029150D+00 Y= 3.810797994044D+00 Z= -2.418710692765D+00
I= 9 X= -2.014586514679D+00 Y= -2.207022191707D+00 Z= 4.856533767207D+00
I= 10 X= -3.762072951233D+00 Y= -2.733344581805D+00 Z= 5.485557574776D+00

I= 11 X= -1.257592652535D+00 Y= -4.245038466745D+00 Z= 4.502265343074D+00
I= 12 X= -9.066906519598D-01 Y= -1.013356185147D+00 Z= 6.212957948890D+00
I= 13 X= -1.850764583213D+00 Y= 3.442048965220D+00 Z= 4.213029462509D+00
I= 14 X= -3.599903203780D+00 Y= 3.405085933182D+00 Z= 5.251805279439D+00
I= 15 X= -5.523971969021D-01 Y= 3.115690114858D+00 Z= 5.436630160603D+00
I= 16 X= -1.316565066600D+00 Y= 5.469558541413D+00 Z= 3.996364945629D+00
I= 17 X= -2.406080484443D+00 Y= 5.244909398473D+00 Z= -1.737470356877D+00
I= 18 X= -4.458428597867D+00 Y= 5.871764645114D+00 Z= -2.070526425644D+00
I= 19 X= -1.156591946988D+00 Y= 6.520087995925D+00 Z= -2.861752108917D-01
I= 20 X= -1.641136708443D+00 Y= 5.643657594434D+00 Z= -3.887003704967D+00
I= 21 X= -3.635732692538D+00 Y= -1.979671287864D-01 Z= -4.502357879680D+00
I= 22 X= -5.532818254874D+00 Y= -6.139620653727D-01 Z= -4.286552115383D+00
I= 23 X= -3.633487257792D+00 Y= 2.016047134028D+00 Z= -5.286515474785D+00
I= 24 X= -2.442752125480D+00 Y= -1.590911927162D+00 Z= -5.540826360431D+00
I= 25 X= -3.122360105558D+00 Y= -4.614185135376D+00 Z= -7.715851814112D-01
I= 26 X= -2.500140202939D+00 Y= -5.250923744856D+00 Z= -3.164261839439D+00
I= 27 X= -2.017877795486D+00 Y= -5.907343611341D+00 Z= 5.194228797234D-01
I= 28 X= -5.206722115556D+00 Y= -5.125737939170D+00 Z= -9.633853781367D-01
I= 29 X= 3.673110327142D+00 Y= -3.601858253744D+00 Z= -1.580245785997D+00
I= 30 X= 3.673072171878D+00 Y= -3.335936691272D+00 Z= 1.006968675431D+00
I= 31 X= 2.811808407759D+00 Y= -5.110268383307D+00 Z= -2.429439169771D+00
I= 32 X= 5.117064304804D+00 Y= -2.910359831946D+00 Z= -3.086407805357D+00
I= 33 X= 4.890625981571D+00 Y= -1.986689308816D+00 Z= 2.433644072590D+00
I= 34 X= 2.423375267105D+00 Y= -4.463143524221D+00 Z= 2.104574043184D+00
I= 35 X= 1.106187722424D+00 Y= -1.221358054026D-01 Z= -4.053442143256D-01
I= 36 X= 3.877350600185D+00 Y= 2.521680152949D+00 Z= 1.307582769216D+00
I= 37 X= 4.626192694744D+00 Y= 1.153617746872D+00 Z= 2.910571556733D+00
I= 38 X= 3.012439396432D+00 Y= 4.152708392578D+00 Z= 2.336355062597D+00

Forward Direction:

Total Energy: -656.4396589 Hartrees

Potential Energy: -656.5816719 Hartress

Kinetic Energy: 0.1420130 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.967962739300D+12 Y= -8.957751525231D+09 Z= 1.082303633514D+13
I= 1 X= 2.487405063923D+12 Y= 1.033963249252D+13 Z= 1.581514867771D+13
I= 2 X= -5.295898169183D+11 Y= -4.696699656317D+12 Z= -1.647604707625D+13
I= 3 X= -2.053239181666D+12 Y= -1.061299291297D+13 Z= 1.598692042838D+13
I= 4 X= 1.778534674540D+13 Y= -6.213877519205D+12 Z= -4.279105310889D+12
I= 5 X= -1.308386920339D+13 Y= -2.796783375199D+11 Z= 1.181421966295D+13
I= 6 X= -1.384991711837D+13 Y= -2.959234724489D+13 Z= 7.806959094793D+12
I= 7 X= -4.911080161778D+13 Y= 7.400586312600D+13 Z= 3.290708495779D+13
I= 8 X= 1.668992882932D+12 Y= -7.132130824930D+12 Z= 4.174529250689D+12
I= 9 X= -2.190843265185D+13 Y= 2.190840600928D+13 Z= -1.072009541442D+13
I= 10 X= 4.397136614924D+13 Y= 1.420235734491D+13 Z= -2.085093906647D+13
I= 11 X= 8.905676844049D+13 Y= -1.137669627566D+13 Z= -1.247694908909D+13
I= 12 X= 5.159717994137D+13 Y= 7.029277387300D+12 Z= -1.234350911020D+13
I= 13 X= 2.920929499369D+12 Y= -1.876777850399D+12 Z= 2.028467067309D+13
I= 14 X= -3.197417838653D+13 Y= -4.780231675870D+13 Z= -1.607314106033D+13
I= 15 X= 3.345243824717D+13 Y= -1.563999382740D+13 Z= -3.806784213646D+13
I= 16 X= 8.591109997627D+13 Y= -1.318053510659D+13 Z= -2.931516028819D+13
I= 17 X= -2.421359548155D+11 Y= -1.483475753759D+13 Z= 3.472760158001D+12
I= 18 X= 3.978274771823D+13 Y= 4.011548706786D+13 Z= -2.092686179524D+13
I= 19 X= -7.063786080855D+13 Y= -7.370630911940D+13 Z= 2.272341647607D+13
I= 20 X= -8.693575771231D+13 Y= 7.628447904488D+13 Z= -5.224067828074D+13
I= 21 X= -2.195723715385D+13 Y= 4.815806554928D+12 Z= -1.415458350093D+12
I= 22 X= 7.620736726288D+13 Y= -2.584962872462D+12 Z= -3.036954589046D+13
I= 23 X= -6.062280242607D+11 Y= -1.196005842767D+14 Z= -1.572169628281D+13
I= 24 X= 4.405060105772D+13 Y= -7.907960030240D+13 Z= -6.031692867288D+13
I= 25 X= 1.929737755960D+13 Y= -6.818974911165D+12 Z= 1.338659063325D+13
I= 26 X= -3.934691108197D+13 Y= 3.748857720210D+13 Z= -3.659144644293D+13

I= 27 X= -4.247133762672D+12 Y= 3.164544676551D+13 Z= 2.898481936045D+12
I= 28 X= -1.088798098327D+14 Y= 9.989455577281D+12 Z= -9.675644911321D+13
I= 29 X= -6.598083815423D+11 Y= 2.391696245047D+12 Z= -2.201356373936D+13
I= 30 X= -6.257756237270D+12 Y= 8.421575987549D+12 Z= 3.853289579819D+12
I= 31 X= -1.294803820442D+13 Y= 5.189091930793D+12 Z= -9.740510740963D+13
I= 32 X= -1.856250334181D+13 Y= -6.821875105656D+13 Z= 6.232079175157D+13
I= 33 X= -5.697885696707D+13 Y= 1.443721616275D+13 Z= 4.727940831824D+13
I= 34 X= 1.047907919006D+12 Y= 6.687300769686D+13 Z= -7.822948126860D+13
I= 35 X= 2.314307239612D+12 Y= 5.753791060690D+11 Z= -3.484748278073D+11
I= 36 X= -6.680137115067D+12 Y= 6.247370881084D+12 Z= -4.169094544929D+12
I= 37 X= 7.278017069786D+13 Y= -1.311067092935D+14 Z= 8.447150593542D+13
I= 38 X= 1.488413577012D+13 Y= 5.844807267069D+13 Z= -4.428637894018D+13

Backward Direction:

Total Energy: -656.4396584 Hartrees

Potential Energy: -656.5816719 Hartress

Kinetic Energy: 0.1420135 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.786972277898D+12 Y= -2.453050472105D+11 Z= 1.091552530111D+13
I= 1 X= 2.208249452461D+12 Y= 9.731866488335D+12 Z= 1.545030504578D+13
I= 2 X= -7.894085468617D+11 Y= -4.457868745547D+12 Z= -1.686057495120D+13
I= 3 X= -2.585594332158D+12 Y= -1.060054493618D+13 Z= 1.521559253959D+13
I= 4 X= 1.869588119965D+13 Y= -6.295113740656D+12 Z= -4.884170096870D+12
I= 5 X= -1.458661797425D+13 Y= -2.416751356680D+12 Z= 7.547521107867D+12
I= 6 X= 1.981140377266D+13 Y= 8.836092539659D+12 Z= 2.295235520270D+13
I= 7 X= -4.296256030335D+13 Y= 7.982693983704D+13 Z= 3.328323300933D+13
I= 8 X= 9.433967929351D+12 Y= -8.555530893713D+11 Z= 4.896926436214D+12
I= 9 X= -2.161903815071D+13 Y= 2.204431110643D+13 Z= -1.104720643546D+13
I= 10 X= 4.402429408789D+13 Y= 1.487494639464D+13 Z= -2.163060916164D+13
I= 11 X= 8.897318557398D+13 Y= -1.138404873789D+13 Z= -1.249320215434D+13
I= 12 X= 5.176678545722D+13 Y= 7.074704195266D+12 Z= -1.250456680160D+13

I= 13 X= 2.978297736824D+12 Y= -1.904691039418D+12 Z= 2.016392812032D+13
I= 14 X= -3.187664830731D+13 Y= -4.797427985810D+13 Z= -1.604761599849D+13
I= 15 X= 3.363179664613D+13 Y= -1.580449646617D+13 Z= -3.836484647158D+13
I= 16 X= 8.589860593012D+13 Y= -1.312766380618D+13 Z= -2.927334499628D+13
I= 17 X= -1.542829694299D+11 Y= -1.502863600569D+13 Z= 3.453560551850D+12
I= 18 X= 3.980127107216D+13 Y= 3.980639335049D+13 Z= -2.118042384954D+13
I= 19 X= -7.082358026013D+13 Y= -7.376817684734D+13 Z= 2.291492220711D+13
I= 20 X= -8.680678857485D+13 Y= 7.611124196477D+13 Z= -5.226280093321D+13
I= 21 X= -2.206778415549D+13 Y= 4.746358457463D+12 Z= -1.685320431333D+12
I= 22 X= 7.618761161994D+13 Y= -2.273735442543D+12 Z= -3.145105552808D+13
I= 23 X= -2.044013642947D+11 Y= -1.197754951129D+14 Z= -1.584710256486D+13
I= 24 X= 4.385688662191D+13 Y= -7.918839832090D+13 Z= -6.063600984525D+13
I= 25 X= 1.917723514818D+13 Y= -6.940343868410D+12 Z= 1.332459385817D+13
I= 26 X= -3.964407591061D+13 Y= 3.716350183577D+13 Z= -3.662770449260D+13
I= 27 X= -3.999469274164D+12 Y= 3.185396016153D+13 Z= 2.826604847201D+12
I= 28 X= -1.088675374012D+14 Y= 9.621614374468D+12 Z= -9.649607554953D+13
I= 29 X= -1.216202493155D+12 Y= 2.547983014830D+12 Z= -2.220871130049D+13
I= 30 X= -6.224990687480D+12 Y= 8.313899678604D+12 Z= 3.611613570432D+12
I= 31 X= -1.333271198268D+13 Y= 5.075288135225D+12 Z= -9.739308771097D+13
I= 32 X= -1.968827600251D+13 Y= -6.728386530388D+13 Z= 6.165054084407D+13
I= 33 X= -5.694413793778D+13 Y= 1.430114059297D+13 Z= 4.708691249726D+13
I= 34 X= 1.410612095944D+12 Y= 6.662048358340D+13 Z= -7.829889980495D+13
I= 35 X= 2.308254292280D+12 Y= 7.167572054844D+11 Z= 5.484821192948D+11
I= 36 X= -8.636260191379D+12 Y= 3.776626255256D+12 Z= -5.070731683428D+12
I= 37 X= 7.452521353297D+13 Y= -1.302208126954D+14 Z= 8.229515824935D+13
I= 38 X= 1.583978892150D+13 Y= 5.834849186485D+13 Z= -4.591172850621D+13

Seed: 22402754432

CM Start Point Coordinates: bohr

I= 0 X= -2.241453188187D+00 Y= 2.324612814668D+00 Z= -7.276585752778D-01

I= 1 X= -2.948263084966D+00 Y= -9.983544852328D-02 Z= -1.896983224470D+00
I= 2 X= -1.949638523999D+00 Y= 1.670790243826D+00 Z= 2.021938748936D+00
I= 3 X= -2.640302755890D+00 Y= -2.126403887036D+00 Z= -1.166051757549D-01
I= 4 X= -2.236174494422D+00 Y= -1.082895220918D+00 Z= 2.385257756100D+00
I= 5 X= 4.945097339488D+00 Y= 2.253043613737D+00 Z= -1.080110675789D+00
I= 6 X= 2.372900077200D+00 Y= 8.223364898755D-01 Z= -2.880328837131D+00
I= 7 X= 6.437976514350D+00 Y= 1.001022071770D+00 Z= -1.598545023513D+00
I= 8 X= 4.504508050525D+00 Y= 3.871219076277D+00 Z= -2.624667735194D+00
I= 9 X= -2.082459874095D+00 Y= -2.379121598909D+00 Z= 4.745027170373D+00
I= 10 X= -3.991621300494D+00 Y= -3.013780760537D+00 Z= 5.614191829856D+00
I= 11 X= -8.931154665010D-01 Y= -4.299508535126D+00 Z= 4.467379287654D+00
I= 12 X= -1.174178652972D+00 Y= -1.029303805830D+00 Z= 6.585774165744D+00
I= 13 X= -1.835106642603D+00 Y= 3.417244850727D+00 Z= 4.181107188876D+00
I= 14 X= -3.716891828189D+00 Y= 3.010300725559D+00 Z= 5.470257576561D+00
I= 15 X= -7.549573135827D-02 Y= 2.974826468787D+00 Z= 5.469269767658D+00
I= 16 X= -2.144898281818D+00 Y= 5.483049708205D+00 Z= 3.680319272868D+00
I= 17 X= -2.295757317031D+00 Y= 4.809979215623D+00 Z= -1.874144270347D+00
I= 18 X= -4.435096036312D+00 Y= 5.718021657867D+00 Z= -1.823452917281D+00
I= 19 X= -1.171913224991D+00 Y= 6.384647610523D+00 Z= -8.376203335351D-01
I= 20 X= -1.678066114526D+00 Y= 4.744199467354D+00 Z= -3.772444615032D+00
I= 21 X= -3.494748308453D+00 Y= -3.899709678215D-02 Z= -4.618114775041D+00
I= 22 X= -5.559571268697D+00 Y= -5.354279347297D-01 Z= -4.575087513686D+00
I= 23 X= -3.056389279594D+00 Y= 1.858726638611D+00 Z= -5.364412788311D+00
I= 24 X= -2.536979498300D+00 Y= -1.673220280351D+00 Z= -5.970272218671D+00
I= 25 X= -3.155512918476D+00 Y= -4.629309219210D+00 Z= -6.522996332610D-01
I= 26 X= -3.418694843745D+00 Y= -5.406115847399D+00 Z= -2.797309361722D+00
I= 27 X= -1.767929069813D+00 Y= -6.048461482160D+00 Z= 2.479093942450D-01
I= 28 X= -4.946482502546D+00 Y= -5.098394794882D+00 Z= 2.711674727825D-01
I= 29 X= 2.989551191519D+00 Y= -3.714549588738D+00 Z= -1.698139200234D+00
I= 30 X= 4.110033381050D+00 Y= -3.131578299957D+00 Z= 7.670354074606D-01

I= 31 X= 1.142800829226D+00 Y= -4.877681187581D+00 Z= -1.945402226996D+00
I= 32 X= 4.288202757428D+00 Y= -3.476278361422D+00 Z= -3.427069457248D+00
I= 33 X= 5.914007776473D+00 Y= -2.358704310265D+00 Z= 8.141142294307D-01
I= 34 X= 3.101773350788D+00 Y= -4.149806478119D+00 Z= 2.485181176224D+00
I= 35 X= 1.093164474004D+00 Y= -2.829171065918D-03 Z= -3.605310806238D-01
I= 36 X= 3.866268123697D+00 Y= 2.706415701273D+00 Z= 1.438951637985D+00
I= 37 X= 4.950753991894D+00 Y= 2.075265442265D+00 Z= 3.051409676325D+00
I= 38 X= 3.021947176100D+00 Y= 4.557270594872D+00 Z= 2.036703744103D+00

Forward Direction:

Total Energy: -656.4399922 Hartrees

Potential Energy: -656.6314769 Hartress

Kinetic Energy: 0.1914847 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.831465174878D+13 Y= -1.973350118754D+13 Z= 2.264997692881D+13
I= 1 X= -1.106138837384D+13 Y= -1.550926789268D+12 Z= 1.625169592431D+13
I= 2 X= 5.432022909947D+12 Y= 5.411997184579D+12 Z= 8.120824322153D+12
I= 3 X= 1.049262701984D+13 Y= -8.831423647848D+12 Z= 4.564266076969D+12
I= 4 X= -3.061378634638D+12 Y= 1.352265955289D+13 Z= -1.289354498003D+13
I= 5 X= 1.235145317805D+13 Y= 2.603913478459D+13 Z= -4.778495320064D+12
I= 6 X= -1.782280542225D+13 Y= -2.807661235675D+13 Z= -8.264335234396D+13
I= 7 X= -5.486510064483D+13 Y= 5.098914896469D+12 Z= 2.725264493800D+13
I= 8 X= 8.753591683445D+13 Y= -7.454109568790D+13 Z= -4.167333831881D+13
I= 9 X= -4.904232425534D+12 Y= 2.805973931696D+12 Z= 6.720066032657D+12
I= 10 X= 8.010892542540D+13 Y= -1.694215909038D+13 Z= -3.224449443589D+13
I= 11 X= 1.318411727066D+13 Y= -6.238464158256D+13 Z= -4.406553607876D+13
I= 12 X= -2.910654220702D+13 Y= 6.269011460261D+12 Z= -5.389709122004D+13
I= 13 X= 1.150602651984D+13 Y= -7.115362146275D+12 Z= -3.472893903536D+13
I= 14 X= -3.295556867006D+13 Y= -3.196555265155D+13 Z= 5.712439325374D+13
I= 15 X= 3.905237927747D+12 Y= 4.777206956874D+13 Z= 1.259730806606D+14
I= 16 X= 5.876340816588D+13 Y= -4.411423288346D+13 Z= 1.605301764715D+13

I= 17 X= -1.614477692075D+13 Y= -8.342477347499D+12 Z= -2.463319422874D+13
I= 18 X= 9.875816598141D+13 Y= 4.403455831630D+13 Z= 3.221430958110D+13
I= 19 X= 2.360368667786D+13 Y= -2.254202966179D+13 Z= 6.394111811567D+13
I= 20 X= 3.019621604449D+13 Y= -6.225126907601D+13 Z= -3.078250189095D+13
I= 21 X= 6.872442105453D+12 Y= -2.079787215530D+13 Z= -3.416144996314D+12
I= 22 X= 3.339073094086D+13 Y= 5.805947503589D+13 Z= -7.294764360204D+13
I= 23 X= -6.559671356253D+13 Y= -2.041394024651D+13 Z= 8.846349685374D+13
I= 24 X= -4.958956906455D+13 Y= 9.716782434741D+13 Z= 2.131181073651D+13
I= 25 X= 4.504872419080D+12 Y= 1.017119321595D+12 Z= 1.076974753878D+13
I= 26 X= -5.326181957100D+13 Y= 1.332055516473D+13 Z= -6.086535255936D+13
I= 27 X= -1.434426677603D+14 Y= 8.822764352760D+13 Z= -8.083896914474D+13
I= 28 X= 6.567220511977D+13 Y= -1.220140362375D+14 Z= 2.166703379663D+13
I= 29 X= -1.170531128683D+13 Y= -6.504422961710D+12 Z= -1.868419825387D+13
I= 30 X= -9.149609973894D+12 Y= 8.229097503373D+12 Z= 1.456708588758D+13
I= 31 X= -9.900300770970D+12 Y= -1.253434299407D+14 Z= 2.058596029309D+13
I= 32 X= 9.063591531430D+13 Y= 7.712665782042D+13 Z= -6.373840491761D+13
I= 33 X= 2.647850050852D+13 Y= 5.109017791153D+13 Z= 8.717585600190D+13
I= 34 X= 5.628449061783D+12 Y= 3.833351820064D+12 Z= -3.334947547570D+13
I= 35 X= -2.117297844454D+12 Y= 1.757724902747D+12 Z= 1.645820751333D+12
I= 36 X= -8.721748387226D+12 Y= -4.857233852946D+12 Z= -5.178839432782D+12
I= 37 X= 1.766229703354D+13 Y= 4.556450282880D+13 Z= 3.574753023954D+13
I= 38 X= -1.906175934615D+13 Y= 1.401078492669D+14 Z= 7.759853212627D+13

Backward Direction:

Total Energy: -656.4400323 Hartrees

Potential Energy: -656.6314769 Hartress

Kinetic Energy: 0.1914446 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.799715356831D+13 Y= -2.014810776817D+13 Z= 2.281222348077D+13

I= 1 X= -1.155109041876D+13 Y= -2.617085739913D+12 Z= 1.561167772469D+13

I= 2 X= 4.976242128899D+12 Y= 5.830960587304D+12 Z= 7.446275510185D+12

I= 3 X= 9.558755752308D+12 Y= -8.809587083717D+12 Z= 3.211182607074D+12
I= 4 X= -1.464095386288D+12 Y= 1.338015285740D+13 Z= -1.395496538519D+13
I= 5 X= 9.715292157313D+12 Y= 2.229022564217D+13 Z= -1.226324902850D+13
I= 6 X= 4.122676021570D+13 Y= 3.933555737635D+13 Z= -5.607490411057D+13
I= 7 X= -4.407969562790D+13 Y= 1.531039923777D+13 Z= 2.791249364748D+13
I= 8 X= 1.011574382649D+14 Y= -6.353055958783D+13 Z= -4.040609036747D+13
I= 9 X= -4.396569058635D+12 Y= 3.044382187603D+12 Z= 6.146239357854D+12
I= 10 X= 8.020177298702D+13 Y= -1.576228587248D+13 Z= -3.361221202994D+13
I= 11 X= 1.303749403859D+13 Y= -6.239753945825D+13 Z= -4.409404762731D+13
I= 12 X= -2.880901580843D+13 Y= 6.348700357909D+12 Z= -5.417962280927D+13
I= 13 X= 1.160666337775D+13 Y= -7.164328188824D+12 Z= -3.494074876768D+13
I= 14 X= -3.278447886455D+13 Y= -3.226721478953D+13 Z= 5.716916997831D+13
I= 15 X= 4.219873095661D+12 Y= 4.748349475389D+13 Z= 1.254520679201D+14
I= 16 X= 5.874149078362D+13 Y= -4.402148466867D+13 Z= 1.612637111741D+13
I= 17 X= -1.599066292543D+13 Y= -8.682584001743D+12 Z= -2.466687467217D+13
I= 18 X= 9.879066014028D+13 Y= 4.349233807914D+13 Z= 3.176950444345D+13
I= 19 X= 2.327789277766D+13 Y= -2.265055965943D+13 Z= 6.427706243968D+13
I= 20 X= 3.042245705556D+13 Y= -6.255516607030D+13 Z= -3.082131005366D+13
I= 21 X= 6.678517667301D+12 Y= -2.091969981802D+13 Z= -3.889544084087D+12
I= 22 X= 3.335607506695D+13 Y= 5.860543827955D+13 Z= -7.484485596156D+13
I= 23 X= -6.489181879199D+13 Y= -2.072077339072D+13 Z= 8.824350588891D+13
I= 24 X= -4.992938796456D+13 Y= 9.697696803545D+13 Z= 2.075207023114D+13
I= 25 X= 4.294115471145D+12 Y= 8.042107355906D+11 Z= 1.066099118084D+13
I= 26 X= -5.378311385671D+13 Y= 1.275029949776D+13 Z= -6.092895736906D+13
I= 27 X= -1.430082082580D+14 Y= 8.859342315692D+13 Z= -8.096505780906D+13
I= 28 X= 6.569373373909D+13 Y= -1.226593128628D+14 Z= 2.212378789019D+13
I= 29 X= -1.268135232150D+13 Y= -6.230260638830D+12 Z= -1.902653118444D+13
I= 30 X= -9.092131793378D+12 Y= 8.040208919566D+12 Z= 1.414313154229D+13
I= 31 X= -1.057510552605D+13 Y= -1.255430675218D+14 Z= 2.060704555977D+13
I= 32 X= 8.866105560414D+13 Y= 7.876665875473D+13 Z= -6.491417650901D+13

I= 33 X= 2.653940553002D+13 Y= 5.085147059992D+13 Z= 8.683817482472D+13
I= 34 X= 6.264714173628D+12 Y= 3.390367445260D+12 Z= -3.347125128096D+13
I= 35 X= -2.127916081644D+12 Y= 2.005734046932D+12 Z= 3.219285984299D+12
I= 36 X= -1.215323042242D+13 Y= -9.191478412586D+12 Z= -6.760514779598D+12
I= 37 X= 2.072349661285D+13 Y= 4.711856570819D+13 Z= 3.192972446107D+13
I= 38 X= -1.738532770210D+13 Y= 1.399331620274D+14 Z= 7.474730159110D+13

Seed: 22676000783

CM Start Point Coordinates: bohr

I= 0 X= -2.354196934760D+00 Y= 2.413098466383D+00 Z= -5.003039887492D-01
I= 1 X= -2.622744366639D+00 Y= 2.523044007125D-02 Z= -2.039016958940D+00
I= 2 X= -2.142508122030D+00 Y= 1.658456168879D+00 Z= 2.066709993443D+00
I= 3 X= -2.563875572977D+00 Y= -1.980244319109D+00 Z= -2.555569442641D-01
I= 4 X= -2.084371758393D+00 Y= -9.464919987094D-01 Z= 2.341095590165D+00
I= 5 X= 4.075399682154D+00 Y= 2.604096573728D+00 Z= -1.301034617842D+00
I= 6 X= 2.408240869417D+00 Y= 3.681804710413D-01 Z= -3.261222173846D+00
I= 7 X= 5.783849355033D+00 Y= 1.925958936781D+00 Z= -1.653621255849D+00
I= 8 X= 3.161609536208D+00 Y= 4.157647013499D+00 Z= -2.411507505067D+00
I= 9 X= -1.921744440601D+00 Y= -2.473846132936D+00 Z= 4.750830200973D+00
I= 10 X= -3.920759736735D+00 Y= -2.881729170338D+00 Z= 5.556873768687D+00
I= 11 X= -9.112206204248D-01 Y= -4.624342272353D+00 Z= 4.589931449416D+00
I= 12 X= -5.910683133193D-01 Y= -1.362128363790D+00 Z= 5.881116461364D+00
I= 13 X= -1.755123961283D+00 Y= 3.649072997561D+00 Z= 4.257918051532D+00
I= 14 X= -3.612848952997D+00 Y= 3.367021349161D+00 Z= 5.245538787108D+00
I= 15 X= -2.185275086906D-01 Y= 2.893302720473D+00 Z= 5.435322103219D+00
I= 16 X= -1.253766100561D+00 Y= 5.363821336850D+00 Z= 3.710984703388D+00
I= 17 X= -2.342471348673D+00 Y= 5.054510669058D+00 Z= -1.810717920801D+00
I= 18 X= -4.093869122285D+00 Y= 6.030026632143D+00 Z= -1.353410096686D+00
I= 19 X= -4.755438259813D-01 Y= 6.127621954817D+00 Z= -1.095889165175D+00
I= 20 X= -1.783197003842D+00 Y= 4.595518061793D+00 Z= -3.660525288913D+00

I= 21 X= -3.226012616220D+00 Y= -2.229104473922D-01 Z= -4.778623643623D+00
I= 22 X= -5.102495599521D+00 Y= -1.425909655109D-01 Z= -4.959207357595D+00
I= 23 X= -2.155156965162D+00 Y= 9.374590668466D-01 Z= -6.083684388151D+00
I= 24 X= -3.294774453282D+00 Y= -2.546603945420D+00 Z= -5.471105166171D+00
I= 25 X= -2.708548560016D+00 Y= -4.714159946921D+00 Z= -7.030614676257D-01
I= 26 X= -3.415256747291D+00 Y= -5.015461096540D+00 Z= -2.721483443876D+00
I= 27 X= -8.369678405754D-01 Y= -5.846306959960D+00 Z= -7.045395273986D-02
I= 28 X= -4.147628590758D+00 Y= -5.240413460323D+00 Z= 8.532159131082D-01
I= 29 X= 2.587701100786D+00 Y= -3.859836049327D+00 Z= -1.651456530325D+00
I= 30 X= 3.463181888714D+00 Y= -3.488755855504D+00 Z= 8.955545972246D-01
I= 31 X= 1.066426582812D+00 Y= -4.992386054375D+00 Z= -2.282980999511D+00
I= 32 X= 4.159769262980D+00 Y= -3.232477577122D+00 Z= -2.996770859344D+00
I= 33 X= 5.358762374164D+00 Y= -2.981591850829D+00 Z= 1.177694531348D+00
I= 34 X= 2.574546287276D+00 Y= -4.629442139898D+00 Z= 2.533944598105D+00
I= 35 X= 1.163089235001D+00 Y= -2.001391081006D-02 Z= -3.215938635360D-01
I= 36 X= 3.895996086973D+00 Y= 2.626086332552D+00 Z= 1.318457220791D+00
I= 37 X= 5.184411039308D+00 Y= 1.422166803015D+00 Z= 2.528223403982D+00
I= 38 X= 2.845416300353D+00 Y= 4.250683015548D+00 Z= 2.497485311660D+00

Forward Direction:

Total Energy: -656.4375491 Hartrees

Potential Energy: -656.6160054 Hartress

Kinetic Energy: 0.1784564 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.141387224845D+11 Y= -2.367524790242D+13 Z= 6.036877193077D+12
I= 1 X= 1.327099881124D+13 Y= 5.895513831896D+12 Z= -7.248102119250D+12
I= 2 X= 1.483881794733D+13 Y= 3.694155767085D+11 Z= -3.978945465638D+13
I= 3 X= -9.991561126140D+12 Y= -1.897390395301D+13 Z= -9.329953526073D+12
I= 4 X= -7.014826512558D+12 Y= 1.953975742581D+13 Z= -3.167865088171D+12
I= 5 X= -9.564425608072D+12 Y= 4.503304536949D+12 Z= 2.134709060672D+13
I= 6 X= 1.929203585154D+13 Y= -3.535363321033D+13 Z= -1.638937127977D+13

I= 7 X= 7.326131716602D+13 Y= 2.872225379565D+13 Z= -6.817857419897D+13
I= 8 X= 4.580634787739D+12 Y= -6.631421316760D+13 Z= -7.876912198464D+13
I= 9 X= 2.751989332153D+12 Y= -3.402619478989D+13 Z= -1.345778658673D+11
I= 10 X= -6.981292295316D+12 Y= 5.647362036463D+13 Z= 1.740963341809D+13
I= 11 X= -1.190568265717D+13 Y= 4.365605973539D+12 Z= -3.973059913356D+13
I= 12 X= -1.037771274730D+14 Y= -1.647731465707D+13 Z= -4.735782832991D+13
I= 13 X= 9.434936477796D+12 Y= 8.100866971709D+12 Z= -1.435608175490D+12
I= 14 X= -2.322666814477D+13 Y= -2.241145719954D+13 Z= 6.217618756376D+13
I= 15 X= -4.807231012886D+13 Y= 1.758819955509D+13 Z= -4.595763751448D+13
I= 16 X= -2.052622369363D+13 Y= -1.459349329656D+14 Z= 3.634036170514D+13
I= 17 X= -1.087886231585D+13 Y= 1.542017183273D+12 Z= -2.222308227967D+13
I= 18 X= 1.380366944287D+14 Y= 1.346482823645D+13 Z= -1.601026795447D+13
I= 19 X= 5.862321649518D+13 Y= 4.705042162122D+13 Z= 3.130738800616D+13
I= 20 X= 2.261079048687D+13 Y= -3.999612420169D+13 Z= 7.398661367803D+13
I= 21 X= 1.311977703563D+13 Y= 1.983743188022D+13 Z= 2.598708944041D+13
I= 22 X= -3.230250431025D+13 Y= 1.794097657351D+13 Z= -5.697719262032D+12
I= 23 X= 3.697900649609D+13 Y= 5.025244524466D+13 Z= -1.737854198232D+14
I= 24 X= -2.325653374484D+13 Y= -1.039309029269D+13 Z= 1.320498754377D+13
I= 25 X= -1.354130279816D+13 Y= 8.760982728532D+12 Z= 1.173321371432D+13
I= 26 X= 2.932461131791D+13 Y= 3.083094255163D+13 Z= 7.910414005542D+12
I= 27 X= 3.744858583409D+13 Y= 4.556730384167D+13 Z= -4.712332034400D+13
I= 28 X= 4.157168483085D+13 Y= 2.932677265392D+13 Z= -4.573203344492D+12
I= 29 X= 8.017323067028D+12 Y= -2.933546074508D+12 Z= 2.294459294129D+13
I= 30 X= -2.352873166757D+13 Y= -6.632546468664D+12 Z= 6.511690833601D+12
I= 31 X= -6.444696355998D+13 Y= -6.746633107461D+12 Z= 3.725223215191D+13
I= 32 X= 7.905400287371D+13 Y= 2.917418207353D+13 Z= -1.444647652260D+14
I= 33 X= 4.550010443856D+13 Y= 4.379706044824D+13 Z= -6.429088686417D+13
I= 34 X= 1.485534591666D+13 Y= 3.484056621358D+13 Z= -1.097642883488D+14
I= 35 X= -2.268346724045D+11 Y= 1.424725953001D+12 Z= 2.948512379664D+12
I= 36 X= -1.474529817128D+13 Y= -1.597702683114D+12 Z= 1.037046936006D+13

I= 37 X= 4.180427994448D+13 Y= 1.619409243403D+13 Z= -3.250965685164D+13

I= 38 X= 4.235465742081D+13 Y= -3.775372307677D+13 Z= 5.673873233527D+13

Backward Direction:

Total Energy: -656.4375276 Hartrees

Potential Energy: -656.6160054 Hartress

Kinetic Energy: 0.1784778 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.001110946638D+11 Y= -2.382415144787D+13 Z= 6.095147099586D+12

I= 1 X= 1.309512516688D+13 Y= 5.512609037541D+12 Z= -7.477960938160D+12

I= 2 X= 1.467512692746D+13 Y= 5.198838500132D+11 Z= -4.003171494359D+13

I= 3 X= -1.032695556702D+13 Y= -1.896606147855D+13 Z= -9.815905594460D+12

I= 4 X= -6.441171510994D+12 Y= 1.948857697444D+13 Z= -3.549068061544D+12

I= 5 X= -1.051118752583D+13 Y= 3.156905592698D+12 Z= 1.865898478748D+13

I= 6 X= 4.049934436117D+13 Y= -1.114294401317D+13 Z= -6.847467419345D+12

I= 7 X= 7.713483273128D+13 Y= 3.238964908108D+13 Z= -6.794159336753D+13

I= 8 X= 9.472725092040D+12 Y= -6.235984308414D+13 Z= -7.831399724447D+13

I= 9 X= 2.934313681987D+12 Y= -3.394057184692D+13 Z= -3.406643825849D+11

I= 10 X= -6.947946633648D+12 Y= 5.689736497384D+13 Z= 1.691842558841D+13

I= 11 X= -1.195834152785D+13 Y= 4.360973761647D+12 Z= -3.974083889392D+13

I= 12 X= -1.036702726110D+14 Y= -1.644869485882D+13 Z= -4.745929792364D+13

I= 13 X= 9.471079619051D+12 Y= 8.083281102575D+12 Z= -1.511678410319D+12

I= 14 X= -2.316522223757D+13 Y= -2.251979740559D+13 Z= 6.219226886697D+13

I= 15 X= -4.795931073414D+13 Y= 1.748455958313D+13 Z= -4.614475621611D+13

I= 16 X= -2.053409519284D+13 Y= -1.459016229783D+14 Z= 3.636670617674D+13

I= 17 X= -1.082351317025D+13 Y= 1.419869854473D+12 Z= -2.223517841524D+13

I= 18 X= 1.380483645178D+14 Y= 1.327009298806D+13 Z= -1.617001713137D+13

I= 19 X= 5.850620951829D+13 Y= 4.701144370733D+13 Z= 3.142804045797D+13

I= 20 X= 2.269204362090D+13 Y= -4.010526704014D+13 Z= 7.397267596209D+13

I= 21 X= 1.305013020111D+13 Y= 1.979367818270D+13 Z= 2.581707090820D+13

I= 22 X= -3.231495076485D+13 Y= 1.813705611159D+13 Z= -6.379092061932D+12

I= 23 X= 3.723216536691D+13 Y= 5.014224790117D+13 Z= -1.738644283013D+14
I= 24 X= -2.337857773681D+13 Y= -1.046163523105D+13 Z= 1.300395999562D+13
I= 25 X= -1.361699492978D+13 Y= 8.684517844891D+12 Z= 1.169415450264D+13
I= 26 X= 2.913739150617D+13 Y= 3.062613853756D+13 Z= 7.887570691724D+12
I= 27 X= 3.760461943741D+13 Y= 4.569867147930D+13 Z= -4.716860436338D+13
I= 28 X= 4.157941671342D+13 Y= 2.909502530053D+13 Z= -4.409162761945D+12
I= 29 X= 7.666783598021D+12 Y= -2.835082268311D+12 Z= 2.282164605684D+13
I= 30 X= -2.350808871499D+13 Y= -6.700384706471D+12 Z= 6.359430091584D+12
I= 31 X= -6.468931576620D+13 Y= -6.818331782044D+12 Z= 3.725980480313D+13
I= 32 X= 7.834474347657D+13 Y= 2.976317888416D+13 Z= -1.448870367597D+14
I= 33 X= 4.552197812910D+13 Y= 4.371133010594D+13 Z= -6.441216309286D+13
I= 34 X= 1.508385682857D+13 Y= 3.468147094299D+13 Z= -1.098080234154D+14
I= 35 X= -2.306481506725D+11 Y= 1.513796996503D+12 Z= 3.513613278548D+12
I= 36 X= -1.597769501258D+13 Y= -3.154321440816D+12 Z= 9.802419845966D+12
I= 37 X= 4.290369199213D+13 Y= 1.675222508841D+13 Z= -3.388079961999D+13
I= 38 X= 4.295673810788D+13 Y= -3.781646098556D+13 Z= 5.571472944722D+13

Seed: 23239193623

CM Start Point Coordinates: bohr

I= 0 X= -2.428232309649D+00 Y= 2.269192768021D+00 Z= -5.495460774464D-01
I= 1 X= -2.970092217797D+00 Y= -1.858580947634D-02 Z= -1.897787449033D+00
I= 2 X= -2.116087560224D+00 Y= 1.745035066561D+00 Z= 2.170663371156D+00
I= 3 X= -2.624361751457D+00 Y= -2.147467448882D+00 Z= -1.289592591219D-01
I= 4 X= -2.111354365558D+00 Y= -8.763252395633D-01 Z= 2.468447709838D+00
I= 5 X= 4.705344750317D+00 Y= 2.487973003027D+00 Z= -1.163395907189D+00
I= 6 X= 2.316535968487D+00 Y= 9.329693227286D-01 Z= -3.297592303774D+00
I= 7 X= 6.267525344683D+00 Y= 1.051403320567D+00 Z= -1.778526026890D+00
I= 8 X= 4.571621952111D+00 Y= 4.242496325916D+00 Z= -2.508045179704D+00
I= 9 X= -2.236012899056D+00 Y= -2.477714987119D+00 Z= 4.673375513781D+00
I= 10 X= -4.285194451025D+00 Y= -3.249307096423D+00 Z= 5.004234286624D+00

I= 11 X= -1.187423062220D+00 Y= -4.114762730429D+00 Z= 4.464330874115D+00
I= 12 X= -1.744317262919D+00 Y= -1.482666419769D+00 Z= 6.544001907771D+00
I= 13 X= -1.949931998969D+00 Y= 3.522785700496D+00 Z= 4.263771068680D+00
I= 14 X= -3.659688239343D+00 Y= 2.923004054761D+00 Z= 5.902649429537D+00
I= 15 X= 1.894541474950D-01 Y= 3.334422959671D+00 Z= 5.296200241932D+00
I= 16 X= -2.497059756873D+00 Y= 5.879562068383D+00 Z= 3.423709543083D+00
I= 17 X= -2.061691998552D+00 Y= 4.756698290890D+00 Z= -1.683070209735D+00
I= 18 X= -3.953811845261D+00 Y= 6.190537758201D+00 Z= -1.491492965880D+00
I= 19 X= -6.499544032189D-01 Y= 5.985574819740D+00 Z= -9.852023456794D-01
I= 20 X= -1.913265493834D+00 Y= 4.458408184028D+00 Z= -3.891096213690D+00
I= 21 X= -3.749892545058D+00 Y= 8.957931891896D-03 Z= -4.709387083968D+00
I= 22 X= -6.021042206914D+00 Y= 6.009507098417D-01 Z= -4.489302562953D+00
I= 23 X= -2.481077619766D+00 Y= 1.494888781430D+00 Z= -5.799190353760D+00
I= 24 X= -3.631634004263D+00 Y= -1.866910969789D+00 Z= -5.554971049750D+00
I= 25 X= -3.058492061727D+00 Y= -4.859449638666D+00 Z= -5.677822709635D-01
I= 26 X= -3.405168737161D+00 Y= -5.198073481153D+00 Z= -2.686403399133D+00
I= 27 X= -1.156162951282D+00 Y= -5.685081063832D+00 Z= -1.542159035675D-01
I= 28 X= -4.731050397407D+00 Y= -5.756024294069D+00 Z= 8.289821817037D-01
I= 29 X= 3.211055846619D+00 Y= -3.687078344393D+00 Z= -1.524815216526D+00
I= 30 X= 3.676313195919D+00 Y= -3.129664933523D+00 Z= 1.027237398404D+00
I= 31 X= 1.871900694421D+00 Y= -4.660173767132D+00 Z= -2.203912564971D+00
I= 32 X= 4.924690187713D+00 Y= -3.138053235505D+00 Z= -2.652486934604D+00
I= 33 X= 5.637869797662D+00 Y= -2.423493394854D+00 Z= 1.391199727368D+00
I= 34 X= 2.687521637957D+00 Y= -4.290426725266D+00 Z= 2.505726530755D+00
I= 35 X= 1.198077301292D+00 Y= -1.962056262763D-02 Z= -4.520675150063D-01
I= 36 X= 3.820638013956D+00 Y= 2.507741770561D+00 Z= 1.317735073861D+00
I= 37 X= 5.112217419424D+00 Y= 1.267610026914D+00 Z= 2.396909646010D+00
I= 38 X= 3.198699408917D+00 Y= 4.290853511769D+00 Z= 1.879783736842D+00

Forward Direction:

Total Energy: -656.4361271 Hartrees

Potential Energy: -656.5952592 Hartress

Kinetic Energy: 0.1591321 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.187916816717D+13 Y= 7.335098033131D+12 Z= 2.362042254132D+12
I= 1 X= 2.479298763835D+12 Y= -1.114879184375D+13 Z= -7.374116171194D+12
I= 2 X= -1.085824937634D+12 Y= -1.258715032342D+13 Z= -1.988347709696D+13
I= 3 X= -1.460772925090D+13 Y= 3.410437149964D+12 Z= -7.544898442247D+12
I= 4 X= 1.568003381748D+13 Y= -2.639242699465D+13 Z= 1.827510308489D+13
I= 5 X= 1.962196789862D+12 Y= 2.910483560431D+12 Z= -7.091926808667D+12
I= 6 X= 1.653178596013D+13 Y= -2.927287918721D+13 Z= -7.896788941720D+13
I= 7 X= 7.056098678893D+13 Y= -9.006507411046D+13 Z= -1.401300166182D+13
I= 8 X= 2.504645239867D+13 Y= -3.102151202245D+13 Z= 1.074121897091D+14
I= 9 X= -1.032412153175D+13 Y= 1.670746262697D+13 Z= -1.685781282095D+13
I= 10 X= -4.228333335809D+13 Y= -2.198639858594D+13 Z= 1.323048750928D+14
I= 11 X= 2.522819219217D+12 Y= 7.483213245464D+13 Z= -5.823103920456D+13
I= 12 X= -1.727643026692D+13 Y= -4.471263073002D+13 Z= 5.639701745693D+13
I= 13 X= -1.224679381919D+13 Y= 2.873449201732D+12 Z= 1.734373705279D+13
I= 14 X= -2.918489597796D+13 Y= -1.826031907024D+13 Z= 2.251460538193D+13
I= 15 X= -4.692289207654D+13 Y= -3.127571789626D+13 Z= 5.004293325809D+13
I= 16 X= 4.311447164552D+13 Y= 1.492686806693D+14 Z= -5.808550072655D+13
I= 17 X= 7.072439700375D+12 Y= 1.199307686735D+13 Z= 2.999959538280D+13
I= 18 X= 5.517893611764D+13 Y= 2.358051590575D+13 Z= -1.730011760563D+13
I= 19 X= -2.787607085712D+13 Y= 2.508827174512D+13 Z= -1.046789403695D+14
I= 20 X= 6.570292643532D+13 Y= 4.913460803891D+13 Z= -4.235252336712D+13
I= 21 X= -1.008748925898D+13 Y= -4.173945734947D+12 Z= -3.881440153695D+12
I= 22 X= 4.620520732452D+13 Y= 4.138308160390D+13 Z= 1.565056057655D+13
I= 23 X= 2.105942047959D+13 Y= 8.016090268064D+12 Z= -4.768703037382D+12
I= 24 X= 7.529504989820D+13 Y= -6.726880809498D+13 Z= -8.429521391261D+12
I= 25 X= 4.230294624751D+12 Y= 6.702256864868D+12 Z= -5.522855068153D+12
I= 26 X= 2.346457217399D+13 Y= -2.995389378061D+12 Z= 2.474555425536D+13

I= 27 X= -7.929071631016D+13 Y= 1.000747099168D+13 Z= 6.409060238981D+13
I= 28 X= -4.844579890759D+13 Y= -7.436483894340D+13 Z= 2.171891875799D+13
I= 29 X= 8.674249696519D+12 Y= -2.923157107378D+12 Z= 2.165504175107D+11
I= 30 X= 2.255709526491D+13 Y= -5.078020216433D+12 Z= 2.136150131143D+13
I= 31 X= -7.661731028040D+13 Y= -7.908603929452D+13 Z= -1.153013524488D+14
I= 32 X= 1.883283528806D+12 Y= 3.373259267902D+13 Z= -6.408247014633D+13
I= 33 X= -4.366912191341D+12 Y= -8.490953023072D+12 Z= -4.503476428783D+13
I= 34 X= -6.618663712551D+12 Y= -5.258356075387D+13 Z= -2.329479268334D+13
I= 35 X= 6.967784103920D+11 Y= 2.678252302626D+12 Z= -1.565246011816D+12
I= 36 X= -1.147481971742D+13 Y= 2.378399327955D+12 Z= -1.601531249896D+12
I= 37 X= 7.906359003514D+13 Y= -4.118821650415D+13 Z= 3.713081539956D+13
I= 38 X= -1.101307838908D+14 Y= -7.670092211713D+11 Z= 2.659244564423D+13

Backward Direction:

Total Energy: -656.4361129 Hartrees

Potential Energy: -656.5952592 Hartress

Kinetic Energy: 0.1591464 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.201021609756D+13 Y= 7.163968439653D+12 Z= 2.429009802676D+12
I= 1 X= 2.277173387159D+12 Y= -1.158885081900D+13 Z= -7.638284805037D+12
I= 2 X= -1.273949254443D+12 Y= -1.241422244474D+13 Z= -2.016189830084D+13
I= 3 X= -1.499318625260D+13 Y= 3.419450230507D+12 Z= -8.103386015695D+12
I= 4 X= 1.633931527794D+13 Y= -2.645124688281D+13 Z= 1.783699995215D+13
I= 5 X= 8.741167083026D+11 Y= 1.363114740359D+12 Z= -1.018127202130D+13
I= 6 X= 4.090459767241D+13 Y= -1.448387974552D+12 Z= -6.800171584230D+13
I= 7 X= 7.501268161358D+13 Y= -8.585026605255D+13 Z= -1.374064794968D+13
I= 8 X= 3.066875924586D+13 Y= -2.647689395006D+13 Z= 1.079352485202D+14
I= 9 X= -1.011458258649D+13 Y= 1.680586605353D+13 Z= -1.709466078640D+13
I= 10 X= -4.224501036472D+13 Y= -2.149940384934D+13 Z= 1.317403472612D+14
I= 11 X= 2.462300226044D+12 Y= 7.482680882812D+13 Z= -5.824280739610D+13
I= 12 X= -1.715362572925D+13 Y= -4.467973900330D+13 Z= 5.628040204115D+13

I= 13 X= -1.220525578126D+13 Y= 2.853238381255D+12 Z= 1.725631221548D+13
I= 14 X= -2.911427836294D+13 Y= -1.838483065077D+13 Z= 2.253308705750D+13
I= 15 X= -4.679302585844D+13 Y= -3.139482765703D+13 Z= 4.982788433303D+13
I= 16 X= 4.310542520614D+13 Y= 1.493069626579D+14 Z= -5.805522395238D+13
I= 17 X= 7.136050523165D+12 Y= 1.185269724962D+13 Z= 2.998569372028D+13
I= 18 X= 5.519234814086D+13 Y= 2.335671355262D+13 Z= -1.748371170762D+13
I= 19 X= -2.801054285625D+13 Y= 2.504347580073D+13 Z= -1.045402787588D+14
I= 20 X= 6.579630780880D+13 Y= 4.900917402265D+13 Z= -4.236854149793D+13
I= 21 X= -1.016753190951D+13 Y= -4.224230315933D+12 Z= -4.076836457130D+12
I= 22 X= 4.619090305337D+13 Y= 4.160842889389D+13 Z= 1.486748284819D+13
I= 23 X= 2.135036703504D+13 Y= 7.889444350988D+12 Z= -4.859504693417D+12
I= 24 X= 7.515478904972D+13 Y= -6.734758437247D+13 Z= -8.660555265584D+12
I= 25 X= 4.143304325812D+12 Y= 6.614378472394D+12 Z= -5.567744443490D+12
I= 26 X= 2.324940704664D+13 Y= -3.230763404910D+12 Z= 2.471930125248D+13
I= 27 X= -7.911139238754D+13 Y= 1.015844717977D+13 Z= 6.403855907147D+13
I= 28 X= -4.843691292529D+13 Y= -7.463117800490D+13 Z= 2.190744481237D+13
I= 29 X= 8.271387047556D+12 Y= -2.809996128251D+12 Z= 7.525189980314D+10
I= 30 X= 2.258081948287D+13 Y= -5.155984310999D+12 Z= 2.118651341160D+13
I= 31 X= -7.689583712557D+13 Y= -7.916844005533D+13 Z= -1.152926494677D+14
I= 32 X= 1.068156720078D+12 Y= 3.440950593921D+13 Z= -6.456777193092D+13
I= 33 X= -4.341773534463D+12 Y= -8.589479884195D+12 Z= -4.517414278406D+13
I= 34 X= -6.356044176134D+12 Y= -5.276640333436D+13 Z= -2.334505585785D+13
I= 35 X= 6.923957143181D+11 Y= 2.780618511633D+12 Z= -9.157954789973D+11
I= 36 X= -1.289116994256D+13 Y= 5.894322907247D+11 Z= -2.254370522796D+12
I= 37 X= 8.032710552424D+13 Y= -4.054677432573D+13 Z= 3.555500937303D+13
I= 38 X= -1.094388337934D+14 Y= -8.391116846853D+11 Z= 2.541559524050D+13

Seed: 23251358091

CM Start Point Coordinates: bohr

I= 0 X= -2.386299657621D+00 Y= 2.499942732530D+00 Z= -5.773071847309D-01

I= 1 X= -2.708547526818D+00 Y= 1.342190228580D-01 Z= -2.025834527863D+00
I= 2 X= -2.165603745036D+00 Y= 1.704086400102D+00 Z= 2.115227449873D+00
I= 3 X= -2.560080820320D+00 Y= -1.973412277552D+00 Z= -3.835865580358D-01
I= 4 X= -2.132790198368D+00 Y= -8.967273193550D-01 Z= 2.259465383136D+00
I= 5 X= 4.245768213531D+00 Y= 2.195452438761D+00 Z= -1.906566825148D+00
I= 6 X= 2.117320752814D+00 Y= -2.044012943363D-01 Z= -2.974075312841D+00
I= 7 X= 5.933657499640D+00 Y= 1.018089315462D+00 Z= -2.294350539976D+00
I= 8 X= 3.362524422985D+00 Y= 3.449933125703D+00 Z= -3.140655376707D+00
I= 9 X= -1.843804049630D+00 Y= -2.583340200483D+00 Z= 4.677085865248D+00
I= 10 X= -3.710226534229D+00 Y= -3.929760380871D+00 Z= 5.105182995975D+00
I= 11 X= -5.225472040590D-01 Y= -4.408986511487D+00 Z= 3.976662221184D+00
I= 12 X= -1.158639587549D+00 Y= -1.651892728152D+00 Z= 6.253670433882D+00
I= 13 X= -2.064019500102D+00 Y= 3.511719288872D+00 Z= 4.426843680236D+00
I= 14 X= -3.970338365397D+00 Y= 3.458611595774D+00 Z= 5.406848993644D+00
I= 15 X= -4.548166930527D-01 Y= 2.708669421731D+00 Z= 5.671714402469D+00
I= 16 X= -1.266754493238D+00 Y= 5.491007309767D+00 Z= 3.740942897138D+00
I= 17 X= -2.298004732699D+00 Y= 5.038603182947D+00 Z= -1.374800868931D+00
I= 18 X= -4.185629527698D+00 Y= 5.697865436895D+00 Z= -1.467336789768D+00
I= 19 X= -1.106714299926D+00 Y= 6.534624816949D+00 Z= -2.665926578038D-01
I= 20 X= -1.649133903581D+00 Y= 5.529953547921D+00 Z= -3.416063657827D+00
I= 21 X= -3.532883509331D+00 Y= -1.722220717718D-01 Z= -4.698863998653D+00
I= 22 X= -5.467438875169D+00 Y= -2.613503989232D-01 Z= -5.120925934271D+00
I= 23 X= -3.357520499262D+00 Y= 1.834135822316D+00 Z= -5.825955666489D+00
I= 24 X= -2.529871747534D+00 Y= -1.678338784703D+00 Z= -5.788017576117D+00
I= 25 X= -3.210060199453D+00 Y= -4.560805065978D+00 Z= -1.021650787008D+00
I= 26 X= -2.458797160652D+00 Y= -4.910252707118D+00 Z= -3.010611261113D+00
I= 27 X= -2.237910806196D+00 Y= -5.545317152868D+00 Z= 4.415693969328D-01
I= 28 X= -5.203310934131D+00 Y= -4.908200903843D+00 Z= -1.295784323352D+00
I= 29 X= 3.254623470953D+00 Y= -3.762283100593D+00 Z= -1.223939189363D+00
I= 30 X= 3.804056838000D+00 Y= -3.093684212562D+00 Z= 1.356615587564D+00

I= 31 X= 1.943198579916D+00 Y= -5.418181298372D+00 Z= -1.308622157108D+00
I= 32 X= 4.571039893067D+00 Y= -3.679659335004D+00 Z= -2.838607287770D+00
I= 33 X= 5.302994452190D+00 Y= -2.214119291982D+00 Z= 1.907850242256D+00
I= 34 X= 2.674685613255D+00 Y= -3.910971085008D+00 Z= 3.030296261376D+00
I= 35 X= 1.166199399103D+00 Y= -7.101642999338D-02 Z= -2.893775057724D-01
I= 36 X= 4.045157979324D+00 Y= 2.618293488847D+00 Z= 8.313322904181D-01
I= 37 X= 5.225337363987D+00 Y= 1.999651873405D+00 Z= 2.309437813810D+00
I= 38 X= 2.812979096172D+00 Y= 4.393451031719D+00 Z= 1.230950521668D+00

Forward Direction:

Total Energy: -656.4319312 Hartrees

Potential Energy: -656.6442690 Hartress

Kinetic Energy: 0.2123377 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.722577698446D+12 Y= 1.201351969608D+13 Z= -1.613202869869D+13
I= 1 X= -6.340227149379D+12 Y= -1.240809625447D+13 Z= 7.567560413013D+12
I= 2 X= 1.975617637122D+13 Y= -4.159848006884D+12 Z= 2.294977081406D+13
I= 3 X= 1.625679036893D+12 Y= 5.063710732921D+12 Z= 1.422912484831D+13
I= 4 X= -2.015456552617D+13 Y= 3.103194828537D+13 Z= -3.545344162578D+13
I= 5 X= -2.889213737222D+13 Y= -8.005435508176D+12 Z= 2.364300599795D+13
I= 6 X= 2.870229617994D+13 Y= -3.888299691803D+13 Z= -4.779760984183D+13
I= 7 X= -1.272012518765D+13 Y= 1.900212580965D+13 Z= 3.816830848926D+13
I= 8 X= -2.404903678614D+13 Y= 1.579046281128D+14 Z= -2.342325455817D+12
I= 9 X= 1.500436965953D+13 Y= -8.700818968115D+12 Z= -4.238104063473D+12
I= 10 X= 3.906288862424D+13 Y= -2.390536688107D+13 Z= 2.471158027930D+13
I= 11 X= 7.306583681176D+12 Y= 3.725339090509D+13 Z= -1.536018740279D+13
I= 12 X= -6.104967685825D+13 Y= -1.152102370668D+14 Z= -5.345499967252D+13
I= 13 X= 1.324208313571D+13 Y= -1.155618645575D+13 Z= -1.425829857638D+13
I= 14 X= -3.834365598696D+13 Y= -2.891493563171D+13 Z= 6.065202601428D+13
I= 15 X= -1.656059683096D+13 Y= 5.964724057639D+13 Z= -1.551695269923D+13
I= 16 X= 2.481180332924D+13 Y= -2.036768333616D+14 Z= 1.598810184938D+13

I= 17 X= 1.321243046452D+13 Y= -1.791597323082D+13 Z= 1.017036904802D+12
I= 18 X= -1.058706108409D+14 Y= 3.823701874591D+13 Z= 4.842710615523D+13
I= 19 X= 3.877582861550D+13 Y= 1.673537785481D+13 Z= 7.746818908774D+13
I= 20 X= -6.140226293233D+13 Y= -1.409230216368D+13 Z= 3.481945388739D+13
I= 21 X= 2.393423561421D+13 Y= 3.094511506968D+13 Z= 9.551147991746D+11
I= 22 X= 3.628770493023D+13 Y= -2.305456442514D+12 Z= 4.693140091829D+13
I= 23 X= -8.020103631362D+13 Y= -1.338714290956D+14 Z= 3.056422424388D+13
I= 24 X= -8.669227375800D+12 Y= 4.946738729688D+13 Z= 4.030237870947D+13
I= 25 X= -1.819475626710D+13 Y= -1.270836106097D+13 Z= 4.959984214351D+12
I= 26 X= -1.631388281223D+13 Y= -3.824992811837D+13 Z= 8.590228461596D+13
I= 27 X= 9.091158939168D+13 Y= -1.170309270032D+14 Z= 4.636842992458D+13
I= 28 X= -2.326680756002D+13 Y= 3.547437662288D+13 Z= -4.746779860781D+12
I= 29 X= 2.667270769812D+12 Y= 2.156721476514D+12 Z= -1.091777404152D+13
I= 30 X= 1.112210848631D+13 Y= 1.790715384509D+13 Z= 1.309630522309D+12
I= 31 X= 4.749113431342D+13 Y= -6.260446015737D+13 Z= -1.196450003239D+13
I= 32 X= -1.038171446037D+14 Y= -3.479592906868D+13 Z= 7.239259716527D+13
I= 33 X= 2.093699347472D+12 Y= -2.319322166067D+12 Z= -1.196108123392D+14
I= 34 X= -2.718974410736D+13 Y= -3.710500377156D+13 Z= -1.693328758415D+12
I= 35 X= -8.845363192325D+11 Y= 1.977490652563D+12 Z= -2.599409168905D+12
I= 36 X= 1.572575619566D+13 Y= 2.912213990917D+12 Z= 2.820282682964D+12
I= 37 X= -1.144861623371D+14 Y= 1.938413427418D+13 Z= -9.735965984116D+12
I= 38 X= 4.033544878169D+13 Y= -9.848572563286D+13 Z= -5.662443151356D+13

Backward Direction:

Total Energy: -656.4319359 Hartrees

Potential Energy: -656.6442690 Hartress

Kinetic Energy: 0.2123331 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.911422817897D+12 Y= 1.176691535665D+13 Z= -1.603552587954D+13

I= 1 X= -6.631497609955D+12 Y= -1.304223820143D+13 Z= 7.186883229602D+12

I= 2 X= 1.948508197850D+13 Y= -3.910652267468D+12 Z= 2.254855512665D+13

I= 3 X= 1.070220637011D+12 Y= 5.076698928179D+12 Z= 1.342432272566D+13
I= 4 X= -1.920451552803D+13 Y= 3.094718655868D+13 Z= -3.608476512732D+13
I= 5 X= -3.046010271470D+13 Y= -1.023525362653D+13 Z= 1.919114045605D+13
I= 6 X= 6.382445740126D+13 Y= 1.213167519555D+12 Z= -3.199493098709D+13
I= 7 X= -6.305061339585D+12 Y= 2.507582669646D+13 Z= 3.856078068684D+13
I= 8 X= -1.594707589189D+13 Y= 1.644535979459D+14 Z= -1.588577542968D+12
I= 9 X= 1.530632335752D+13 Y= -8.559015838738D+12 Z= -4.579411111941D+12
I= 10 X= 3.911811353711D+13 Y= -2.320358868757D+13 Z= 2.389807390524D+13
I= 11 X= 7.219373476182D+12 Y= 3.724571936429D+13 Z= -1.537714581620D+13
I= 12 X= -6.087271077699D+13 Y= -1.151628388113D+14 Z= -5.362304696511D+13
I= 13 X= 1.330194105232D+13 Y= -1.158531102627D+13 Z= -1.438428113796D+13
I= 14 X= -3.824189328218D+13 Y= -2.909436161754D+13 Z= 6.067865881094D+13
I= 15 X= -1.637345460809D+13 Y= 5.947559882040D+13 Z= -1.582684647933D+13
I= 16 X= 2.479876706065D+13 Y= -2.036216675407D+14 Z= 1.603173185037D+13
I= 17 X= 1.330409611297D+13 Y= -1.811826567131D+13 Z= 9.970040723355D+11
I= 18 X= -1.058512835996D+14 Y= 3.791451093104D+13 Z= 4.816253998183D+13
I= 19 X= 3.858204928704D+13 Y= 1.667082517852D+13 Z= 7.766800581541D+13
I= 20 X= -6.126769678193D+13 Y= -1.427305741686D+13 Z= 3.479637114868D+13
I= 21 X= 2.381889107056D+13 Y= 3.087265304957D+13 Z= 6.735411929407D+11
I= 22 X= 3.626709192542D+13 Y= -1.980722314215D+12 Z= 4.580295572542D+13
I= 23 X= -7.978177111212D+13 Y= -1.340539307439D+14 Z= 3.043337555690D+13
I= 24 X= -8.871348658753D+12 Y= 4.935386764461D+13 Z= 3.996944999199D+13
I= 25 X= -1.832011263762D+13 Y= -1.283499721194D+13 Z= 4.895296891430D+12
I= 26 X= -1.662394406121D+13 Y= -3.858911116747D+13 Z= 8.586445303723D+13
I= 27 X= 9.117000207443D+13 Y= -1.168133645099D+14 Z= 4.629343350260D+13
I= 28 X= -2.325400252466D+13 Y= 3.509057177928D+13 Z= -4.475106555174D+12
I= 29 X= 2.086730163361D+12 Y= 2.319790809963D+12 Z= -1.112139065219D+13
I= 30 X= 1.115629599987D+13 Y= 1.779480457998D+13 Z= 1.057466213905D+12
I= 31 X= 4.708976639079D+13 Y= -6.272320283191D+13 Z= -1.195195870156D+13
I= 32 X= -1.049917737541D+14 Y= -3.382047096633D+13 Z= 7.169325858520D+13

I= 33 X= 2.129925114587D+12 Y= -2.461303170896D+12 Z= -1.198116621276D+14
I= 34 X= -2.681129922657D+13 Y= -3.736848697380D+13 Z= -1.765759935477D+12
I= 35 X= -8.908519537924D+11 Y= 2.125004305729D+12 Z= -1.663525915877D+12
I= 36 X= 1.368474092272D+13 Y= 3.342435255790D+11 Z= 1.879516125296D+12
I= 37 X= -1.126653878092D+14 Y= 2.030847717911D+13 Z= -1.200676321337D+13
I= 38 X= 4.133257554948D+13 Y= -9.858962806382D+13 Z= -5.832031830645D+13

Seed: 25612201332

CM Start Point Coordinates: bohr

I= 0 X= -2.137650388999D+00 Y= 2.394866146625D+00 Z= -4.467868160046D-01
I= 1 X= -2.664937482801D+00 Y= 6.216440409641D-02 Z= -1.973219319812D+00
I= 2 X= -2.113482233894D+00 Y= 1.664660279135D+00 Z= 2.157400596205D+00
I= 3 X= -2.689168274773D+00 Y= -2.008422255650D+00 Z= -3.288069871200D-01
I= 4 X= -2.322823423137D+00 Y= -1.058665672009D+00 Z= 2.184645159482D+00
I= 5 X= 4.215575594314D+00 Y= 2.519484818615D+00 Z= -1.883038781014D+00
I= 6 X= 2.080433762373D+00 Y= 3.285791502116D-01 Z= -3.359619211790D+00
I= 7 X= 5.520708032702D+00 Y= 1.480077466887D+00 Z= -2.715312334026D+00
I= 8 X= 3.222938069606D+00 Y= 4.241564603625D+00 Z= -2.789840998389D+00
I= 9 X= -2.101698731147D+00 Y= -2.665223184667D+00 Z= 4.493478482975D+00
I= 10 X= -4.252666260696D+00 Y= -3.307469242936D+00 Z= 4.793177614563D+00
I= 11 X= -8.740219383875D-01 Y= -4.306807687389D+00 Z= 3.958238908266D+00
I= 12 X= -1.542107156568D+00 Y= -1.598371359481D+00 Z= 6.552125254050D+00
I= 13 X= -1.925900774122D+00 Y= 3.396922426718D+00 Z= 4.474588003868D+00
I= 14 X= -3.873182197894D+00 Y= 3.428100319240D+00 Z= 5.098829807341D+00
I= 15 X= -7.297733682820D-01 Y= 2.440307272157D+00 Z= 5.857269113906D+00
I= 16 X= -1.102520578926D+00 Y= 4.909368487235D+00 Z= 3.898536224880D+00
I= 17 X= -1.900243988069D+00 Y= 5.199577661364D+00 Z= -1.644135677225D+00
I= 18 X= -3.344696561103D+00 Y= 6.580298812543D+00 Z= -5.652951880678D-01
I= 19 X= 2.075524943394D-01 Y= 6.128137720954D+00 Z= -1.238433836706D+00
I= 20 X= -2.232846807760D+00 Y= 4.591983106121D+00 Z= -3.698734236914D+00

I= 21 X= -3.814785965102D+00 Y= -2.093955177121D-01 Z= -4.584700250697D+00
I= 22 X= -5.716211349085D+00 Y= 3.873356825204D-01 Z= -4.517666298644D+00
I= 23 X= -2.881776027461D+00 Y= 1.077797363056D+00 Z= -5.733980139098D+00
I= 24 X= -3.392959740107D+00 Y= -2.310794790486D+00 Z= -5.182923244631D+00
I= 25 X= -3.213046226043D+00 Y= -4.691305681895D+00 Z= -7.938271587029D-01
I= 26 X= -2.163323697310D+00 Y= -5.403927033286D+00 Z= -2.642042548636D+00
I= 27 X= -2.517387681252D+00 Y= -5.859357600126D+00 Z= 6.008473125800D-01
I= 28 X= -5.362080839836D+00 Y= -4.917227430642D+00 Z= -7.774194836130D-01
I= 29 X= 3.666506411622D+00 Y= -3.398675483225D+00 Z= -1.290328526339D+00
I= 30 X= 3.486310566330D+00 Y= -2.969307708225D+00 Z= 1.514966798121D+00
I= 31 X= 2.862116598735D+00 Y= -4.912496843752D+00 Z= -2.404589873814D+00
I= 32 X= 5.580064283545D+00 Y= -2.786866009377D+00 Z= -2.158553896061D+00
I= 33 X= 4.867601511532D+00 Y= -1.733196875852D+00 Z= 2.263486800207D+00
I= 34 X= 2.346504569938D+00 Y= -4.363191220639D+00 Z= 2.691751164240D+00
I= 35 X= 1.133547988378D+00 Y= -9.624847589141D-02 Z= -3.237352333077D-01
I= 36 X= 4.158939922457D+00 Y= 2.582303108703D+00 Z= 7.725812027565D-01
I= 37 X= 5.971615004352D+00 Y= 1.800514155968D+00 Z= 1.648609658826D+00
I= 38 X= 2.989285867528D+00 Y= 4.181677035568D+00 Z= 1.890156169763D+00

Forward Direction:

Total Energy: -656.4342725 Hartrees

Potential Energy: -656.6230598 Hartress

Kinetic Energy: 0.1887873 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.946917975751D+13 Y= 1.477565505191D+12 Z= 2.972561839034D+13
I= 1 X= 1.674846718174D+13 Y= -2.497404454086D+13 Z= 7.773442742247D+12
I= 2 X= -1.722562195329D+13 Y= -1.792314714517D+13 Z= -1.341400457846D+13
I= 3 X= 1.376350179889D+13 Y= -7.031324377803D+12 Z= -1.116111318730D+13
I= 4 X= 6.562693178563D+12 Y= 7.205080147233D+12 Z= 7.001360180704D+12
I= 5 X= -7.254146123421D+12 Y= 4.990859696599D+12 Z= 1.401693148762D+13
I= 6 X= 7.669131424796D+13 Y= -8.753813799745D+13 Z= -5.573557172548D+13

I= 7 X= -1.819892144076D+13 Y= 2.680368406477D+13 Z= -3.443790581646D+13
I= 8 X= -3.264342124292D+12 Y= 1.029444906334D+14 Z= -6.290264174365D+13
I= 9 X= -1.915068530771D+13 Y= -1.467216807240D+12 Z= 2.106215151229D+12
I= 10 X= 1.092814681967D+14 Y= 6.728129862478D+13 Z= -9.295140769644D+13
I= 11 X= 9.253016511765D+12 Y= -5.933626384503D+13 Z= 5.179391136309D+13
I= 12 X= 2.177427276609D+13 Y= -8.727220894473D+12 Z= 3.926025012085D+13
I= 13 X= -2.446127611337D+12 Y= -8.320220151720D+12 Z= 4.815143432449D+12
I= 14 X= 5.535096164748D+13 Y= 5.538531414140D+13 Z= 1.295632095701D+12
I= 15 X= -6.289022427299D+13 Y= -6.452524302025D+13 Z= -1.411269486633D+14
I= 16 X= -1.907705289840D+13 Y= 6.547435320795D+12 Z= 3.599655583155D+13
I= 17 X= 1.316123594179D+10 Y= 9.351658363694D+12 Z= -3.551284835693D+13
I= 18 X= -1.127544585470D+14 Y= 3.719507836760D+13 Z= 3.647952854948D+13
I= 19 X= 8.070026711991D+11 Y= 3.997294879648D+12 Z= -2.199287893090D+12
I= 20 X= -2.262652672402D+11 Y= -9.104635210818D+12 Z= 1.072524431804D+14
I= 21 X= -3.904181584161D+12 Y= -1.845674956194D+13 Z= -7.884259306298D+12
I= 22 X= 1.115374640472D+14 Y= -2.800052191428D+13 Z= -1.659524319757D+13
I= 23 X= -9.473117846801D+13 Y= 8.832701388045D+13 Z= -3.405158030608D+13
I= 24 X= -6.702364064934D+13 Y= -4.630366158702D+13 Z= 8.410865335883D+13
I= 25 X= -2.907536403981D+12 Y= 2.783843153594D+13 Z= 1.717003340373D+13
I= 26 X= 2.859898911242D+13 Y= 1.331482919173D+13 Z= -4.289372139620D+13
I= 27 X= -4.576684491103D+12 Y= -7.132650825026D+13 Z= -2.766762422549D+13
I= 28 X= -8.262401206094D+13 Y= -7.931763117721D+13 Z= 7.744385930579D+13
I= 29 X= -1.268946276115D+13 Y= -5.806092328093D+12 Z= -1.847049638520D+13
I= 30 X= 1.388957002612D+13 Y= 6.241372554439D+10 Z= 3.708193030028D+12
I= 31 X= 1.167213528788D+14 Y= 8.333276743293D+13 Z= 4.752666833784D+13
I= 32 X= -9.715826024719D+11 Y= 2.310358053131D+13 Z= 3.293946558514D+13
I= 33 X= 3.245341606800D+13 Y= 5.952005472264D+13 Z= 9.804189358344D+13
I= 34 X= -5.259138949802D+13 Y= 1.135064392148D+13 Z= 4.076865256941D+13
I= 35 X= -9.350771552583D+11 Y= 3.866028003210D+12 Z= 4.619161205291D+10
I= 36 X= 5.736923457460D+12 Y= -1.188474580085D+13 Z= -8.465544382180D+12

I= 37 X= -7.493595637888D+13 Y= 1.925505600092D+13 Z= -2.239174125593D+13

I= 38 X= 5.926007683736D+11 Y= -3.859180975580D+12 Z= -2.237479764229D+13

Backward Direction:

Total Energy: -656.4342778 Hartrees

Potential Energy: -656.6230598 Hartress

Kinetic Energy: 0.1887819 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.934824921206D+13 Y= 1.319647748447D+12 Z= 2.978741579708D+13

I= 1 X= 1.656194662976D+13 Y= -2.538012933806D+13 Z= 7.529668903258D+12

I= 2 X= -1.739922237587D+13 Y= -1.776356993753D+13 Z= -1.367093063812D+13

I= 3 X= 1.340780350124D+13 Y= -7.023007141715D+12 Z= -1.167648345737D+13

I= 4 X= 7.171075676906D+12 Y= 7.150801371173D+12 Z= 6.597080227936D+12

I= 5 X= -8.258222402901D+12 Y= 3.562953466448D+12 Z= 1.116609513843D+13

I= 6 X= 9.918245486260D+13 Y= -6.186180029044D+13 Z= -4.561602725992D+13

I= 7 X= -1.409091390279D+13 Y= 3.069309337076D+13 Z= -3.418657881838D+13

I= 8 X= 1.923901865075D+12 Y= 1.071382474039D+14 Z= -6.241996500350D+13

I= 9 X= -1.895732354504D+13 Y= -1.376410489353D+12 Z= 1.887652724017D+12

I= 10 X= 1.093168325130D+14 Y= 6.773069556529D+13 Z= -9.347235189424D+13

I= 11 X= 9.197169810238D+12 Y= -5.934117646235D+13 Z= 5.178305171794D+13

I= 12 X= 2.188759634525D+13 Y= -8.696868525703D+12 Z= 3.915263785062D+13

I= 13 X= -2.407796462631D+12 Y= -8.338870622164D+12 Z= 4.734468114382D+12

I= 14 X= 5.541612732538D+13 Y= 5.527041532050D+13 Z= 1.312686917621D+12

I= 15 X= -6.277038420461D+13 Y= -6.463515706786D+13 Z= -1.413253950185D+14

I= 16 X= -1.908540091457D+13 Y= 6.582761796498D+12 Z= 3.602449512771D+13

I= 17 X= 7.186106680080D+10 Y= 9.222116570873D+12 Z= -3.552567676076D+13

I= 18 X= -1.127420819850D+14 Y= 3.698855438031D+13 Z= 3.631010859170D+13

I= 19 X= 6.829124089730D+11 Y= 3.955957351090D+12 Z= -2.071331473681D+12

I= 20 X= -1.400932845199D+11 Y= -9.220385259849D+12 Z= 1.072376617104D+14

I= 21 X= -3.978044647290D+12 Y= -1.850315198736D+13 Z= -8.064570293425D+12

I= 22 X= 1.115242641176D+14 Y= -2.779257226875D+13 Z= -1.731786443106D+13

I= 23 X= -9.446269406733D+13 Y= 8.821014549949D+13 Z= -3.413537173685D+13
I= 24 X= -6.715307284015D+13 Y= -4.637635604356D+13 Z= 8.389545615191D+13
I= 25 X= -2.987810730717D+12 Y= 2.775733767946D+13 Z= 1.712860965220D+13
I= 26 X= 2.840043552557D+13 Y= 1.309762690710D+13 Z= -4.291794756574D+13
I= 27 X= -4.411205039505D+12 Y= -7.118718798663D+13 Z= -2.771564960659D+13
I= 28 X= -8.261581211600D+13 Y= -7.956340787427D+13 Z= 7.761783044985D+13
I= 29 X= -1.306122292553D+13 Y= -5.701667793902D+12 Z= -1.860088613427D+13
I= 30 X= 1.391146264704D+13 Y= -9.531251958051D+09 Z= 3.546714843937D+12
I= 31 X= 1.164643293347D+14 Y= 8.325672831536D+13 Z= 4.753469941499D+13
I= 32 X= -1.723778611187D+12 Y= 2.372823358738D+13 Z= 3.249163088994D+13
I= 33 X= 3.247661392460D+13 Y= 5.942913450005D+13 Z= 9.791327561978D+13
I= 34 X= -5.234904515915D+13 Y= 1.118191746522D+13 Z= 4.072226989430D+13
I= 35 X= -9.391214911041D+11 Y= 3.960491162834D+12 Z= 6.455021646384D+11
I= 36 X= 4.429920702887D+12 Y= -1.353559797536D+13 Z= -9.067982050440D+12
I= 37 X= -7.376998895079D+13 Y= 1.984697647242D+13 Z= -2.384588923605D+13
I= 38 X= 1.231129764539D+12 Y= -3.925716863015D+12 Z= -2.346079084531D+13

Seed: 25704926461

CM Start Point Coordinates: bohr

I= 0 X= -2.265733303664D+00 Y= 2.194446219218D+00 Z= -7.287480140171D-01
I= 1 X= -2.786395625642D+00 Y= -1.928177476166D-01 Z= -1.900292857037D+00
I= 2 X= -2.047891305701D+00 Y= 1.781857071927D+00 Z= 1.823507888877D+00
I= 3 X= -2.608149846163D+00 Y= -2.143378033900D+00 Z= -1.448189027585D-01
I= 4 X= -1.983679734636D+00 Y= -7.831250184582D-01 Z= 2.347810657119D+00
I= 5 X= 4.550672351212D+00 Y= 2.649715051608D+00 Z= -6.788886080971D-01
I= 6 X= 2.582027028046D+00 Y= 8.635028878775D-01 Z= -3.019014976589D+00
I= 7 X= 5.997951137369D+00 Y= 1.050495015229D+00 Z= -1.407236071395D+00
I= 8 X= 4.291325514141D+00 Y= 4.344286217554D+00 Z= -1.921313314791D+00
I= 9 X= -1.699689455482D+00 Y= -2.315763164851D+00 Z= 4.771457109771D+00
I= 10 X= -3.523990634422D+00 Y= -2.128273039495D+00 Z= 6.117665522498D+00

I= 11 X= -1.441895274330D+00 Y= -4.284403336799D+00 Z= 4.359825354102D+00
I= 12 X= -3.459496189551D-02 Y= -1.642036515228D+00 Z= 5.940018301628D+00
I= 13 X= -1.679205168403D+00 Y= 3.747070316094D+00 Z= 3.900198720992D+00
I= 14 X= -3.539820058867D+00 Y= 4.487396167843D+00 Z= 4.970555984165D+00
I= 15 X= -3.871445351408D-01 Y= 3.068266751235D+00 Z= 5.062444437758D+00
I= 16 X= -7.185945709500D-01 Y= 5.447960082552D+00 Z= 3.227540485657D+00
I= 17 X= -2.382081738141D+00 Y= 4.813831162061D+00 Z= -2.061018969548D+00
I= 18 X= -4.757154874822D+00 Y= 4.867723195011D+00 Z= -3.019247442614D+00
I= 19 X= -2.076131097384D+00 Y= 6.488874726891D+00 Z= -5.118427292682D-01
I= 20 X= -6.258675409666D-01 Y= 4.718508641318D+00 Z= -3.597854988970D+00
I= 21 X= -3.865846348648D+00 Y= -2.450535448996D-01 Z= -4.443716352276D+00
I= 22 X= -5.958835868872D+00 Y= -6.403792385890D-01 Z= -4.639843867071D+00
I= 23 X= -3.498365604020D+00 Y= 1.376773885184D+00 Z= -5.496752494872D+00
I= 24 X= -3.427505128239D+00 Y= -1.795219200279D+00 Z= -5.516654136032D+00
I= 25 X= -2.932778635958D+00 Y= -4.763321688765D+00 Z= -7.112907216104D-01
I= 26 X= -2.518613823373D+00 Y= -5.357810393755D+00 Z= -2.884097378200D+00
I= 27 X= -1.475578312818D+00 Y= -6.149031565286D+00 Z= 1.660998958700D-01
I= 28 X= -4.755631217175D+00 Y= -5.577222302946D+00 Z= -4.383861379250D-02
I= 29 X= 3.013484962629D+00 Y= -3.364535348768D+00 Z= -1.969869560626D+00
I= 30 X= 3.402936072590D+00 Y= -3.633674212185D+00 Z= 6.596704440566D-01
I= 31 X= 1.657866277158D+00 Y= -4.561454419548D+00 Z= -2.809574425638D+00
I= 32 X= 4.491530108939D+00 Y= -2.639811940286D+00 Z= -2.977579722520D+00
I= 33 X= 5.287463606893D+00 Y= -2.695978861893D+00 Z= 1.341448003765D+00
I= 34 X= 2.334529501034D+00 Y= -4.760212388600D+00 Z= 2.025787435954D+00
I= 35 X= 1.126617404058D+00 Y= 1.907684553475D-02 Z= -3.402364537970D-01
I= 36 X= 3.959814590076D+00 Y= 2.166839756220D+00 Z= 1.928923026099D+00
I= 37 X= 5.206290996556D+00 Y= 9.078485601904D-01 Z= 3.319995088005D+00
I= 38 X= 2.882285224952D+00 Y= 3.709059718358D+00 Z= 2.798725370750D+00

Forward Direction:

Total Energy: -656.4308871 Hartrees

Potential Energy: -656.6198561 Hartress

Kinetic Energy: 0.1889690 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.958087112099D+13 Y= 5.549284338429D+12 Z= 2.900899920268D+13
I= 1 X= 6.585711968672D+12 Y= -1.915473370968D+13 Z= -1.141862700841D+13
I= 2 X= 1.594060198727D+13 Y= 1.428924323682D+13 Z= -7.656448912912D+12
I= 3 X= -5.917842743137D+12 Y= 8.263559516807D+11 Z= 1.160113961291D+13
I= 4 X= -1.577507597376D+12 Y= -1.618400325182D+13 Z= 6.201373345706D+12
I= 5 X= 1.680131652693D+13 Y= 1.242510847887D+13 Z= -3.010166063922D+13
I= 6 X= 2.142197889818D+13 Y= -7.570958917113D+13 Z= 6.387920884572D+13
I= 7 X= -2.738211135672D+13 Y= -6.427977954533D+13 Z= -2.993570393194D+13
I= 8 X= -1.037768907157D+13 Y= -4.018600113981D+13 Z= 1.028690706291D+14
I= 9 X= 6.547946608971D+11 Y= 2.849231413294D+12 Z= -3.653113637152D+12
I= 10 X= -1.319346672426D+14 Y= 1.584598555559D+13 Z= 4.911552146470D+13
I= 11 X= -1.943785397781D+13 Y= -8.289911263206D+12 Z= -9.173049615301D+13
I= 12 X= 1.758448731718D+13 Y= 1.360775112149D+13 Z= 8.488416055672D+13
I= 13 X= -1.878721842820D+13 Y= 7.813656161135D+12 Z= 6.723602969741D+12
I= 14 X= 1.114411256999D+13 Y= -8.423291330706D+13 Z= 1.297935515110D+13
I= 15 X= 3.927472440035D+13 Y= 7.265073275243D+13 Z= -7.534157032230D+12
I= 16 X= 1.009781690576D+14 Y= -1.423595630657D+14 Z= -8.637716288257D+13
I= 17 X= 3.997034367627D+12 Y= -5.738548238168D+12 Z= -3.007299446205D+12
I= 18 X= -9.627887214894D+13 Y= 8.302224176116D+13 Z= -1.981688698679D+13
I= 19 X= 6.311812017942D+13 Y= 5.984201697739D+11 Z= 9.154536371611D+12
I= 20 X= -1.989583936716D+13 Y= 5.572235470211D+13 Z= 1.218383833917D+12
I= 21 X= -1.010356559509D+12 Y= -2.857794683012D+13 Z= -7.445918026286D+10
I= 22 X= 8.779932101078D+13 Y= -2.233704023588D+13 Z= 7.582708449409D+11
I= 23 X= 3.987272751667D+13 Y= 4.379608375943D+13 Z= 1.824921947729D+13
I= 24 X= -3.593694050612D+13 Y= 3.567854516021D+13 Z= 2.049200302594D+13
I= 25 X= -8.173216628604D+12 Y= 8.483631341881D+12 Z= -8.093011259379D+12
I= 26 X= -4.600508457264D+13 Y= -1.795392662563D+13 Z= 9.215492556253D+13

I= 27 X= 2.478467869993D+13 Y= -3.895581869331D+13 Z= -3.317267633601D+13
I= 28 X= -7.511813795580D+13 Y= 1.983196982125D+13 Z= 3.462477476038D+13
I= 29 X= 6.632562851062D+12 Y= -1.802512696645D+12 Z= 6.261416775874D+12
I= 30 X= 5.388176954110D+12 Y= 1.521706498237D+13 Z= -9.901525490230D+12
I= 31 X= 4.770699572200D+13 Y= 1.327731260606D+14 Z= 4.438781156893D+13
I= 32 X= 4.723041342438D+13 Y= -7.113510850011D+12 Z= -3.293471784011D+13
I= 33 X= -1.240119133747D+14 Y= -5.081436403494D+13 Z= 2.801997937695D+13
I= 34 X= 8.114112919134D+13 Y= 6.070543910963D+13 Z= -9.954759795512D+13
I= 35 X= -2.881304348763D+12 Y= -1.695219118903D+11 Z= -1.967757503279D+12
I= 36 X= -9.180190026593D+12 Y= -1.111644923030D+13 Z= 1.256011769291D+13
I= 37 X= -1.829468884748D+12 Y= 1.037548257684D+14 Z= 1.032052724846D+12
I= 38 X= -6.798497087719D+13 Y= 1.115927235647D+14 Z= 5.659919782182D+13

Backward Direction:

Total Energy: -656.4309040 Hartrees

Potential Energy: -656.6198561 Hartress

Kinetic Energy: 0.1889521 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.947677431328D+13 Y= 5.413349003571D+12 Z= 2.906219430606D+13
I= 1 X= 6.425155394886D+12 Y= -1.950429081007D+13 Z= -1.162846711456D+13
I= 2 X= 1.579116703847D+13 Y= 1.442660702526D+13 Z= -7.877610426188D+12
I= 3 X= -6.224027231487D+12 Y= 8.335154172327D+11 Z= 1.115750976614D+13
I= 4 X= -1.053812983727D+12 Y= -1.623072632925D+13 Z= 5.853369851682D+12
I= 5 X= 1.593700937926D+13 Y= 1.119596923275D+13 Z= -3.255565570164D+13
I= 6 X= 4.078231434454D+13 Y= -5.360744150733D+13 Z= 7.259009544628D+13
I= 7 X= -2.384594547913D+13 Y= -6.093178265087D+13 Z= -2.971936208073D+13
I= 8 X= -5.911657502229D+12 Y= -3.657602247395D+13 Z= 1.032845579395D+14
I= 9 X= 8.212401370139D+11 Y= 2.927397337467D+12 Z= -3.841251800969D+12
I= 10 X= -1.319042257023D+14 Y= 1.623282567986D+13 Z= 4.866709358324D+13
I= 11 X= -1.948592673378D+13 Y= -8.294140039224D+12 Z= -9.173984411312D+13
I= 12 X= 1.768203606080D+13 Y= 1.363387838290D+13 Z= 8.479152810050D+13

I= 13 X= -1.875422304105D+13 Y= 7.797601868080D+12 Z= 6.654157795054D+12
I= 14 X= 1.120020707286D+13 Y= -8.433181802266D+13 Z= 1.299403590887D+13
I= 15 X= 3.937788252598D+13 Y= 7.255611893070D+13 Z= -7.704979313018D+12
I= 16 X= 1.009709830916D+14 Y= -1.423291540958D+14 Z= -8.635311278258D+13
I= 17 X= 4.047563084255D+12 Y= -5.850057591397D+12 Z= -3.018342115891D+12
I= 18 X= -9.626821842247D+13 Y= 8.284446626672D+13 Z= -1.996272338955D+13
I= 19 X= 6.301130349937D+13 Y= 5.628369032004D+11 Z= 9.264681045577D+12
I= 20 X= -1.982166267143D+13 Y= 5.562271725829D+13 Z= 1.205659982703D+12
I= 21 X= -1.073937757347D+12 Y= -2.861788995997D+13 Z= -2.296705697119D+11
I= 22 X= 8.778795853515D+13 Y= -2.215803753829D+13 Z= 1.362397174018D+11
I= 23 X= 4.010383843641D+13 Y= 4.369548365387D+13 Z= 1.817709195448D+13
I= 24 X= -3.604835552566D+13 Y= 3.561596989205D+13 Z= 2.030848323583D+13
I= 25 X= -8.242316629045D+12 Y= 8.413825887196D+12 Z= -8.128668754636D+12
I= 26 X= -4.617599915653D+13 Y= -1.814089398531D+13 Z= 9.213407171938D+13
I= 27 X= 2.492712313025D+13 Y= -3.883589205342D+13 Z= -3.321401650236D+13
I= 28 X= -7.511107945264D+13 Y= 1.962040567227D+13 Z= 3.477452883531D+13
I= 29 X= 6.312552337122D+12 Y= -1.712624237076D+12 Z= 6.149177501292D+12
I= 30 X= 5.407022085842D+12 Y= 1.515513486779D+13 Z= -1.004052563891D+13
I= 31 X= 4.748575029318D+13 Y= 1.327076717179D+14 Z= 4.439472470450D+13
I= 32 X= 4.658292438245D+13 Y= -6.575810567760D+12 Z= -3.332021318256D+13
I= 33 X= -1.239919446962D+14 Y= -5.089262800988D+13 Z= 2.790926525023D+13
I= 34 X= 8.134973878527D+13 Y= 6.056019966001D+13 Z= -9.958752408174D+13
I= 35 X= -2.884785706193D+12 Y= -8.820818539608D+10 Z= -1.451872002722D+12
I= 36 X= -1.030525576741D+13 Y= -1.253749996264D+13 Z= 1.204154037658D+13
I= 37 X= -8.258061155739D+11 Y= 1.042643498986D+14 Z= -2.196753779022D+11
I= 38 X= -6.743532621130D+13 Y= 1.115354495876D+14 Z= 5.566437672390D+13

Seed: 27693154100

CM Start Point Coordinates: bohr

I= 0 X= -2.322883618915D+00 Y= 2.460709443027D+00 Z= -5.976314921952D-01

I= 1 X= -2.984854402562D+00 Y= 6.584784421506D-02 Z= -1.964972005159D+00
I= 2 X= -1.896867704586D+00 Y= 1.622640755649D+00 Z= 2.033022732564D+00
I= 3 X= -2.526435700021D+00 Y= -2.014392299498D+00 Z= -4.066531811477D-01
I= 4 X= -2.078382207439D+00 Y= -1.104227027834D+00 Z= 2.199129740329D+00
I= 5 X= 4.101837067187D+00 Y= 2.482372752482D+00 Z= -1.617909775963D+00
I= 6 X= 2.621954147996D+00 Y= 1.409359839171D-04 Z= -3.099323472848D+00
I= 7 X= 5.773204777476D+00 Y= 1.786123956736D+00 Z= -2.207414089916D+00
I= 8 X= 3.554302040529D+00 Y= 3.573247527947D+00 Z= -3.408565929915D+00
I= 9 X= -2.153365027523D+00 Y= -2.668961541965D+00 Z= 4.475432683735D+00
I= 10 X= -3.939671298107D+00 Y= -3.212801191246D+00 Z= 4.921268455824D+00
I= 11 X= -1.655235331505D+00 Y= -4.689778225147D+00 Z= 3.939136455458D+00
I= 12 X= -1.249742463928D+00 Y= -2.028404119098D+00 Z= 6.080059820584D+00
I= 13 X= -1.322455321970D+00 Y= 3.335165072779D+00 Z= 4.221250176268D+00
I= 14 X= -3.262097052140D+00 Y= 3.734693885066D+00 Z= 5.091461484178D+00
I= 15 X= 1.763171193761D-01 Y= 2.423222310271D+00 Z= 5.565610433359D+00
I= 16 X= -6.032275504115D-01 Y= 5.015958790196D+00 Z= 3.448368963587D+00
I= 17 X= -2.352739689352D+00 Y= 5.043824098583D+00 Z= -1.597638997266D+00
I= 18 X= -4.482639199388D+00 Y= 5.540256901311D+00 Z= -2.188664078254D+00
I= 19 X= -1.680289955098D+00 Y= 6.150100409761D+00 Z= 3.751142528998D-01
I= 20 X= -8.549799680088D-01 Y= 5.405239663672D+00 Z= -3.068982981506D+00
I= 21 X= -3.802687184881D+00 Y= 2.983595015533D-01 Z= -4.646619345850D+00
I= 22 X= -6.052456700514D+00 Y= 1.705170570591D+00 Z= -4.737519783960D+00
I= 23 X= -2.278463281424D+00 Y= 1.318268759726D+00 Z= -5.988368915572D+00
I= 24 X= -4.414461690766D+00 Y= -1.741601965238D+00 Z= -5.991488417073D+00
I= 25 X= -3.237842100627D+00 Y= -4.834538085168D+00 Z= -8.688676426550D-01
I= 26 X= -3.613451696255D+00 Y= -5.064298540000D+00 Z= -2.976519649556D+00
I= 27 X= -2.110629205391D+00 Y= -6.365665942158D+00 Z= 8.011885459551D-02
I= 28 X= -5.012083804482D+00 Y= -4.885055685725D+00 Z= 1.142918976987D-02
I= 29 X= 3.390253683654D+00 Y= -3.685056030008D+00 Z= -9.360172009066D-01
I= 30 X= 3.632170738738D+00 Y= -2.702430922261D+00 Z= 1.701466043684D+00

I= 31 X= 1.718436079684D+00 Y= -4.974359363877D+00 Z= -1.349855920831D+00
I= 32 X= 4.559888567511D+00 Y= -3.284509400190D+00 Z= -2.434634514877D+00
I= 33 X= 5.249546152584D+00 Y= -1.948801663272D+00 Z= 2.188123894304D+00
I= 34 X= 2.555141732148D+00 Y= -3.465719478069D+00 Z= 3.275614963755D+00
I= 35 X= 1.217923050599D+00 Y= -1.625104048541D-01 Z= -3.581907327683D-01
I= 36 X= 3.735506719302D+00 Y= 2.925734709686D+00 Z= 9.635870954529D-01
I= 37 X= 5.251606226483D+00 Y= 2.450313350138D+00 Z= 2.380447910784D+00
I= 38 X= 2.302113817297D+00 Y= 4.565076541840D+00 Z= 1.452556628590D+00

Forward Direction:

Total Energy: -656.4387536 Hartrees

Potential Energy: -656.5966937 Hartress

Kinetic Energy: 0.1579401 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.683014739521D+12 Y= 8.590937317379D+11 Z= 1.636225557424D+13
I= 1 X= 1.150310839580D+13 Y= 1.956984815273D+13 Z= 9.425862966858D+12
I= 2 X= 5.060319580764D+12 Y= -1.288661207607D+13 Z= -1.133760928121D+13
I= 3 X= 1.679583892646D+13 Y= 1.064458621997D+13 Z= 1.735791619159D+13
I= 4 X= 4.409466303198D+11 Y= 1.353775708731D+13 Z= 3.010757386615D+12
I= 5 X= 5.152536385097D+12 Y= -1.614813463465D+13 Z= -1.942121825937D+13
I= 6 X= -6.395549462168D+13 Y= 3.628221828939D+13 Z= -1.237151058825D+14
I= 7 X= -1.077460158612D+13 Y= 8.381817601302D+13 Z= 9.638371152532D+13
I= 8 X= 1.144934155067D+13 Y= 3.444642324078D+13 Z= -7.359408939493D+13
I= 9 X= 1.417461280763D+11 Y= -3.840913604599D+12 Z= 1.876024939933D+13
I= 10 X= 3.377041793326D+13 Y= 6.363778033320D+13 Z= 1.023458534999D+13
I= 11 X= -8.253376696911D+12 Y= -1.553675033045D+13 Z= -4.489902835274D+13
I= 12 X= -4.802133790592D+13 Y= 1.738829072327D+13 Z= -1.138357551082D+13
I= 13 X= 6.949017548198D+12 Y= -1.455957193019D+13 Z= -7.187726570910D+12
I= 14 X= -5.687552021901D+13 Y= 2.851804137787D+13 Z= 6.100272176370D+13
I= 15 X= -1.191508105143D+13 Y= 5.293399919234D+12 Z= -1.391257796833D+13
I= 16 X= -2.636723275815D+13 Y= -5.937267866765D+13 Z= 9.582415386980D+13

I= 17 X= 1.330330630644D+13 Y= 1.747664870321D+12 Z= 1.285934669604D+13
I= 18 X= -1.365817478281D+13 Y= -5.134281693525D+13 Z= -6.897139676975D+13
I= 19 X= 1.947960869461D+13 Y= 6.192608287782D+13 Z= 3.600850629767D+13
I= 20 X= -1.537152164724D+12 Y= -2.067360511662D+13 Z= -9.156318047160D+13
I= 21 X= 1.074314751627D+10 Y= -1.828452952649D+13 Z= -8.074350246923D+12
I= 22 X= 9.185491717449D+13 Y= 4.074400967141D+13 Z= -6.148007685872D+12
I= 23 X= -3.237320013542D+12 Y= 7.322215649346D+13 Z= -6.647242065001D+13
I= 24 X= -7.055836024485D+13 Y= 2.192076564310D+13 Z= -3.338014130523D+13
I= 25 X= 1.229807181606D+12 Y= -1.156542642503D+12 Z= 1.570429013019D+13
I= 26 X= 1.715212477526D+13 Y= -1.268917104002D+14 Z= -8.437512429504D+13
I= 27 X= -2.529350692920D+13 Y= 4.630224185114D+13 Z= -1.408233753300D+14
I= 28 X= -1.198693529960D+14 Y= 5.502926400889D+13 Z= 8.876725514777D+12
I= 29 X= 8.044168552871D+12 Y= -9.501189115980D+12 Z= -1.325673609619D+13
I= 30 X= -2.306939487366D+13 Y= 7.425120268982D+12 Z= 1.099522704768D+13
I= 31 X= -3.167763221172D+13 Y= 3.711700301072D+13 Z= 1.346458212067D+13
I= 32 X= -5.285861076515D+13 Y= -1.207163222567D+13 Z= 6.107793730851D+12
I= 33 X= 3.716161528200D+13 Y= -1.968091829711D+13 Z= -1.278188581821D+12
I= 34 X= 3.254929496076D+13 Y= 2.756041815086D+13 Z= -1.404081146901D+14
I= 35 X= -1.182155497898D+12 Y= -5.678442302685D+10 Z= -8.338296050490D+11
I= 36 X= -6.999032051467D+12 Y= -3.301521130125D+12 Z= 5.146698484260D+12
I= 37 X= 1.313373913078D+13 Y= -7.030204097249D+13 Z= 3.005016876179D+13
I= 38 X= -3.011834628855D+13 Y= 5.679056571283D+13 Z= 2.866138038967D+13

Backward Direction:

Total Energy: -656.4387854 Hartrees

Potential Energy: -656.5966937 Hartress

Kinetic Energy: 0.1579083 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.786970784276D+12 Y= 7.233422122114D+11 Z= 1.641537874462D+13

I= 1 X= 1.134276893327D+13 Y= 1.922076373367D+13 Z= 9.216306613807D+12

I= 2 X= 4.911086703251D+12 Y= -1.274943403575D+13 Z= -1.155847173349D+13

I= 3 X= 1.649006847028D+13 Y= 1.065173600179D+13 Z= 1.691488623307D+13
I= 4 X= 9.639330896704D+11 Y= 1.349109718998D+13 Z= 2.663224473928D+12
I= 5 X= 4.289397978516D+12 Y= -1.737561180269D+13 Z= -2.187189495902D+13
I= 6 X= -4.462133877945D+13 Y= 5.835447879070D+13 Z= -1.150159983943D+14
I= 7 X= -7.243217414517D+12 Y= 8.716164564702D+13 Z= 9.659976083322D+13
I= 8 X= 1.590933402390D+13 Y= 3.805152039162D+13 Z= -7.317916391621D+13
I= 9 X= 3.079665308294D+11 Y= -3.762853380321D+12 Z= 1.857236564004D+13
I= 10 X= 3.380081830699D+13 Y= 6.402409735735D+13 Z= 9.786763852189D+12
I= 11 X= -8.301384439409D+12 Y= -1.554097337675D+13 Z= -4.490836367556D+13
I= 12 X= -4.792392107018D+13 Y= 1.741438265875D+13 Z= -1.147608270744D+13
I= 13 X= 6.981968318405D+12 Y= -1.457560451405D+13 Z= -7.257077840490D+12
I= 14 X= -5.681950156949D+13 Y= 2.841927041050D+13 Z= 6.101738267424D+13
I= 15 X= -1.181206242071D+13 Y= 5.198914032753D+12 Z= -1.408316926161D+13
I= 16 X= -2.637440900508D+13 Y= -5.934231081919D+13 Z= 9.584817144680D+13
I= 17 X= 1.335376669449D+13 Y= 1.636306302470D+12 Z= 1.284831896058D+13
I= 18 X= -1.364753546385D+13 Y= -5.152035203418D+13 Z= -6.911703597256D+13
I= 19 X= 1.937293644750D+13 Y= 6.189054771790D+13 Z= 3.611850202379D+13
I= 20 X= -1.463075771377D+12 Y= -2.077310782756D+13 Z= -9.157588713470D+13
I= 21 X= -5.275207371481D+10 Y= -1.832441864251D+13 Z= -8.229351755304D+12
I= 22 X= 9.184357006375D+13 Y= 4.092277031940D+13 Z= -6.769197682642D+12
I= 23 X= -3.006521610550D+12 Y= 7.312169242118D+13 Z= -6.654445063982D+13
I= 24 X= -7.066962459445D+13 Y= 2.185827499407D+13 Z= -3.356341293517D+13
I= 25 X= 1.160800616018D+12 Y= -1.226253701706D+12 Z= 1.566868085350D+13
I= 26 X= 1.698144129395D+13 Y= -1.270784249308D+14 Z= -8.439594993873D+13
I= 27 X= -2.515125510951D+13 Y= 4.642200632675D+13 Z= -1.408646595975D+14
I= 28 X= -1.198623040381D+14 Y= 5.481798592860D+13 Z= 9.026277089126D+12
I= 29 X= 7.724590766104D+12 Y= -9.411422205140D+12 Z= -1.336882359667D+13
I= 30 X= -2.305057522449D+13 Y= 7.363273898404D+12 Z= 1.085641486009D+13
I= 31 X= -3.189857846519D+13 Y= 3.705163717688D+13 Z= 1.347148591007D+13
I= 32 X= -5.350522425079D+13 Y= -1.153465903491D+13 Z= 5.722819666612D+12

I= 33 X= 3.718155695436D+13 Y= -1.975907644121D+13 Z= -1.388752995226D+12
I= 34 X= 3.275762247045D+13 Y= 2.741537510494D+13 Z= -1.404479868298D+14
I= 35 X= -1.185632147571D+12 Y= 2.441934864612D+10 Z= -3.186416999743D+11
I= 36 X= -8.122576446191D+12 Y= -4.720650277325D+12 Z= 4.628822402972D+12
I= 37 X= 1.413604472060D+13 Y= -6.979320583327D+13 Z= 2.880013328594D+13
I= 38 X= -2.956944486594D+13 Y= 5.673336918222D+13 Z= 2.772782338444D+13

Seed: 2820608934

CM Start Point Coordinates: bohr

I= 0 X= -2.520356461576D+00 Y= 2.323468711583D+00 Z= -4.036383656379D-01
I= 1 X= -2.976976460236D+00 Y= 1.596107184439D-01 Z= -1.877484212102D+00
I= 2 X= -1.689596645884D+00 Y= 1.687721006582D+00 Z= 2.150460395905D+00
I= 3 X= -2.593233980356D+00 Y= -2.160165454600D+00 Z= -3.253983343786D-01
I= 4 X= -2.098310101953D+00 Y= -1.072896986661D+00 Z= 2.228530041396D+00
I= 5 X= 4.530593753671D+00 Y= 2.309995048195D+00 Z= -1.797333920711D+00
I= 6 X= 1.975380850713D+00 Y= 4.415584789895D-01 Z= -3.089893062952D+00
I= 7 X= 5.833912238375D+00 Y= 7.619276580142D-01 Z= -2.336803721615D+00
I= 8 X= 4.228972256143D+00 Y= 3.990621989404D+00 Z= -3.077238691302D+00
I= 9 X= -2.278682139898D+00 Y= -2.318070713579D+00 Z= 4.800497391372D+00
I= 10 X= -4.361784328598D+00 Y= -1.470711303528D+00 Z= 5.749106444672D+00
I= 11 X= -2.464489462595D+00 Y= -4.412291477280D+00 Z= 4.746274406699D+00
I= 12 X= -6.854520396088D-01 Y= -1.479044693559D+00 Z= 6.019548826122D+00
I= 13 X= -1.279246885685D+00 Y= 3.232818112476D+00 Z= 4.379187546955D+00
I= 14 X= -3.088489613748D+00 Y= 3.619119625198D+00 Z= 5.012878967514D+00
I= 15 X= -4.585884043324D-01 Y= 1.978233434215D+00 Z= 5.795267652999D+00
I= 16 X= -1.971213163763D-01 Y= 5.104917047553D+00 Z= 4.138950549814D+00
I= 17 X= -2.485963738258D+00 Y= 5.033195329503D+00 Z= -1.344203895513D+00
I= 18 X= -4.504646740945D+00 Y= 5.224124419162D+00 Z= -1.758802156640D+00
I= 19 X= -1.630316348091D+00 Y= 6.434100837748D+00 Z= 1.411016587119D-01
I= 20 X= -1.665412848815D+00 Y= 5.035480591287D+00 Z= -3.218082793480D+00

I= 21 X= -3.483043942903D+00 Y= 7.338500619999D-02 Z= -4.795364480787D+00
I= 22 X= -5.551422395520D+00 Y= -1.139239191040D+00 Z= -5.158217115079D+00
I= 23 X= -3.728041864875D+00 Y= 2.250974584155D+00 Z= -5.903981877222D+00
I= 24 X= -1.919505265507D+00 Y= -9.221966646947D-01 Z= -6.012318873386D+00
I= 25 X= -2.796012171881D+00 Y= -4.764624426603D+00 Z= -1.171506995963D+00
I= 26 X= -2.005076364200D+00 Y= -4.979573901504D+00 Z= -3.092546266458D+00
I= 27 X= -2.121049417663D+00 Y= -6.246687421015D+00 Z= 2.835401480826D-01
I= 28 X= -5.149652660449D+00 Y= -5.399997172291D+00 Z= -1.390130937990D+00
I= 29 X= 3.622170662214D+00 Y= -3.740062430829D+00 Z= -8.861162462280D-01
I= 30 X= 3.499715410497D+00 Y= -2.886918756368D+00 Z= 1.586552757153D+00
I= 31 X= 2.079547619573D+00 Y= -4.993281948318D+00 Z= -1.853394765253D+00
I= 32 X= 5.163251193731D+00 Y= -3.363861067550D+00 Z= -2.419876810904D+00
I= 33 X= 4.886236429320D+00 Y= -1.684143318996D+00 Z= 2.616672433842D+00
I= 34 X= 2.078197999301D+00 Y= -3.716989340259D+00 Z= 2.771064194242D+00
I= 35 X= 1.052463830607D+00 Y= -6.542665590870D-02 Z= -4.034875969683D-01
I= 36 X= 3.961963723266D+00 Y= 2.600204456125D+00 Z= 7.978329298532D-01
I= 37 X= 5.263896108625D+00 Y= 1.735963213861D+00 Z= 1.930702791063D+00
I= 38 X= 2.802660944174D+00 Y= 4.224026611547D+00 Z= 1.511814977692D+00

Forward Direction:

Total Energy: -656.4202292 Hartrees

Potential Energy: -656.6239587 Hartress

Kinetic Energy: 0.2037295 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.220890299759D+13 Y= 5.609844712262D+12 Z= 6.780930742522D+11
I= 1 X= 3.680461921967D+12 Y= -1.691706541974D+12 Z= 1.142375439673D+13
I= 2 X= 4.549013328350D+12 Y= 2.263390702133D+13 Z= 1.109048706327D+13
I= 3 X= 1.240234199253D+13 Y= 1.776878179547D+13 Z= 6.206817938624D+12
I= 4 X= -1.077041321435D+13 Y= -3.674573259088D+13 Z= -1.547694394812D+13
I= 5 X= -1.801756633196D+12 Y= 2.290080306870D+12 Z= 1.347166898658D+12
I= 6 X= -5.596253498133D+11 Y= -9.656817476109D+13 Z= -5.889162200133D+13

I= 7 X= 1.750854237543D+14 Y= -2.151144220326D+13 Z= -6.607117164588D+13
I= 8 X= 8.713801188925D+13 Y= 1.415984946752D+12 Z= -5.019721000239D+13
I= 9 X= 1.367782596692D+13 Y= 3.281565258092D+12 Z= 1.138470713383D+13
I= 10 X= 1.391638806452D+13 Y= 3.708709722745D+13 Z= -7.872248407601D+13
I= 11 X= -3.905919525367D+13 Y= 1.667088899460D+13 Z= -4.602035294184D+13
I= 12 X= -1.086233065126D+14 Y= -1.161111112195D+13 Z= -1.964586629305D+13
I= 13 X= 5.826530576872D+12 Y= 2.516604080599D+13 Z= 7.912800616764D+12
I= 14 X= 1.454443602892D+13 Y= 2.488255905411D+13 Z= 1.530158491867D+13
I= 15 X= -7.938776906163D+12 Y= 7.901660031776D+13 Z= -4.134857851809D+13
I= 16 X= -7.190142405845D+13 Y= -1.277256064215D+14 Z= 6.930278105057D+13
I= 17 X= 9.950716306529D+11 Y= -8.306325764163D+11 Z= -2.779944783729D+13
I= 18 X= 9.225403813425D+13 Y= -3.841866114629D+13 Z= 8.350973356388D+12
I= 19 X= -9.707030476888D+12 Y= -6.063837268707D+13 Z= 5.253051145365D+13
I= 20 X= 9.397111515788D+12 Y= -1.661924479776D+13 Z= -3.986298461073D+13
I= 21 X= -2.924918860983D+13 Y= -7.356866665707D+12 Z= 4.117437882073D+12
I= 22 X= 1.089555736683D+14 Y= -5.101728052310D+13 Z= 4.175687978847D+12
I= 23 X= 5.165380455220D+13 Y= -3.679526985341D+13 Z= -5.693026794732D+13
I= 24 X= 3.440362477564D+13 Y= 3.217656103217D+13 Z= -3.224477462486D+13
I= 25 X= -1.642622672415D+13 Y= -9.518132297458D+12 Z= 2.783315144967D+13
I= 26 X= -2.713742590125D+13 Y= -1.233092361495D+14 Z= -1.214250675358D+14
I= 27 X= 3.470510877833D+13 Y= 1.845161830331D+13 Z= -7.025912572935D+13
I= 28 X= 3.943530871051D+13 Y= 1.534100181192D+13 Z= -7.339113086097D+13
I= 29 X= -1.179172489446D+13 Y= -5.965307246084D+12 Z= -1.227671681815D+13
I= 30 X= 1.718788385552D+13 Y= 2.070480382334D+13 Z= -1.335392445320D+13
I= 31 X= -5.504565236764D+13 Y= 3.515385075164D+12 Z= -3.124993964318D+13
I= 32 X= 1.764621183775D+13 Y= -2.641048932241D+13 Z= 5.353777654969D+12
I= 33 X= -1.546897999070D+14 Y= 1.152397250750D+13 Z= -1.085257522581D+13
I= 34 X= 2.106021070943D+13 Y= 1.022457495701D+13 Z= 1.299489916558D+14
I= 35 X= -5.892993849437D+11 Y= -1.298355603735D+12 Z= 2.096294436784D+12
I= 36 X= 9.368356395385D+12 Y= -4.179909367299D+12 Z= 1.532915063497D+13

I= 37 X= 7.191767351609D+13 Y= 9.397717280387D+12 Z= -2.533987389899D+13

I= 38 X= -6.390770746254D+13 Y= 1.123935991298D+14 Z= -1.490594200744D+13

Backward Direction:

Total Energy: -656.4202023 Hartrees

Potential Energy: -656.6239587 Hartress

Kinetic Energy: 0.2037564 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.250745311740D+13 Y= 5.219981549675D+12 Z= 8.306568710392D+11

I= 1 X= 3.219984939009D+12 Y= -2.694237904428D+12 Z= 1.082193201657D+13

I= 2 X= 4.120433212022D+12 Y= 2.302786699363D+13 Z= 1.045619483275D+13

I= 3 X= 1.152420348446D+13 Y= 1.778931516883D+13 Z= 4.934485504328D+12

I= 4 X= -9.268454665392D+12 Y= -3.687973459117D+13 Z= -1.647501955791D+13

I= 5 X= -4.280593485617D+12 Y= -1.235096672906D+12 Z= -5.690902167852D+12

I= 6 X= 5.496590527071D+13 Y= -3.317911415887D+13 Z= -3.390875938441D+13

I= 7 X= 1.852271636642D+14 Y= -1.190937180546D+13 Z= -6.545070222694D+13

I= 8 X= 9.994661085703D+13 Y= 1.176942027926D+13 Z= -4.900559048836D+13

I= 9 X= 1.415519235148D+13 Y= 3.505745483645D+12 Z= 1.084512601692D+13

I= 10 X= 1.400369455229D+13 Y= 3.819655646641D+13 Z= -8.000857727584D+13

I= 11 X= -3.919706811210D+13 Y= 1.665876086170D+13 Z= -4.604716293808D+13

I= 12 X= -1.083435362651D+14 Y= -1.153617799826D+13 Z= -1.991153660051D+13

I= 13 X= 5.921161498106D+12 Y= 2.511999702103D+13 Z= 7.713631536048D+12

I= 14 X= 1.470531531995D+13 Y= 2.459889989106D+13 Z= 1.534368940646D+13

I= 15 X= -7.642918930735D+12 Y= 7.874524743434D+13 Z= -4.183849759995D+13

I= 16 X= -7.192203343006D+13 Y= -1.276383933579D+14 Z= 6.937175684137D+13

I= 17 X= 1.139988214644D+12 Y= -1.150441915781D+12 Z= -2.783111826001D+13

I= 18 X= 9.228459306265D+13 Y= -3.892852206960D+13 Z= 7.932713859266D+12

I= 19 X= -1.001338121530D+13 Y= -6.074042567625D+13 Z= 5.284640688325D+13

I= 20 X= 9.609850621107D+12 Y= -1.690500544299D+13 Z= -3.989947669162D+13

I= 21 X= -2.943153977755D+13 Y= -7.471423742231D+12 Z= 3.672290905539D+12

I= 22 X= 1.089229860339D+14 Y= -5.050389996549D+13 Z= 2.391699864816D+12

I= 23 X= 5.231663171974D+13 Y= -3.708379141247D+13 Z= -5.713713000766D+13
I= 24 X= 3.408408602184D+13 Y= 3.199709488732D+13 Z= -3.277111022264D+13
I= 25 X= -1.662440585268D+13 Y= -9.718334653821D+12 Z= 2.773088559345D+13
I= 26 X= -2.762760971382D+13 Y= -1.238454593760D+14 Z= -1.214848764532D+14
I= 27 X= 3.511364006144D+13 Y= 1.879556847609D+13 Z= -7.037768951396D+13
I= 28 X= 3.945555251748D+13 Y= 1.473423481210D+13 Z= -7.296163552352D+13
I= 29 X= -1.270951651267D+13 Y= -5.707506730619D+12 Z= -1.259861956964D+13
I= 30 X= 1.724193177875D+13 Y= 2.052718797205D+13 Z= -1.375257751319D+13
I= 31 X= -5.568018526855D+13 Y= 3.327661719075D+12 Z= -3.123011273185D+13
I= 32 X= 1.578921031415D+13 Y= -2.486836244720D+13 Z= 4.248175252796D+12
I= 33 X= -1.546325296569D+14 Y= 1.129951107198D+13 Z= -1.117010383677D+13
I= 34 X= 2.165850398403D+13 Y= 9.808027568121D+12 Z= 1.298344833391D+14
I= 35 X= -5.992839337405D+11 Y= -1.065147464074D+12 Z= 3.575856412041D+12
I= 36 X= 6.141662705962D+12 Y= -8.255489371279D+12 Z= 1.384186851791D+13
I= 37 X= 7.479618293496D+13 Y= 1.085903482175D+13 Z= -2.892983581269D+13
I= 38 X= -6.233132403640D+13 Y= 1.122293370971D+14 Z= -1.758701318807D+13

Seed: 28766904189

CM Start Point Coordinates: bohr

I= 0 X= -2.243595113761D+00 Y= 2.400713916693D+00 Z= -4.809381481111D-01
I= 1 X= -3.022327708680D+00 Y= 2.675779913055D-01 Z= -1.981389538556D+00
I= 2 X= -1.969343332393D+00 Y= 1.530089237105D+00 Z= 2.231959392831D+00
I= 3 X= -2.703325394280D+00 Y= -1.818705991927D+00 Z= -4.013809068641D-01
I= 4 X= -2.241055278355D+00 Y= -1.034559975669D+00 Z= 2.052248518577D+00
I= 5 X= 4.283251179188D+00 Y= 2.406315997090D+00 Z= -2.440491149845D+00
I= 6 X= 1.963696811042D+00 Y= -4.741932291241D-01 Z= -3.038355838684D+00
I= 7 X= 5.799434571715D+00 Y= 1.183232901469D+00 Z= -2.982696199181D+00
I= 8 X= 3.760306213182D+00 Y= 3.647742948160D+00 Z= -3.702695130849D+00
I= 9 X= -2.347602230283D+00 Y= -2.657867548102D+00 Z= 4.401567637838D+00
I= 10 X= -4.610914883176D+00 Y= -3.115127904656D+00 Z= 5.116404579938D+00

I= 11 X= -1.841135536727D+00 Y= -4.500929915317D+00 Z= 4.154219203408D+00
I= 12 X= -1.310775271977D+00 Y= -1.595723575589D+00 Z= 5.934917265907D+00
I= 13 X= -1.438512031916D+00 Y= 3.364974045171D+00 Z= 4.584403036577D+00
I= 14 X= -2.922252282025D+00 Y= 3.614670168661D+00 Z= 6.016033228288D+00
I= 15 X= 3.014954931571D-01 Y= 2.445330539006D+00 Z= 5.469404807205D+00
I= 16 X= -1.147699146859D+00 Y= 5.371303355470D+00 Z= 3.694007237966D+00
I= 17 X= -2.437597072840D+00 Y= 5.072762018672D+00 Z= -1.263245385891D+00
I= 18 X= -4.551722119802D+00 Y= 5.304312192273D+00 Z= -7.235213226830D-01
I= 19 X= -1.172736905003D+00 Y= 6.644699811285D+00 Z= 2.923950157110D-02
I= 20 X= -2.185732495417D+00 Y= 5.352484206694D+00 Z= -3.393446038096D+00
I= 21 X= -3.462534432641D+00 Y= 2.265603948529D-01 Z= -4.751604159260D+00
I= 22 X= -5.564754283977D+00 Y= -4.045476075326D-01 Z= -5.429480201561D+00
I= 23 X= -2.866353592163D+00 Y= 1.950899800969D+00 Z= -5.543627563752D+00
I= 24 X= -2.607830047556D+00 Y= -1.451961320080D+00 Z= -5.873224361768D+00
I= 25 X= -2.947043908772D+00 Y= -4.591891190805D+00 Z= -1.285639191626D+00
I= 26 X= -2.539118951971D+00 Y= -4.544333927060D+00 Z= -3.406209053696D+00
I= 27 X= -1.396817803136D+00 Y= -5.753491904723D+00 Z= -2.437376096531D-02
I= 28 X= -4.823065293733D+00 Y= -5.599604726322D+00 Z= -7.111078903304D-01
I= 29 X= 3.782716325152D+00 Y= -3.645822073168D+00 Z= -7.369900977357D-01
I= 30 X= 3.615670522883D+00 Y= -3.055791574102D+00 Z= 1.947985094986D+00
I= 31 X= 2.517010717015D+00 Y= -5.415475481620D+00 Z= -1.415492706755D+00
I= 32 X= 5.711783392604D+00 Y= -3.307978844695D+00 Z= -1.466543385373D+00
I= 33 X= 5.403044450544D+00 Y= -2.317346635197D+00 Z= 2.531842685886D+00
I= 34 X= 2.598096397302D+00 Y= -3.707017116674D+00 Z= 3.472001404373D+00
I= 35 X= 1.082497453363D+00 Y= -1.705702933038D-01 Z= -2.476843519016D-01
I= 36 X= 4.096451963957D+00 Y= 3.024791997896D+00 Z= 1.481905722023D-01
I= 37 X= 5.456817715291D+00 Y= 2.105842532344D+00 Z= 1.462976684548D+00
I= 38 X= 3.076303766818D+00 Y= 4.252412045316D+00 Z= 1.012273973738D+00

Forward Direction:

Total Energy: -656.4401012 Hartrees

Potential Energy: -656.6076346 Hartress

Kinetic Energy: 0.1675333 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.738326635310D+11 Y= 1.923997732633D+12 Z= 6.910032421387D+12
I= 1 X= -2.029639011266D+13 Y= 1.918233010364D+13 Z= 4.163846206353D+12
I= 2 X= -3.925753280522D+12 Y= -3.002485425162D+12 Z= -1.525800346305D+13
I= 3 X= 1.579664181116D+13 Y= -5.287528925127D+12 Z= 1.602638983081D+13
I= 4 X= -1.795293624862D+13 Y= 4.196808364325D+12 Z= -1.921302338379D+13
I= 5 X= 2.289999288860D+12 Y= 1.117103022541D+13 Z= 7.652875690110D+12
I= 6 X= 4.571180531198D+13 Y= -5.238686170261D+13 Z= -4.495736837666D+13
I= 7 X= -7.365093336810D+13 Y= -4.101867359873D+13 Z= 4.510882181203D+13
I= 8 X= -4.992327871475D+13 Y= 8.039842595551D+13 Z= -6.958253285136D+12
I= 9 X= 1.146096215326D+13 Y= 1.060875834757D+13 Z= 1.586975030976D+13
I= 10 X= -7.794972799869D+12 Y= -7.548620555406D+13 Z= -9.221683601480D+12
I= 11 X= -6.339758633919D+13 Y= -1.508937079662D+14 Z= 1.157106795754D+13
I= 12 X= -6.768164053001D+13 Y= 7.425563279595D+12 Z= 8.581554826966D+13
I= 13 X= 3.795544608189D+11 Y= -1.851622753739D+13 Z= 1.238166766930D+13
I= 14 X= -1.483685496508D+13 Y= -7.572402347235D+12 Z= 3.207104683778D+13
I= 15 X= -1.531101863242D+13 Y= -3.410370342331D+12 Z= 8.001551209381D+13
I= 16 X= 3.843672022946D+13 Y= 1.417385580721D+14 Z= -4.624035429481D+13
I= 17 X= -3.699442175365D+12 Y= -1.269549379145D+12 Z= -2.191332965502D+13
I= 18 X= -2.601671402180D+13 Y= -3.242539590104D+13 Z= -6.455719293977D+13
I= 19 X= 1.138365571390D+14 Y= -2.968860089490D+13 Z= 2.961312430328D+13
I= 20 X= -5.280775709181D+13 Y= 1.632903038030D+13 Z= -3.615386856731D+12
I= 21 X= -7.357583096251D+12 Y= -1.884411064142D+13 Z= -4.249860289881D+12
I= 22 X= -6.503148142365D+12 Y= -2.155763722981D+13 Z= 4.854024419893D+13
I= 23 X= 8.825579846357D+13 Y= 1.110872759930D+14 Z= -4.447053166129D+13
I= 24 X= 2.996340107148D+13 Y= -7.269068997808D+13 Z= -4.560962714612D+13
I= 25 X= -1.049802881155D+13 Y= -2.469746500716D+12 Z= -1.970962506615D+12
I= 26 X= -2.658913468160D+12 Y= 8.456315534881D+13 Z= 5.984011332423D+13

I= 27 X= -1.461914572783D+13 Y= -7.390059560699D+13 Z= -6.754304618743D+13
I= 28 X= 2.323229374328D+13 Y= -2.181934297995D+13 Z= 2.590856205604D+13
I= 29 X= -6.462004320923D+12 Y= -5.484633046467D+12 Z= -1.654310818287D+13
I= 30 X= 1.077925326935D+13 Y= 4.364434735925D+12 Z= 1.517727390387D+13
I= 31 X= 9.788013702846D+13 Y= 1.178279917258D+14 Z= -1.259596275057D+13
I= 32 X= -9.748533561884D+13 Y= -6.142148037461D+13 Z= 4.768761759157D+12
I= 33 X= 5.008426480376D+13 Y= -2.916602008182D+13 Z= -2.193461351774D+13
I= 34 X= 3.663880970133D+12 Y= -6.255167103227D+13 Z= 6.179044787163D+13
I= 35 X= 3.638402568328D+12 Y= 2.727008045494D+12 Z= -1.102979178809D+12
I= 36 X= -1.252969863552D+12 Y= 5.957963633960D+12 Z= -1.930426073079D+12
I= 37 X= 5.193616923784D+13 Y= -9.331605405096D+13 Z= 3.996221055666D+13
I= 38 X= -4.422014463759D+13 Y= -3.864435844536D+13 Z= -1.018822470689D+13

Backward Direction:

Total Energy: -656.4400785 Hartrees

Potential Energy: -656.6076346 Hartress

Kinetic Energy: 0.1675560 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.285747083832D+12 Y= 1.516682731248D+12 Z= 7.069425585592D+12
I= 1 X= -2.077747989133D+13 Y= 1.813492141891D+13 Z= 3.535083843577D+12
I= 2 X= -4.373518361344D+12 Y= -2.590890226035D+12 Z= -1.592068915677D+13
I= 3 X= 1.487919430273D+13 Y= -5.266076395347D+12 Z= 1.469710269781D+13
I= 4 X= -1.638374401505D+13 Y= 4.056807896548D+12 Z= -2.025577685908D+13
I= 5 X= -2.998002373166D+11 Y= 7.488052195724D+12 Z= 2.997544435095D+11
I= 6 X= 1.037228812408D+14 Y= 1.383974732510D+13 Z= -1.885617269286D+13
I= 7 X= -6.305520853139D+13 Y= -3.098677604070D+13 Z= 4.575706592735D+13
I= 8 X= -3.654131551872D+13 Y= 9.121532255133D+13 Z= -5.713292106461D+12
I= 9 X= 1.195969737332D+13 Y= 1.084297377926D+13 Z= 1.530601537998D+13
I= 10 X= -7.703758120218D+12 Y= -7.432708246515D+13 Z= -1.056534748497D+13
I= 11 X= -6.354163095023D+13 Y= -1.509063789975D+14 Z= 1.154305783935D+13
I= 12 X= -6.738934663398D+13 Y= 7.503850711555D+12 Z= 8.553798549459D+13

I= 13 X= 4.784214410214D+11 Y= -1.856433242647D+13 Z= 1.217358298134D+13
I= 14 X= -1.466877407453D+13 Y= -7.868759237189D+12 Z= 3.211503609200D+13
I= 15 X= -1.500191686450D+13 Y= -3.693870066686D+12 Z= 7.950366226962D+13
I= 16 X= 3.841518829297D+13 Y= 1.418296751435D+14 Z= -4.616829087046D+13
I= 17 X= -3.548038542977D+12 Y= -1.603674665949D+12 Z= -2.194641777235D+13
I= 18 X= -2.598479133161D+13 Y= -3.295808024656D+13 Z= -6.499417540762D+13
I= 19 X= 1.135164929114D+14 Y= -2.979522218310D+13 Z= 2.994316048175D+13
I= 20 X= -5.258549492076D+13 Y= 1.603047794238D+13 Z= -3.653512465899D+12
I= 21 X= -7.548097031017D+12 Y= -1.896379575120D+13 Z= -4.714933828431D+12
I= 22 X= -6.537194527604D+12 Y= -2.102127570554D+13 Z= 4.667639762372D+13
I= 23 X= 8.894829643247D+13 Y= 1.107858390535D+14 Z= -4.468665369900D+13
I= 24 X= 2.962955848467D+13 Y= -7.287818974463D+13 Z= -4.615952363431D+13
I= 25 X= -1.070507923387D+13 Y= -2.678910717508D+12 Z= -2.077806194508D+12
I= 26 X= -3.171039879217D+12 Y= 8.400292862652D+13 Z= 5.977762712132D+13
I= 27 X= -1.419232694895D+13 Y= -7.354124884982D+13 Z= -6.766691736486D+13
I= 28 X= 2.325344374330D+13 Y= -2.245327129505D+13 Z= 2.635728333483D+13
I= 29 X= -7.420879971661D+12 Y= -5.215292347901D+12 Z= -1.687942059151D+13
I= 30 X= 1.083572059623D+13 Y= 4.178868088535D+12 Z= 1.476077553512D+13
I= 31 X= 9.721719988994D+13 Y= 1.176318651188D+14 Z= -1.257524830317D+13
I= 32 X= -9.942546397565D+13 Y= -5.981032172128D+13 Z= 3.613668161357D+12
I= 33 X= 5.014409870414D+13 Y= -2.940052930837D+13 Z= -2.226635598554D+13
I= 34 X= 4.288956251976D+12 Y= -6.298686475000D+13 Z= 6.167081370546D+13
I= 35 X= 3.627971070939D+12 Y= 2.970655515940D+12 Z= 4.428139206162D+11
I= 36 X= -4.624103296539D+12 Y= 1.699944333631D+12 Z= -3.484284897996D+12
I= 37 X= 5.494353227742D+13 Y= -9.178932207859D+13 Z= 3.621154755643D+13
I= 38 X= -4.257319597257D+13 Y= -3.881597350382D+13 Z= -1.298931138099D+13

Seed: 28801055485

CM Start Point Coordinates: bohr

I= 0 X= -2.107220603189D+00 Y= 2.305312964282D+00 Z= -5.331418085446D-01

I= 1 X= -2.874414283892D+00 Y= 6.388447098391D-02 Z= -1.892876399868D+00
I= 2 X= -1.885293072112D+00 Y= 1.575149600514D+00 Z= 2.131680845058D+00
I= 3 X= -2.709343989140D+00 Y= -2.153972070738D+00 Z= -2.544454572310D-01
I= 4 X= -2.278084898857D+00 Y= -1.007584470609D+00 Z= 2.302062257554D+00
I= 5 X= 3.888146918697D+00 Y= 2.966358356525D+00 Z= -1.844481615471D+00
I= 6 X= 2.201953339684D+00 Y= 2.893123932745D-01 Z= -3.294370803700D+00
I= 7 X= 5.771475536449D+00 Y= 2.530344811980D+00 Z= -3.131552202054D+00
I= 8 X= 2.290398688065D+00 Y= 4.502438903242D+00 Z= -2.706331665993D+00
I= 9 X= -2.459235296001D+00 Y= -2.436069891215D+00 Z= 4.653645040693D+00
I= 10 X= -4.313803748487D+00 Y= -2.392498353215D+00 Z= 5.189465188437D+00
I= 11 X= -1.558633269115D+00 Y= -4.243454397504D+00 Z= 4.434996586931D+00
I= 12 X= -1.074405959308D+00 Y= -1.632519121741D+00 Z= 5.996486520365D+00
I= 13 X= -1.668718949842D+00 Y= 3.529873622373D+00 Z= 4.159367907567D+00
I= 14 X= -3.595200466146D+00 Y= 3.774018780563D+00 Z= 5.092119674543D+00
I= 15 X= -5.016867958639D-01 Y= 2.993745579831D+00 Z= 5.986584776503D+00
I= 16 X= -1.164198128934D+00 Y= 5.360280227618D+00 Z= 3.682483669150D+00
I= 17 X= -2.053757254606D+00 Y= 5.017355853099D+00 Z= -1.466689314609D+00
I= 18 X= -3.552867770939D+00 Y= 6.653385697569D+00 Z= -9.434962751919D-02
I= 19 X= 2.786881139627D-01 Y= 5.994924526219D+00 Z= -1.220246808635D+00
I= 20 X= -2.673579377577D+00 Y= 4.997898403610D+00 Z= -3.654930106188D+00
I= 21 X= -3.493214251697D+00 Y= -6.768881623768D-03 Z= -4.600411522637D+00
I= 22 X= -5.583536685130D+00 Y= 3.241803370529D-01 Z= -4.861432237896D+00
I= 23 X= -2.609499852164D+00 Y= 1.314757459953D+00 Z= -5.612421164051D+00
I= 24 X= -3.140428117066D+00 Y= -1.784989262652D+00 Z= -5.583713669606D+00
I= 25 X= -3.098749230148D+00 Y= -4.787373967706D+00 Z= -8.934177823516D-01
I= 26 X= -2.688051634884D+00 Y= -5.298115103471D+00 Z= -2.974926299214D+00
I= 27 X= -1.920896610626D+00 Y= -6.019996520250D+00 Z= 3.795081359943D-01
I= 28 X= -5.150191500534D+00 Y= -5.302715590443D+00 Z= -5.826384899042D-01
I= 29 X= 3.519276307052D+00 Y= -3.551449940809D+00 Z= -1.272803898760D+00
I= 30 X= 3.544236270163D+00 Y= -3.254308691921D+00 Z= 1.388776867248D+00

I= 31 X= 2.241314141238D+00 Y= -4.670109747193D+00 Z= -2.404353461925D+00
I= 32 X= 5.209267751941D+00 Y= -2.856983070285D+00 Z= -2.212564087987D+00
I= 33 X= 5.030936330402D+00 Y= -2.337187033207D+00 Z= 2.368855419492D+00
I= 34 X= 2.162132199577D+00 Y= -4.376398000234D+00 Z= 2.649747385284D+00
I= 35 X= 1.191500405073D+00 Y= -1.346539815319D-01 Z= -3.385454500955D-01
I= 36 X= 3.916059662452D+00 Y= 2.584276775933D+00 Z= 9.219196116255D-01
I= 37 X= 5.920251340266D+00 Y= 1.787808800350D+00 Z= 1.723765432366D+00
I= 38 X= 2.975809041776D+00 Y= 4.083320831461D+00 Z= 2.067865139359D+00

Forward Direction:

Total Energy: -656.4382827 Hartrees

Potential Energy: -656.6298109 Hartress

Kinetic Energy: 0.1915282 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.656893657006D+13 Y= 1.968166641147D+13 Z= -1.340107344481D+13
I= 1 X= 1.518607630710D+13 Y= -1.600212278047D+10 Z= 9.559877036534D+12
I= 2 X= 6.650366299375D+12 Y= 2.720353517037D+13 Z= 1.710425519040D+13
I= 3 X= -6.846008964696D+12 Y= -2.314887315669D+13 Z= 6.434619771963D+12
I= 4 X= -1.551039729791D+13 Y= -7.583717470904D+12 Z= -1.463152845180D+13
I= 5 X= 2.072409487509D+13 Y= -8.319023026506D+12 Z= 1.403459458635D+13
I= 6 X= -7.195964339290D+12 Y= -6.358113018783D+12 Z= -7.674053198492D+13
I= 7 X= -6.190595046913D+13 Y= 7.279396139726D+13 Z= -1.011639320491D+13
I= 8 X= -5.829935337252D+13 Y= 9.371306013546D+13 Z= 3.207935449667D+13
I= 9 X= 3.014521987188D+12 Y= 5.494515154570D+12 Z= -1.633039199223D+13
I= 10 X= -1.197937597451D+14 Y= 4.199498400916D+13 Z= 1.131137631026D+14
I= 11 X= -2.711457257174D+13 Y= 1.007672626668D+14 Z= -8.939466132544D+12
I= 12 X= -1.926188955101D+13 Y= -9.819659686736D+13 Z= 1.168714218579D+13
I= 13 X= -1.164526381168D+13 Y= -1.169453962815D+12 Z= -3.739098409750D+11
I= 14 X= 5.238728042764D+13 Y= 6.359003687220D+13 Z= -3.786480138435D+13
I= 15 X= 1.242346417819D+13 Y= 4.077451087155D+13 Z= 3.754962178273D+13
I= 16 X= -7.238696744046D+13 Y= -1.480185855589D+13 Z= 5.322499471886D+13

I= 17 X= 2.290598565291D+13 Y= 4.843747755670D+12 Z= 1.814503499026D+13
I= 18 X= -1.525507539274D+14 Y= -1.624210574404D+13 Z= -5.335941015848D+13
I= 19 X= -1.972857384636D+13 Y= -4.812394158928D+12 Z= -5.011322711681D+13
I= 20 X= -9.288788041258D+13 Y= -6.500079076699D+13 Z= -6.889539255874D+13
I= 21 X= -7.716992764717D+12 Y= 2.104042380849D+12 Z= -1.088761075243D+13
I= 22 X= 9.163417403712D+13 Y= 4.811640602541D+13 Z= 2.279257197229D+13
I= 23 X= -5.130722591084D+13 Y= 2.018450421918D+13 Z= -4.206347997624D+13
I= 24 X= 1.233588046796D+13 Y= 6.232957650266D+13 Z= 6.853409540980D+13
I= 25 X= 9.274058600472D+12 Y= 1.176418278800D+12 Z= -8.938062163903D+12
I= 26 X= -5.685978177135D+13 Y= 2.914139965186D+13 Z= 3.908971577377D+13
I= 27 X= 8.615239293082D+13 Y= -8.894063658523D+13 Z= 1.206142890980D+14
I= 28 X= -3.119178373894D+13 Y= 4.670854997079D+13 Z= 1.903730403866D+13
I= 29 X= 7.426663379715D+12 Y= -4.605066726092D+11 Z= 9.405027181926D+12
I= 30 X= 1.145727916322D+13 Y= 9.867301529526D+12 Z= 1.027779492440D+13
I= 31 X= -2.211832131680D+13 Y= 3.591763450972D+12 Z= -3.802238286037D+13
I= 32 X= -1.173459274129D+14 Y= -3.960380872666D+13 Z= -9.787325543361D+13
I= 33 X= -5.707348050027D+13 Y= 1.108860162172D+12 Z= -1.095100640693D+13
I= 34 X= -3.402462898553D+13 Y= -8.997203120531D+13 Z= 1.116487094373D+14
I= 35 X= 1.044531063963D+12 Y= -3.355460192026D+12 Z= -3.484610639461D+12
I= 36 X= 1.839381810216D+13 Y= -1.565281002436D+13 Z= -1.057943310699D+12
I= 37 X= 3.389777758827D+13 Y= -6.378330576396D+13 Z= -1.727441635967D+13
I= 38 X= -7.009299839648D+13 Y= 3.856503180711D+13 Z= 8.355015380883D+12

Backward Direction:

Total Energy: -656.4382518 Hartrees

Potential Energy: -656.6298109 Hartress

Kinetic Energy: 0.1915591 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.686250447248D+13 Y= 1.929830930356D+13 Z= -1.325105564002D+13

I= 1 X= 1.473328378518D+13 Y= -1.001803195860D+12 Z= 8.968097895718D+12

I= 2 X= 6.228938346751D+12 Y= 2.759092072050D+13 Z= 1.648054805784D+13

I= 3 X= -7.709493059708D+12 Y= -2.312868244482D+13 Z= 5.183520079832D+12
I= 4 X= -1.403350350334D+13 Y= -7.715483239679D+12 Z= -1.561294812986D+13
I= 5 X= 1.828662496534D+13 Y= -1.178537168952D+13 Z= 7.113977140307D+12
I= 6 X= 4.740295367207D+13 Y= 5.597310802269D+13 Z= -5.217458452872D+13
I= 7 X= -5.193345638075D+13 Y= 8.223579200647D+13 Z= -9.506278208755D+12
I= 8 X= -4.570450489705D+13 Y= 1.038937168640D+14 Z= 3.325108821142D+13
I= 9 X= 3.483922062048D+12 Y= 5.714954250033D+12 Z= -1.686096855459D+13
I= 10 X= -1.197079102326D+14 Y= 4.308592855431D+13 Z= 1.118491322790D+14
I= 11 X= -2.725014461658D+13 Y= 1.007553369273D+14 Z= -8.965828718929D+12
I= 12 X= -1.898678811966D+13 Y= -9.812291423268D+13 Z= 1.142590540160D+13
I= 13 X= -1.155221209261D+13 Y= -1.214729367787D+12 Z= -5.697551789952D+11
I= 14 X= 5.254547495373D+13 Y= 6.331111141829D+13 Z= -3.782339954412D+13
I= 15 X= 1.271438486028D+13 Y= 4.050768633681D+13 Z= 3.706787850129D+13
I= 16 X= -7.240723288742D+13 Y= -1.471610090490D+13 Z= 5.329281944193D+13
I= 17 X= 2.304848386349D+13 Y= 4.529275409388D+12 Z= 1.811389308530D+13
I= 18 X= -1.525207089021D+14 Y= -1.674345809046D+13 Z= -5.377068972152D+13
I= 19 X= -2.002981219636D+13 Y= -4.912744082008D+12 Z= -4.980260336215D+13
I= 20 X= -9.267869150218D+13 Y= -6.528178262374D+13 Z= -6.893127566172D+13
I= 21 X= -7.896300846369D+12 Y= 1.991397037689D+12 Z= -1.132532909568D+13
I= 22 X= 9.160213022817D+13 Y= 4.862121926556D+13 Z= 2.103835513464D+13
I= 23 X= -5.065546003060D+13 Y= 1.990079751681D+13 Z= -4.226688991634D+13
I= 24 X= 1.202167419042D+13 Y= 6.215310529540D+13 Z= 6.801654332407D+13
I= 25 X= 9.079186695954D+12 Y= 9.795569077789D+11 Z= -9.038621403327D+12
I= 26 X= -5.734178538081D+13 Y= 2.861412494100D+13 Z= 3.903090495272D+13
I= 27 X= 8.655410661940D+13 Y= -8.860242627651D+13 Z= 1.204977039163D+14
I= 28 X= -3.117187776102D+13 Y= 4.611190873988D+13 Z= 1.945963194057D+13
I= 29 X= 6.524187909830D+12 Y= -2.070083434721D+11 Z= 9.088496358184D+12
I= 30 X= 1.151042513248D+13 Y= 9.692649739524D+12 Z= 9.885794605500D+12
I= 31 X= -2.274226510347D+13 Y= 3.407172832103D+12 Z= -3.800288682103D+13
I= 32 X= -1.191719392093D+14 Y= -3.808741693676D+13 Z= -9.896040749109D+13

I= 33 X= -5.701716597699D+13 Y= 8.881445502130D+11 Z= -1.126323608653D+13
I= 34 X= -3.343632005805D+13 Y= -9.038162723419D+13 Z= 1.115361120412D+14
I= 35 X= 1.034713137754D+12 Y= -3.126143840573D+12 Z= -2.029739662673D+12
I= 36 X= 1.522097162545D+13 Y= -1.966037656140D+13 Z= -2.520405595094D+12
I= 37 X= 3.672825031065D+13 Y= -6.234637475729D+13 Z= -2.080446882495D+13
I= 38 X= -6.854292172855D+13 Y= 3.840351098670D+13 Z= 5.718686041203D+12

Seed: 29461475743

CM Start Point Coordinates: bohr

I= 0 X= -2.277142533219D+00 Y= 2.369622252300D+00 Z= -5.939761334575D-01
I= 1 X= -2.688950440860D+00 Y= 5.857268764421D-02 Z= -1.990097416546D+00
I= 2 X= -1.849338657067D+00 Y= 1.585501630137D+00 Z= 2.116854018758D+00
I= 3 X= -2.576603056424D+00 Y= -2.029211999525D+00 Z= -3.938492249595D-01
I= 4 X= -2.059296909554D+00 Y= -1.001915485734D+00 Z= 2.127837083583D+00
I= 5 X= 3.705907829886D+00 Y= 2.832120658238D+00 Z= -1.973770400243D+00
I= 6 X= 2.183515191775D+00 Y= -8.077540274056D-02 Z= -3.049717770272D+00
I= 7 X= 5.519433530519D+00 Y= 2.165263170312D+00 Z= -3.316573799305D+00
I= 8 X= 2.258233690666D+00 Y= 4.267954338216D+00 Z= -2.893721152063D+00
I= 9 X= -2.218934662427D+00 Y= -2.522924820811D+00 Z= 4.453751357920D+00
I= 10 X= -4.075855680509D+00 Y= -1.766975084714D+00 Z= 5.574718551248D+00
I= 11 X= -2.376140298450D+00 Y= -4.855145002025D+00 Z= 4.085974412027D+00
I= 12 X= -4.684420499172D-01 Y= -2.453836315461D+00 Z= 5.994428473031D+00
I= 13 X= -1.842044793314D+00 Y= 3.203754967432D+00 Z= 4.552043572825D+00
I= 14 X= -3.797875827486D+00 Y= 4.033004320947D+00 Z= 4.974280576832D+00
I= 15 X= -8.466828852299D-01 Y= 2.380762166934D+00 Z= 6.280611964366D+00
I= 16 X= -6.734549740994D-01 Y= 5.074887359443D+00 Z= 3.910094460980D+00
I= 17 X= -2.096167119186D+00 Y= 4.910981505572D+00 Z= -1.580140781766D+00
I= 18 X= -3.846760248856D+00 Y= 6.432918648185D+00 Z= -8.756567083016D-01
I= 19 X= -3.330378531005D-01 Y= 6.078795138815D+00 Z= -8.858123839491D-01
I= 20 X= -2.143647283686D+00 Y= 4.809686425098D+00 Z= -3.532411546710D+00

I= 21 X= -3.623471895139D+00 Y= -6.199219124654D-02 Z= -4.699915264592D+00
I= 22 X= -5.623643687291D+00 Y= 6.423697078153D-01 Z= -5.045956458903D+00
I= 23 X= -2.382494495151D+00 Y= 1.206105324220D+00 Z= -6.003681323699D+00
I= 24 X= -3.798521073826D+00 Y= -2.146074037774D+00 Z= -5.352539579375D+00
I= 25 X= -3.215020952768D+00 Y= -4.716217192334D+00 Z= -9.165366597612D-01
I= 26 X= -2.631605515939D+00 Y= -5.299401430168D+00 Z= -2.821455395330D+00
I= 27 X= -2.518088850779D+00 Y= -6.078424934579D+00 Z= 6.775241679201D-01
I= 28 X= -5.674374965581D+00 Y= -4.507818822717D+00 Z= -1.125629182512D+00
I= 29 X= 3.374505328635D+00 Y= -3.563510477986D+00 Z= -9.857439710907D-01
I= 30 X= 3.554328709219D+00 Y= -3.143111621801D+00 Z= 1.633175401845D+00
I= 31 X= 2.150072744973D+00 Y= -4.922629803919D+00 Z= -1.847245036554D+00
I= 32 X= 4.972817143263D+00 Y= -3.305094767692D+00 Z= -2.125418415290D+00
I= 33 X= 5.421513245128D+00 Y= -2.500450864237D+00 Z= 2.315323271023D+00
I= 34 X= 2.747057539808D+00 Y= -4.138370850848D+00 Z= 3.154288626586D+00
I= 35 X= 1.174173953037D+00 Y= -6.758353167709D-02 Z= -3.088934674696D-01
I= 36 X= 4.277137989543D+00 Y= 2.606220006142D+00 Z= 7.647392025530D-01
I= 37 X= 6.208998871031D+00 Y= 1.529433346111D+00 Z= 1.270757671073D+00
I= 38 X= 3.371687957034D+00 Y= 4.048994382083D+00 Z= 2.239454769502D+00

Forward Direction:

Total Energy: -656.4294854 Hartrees

Potential Energy: -656.6195926 Hartress

Kinetic Energy: 0.1901073 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.002556125267D+12 Y= 1.491453162004D+13 Z= -3.005900055802D+13
I= 1 X= 8.670452460575D+12 Y= 7.406005341441D+12 Z= -3.426390122860D+13
I= 2 X= -2.037952598174D+13 Y= -1.251835749549D+12 Z= 2.321800885509D+12
I= 3 X= -1.274867559464D+11 Y= -1.009118849084D+13 Z= 3.691146669355D+13
I= 4 X= -5.980152912257D+12 Y= 1.128777866205D+13 Z= -8.113392745860D+11
I= 5 X= 1.259811524243D+13 Y= -5.871967476924D+12 Z= 2.377340886415D+13
I= 6 X= 1.466265500932D+13 Y= -1.197203195262D+13 Z= -6.477403183986D+13

I= 7 X= -2.341349356521D+13 Y= 7.048630336217D+13 Z= -7.091750820685D+13
I= 8 X= -1.049209279269D+13 Y= -6.452147000587D+13 Z= -1.064787435913D+14
I= 9 X= -1.553984150786D+13 Y= -4.523060688615D+12 Z= 2.762597083170D+13
I= 10 X= 4.833937139805D+13 Y= 8.142315318371D+13 Z= -4.156775022099D+12
I= 11 X= 2.546749757761D+12 Y= -3.058558467142D+13 Z= -2.587990036638D+12
I= 12 X= -3.554723244792D+13 Y= 3.440181260001D+13 Z= 1.051558153114D+13
I= 13 X= -1.469211157645D+13 Y= 7.184647198772D+12 Z= 1.643597498353D+13
I= 14 X= -8.702930583085D+12 Y= -4.115384561877D+13 Z= -2.889838758105D+13
I= 15 X= 7.381235215525D+13 Y= -9.997559068496D+13 Z= 1.314256268267D+14
I= 16 X= -1.368805999944D+12 Y= 4.788547206355D+13 Z= 1.976156320603D+12
I= 17 X= -2.549439249430D+12 Y= -2.203302357285D+13 Z= 5.294321570789D+12
I= 18 X= 8.568368688474D+13 Y= 4.003370758004D+13 Z= -4.177146046340D+13
I= 19 X= -6.414237312264D+13 Y= -7.030730248807D+13 Z= -3.666124486378D+13
I= 20 X= -3.730348349748D+13 Y= 9.182923171208D+12 Z= 3.851476727269D+13
I= 21 X= -1.004879933461D+13 Y= 2.808250544159D+10 Z= 7.535599288368D+12
I= 22 X= 1.592984915267D+14 Y= 1.721193010538D+13 Z= -1.195044355608D+13
I= 23 X= 4.785625427868D+13 Y= 3.968038643052D+13 Z= 4.268079518260D+12
I= 24 X= -6.021373821730D+13 Y= 1.520686688910D+13 Z= 6.240893745029D+12
I= 25 X= -1.084191521205D+12 Y= -2.411729644735D+12 Z= -2.114773712171D+13
I= 26 X= -1.985402778649D+13 Y= 2.703092691369D+12 Z= 5.547280512734D+13
I= 27 X= -3.891622744424D+13 Y= 5.894848998667D+12 Z= 2.561600460470D+13
I= 28 X= -3.587149739984D+12 Y= 1.354910641833D+13 Z= 1.159261404306D+13
I= 29 X= -1.690959057359D+13 Y= -1.439728145003D+13 Z= -2.904057092965D+12
I= 30 X= -1.873272952134D+12 Y= 5.573838985537D+12 Z= 1.019899473248D+13
I= 31 X= 4.756052931484D+13 Y= -2.878918533119D+13 Z= -1.980997756211D+13
I= 32 X= 4.263148867087D+13 Y= 3.771976040882D+13 Z= 3.250323902591D+13
I= 33 X= 3.500728037082D+13 Y= -1.824979167199D+13 Z= -2.788951052109D+13
I= 34 X= 9.021939213280D+13 Y= 8.075374689104D+13 Z= -2.253049424144D+14
I= 35 X= 1.484656063045D+12 Y= 1.213164488365D+12 Z= -7.916189449914D+10
I= 36 X= 1.317772126052D+13 Y= -2.527726059767D+12 Z= -1.425881283438D+13

I= 37 X= 9.655782998166D+13 Y= -7.160004371778D+13 Z= 7.258103925035D+13

I= 38 X= -4.766098669117D+13 Y= 1.614856194903D+13 Z= -5.877191073892D+13

Backward Direction:

Total Energy: -656.4294551 Hartrees

Potential Energy: -656.6195926 Hartress

Kinetic Energy: 0.1901375 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.693691268432D+12 Y= 1.451119890902D+13 Z= -2.990116576993D+13

I= 1 X= 8.194066262381D+12 Y= 6.368837096240D+12 Z= -3.488651622671D+13

I= 2 X= -2.082291329550D+13 Y= -8.442646864166D+11 Z= 1.665594222265D+12

I= 3 X= -1.035964447372D+12 Y= -1.006994570100D+13 Z= 3.559517590501D+13

I= 4 X= -4.426302558347D+12 Y= 1.114914696873D+13 Z= -1.843897823310D+12

I= 5 X= 1.003363600083D+13 Y= -9.518937296666D+12 Z= 1.649217855473D+13

I= 6 X= 7.210656081886D+13 Y= 5.360708428248D+13 Z= -3.892802566971D+13

I= 7 X= -1.292136236668D+13 Y= 8.042011977669D+13 Z= -7.027560192448D+13

I= 8 X= 2.759035911906D+12 Y= -5.381032942985D+13 Z= -1.052459543066D+14

I= 9 X= -1.504598238722D+13 Y= -4.291135164743D+12 Z= 2.706774749779D+13

I= 10 X= 4.842969427322D+13 Y= 8.257094360093D+13 Z= -5.487302009342D+12

I= 11 X= 2.404113469763D+12 Y= -3.059813182688D+13 Z= -2.615726301406D+12

I= 12 X= -3.525779630472D+13 Y= 3.447933462181D+13 Z= 1.024073246771D+13

I= 13 X= -1.459421120959D+13 Y= 7.137012627921D+12 Z= 1.622992472399D+13

I= 14 X= -8.536493005122D+12 Y= -4.144730504617D+13 Z= -2.885482841415D+13

I= 15 X= 7.411843185160D+13 Y= -1.002563186514D+14 Z= 1.309187813229D+14

I= 16 X= -1.390127413069D+12 Y= 4.797569829031D+13 Z= 2.047515184306D+12

I= 17 X= -2.399515881125D+12 Y= -2.236388213950D+13 Z= 5.261556955214D+12

I= 18 X= 8.571529746992D+13 Y= 3.950623124892D+13 Z= -4.220417057917D+13

I= 19 X= -6.445930811229D+13 Y= -7.041288135564D+13 Z= -3.633443543594D+13

I= 20 X= -3.708339437475D+13 Y= 8.887289661577D+12 Z= 3.847701439791D+13

I= 21 X= -1.023745062941D+13 Y= -9.043245190960D+10 Z= 7.075072739850D+12

I= 22 X= 1.592647780090D+14 Y= 1.774304766611D+13 Z= -1.379606743506D+13

I= 23 X= 4.854198174447D+13 Y= 3.938189661565D+13 Z= 4.054070490252D+12
I= 24 X= -6.054431685435D+13 Y= 1.502120029135D+13 Z= 5.696373552894D+12
I= 25 X= -1.289217624327D+12 Y= -2.618848878809D+12 Z= -2.125353620498D+13
I= 26 X= -2.036114717471D+13 Y= 2.148343259774D+12 Z= 5.541092984773D+13
I= 27 X= -3.849358164536D+13 Y= 6.250682448088D+12 Z= 2.549334451256D+13
I= 28 X= -3.566206522201D+12 Y= 1.292137597939D+13 Z= 1.203694820211D+13
I= 29 X= -1.785909136416D+13 Y= -1.413057407416D+13 Z= -3.237081400690D+12
I= 30 X= -1.817357703859D+12 Y= 5.390086608559D+12 Z= 9.786568438738D+12
I= 31 X= 4.690407366824D+13 Y= -2.898339442006D+13 Z= -1.978946564307D+13
I= 32 X= 4.071032881292D+13 Y= 3.931516688298D+13 Z= 3.135943869663D+13
I= 33 X= 3.506652927880D+13 Y= -1.848200811841D+13 Z= -2.821800956431D+13
I= 34 X= 9.083835609290D+13 Y= 8.032280802564D+13 Z= -2.254234069280D+14
I= 35 X= 1.474326553925D+12 Y= 1.454429835257D+12 Z= 1.451518097154D+12
I= 36 X= 9.839547157855D+12 Y= -6.744115012437D+12 Z= -1.579747969352D+13
I= 37 X= 9.953579024812D+13 Y= -7.008823849515D+13 Z= 6.886704621419D+13
I= 38 X= -4.603014012268D+13 Y= 1.597862475847D+13 Z= -6.154561138718D+13

Seed: 30047930840

CM Start Point Coordinates: bohr

I= 0 X= -2.463821275101D+00 Y= 2.345698289588D+00 Z= -4.602381604126D-01
I= 1 X= -2.763656526715D+00 Y= 1.823317673000D-01 Z= -1.835668776517D+00
I= 2 X= -2.034922446444D+00 Y= 1.605199845908D+00 Z= 1.975915520207D+00
I= 3 X= -2.564827279669D+00 Y= -1.999258847277D+00 Z= -2.074197495209D-01
I= 4 X= -2.150808573686D+00 Y= -9.827338734319D-01 Z= 2.300835093349D+00
I= 5 X= 4.193028738150D+00 Y= 2.592745756795D+00 Z= -1.592166977002D+00
I= 6 X= 2.338305220947D+00 Y= 1.155599606110D-01 Z= -2.919523780405D+00
I= 7 X= 5.702847961584D+00 Y= 1.724186256744D+00 Z= -2.741972784743D+00
I= 8 X= 2.962928674732D+00 Y= 4.513278967306D+00 Z= -2.244775802959D+00
I= 9 X= -1.957924296378D+00 Y= -2.559620584713D+00 Z= 4.786180970438D+00
I= 10 X= -4.178539531253D+00 Y= -2.687609434512D+00 Z= 5.079599339805D+00

I= 11 X= -1.493416241364D+00 Y= -4.498109112431D+00 Z= 4.312332761196D+00
I= 12 X= -1.100194797157D+00 Y= -1.542792226890D+00 Z= 6.256837199006D+00
I= 13 X= -1.844015220728D+00 Y= 3.443132490440D+00 Z= 4.263162119533D+00
I= 14 X= -3.756284066483D+00 Y= 3.169855357735D+00 Z= 5.271211281152D+00
I= 15 X= -5.095127500028D-01 Y= 2.988860150916D+00 Z= 5.239696333214D+00
I= 16 X= -1.803115927768D+00 Y= 5.409859232056D+00 Z= 3.401570910931D+00
I= 17 X= -2.308583969578D+00 Y= 4.840096107524D+00 Z= -1.720552390327D+00
I= 18 X= -3.940011772188D+00 Y= 5.727399649724D+00 Z= -1.682166814186D+00
I= 19 X= -1.053396248922D+00 Y= 6.300619316793D+00 Z= -7.076983998688D-01
I= 20 X= -1.467859316981D+00 Y= 4.689693142247D+00 Z= -3.559430336627D+00
I= 21 X= -3.136424178398D+00 Y= 7.569756471947D-02 Z= -4.637331673598D+00
I= 22 X= -5.014231044563D+00 Y= 2.209862225379D-01 Z= -5.542829531572D+00
I= 23 X= -2.224752853400D+00 Y= 1.235215792560D+00 Z= -6.011513640010D+00
I= 24 X= -2.503829966175D+00 Y= -1.788441016437D+00 Z= -5.083124031263D+00
I= 25 X= -2.959193749052D+00 Y= -4.752862697813D+00 Z= -6.455252831765D-01
I= 26 X= -2.677019481293D+00 Y= -5.228899337757D+00 Z= -2.428547936753D+00
I= 27 X= -1.650565354608D+00 Y= -5.561211312178D+00 Z= 8.840591101441D-01
I= 28 X= -4.575381193803D+00 Y= -5.225629831357D+00 Z= 5.935128836226D-01
I= 29 X= 3.214697930744D+00 Y= -3.659458867528D+00 Z= -1.385356945235D+00
I= 30 X= 3.543966874716D+00 Y= -3.438607405019D+00 Z= 1.134498576137D+00
I= 31 X= 1.357672580405D+00 Y= -4.723062402190D+00 Z= -1.985008543196D+00
I= 32 X= 4.127952212833D+00 Y= -3.473005075592D+00 Z= -3.197792825858D+00
I= 33 X= 5.444922375638D+00 Y= -2.495907227073D+00 Z= 1.883083879227D+00
I= 34 X= 2.378009944667D+00 Y= -4.468625265661D+00 Z= 2.622580879047D+00
I= 35 X= 1.110310414974D+00 Y= 4.893546494828D-03 Z= -3.767707319377D-01
I= 36 X= 4.133251647734D+00 Y= 2.347547449614D+00 Z= 1.109276387250D+00
I= 37 X= 5.664036887630D+00 Y= 1.302299750262D+00 Z= 2.238351465736D+00
I= 38 X= 2.945281226398D+00 Y= 3.320653110267D+00 Z= 2.052218112090D+00

Forward Direction:

Total Energy: -656.4251097 Hartrees

Potential Energy: -656.5819142 Hartress

Kinetic Energy: 0.1568044 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.483853851582D+13 Y= 1.288036727101D+13 Z= -8.007099933847D+12
I= 1 X= -4.736486330774D+12 Y= -1.068946676687D+13 Z= -9.168626976015D+12
I= 2 X= 7.670972562897D+12 Y= 5.194680435385D+12 Z= 3.118057101240D+12
I= 3 X= -2.067665579865D+12 Y= 2.064761982282D+12 Z= 1.631107842745D+12
I= 4 X= 9.380856939912D+12 Y= -8.231419961815D+12 Z= 2.444203252303D+13
I= 5 X= 1.332068333997D+13 Y= 2.822918926204D+12 Z= 4.004752976974D+12
I= 6 X= -1.063624368133D+12 Y= -3.510026650220D+13 Z= -4.867727244572D+13
I= 7 X= 1.030240523214D+13 Y= -5.825237181607D+13 Z= -1.219589393826D+14
I= 8 X= -4.553567946842D+13 Y= 1.137962363485D+13 Z= -7.510155972040D+13
I= 9 X= 7.760291048242D+12 Y= 1.731333140174D+13 Z= 4.834651375486D+12
I= 10 X= 1.124658546681D+14 Y= -5.573937775139D+13 Z= -5.320121732637D+13
I= 11 X= -6.500983594845D+13 Y= -3.316144544140D+13 Z= 6.551652213193D+13
I= 12 X= -9.316908343610D+13 Y= -3.450519731766D+13 Z= -7.061400953023D+12
I= 13 X= 3.022661562251D+12 Y= -3.010079033122D+12 Z= -1.560740831735D+12
I= 14 X= -5.077292764694D+13 Y= -1.933551518474D+13 Z= -1.602351440282D+13
I= 15 X= 1.436243735747D+13 Y= 3.916620236934D+13 Z= -9.436698774203D+12
I= 16 X= 7.526796321251D+13 Y= -4.935471720090D+13 Z= -9.068434066992D+13
I= 17 X= -7.158763460501D+12 Y= 4.096330595822D+12 Z= 1.382715239751D+13
I= 18 X= 2.687629842129D+13 Y= 8.981268018226D+13 Z= -2.578739788186D+13
I= 19 X= -6.083826789002D+12 Y= 3.823992062948D+13 Z= -2.342638343740D+12
I= 20 X= -1.353517221803D+12 Y= 2.171348912544D+13 Z= -5.004489868617D+13
I= 21 X= 1.773694277019D+13 Y= -1.439260426984D+11 Z= -1.636895067410D+13
I= 22 X= -5.281726914926D+13 Y= -2.453117731097D+13 Z= -1.565536495926D+13
I= 23 X= -1.331512929088D+14 Y= -9.737371345023D+13 Z= 5.052172741717D+13
I= 24 X= 3.641042518503D+13 Y= -3.233912688217D+13 Z= 5.392987905871D+13
I= 25 X= -1.189684380287D+13 Y= 1.836783140467D+13 Z= 6.435044807232D+12
I= 26 X= -2.266101169263D+13 Y= 1.554206966757D+13 Z= -1.024044613731D+14

I= 27 X= -6.224997763140D+13 Y= 3.194829291884D+13 Z= -1.055200284188D+14
I= 28 X= -5.668796755456D+13 Y= -7.123284959457D+13 Z= -2.979707593863D+12
I= 29 X= -7.569913504278D+12 Y= 3.703328851033D+12 Z= -1.433872055607D+13
I= 30 X= 2.088975176188D+13 Y= 5.178393417560D+12 Z= -1.137412926681D+13
I= 31 X= 7.093911600582D+13 Y= 1.431865756740D+14 Z= -1.988589400713D+13
I= 32 X= -3.535906069730D+13 Y= 2.420346187922D+13 Z= 7.662217893099D+12
I= 33 X= 1.249750153958D+13 Y= 1.691670774381D+13 Z= 1.210899524807D+14
I= 34 X= -1.633992338657D+13 Y= 3.404480356253D+13 Z= 2.834749223612D+13
I= 35 X= -3.491072210215D+12 Y= -3.418352466284D+12 Z= 4.029241771745D+12
I= 36 X= -7.387608567635D+12 Y= -1.817442335545D+13 Z= -7.073658199928D+11
I= 37 X= -1.746242034588D+13 Y= 6.089446309194D+13 Z= -2.907648919194D+12
I= 38 X= 1.642613230227D+13 Y= -4.063737510936D+13 Z= 4.968897756055D+13

Backward Direction:

Total Energy: -656.4250987 Hartrees

Potential Energy: -656.5819142 Hartress

Kinetic Energy: 0.1568154 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.461032498733D+13 Y= 1.258235349743D+13 Z= -7.890479239676D+12
I= 1 X= -5.088477738174D+12 Y= -1.145580783937D+13 Z= -9.628663665059D+12
I= 2 X= 7.343363313720D+12 Y= 5.495825834514D+12 Z= 2.633200261249D+12
I= 3 X= -2.738919999572D+12 Y= 2.080457817805D+12 Z= 6.585291896736D+11
I= 4 X= 1.052896319136D+13 Y= -8.333851906118D+12 Z= 2.367909745517D+13
I= 5 X= 1.142584537067D+13 Y= 1.282521985523D+11 Z= -1.375189832191D+12
I= 6 X= 4.138042902639D+13 Y= 1.335471704799D+13 Z= -2.958022027880D+13
I= 7 X= 1.805481291675D+13 Y= -5.091249078861D+13 Z= -1.214846487837D+14
I= 8 X= -3.574470849818D+13 Y= 1.929385258853D+13 Z= -7.419067851228D+13
I= 9 X= 8.125192817399D+12 Y= 1.748469612984D+13 Z= 4.422192286955D+12
I= 10 X= 1.125325922717D+14 Y= -5.489130035801D+13 Z= -5.418431480409D+13
I= 11 X= -6.511522680481D+13 Y= -3.317071625961D+13 Z= 6.549602841009D+13
I= 12 X= -9.295522536863D+13 Y= -3.444791797841D+13 Z= -7.264480946407D+12

I= 13 X= 3.094998016149D+12 Y= -3.045275181664D+12 Z= -1.712986890068D+12
I= 14 X= -5.064995054166D+13 Y= -1.955234598065D+13 Z= -1.599132948417D+13
I= 15 X= 1.458859298822D+13 Y= 3.895877857758D+13 Z= -9.811195894990D+12
I= 16 X= 7.525220928014D+13 Y= -4.928805100123D+13 Z= -9.063161515451D+13
I= 17 X= -7.047988343612D+12 Y= 3.851866391157D+12 Z= 1.380294333431D+13
I= 18 X= 2.689965479255D+13 Y= 8.942293938586D+13 Z= -2.610711798086D+13
I= 19 X= -6.318003162813D+12 Y= 3.816191070214D+13 Z= -2.101165960215D+12
I= 20 X= -1.190898157086D+12 Y= 2.149505195169D+13 Z= -5.007279346152D+13
I= 21 X= 1.759755242451D+13 Y= -2.314941688655D+11 Z= -1.670922373044D+13
I= 22 X= -5.284217933980D+13 Y= -2.413874608896D+13 Z= -1.701905632014D+13
I= 23 X= -1.326446237942D+14 Y= -9.759426108894D+13 Z= 5.036360079598D+13
I= 24 X= 3.616616781026D+13 Y= -3.247631189676D+13 Z= 5.352754492500D+13
I= 25 X= -1.204833313395D+13 Y= 1.821479550568D+13 Z= 6.356872163967D+12
I= 26 X= -2.303571118371D+13 Y= 1.513217736747D+13 Z= -1.024501796749D+14
I= 27 X= -6.193769384823D+13 Y= 3.221121051880D+13 Z= -1.056106592901D+14
I= 28 X= -5.667249306959D+13 Y= -7.169666596597D+13 Z= -2.651398748008D+12
I= 29 X= -8.271478999912D+12 Y= 3.900393134250D+12 Z= -1.458478497761D+13
I= 30 X= 2.093106632383D+13 Y= 5.042622780486D+12 Z= -1.167886209060D+13
I= 31 X= 7.045407519776D+13 Y= 1.430430787996D+14 Z= -1.987073819598D+13
I= 32 X= -3.677856395735D+13 Y= 2.538227304359D+13 Z= 6.817088691223D+12
I= 33 X= 1.254127926895D+13 Y= 1.674512805831D+13 Z= 1.208472316784D+14
I= 34 X= -1.588258436751D+13 Y= 3.372639220303D+13 Z= 2.825996138214D+13
I= 35 X= -3.498704458907D+12 Y= -3.240086745742D+12 Z= 5.160227946430D+12
I= 36 X= -9.854112852358D+12 Y= -2.128982150512D+13 Z= -1.844253316843D+12
I= 37 X= -1.526207023179D+13 Y= 6.201150310871D+13 Z= -5.651837645900D+12
I= 38 X= 1.763112938532D+13 Y= -4.076293800764D+13 Z= 4.763955044369D+13

Seed: 3117303747

CM Start Point Coordinates: bohr

I= 0 X= -2.333373186874D+00 Y= 2.403336132100D+00 Z= -5.577833252062D-01

I= 1 X= -2.854188855719D+00 Y= 1.279252914569D-01 Z= -2.008025198348D+00
I= 2 X= -2.156766004625D+00 Y= 1.717427740883D+00 Z= 2.034376076318D+00
I= 3 X= -2.665510050348D+00 Y= -1.963638410864D+00 Z= -3.145571574337D-01
I= 4 X= -2.114649573566D+00 Y= -8.723380851221D-01 Z= 2.268178723035D+00
I= 5 X= 4.607737299491D+00 Y= 2.537636973335D+00 Z= -1.004201988310D+00
I= 6 X= 2.809362983113D+00 Y= 3.822937402584D-01 Z= -2.775822357515D+00
I= 7 X= 6.178624805019D+00 Y= 1.017859001735D+00 Z= -1.488143182339D+00
I= 8 X= 4.666840235160D+00 Y= 4.019008361643D+00 Z= -2.624993797262D+00
I= 9 X= -1.887843835533D+00 Y= -2.414357882139D+00 Z= 4.654793563005D+00
I= 10 X= -3.738020195972D+00 Y= -2.392379150746D+00 Z= 5.993413521622D+00
I= 11 X= -1.522304814092D+00 Y= -4.417926779226D+00 Z= 4.405747363638D+00
I= 12 X= -2.446315506767D-01 Y= -1.779019456634D+00 Z= 5.761471599081D+00
I= 13 X= -1.717658640450D+00 Y= 3.435802824426D+00 Z= 4.254957040192D+00
I= 14 X= -3.362946093263D+00 Y= 3.917158921287D+00 Z= 5.528791398941D+00
I= 15 X= -1.533340482920D-01 Y= 2.423813720825D+00 Z= 5.270198652794D+00
I= 16 X= -8.836143882510D-01 Y= 5.358303581254D+00 Z= 3.680488678859D+00
I= 17 X= -2.130635355802D+00 Y= 5.090213164722D+00 Z= -1.734578542111D+00
I= 18 X= -3.902352360238D+00 Y= 6.270946810900D+00 Z= -1.181049726346D+00
I= 19 X= -2.843498147140D-01 Y= 6.284782064005D+00 Z= -1.522469558044D+00
I= 20 X= -1.816911247113D+00 Y= 4.890012706050D+00 Z= -3.737310271460D+00
I= 21 X= -3.726208604543D+00 Y= -3.951907880220D-01 Z= -4.797055952122D+00
I= 22 X= -5.767357855343D+00 Y= -1.546793969752D+00 Z= -4.481871753857D+00
I= 23 X= -3.947602990625D+00 Y= 1.732032065250D+00 Z= -6.133443429628D+00
I= 24 X= -2.277119733277D+00 Y= -1.821905172903D+00 Z= -5.532325116904D+00
I= 25 X= -3.022100735746D+00 Y= -4.720688757114D+00 Z= -7.454890558429D-01
I= 26 X= -3.108942947505D+00 Y= -4.702997186174D+00 Z= -2.714589583787D+00
I= 27 X= -1.315021662471D+00 Y= -5.733239378489D+00 Z= 2.125912714271D-01
I= 28 X= -4.618468184910D+00 Y= -5.291447067664D+00 Z= 2.818996506656D-01
I= 29 X= 2.916260975298D+00 Y= -3.761354565092D+00 Z= -1.510633374384D+00
I= 30 X= 3.951709216406D+00 Y= -2.964493354594D+00 Z= 8.438773554627D-01

I= 31 X= 1.202712830044D+00 Y= -5.039808370716D+00 Z= -1.991641259398D+00
I= 32 X= 4.182377952588D+00 Y= -3.701189747277D+00 Z= -3.325262015869D+00
I= 33 X= 6.020547701914D+00 Y= -2.000134965154D+00 Z= 9.908319919874D-01
I= 34 X= 3.640283553552D+00 Y= -3.696511105858D+00 Z= 2.844115832562D+00
I= 35 X= 1.111656517184D+00 Y= -1.023181347485D-01 Z= -3.688816457309D-01
I= 36 X= 3.696827933635D+00 Y= 2.606324920307D+00 Z= 1.557267516739D+00
I= 37 X= 4.641251266096D+00 Y= 1.810801621499D+00 Z= 3.238962425441D+00
I= 38 X= 2.451969036615D+00 Y= 4.621370112242D+00 Z= 1.945892470235D+00

Forward Direction:

Total Energy: -656.4371124 Hartrees

Potential Energy: -656.6192845 Hartress

Kinetic Energy: 0.1821721 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.050236465275D+12 Y= 1.406182421267D+13 Z= -8.295414030843D+12
I= 1 X= -8.180570886950D+11 Y= -1.476116714153D+13 Z= -1.940648685923D+12
I= 2 X= 1.805889713636D+13 Y= 5.222469093421D+11 Z= 1.657114548178D+13
I= 3 X= -1.038149248624D+13 Y= -9.748570668108D+12 Z= -4.643648077891D+12
I= 4 X= -8.075566691344D+12 Y= 1.476731008152D+13 Z= -9.328595079638D+12
I= 5 X= 1.915289296163D+13 Y= 1.002023420004D+13 Z= -1.852237843876D+13
I= 6 X= -6.716566400877D+13 Y= -3.105408011540D+13 Z= 6.168879783207D+13
I= 7 X= -1.317910992472D+14 Y= -2.505671389627D+13 Z= 9.313833581760D+13
I= 8 X= -1.085142193554D+14 Y= -2.791811436530D+12 Z= 7.207557688866D+13
I= 9 X= 6.947502266654D+12 Y= -1.468951010651D+13 Z= -1.418556617954D+13
I= 10 X= 1.080214133642D+13 Y= -5.019654236038D+13 Z= -1.267087690838D+13
I= 11 X= -3.258586860522D+13 Y= -8.713557929337D+13 Z= -3.627938835794D+13
I= 12 X= 9.804799299564D+13 Y= 1.091570295734D+14 Z= 1.122894825954D+14
I= 13 X= -8.370643157391D+12 Y= 2.323557777994D+12 Z= 8.473655720373D+12
I= 14 X= 6.621878749500D+13 Y= 1.072117345079D+14 Z= 5.251649314152D+13
I= 15 X= -6.915783875743D+13 Y= 3.007250602023D+13 Z= 8.140701502441D+13
I= 16 X= -6.511581181563D+13 Y= -1.614357909273D+14 Z= 1.221973037255D+13

I= 17 X= 8.717514018070D+12 Y= -1.940962619808D+12 Z= -1.123503903572D+13
I= 18 X= 4.082162596893D+13 Y= 2.584120765239D+13 Z= 1.240543895364D+13
I= 19 X= -3.612485142760D+13 Y= -4.544209552788D+13 Z= -6.069025770458D+13
I= 20 X= 2.419962051420D+13 Y= -9.070207654313D+13 Z= 1.038615980808D+14
I= 21 X= -1.182924334885D+12 Y= -6.279720551524D+12 Z= -9.970567423155D+12
I= 22 X= 8.780256864011D+12 Y= -2.386031959885D+13 Z= -1.477606891786D+13
I= 23 X= -1.555566989482D+12 Y= -6.977814856986D+13 Z= 7.123266939169D+13
I= 24 X= -4.234306276740D+13 Y= 7.430340321116D+13 Z= 5.259864852687D+13
I= 25 X= -4.266694179435D+12 Y= -3.983127923694D+11 Z= -3.229160398218D+13
I= 26 X= -1.996941494792D+13 Y= 4.376692356668D+13 Z= 9.502053286752D+13
I= 27 X= 8.537264150157D+13 Y= -3.766183440684D+13 Z= 4.848612258059D+13
I= 28 X= -3.297320963243D+13 Y= 4.292909368789D+13 Z= -2.038337843305D+13
I= 29 X= -3.778817307050D+12 Y= -9.973685019436D+12 Z= -4.987115889638D+12
I= 30 X= -4.941977273578D+12 Y= 5.982343668259D+12 Z= -1.809026766676D+13
I= 31 X= -6.209586668428D+13 Y= 2.718328461636D+13 Z= -6.057450891356D+13
I= 32 X= 3.007607209613D+13 Y= -2.273946765903D+13 Z= 3.730160860646D+13
I= 33 X= -1.665413135087D+13 Y= 2.888563936905D+13 Z= 9.236599813016D+13
I= 34 X= -5.379337952731D+12 Y= 2.922988607541D+13 Z= 7.062863635318D+13
I= 35 X= 1.688650743441D+12 Y= 3.060102197712D+12 Z= 4.285924239008D+12
I= 36 X= 1.306897378273D+13 Y= -8.330877245305D+12 Z= -1.165744695742D+12
I= 37 X= -8.680541414289D+13 Y= 6.890340664374D+12 Z= 1.507064778295D+13
I= 38 X= -2.140413570725D+13 Y= 2.955407131281D+13 Z= -1.142188000440D+13

Backward Direction:

Total Energy: -656.4371115 Hartrees

Potential Energy: -656.6192845 Hartress

Kinetic Energy: 0.1821730 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.423549360154D+12 Y= 1.357433170768D+13 Z= -8.104645283572D+12

I= 1 X= -1.393846491817D+12 Y= -1.601475191614D+13 Z= -2.693179130853D+12

I= 2 X= 1.752299219714D+13 Y= 1.014862143797D+12 Z= 1.577801410248D+13

I= 3 X= -1.147953401255D+13 Y= -9.722895337879D+12 Z= -6.234597376650D+12
I= 4 X= -6.197488418927D+12 Y= 1.459975136507D+13 Z= -1.057660829354D+13
I= 5 X= 1.605330700032D+13 Y= 5.612284130651D+12 Z= -2.732291730939D+13
I= 6 X= 2.264542762852D+12 Y= 4.820883796034D+13 Z= 9.292785665482D+13
I= 7 X= -1.191096698009D+14 Y= -1.305009773555D+13 Z= 9.391418288616D+13
I= 8 X= -9.249809731563D+13 Y= 1.015432609514D+13 Z= 7.356560117658D+13
I= 9 X= 7.544410508827D+12 Y= -1.440919077896D+13 Z= -1.486026893432D+13
I= 10 X= 1.091131106947D+13 Y= -4.880925287773D+13 Z= -1.427903294282D+13
I= 11 X= -3.275826751947D+13 Y= -8.715074454672D+13 Z= -3.631291209864D+13
I= 12 X= 9.839782316504D+13 Y= 1.092507274126D+14 Z= 1.119572832639D+14
I= 13 X= -8.252314806421D+12 Y= 2.265983731224D+12 Z= 8.224610815125D+12
I= 14 X= 6.641995409606D+13 Y= 1.068570415524D+14 Z= 5.256914141009D+13
I= 15 X= -6.878789217671D+13 Y= 2.973320108317D+13 Z= 8.079441064920D+13
I= 16 X= -6.514158218174D+13 Y= -1.613267380071D+14 Z= 1.230597904352D+13
I= 17 X= 8.898720544243D+12 Y= -2.340858456908D+12 Z= -1.127464034796D+13
I= 18 X= 4.085983245108D+13 Y= 2.520366760358D+13 Z= 1.188243912317D+13
I= 19 X= -3.650791837487D+13 Y= -4.556970458366D+13 Z= -6.029525590327D+13
I= 20 X= 2.446563364158D+13 Y= -9.105939722802D+13 Z= 1.038159676555D+14
I= 21 X= -1.410939793294D+12 Y= -6.422964952997D+12 Z= -1.052718788685D+13
I= 22 X= 8.739508648762D+12 Y= -2.321837852848D+13 Z= -1.700680245454D+13
I= 23 X= -7.267549677630D+11 Y= -7.013892155831D+13 Z= 7.097400503219D+13
I= 24 X= -4.274262026423D+13 Y= 7.407899524256D+13 Z= 5.194050822530D+13
I= 25 X= -4.514501225815D+12 Y= -6.486497257376D+11 Z= -3.241947920446D+13
I= 26 X= -2.058235036777D+13 Y= 4.309641958000D+13 Z= 9.494574662848D+13
I= 27 X= 8.588347698342D+13 Y= -3.723175241100D+13 Z= 4.833786811102D+13
I= 28 X= -3.294789637916D+13 Y= 4.217038041204D+13 Z= -1.984632907550D+13
I= 29 X= -4.926441851516D+12 Y= -9.651326224861D+12 Z= -5.389629369974D+12
I= 30 X= -4.874394697128D+12 Y= 5.760249341874D+12 Z= -1.858875122941D+13
I= 31 X= -6.288929900097D+13 Y= 2.694855167233D+13 Z= -6.054971695648D+13
I= 32 X= 2.775404116372D+13 Y= -2.081116212599D+13 Z= 3.591914179555D+13

I= 33 X= -1.658251951266D+13 Y= 2.860496841232D+13 Z= 9.196895416434D+13
I= 34 X= -4.631220373307D+12 Y= 2.870902709263D+13 Z= 7.048545292091D+13
I= 35 X= 1.676165869352D+12 Y= 3.351710205085D+12 Z= 6.135997398095D+12
I= 36 X= 9.034253040016D+12 Y= -1.342706199423D+13 Z= -3.025471271201D+12
I= 37 X= -8.320606980816D+13 Y= 8.717600630829D+12 Z= 1.058168936743D+13
I= 38 X= -1.943299511758D+13 Y= 2.934867486609D+13 Z= -1.477434371541D+13

Seed: 3126505819

CM Start Point Coordinates: bohr

I= 0 X= -2.556557069976D+00 Y= 2.186477224211D+00 Z= -7.537443479591D-01
I= 1 X= -2.886991484778D+00 Y= -8.259103335799D-02 Z= -2.030301437109D+00
I= 2 X= -2.094355217343D+00 Y= 1.766154088714D+00 Z= 1.975069559632D+00
I= 3 X= -2.519860294640D+00 Y= -2.009402556356D+00 Z= -1.383598481249D-01
I= 4 X= -2.031963805517D+00 Y= -8.450503533708D-01 Z= 2.351548178518D+00
I= 5 X= 4.836244778988D+00 Y= 2.432135533675D+00 Z= -4.263831271451D-01
I= 6 X= 2.804706616966D+00 Y= 1.151598280983D+00 Z= -3.054644180007D+00
I= 7 X= 6.417463815100D+00 Y= 1.082115020703D+00 Z= -8.645297837128D-01
I= 8 X= 5.002028649827D+00 Y= 4.190930461265D+00 Z= -1.517730618223D+00
I= 9 X= -1.755520805178D+00 Y= -2.069802296091D+00 Z= 4.996910955240D+00
I= 10 X= -3.760955930385D+00 Y= -1.522118737196D+00 Z= 6.090705721278D+00
I= 11 X= -1.230435890670D+00 Y= -4.106018251694D+00 Z= 5.071516885258D+00
I= 12 X= -3.518490064738D-01 Y= -8.038669753913D-01 Z= 6.002011456318D+00
I= 13 X= -1.967060462836D+00 Y= 3.825539816359D+00 Z= 3.977160232439D+00
I= 14 X= -4.159427958193D+00 Y= 3.449013100438D+00 Z= 5.163729024099D+00
I= 15 X= -3.649702852504D-01 Y= 3.479735416696D+00 Z= 5.390385904117D+00
I= 16 X= -2.175489659970D+00 Y= 5.744437096342D+00 Z= 3.049179500475D+00
I= 17 X= -2.429119780870D+00 Y= 4.848088449001D+00 Z= -1.846992580619D+00
I= 18 X= -4.390848535235D+00 Y= 5.951088645934D+00 Z= -1.283905317314D+00
I= 19 X= -9.351223592480D-01 Y= 6.125472768402D+00 Z= -9.390557472032D-01
I= 20 X= -2.009949186215D+00 Y= 4.197917942754D+00 Z= -3.687066964713D+00

I= 21 X= -3.678349695837D+00 Y= -3.762224391464D-01 Z= -4.577109853448D+00
I= 22 X= -5.960486278156D+00 Y= -3.165371538981D-01 Z= -4.942962126767D+00
I= 23 X= -3.051371835019D+00 Y= 1.111240361283D+00 Z= -5.946201597211D+00
I= 24 X= -3.036095555422D+00 Y= -2.073436712551D+00 Z= -5.483673329711D+00
I= 25 X= -2.907366410225D+00 Y= -4.636801153740D+00 Z= -4.513851506656D-01
I= 26 X= -3.292648448633D+00 Y= -5.137195908216D+00 Z= -2.736057312956D+00
I= 27 X= -9.477107575499D-01 Y= -5.794977237316D+00 Z= 1.674031846302D-01
I= 28 X= -4.728096904238D+00 Y= -5.391593830170D+00 Z= 3.989960756325D-01
I= 29 X= 3.218491686491D+00 Y= -3.419615276435D+00 Z= -2.161699416077D+00
I= 30 X= 3.712583032471D+00 Y= -3.472655698799D+00 Z= 4.205307596930D-01
I= 31 X= 1.851282361286D+00 Y= -4.537912312190D+00 Z= -2.906174943691D+00
I= 32 X= 4.572688197919D+00 Y= -2.548099300919D+00 Z= -3.855520756684D+00
I= 33 X= 5.507319853865D+00 Y= -2.763859351998D+00 Z= 8.725692427597D-01
I= 34 X= 2.602042111457D+00 Y= -4.608052836289D+00 Z= 1.584518689731D+00
I= 35 X= 1.071422022049D+00 Y= -4.542199766648D-02 Z= -4.199834485432D-01
I= 36 X= 4.131991694213D+00 Y= 2.121839473126D+00 Z= 2.049128601015D+00
I= 37 X= 5.200147758579D+00 Y= 6.666580178859D-01 Z= 3.207668159841D+00
I= 38 X= 3.341544502839D+00 Y= 3.899165063230D+00 Z= 2.804448811276D+00

Forward Direction:

Total Energy: -656.4446579 Hartrees

Potential Energy: -656.6196918 Hartress

Kinetic Energy: 0.1750339 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.661493264765D+13 Y= -3.136119961552D+11 Z= 4.199146019787D+12
I= 1 X= 1.538376888171D+13 Y= 1.054912538892D+13 Z= -1.099010082544D+12
I= 2 X= -1.389325396747D+12 Y= -1.686541426147D+12 Z= 1.067169694947D+13
I= 3 X= 2.409669759798D+13 Y= 2.164605418404D+13 Z= -9.559240913641D+11
I= 4 X= -6.577899001489D+12 Y= -1.136363222589D+13 Z= -1.441047135965D+13
I= 5 X= -2.177544843902D+13 Y= 1.725569293706D+13 Z= 1.270120942079D+13
I= 6 X= -5.595918934668D+13 Y= -2.226125499697D+13 Z= 1.870536868045D+13

I= 7 X= 1.483807027092D+14 Y= -6.871117963455D+13 Z= 2.790151889936D+13
I= 8 X= 3.996769835515D+13 Y= 1.167962944239D+13 Z= -7.104203303405D+12
I= 9 X= -8.791179409844D+12 Y= -8.942502951605D+11 Z= 2.907865634269D+13
I= 10 X= 9.387899092746D+13 Y= -7.246186456913D+13 Z= -2.399463562800D+13
I= 11 X= -2.959066506814D+13 Y= 2.461460279092D+12 Z= -6.158555760099D+13
I= 12 X= -4.374316333460D+12 Y= 9.073880442129D+13 Z= -1.134156751634D+14
I= 13 X= -4.943496423771D+12 Y= -1.729602871546D+12 Z= -2.166594097425D+13
I= 14 X= -3.443555973370D+13 Y= 1.729509380260D+13 Z= 9.965389321561D+12
I= 15 X= 1.194426598770D+12 Y= -1.957762200390D+13 Z= 8.914592730686D+13
I= 16 X= -3.705327020004D+13 Y= -4.557182177508D+13 Z= 2.603161689494D+13
I= 17 X= 7.065010096672D+12 Y= 1.125244328856D+12 Z= -1.208266039270D+12
I= 18 X= 1.242478121386D+14 Y= 1.637980423011D+13 Z= 6.327912198955D+13
I= 19 X= -7.298495755819D+13 Y= 4.461226242009D+13 Z= 4.003491097036D+13
I= 20 X= -2.380692804347D+13 Y= -2.016291953176D+13 Z= 6.067342772554D+13
I= 21 X= -1.662567314954D+13 Y= 1.284985097135D+13 Z= 6.338585812173D+12
I= 22 X= 5.019803984825D+13 Y= -1.918344973200D+13 Z= -5.663016610528D+13
I= 23 X= -4.514783471995D+13 Y= -7.266773612061D+13 Z= 3.741804019956D+13
I= 24 X= 9.984242829850D+12 Y= -9.466702937807D+13 Z= -2.635549927732D+12
I= 25 X= -1.893864276287D+13 Y= -2.881905515428D+13 Z= 9.269920563805D+12
I= 26 X= 6.108157268139D+13 Y= 7.625638145252D+12 Z= -1.343431344131D+14
I= 27 X= -6.607670452936D+13 Y= -2.566090322385D+13 Z= -5.031032357667D+13
I= 28 X= 8.157776490358D+12 Y= -2.212319784404D+13 Z= -2.310318438073D+12
I= 29 X= -2.713244656687D+12 Y= 1.375700254138D+13 Z= -2.907772672379D+13
I= 30 X= -3.205275226596D+12 Y= -2.264593459224D+12 Z= 4.785515013445D+12
I= 31 X= 1.584442407502D+13 Y= -4.340569792554D+13 Z= 8.656587926936D+13
I= 32 X= 4.369155571475D+13 Y= -4.812773092655D+13 Z= 9.715541998039D+13
I= 33 X= -2.106212902860D+13 Y= -2.457864610780D+13 Z= -2.159782678870D+13
I= 34 X= -4.022695651163D+13 Y= 4.294742190938D+13 Z= -1.022927318292D+14
I= 35 X= 3.242895990631D+12 Y= 2.022376851589D+11 Z= 3.894774552065D+11
I= 36 X= 5.972332807089D+12 Y= 1.644458272355D+12 Z= -2.201946884853D+13

I= 37 X= 5.297019601759D+13 Y= -4.568167850380D+13 Z= 8.242211860311D+13

I= 38 X= 3.411948021928D+13 Y= 1.233804228935D+13 Z= 5.661064635298D+13

Backward Direction:

Total Energy: -656.4445852 Hartrees

Potential Energy: -656.6196918 Hartress

Kinetic Energy: 0.1751065 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.689335598680D+13 Y= -6.771925008690D+11 Z= 4.341424715398D+12

I= 1 X= 1.495433499299D+13 Y= 9.614179763046D+12 Z= -1.660260555248D+12

I= 2 X= -1.789012750926D+12 Y= -1.319140299160D+12 Z= 1.008016558410D+13

I= 3 X= 2.327775887138D+13 Y= 2.166520329863D+13 Z= -2.142482127468D+12

I= 4 X= -5.177195117423D+12 Y= -1.148860047087D+13 Z= -1.534126161606D+13

I= 5 X= -2.408717429425D+13 Y= 1.396816606202D+13 Z= 6.137612376017D+12

I= 6 X= -4.176917076323D+12 Y= 3.685442671563D+13 Z= 4.200400949801D+13

I= 7 X= 1.578387363646D+14 Y= -5.975643362965D+13 Z= 2.848015932489D+13

I= 8 X= 5.191280453099D+13 Y= 2.133508705559D+13 Z= -5.992916914660D+12

I= 9 X= -8.345994715626D+12 Y= -6.851831985713D+11 Z= 2.857545113285D+13

I= 10 X= 9.396041163934D+13 Y= -7.142719961317D+13 Z= -2.519402675836D+13

I= 11 X= -2.971924322010D+13 Y= 2.450149759689D+12 Z= -6.161056019167D+13

I= 12 X= -4.113406830509D+12 Y= 9.080868592433D+13 Z= -1.136634352771D+14

I= 13 X= -4.855245052100D+12 Y= -1.772542610198D+12 Z= -2.185168305556D+13

I= 14 X= -3.428552613893D+13 Y= 1.703055753590D+13 Z= 1.000465532397D+13

I= 15 X= 1.470339281131D+12 Y= -1.983068160346D+13 Z= 8.868903616696D+13

I= 16 X= -3.707249020247D+13 Y= -4.549048817832D+13 Z= 2.609594267484D+13

I= 17 X= 7.200157121243D+12 Y= 8.269949629407D+11 Z= -1.237801395991D+12

I= 18 X= 1.242763072094D+14 Y= 1.590431562190D+13 Z= 6.288905949250D+13

I= 19 X= -7.327065564193D+13 Y= 4.451708933492D+13 Z= 4.032951027800D+13

I= 20 X= -2.360853076117D+13 Y= -2.042941559966D+13 Z= 6.063939574518D+13

I= 21 X= -1.679573109878D+13 Y= 1.274301677009D+13 Z= 5.923448456583D+12

I= 22 X= 5.016764911116D+13 Y= -1.870467876451D+13 Z= -5.829388650836D+13

I= 23 X= -4.452969209657D+13 Y= -7.293680697847D+13 Z= 3.722512376204D+13
I= 24 X= 9.686245806296D+12 Y= -9.483439679748D+13 Z= -3.126402567520D+12
I= 25 X= -1.912346162530D+13 Y= -2.900576085237D+13 Z= 9.174548968237D+12
I= 26 X= 6.062443464697D+13 Y= 7.125564452272D+12 Z= -1.343989113084D+14
I= 27 X= -6.569571440979D+13 Y= -2.534014048154D+13 Z= -5.042089438191D+13
I= 28 X= 8.176655561967D+12 Y= -2.268905959282D+13 Z= -1.909777561731D+12
I= 29 X= -3.569163275136D+12 Y= 1.399742341219D+13 Z= -2.937792837354D+13
I= 30 X= -3.154870948503D+12 Y= -2.430235324550D+12 Z= 4.413737184000D+12
I= 31 X= 1.525266826441D+13 Y= -4.358076589395D+13 Z= 8.658436954621D+13
I= 32 X= 4.195974410435D+13 Y= -4.668956667117D+13 Z= 9.612435185725D+13
I= 33 X= -2.100871965471D+13 Y= -2.478797545591D+13 Z= -2.189394918483D+13
I= 34 X= -3.966899723165D+13 Y= 4.255895609337D+13 Z= -1.023995205587D+14
I= 35 X= 3.233584550345D+12 Y= 4.197240790304D+11 Z= 1.769294634330D+12
I= 36 X= 2.963166946933D+12 Y= -2.156366161124D+12 Z= -2.340648571601D+13
I= 37 X= 5.565465047720D+13 Y= -4.431887580842D+13 Z= 7.907417428006D+13
I= 38 X= 3.558959162668D+13 Y= 1.218485399330D+13 Z= 5.411031982217D+13

Seed: 31995162837

CM Start Point Coordinates: bohr

I= 0 X= -2.512733244691D+00 Y= 2.214807842580D+00 Z= -6.107598628332D-01
I= 1 X= -2.814735540646D+00 Y= -7.148513014117D-02 Z= -1.905023316821D+00
I= 2 X= -2.000883647872D+00 Y= 1.761219710585D+00 Z= 2.139899513588D+00
I= 3 X= -2.513835740919D+00 Y= -1.884703477515D+00 Z= -1.625922280535D-01
I= 4 X= -1.855286058190D+00 Y= -1.003474138013D+00 Z= 2.263264973173D+00
I= 5 X= 4.955218848566D+00 Y= 2.079498451617D+00 Z= -1.411609626695D+00
I= 6 X= 2.237080404395D+00 Y= 8.161530639897D-01 Z= -3.352865402547D+00
I= 7 X= 6.532970112900D+00 Y= 4.828958472070D-01 Z= -1.792499488875D+00
I= 8 X= 4.657938923523D+00 Y= 3.869614736450D+00 Z= -2.752397254303D+00
I= 9 X= -2.239602116209D+00 Y= -2.497076221937D+00 Z= 4.684636009587D+00
I= 10 X= -4.286587010629D+00 Y= -2.317315352301D+00 Z= 5.533127992016D+00

I= 11 X= -1.999171177896D+00 Y= -4.302470894169D+00 Z= 4.387668541470D+00
I= 12 X= -7.263476798389D-01 Y= -1.712712005842D+00 Z= 6.042724608773D+00
I= 13 X= -1.983942654829D+00 Y= 3.714108537257D+00 Z= 4.237495069699D+00
I= 14 X= -3.789204620794D+00 Y= 3.671687837427D+00 Z= 5.022683571979D+00
I= 15 X= -7.287094491662D-01 Y= 2.896919771428D+00 Z= 5.844948017704D+00
I= 16 X= -1.505685129859D+00 Y= 5.532803988545D+00 Z= 3.638328248945D+00
I= 17 X= -2.868906246288D+00 Y= 5.103619470976D+00 Z= -1.355511765081D+00
I= 18 X= -4.651237824809D+00 Y= 5.926242917930D+00 Z= -7.177387106637D-01
I= 19 X= -1.309894930087D+00 Y= 6.430879207478D+00 Z= -4.225039341110D-01
I= 20 X= -3.015716845069D+00 Y= 4.920187120308D+00 Z= -3.619269710870D+00
I= 21 X= -3.493125356625D+00 Y= 3.288801947609D-02 Z= -4.653404718420D+00
I= 22 X= -5.757372240552D+00 Y= 2.601566709396D-01 Z= -4.758802244806D+00
I= 23 X= -2.716892167932D+00 Y= 1.540876978825D+00 Z= -5.748661463761D+00
I= 24 X= -3.149642408961D+00 Y= -1.953336461502D+00 Z= -5.513475514457D+00
I= 25 X= -3.039293986845D+00 Y= -4.617710430775D+00 Z= -7.968141867982D-01
I= 26 X= -2.915780353060D+00 Y= -5.072317937680D+00 Z= -2.722401802565D+00
I= 27 X= -1.660971916648D+00 Y= -5.883720572566D+00 Z= 4.448447925750D-02
I= 28 X= -4.723289873061D+00 Y= -5.356555782371D+00 Z= -1.997156439740D-01
I= 29 X= 3.208824824867D+00 Y= -3.611986255080D+00 Z= -1.456870491116D+00
I= 30 X= 3.652294959572D+00 Y= -3.069391884954D+00 Z= 1.087592519789D+00
I= 31 X= 1.809964970377D+00 Y= -5.233890300721D+00 Z= -2.127854811447D+00
I= 32 X= 5.027255740182D+00 Y= -3.535226374307D+00 Z= -2.596126900942D+00
I= 33 X= 5.499505004593D+00 Y= -2.448391188545D+00 Z= 1.971926946935D+00
I= 34 X= 2.527317114391D+00 Y= -3.836857922554D+00 Z= 2.849986653548D+00
I= 35 X= 1.170057225635D+00 Y= -1.119736196524D-01 Z= -4.054607342668D-01
I= 36 X= 4.048219012591D+00 Y= 2.696312326267D+00 Z= 1.119657923221D+00
I= 37 X= 4.840168524354D+00 Y= 2.078364543105D+00 Z= 3.017814137655D+00
I= 38 X= 2.946900835640D+00 Y= 4.578529700214D+00 Z= 1.507283171109D+00

Forward Direction:

Total Energy: -656.4442728 Hartrees

Potential Energy: -656.6329898 Hartress

Kinetic Energy: 0.1887169 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.172677465483D+12 Y= -1.098333480121D+13 Z= -1.059712744722D+13
I= 1 X= -6.531323937871D+12 Y= 1.803203752465D+13 Z= -1.082966515965D+13
I= 2 X= 6.313011896400D+12 Y= 9.058762070469D+12 Z= 2.244262526032D+13
I= 3 X= 2.973400888178D+12 Y= -1.022411002837D+13 Z= 1.388311893792D+13
I= 4 X= 4.800861588788D+12 Y= -5.351987090877D+12 Z= -1.689382901337D+13
I= 5 X= 9.619388823593D+12 Y= -9.575380122722D+12 Z= 7.007002516593D+11
I= 6 X= 3.794041817749D+13 Y= -2.654341483305D+13 Z= -5.212657962915D+13
I= 7 X= -8.241167595518D+13 Y= 3.545630846182D+13 Z= -5.142273976876D+13
I= 8 X= 2.701510233258D+13 Y= -8.444063232928D+12 Z= -7.385713225231D+13
I= 9 X= 7.400291402045D+11 Y= -5.633026564501D+12 Z= 9.265777760815D+12
I= 10 X= 4.182868355629D+13 Y= -4.944128979597D+13 Z= -3.206215208307D+13
I= 11 X= -7.960393678861D+13 Y= 1.250884321989D+14 Z= -5.206363344324D+13
I= 12 X= -2.748437461185D+13 Y= -8.673416531336D+12 Z= -4.483914456380D+13
I= 13 X= 6.921969744320D+12 Y= 1.155497186979D+13 Z= 1.517722558472D+13
I= 14 X= -5.229132467790D+13 Y= 1.076853818294D+14 Z= 8.433626403387D+12
I= 15 X= 5.364416843113D+13 Y= -8.137723109292D+13 Z= 1.493983835588D+13
I= 16 X= -5.983164099306D+13 Y= -5.731198225305D+13 Z= 2.183240900265D+13
I= 17 X= 6.810352116910D+12 Y= 2.799509446055D+13 Z= 2.413271198554D+13
I= 18 X= 3.450209011214D+13 Y= -8.596241122849D+13 Z= -8.565241031476D+12
I= 19 X= -7.881119104456D+13 Y= -4.256376972031D+13 Z= -1.243495362221D+14
I= 20 X= -1.538173649571D+13 Y= -2.426124803744D+13 Z= -1.978298580483D+13
I= 21 X= 4.547619322700D+12 Y= -1.102335561678D+13 Z= 1.090372066229D+13
I= 22 X= 2.521678532004D+13 Y= 2.632650432772D+13 Z= -1.688635144742D+13
I= 23 X= -4.051056073597D+13 Y= 9.034545611326D+12 Z= -2.768379840537D+13
I= 24 X= -8.869407562312D+12 Y= -8.938251737699D+13 Z= -1.694038683270D+14
I= 25 X= 2.494061229538D+13 Y= -6.138547857341D+12 Z= -8.504065225725D+12
I= 26 X= -1.556037116027D+13 Y= 2.066044030206D+13 Z= -1.147162347900D+13

I= 27 X= -2.528648539715D+13 Y= 6.352384711310D+13 Z= -4.729446020896D+12
I= 28 X= -9.254695768795D+13 Y= -3.233488491711D+13 Z= 5.170751582125D+13
I= 29 X= -1.144111137280D+13 Y= 9.295121930570D+12 Z= -3.248968140312D+12
I= 30 X= 2.152250799909D+12 Y= -8.602187980096D+11 Z= -9.946072527934D+11
I= 31 X= -7.662256609329D+12 Y= -6.581484114238D+12 Z= 1.078228830691D+14
I= 32 X= -1.535125604393D+13 Y= 9.798047550907D+13 Z= 9.082267709173D+12
I= 33 X= -3.116293679178D+13 Y= -3.394521509352D+13 Z= 4.013770541247D+12
I= 34 X= -1.645082920215D+14 Y= 1.960113498473D+12 Z= 1.123062932758D+14
I= 35 X= -6.051550427457D+11 Y= -3.457740529017D+12 Z= -1.538847611420D+12
I= 36 X= -1.169102840069D+13 Y= 2.253220870146D+13 Z= 1.205182516114D+12
I= 37 X= 7.024689005672D+13 Y= 6.509127398331D+13 Z= -5.137453910298D+12
I= 38 X= 1.164088135265D+14 Y= -1.134640925365D+14 Z= -3.399945813663D+13

Backward Direction:

Total Energy: -656.4442694 Hartrees

Potential Energy: -656.6329898 Hartress

Kinetic Energy: 0.1887203 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.268434746873D+12 Y= -1.110837992557D+13 Z= -1.054819397343D+13
I= 1 X= -6.679017811992D+12 Y= 1.771048455381D+13 Z= -1.102269430661D+13
I= 2 X= 6.175548656301D+12 Y= 9.185121208715D+12 Z= 2.223918169914D+13
I= 3 X= 2.691745812545D+12 Y= -1.021752413250D+13 Z= 1.347502968639D+13
I= 4 X= 5.282601363267D+12 Y= -5.394967035394D+12 Z= -1.721395284066D+13
I= 5 X= 8.824324066816D+12 Y= -1.070604911772D+13 Z= -1.556697470812D+12
I= 6 X= 5.574973564140D+13 Y= -6.211940438181D+12 Z= -4.411354982940D+13
I= 7 X= -7.915880356245D+13 Y= 3.853608668710D+13 Z= -5.122372975284D+13
I= 8 X= 3.112334592065D+13 Y= -5.123291425708D+12 Z= -7.347493094921D+13
I= 9 X= 8.931401393453D+11 Y= -5.561122761760D+12 Z= 9.092711942863D+12
I= 10 X= 4.185668633319D+13 Y= -4.908544066338D+13 Z= -3.247465497588D+13
I= 11 X= -7.964815827986D+13 Y= 1.250845422145D+14 Z= -5.207223250758D+13
I= 12 X= -2.739464080223D+13 Y= -8.649382398438D+12 Z= -4.492435593465D+13

I= 13 X= 6.952321766486D+12 Y= 1.154020373782D+13 Z= 1.511334388208D+13
I= 14 X= -5.223972408502D+13 Y= 1.075944006884D+14 Z= 8.447131041240D+12
I= 15 X= 5.373906223258D+13 Y= -8.146426510384D+13 Z= 1.478270119185D+13
I= 16 X= -5.983825126563D+13 Y= -5.728400944225D+13 Z= 2.185453236929D+13
I= 17 X= 6.856832816399D+12 Y= 2.789251847455D+13 Z= 2.412255398186D+13
I= 18 X= 3.451189033242D+13 Y= -8.612594456139D+13 Z= -8.699394022905D+12
I= 19 X= -7.890945030293D+13 Y= -4.259650230570D+13 Z= -1.242482155881D+14
I= 20 X= -1.531350232806D+13 Y= -2.435290320748D+13 Z= -1.979469031479D+13
I= 21 X= 4.489131817394D+12 Y= -1.106009877393D+13 Z= 1.076094374936D+13
I= 22 X= 2.520633312881D+13 Y= 2.649116655302D+13 Z= -1.745854968296D+13
I= 23 X= -4.029796484573D+13 Y= 8.942004900315D+12 Z= -2.775014756213D+13
I= 24 X= -8.971896761580D+12 Y= -8.944007953845D+13 Z= -1.695726857649D+14
I= 25 X= 2.487704811190D+13 Y= -6.202760973202D+12 Z= -8.536866086027D+12
I= 26 X= -1.571759323842D+13 Y= 2.048845149751D+13 Z= -1.149080664912D+13
I= 27 X= -2.515545263876D+13 Y= 6.363416605315D+13 Z= -4.767474295704D+12
I= 28 X= -9.254046466872D+13 Y= -3.252950000636D+13 Z= 5.184527261373D+13
I= 29 X= -1.173548482789D+13 Y= 9.377809141743D+12 Z= -3.352215569251D+12
I= 30 X= 2.169586187535D+12 Y= -9.171874929435D+11 Z= -1.122471656235D+12
I= 31 X= -7.865777364618D+12 Y= -6.641694701094D+12 Z= 1.078292423717D+14
I= 32 X= -1.594687267866D+13 Y= 9.847509891685D+13 Z= 8.727655622666D+12
I= 33 X= -3.114456787342D+13 Y= -3.401720909028D+13 Z= 3.911926076336D+12
I= 34 X= -1.643163948040D+14 Y= 1.826509650091D+12 Z= 1.122695657547D+14
I= 35 X= -6.083574975223D+11 Y= -3.382941103751D+12 Z= -1.064291337480D+12
I= 36 X= -1.272596154996D+13 Y= 2.122500285695D+13 Z= 7.281500752503D+11
I= 37 X= 7.117014621566D+13 Y= 6.555997851738D+13 Z= -6.288902096518D+12
I= 38 X= 1.169144244153D+14 Y= -1.135167781153D+14 Z= -3.485938774453D+13

Seed: 3292668439

CM Start Point Coordinates: bohr

I= 0 X= -2.314264950691D+00 Y= 2.386875914306D+00 Z= -5.912423549943D-01

I= 1 X= -2.958507062756D+00 Y= 1.151924134325D-01 Z= -2.051930248151D+00
I= 2 X= -2.167724476009D+00 Y= 1.800871576994D+00 Z= 2.110466838840D+00
I= 3 X= -2.468417397284D+00 Y= -2.087587084314D+00 Z= -2.624726131395D-01
I= 4 X= -2.242316648666D+00 Y= -9.946656321844D-01 Z= 2.144413323052D+00
I= 5 X= 4.556521343859D+00 Y= 2.271580931336D+00 Z= -1.420918970008D+00
I= 6 X= 2.277796585828D+00 Y= 6.805303123968D-01 Z= -3.227366048925D+00
I= 7 X= 5.988685915101D+00 Y= 9.301507350353D-01 Z= -2.206373673011D+00
I= 8 X= 4.011049390223D+00 Y= 4.378916800509D+00 Z= -2.373404236861D+00
I= 9 X= -2.420418965109D+00 Y= -2.333109149781D+00 Z= 4.685130987623D+00
I= 10 X= -4.256576130354D+00 Y= -1.829438164783D+00 Z= 5.268481007459D+00
I= 11 X= -2.489676987914D+00 Y= -4.703704280371D+00 Z= 4.425804429747D+00
I= 12 X= -1.565749413550D+00 Y= -1.518322126591D+00 Z= 6.102642659265D+00
I= 13 X= -1.531393364985D+00 Y= 3.382666869417D+00 Z= 4.362835061595D+00
I= 14 X= -3.265611912186D+00 Y= 4.056729460727D+00 Z= 5.224832412348D+00
I= 15 X= 2.502067100448D-03 Y= 2.312718058929D+00 Z= 5.618810375109D+00
I= 16 X= -4.611363522988D-01 Y= 5.084377541495D+00 Z= 3.573578749480D+00
I= 17 X= -2.692429054719D+00 Y= 4.987061048555D+00 Z= -1.575624508400D+00
I= 18 X= -4.611279546243D+00 Y= 5.638470627489D+00 Z= -1.602014657830D+00
I= 19 X= -1.798820589207D+00 Y= 6.499947561648D+00 Z= -2.532602317411D-01
I= 20 X= -1.717907242558D+00 Y= 5.071394729451D+00 Z= -3.620677539268D+00
I= 21 X= -3.839265296389D+00 Y= -3.417015702646D-02 Z= -4.655742589457D+00
I= 22 X= -5.879951172506D+00 Y= -8.943055506641D-03 Z= -4.547584070581D+00
I= 23 X= -3.423558855298D+00 Y= 1.489618498791D+00 Z= -5.603194703574D+00
I= 24 X= -2.917328608930D+00 Y= -1.647722368171D+00 Z= -5.743903831517D+00
I= 25 X= -2.764264044081D+00 Y= -4.874920165132D+00 Z= -7.689710504367D-01
I= 26 X= -2.871668371261D+00 Y= -4.938495605142D+00 Z= -2.895324158480D+00
I= 27 X= -1.116287815655D+00 Y= -5.683507710698D+00 Z= 2.901214449219D-01
I= 28 X= -4.657308833179D+00 Y= -5.510916918193D+00 Z= 1.762763633044D-01
I= 29 X= 3.339914607603D+00 Y= -3.689801143999D+00 Z= -1.465981083055D+00
I= 30 X= 3.568857444772D+00 Y= -3.103145251661D+00 Z= 1.238955731766D+00

I= 31 X= 2.206249926029D+00 Y= -5.138959640751D+00 Z= -2.407292141996D+00
I= 32 X= 5.061507115341D+00 Y= -3.376226463048D+00 Z= -2.513634298662D+00
I= 33 X= 5.404770676014D+00 Y= -2.316330857840D+00 Z= 1.919876839095D+00
I= 34 X= 2.277733344405D+00 Y= -3.751183548058D+00 Z= 2.489128658784D+00
I= 35 X= 1.191633510928D+00 Y= -6.746281344107D-02 Z= -3.588559568429D-01
I= 36 X= 4.181508601314D+00 Y= 2.630760459952D+00 Z= 1.106139316491D+00
I= 37 X= 5.260493249150D+00 Y= 1.894219661997D+00 Z= 2.780520571172D+00
I= 38 X= 2.987124287900D+00 Y= 3.826331167481D+00 Z= 1.770552732094D+00

Forward Direction:

Total Energy: -656.4398218 Hartrees

Potential Energy: -656.6175869 Hartress

Kinetic Energy: 0.1777651 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.582104601306D+12 Y= 3.974415679957D+13 Z= -6.373113888822D+12
I= 1 X= 3.057017088336D+12 Y= 7.332473049798D+11 Z= -7.255712381761D+12
I= 2 X= -2.121349491100D+13 Y= -9.597297943432D+12 Z= -1.623064593928D+13
I= 3 X= -7.673786516617D+11 Y= -3.785469760253D+13 Z= 1.199772201120D+13
I= 4 X= -9.336496869238D+12 Y= 1.122390019610D+13 Z= 1.346654366896D+13
I= 5 X= 5.180075261349D+12 Y= 7.385431627533D+12 Z= -4.664900059236D+12
I= 6 X= 5.328877937328D+13 Y= -2.477631526965D+13 Z= -6.322743226835D+13
I= 7 X= -3.944793317740D+13 Y= -6.397318027854D+13 Z= 2.391744565702D+13
I= 8 X= -3.388803602663D+13 Y= -5.747624768840D+13 Z= -1.860119901706D+13
I= 9 X= -1.260403100096D+13 Y= -9.034180665803D+12 Z= -2.294543788977D+13
I= 10 X= 5.367060796507D+13 Y= 8.532358545591D+13 Z= -3.629391203643D+12
I= 11 X= 1.124390649881D+13 Y= -1.575956952515D+14 Z= 1.053138968774D+13
I= 12 X= -2.085345596010D+13 Y= 1.163971905310D+13 Z= 1.453725535038D+14
I= 13 X= 1.522370690686D+13 Y= 1.089773452452D+13 Z= 5.573447046682D+12
I= 14 X= 2.473580934954D+13 Y= 2.204385781077D+13 Z= 1.071306450100D+13
I= 15 X= -3.800794971517D+13 Y= -1.856257032445D+13 Z= 2.296064171360D+13
I= 16 X= -3.012554875237D+13 Y= -8.925464364276D+13 Z= 8.684830516152D+12

I= 17 X= -4.911262468609D+12 Y= 4.686224616163D+12 Z= 2.320520160089D+13
I= 18 X= -8.835864602394D+12 Y= 6.438238401890D+13 Z= -1.372638444688D+13
I= 19 X= 6.417870845479D+13 Y= 8.513667219633D+13 Z= 3.014173998039D+11
I= 20 X= 1.508110838535D+13 Y= -3.398796773745D+13 Z= -9.966957587978D+13
I= 21 X= 6.084121619812D+12 Y= -5.283329370021D+12 Z= -1.711183768066D+13
I= 22 X= -1.176226245001D+13 Y= 5.315788470409D+12 Z= 4.213585077971D+13
I= 23 X= 1.870397739701D+12 Y= -9.396958759117D+13 Z= 5.142196456669D+13
I= 24 X= -7.722519318220D+13 Y= 8.850104024244D+13 Z= -2.684960399382D+13
I= 25 X= -1.007502351573D+13 Y= -1.109118880919D+12 Z= -1.235240667601D+13
I= 26 X= -4.685506679791D+13 Y= 7.689222300920D+13 Z= 1.065563922305D+14
I= 27 X= -1.246785258085D+13 Y= 5.305026806819D+13 Z= -5.674021838798D+13
I= 28 X= 2.326695735247D+13 Y= 5.951628511756D+13 Z= -1.045338931715D+13
I= 29 X= -8.213467274471D+12 Y= -1.594761127286D+13 Z= 2.744013199480D+12
I= 30 X= -1.857681528621D+13 Y= 1.804794296599D+13 Z= 1.738568253852D+13
I= 31 X= 7.184877341284D+13 Y= 1.852186790823D+13 Z= 2.524862917060D+13
I= 32 X= 9.870553735264D+13 Y= 2.655822044409D+13 Z= -8.496485361975D+13
I= 33 X= -3.615543351984D+13 Y= -2.262348513914D+13 Z= -7.392365420599D+13
I= 34 X= 7.264785445542D+13 Y= 1.196554050992D+13 Z= -6.485398023569D+13
I= 35 X= 3.826681371964D+12 Y= 1.728559483835D+11 Z= 1.469568778692D+12
I= 36 X= 1.840901396395D+13 Y= -1.270522031055D+13 Z= 6.530610447332D+12
I= 37 X= 4.273847531169D+13 Y= -5.846697509683D+13 Z= 1.982668586686D+13
I= 38 X= -6.440865909371D+13 Y= -1.994595481180D+13 Z= -2.927459862301D+13

Backward Direction:

Total Energy: -656.4397877 Hartrees

Potential Energy: -656.6175869 Hartress

Kinetic Energy: 0.1777991 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.763583902163D+12 Y= 3.950717115210D+13 Z= -6.280375119800D+12

I= 1 X= 2.777107502481D+12 Y= 1.238397824120D+11 Z= -7.621541423076D+12

I= 2 X= -2.147401538664D+13 Y= -9.357821973039D+12 Z= -1.661621238966D+13

I= 3 X= -1.301171645672D+12 Y= -3.784221600542D+13 Z= 1.122431083670D+13
I= 4 X= -8.423503146393D+12 Y= 1.114244456291D+13 Z= 1.285984465752D+13
I= 5 X= 3.673267707827D+12 Y= 5.242586569626D+12 Z= -8.943122570767D+12
I= 6 X= 8.704101637303D+13 Y= 1.375591616533D+13 Z= -4.804112984923D+13
I= 7 X= -3.328308603002D+13 Y= -5.813638137965D+13 Z= 2.429460964806D+13
I= 8 X= -2.610208849668D+13 Y= -5.118271750219D+13 Z= -1.787685070662D+13
I= 9 X= -1.231385487166D+13 Y= -8.897908504380D+12 Z= -2.327343240931D+13
I= 10 X= 5.372367885730D+13 Y= 8.599799110137D+13 Z= -4.411167120018D+12
I= 11 X= 1.116009788810D+13 Y= -1.576030675607D+14 Z= 1.051509272474D+13
I= 12 X= -2.068339235035D+13 Y= 1.168526856027D+13 Z= 1.452110608177D+14
I= 13 X= 1.528123008962D+13 Y= 1.086974594575D+13 Z= 5.452378377158D+12
I= 14 X= 2.483360284621D+13 Y= 2.187143026017D+13 Z= 1.073865850374D+13
I= 15 X= -3.782810688613D+13 Y= -1.872751727159D+13 Z= 2.266283519785D+13
I= 16 X= -3.013807654774D+13 Y= -8.920162954625D+13 Z= 8.726758742784D+12
I= 17 X= -4.823172201015D+12 Y= 4.491822501337D+12 Z= 2.318595014045D+13
I= 18 X= -8.817291217855D+12 Y= 6.407245547429D+13 Z= -1.398063133610D+13
I= 19 X= 6.399248740205D+13 Y= 8.507463737204D+13 Z= 4.934403719976D+11
I= 20 X= 1.521042584428D+13 Y= -3.416167271023D+13 Z= -9.969175827599D+13
I= 21 X= 5.973276037597D+12 Y= -5.352965041281D+12 Z= -1.738242863469D+13
I= 22 X= -1.178207145538D+13 Y= 5.627856485214D+12 Z= 4.105142009118D+13
I= 23 X= 2.273309682855D+12 Y= -9.414497084099D+13 Z= 5.129621957296D+13
I= 24 X= -7.741943081521D+13 Y= 8.839194837397D+13 Z= -2.716954697473D+13
I= 25 X= -1.019549041921D+13 Y= -1.230815645193D+12 Z= -1.241457089830D+13
I= 26 X= -4.715303424927D+13 Y= 7.656626964321D+13 Z= 1.065200362556D+14
I= 27 X= -1.221951917136D+13 Y= 5.325934463259D+13 Z= -5.681228961025D+13
I= 28 X= 2.327926293128D+13 Y= 5.914745041467D+13 Z= -1.019231250459D+13
I= 29 X= -8.771364153733D+12 Y= -1.579090238663D+13 Z= 2.548338564486D+12
I= 30 X= -1.854396124058D+13 Y= 1.793997583396D+13 Z= 1.714335378606D+13
I= 31 X= 7.146306066704D+13 Y= 1.840775673882D+13 Z= 2.526068133265D+13
I= 32 X= 9.757672408680D+13 Y= 2.749563123778D+13 Z= -8.563691481036D+13

I= 33 X= -3.612062072131D+13 Y= -2.275992824272D+13 Z= -7.411666993688D+13
I= 34 X= 7.301153826508D+13 Y= 1.171233435345D+13 Z= -6.492358626612D+13
I= 35 X= 3.820612076398D+12 Y= 3.146158973287D+11 Z= 2.368948323425D+12
I= 36 X= 1.644760758245D+13 Y= -1.518263818854D+13 Z= 5.626538070773D+12
I= 37 X= 4.448823134526D+13 Y= -5.757868577772D+13 Z= 1.764446006776D+13
I= 38 X= -6.345042481137D+13 Y= -2.004580457632D+13 Z= -3.090433811228D+13

Seed: 33076722442

CM Start Point Coordinates: bohr

I= 0 X= -2.341509245685D+00 Y= 2.355803988242D+00 Z= -6.543685860164D-01
I= 1 X= -2.682871356934D+00 Y= -5.978244182248D-02 Z= -1.940291845597D+00
I= 2 X= -2.090715226297D+00 Y= 1.830339725673D+00 Z= 1.950834092801D+00
I= 3 X= -2.543906479014D+00 Y= -2.083609762938D+00 Z= -9.248403974080D-02
I= 4 X= -1.943214149015D+00 Y= -7.655260595467D-01 Z= 2.375892016395D+00
I= 5 X= 4.421247427695D+00 Y= 2.436341157970D+00 Z= -7.896871626130D-01
I= 6 X= 2.746604841764D+00 Y= 4.683643741927D-01 Z= -2.685660609120D+00
I= 7 X= 6.157906914208D+00 Y= 1.319925874354D+00 Z= -1.545467036948D+00
I= 8 X= 3.786232076327D+00 Y= 4.251909685270D+00 Z= -1.783119981591D+00
I= 9 X= -1.816852827382D+00 Y= -2.470241144855D+00 Z= 4.799094029864D+00
I= 10 X= -3.802941795294D+00 Y= -2.821978834796D+00 Z= 5.479326159005D+00
I= 11 X= -2.583412486845D-01 Y= -4.078668834152D+00 Z= 4.266838951782D+00
I= 12 X= -1.064655555110D+00 Y= -9.279392768862D-01 Z= 6.592365419643D+00
I= 13 X= -1.842766686025D+00 Y= 3.689276782381D+00 Z= 4.134550478078D+00
I= 14 X= -3.916514976545D+00 Y= 3.810378762284D+00 Z= 5.202559832108D+00
I= 15 X= -8.350470657814D-02 Y= 3.503187969614D+00 Z= 5.343042103127D+00
I= 16 X= -1.786538886457D+00 Y= 5.778050266644D+00 Z= 3.148731793698D+00
I= 17 X= -2.520117383236D+00 Y= 4.879721494211D+00 Z= -1.845063124491D+00
I= 18 X= -4.223614883081D+00 Y= 6.008395728135D+00 Z= -1.193239015939D+00
I= 19 X= -2.532711649925D-01 Y= 5.785106434303D+00 Z= -1.156817880749D+00
I= 20 X= -2.182177892924D+00 Y= 5.038311079969D+00 Z= -3.912133438330D+00

I= 21 X= -3.130348322641D+00 Y= -4.378736977797D-01 Z= -4.664214521109D+00
I= 22 X= -5.367467600422D+00 Y= -9.817961890069D-01 Z= -4.884558782577D+00
I= 23 X= -2.753505734578D+00 Y= 1.266836159401D+00 Z= -6.074326946916D+00
I= 24 X= -1.929508220801D+00 Y= -1.985068968523D+00 Z= -5.376781181704D+00
I= 25 X= -3.273957669982D+00 Y= -4.872039914252D+00 Z= -4.943484441107D-01
I= 26 X= -2.478047899753D+00 Y= -5.465540758715D+00 Z= -2.488848719856D+00
I= 27 X= -2.780918916467D+00 Y= -6.192470301012D+00 Z= 1.275634201375D+00
I= 28 X= -5.420075564129D+00 Y= -4.644579583436D+00 Z= -6.254725562175D-01
I= 29 X= 2.679788237150D+00 Y= -3.772114835602D+00 Z= -2.094694663412D+00
I= 30 X= 3.706764303883D+00 Y= -3.480266053690D+00 Z= 3.757199556258D-01
I= 31 X= 6.988285322167D-01 Y= -4.736605133610D+00 Z= -2.676860140943D+00
I= 32 X= 3.943762827158D+00 Y= -3.466216317996D+00 Z= -3.634717428965D+00
I= 33 X= 5.680245225567D+00 Y= -2.709263146560D+00 Z= 4.777504479727D-01
I= 34 X= 2.936929625354D+00 Y= -4.275052590820D+00 Z= 1.938854077646D+00
I= 35 X= 1.173380984645D+00 Y= 1.473500072146D-02 Z= -3.470111147758D-01
I= 36 X= 3.702309346576D+00 Y= 2.567431674711D+00 Z= 1.811188085023D+00
I= 37 X= 4.936078225496D+00 Y= 1.434046940926D+00 Z= 3.222209983314D+00
I= 38 X= 2.817731458622D+00 Y= 4.289598985568D+00 Z= 2.324629251183D+00

Forward Direction:

Total Energy: -656.4333400 Hartrees

Potential Energy: -656.6016481 Hartress

Kinetic Energy: 0.1683081 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.699331808762D+12 Y= 5.705353098966D+12 Z= -1.669167170654D+13
I= 1 X= 2.987680750795D+11 Y= -1.277245379663D+13 Z= 9.420127660363D+12
I= 2 X= 2.238954525266D+11 Y= 4.255978317863D+12 Z= 5.296692421753D+12
I= 3 X= 1.702342725415D+12 Y= 1.213795089079D+13 Z= 1.068580629477D+13
I= 4 X= -1.811664131461D+13 Y= -5.041811729365D+12 Z= -2.055347461882D+13
I= 5 X= 1.577941463343D+13 Y= -1.853028017271D+13 Z= 8.496910497541D+12
I= 6 X= -3.775300435503D+13 Y= -1.982808996996D+13 Z= 8.863913796158D+12

I= 7 X= -7.168445039958D+13 Y= 9.464289551313D+13 Z= -3.671742700764D+13
I= 8 X= -4.440755523104D+13 Y= -8.575392203170D+13 Z= -1.244344839737D+14
I= 9 X= -9.908587558589D+12 Y= 4.331616925000D+12 Z= 9.663464652328D+12
I= 10 X= 1.556397642724D+13 Y= 6.105242097857D+12 Z= -1.436034631033D+13
I= 11 X= 3.714489270565D+13 Y= -6.881612218806D+13 Z= -1.900742099461D+13
I= 12 X= 6.425913080885D+13 Y= 1.112637798538D+13 Z= 1.133053499610D+14
I= 13 X= 4.851512407522D+12 Y= -4.592678271891D+12 Z= 1.294861561712D+13
I= 14 X= 1.294866989822D+14 Y= 2.972049401632D+13 Z= 2.362156174719D+13
I= 15 X= -1.955463292817D+13 Y= 2.665387921023D+13 Z= 3.201386863789D+13
I= 16 X= 1.985399929386D+13 Y= 6.097436272821D+13 Z= 3.815234401742D+13
I= 17 X= -1.264975093102D+12 Y= -6.570124316713D+12 Z= 1.594484950046D+13
I= 18 X= 7.527676815255D+12 Y= 2.535635059295D+13 Z= 3.729258118963D+13
I= 19 X= 7.051327229869D+13 Y= -1.403040103262D+12 Z= -2.265116844722D+13
I= 20 X= 7.601581067834D+13 Y= 1.652745949189D+13 Z= -7.016418248432D+13
I= 21 X= 1.647748131218D+13 Y= 8.788502401576D+12 Z= 4.425910782216D+12
I= 22 X= 3.486352725847D+13 Y= 3.367597269779D+13 Z= -4.617049314338D+13
I= 23 X= -5.080372536461D+13 Y= 3.101851184601D+13 Z= 4.387776763274D+12
I= 24 X= -5.031836264551D+13 Y= -1.866918921739D+14 Z= -2.773702997789D+13
I= 25 X= 2.341619357037D+13 Y= 1.085614664906D+13 Z= -2.080042467021D+13
I= 26 X= -8.679961438708D+13 Y= -3.082338807576D+13 Z= 4.994559832320D+12
I= 27 X= 1.605478907868D+13 Y= -5.447302897953D+13 Z= 2.202605206942D+13
I= 28 X= -1.084568988050D+14 Y= -1.870038122944D+13 Z= -1.414866783578D+13
I= 29 X= -1.578433765809D+13 Y= -3.239401743949D+12 Z= 6.792312471720D+11
I= 30 X= 4.597615512987D+11 Y= -3.047460973137D+12 Z= 1.283883844910D+13
I= 31 X= 8.527079848514D+13 Y= 8.061184855391D+13 Z= -3.151492598443D+13
I= 32 X= 2.169965101443D+13 Y= 5.185443041147D+13 Z= -2.247441760609D+13
I= 33 X= -7.476556470439D+13 Y= -4.863835557807D+12 Z= 6.293364206203D+13
I= 34 X= 9.305528743870D+13 Y= 7.423914774687D+13 Z= -5.350709069616D+13
I= 35 X= -1.710621480086D+12 Y= 2.004065868483D+11 Z= -3.954354979466D+12
I= 36 X= -1.674506979635D+13 Y= -1.929675218913D+12 Z= 2.065819101212D+12

I= 37 X= 6.883356062850D+13 Y= -4.593562415753D+13 Z= 1.000585659407D+14

I= 38 X= -5.341989990903D+12 Y= 6.920077942589D+13 Z= 2.915876980107D+13

Backward Direction:

Total Energy: -656.4333334 Hartrees

Potential Energy: -656.6016481 Hartress

Kinetic Energy: 0.1683147 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.032063534894D+12 Y= 5.270853715252D+12 Z= -1.652164057305D+13

I= 1 X= -2.144298482207D+11 Y= -1.388976699893D+13 Z= 8.749401420039D+12

I= 2 X= -2.537536665478D+11 Y= 4.695043562107D+12 Z= 4.589778792208D+12

I= 3 X= 7.236643640547D+11 Y= 1.216083517158D+13 Z= 9.267801952261D+12

I= 4 X= -1.644272049928D+13 Y= -5.191155889897D+12 Z= -2.166582192079D+13

I= 5 X= 1.301677074414D+13 Y= -2.245906178030D+13 Z= 6.530386949555D+11

I= 6 X= 2.412975636780D+13 Y= 5.081851215848D+13 Z= 3.670711479265D+13

I= 7 X= -6.038156221376D+13 Y= 1.053443263388D+14 Z= -3.602591879294D+13

I= 8 X= -3.013247391163D+13 Y= -7.421510098248D+13 Z= -1.231064335327D+14

I= 9 X= -9.376566532677D+12 Y= 4.581463996876D+12 Z= 9.062105803545D+12

I= 10 X= 1.566127881323D+13 Y= 7.341725566969D+12 Z= -1.579368691955D+13

I= 11 X= 3.699123449318D+13 Y= -6.882963888876D+13 Z= -1.903730052124D+13

I= 12 X= 6.457093252419D+13 Y= 1.120989035581D+13 Z= 1.130092625286D+14

I= 13 X= 4.956977815509D+12 Y= -4.643993702145D+12 Z= 1.272664326450D+13

I= 14 X= 1.296659976688D+14 Y= 2.940435814382D+13 Z= 2.366848685837D+13

I= 15 X= -1.922490157455D+13 Y= 2.635145858651D+13 Z= 3.146785773224D+13

I= 16 X= 1.983103031536D+13 Y= 6.107156098759D+13 Z= 3.822921698567D+13

I= 17 X= -1.103466716072D+12 Y= -6.926549272130D+12 Z= 1.590955306734D+13

I= 18 X= 7.561730040764D+12 Y= 2.478811466042D+13 Z= 3.682643432473D+13

I= 19 X= 7.017184684454D+13 Y= -1.516777343973D+12 Z= -2.229910551473D+13

I= 20 X= 7.625290671598D+13 Y= 1.620898153726D+13 Z= -7.020485261752D+13

I= 21 X= 1.627425239108D+13 Y= 8.660829454966D+12 Z= 3.929798030213D+12

I= 22 X= 3.482720859992D+13 Y= 3.424813123613D+13 Z= -4.815873365660D+13

I= 23 X= -5.006500977678D+13 Y= 3.069695686813D+13 Z= 4.157230644665D+12
I= 24 X= -5.067448604411D+13 Y= -1.868919057627D+14 Z= -2.832362680154D+13
I= 25 X= 2.319532451555D+13 Y= 1.063302271883D+13 Z= -2.091439915283D+13
I= 26 X= -8.734592034383D+13 Y= -3.142100458465D+13 Z= 4.927903271937D+12
I= 27 X= 1.651009393304D+13 Y= -5.408969926753D+13 Z= 2.189391367896D+13
I= 28 X= -1.084343372393D+14 Y= -1.937661819269D+13 Z= -1.366999870082D+13
I= 29 X= -1.680720909224D+13 Y= -2.952085127392D+12 Z= 3.204732007240D+11
I= 30 X= 5.199975317256D+11 Y= -3.245412420863D+12 Z= 1.239454279658D+13
I= 31 X= 8.456361663014D+13 Y= 8.040263236875D+13 Z= -3.149282904848D+13
I= 32 X= 1.963003763743D+13 Y= 5.357311850546D+13 Z= -2.370660266066D+13
I= 33 X= -7.470173746648D+13 Y= -5.113996036300D+12 Z= 6.257975895612D+13
I= 34 X= 9.372208052100D+13 Y= 7.377490900724D+13 Z= -5.363470930309D+13
I= 35 X= -1.721749180005D+12 Y= 4.603151971435D+11 Z= -2.305394966488D+12
I= 36 X= -2.034119416062D+13 Y= -6.471876606454D+12 Z= 4.082550529452D+11
I= 37 X= 7.204163640411D+13 Y= -4.430699742011D+13 Z= 9.605758203843D+13
I= 38 X= -3.585123241668D+12 Y= 6.901771070177D+13 Z= 2.617073737112D+13

Seed: 33848100429

CM Start Point Coordinates: bohr

I= 0 X= -2.284033875554D+00 Y= 2.263477516796D+00 Z= -5.275606433121D-01
I= 1 X= -2.737401410556D+00 Y= -2.840936079137D-02 Z= -2.011952691127D+00
I= 2 X= -2.142174825310D+00 Y= 1.705974952259D+00 Z= 2.144472725295D+00
I= 3 X= -2.592688978132D+00 Y= -1.876681686719D+00 Z= -1.735508320584D-01
I= 4 X= -2.045331084737D+00 Y= -9.867499178147D-01 Z= 2.331832596239D+00
I= 5 X= 4.777647436921D+00 Y= 2.444563624460D+00 Z= -1.029814703187D+00
I= 6 X= 2.400732186200D+00 Y= 5.813884882605D-01 Z= -2.919860211566D+00
I= 7 X= 6.400514479282D+00 Y= 1.515598700392D+00 Z= -1.748270566263D+00
I= 8 X= 4.150009003030D+00 Y= 3.833956628684D+00 Z= -2.311095505755D+00
I= 9 X= -1.867560739661D+00 Y= -2.509424393130D+00 Z= 4.697550182387D+00
I= 10 X= -3.730046400319D+00 Y= -2.701548878376D+00 Z= 5.685513313201D+00

I= 11 X= -7.444353292695D-01 Y= -4.478023669627D+00 Z= 4.729167079216D+00
I= 12 X= -5.975277168960D-01 Y= -1.002334539960D+00 Z= 5.808475646822D+00
I= 13 X= -1.982750069775D+00 Y= 3.647877413906D+00 Z= 4.088146781334D+00
I= 14 X= -3.864740651691D+00 Y= 3.866292957449D+00 Z= 4.928446513500D+00
I= 15 X= -4.939874480943D-01 Y= 3.243554041961D+00 Z= 5.805158104688D+00
I= 16 X= -1.332930004010D+00 Y= 5.719042032740D+00 Z= 3.206104755464D+00
I= 17 X= -2.391652607365D+00 Y= 4.829036513817D+00 Z= -1.764625291993D+00
I= 18 X= -4.111428622284D+00 Y= 5.510320059001D+00 Z= -1.658443446398D+00
I= 19 X= -1.127052596935D+00 Y= 5.964726328572D+00 Z= -6.802833210995D-01
I= 20 X= -2.048726450305D+00 Y= 4.482274955204D+00 Z= -3.908386811837D+00
I= 21 X= -3.260342808962D+00 Y= -3.496806205427D-01 Z= -4.615278021532D+00
I= 22 X= -5.303501444203D+00 Y= -6.453290542171D-01 Z= -5.046806697610D+00
I= 23 X= -2.737664246339D+00 Y= 1.671993974666D+00 Z= -5.871063735069D+00
I= 24 X= -2.173985447961D+00 Y= -1.934308092380D+00 Z= -5.645455521824D+00
I= 25 X= -3.104474069786D+00 Y= -4.644550333425D+00 Z= -6.768348616776D-01
I= 26 X= -3.774672266931D+00 Y= -5.150733466038D+00 Z= -2.608687168331D+00
I= 27 X= -1.827416248645D+00 Y= -6.230123660073D+00 Z= 2.231809852339D-01
I= 28 X= -4.903794700384D+00 Y= -4.955566371569D+00 Z= 1.902825812557D-01
I= 29 X= 2.809968182649D+00 Y= -3.791825279693D+00 Z= -1.734522082996D+00
I= 30 X= 3.751907023845D+00 Y= -3.011944941314D+00 Z= 5.370748648065D-01
I= 31 X= 8.719621767619D-01 Y= -4.969571620667D+00 Z= -1.868704665788D+00
I= 32 X= 3.618246140984D+00 Y= -3.338856524990D+00 Z= -3.891608589978D+00
I= 33 X= 6.044539065311D+00 Y= -2.330446600013D+00 Z= 6.388945846711D-01
I= 34 X= 3.376561246774D+00 Y= -3.960471457304D+00 Z= 2.401528690169D+00
I= 35 X= 1.095174364661D+00 Y= -1.314582289286D-02 Z= -3.265895354705D-01
I= 36 X= 3.998531964150D+00 Y= 2.444738179513D+00 Z= 1.508280511980D+00
I= 37 X= 5.474095831020D+00 Y= 1.088010275048D+00 Z= 2.693970566169D+00
I= 38 X= 2.610747699250D+00 Y= 3.938309218530D+00 Z= 2.174397327012D+00

Forward Direction:

Total Energy: -656.4419405 Hartrees

Potential Energy: -656.6151223 Hartress

Kinetic Energy: 0.1731819 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.127462177164D+13 Y= 1.706351508039D+13 Z= 7.824966089752D+12
I= 1 X= 1.723909244022D+13 Y= -9.342929127640D+12 Z= -1.465494337925D+13
I= 2 X= -1.811683441482D+12 Y= -6.234042390089D+12 Z= 1.917669502035D+13
I= 3 X= 8.362823233096D+12 Y= -9.162738122210D+12 Z= 6.078834666096D+12
I= 4 X= -5.363052395355D+12 Y= 2.199218391235D+13 Z= -1.339853384124D+13
I= 5 X= -6.086291556144D+12 Y= 2.072092629276D+13 Z= 1.259880697259D+13
I= 6 X= -7.210759350255D+13 Y= -7.505342708438D+13 Z= 5.989740779123D+13
I= 7 X= 1.209198133397D+14 Y= -1.344524403090D+14 Z= 8.612666961264D+13
I= 8 X= -4.409843783116D+12 Y= -1.245251710694D+13 Z= 3.198803378033D+13
I= 9 X= 9.634932440100D+11 Y= 1.006063060317D+13 Z= 1.507753310148D+12
I= 10 X= -1.479332863673D+13 Y= -4.414292158745D+13 Z= 1.738621988287D+13
I= 11 X= -4.559120651763D+12 Y= -3.113135460089D+13 Z= -4.004409756861D+13
I= 12 X= 8.567745081009D+12 Y= -7.024705326029D+12 Z= -3.930927515308D+13
I= 13 X= -3.486015040475D+12 Y= 2.392969843926D+13 Z= -3.001553950832D+13
I= 14 X= 1.309070643697D+13 Y= -3.218777394075D+13 Z= 6.239756337393D+13
I= 15 X= 6.543182879490D+13 Y= 4.833633896858D+13 Z= 1.108633612983D+13
I= 16 X= -3.252837239092D+13 Y= -3.374419791828D+13 Z= 1.195331558357D+14
I= 17 X= -1.061175463324D+13 Y= -1.478284533900D+13 Z= -1.768336577537D+13
I= 18 X= 1.716079687636D+13 Y= 4.899957620046D+13 Z= 1.800376134663D+13
I= 19 X= 5.267872087172D+12 Y= -4.212666198750D+13 Z= -1.982891747718D+13
I= 20 X= -5.474110216229D+12 Y= -8.947994165344D+12 Z= 1.694507369081D+14
I= 21 X= -1.454062178629D+13 Y= -2.333004835510D+13 Z= 1.030056948856D+12
I= 22 X= -2.209358978126D+13 Y= 8.894729015066D+13 Z= -7.034584245543D+12
I= 23 X= -2.505399183719D+13 Y= 6.986407316149D+13 Z= 9.355882085609D+12
I= 24 X= 1.104747518248D+14 Y= -5.601114828930D+13 Z= 7.474122201329D+13
I= 25 X= -1.164713359634D+13 Y= 1.994898017681D+13 Z= -1.427564952398D+13
I= 26 X= -2.992957790966D+13 Y= -3.779517437165D+13 Z= -1.394412236007D+14

I= 27 X= -1.543443084730D+13 Y= -4.134158862784D+13 Z= 9.861113073728D+13
I= 28 X= 2.064968987767D+13 Y= -5.128663427161D+13 Z= 2.747146664327D+12
I= 29 X= 1.202352775703D+13 Y= 5.579760017160D+11 Z= -7.548822746379D+12
I= 30 X= 9.515614132748D+12 Y= 8.440170587355D+12 Z= 1.343870460742D+13
I= 31 X= -8.131443944012D+13 Y= -4.308379983122D+13 Z= -1.755225003187D+13
I= 32 X= -1.561689634458D+13 Y= -2.106948808735D+12 Z= -5.530829560204D+13
I= 33 X= -9.107555795879D+13 Y= -8.513060411138D+13 Z= 7.237874156205D+12
I= 34 X= 1.439689034892D+13 Y= 2.106321913399D+12 Z= 2.711554928463D+13
I= 35 X= 2.271130750163D+12 Y= -2.009095168930D+12 Z= -1.052515124492D+12
I= 36 X= 6.224491560392D+12 Y= -2.182220773409D+12 Z= 4.352881165534D+12
I= 37 X= 1.583415121967D+13 Y= 2.052403288458D+13 Z= 2.087634704804D+13
I= 38 X= -8.437104016456D+13 Y= -2.239446306631D+13 Z= -1.469185158330D+13

Backward Direction:

Total Energy: -656.4420482 Hartrees

Potential Energy: -656.6151223 Hartress

Kinetic Energy: 0.1730741 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.187213027918D+13 Y= 1.628325561966D+13 Z= 8.130302312696D+12
I= 1 X= 1.631750877262D+13 Y= -1.134936281066D+13 Z= -1.585941113034D+13
I= 2 X= -2.669429757870D+12 Y= -5.445583706627D+12 Z= 1.790724316579D+13
I= 3 X= 6.605345360357D+12 Y= -9.121643295850D+12 Z= 3.532429886964D+12
I= 4 X= -2.357081374427D+12 Y= 2.172399666427D+13 Z= -1.539604992622D+13
I= 5 X= -1.104735506352D+13 Y= 1.366575166585D+13 Z= -1.486955695526D+12
I= 6 X= 3.901939872375D+13 Y= 5.181137845662D+13 Z= 1.098972970096D+14
I= 7 X= 1.412171619564D+14 Y= -1.152351687077D+14 Z= 8.736845694021D+13
I= 8 X= 2.122486986765D+13 Y= 8.268511848785D+12 Z= 3.437290234803D+13
I= 9 X= 1.918878816412D+12 Y= 1.050929762140D+13 Z= 4.278532013371D+11
I= 10 X= -1.461859627220D+13 Y= -4.192248592061D+13 Z= 1.481227474332D+13
I= 11 X= -4.835054910670D+12 Y= -3.115562746560D+13 Z= -4.009775422544D+13
I= 12 X= 9.127668145937D+12 Y= -6.874736613552D+12 Z= -3.984097908021D+13

I= 13 X= -3.296623788491D+12 Y= 2.383754790480D+13 Z= -3.041415003515D+13
I= 14 X= 1.341268501682D+13 Y= -3.275548017832D+13 Z= 6.248182991712D+13
I= 15 X= 6.602394932379D+13 Y= 4.779326213563D+13 Z= 1.010582800844D+13
I= 16 X= -3.256961932147D+13 Y= -3.356965251908D+13 Z= 1.196712017420D+14
I= 17 X= -1.032172328926D+13 Y= -1.542290135357D+13 Z= -1.774674992669D+13
I= 18 X= 1.722194852208D+13 Y= 4.797915711551D+13 Z= 1.716667039642D+13
I= 19 X= 4.654751662629D+12 Y= -4.233090753315D+13 Z= -1.919669464325D+13
I= 20 X= -5.048341080455D+12 Y= -9.519906228541D+12 Z= 1.693777028165D+14
I= 21 X= -1.490557348636D+13 Y= -2.355931916327D+13 Z= 1.391542595978D+11
I= 22 X= -2.215880961409D+13 Y= 8.997475331578D+13 Z= -1.060500006879D+13
I= 23 X= -2.372743108606D+13 Y= 6.928663548643D+13 Z= 8.941875078030D+12
I= 24 X= 1.098352373403D+14 Y= -5.637032600056D+13 Z= 7.368783105377D+13
I= 25 X= -1.204376285955D+13 Y= 1.954830168568D+13 Z= -1.448032108409D+13
I= 26 X= -3.091061588255D+13 Y= -3.886835411293D+13 Z= -1.395609232371D+14
I= 27 X= -1.461680962332D+13 Y= -4.065321793815D+13 Z= 9.837384102396D+13
I= 28 X= 2.069020518170D+13 Y= -5.250099800274D+13 Z= 3.606724695868D+12
I= 29 X= 1.018668944463D+13 Y= 1.073929574391D+12 Z= -8.193068450492D+12
I= 30 X= 9.623783890603D+12 Y= 8.084695996671D+12 Z= 1.264085333149D+13
I= 31 X= -8.258437295985D+13 Y= -4.345950325119D+13 Z= -1.751256909078D+13
I= 32 X= -1.933343883426D+13 Y= 9.794137950096D+11 Z= -5.752101230771D+13
I= 33 X= -9.096093913099D+13 Y= -8.557983392656D+13 Z= 6.602382718845D+12
I= 34 X= 1.559429505875D+13 Y= 1.272657501445D+12 Z= 2.688637607035D+13
I= 35 X= 2.251147998663D+12 Y= -1.542359978790D+12 Z= 1.908632121967D+12
I= 36 X= -2.333083121846D+11 Y= -1.033895412521D+13 Z= 1.376283080043D+12
I= 37 X= 2.159510641173D+13 Y= 2.344866631102D+13 Z= 1.369151395784D+13
I= 38 X= -8.121611761347D+13 Y= -2.272321175951D+13 Z= -2.005766029694D+13

Seed: 33982230834

CM Start Point Coordinates: bohr

I= 0 X= -2.187514531852D+00 Y= 2.217244653830D+00 Z= -7.215549841069D-01

I= 1 X= -2.751424272606D+00 Y= -1.427947300504D-01 Z= -1.922227418891D+00
I= 2 X= -2.064914217418D+00 Y= 1.721974050029D+00 Z= 2.103254821010D+00
I= 3 X= -2.634661210160D+00 Y= -1.947382624186D+00 Z= -1.353101135687D-01
I= 4 X= -2.019067454649D+00 Y= -9.470347504816D-01 Z= 2.424766518476D+00
I= 5 X= 3.970215650695D+00 Y= 2.925465602245D+00 Z= -1.261600473312D+00
I= 6 X= 2.195077265858D+00 Y= 4.836107775202D-01 Z= -3.227741508328D+00
I= 7 X= 5.711213458182D+00 Y= 2.452090919994D+00 Z= -2.935574609651D+00
I= 8 X= 2.881263665750D+00 Y= 4.576483955189D+00 Z= -1.885051968980D+00
I= 9 X= -1.668300727124D+00 Y= -2.261478054136D+00 Z= 4.936772411585D+00
I= 10 X= -3.509740844249D+00 Y= -2.059729442476D+00 Z= 6.048760779439D+00
I= 11 X= -1.158118771188D+00 Y= -4.204662016351D+00 Z= 4.484311971419D+00
I= 12 X= -2.578924651706D-01 Y= -1.371250872748D+00 Z= 5.676502953740D+00
I= 13 X= -2.136237763320D+00 Y= 3.688060847494D+00 Z= 4.099481010529D+00
I= 14 X= -4.131144073596D+00 Y= 3.824622099604D+00 Z= 4.684125841536D+00
I= 15 X= -8.761491859420D-01 Y= 3.139770944576D+00 Z= 5.687937040316D+00
I= 16 X= -1.394497966222D+00 Y= 5.531093430797D+00 Z= 3.605398072626D+00
I= 17 X= -1.759777393999D+00 Y= 4.905817780640D+00 Z= -1.680502849334D+00
I= 18 X= -3.506955279712D+00 Y= 6.434276482195D+00 Z= -8.639736438730D-01
I= 19 X= 1.372896375573D-01 Y= 5.925834528543D+00 Z= -1.304785863953D+00
I= 20 X= -2.333746400838D+00 Y= 4.479790687871D+00 Z= -4.000842324887D+00
I= 21 X= -3.244436848420D+00 Y= -4.698205620127D-01 Z= -4.805476512053D+00
I= 22 X= -5.521687539096D+00 Y= -4.601786532010D-01 Z= -4.893340898508D+00
I= 23 X= -2.378534652725D+00 Y= 8.848492036496D-01 Z= -6.105922525338D+00
I= 24 X= -2.652009073535D+00 Y= -2.413536958197D+00 Z= -5.451499704945D+00
I= 25 X= -3.276084748967D+00 Y= -4.666614664661D+00 Z= -7.452220439308D-01
I= 26 X= -2.525030833563D+00 Y= -4.898772353790D+00 Z= -2.740614351096D+00
I= 27 X= -2.435548848270D+00 Y= -6.303880439082D+00 Z= 5.781749012914D-01
I= 28 X= -5.727609864109D+00 Y= -4.431254894476D+00 Z= -1.364895649767D+00
I= 29 X= 3.274237991408D+00 Y= -3.540962550159D+00 Z= -1.971303062519D+00
I= 30 X= 3.585266748458D+00 Y= -3.507420873442D+00 Z= 6.605614621802D-01

I= 31 X= 2.321465037879D+00 Y= -4.872807937139D+00 Z= -2.812252642246D+00
I= 32 X= 4.859749074233D+00 Y= -2.888415159513D+00 Z= -3.157619591624D+00
I= 33 X= 5.335838956857D+00 Y= -2.757481560042D+00 Z= 1.706913623449D+00
I= 34 X= 2.664146061153D+00 Y= -4.827417250326D+00 Z= 1.971921834636D+00
I= 35 X= 1.071054754607D+00 Y= -4.326274727070D-02 Z= -2.737176540005D-01
I= 36 X= 4.005328702822D+00 Y= 2.296144286815D+00 Z= 1.458483812847D+00
I= 37 X= 5.609876465302D+00 Y= 1.208150418154D+00 Z= 2.292846609189D+00
I= 38 X= 3.390353113049D+00 Y= 3.737079282373D+00 Z= 2.901265299416D+00

Forward Direction:

Total Energy: -656.4309392 Hartrees

Potential Energy: -656.5885644 Hartress

Kinetic Energy: 0.1576252 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.144537705953D+12 Y= 8.012496430888D+12 Z= 3.084249160236D+12
I= 1 X= 2.237025956276D+13 Y= -4.509441579077D+12 Z= -9.106000963945D+12
I= 2 X= -9.629676708169D+12 Y= -9.517970633431D+12 Z= 3.819391279094D+12
I= 3 X= 1.148674363765D+13 Y= 1.401983246831D+12 Z= 5.004144891588D+12
I= 4 X= -9.028101158600D+11 Y= -1.460149191368D+13 Z= 1.345850601823D+13
I= 5 X= 1.640076509456D+12 Y= 1.091149616337D+13 Z= -1.134685957741D+13
I= 6 X= -3.106898157592D+13 Y= -6.315457664681D+13 Z= 1.426648770659D+13
I= 7 X= 1.284322250339D+14 Y= 1.415017211288D+12 Z= -5.321448418470D+13
I= 8 X= 3.009510526127D+13 Y= 4.252122501097D+13 Z= -6.026057810661D+13
I= 9 X= 4.050731746293D+12 Y= 1.952035283086D+13 Z= -2.318851868563D+13
I= 10 X= -4.765582213740D+13 Y= -8.564266951904D+11 Z= 8.524557595887D+13
I= 11 X= 2.589178890545D+10 Y= -4.217505260829D+13 Z= 1.665333224209D+13
I= 12 X= 1.274159510735D+13 Y= 2.280738769508D+13 Z= -2.836744261203D+13
I= 13 X= -2.217690177700D+12 Y= 1.941379307477D+13 Z= -1.011975525408D+13
I= 14 X= 1.298149351791D+14 Y= 8.251498709382D+13 Z= -8.656342714212D+13
I= 15 X= 3.325607832195D+13 Y= -2.434896939581D+13 Z= 4.800886021588D+13
I= 16 X= -6.269168302606D+13 Y= -4.744103760891D+13 Z= 2.358080586528D+13

I= 17 X= -2.440612043582D+13 Y= -1.674953014670D+13 Z= -2.079642357309D+12
I= 18 X= 2.904627081500D+13 Y= -1.986139105354D+13 Z= -9.025826797904D+12
I= 19 X= 2.431937258752D+13 Y= -8.867070310742D+13 Z= 4.969524009580D+13
I= 20 X= 2.303883869981D+13 Y= 2.954443184051D+13 Z= 1.123957176823D+14
I= 21 X= 5.634691548420D+12 Y= -8.064104236737D+12 Z= 6.093625356574D+12
I= 22 X= -6.481652608261D+13 Y= -1.034848049414D+13 Z= 5.274692445473D+13
I= 23 X= 8.860077035866D+13 Y= 4.426583750599D+13 Z= 1.228865273778D+13
I= 24 X= 4.231064437626D+13 Y= 1.408434409194D+14 Z= 4.189757731626D+13
I= 25 X= 3.040260190922D+12 Y= 2.920655306532D+12 Z= 1.429116167483D+13
I= 26 X= -2.663598955170D+13 Y= 4.806797413428D+13 Z= -2.220121116915D+13
I= 27 X= -2.703101096974D+12 Y= -2.186954722518D+13 Z= -3.605727734699D+13
I= 28 X= -1.209805652012D+14 Y= -6.970775312855D+13 Z= -5.264124832045D+13
I= 29 X= 2.591544184308D+12 Y= -3.271741347419D+12 Z= -3.381394702888D+12
I= 30 X= 4.556747634839D+12 Y= -2.058187225559D+12 Z= -7.723415459242D+11
I= 31 X= -6.322002759652D+13 Y= 1.172624078345D+13 Z= -1.075810158125D+13
I= 32 X= -6.259663537280D+13 Y= 5.082341404009D+12 Z= 8.004318598555D+13
I= 33 X= 6.339034326379D+13 Y= 1.170376038896D+12 Z= 1.340788074355D+14
I= 34 X= 6.454640855577D+12 Y= -5.785339147761D+13 Z= -3.662156373126D+12
I= 35 X= -2.311849890027D+12 Y= 1.394165741238D+11 Z= 6.509137520359D+11
I= 36 X= -7.587481953807D+12 Y= -4.975721479261D+12 Z= -2.125574931578D+13
I= 37 X= 2.754305483140D+13 Y= -4.897490652993D+13 Z= 6.112036784373D+13
I= 38 X= 3.788452619613D+13 Y= 6.973063318148D+13 Z= -1.304916263344D+13

Backward Direction:

Total Energy: -656.4309505 Hartrees

Potential Energy: -656.5885644 Hartress

Kinetic Energy: 0.1576139 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.287161350230D+12 Y= 7.826250633587D+12 Z= 3.157132081051D+12

I= 1 X= 2.215028006525D+13 Y= -4.988371805114D+12 Z= -9.393504117569D+12

I= 2 X= -9.834418404254D+12 Y= -9.329767704922D+12 Z= 3.516376598414D+12

I= 3 X= 1.106723848239D+13 Y= 1.411792469508D+12 Z= 4.396325043785D+12
I= 4 X= -1.852930642508D+11 Y= -1.466550747537D+13 Z= 1.298170439892D+13
I= 5 X= 4.558842344777D+11 Y= 9.227445299718D+12 Z= -1.470909255536D+13
I= 6 X= -4.543272825842D+12 Y= -3.287229495145D+13 Z= 2.620132435058D+13
I= 7 X= 1.332771465687D+14 Y= 6.002127324015D+12 Z= -5.291807295295D+13
I= 8 X= 3.621404121536D+13 Y= 4.746727788340D+13 Z= -5.969131651051D+13
I= 9 X= 4.278779666495D+12 Y= 1.962744841948D+13 Z= -2.344628788376D+13
I= 10 X= -4.761411399998D+13 Y= -3.264147777001D+11 Z= 8.463118230164D+13
I= 11 X= -3.997296664993D+10 Y= -4.218084647949D+13 Z= 1.664052454282D+13
I= 12 X= 1.287524720747D+13 Y= 2.284318481135D+13 Z= -2.849435888451D+13
I= 13 X= -2.172483003671D+12 Y= 1.939179699429D+13 Z= -1.021490249457D+13
I= 14 X= 1.298917905856D+14 Y= 8.237947716916D+13 Z= -8.654331294955D+13
I= 15 X= 3.339741587161D+13 Y= -2.447860034687D+13 Z= 4.777481561138D+13
I= 16 X= -6.270152855625D+13 Y= -4.739937409785D+13 Z= 2.361375704492D+13
I= 17 X= -2.433689074841D+13 Y= -1.690230976460D+13 Z= -2.094771982149D+12
I= 18 X= 2.906086754501D+13 Y= -2.010496229655D+13 Z= -9.225638116398D+12
I= 19 X= 2.417302241967D+13 Y= -8.871945596302D+13 Z= 4.984614994886D+13
I= 20 X= 2.314046863026D+13 Y= 2.940791799589D+13 Z= 1.123782846376D+14
I= 21 X= 5.547578577678D+12 Y= -8.118830550768D+12 Z= 5.880969325623D+12
I= 22 X= -6.483209387771D+13 Y= -1.010322785641D+13 Z= 5.189467597570D+13
I= 23 X= 8.891741677255D+13 Y= 4.412800471705D+13 Z= 1.218983040012D+13
I= 24 X= 4.215799402460D+13 Y= 1.407577061853D+14 Z= 4.164613577874D+13
I= 25 X= 2.945585871727D+12 Y= 2.825014447818D+12 Z= 1.424230713227D+13
I= 26 X= -2.687016062633D+13 Y= 4.781180906913D+13 Z= -2.222978315052D+13
I= 27 X= -2.507937151683D+12 Y= -2.170523502577D+13 Z= -3.611391775458D+13
I= 28 X= -1.209708943088D+14 Y= -6.999761842548D+13 Z= -5.243606940141D+13
I= 29 X= 2.153095907412D+12 Y= -3.148584642589D+12 Z= -3.535174387689D+12
I= 30 X= 4.582567459566D+12 Y= -2.143038036074D+12 Z= -9.627864607385D+11
I= 31 X= -6.352315725218D+13 Y= 1.163656140655D+13 Z= -1.074862984670D+13
I= 32 X= -6.348376389161D+13 Y= 5.819047705487D+12 Z= 7.951501656809D+13

I= 33 X= 6.341770246506D+13 Y= 1.063146115003D+12 Z= 1.339271173701D+14
I= 34 X= 6.740458079370D+12 Y= -5.805238488830D+13 Z= -3.716859387736D+12
I= 35 X= -2.316619718221D+12 Y= 2.508249858734D+11 Z= 1.357731491180D+12
I= 36 X= -9.128941099899D+12 Y= -6.922711395167D+12 Z= -2.196625512779D+13
I= 37 X= 2.891817906179D+13 Y= -4.827680454155D+13 Z= 5.940536785689D+13
I= 38 X= 3.863759756874D+13 Y= 6.965216176885D+13 Z= -1.432996648114D+13

Seed: 34740595451

CM Start Point Coordinates: bohr

I= 0 X= -2.243386068447D+00 Y= 2.361613484637D+00 Z= -5.357319440030D-01
I= 1 X= -2.772516217781D+00 Y= 1.064799787226D-01 Z= -2.066120270485D+00
I= 2 X= -2.095814781553D+00 Y= 1.853617132124D+00 Z= 2.061832872841D+00
I= 3 X= -2.525570367189D+00 Y= -1.798031140427D+00 Z= -8.579329988933D-02
I= 4 X= -1.999991818369D+00 Y= -7.778237688946D-01 Z= 2.298109686565D+00
I= 5 X= 4.587197545027D+00 Y= 2.408652120169D+00 Z= -1.090325085079D+00
I= 6 X= 2.582069241905D+00 Y= 6.726415995835D-01 Z= -3.230785117863D+00
I= 7 X= 6.191521327398D+00 Y= 1.318547386471D+00 Z= -1.849893019814D+00
I= 8 X= 4.093619442026D+00 Y= 4.022822057214D+00 Z= -1.869044841562D+00
I= 9 X= -1.844201073233D+00 Y= -2.310052911044D+00 Z= 4.822167103372D+00
I= 10 X= -3.577691996985D+00 Y= -1.441066562638D+00 Z= 5.942051350490D+00
I= 11 X= -1.667055432953D+00 Y= -4.180369372845D+00 Z= 4.515971855058D+00
I= 12 X= 2.329223213789D-01 Y= -1.677913447919D+00 Z= 5.702472795634D+00
I= 13 X= -1.944557812553D+00 Y= 3.499472765943D+00 Z= 4.158349509667D+00
I= 14 X= -3.757011979798D+00 Y= 3.430920502970D+00 Z= 4.946749073690D+00
I= 15 X= -3.412545139745D-01 Y= 2.714274338470D+00 Z= 5.646568280549D+00
I= 16 X= -1.712308215948D+00 Y= 5.432054623843D+00 Z= 3.636103386630D+00
I= 17 X= -2.449540993659D+00 Y= 4.982170886206D+00 Z= -1.598606713507D+00
I= 18 X= -4.373908660183D+00 Y= 5.849689618689D+00 Z= -1.305080849846D+00
I= 19 X= -1.234604041986D+00 Y= 6.182315140803D+00 Z= -6.121419355270D-01
I= 20 X= -1.710849371146D+00 Y= 4.719914597038D+00 Z= -3.596932989628D+00

I= 21 X= -3.777144853046D+00 Y= -2.657930207342D-01 Z= -4.650472582976D+00
I= 22 X= -5.650750462144D+00 Y= 5.361307452257D-01 Z= -4.815794111227D+00
I= 23 X= -2.159589913355D+00 Y= 6.719762803194D-01 Z= -5.887398266890D+00
I= 24 X= -3.488792229516D+00 Y= -2.551234206192D+00 Z= -5.160960726664D+00
I= 25 X= -2.755917907820D+00 Y= -4.632810607403D+00 Z= -9.100567085030D-01
I= 26 X= -2.917560040980D+00 Y= -4.932827149019D+00 Z= -3.039235388491D+00
I= 27 X= -8.023987946605D-01 Y= -5.743055813202D+00 Z= -2.765201340265D-01
I= 28 X= -4.556076298623D+00 Y= -5.744678756698D+00 Z= 9.314852441596D-02
I= 29 X= 3.248538165776D+00 Y= -3.703651864345D+00 Z= -1.559027713204D+00
I= 30 X= 3.467748017968D+00 Y= -3.281255908014D+00 Z= 9.707365878486D-01
I= 31 X= 1.838211311036D+00 Y= -4.626745697542D+00 Z= -2.620702956434D+00
I= 32 X= 4.660973461789D+00 Y= -3.054265717570D+00 Z= -2.822293611533D+00
I= 33 X= 5.015416852007D+00 Y= -1.850254449299D+00 Z= 1.422705058164D+00
I= 34 X= 2.448310170464D+00 Y= -4.284750748662D+00 Z= 2.410216049836D+00
I= 35 X= 1.099919714084D+00 Y= -1.143436629911D-01 Z= -3.936726464334D-01
I= 36 X= 3.937554946572D+00 Y= 2.428804611156D+00 Z= 1.366476143137D+00
I= 37 X= 5.032004416629D+00 Y= 1.730931716521D+00 Z= 3.196683225922D+00
I= 38 X= 2.703681479172D+00 Y= 4.104584250227D+00 Z= 1.888359214723D+00

Forward Direction:

Total Energy: -656.4320278 Hartrees

Potential Energy: -656.6149620 Hartress

Kinetic Energy: 0.1829342 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.219314098292D+13 Y= 1.816747336244D+13 Z= 1.772099854358D+13
I= 1 X= -1.430058165545D+13 Y= -3.724353180261D+12 Z= -7.192567366674D+12
I= 2 X= 5.126978844887D+12 Y= -8.661671214170D+12 Z= -1.832540335606D+13
I= 3 X= -2.024507410486D+12 Y= 4.562774125803D+12 Z= -1.179755557245D+13
I= 4 X= -2.376525355413D+12 Y= -4.892238514986D+12 Z= -4.119364959743D+12
I= 5 X= 7.912549995637D+12 Y= -1.573909511211D+13 Z= 1.060802341449D+13
I= 6 X= -1.716916127022D+13 Y= -3.023877392250D+13 Z= 1.002916057979D+13

I= 7 X= 6.766824501935D+13 Y= -9.269484441122D+12 Z= -1.750074539846D+13
I= 8 X= -1.843318488157D+13 Y= 3.826864738322D+13 Z= 1.210409101332D+13
I= 9 X= 1.726655114028D+13 Y= -1.452034658159D+13 Z= 1.880264608101D+13
I= 10 X= -5.643551390165D+13 Y= -6.097889650722D+13 Z= -8.411086359057D+13
I= 11 X= -3.621373674405D+13 Y= 1.405689542257D+14 Z= -1.015569321253D+11
I= 12 X= -6.865781846912D+13 Y= -1.791770399092D+13 Z= -3.300959435234D+13
I= 13 X= 1.944565746406D+13 Y= -1.784701288215D+13 Z= -2.828464975007D+12
I= 14 X= -7.206341018809D+13 Y= 8.393638732139D+13 Z= 3.860122426723D+13
I= 15 X= -3.011870413781D+13 Y= -3.266327521160D+13 Z= 2.346122927012D+13
I= 16 X= -4.119496693417D+12 Y= 5.254141257646D+13 Z= 2.087052289703D+13
I= 17 X= -8.579011080108D+12 Y= 1.959281995380D+12 Z= -1.142645724339D+12
I= 18 X= 2.098294656872D+12 Y= -2.356763619648D+13 Z= 6.629989563869D+12
I= 19 X= -1.106187106883D+13 Y= 3.872782968398D+13 Z= -6.401391174625D+12
I= 20 X= -1.141913745266D+13 Y= 6.048630600155D+13 Z= -1.875219302645D+14
I= 21 X= -5.931328544637D+12 Y= -1.612438476333D+12 Z= -2.968488281897D+12
I= 22 X= 6.973902063537D+13 Y= 4.144257704288D+13 Z= 1.861976195163D+13
I= 23 X= 1.535064315380D+12 Y= -2.599014977021D+13 Z= -2.358737015287D+13
I= 24 X= 5.405189959853D+13 Y= 1.323618688288D+14 Z= 5.570180121016D+13
I= 25 X= -2.833908710890D+12 Y= -2.474846432687D+12 Z= 6.366981728475D+12
I= 26 X= -6.326160414956D+13 Y= -1.457626605920D+13 Z= -1.209607557411D+14
I= 27 X= 3.562243603354D+13 Y= 2.527294361121D+13 Z= 1.540268323224D+14
I= 28 X= -1.602080493949D+13 Y= 6.519328083930D+12 Z= 4.922184998497D+13
I= 29 X= -1.279329314849D+13 Y= -1.987304077633D+13 Z= 1.953686148050D+13
I= 30 X= -1.970539809421D+12 Y= 1.724294522226D+13 Z= -8.181061177176D+12
I= 31 X= 8.842343599342D+13 Y= 3.806002708626D+13 Z= -3.957673407300D+13
I= 32 X= 6.595302140362D+13 Y= -3.246349599695D+13 Z= -6.232094946453D+13
I= 33 X= 2.685760894698D+13 Y= 4.156592362918D+13 Z= 4.923842236781D+13
I= 34 X= 8.175812957851D+12 Y= -1.654704064547D+13 Z= 1.195836220167D+14
I= 35 X= -8.384117803787D+11 Y= -1.377577021589D+12 Z= -3.623748228677D+12
I= 36 X= -2.600544187157D+11 Y= 1.093130625658D+13 Z= 1.146154339759D+13

I= 37 X= -1.018250458014D+14 Y= 1.118716289448D+14 Z= -6.876509229666D+13

I= 38 X= 4.279308207804D+13 Y= 2.762365439035D+13 Z= 1.230795632918D+14

Backward Direction:

Total Energy: -656.4320307 Hartrees

Potential Energy: -656.6149620 Hartress

Kinetic Energy: 0.1829313 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.197149404237D+13 Y= 1.787803460055D+13 Z= 1.783426360781D+13

I= 1 X= -1.464244490603D+13 Y= -4.468643649036D+12 Z= -7.639367015993D+12

I= 2 X= 4.808796185668D+12 Y= -8.369190936103D+12 Z= -1.879630898520D+13

I= 3 X= -2.676447240074D+12 Y= 4.578018331087D+12 Z= -1.274214936601D+13

I= 4 X= -1.261454572009D+12 Y= -4.991723095554D+12 Z= -4.860347427551D+12

I= 5 X= 6.072233862421D+12 Y= -1.835622582981D+13 Z= 5.382882421444D+12

I= 6 X= 2.405361212886D+13 Y= 1.682197186614D+13 Z= 2.857671650593D+13

I= 7 X= 7.519758587441D+13 Y= -2.140800252748D+12 Z= -1.704010197885D+13

I= 8 X= -8.923938105977D+12 Y= 4.595515328327D+13 Z= 1.298876263678D+13

I= 9 X= 1.762095327050D+13 Y= -1.435391267989D+13 Z= 1.840205504063D+13

I= 10 X= -5.637069658892D+13 Y= -6.015522158907D+13 Z= -8.506567352518D+13

I= 11 X= -3.631609509143D+13 Y= 1.405599501647D+14 Z= -1.214609758823D+11

I= 12 X= -6.845011391287D+13 Y= -1.786207280625D+13 Z= -3.320683095680D+13

I= 13 X= 1.951591251352D+13 Y= -1.788119630218D+13 Z= -2.976330323611D+12

I= 14 X= -7.194397160887D+13 Y= 8.372579559883D+13 Z= 3.863248310771D+13

I= 15 X= -2.989905588082D+13 Y= -3.286473062209D+13 Z= 2.309750787872D+13

I= 16 X= -4.134797317924D+12 Y= 5.260616052780D+13 Z= 2.092173128939D+13

I= 17 X= -8.471423391460D+12 Y= 1.721851973885D+12 Z= -1.166158198254D+12

I= 18 X= 2.120978976864D+12 Y= -2.394616263899D+13 Z= 6.319469048458D+12

I= 19 X= -1.128930928416D+13 Y= 3.865206440422D+13 Z= -6.166866883151D+12

I= 20 X= -1.126119756736D+13 Y= 6.027415411090D+13 Z= -1.875490223996D+14

I= 21 X= -6.066708085558D+12 Y= -1.697486927526D+12 Z= -3.298970363825D+12

I= 22 X= 6.971482721170D+13 Y= 4.182371649554D+13 Z= 1.729530927967D+13

I= 23 X= 2.027154596252D+12 Y= -2.620435139602D+13 Z= -2.374094685815D+13
I= 24 X= 5.381467046203D+13 Y= 1.322286311614D+14 Z= 5.531104378711D+13
I= 25 X= -2.981039104658D+12 Y= -2.623478896254D+12 Z= 6.291058416361D+12
I= 26 X= -6.362552209843D+13 Y= -1.497436417095D+13 Z= -1.210051585523D+14
I= 27 X= 3.592573420231D+13 Y= 2.552829604461D+13 Z= 1.539388092474D+14
I= 28 X= -1.600577571186D+13 Y= 6.068857518721D+12 Z= 4.954071212311D+13
I= 29 X= -1.347467188651D+13 Y= -1.968164679729D+13 Z= 1.929787728599D+13
I= 30 X= -1.930414027421D+12 Y= 1.711108123441D+13 Z= -8.477025657294D+12
I= 31 X= 8.795235168736D+13 Y= 3.792065917288D+13 Z= -3.956201434980D+13
I= 32 X= 6.457436275379D+13 Y= -3.131860379914D+13 Z= -6.314176102234D+13
I= 33 X= 2.690012702220D+13 Y= 4.139928095951D+13 Z= 4.900268558408D+13
I= 34 X= 8.619992561523D+12 Y= -1.685629007173D+13 Z= 1.194986097667D+14
I= 35 X= -8.458244201132D+11 Y= -1.204440696945D+12 Z= -2.525304911856D+12
I= 36 X= -2.655587811263D+12 Y= 7.905550191255D+12 Z= 1.035736856295D+13
I= 37 X= -9.968800829201D+13 Y= 1.129565273893D+14 Z= -7.143032007215D+13
I= 38 X= 4.396340672348D+13 Y= 2.750170442551D+13 Z= 1.210891061380D+14

Seed: 34894387040

CM Start Point Coordinates: bohr

I= 0 X= -2.395950504115D+00 Y= 2.367037696724D+00 Z= -3.554425585372D-01
I= 1 X= -2.744392058285D+00 Y= 2.089604970715D-01 Z= -1.960409816419D+00
I= 2 X= -1.929261199720D+00 Y= 1.620026837000D+00 Z= 2.184993317156D+00
I= 3 X= -2.618794552956D+00 Y= -1.958837882605D+00 Z= -3.094073930823D-01
I= 4 X= -2.034463479102D+00 Y= -1.220501343560D+00 Z= 2.183720813118D+00
I= 5 X= 4.081420188259D+00 Y= 2.410197914046D+00 Z= -1.968177615852D+00
I= 6 X= 2.204625175330D+00 Y= 1.453176369936D-01 Z= -3.166189723376D+00
I= 7 X= 5.957860501697D+00 Y= 1.283303017499D+00 Z= -2.662649741740D+00
I= 8 X= 3.154325988372D+00 Y= 3.679816803355D+00 Z= -3.287476193597D+00
I= 9 X= -2.095520614764D+00 Y= -2.795325416441D+00 Z= 4.509537602575D+00
I= 10 X= -4.139744123796D+00 Y= -3.106943988280D+00 Z= 5.111774770669D+00

I= 11 X= -6.406477546308D-01 Y= -4.414327132035D+00 Z= 4.606838829756D+00
I= 12 X= -2.038043048954D+00 Y= -1.465310512488D+00 Z= 6.233520182389D+00
I= 13 X= -1.694947772951D+00 Y= 3.119008647929D+00 Z= 4.540214881593D+00
I= 14 X= -3.472843583153D+00 Y= 4.021253772078D+00 Z= 5.404504541476D+00
I= 15 X= -4.619670524423D-01 Y= 2.082870934930D+00 Z= 6.122597018976D+00
I= 16 X= -1.092085002119D+00 Y= 5.082079680591D+00 Z= 4.087872517099D+00
I= 17 X= -2.429727656533D+00 Y= 4.818928866228D+00 Z= -1.616636338505D+00
I= 18 X= -4.292206552041D+00 Y= 5.200958434653D+00 Z= -2.149956123279D+00
I= 19 X= -2.061037497540D+00 Y= 6.626987694101D+00 Z= 8.726422696277D-02
I= 20 X= -9.910312542889D-01 Y= 5.080524460757D+00 Z= -3.268597112451D+00
I= 21 X= -3.333248574720D+00 Y= 2.092953388575D-01 Z= -4.810775841387D+00
I= 22 X= -5.306732130076D+00 Y= 6.019783422869D-01 Z= -5.069432112247D+00
I= 23 X= -2.319200688934D+00 Y= 1.873626404317D+00 Z= -5.718419527981D+00
I= 24 X= -2.512136638381D+00 Y= -1.725237717276D+00 Z= -5.629393108139D+00
I= 25 X= -3.522594099261D+00 Y= -4.537564481851D+00 Z= -8.064157773751D-01
I= 26 X= -4.129580864236D+00 Y= -4.994413972622D+00 Z= -2.911441759745D+00
I= 27 X= -1.801114734808D+00 Y= -5.531192909816D+00 Z= -1.003890576216D-01
I= 28 X= -5.302122297860D+00 Y= -4.946477468684D+00 Z= 2.483791653736D-01
I= 29 X= 3.197476093154D+00 Y= -3.889878393144D+00 Z= -7.793442042225D-01
I= 30 X= 3.535156010217D+00 Y= -2.868967890540D+00 Z= 1.590641254464D+00
I= 31 X= 1.796837905593D+00 Y= -5.551240959648D+00 Z= -1.456637095932D+00
I= 32 X= 4.765823472946D+00 Y= -3.266292800475D+00 Z= -2.141112588724D+00
I= 33 X= 5.161125757284D+00 Y= -1.793008098624D+00 Z= 2.214324983661D+00
I= 34 X= 2.576877128031D+00 Y= -3.657571495646D+00 Z= 3.400859366384D+00
I= 35 X= 1.243924181242D+00 Y= -7.275435301012D-02 Z= -3.929053602085D-01
I= 36 X= 3.905409632985D+00 Y= 3.010505485707D+00 Z= 6.718640054855D-01
I= 37 X= 5.179843039095D+00 Y= 2.195915715855D+00 Z= 2.100943125903D+00
I= 38 X= 2.765425862639D+00 Y= 4.137319248952D+00 Z= 1.454833309272D+00

Forward Direction:

Total Energy: -656.4422940 Hartrees

Potential Energy: -656.6194233 Hartress

Kinetic Energy: 0.1771292 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.114499800611D+12 Y= 1.583248387728D+13 Z= 3.160509118308D+12
I= 1 X= 1.003369349403D+13 Y= 8.435398251858D+11 Z= 8.145767437815D+12
I= 2 X= -2.202767127661D+13 Y= -3.207840094828D+13 Z= -1.587901181465D+13
I= 3 X= -2.625294643227D+12 Y= -9.878634317434D+12 Z= -1.695693003627D+12
I= 4 X= -6.613508838902D+12 Y= 8.364552404359D+12 Z= 2.566634922679D+11
I= 5 X= 1.028271421003D+13 Y= -1.876211227840D+13 Z= 2.069494024223D+13
I= 6 X= 1.243054230856D+13 Y= -9.298311735790D+13 Z= -9.067934767153D+13
I= 7 X= -7.655414354849D+12 Y= 2.734117545455D+13 Z= -4.495223430321D+13
I= 8 X= -3.632543412017D+13 Y= 2.707431340223D+13 Z= -1.206498757951D+14
I= 9 X= 5.611826866473D+12 Y= -5.336116059292D+12 Z= -5.195007516149D+11
I= 10 X= -7.533538786569D+13 Y= 2.277611267958D+13 Z= 1.237125911407D+13
I= 11 X= 3.427448076439D+13 Y= -1.615216492983D+13 Z= -9.490257669308D+13
I= 12 X= 2.018730777772D+13 Y= 6.610742387774D+13 Z= 6.386663571748D+13
I= 13 X= 7.123164003659D+12 Y= 1.252538972322D+13 Z= -1.523417072157D+13
I= 14 X= -2.021467965323D+13 Y= -3.384441220545D+13 Z= -1.832357819722D+13
I= 15 X= -2.860784929952D+13 Y= -6.462097876957D+13 Z= 1.879464304509D+13
I= 16 X= -9.789611750508D+13 Y= 2.916616523852D+12 Z= 1.189660061375D+14
I= 17 X= 1.410438259140D+13 Y= -7.107937253163D+12 Z= 5.338265072154D+12
I= 18 X= 6.488785380057D+13 Y= -1.092796791684D+13 Z= -1.165860838679D+13
I= 19 X= 3.987504497771D+13 Y= 9.207798013590D+12 Z= -1.892748391573D+13
I= 20 X= -2.722958832709D+13 Y= -3.725612274888D+13 Z= 5.783796300722D+13
I= 21 X= 5.968243926066D+12 Y= -3.227676963619D+12 Z= -2.379405086885D+13
I= 22 X= 4.489423265048D+13 Y= 2.195582947628D+13 Z= 5.689924605186D+13
I= 23 X= -1.882015811213D+13 Y= 5.836138857802D+13 Z= 5.906079309375D+13
I= 24 X= -8.718411142149D+13 Y= 5.887915275472D+13 Z= 1.404583308444D+14
I= 25 X= -1.284109911837D+13 Y= 2.441716555480D+13 Z= -9.432070771507D+12
I= 26 X= -4.565737990927D+13 Y= 4.088122446863D+13 Z= 7.905353516619D+13

I= 27 X= 1.233895355155D+14 Y= -1.370021601004D+14 Z= 7.977387763097D+13
I= 28 X= 2.763200622415D+12 Y= -1.341444285887D+13 Z= 3.356059785690D+12
I= 29 X= -3.248740562368D+12 Y= -2.908751043802D+12 Z= -2.182552707651D+12
I= 30 X= 1.355704801410D+13 Y= -1.298364389186D+13 Z= -8.763633731856D+12
I= 31 X= 7.052143071611D+13 Y= 5.680746331115D+13 Z= 6.815534179262D+13
I= 32 X= 4.962096765793D+13 Y= 4.711076229277D+13 Z= 3.752861104110D+13
I= 33 X= -5.162279910922D+13 Y= -3.723187414883D+13 Z= 3.463873573078D+12
I= 34 X= -7.750286223713D+13 Y= -2.424123367131D+13 Z= -1.013549218395D+13
I= 35 X= 3.278925375681D+11 Y= 2.151513919687D+12 Z= 1.117301836626D+11
I= 36 X= -2.128056990991D+13 Y= 1.323236503251D+13 Z= 4.474495967029D+12
I= 37 X= -2.742895821457D+12 Y= 7.911538526973D+12 Z= -7.416028715954D+13
I= 38 X= 7.858086766371D+13 Y= 3.884674100834D+12 Z= 9.525445717301D+13

Backward Direction:

Total Energy: -656.4423131 Hartrees

Potential Energy: -656.6194233 Hartress

Kinetic Energy: 0.1771102 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.576703766690D+12 Y= 1.513020024702D+13 Z= 3.435331330267D+12
I= 1 X= 9.204209001483D+12 Y= -9.623793604423D+11 Z= 7.061669100281D+12
I= 2 X= -2.279969805253D+13 Y= -3.136873749150D+13 Z= -1.702160001872D+13
I= 3 X= -4.207137609072D+12 Y= -9.841646334050D+12 Z= -3.987620858131D+12
I= 4 X= -3.907941849514D+12 Y= 8.123166655570D+12 Z= -1.541229281490D+12
I= 5 X= 5.817438408535D+12 Y= -2.511222258726D+13 Z= 8.016849127395D+12
I= 6 X= 1.124519728735D+14 Y= 2.120335601226D+13 Z= -4.567623593815D+13
I= 7 X= 1.061350307488D+13 Y= 4.463795419823D+13 Z= -4.383454594688D+13
I= 8 X= -1.325254535135D+13 Y= 4.572457035292D+13 Z= -1.185033409045D+14
I= 9 X= 6.471735243627D+12 Y= -4.932286926028D+12 Z= -1.491480210442D+12
I= 10 X= -7.517811751070D+13 Y= 2.477464740026D+13 Z= 1.005454317676D+13
I= 11 X= 3.402612219611D+13 Y= -1.617401205588D+13 Z= -9.495087113250D+13
I= 12 X= 2.069127451493D+13 Y= 6.624240535317D+13 Z= 6.338806803805D+13

I= 13 X= 7.293628295116D+12 Y= 1.244244832276D+13 Z= -1.559294579684D+13
I= 14 X= -1.992487825022D+13 Y= -3.435538428132D+13 Z= -1.824773289036D+13
I= 15 X= -2.807490278742D+13 Y= -6.510978280526D+13 Z= 1.791212275696D+13
I= 16 X= -9.793324239033D+13 Y= 3.073718591116D+12 Z= 1.190902563194D+14
I= 17 X= 1.436542942963D+13 Y= -7.684028776602D+12 Z= 5.281215265201D+12
I= 18 X= 6.494289420921D+13 Y= -1.184641063588D+13 Z= -1.241204401669D+13
I= 19 X= 3.932319721043D+13 Y= 9.023963901383D+12 Z= -1.835844276133D+13
I= 20 X= -2.684636875261D+13 Y= -3.777088033787D+13 Z= 5.777222762765D+13
I= 21 X= 5.639763959136D+12 Y= -3.434035416762D+12 Z= -2.459592051196D+13
I= 22 X= 4.483553061602D+13 Y= 2.288061232446D+13 Z= 5.368564248606D+13
I= 23 X= -1.762616822361D+13 Y= 5.784165757860D+13 Z= 5.868816019436D+13
I= 24 X= -8.775971553260D+13 Y= 5.855586974260D+13 Z= 1.395102113238D+14
I= 25 X= -1.319809092821D+13 Y= 2.405652917783D+13 Z= -9.616288322473D+12
I= 26 X= -4.654037709590D+13 Y= 3.991529377279D+13 Z= 7.894579782060D+13
I= 27 X= 1.241254471382D+14 Y= -1.363825822696D+14 Z= 7.956030165703D+13
I= 28 X= 2.799666995793D+12 Y= -1.450744821504D+13 Z= 4.129735218995D+12
I= 29 X= -4.902013024741D+12 Y= -2.444359690296D+12 Z= -2.762415221268D+12
I= 30 X= 1.365440774404D+13 Y= -1.330359385562D+13 Z= -9.481751125323D+12
I= 31 X= 6.937840897451D+13 Y= 5.646930609952D+13 Z= 6.819105718728D+13
I= 32 X= 4.627584070449D+13 Y= 4.988868686814D+13 Z= 3.553702387966D+13
I= 33 X= -5.151963480628D+13 Y= -3.763620983623D+13 Z= 2.891890453073D+12
I= 34 X= -7.642512108953D+13 Y= -2.499158518349D+13 Z= -1.034176280205D+13
I= 35 X= 3.099067773781D+11 Y= 2.571605568758D+12 Z= 2.776952896838D+12
I= 36 X= -2.709300457309D+13 Y= 5.890781118835D+12 Z= 1.795366505854D+12
I= 37 X= 2.442333869388D+12 Y= 1.054389646017D+13 Z= -8.062709841236D+13
I= 38 X= 8.142050059637D+13 Y= 3.588779161012D+12 Z= 9.042488469479D+13

Seed: 37466053161

CM Start Point Coordinates: bohr

I= 0 X= -2.547833816944D+00 Y= 2.321319852721D+00 Z= -4.781518337903D-01

I= 1 X= -2.823848756819D+00 Y= 8.048069223718D-02 Z= -1.910370878160D+00
I= 2 X= -1.936202311422D+00 Y= 1.754484019033D+00 Z= 2.033310549275D+00
I= 3 X= -2.698759863606D+00 Y= -1.914646169465D+00 Z= -1.071371756815D-01
I= 4 X= -2.078701351847D+00 Y= -9.608246669126D-01 Z= 2.336580962843D+00
I= 5 X= 4.905604713331D+00 Y= 2.259386009308D+00 Z= -9.898648143170D-01
I= 6 X= 2.386753711399D+00 Y= 1.012104456492D+00 Z= -3.221103165984D+00
I= 7 X= 6.266059429817D+00 Y= 5.786834737604D-01 Z= -1.290749076732D+00
I= 8 X= 4.780658265763D+00 Y= 3.924846955103D+00 Z= -2.652567131568D+00
I= 9 X= -1.952055693478D+00 Y= -2.550481580232D+00 Z= 4.718192959464D+00
I= 10 X= -3.829166925792D+00 Y= -2.844163232607D+00 Z= 5.409852755317D+00
I= 11 X= -1.287348923366D+00 Y= -4.313582060143D+00 Z= 4.139865458682D+00
I= 12 X= -8.260097598514D-01 Y= -1.787139702634D+00 Z= 6.173350176056D+00
I= 13 X= -1.647681970716D+00 Y= 3.597389085985D+00 Z= 3.991618434795D+00
I= 14 X= -3.545736885062D+00 Y= 4.497851237006D+00 Z= 4.876944256881D+00
I= 15 X= -5.612617466334D-01 Y= 2.902009355617D+00 Z= 5.727682347259D+00
I= 16 X= -5.593561149326D-01 Y= 5.185846091754D+00 Z= 3.352956847060D+00
I= 17 X= -2.513561754117D+00 Y= 4.930332539932D+00 Z= -1.638946995050D+00
I= 18 X= -4.143174438275D+00 Y= 6.272957733511D+00 Z= -4.946650139013D-01
I= 19 X= -7.310130423976D-01 Y= 6.145769858007D+00 Z= -1.694778901225D+00
I= 20 X= -3.136124398156D+00 Y= 4.575130947107D+00 Z= -3.949815418697D+00
I= 21 X= -3.445967267110D+00 Y= -5.127709162261D-01 Z= -4.629540289333D+00
I= 22 X= -5.504043842710D+00 Y= -1.640570077059D+00 Z= -4.980838670193D+00
I= 23 X= -3.546471673322D+00 Y= 1.570637474881D+00 Z= -5.699526387556D+00
I= 24 X= -1.890472624824D+00 Y= -2.137842784636D+00 Z= -5.471522933977D+00
I= 25 X= -3.191342653429D+00 Y= -4.580967063641D+00 Z= -7.809455782442D-01
I= 26 X= -2.742645088154D+00 Y= -5.101165683737D+00 Z= -2.749929764481D+00
I= 27 X= -2.134036493515D+00 Y= -5.813061885190D+00 Z= 1.520333701786D-01
I= 28 X= -5.328493471319D+00 Y= -4.888168488541D+00 Z= -7.399206618561D-01
I= 29 X= 3.001765767047D+00 Y= -3.587660726848D+00 Z= -1.641275341723D+00
I= 30 X= 3.784377240479D+00 Y= -2.937713156659D+00 Z= 6.903476532197D-01

I= 31 X= 1.214572085341D+00 Y= -4.911397031317D+00 Z= -1.881227339005D+00
I= 32 X= 4.098651906703D+00 Y= -3.389992882532D+00 Z= -3.396353142876D+00
I= 33 X= 5.773133079894D+00 Y= -2.458073380632D+00 Z= 1.141408683230D+00
I= 34 X= 2.834233349320D+00 Y= -4.179926515113D+00 Z= 2.324056983090D+00
I= 35 X= 1.153856460799D+00 Y= -4.484055951060D-02 Z= -3.741999491999D-01
I= 36 X= 3.721135221698D+00 Y= 2.548573167211D+00 Z= 1.590730514270D+00
I= 37 X= 4.360326753482D+00 Y= 1.660972917683D+00 Z= 3.554388846963D+00
I= 38 X= 2.434418183622D+00 Y= 4.395580591531D+00 Z= 1.660580584088D+00

Forward Direction:

Total Energy: -656.4300452 Hartrees

Potential Energy: -656.6048472 Hartress

Kinetic Energy: 0.1748021 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.392899393085D+12 Y= 5.478761381802D+12 Z= 6.093234381661D+11
I= 1 X= 5.339236562076D+12 Y= -1.705010020735D+13 Z= -1.769814011386D+13
I= 2 X= -1.200251317863D+13 Y= -2.630021279784D+13 Z= 2.552801972716D+13
I= 3 X= 4.661889371201D+12 Y= -2.542232662481D+13 Z= -1.370508633555D+13
I= 4 X= -1.297179273025D+12 Y= 1.056839085122D+13 Z= 3.952672225035D+13
I= 5 X= 3.539617664681D+12 Y= 1.985651777225D+13 Z= 2.099015256488D+13
I= 6 X= -2.142772450532D+13 Y= -3.035227360011D+13 Z= 2.751950900888D+13
I= 7 X= 2.662092174008D+13 Y= -4.314858933522D+12 Z= -6.661815032372D+13
I= 8 X= 1.143740312217D+13 Y= 7.928000488794D+12 Z= -4.792664393255D+13
I= 9 X= 8.747624565825D+12 Y= 1.010367911931D+13 Z= -1.023744888146D+13
I= 10 X= -1.124303710799D+14 Y= 6.953294950707D+13 Z= -2.756292280512D+13
I= 11 X= 3.263556594824D+13 Y= -8.382493896372D+13 Z= -5.046153007788D+12
I= 12 X= -5.167884002708D+13 Y= 4.840681080189D+13 Z= 6.051674784145D+12
I= 13 X= -6.686399276119D+12 Y= -4.020002046843D+12 Z= 1.645432030149D+11
I= 14 X= 3.155321139792D+13 Y= 4.647412262714D+12 Z= -6.593743240815D+13
I= 15 X= 8.755599918207D+13 Y= -3.134743805749D+13 Z= 7.278678131338D+13
I= 16 X= 8.928259112984D+12 Y= 1.189353740255D+12 Z= -3.822096074275D+13

I= 17 X= -3.177394608156D+12 Y= -1.478628152891D+13 Z= 6.188751211364D+11
I= 18 X= -7.928249110481D+13 Y= 2.656978542112D+13 Z= -5.684974456337D+13
I= 19 X= 3.569554563389D+13 Y= 2.127640403044D+13 Z= 5.265314997335D+13
I= 20 X= -1.605649704598D+13 Y= -1.527367225013D+13 Z= -2.205588747998D+13
I= 21 X= 7.672874404610D+12 Y= 1.511217181598D+12 Z= 2.586965561842D+12
I= 22 X= -8.395840839175D+13 Y= 6.203499257130D+13 Z= -5.582391040854D+13
I= 23 X= -7.581784676933D+13 Y= 9.291570743538D+12 Z= 1.372132580257D+13
I= 24 X= 1.453355030018D+14 Y= -6.549444370328D+13 Z= 7.247556386517D+13
I= 25 X= -9.653891199485D+12 Y= 2.760847633843D+13 Z= 3.840437459205D+12
I= 26 X= 2.893463103048D+13 Y= -1.035634570618D+14 Z= -1.289185380948D+14
I= 27 X= 2.244828125949D+12 Y= -7.236867340232D+12 Z= 1.508679472640D+13
I= 28 X= 1.620262776224D+13 Y= 6.835910143485D+13 Z= -2.157112491124D+13
I= 29 X= 1.104185704984D+13 Y= 2.358070453951D+13 Z= 1.757317681897D+13
I= 30 X= 8.212304433197D+12 Y= -2.703447589159D+12 Z= -5.474703261009D+12
I= 31 X= -1.241629243807D+12 Y= -3.372891703124D+13 Z= -3.296978240418D+13
I= 32 X= 6.416333834437D+13 Y= 6.169200043121D+13 Z= -1.179111745495D+14
I= 33 X= -2.369813391309D+13 Y= -1.174977465615D+14 Z= -3.623524047625D+13
I= 34 X= -6.137626553158D+13 Y= 6.665624962213D+12 Z= 5.945570490141D+13
I= 35 X= -7.795315515889D+11 Y= -1.800130708983D+11 Z= -3.644884696580D+12
I= 36 X= -7.626009053127D+12 Y= 8.442927076084D+12 Z= 7.316390887785D+12
I= 37 X= -6.463592928869D+12 Y= 2.126792983030D+13 Z= -4.361426597873D+13
I= 38 X= 4.576360738418D+13 Y= -9.869493939612D+13 Z= -3.332065402119D+13

Backward Direction:

Total Energy: -656.4300400 Hartrees

Potential Energy: -656.6048472 Hartress

Kinetic Energy: 0.1748072 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.718414095664D+12 Y= 5.053686383559D+12 Z= 7.756665604071D+11

I= 1 X= 4.837170011783D+12 Y= -1.814317864722D+13 Z= -1.835431815732D+13

I= 2 X= -1.246980198629D+13 Y= -2.587067097187D+13 Z= 2.483643920673D+13

I= 3 X= 3.704438752439D+12 Y= -2.539993870930D+13 Z= -1.509233386116D+13
I= 4 X= 3.404338409068D+11 Y= 1.042228599917D+13 Z= 3.843850200003D+13
I= 5 X= 8.368961140642D+11 Y= 1.601295227942D+13 Z= 1.331641602371D+13
I= 6 X= 3.911278587299D+13 Y= 3.876198858533D+13 Z= 5.475878500723D+13
I= 7 X= 3.767864786021D+13 Y= 6.154455563435D+12 Z= -6.594164106701D+13
I= 8 X= 2.540285486862D+13 Y= 1.921654203572D+13 Z= -4.662739918947D+13
I= 9 X= 9.268105943164D+12 Y= 1.034810695461D+13 Z= -1.082576412774D+13
I= 10 X= -1.123351792050D+14 Y= 7.074261338096D+13 Z= -2.896517395162D+13
I= 11 X= 3.248524062496D+13 Y= -8.383816248946D+13 Z= -5.075384443254D+12
I= 12 X= -5.137380136761D+13 Y= 4.848851177298D+13 Z= 5.762009551785D+12
I= 13 X= -6.583221436994D+12 Y= -4.070204434586D+12 Z= -5.261452058781D+10
I= 14 X= 3.172862105306D+13 Y= 4.338133438125D+12 Z= -6.589152511134D+13
I= 15 X= 8.787857859298D+13 Y= -3.164329910763D+13 Z= 7.225261350361D+13
I= 16 X= 8.905788329985D+12 Y= 1.284443755977D+12 Z= -3.814575516507D+13
I= 17 X= -3.019389380507D+12 Y= -1.513497555152D+13 Z= 5.843442741992D+11
I= 18 X= -7.924917649995D+13 Y= 2.601387464745D+13 Z= -5.730578060914D+13
I= 19 X= 3.536152577428D+13 Y= 2.116513377319D+13 Z= 5.299757658365D+13
I= 20 X= -1.582454367485D+13 Y= -1.558524235216D+13 Z= -2.209567547287D+13
I= 21 X= 7.474053560477D+12 Y= 1.386313488164D+12 Z= 2.101613601846D+12
I= 22 X= -8.399393929302D+13 Y= 6.259474086519D+13 Z= -5.776902555504D+13
I= 23 X= -7.509515408164D+13 Y= 8.976990361759D+12 Z= 1.349578027901D+13
I= 24 X= 1.449871039948D+14 Y= -6.569011895380D+13 Z= 7.190169045278D+13
I= 25 X= -9.869969558027D+12 Y= 2.739019201486D+13 Z= 3.728935108798D+12
I= 26 X= 2.840017456107D+13 Y= -1.041481111392D+14 Z= -1.289837488582D+14
I= 27 X= 2.690257315188D+12 Y= -6.861852128902D+12 Z= 1.495752244448D+13
I= 28 X= 1.622469995863D+13 Y= 6.769753219426D+13 Z= -2.110283821148D+13
I= 29 X= 1.004117191843D+13 Y= 2.386178919900D+13 Z= 1.722220031017D+13
I= 30 X= 8.271233882257D+12 Y= -2.897105428307D+12 Z= -5.909362045631D+12
I= 31 X= -1.933472169332D+12 Y= -3.393359526751D+13 Z= -3.294816475771D+13
I= 32 X= 6.213861532680D+13 Y= 6.337340981490D+13 Z= -1.191166332444D+14

I= 33 X= -2.363569110011D+13 Y= -1.177424810033D+14 Z= -3.658144778008D+13
I= 34 X= -6.072393533839D+13 Y= 6.211455656534D+12 Z= 5.933085437002D+13
I= 35 X= -7.904178891166D+11 Y= 7.425806566574D+10 Z= -2.031690980141D+12
I= 36 X= -1.114413270987D+13 Y= 3.999247010134D+12 Z= 5.694779759775D+12
I= 37 X= -3.325101007075D+12 Y= 2.286123130345D+13 Z= -4.752846768023D+13
I= 38 X= 4.748236731499D+13 Y= -9.887403732189D+13 Z= -3.624387538525D+13

Seed: 37615231480

CM Start Point Coordinates: bohr

I= 0 X= -2.28546555216D+00 Y= 2.225843298464D+00 Z= -4.411050018420D-01
I= 1 X= -2.818515169481D+00 Y= -4.014294637215D-02 Z= -1.993894048656D+00
I= 2 X= -2.110784068534D+00 Y= 1.691879845490D+00 Z= 2.120655099668D+00
I= 3 X= -2.559736801797D+00 Y= -1.935544413057D+00 Z= -2.135012957568D-01
I= 4 X= -2.247437727734D+00 Y= -9.092734417974D-01 Z= 2.279615886722D+00
I= 5 X= 4.546422932357D+00 Y= 2.516199710313D+00 Z= -1.646882347101D+00
I= 6 X= 2.265161392123D+00 Y= 2.242752727559D-01 Z= -2.979418744410D+00
I= 7 X= 6.015583138514D+00 Y= 1.140021027835D+00 Z= -1.860335279890D+00
I= 8 X= 3.863048279131D+00 Y= 3.730396499080D+00 Z= -3.151829240983D+00
I= 9 X= -2.417672225574D+00 Y= -2.490699486993D+00 Z= 4.661118352533D+00
I= 10 X= -4.288159700411D+00 Y= -2.952940510895D+00 Z= 5.582095206837D+00
I= 11 X= -1.426217878893D+00 Y= -4.454217907060D+00 Z= 4.299065033356D+00
I= 12 X= -1.181401671713D+00 Y= -1.659261132716D+00 Z= 6.384948258050D+00
I= 13 X= -1.632874283780D+00 Y= 3.394373098505D+00 Z= 4.269847286719D+00
I= 14 X= -3.466600334983D+00 Y= 3.973759645455D+00 Z= 5.395802084934D+00
I= 15 X= -2.348931942546D-01 Y= 2.562798056632D+00 Z= 5.659695813423D+00
I= 16 X= -6.381509818432D-01 Y= 5.060689079562D+00 Z= 3.756353531173D+00
I= 17 X= -2.380308699052D+00 Y= 4.966065790806D+00 Z= -1.433703088530D+00
I= 18 X= -3.975255889695D+00 Y= 6.342768757670D+00 Z= -1.091398128960D+00
I= 19 X= -9.506295918719D-01 Y= 5.790707575758D+00 Z= -1.046755016585D-03
I= 20 X= -1.810271659336D+00 Y= 4.996687902943D+00 Z= -3.785326498888D+00

I= 21 X= -3.109312442674D+00 Y= -3.032771199447D-01 Z= -4.767558969120D+00
I= 22 X= -5.072388905385D+00 Y= -8.582424395141D-02 Z= -5.130328894085D+00
I= 23 X= -2.383802926546D+00 Y= 1.420828656055D+00 Z= -5.867573900591D+00
I= 24 X= -2.145458024966D+00 Y= -1.999962133274D+00 Z= -5.619039141057D+00
I= 25 X= -3.160029626700D+00 Y= -4.573393601932D+00 Z= -6.072049907906D-01
I= 26 X= -4.051425872578D+00 Y= -5.134906365143D+00 Z= -2.839867165668D+00
I= 27 X= -1.325584182861D+00 Y= -5.870712777656D+00 Z= -3.085074376523D-01
I= 28 X= -5.065378641613D+00 Y= -5.228410331091D+00 Z= 7.800776932521D-01
I= 29 X= 3.186476510412D+00 Y= -3.693854110057D+00 Z= -1.587406937723D+00
I= 30 X= 3.766272979514D+00 Y= -3.097514402714D+00 Z= 9.907651854005D-01
I= 31 X= 1.463519796047D+00 Y= -4.724112789910D+00 Z= -2.327800004624D+00
I= 32 X= 4.476399850899D+00 Y= -3.399252613062D+00 Z= -2.918330080772D+00
I= 33 X= 5.519399435471D+00 Y= -2.224129317139D+00 Z= 1.264411927165D+00
I= 34 X= 2.968865588300D+00 Y= -4.152646938519D+00 Z= 2.417550229997D+00
I= 35 X= 1.152397761496D+00 Y= -5.963182267201D-02 Z= -3.215693184369D-01
I= 36 X= 3.673250983747D+00 Y= 2.831021272562D+00 Z= 9.626302204906D-01
I= 37 X= 4.693271032586D+00 Y= 1.666659435456D+00 Z= 2.445346548941D+00
I= 38 X= 2.790653049900D+00 Y= 4.139535526939D+00 Z= 1.850677432892D+00

Forward Direction:

Total Energy: -656.4472852 Hartrees

Potential Energy: -656.6122373 Hartress

Kinetic Energy: 0.1649521 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.039201155715D+12 Y= -9.317444577888D+11 Z= 5.893407175678D+12
I= 1 X= -4.639819520941D+12 Y= -1.830093027015D+13 Z= 2.361562978346D+13
I= 2 X= 3.727444775796D+12 Y= 2.890059418037D+12 Z= -7.869299338481D+12
I= 3 X= 7.554258207502D+11 Y= 1.551405946449D+13 Z= 1.085045398117D+12
I= 4 X= -3.442887615999D+12 Y= -5.379325126500D+12 Z= 2.699841029377D+13
I= 5 X= -1.092781036093D+13 Y= 2.198249574399D+13 Z= 1.108641551960D+13
I= 6 X= -3.556065922180D+13 Y= 2.287629300211D+13 Z= -8.795029773621D+13

I= 7 X= 8.338703639938D+13 Y= -5.114262541717D+13 Z= -4.885759039697D+12
I= 8 X= -4.604673926611D+13 Y= -3.747325055234D+13 Z= -2.109188516571D+13
I= 9 X= -1.930864492275D+12 Y= -4.585442600818D+12 Z= -9.064768786899D+12
I= 10 X= 1.075495460541D+14 Y= 3.356917122593D+13 Z= -9.492770846297D+13
I= 11 X= -3.677502545094D+13 Y= -1.014421419303D+14 Z= 2.502976806059D+13
I= 12 X= -5.500119886752D+13 Y= 4.048344101383D+12 Z= -9.130621600696D+13
I= 13 X= -9.817992349753D+12 Y= 3.726206937462D+12 Z= 4.258361434977D+12
I= 14 X= 1.967755867629D+13 Y= 3.489170516126D+13 Z= 8.515665060790D+11
I= 15 X= 1.023514514032D+14 Y= -2.807517868339D+13 Z= 1.023005492433D+14
I= 16 X= 3.355622104166D+13 Y= 7.095501161339D+13 Z= 4.253510846267D+13
I= 17 X= -1.062332281408D+12 Y= 7.111791181028D+12 Z= -7.733121894815D+12
I= 18 X= -1.316513521605D+13 Y= 1.708087746851D+13 Z= -4.115307280749D+13
I= 19 X= -4.642979692504D+13 Y= -5.256844535140D+13 Z= 5.642799087393D+13
I= 20 X= -1.157614172520D+13 Y= 3.346952572838D+13 Z= -5.851681503525D+13
I= 21 X= 5.025938710503D+12 Y= -6.535987950700D+11 Z= -2.368349700194D+13
I= 22 X= 2.558238375601D+13 Y= -4.110601476239D+13 Z= 2.723275425305D+13
I= 23 X= 3.001422089653D+13 Y= 2.057187719192D+13 Z= 6.346083527896D+13
I= 24 X= -1.179533049009D+14 Y= 7.540589815363D+13 Z= 1.588291764546D+14
I= 25 X= -1.173997534739D+12 Y= -6.751967479268D+12 Z= -1.423003868983D+13
I= 26 X= 3.765562272021D+13 Y= 4.577415261626D+13 Z= -3.926046551580D+12
I= 27 X= 1.316701367283D+13 Y= 8.653086983418D+12 Z= 3.851773431707D+13
I= 28 X= -4.245631953948D+13 Y= -6.123734573232D+12 Z= 3.298520368356D+13
I= 29 X= -4.511830810801D+12 Y= -2.566847332925D+13 Z= 4.428584931003D+12
I= 30 X= 7.376534205105D+12 Y= 2.778114351405D+12 Z= 7.362758452151D+12
I= 31 X= -1.829126544542D+11 Y= -7.493382249748D+13 Z= -3.554312146918D+13
I= 32 X= 4.288631216789D+13 Y= 9.348282464579D+13 Z= 2.807590398279D+13
I= 33 X= -1.130291536294D+14 Y= -1.367662452424D+13 Z= -9.660960218341D+13
I= 34 X= -5.056510397465D+13 Y= -4.037940095465D+13 Z= -2.309870734270D+13
I= 35 X= 2.705894731703D+12 Y= 6.249326270267D+11 Z= -1.307435167744D+12
I= 36 X= 1.130664872417D+13 Y= -2.446322200024D+12 Z= -3.355810709011D+11

I= 37 X= 2.318557400409D+12 Y= -4.744123757966D+13 Z= -8.903538705472D+13

I= 38 X= -5.858621018141D+13 Y= 9.735703921715D+13 Z= -5.442062664114D+13

Backward Direction:

Total Energy: -656.4472808 Hartrees

Potential Energy: -656.6122373 Hartress

Kinetic Energy: 0.1649565 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.355581923028D+12 Y= -1.344891859403D+12 Z= 6.055082712282D+12

I= 1 X= -5.127798090291D+12 Y= -1.936333694575D+13 Z= 2.297786408528D+13

I= 2 X= 3.273268084498D+12 Y= 3.307548306430D+12 Z= -8.541474120065D+12

I= 3 X= -1.751587481550D+11 Y= 1.553581917601D+13 Z= -2.632759829852D+11

I= 4 X= -1.851225900453D+12 Y= -5.521330279496D+12 Z= 2.594072548716D+13

I= 5 X= -1.355469358746D+13 Y= 1.824678063786D+13 Z= 3.628003904829D+12

I= 6 X= 2.328108538748D+13 Y= 9.005121007806D+13 Z= -6.147535539356D+13

I= 7 X= 9.413448289801D+13 Y= -4.096707971784D+13 Z= -4.228232627718D+12

I= 8 X= -3.247315787113D+13 Y= -2.650146530561D+13 Z= -1.982909721462D+13

I= 9 X= -1.424987814228D+12 Y= -4.347873406091D+12 Z= -9.636575915418D+12

I= 10 X= 1.076420668457D+14 Y= 3.474489196045D+13 Z= -9.629061246030D+13

I= 11 X= -3.692113265478D+13 Y= -1.014549944055D+14 Z= 2.500135685978D+13

I= 12 X= -5.470471958281D+13 Y= 4.127752539699D+12 Z= -9.158775324329D+13

I= 13 X= -9.717709678359D+12 Y= 3.677413227754D+12 Z= 4.047297153513D+12

I= 14 X= 1.984804634225D+13 Y= 3.459110470006D+13 Z= 8.961856455259D+11

I= 15 X= 1.026649792365D+14 Y= -2.836273787924D+13 Z= 1.017813701731D+14

I= 16 X= 3.353438079216D+13 Y= 7.104743340412D+13 Z= 4.260820377312D+13

I= 17 X= -9.087606789830D+11 Y= 6.772881507070D+12 Z= -7.766683802964D+12

I= 18 X= -1.313275542244D+13 Y= 1.654056553859D+13 Z= -4.159631248571D+13

I= 19 X= -4.675444420272D+13 Y= -5.267659337090D+13 Z= 5.676275287909D+13

I= 20 X= -1.135069695272D+13 Y= 3.316669827997D+13 Z= -5.855548658640D+13

I= 21 X= 4.832696779672D+12 Y= -7.749976932964D+11 Z= -2.415522999536D+13

I= 22 X= 2.554784985504D+13 Y= -4.056197299776D+13 Z= 2.534221900223D+13

I= 23 X= 3.071663483951D+13 Y= 2.026612393270D+13 Z= 6.324161856014D+13
I= 24 X= -1.182919278286D+14 Y= 7.521571354984D+13 Z= 1.582714059165D+14
I= 25 X= -1.384012736706D+12 Y= -6.964126747721D+12 Z= -1.433841228609D+13
I= 26 X= 3.713616308756D+13 Y= 4.520590392693D+13 Z= -3.989427505071D+12
I= 27 X= 1.359994413146D+13 Y= 9.017579276682D+12 Z= 3.839208941052D+13
I= 28 X= -4.243486668607D+13 Y= -6.766740195220D+12 Z= 3.344035026934D+13
I= 29 X= -5.484436735356D+12 Y= -2.539527590306D+13 Z= 4.087456817342D+12
I= 30 X= 7.433810093499D+12 Y= 2.589890548670D+12 Z= 6.940296184923D+12
I= 31 X= -8.553424813677D+11 Y= -7.513275746767D+13 Z= -3.552211040891D+13
I= 32 X= 4.091840284543D+13 Y= 9.511705370635D+13 Z= 2.690427044187D+13
I= 33 X= -1.129684629608D+14 Y= -1.391449172531D+13 Z= -9.694609491315D+13
I= 34 X= -4.993107815192D+13 Y= -4.082082627499D+13 Z= -2.322005456697D+13
I= 35 X= 2.695313864387D+12 Y= 8.720689198457D+11 Z= 2.604923584708D+11
I= 36 X= 7.887243562216D+12 Y= -6.765312672649D+12 Z= -1.911689817145D+12
I= 37 X= 5.368983289426D+12 Y= -4.589264412259D+13 Z= -9.283975632255D+13
I= 38 X= -5.691567862969D+13 Y= 9.718296677891D+13 Z= -5.726182246569D+13

Seed: 38791410059

CM Start Point Coordinates: bohr

I= 0 X= -2.156424146905D+00 Y= 2.162471354706D+00 Z= -5.551121569908D-01
I= 1 X= -2.673913250780D+00 Y= 1.606049141104D-02 Z= -1.902674400699D+00
I= 2 X= -1.950018349152D+00 Y= 1.667795906648D+00 Z= 2.030185129695D+00
I= 3 X= -2.510106900241D+00 Y= -2.019476148648D+00 Z= -8.127104728299D-02
I= 4 X= -2.104946880302D+00 Y= -9.017764672030D-01 Z= 2.412146268026D+00
I= 5 X= 4.480789965142D+00 Y= 2.774786342705D+00 Z= -1.164825113902D+00
I= 6 X= 2.340104346188D+00 Y= 1.049838575935D+00 Z= -3.026411811896D+00
I= 7 X= 6.087481722935D+00 Y= 1.912288708270D+00 Z= -1.619960082954D+00
I= 8 X= 3.723675345395D+00 Y= 4.303746814974D+00 Z= -2.387749859692D+00
I= 9 X= -2.146248769828D+00 Y= -2.281766286719D+00 Z= 4.687897259733D+00
I= 10 X= -4.479176821472D+00 Y= -2.861722692865D+00 Z= 5.057093867935D+00

I= 11 X= -1.198948978519D+00 Y= -4.273748794329D+00 Z= 4.617098808803D+00
I= 12 X= -1.859360764364D+00 Y= -1.255087696635D+00 Z= 6.818694053813D+00
I= 13 X= -2.037818189141D+00 Y= 3.403012714260D+00 Z= 4.179103167770D+00
I= 14 X= -4.084445217620D+00 Y= 4.141294887842D+00 Z= 4.380489840584D+00
I= 15 X= -1.596278924430D+00 Y= 2.336228968506D+00 Z= 6.329866698867D+00
I= 16 X= -9.650467137499D-01 Y= 5.016483370564D+00 Z= 3.556423566263D+00
I= 17 X= -2.071711422978D+00 Y= 4.688497067099D+00 Z= -1.686765179914D+00
I= 18 X= -3.860361491941D+00 Y= 5.590965921177D+00 Z= -1.181405007044D+00
I= 19 X= -1.887442633543D-01 Y= 5.596981094406D+00 Z= -8.339881025719D-01
I= 20 X= -1.274722112262D+00 Y= 4.433404841072D+00 Z= -3.927448042862D+00
I= 21 X= -3.673109413368D+00 Y= -2.152396739166D-01 Z= -4.623625112692D+00
I= 22 X= -5.709092510259D+00 Y= -9.974737750023D-01 Z= -4.553528780548D+00
I= 23 X= -3.807947407113D+00 Y= 2.125909603277D+00 Z= -5.504164847853D+00
I= 24 X= -2.438530361509D+00 Y= -1.472203448898D+00 Z= -5.855832296487D+00
I= 25 X= -3.285811384915D+00 Y= -4.739278971547D+00 Z= -5.435496168702D-01
I= 26 X= -3.622804761981D+00 Y= -4.965544155301D+00 Z= -2.472823010720D+00
I= 27 X= -1.898192791331D+00 Y= -5.989681526430D+00 Z= 3.917738362436D-01
I= 28 X= -5.116543267124D+00 Y= -5.089867688620D+00 Z= 7.269692775555D-01
I= 29 X= 2.978004942458D+00 Y= -3.883323343246D+00 Z= -1.595489374756D+00
I= 30 X= 3.874859970997D+00 Y= -3.081698081652D+00 Z= 6.798376839430D-01
I= 31 X= 1.378469184641D+00 Y= -5.078108280922D+00 Z= -1.841651716417D+00
I= 32 X= 4.184526052327D+00 Y= -3.397550277466D+00 Z= -3.298157542818D+00
I= 33 X= 5.767455696232D+00 Y= -2.675133658285D+00 Z= 1.141763246756D+00
I= 34 X= 2.718962267699D+00 Y= -3.805203312069D+00 Z= 2.317787934873D+00
I= 35 X= 1.182393279089D+00 Y= -1.520758559054D-02 Z= -4.338211011305D-01
I= 36 X= 3.831293152059D+00 Y= 2.530471150151D+00 Z= 1.526531401734D+00
I= 37 X= 5.242130549632D+00 Y= 1.573755991400D+00 Z= 2.914608119610D+00
I= 38 X= 2.390067553005D+00 Y= 3.898007360154D+00 Z= 2.510821834391D+00

Forward Direction:

Total Energy: -656.4286449 Hartrees

Potential Energy: -656.6028733 Hartress

Kinetic Energy: 0.1742284 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.421021855301D+12 Y= 1.072275914814D+13 Z= 7.693765604636D+11
I= 1 X= 1.857282622192D+13 Y= -8.530539785968D+12 Z= -1.882193842646D+13
I= 2 X= -1.073588742832D+13 Y= -5.731628295826D+12 Z= 2.725315084315D+12
I= 3 X= -1.522883592143D+13 Y= 5.083621001808D+12 Z= 3.880433673207D+12
I= 4 X= -2.656398958008D+12 Y= 5.203701090043D+12 Z= -2.621614926898D+13
I= 5 X= -1.870441856385D+12 Y= 2.165477032348D+13 Z= 2.107407820718D+12
I= 6 X= -5.051368338576D+13 Y= -3.022609370956D+13 Z= 6.997259775651D+13
I= 7 X= 4.630442776668D+13 Y= -1.580232269245D+13 Z= -2.017683435889D+13
I= 8 X= -1.616464320222D+13 Y= 2.732127341062D+12 Z= -2.462217818248D+13
I= 9 X= 1.879501274758D+13 Y= -1.338243886877D+13 Z= 1.985308436728D+13
I= 10 X= -4.615116486045D+13 Y= -5.176309715540D+13 Z= 1.576821410928D+14
I= 11 X= -3.612058050650D+13 Y= -3.299780362282D+13 Z= 1.025487381677D+13
I= 12 X= -6.347155234982D+13 Y= -1.531178801890D+13 Z= 6.014651979514D+13
I= 13 X= -1.790526684682D+13 Y= 1.433673848330D+12 Z= 2.098002116053D+13
I= 14 X= 5.499762565097D+13 Y= -6.329267189086D+12 Z= -6.302355495405D+13
I= 15 X= 1.951887366330D+13 Y= 3.726638043436D+13 Z= -7.476159909430D+13
I= 16 X= -2.020161102115D+13 Y= 5.823370671056D+13 Z= 2.400580882989D+13
I= 17 X= -3.311317516566D+12 Y= 1.137834668127D+13 Z= -1.026587601518D+13
I= 18 X= 4.125021026657D+13 Y= -1.612693668374D+13 Z= -1.611568852546D+12
I= 19 X= -5.186051305849D+13 Y= -5.735822633663D+13 Z= 1.735832001230D+13
I= 20 X= 4.495691533920D+13 Y= 1.282987265815D+13 Z= -8.291789359386D+13
I= 21 X= 4.305449316410D+12 Y= -3.315605335212D+12 Z= -1.716660086518D+12
I= 22 X= -1.546049912497D+14 Y= 1.621915545437D+13 Z= -6.306788882961D+13
I= 23 X= -2.197852092486D+13 Y= -4.100255123298D+12 Z= 2.453451478625D+13
I= 24 X= -3.385109192195D+12 Y= -3.722213157130D+13 Z= 5.137488350061D+13
I= 25 X= 1.935961378658D+13 Y= -2.684884149079D+12 Z= 4.456527533638D+12
I= 26 X= -1.192916785850D+12 Y= 9.070153074947D+13 Z= 1.308334427652D+13

I= 27 X= -4.207689779519D+13 Y= -3.358853465066D+13 Z= -2.200139024970D+13
I= 28 X= -1.565177443393D+14 Y= 1.633588186022D+13 Z= 9.603158776110D+13
I= 29 X= 2.960604099161D+12 Y= 1.737681040775D+13 Z= 1.985798080622D+13
I= 30 X= 8.819692405332D+12 Y= 2.784715843395D+13 Z= -1.148697002987D+13
I= 31 X= -4.557875383471D+13 Y= -6.180284415910D+13 Z= -8.820123595591D+13
I= 32 X= 9.317365348301D+13 Y= -8.225557239729D+13 Z= -8.095106054367D+13
I= 33 X= -6.136579715078D+13 Y= -5.401233385350D+13 Z= -4.106668879367D+12
I= 34 X= -1.642232524625D+13 Y= -5.554358783033D+13 Z= -2.647100024080D+13
I= 35 X= 9.501780570610D+11 Y= -5.028277007161D+12 Z= 1.629175842794D+12
I= 36 X= -9.873951817316D+12 Y= 1.037802684189D+13 Z= -1.767553439123D+13
I= 37 X= 6.734206681139D+13 Y= -5.639201901942D+13 Z= 5.234949007061D+13
I= 38 X= 8.904989796711D+13 Y= -3.206014845832D+13 Z= -5.367017297202D+13

Backward Direction:

Total Energy: -656.4286824 Hartrees

Potential Energy: -656.6028733 Hartress

Kinetic Energy: 0.1741909 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.208139605638D+12 Y= 1.044476580164D+13 Z= 8.781627303016D+11
I= 1 X= 1.824448143294D+13 Y= -9.245398423016D+12 Z= -1.925107006534D+13
I= 2 X= -1.104148804041D+13 Y= -5.450713704288D+12 Z= 2.273030699451D+12
I= 3 X= -1.585499578350D+13 Y= 5.098262398111D+12 Z= 2.973192399627D+12
I= 4 X= -1.585421947854D+12 Y= 5.108150475598D+12 Z= -2.692783071568D+13
I= 5 X= -3.637985496567D+12 Y= 1.914113004910D+13 Z= -2.911112943055D+12
I= 6 X= -1.092100167390D+13 Y= 1.497370667627D+13 Z= 8.778671887851D+13
I= 7 X= 5.353603232186D+13 Y= -8.955531446520D+12 Z= -1.973440637769D+13
I= 8 X= -7.031425093893D+12 Y= 1.011468209180D+13 Z= -2.377248954577D+13
I= 9 X= 1.913540058824D+13 Y= -1.322258634314D+13 Z= 1.946833408732D+13
I= 10 X= -4.608891065049D+13 Y= -5.097199320309D+13 Z= 1.567650876502D+14
I= 11 X= -3.621889125682D+13 Y= -3.300645162890D+13 Z= 1.023575685250D+13
I= 12 X= -6.327206115707D+13 Y= -1.525835668144D+13 Z= 5.995708261947D+13

I= 13 X= -1.783778992155D+13 Y= 1.400842160872D+12 Z= 2.083800292113D+13
I= 14 X= 5.511234121520D+13 Y= -6.531531393408D+12 Z= -6.299353220182D+13
I= 15 X= 1.972983626983D+13 Y= 3.707289127614D+13 Z= -7.511093767516D+13
I= 16 X= -2.021630661314D+13 Y= 5.829589430459D+13 Z= 2.405499227047D+13
I= 17 X= -3.207984218481D+12 Y= 1.115030546804D+13 Z= -1.028845872321D+13
I= 18 X= 4.127199756836D+13 Y= -1.649049487361D+13 Z= -1.909810306467D+12
I= 19 X= -5.207895757063D+13 Y= -5.743099559443D+13 Z= 1.758357039606D+13
I= 20 X= 4.510860973152D+13 Y= 1.262610999276D+13 Z= -8.294391441289D+13
I= 21 X= 4.175423152348D+12 Y= -3.397290676201D+12 Z= -2.034073758840D+12
I= 22 X= -1.546282279815D+14 Y= 1.658522332563D+13 Z= -6.433996804658D+13
I= 23 X= -2.150588960317D+13 Y= -4.305986472054D+12 Z= 2.438701103829D+13
I= 24 X= -3.612957464801D+12 Y= -3.735010055979D+13 Z= 5.099957798630D+13
I= 25 X= 1.921830143680D+13 Y= -2.827639167726D+12 Z= 4.383606491952D+12
I= 26 X= -1.542444152665D+12 Y= 9.031917482616D+13 Z= 1.304069731279D+13
I= 27 X= -4.178559307696D+13 Y= -3.334327973245D+13 Z= -2.208593259008D+13
I= 28 X= -1.565033094204D+14 Y= 1.590322445178D+13 Z= 9.633784098332D+13
I= 29 X= 2.306169445128D+12 Y= 1.756063600347D+13 Z= 1.962844687819D+13
I= 30 X= 8.858231475180D+12 Y= 2.772050880556D+13 Z= -1.177123104413D+13
I= 31 X= -4.603120983032D+13 Y= -6.193670098273D+13 Z= -8.818709830242D+13
I= 32 X= 9.184951178843D+13 Y= -8.115595321863D+13 Z= -8.173941436088D+13
I= 33 X= -6.132496038910D+13 Y= -5.417238689416D+13 Z= -4.333083814321D+12
I= 34 X= -1.599571004774D+13 Y= -5.584060846229D+13 Z= -2.655265081207D+13
I= 35 X= 9.430585383917D+11 Y= -4.861987094620D+12 Z= 2.684182894260D+12
I= 36 X= -1.217475749769D+13 Y= 7.471919685272D+12 Z= -1.873604631640D+13
I= 37 X= 6.939459842769D+13 Y= -5.535002122641D+13 Z= 4.978965466485D+13
I= 38 X= 9.017394390676D+13 Y= -3.217727610092D+13 Z= -5.558192052885D+13

Seed: 40191278813

CM Start Point Coordinates: bohr

I= 0 X= -2.072662318415D+00 Y= 2.306686514535D+00 Z= -5.627270969776D-01

I= 1 X= -2.634078267203D+00 Y= 1.333950959584D-01 Z= -2.072994010893D+00
I= 2 X= -1.896176102185D+00 Y= 1.724971432899D+00 Z= 2.112537917082D+00
I= 3 X= -2.414092076260D+00 Y= -1.897908471757D+00 Z= -2.291244647864D-01
I= 4 X= -2.032904312759D+00 Y= -8.750031343059D-01 Z= 2.362277753281D+00
I= 5 X= 4.248518458981D+00 Y= 2.549533930384D+00 Z= -1.353714843266D+00
I= 6 X= 2.472042650974D+00 Y= 4.386250353033D-01 Z= -3.142820626646D+00
I= 7 X= 5.872444717811D+00 Y= 1.655035829517D+00 Z= -1.821073278538D+00
I= 8 X= 3.200498112324D+00 Y= 4.032145481861D+00 Z= -2.513497693762D+00
I= 9 X= -2.088797913038D+00 Y= -2.669022418316D+00 Z= 4.518579707404D+00
I= 10 X= -3.761566586218D+00 Y= -2.504226254813D+00 Z= 5.941966044208D+00
I= 11 X= -1.820120896923D+00 Y= -4.797056914140D+00 Z= 4.339573294669D+00
I= 12 X= -5.957794354948D-01 Y= -2.159425755708D+00 Z= 6.000063416830D+00
I= 13 X= -1.893447645954D+00 Y= 3.523809487995D+00 Z= 4.166437704423D+00
I= 14 X= -3.930896580909D+00 Y= 3.883992911554D+00 Z= 4.726481824281D+00
I= 15 X= -7.907827949373D-01 Y= 3.017464600184D+00 Z= 5.597988510069D+00
I= 16 X= -1.536102486881D+00 Y= 5.566459272711D+00 Z= 3.447864821204D+00
I= 17 X= -2.426476617460D+00 Y= 4.837839736244D+00 Z= -1.569022822811D+00
I= 18 X= -4.630222199355D+00 Y= 5.276385055366D+00 Z= -2.245064007101D+00
I= 19 X= -1.653813925825D+00 Y= 6.462049566837D+00 Z= -3.854978923685D-01
I= 20 X= -1.437562532632D+00 Y= 5.049779675497D+00 Z= -3.650328838348D+00
I= 21 X= -3.443813276844D+00 Y= -3.067682598355D-01 Z= -4.650696596981D+00
I= 22 X= -5.766501117017D+00 Y= -1.626922862357D-01 Z= -4.887006229853D+00
I= 23 X= -2.760688470144D+00 Y= 1.294177532038D+00 Z= -5.756394615894D+00
I= 24 X= -2.700913187057D+00 Y= -2.118576655296D+00 Z= -5.277400919136D+00
I= 25 X= -3.425816208260D+00 Y= -4.461523709058D+00 Z= -5.923675035321D-01
I= 26 X= -3.755661306955D+00 Y= -5.419624309999D+00 Z= -2.595252918383D+00
I= 27 X= -2.185127005953D+00 Y= -5.984742705426D+00 Z= 1.218197203725D-01
I= 28 X= -5.535236891337D+00 Y= -4.541852938300D+00 Z= 2.309490000692D-01
I= 29 X= 3.227646402402D+00 Y= -3.741010721267D+00 Z= -1.590696005012D+00
I= 30 X= 3.722402715482D+00 Y= -3.267838900179D+00 Z= 1.009962038482D+00

I= 31 X= 1.823398025697D+00 Y= -5.006179672258D+00 Z= -2.542474361318D+00
I= 32 X= 4.531254773152D+00 Y= -3.206537034023D+00 Z= -3.067445910104D+00
I= 33 X= 5.633191187265D+00 Y= -1.924983913228D+00 Z= 1.384781768262D+00
I= 34 X= 2.756289863896D+00 Y= -4.219126535736D+00 Z= 2.580537323044D+00
I= 35 X= 1.164553602861D+00 Y= -6.353948935578D-02 Z= -3.362282486210D-01
I= 36 X= 3.828358593261D+00 Y= 2.636888240585D+00 Z= 1.264658521369D+00
I= 37 X= 5.514955031336D+00 Y= 1.680211728783D+00 Z= 2.231055055765D+00
I= 38 X= 2.898646923005D+00 Y= 4.293895155299D+00 Z= 2.116814718104D+00

Forward Direction:

Total Energy: -656.4402380 Hartrees

Potential Energy: -656.6493211 Hartress

Kinetic Energy: 0.2090831 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.335530522870D+13 Y= 5.204707527711D+12 Z= 8.401976954152D+12
I= 1 X= -1.173857738077D+13 Y= 2.881563979763D+12 Z= -1.841324286962D+13
I= 2 X= 6.682948049963D+12 Y= -1.104302250836D+13 Z= -7.264099059994D+12
I= 3 X= -7.854793474883D+12 Y= 4.617689049334D+12 Z= 1.203848479340D+12
I= 4 X= -3.758206884640D+11 Y= 2.071437037656D+12 Z= 1.303680507595D+13
I= 5 X= -1.881885820848D+13 Y= 1.936262202483D+12 Z= 1.180682769114D+13
I= 6 X= 2.080896497363D+12 Y= 3.192563859495D+13 Z= -7.636316487555D+13
I= 7 X= 8.071343299334D+13 Y= -7.257974431841D+13 Z= -6.044343211386D+13
I= 8 X= -2.872487887909D+13 Y= -6.146391872886D+13 Z= -7.538005016102D+13
I= 9 X= -2.690931084053D+12 Y= 3.224694359747D+12 Z= 1.030210023997D+13
I= 10 X= 2.015998774883D+13 Y= -3.737414524563D+13 Z= -1.671532276986D+12
I= 11 X= 1.021464919367D+13 Y= -9.163268823553D+13 Z= 2.312699738135D+13
I= 12 X= 9.960044145556D+13 Y= -5.276351800741D+13 Z= 1.803536309384D+13
I= 13 X= -7.113106696952D+12 Y= -5.371424793564D+11 Z= 6.865320954063D+12
I= 14 X= -3.125516642777D+13 Y= -2.436734634364D+13 Z= -3.728630594148D+13
I= 15 X= 1.759063788518D+14 Y= 2.197093945324D+13 Z= 1.181519651312D+14
I= 16 X= 4.484128381768D+13 Y= 9.549677509804D+13 Z= -2.901455969927D+13

I= 17 X= 4.729664413736D+12 Y= 1.008669989101D+12 Z= -1.483260919556D+13
I= 18 X= -1.672208875831D+14 Y= -8.160596860704D+12 Z= -6.363413452192D+13
I= 19 X= 3.518487575083D+13 Y= -5.721268577516D+13 Z= 3.990927204574D+13
I= 20 X= -7.342759789174D+12 Y= -2.320675711965D+13 Z= 4.849530101366D+13
I= 21 X= -1.191821152520D+13 Y= 1.086164848046D+13 Z= 1.499732769722D+13
I= 22 X= -2.076207892020D+13 Y= -7.421333083339D+12 Z= 1.732041428070D+13
I= 23 X= -1.242771304545D+13 Y= -1.136664022942D+14 Z= 5.586437784932D+13
I= 24 X= 8.868457162148D+13 Y= -6.249901448314D+13 Z= 6.961684884079D+13
I= 25 X= 7.170549203783D+12 Y= -4.708708393108D+12 Z= 9.519257910280D+12
I= 26 X= -2.949694874604D+13 Y= -1.346967718531D+14 Z= -6.024835303754D+13
I= 27 X= -1.203694910104D+14 Y= 5.052181052990D+13 Z= -1.516776223891D+14
I= 28 X= 5.917202208240D+13 Y= 8.104008604631D+13 Z= -1.554093381674D+13
I= 29 X= -2.300819029592D+13 Y= -6.870846820748D+12 Z= -1.317127589434D+13
I= 30 X= 8.923424312319D+12 Y= -7.830677849534D+12 Z= 1.386950810318D+12
I= 31 X= -5.833252384792D+12 Y= 5.323155036351D+13 Z= 7.494298361195D+13
I= 32 X= 5.512430333320D+13 Y= 9.450713271010D+12 Z= 5.690207412868D+13
I= 33 X= 1.108366240448D+13 Y= 6.276260801725D+13 Z= 1.021550199534D+14
I= 34 X= 4.102384318487D+13 Y= 1.343512319610D+14 Z= -9.036706195830D+13
I= 35 X= 1.089077379339D+11 Y= 2.486964839961D+12 Z= -3.159554155857D+12
I= 36 X= 5.535210991184D+12 Y= -1.611401077861D+12 Z= -2.547356463371D+12
I= 37 X= 6.841744279132D+13 Y= -4.292351315914D+13 Z= 7.280163569568D+13
I= 38 X= -5.696501969095D+13 Y= 4.750937370311D+12 Z= 3.339556130987D+13

Backward Direction:

Total Energy: -656.4402459 Hartrees

Potential Energy: -656.6493211 Hartress

Kinetic Energy: 0.2090752 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.321492802821D+13 Y= 5.021395259655D+12 Z= 8.473711907218D+12

I= 1 X= -1.195509201511D+13 Y= 2.410177311465D+12 Z= -1.869621760469D+13

I= 2 X= 6.481431210973D+12 Y= -1.085778393647D+13 Z= -7.562341002806D+12

I= 3 X= -8.267691067823D+12 Y= 4.627343768723D+12 Z= 6.056023109096D+11
I= 4 X= 3.303948624853D+11 Y= 2.008429775389D+12 Z= 1.256751348671D+13
I= 5 X= -1.998439844755D+13 Y= 2.787365706222D+11 Z= 8.497552740447D+12
I= 6 X= 2.818880278103D+13 Y= 6.173094860410D+13 Z= -6.461631205699D+13
I= 7 X= 8.548204289471D+13 Y= -6.806488509511D+13 Z= -6.015168960762D+13
I= 8 X= -2.270232136494D+13 Y= -5.659577039268D+13 Z= -7.481975491870D+13
I= 9 X= -2.466475117103D+12 Y= 3.330103101765D+12 Z= 1.004839112650D+13
I= 10 X= 2.020103894967D+13 Y= -3.685248148171D+13 Z= -2.276248691385D+12
I= 11 X= 1.014982186951D+13 Y= -9.163839083411D+13 Z= 2.311439140881D+13
I= 12 X= 9.973198843733D+13 Y= -5.272828472026D+13 Z= 1.791044585381D+13
I= 13 X= -7.068611579312D+12 Y= -5.587921028417D+11 Z= 6.771672363646D+12
I= 14 X= -3.117952155955D+13 Y= -2.450072186071D+13 Z= -3.726650855356D+13
I= 15 X= 1.760454902212D+14 Y= 2.184335029916D+13 Z= 1.179216069235D+14
I= 16 X= 4.483159337400D+13 Y= 9.553778236282D+13 Z= -2.898212753119D+13
I= 17 X= 4.797803673891D+12 Y= 8.582967798821D+11 Z= -1.484750051554D+13
I= 18 X= -1.672065207622D+14 Y= -8.400331646747D+12 Z= -6.383079864218D+13
I= 19 X= 3.504083072962D+13 Y= -5.726067073027D+13 Z= 4.005780494504D+13
I= 20 X= -7.242730617899D+12 Y= -2.334112075690D+13 Z= 4.847814256693D+13
I= 21 X= -1.200395239100D+13 Y= 1.080778415294D+13 Z= 1.478802117828D+13
I= 22 X= -2.077740150813D+13 Y= -7.179943383851D+12 Z= 1.648158944060D+13
I= 23 X= -1.211605408467D+13 Y= -1.138020640956D+14 Z= 5.576711204819D+13
I= 24 X= 8.853432564126D+13 Y= -6.258339882116D+13 Z= 6.936936771671D+13
I= 25 X= 7.077366086762D+12 Y= -4.802842827703D+12 Z= 9.471172869094D+12
I= 26 X= -2.972743143294D+13 Y= -1.349489020961D+14 Z= -6.027647497533D+13
I= 27 X= -1.201774010631D+14 Y= 5.068353467214D+13 Z= -1.517333706596D+14
I= 28 X= 5.918154064624D+13 Y= 8.075478637185D+13 Z= -1.533898663212D+13
I= 29 X= -2.343973263856D+13 Y= -6.749629939983D+12 Z= -1.332263341893D+13
I= 30 X= 8.948837452971D+12 Y= -7.914192188736D+12 Z= 1.199505565059D+12
I= 31 X= -6.131607488932D+12 Y= 5.314328351123D+13 Z= 7.495230615430D+13
I= 32 X= 5.425114784516D+13 Y= 1.017581582245D+13 Z= 5.638222382543D+13

I= 33 X= 1.111059067289D+13 Y= 6.265706705203D+13 Z= 1.020057191325D+14
I= 34 X= 4.130515854447D+13 Y= 1.341553728662D+14 Z= -9.042090336146D+13
I= 35 X= 1.042130385256D+11 Y= 2.596618474999D+12 Z= -2.463869396998D+12
I= 36 X= 4.018031137447D+12 Y= -3.527724246889D+12 Z= -3.246671205463D+12
I= 37 X= 6.977090764357D+13 Y= -4.223640686693D+13 Z= 7.111364841913D+13
I= 38 X= -5.622380983335D+13 Y= 4.673701948593D+12 Z= 3.213493121072D+13

Seed: 40972791204

CM Start Point Coordinates: bohr

I= 0 X= -2.363259638942D+00 Y= 2.328799492319D+00 Z= -4.456884469698D-01
I= 1 X= -2.911878212766D+00 Y= 7.256843268077D-02 Z= -1.896388978301D+00
I= 2 X= -1.926287260104D+00 Y= 1.688517119545D+00 Z= 1.982560507786D+00
I= 3 X= -2.538994817372D+00 Y= -1.961381863767D+00 Z= -2.263457302735D-01
I= 4 X= -1.968706429960D+00 Y= -1.027556671736D+00 Z= 2.358011312901D+00
I= 5 X= 4.470984134625D+00 Y= 2.558868556491D+00 Z= -1.590726308855D+00
I= 6 X= 3.026209322608D+00 Y= 5.556739382623D-03 Z= -3.301044498152D+00
I= 7 X= 6.415758927199D+00 Y= 1.642469929315D+00 Z= -1.765239562627D+00
I= 8 X= 3.907957446759D+00 Y= 3.875252814880D+00 Z= -2.821680088011D+00
I= 9 X= -2.083937662990D+00 Y= -2.860408418724D+00 Z= 4.680182238735D+00
I= 10 X= -4.022452778804D+00 Y= -3.342130727922D+00 Z= 4.786143729377D+00
I= 11 X= -1.014789272049D+00 Y= -4.392740226683D+00 Z= 4.125663912845D+00
I= 12 X= -8.949964680326D-01 Y= -1.961967526702D+00 Z= 6.407715232408D+00
I= 13 X= -1.921752838913D+00 Y= 3.459928261574D+00 Z= 4.360504497021D+00
I= 14 X= -3.803446694383D+00 Y= 3.872270477238D+00 Z= 4.730318546307D+00
I= 15 X= -5.184085127033D-01 Y= 2.452906737259D+00 Z= 6.042500061645D+00
I= 16 X= -1.016236701869D+00 Y= 5.321585255392D+00 Z= 4.134206004149D+00
I= 17 X= -2.247462258863D+00 Y= 4.972415929979D+00 Z= -1.862558413393D+00
I= 18 X= -4.140524808760D+00 Y= 5.431321126526D+00 Z= -2.403802365639D+00
I= 19 X= -1.250308038206D+00 Y= 6.384437736025D+00 Z= -6.774263005871D-01
I= 20 X= -8.685348852276D-01 Y= 5.397315769867D+00 Z= -3.549342875757D+00

I= 21 X= -3.932936595012D+00 Y= 1.781852890386D-02 Z= -4.449164393254D+00
I= 22 X= -6.117124150635D+00 Y= 3.982906751367D-01 Z= -4.540098638367D+00
I= 23 X= -3.014304623853D+00 Y= 1.061961176101D+00 Z= -5.659888680358D+00
I= 24 X= -3.903282743886D+00 Y= -2.019249500959D+00 Z= -5.163204492386D+00
I= 25 X= -3.213434018316D+00 Y= -4.489658792770D+00 Z= -9.882843374958D-01
I= 26 X= -2.960379614115D+00 Y= -4.474123327416D+00 Z= -3.103171367838D+00
I= 27 X= -1.685165474738D+00 Y= -5.906009705760D+00 Z= -3.057596935649D-01
I= 28 X= -5.184344795177D+00 Y= -5.331459868489D+00 Z= -1.638772276364D-01
I= 29 X= 3.370028469851D+00 Y= -3.909434615103D+00 Z= -1.083423116554D+00
I= 30 X= 3.764705655693D+00 Y= -3.198542411122D+00 Z= 1.505879435692D+00
I= 31 X= 1.781010389442D+00 Y= -5.144272399235D+00 Z= -1.672738288698D+00
I= 32 X= 4.785720395474D+00 Y= -3.368508669356D+00 Z= -2.542359824805D+00
I= 33 X= 5.584153837999D+00 Y= -2.258770125769D+00 Z= 2.280984784056D+00
I= 34 X= 2.553684373559D+00 Y= -3.761580136792D+00 Z= 2.928272579364D+00
I= 35 X= 1.163582855175D+00 Y= -3.738027513646D-02 Z= -4.173459921328D-01
I= 36 X= 3.972103791944D+00 Y= 2.695696295751D+00 Z= 1.060911426496D+00
I= 37 X= 4.877582472068D+00 Y= 1.700382460937D+00 Z= 2.511205679426D+00
I= 38 X= 2.135574790219D+00 Y= 4.094635916327D+00 Z= 1.787733341780D+00

Forward Direction:

Total Energy: -656.4291817 Hartrees

Potential Energy: -656.6068642 Hartress

Kinetic Energy: 0.1776824 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.324605003776D+13 Y= -1.890657886419D+13 Z= -6.661353339203D+12
I= 1 X= 2.920511770541D+12 Y= 3.014181254503D+13 Z= 1.141699920988D+13
I= 2 X= -6.269480123767D+12 Y= 2.060762745639D+13 Z= 2.739872186739D+12
I= 3 X= 2.834139525779D+12 Y= -1.933117952566D+13 Z= 6.904829116109D+10
I= 4 X= -5.192105733575D+12 Y= -1.237377685983D+13 Z= 5.672962054063D+12
I= 5 X= 5.247902379432D+12 Y= -1.154253244777D+13 Z= 4.126269688971D+12
I= 6 X= -6.086796533795D+13 Y= -6.176265913086D+11 Z= -3.734165571398D+13

I= 7 X= -2.580688622315D+13 Y= 5.324430821375D+13 Z= 2.914113623740D+13
I= 8 X= 9.006916392550D+13 Y= -8.463070232030D+13 Z= -8.021853596315D+13
I= 9 X= 1.517564363501D+13 Y= 8.009457313950D+12 Z= 2.537899389270D+12
I= 10 X= -3.455365006771D+13 Y= 4.812105322916D+13 Z= -4.970692889008D+13
I= 11 X= -3.133297373556D+13 Y= -2.200028092053D+13 Z= -4.175019639981D+13
I= 12 X= -5.308638894345D+13 Y= 5.009114678563D+12 Z= 4.947857982906D+12
I= 13 X= 5.878592728066D+12 Y= -1.164684427444D+13 Z= 5.274998175355D+12
I= 14 X= 1.067173096463D+14 Y= 5.768999782892D+12 Z= 7.425799600028D+13
I= 15 X= -9.500168762704D+13 Y= -1.810408213738D+13 Z= -6.660672882155D+13
I= 16 X= -2.285863189758D+12 Y= 5.553548208180D+13 Z= 8.571920345352D+13
I= 17 X= -6.813166601116D+12 Y= 1.293388154566D+13 Z= -1.044618083605D+12
I= 18 X= 2.174938719776D+13 Y= 9.949486426896D+12 Z= 3.314950915232D+13
I= 19 X= 9.739700840077D+13 Y= 1.782397512963D+13 Z= 1.429767806407D+14
I= 20 X= 1.278124394936D+13 Y= 1.640513731145D+13 Z= -4.946214150047D+13
I= 21 X= 1.438613664527D+12 Y= 9.599606619468D+12 Z= -4.199119742969D+12
I= 22 X= -5.832837473365D+13 Y= 1.367274835587D+13 Z= -1.759091338074D+13
I= 23 X= 2.009905732458D+13 Y= 3.799308544197D+13 Z= -1.215252445505D+14
I= 24 X= -4.015444430854D+13 Y= -1.492900926971D+13 Z= -8.077123881715D+13
I= 25 X= -1.463412021141D+13 Y= 3.462230865790D+12 Z= -1.581343820628D+13
I= 26 X= 2.350733885867D+12 Y= 4.756876496540D+13 Z= -6.960934078321D+13
I= 27 X= -2.187537264832D+13 Y= -9.843795743558D+13 Z= 6.991969272014D+13
I= 28 X= -1.920888564361D+13 Y= -9.397878237296D+13 Z= 2.445001125218D+13
I= 29 X= 1.280987768289D+13 Y= 2.390437982036D+13 Z= -4.359327909451D+12
I= 30 X= -1.445362562823D+13 Y= -2.223588364998D+13 Z= 4.071873768115D+12
I= 31 X= -1.142185953403D+14 Y= -8.245256231222D+13 Z= -2.572985078818D+13
I= 32 X= 1.715833260004D+13 Y= -4.353151395435D+11 Z= -8.839693402049D+13
I= 33 X= -2.855599136452D+12 Y= 4.585220834399D+12 Z= 1.974945359922D+13
I= 34 X= 6.197777768258D+13 Y= -3.788985373597D+13 Z= -4.476137885983D+13
I= 35 X= -3.627697711518D+12 Y= -1.613948985767D+12 Z= 1.080282759726D+12
I= 36 X= 2.167396366840D+13 Y= 1.519978113341D+13 Z= -3.664375474835D+12

I= 37 X= 1.177265469612D+14 Y= -1.280320343347D+13 Z= 1.452613718470D+14

I= 38 X= -2.123934984918D+13 Y= -1.587598692927D+13 Z= 3.159826436195D+13

Backward Direction:

Total Energy: -656.4292984 Hartrees

Potential Energy: -656.6068642 Hartress

Kinetic Energy: 0.1775658 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.290944290648D+13 Y= -1.934613896348D+13 Z= -6.489341813229D+12

I= 1 X= 2.401336511447D+12 Y= 2.901148573336D+13 Z= 1.073846086384D+13

I= 2 X= -6.752692534555D+12 Y= 2.105180659664D+13 Z= 2.024724967822D+12

I= 3 X= 1.844062266459D+12 Y= -1.930802870592D+13 Z= -1.365471880731D+12

I= 4 X= -3.498688369516D+12 Y= -1.252486046692D+13 Z= 4.547658982375D+12

I= 5 X= 2.453081327751D+12 Y= -1.551707349875D+13 Z= -3.808961530711D+12

I= 6 X= 1.735558441717D+12 Y= 7.085181311146D+13 Z= -9.174158412734D+12

I= 7 X= -1.437235064011D+13 Y= 6.407038112184D+13 Z= 2.984069861143D+13

I= 8 X= 1.045105104736D+14 Y= -7.295748591286D+13 Z= -7.887501740777D+13

I= 9 X= 1.571386123690D+13 Y= 8.262214413798D+12 Z= 1.929536373640D+12

I= 10 X= -3.445521438060D+13 Y= 4.937193831181D+13 Z= -5.115696395662D+13

I= 11 X= -3.148842163231D+13 Y= -2.201395505999D+13 Z= -4.178042394280D+13

I= 12 X= -5.277095560903D+13 Y= 5.093599734604D+12 Z= 4.648321946478D+12

I= 13 X= 5.985286516720D+12 Y= -1.169875738844D+13 Z= 5.050440458331D+12

I= 14 X= 1.068986966659D+14 Y= 5.449181803248D+12 Z= 7.430546766153D+13

I= 15 X= -9.466811581745D+13 Y= -1.841002512458D+13 Z= -6.715909924290D+13

I= 16 X= -2.309099701221D+12 Y= 5.563381243902D+13 Z= 8.579697177426D+13

I= 17 X= -6.649777097082D+12 Y= 1.257330522590D+13 Z= -1.080325622167D+12

I= 18 X= 2.178383705055D+13 Y= 9.374632118970D+12 Z= 3.267793296559D+13

I= 19 X= 9.705160627849D+13 Y= 1.770891315999D+13 Z= 1.433329441295D+14

I= 20 X= 1.302110150310D+13 Y= 1.608294996744D+13 Z= -4.950328534213D+13

I= 21 X= 1.233017688601D+12 Y= 9.470446636081D+12 Z= -4.701010835935D+12

I= 22 X= -5.836511640449D+13 Y= 1.425157095742D+13 Z= -1.960231139466D+13

I= 23 X= 2.084637690616D+13 Y= 3.766778523846D+13 Z= -1.217584758934D+14
I= 24 X= -4.051471555840D+13 Y= -1.513135246134D+13 Z= -8.136466787272D+13
I= 25 X= -1.485756178019D+13 Y= 3.236508158450D+12 Z= -1.592874017572D+13
I= 26 X= 1.798064974647D+12 Y= 4.696418787420D+13 Z= -6.967677370726D+13
I= 27 X= -2.141476475129D+13 Y= -9.805016299095D+13 Z= 6.978601527655D+13
I= 28 X= -1.918606130146D+13 Y= -9.466289562918D+13 Z= 2.493425556104D+13
I= 29 X= 1.177509262589D+13 Y= 2.419504288165D+13 Z= -4.722264495606D+12
I= 30 X= -1.439268806584D+13 Y= -2.243614068588D+13 Z= 3.622403298937D+12
I= 31 X= -1.149340139071D+14 Y= -8.266421528295D+13 Z= -2.570749648607D+13
I= 32 X= 1.506461394954D+13 Y= 1.303390918457D+12 Z= -8.964347062176D+13
I= 33 X= -2.791028487306D+12 Y= 4.332146679309D+12 Z= 1.939144873760D+13
I= 34 X= 6.265233705649D+13 Y= -3.835949957490D+13 Z= -4.489048386720D+13
I= 35 X= -3.638955018438D+12 Y= -1.351013158813D+12 Z= 2.748448597170D+12
I= 36 X= 1.803595439811D+13 Y= 1.060467565948D+13 Z= -5.341245560509D+12
I= 37 X= 1.209719879479D+14 Y= -1.115560770032D+13 Z= 1.412137875450D+14
I= 38 X= -1.946202046396D+13 Y= -1.606118789846D+13 Z= 2.857542961479D+13

Seed: 42986769806

CM Start Point Coordinates: bohr

I= 0 X= -2.216253639748D+00 Y= 2.276392330928D+00 Z= -4.684479474604D-01
I= 1 X= -2.718915775581D+00 Y= 1.376250721179D-01 Z= -2.077453823995D+00
I= 2 X= -2.080921663316D+00 Y= 1.659619672204D+00 Z= 2.089490382640D+00
I= 3 X= -2.642740856440D+00 Y= -1.895761490473D+00 Z= -3.163702165178D-01
I= 4 X= -2.202952914974D+00 Y= -9.512583553342D-01 Z= 2.179160807104D+00
I= 5 X= 4.446007547748D+00 Y= 2.234670251441D+00 Z= -2.035690516628D+00
I= 6 X= 1.996876278738D+00 Y= 3.088296513306D-01 Z= -3.217146685602D+00
I= 7 X= 5.759224221095D+00 Y= 1.043703986306D+00 Z= -2.972196546355D+00
I= 8 X= 3.502519122036D+00 Y= 3.189629526401D+00 Z= -3.572704866177D+00
I= 9 X= -1.854873937647D+00 Y= -2.656947247488D+00 Z= 4.539010676507D+00
I= 10 X= -3.433885524914D+00 Y= -2.530377347913D+00 Z= 5.915013531314D+00

I= 11 X= -1.186808408769D+00 Y= -4.659245966535D+00 Z= 4.252223403680D+00
I= 12 X= -2.191803992011D-01 Y= -1.833412742936D+00 Z= 6.017033301918D+00
I= 13 X= -1.901797539145D+00 Y= 3.403206436691D+00 Z= 4.201867624220D+00
I= 14 X= -3.923877081358D+00 Y= 3.673443017632D+00 Z= 5.027870565246D+00
I= 15 X= -6.454532870674D-01 Y= 2.438018128152D+00 Z= 5.674310615880D+00
I= 16 X= -9.794013884005D-01 Y= 5.481440237521D+00 Z= 3.725470870570D+00
I= 17 X= -2.329388955341D+00 Y= 5.006699285865D+00 Z= -1.143785805275D+00
I= 18 X= -4.074894786429D+00 Y= 6.253592680388D+00 Z= -2.632278010689D-01
I= 19 X= -2.417137934752D-01 Y= 6.018284797665D+00 Z= -6.511962316679D-01
I= 20 X= -2.612158477181D+00 Y= 5.349805759981D+00 Z= -3.085469421868D+00
I= 21 X= -3.503421417037D+00 Y= 1.588315495508D-01 Z= -4.773203678044D+00
I= 22 X= -5.502295234713D+00 Y= -1.381881685586D-01 Z= -4.650718182563D+00
I= 23 X= -3.106737838490D+00 Y= 1.880944129544D+00 Z= -5.696704863034D+00
I= 24 X= -2.967959919079D+00 Y= -1.756517735727D+00 Z= -5.642623900035D+00
I= 25 X= -2.910611569106D+00 Y= -4.605398031476D+00 Z= -1.054699466190D+00
I= 26 X= -2.559459671121D+00 Y= -5.141001216154D+00 Z= -3.196507873823D+00
I= 27 X= -1.148586436179D+00 Y= -5.340022867884D+00 Z= -3.276113463056D-01
I= 28 X= -4.759847570289D+00 Y= -5.719294808855D+00 Z= -4.399733405730D-01
I= 29 X= 3.608238469083D+00 Y= -3.433826605418D+00 Z= -8.198297457532D-01
I= 30 X= 3.310499737553D+00 Y= -3.135730518673D+00 Z= 1.822752743630D+00
I= 31 X= 2.219917896412D+00 Y= -4.965364241372D+00 Z= -2.005279689543D+00
I= 32 X= 5.224418036170D+00 Y= -2.529414254974D+00 Z= -1.951457027093D+00
I= 33 X= 5.029837179753D+00 Y= -1.876975004305D+00 Z= 2.298752777252D+00
I= 34 X= 1.973479999967D+00 Y= -4.359850994402D+00 Z= 2.836332427294D+00
I= 35 X= 1.038630604110D+00 Y= -1.192113035541D-01 Z= -3.346580773190D-01
I= 36 X= 4.267236782349D+00 Y= 2.725608474824D+00 Z= 5.959630362437D-01
I= 37 X= 6.065061694249D+00 Y= 1.974537430081D+00 Z= 1.723033246850D+00
I= 38 X= 3.486070147830D+00 Y= 4.410899065584D+00 Z= 1.763319403038D+00

Forward Direction:

Total Energy: -656.4384327 Hartrees

Potential Energy: -656.6188325 Hartress

Kinetic Energy: 0.1803998 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.406389925460D+12 Y= 5.674569049623D+12 Z= 1.070372395790D+13
I= 1 X= 3.052286291986D+12 Y= -1.391822171626D+13 Z= 1.535342825907D+13
I= 2 X= 1.238572351497D+12 Y= -2.139160472445D+12 Z= 8.251298846221D+12
I= 3 X= -7.503839907650D+12 Y= 1.579333402854D+13 Z= 3.559625507576D+11
I= 4 X= -2.763099873572D+12 Y= -9.227680487971D+12 Z= 7.335971790017D+12
I= 5 X= 2.127444842724D+13 Y= -1.920125772740D+13 Z= 8.410563540502D+12
I= 6 X= 1.455141231070D+13 Y= -2.175295181968D+13 Z= -9.279103036602D+13
I= 7 X= -7.544950451482D+13 Y= 3.951391118898D+13 Z= 8.055665457792D+13
I= 8 X= -4.062902977643D+13 Y= 2.370969195876D+13 Z= -2.628566993332D+12
I= 9 X= -2.830515173522D+13 Y= -1.092972060381D+12 Z= -5.014240717012D+12
I= 10 X= 9.648238736914D+13 Y= 5.683200312256D+13 Z= -2.168575187167D+13
I= 11 X= 8.884235962922D+13 Y= -3.241565889516D+12 Z= -1.337035739923D+13
I= 12 X= 1.544842387788D+13 Y= 5.659934504238D+13 Z= -8.815223872515D+13
I= 13 X= 1.908544790772D+13 Y= 7.220646677582D+12 Z= -3.778051845463D+12
I= 14 X= -1.125301826796D+13 Y= -9.592948660036D+13 Z= 4.113034529282D+13
I= 15 X= -8.829509921035D+13 Y= -1.630588039296D+13 Z= -2.657319481510D+13
I= 16 X= 4.842815780311D+13 Y= -7.270881302263D+13 Z= -7.081813099722D+12
I= 17 X= -5.004524674267D+12 Y= 1.320255191423D+13 Z= 6.032737254598D+12
I= 18 X= 9.250883907571D+13 Y= -1.044526556758D+14 Z= 3.882338729061D+13
I= 19 X= 6.919239990415D+13 Y= 6.199698434019D+13 Z= -2.266878583342D+13
I= 20 X= -1.738070010563D+13 Y= 1.075099515093D+13 Z= 7.737301821993D+13
I= 21 X= 2.628854539077D+12 Y= -6.347423896878D+12 Z= 1.979859145359D+13
I= 22 X= -1.433221860111D+14 Y= 4.211355171938D+13 Z= -7.038563101959D+13
I= 23 X= -6.563371052226D+13 Y= -5.018314903088D+13 Z= -6.056974112473D+13
I= 24 X= 5.430395015815D+13 Y= 9.915221404274D+12 Z= -1.810389363877D+13
I= 25 X= -2.023432716646D+12 Y= -1.709838861022D+13 Z= -1.157583948293D+13
I= 26 X= -6.129614274765D+13 Y= 3.798387840942D+13 Z= 2.136481891357D+12

I= 27 X= -5.268619207107D+13 Y= 7.519260501877D+12 Z= 4.078271946974D+13
I= 28 X= 1.148430597276D+14 Y= -8.515779936466D+13 Z= -6.744031035015D+13
I= 29 X= 1.460816159824D+13 Y= -2.412926676656D+12 Z= -3.894583733351D+12
I= 30 X= 2.362489417381D+13 Y= 5.875011758530D+12 Z= -1.201293928088D+13
I= 31 X= -4.098643504238D+11 Y= -1.073615316161D+13 Z= -9.569896491708D+13
I= 32 X= 5.878760834996D+11 Y= 1.465577202046D+13 Z= 6.619682186331D+13
I= 33 X= -2.132048084882D+13 Y= -6.614822551916D+12 Z= -1.133361047220D+13
I= 34 X= -1.637043167239D+14 Y= -2.901034830797D+13 Z= 7.608107718992D+13
I= 35 X= -3.671801061452D+12 Y= 4.695906576937D+12 Z= -8.324360166156D+11
I= 36 X= 5.067497626890D+12 Y= -1.315153705803D+13 Z= -2.767159962425D+13
I= 37 X= 1.772651793108D+13 Y= 3.950371796623D+13 Z= 6.138334311739D+13
I= 38 X= -1.544775232871D+13 Y= 5.397048117756D+13 Z= 5.262187084918D+13

Backward Direction:

Total Energy: -656.4384183 Hartrees

Potential Energy: -656.6188325 Hartress

Kinetic Energy: 0.1804142 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.631376319728D+12 Y= 5.380769444416D+12 Z= 1.081869553578D+13
I= 1 X= 2.705272341856D+12 Y= -1.467372607405D+13 Z= 1.489989688036D+13
I= 2 X= 9.155957758793D+11 Y= -1.842273525174D+12 Z= 7.773298293671D+12
I= 3 X= -8.165602220328D+12 Y= 1.580880791186D+13 Z= -6.028630124843D+11
I= 4 X= -1.631228819036D+12 Y= -9.328663957729D+12 Z= 6.583825271973D+12
I= 5 X= 1.940640507606D+13 Y= -2.185781957748D+13 Z= 3.106697695373D+12
I= 6 X= 5.639527070887D+13 Y= 2.601683707290D+13 Z= -7.396402675028D+13
I= 7 X= -6.780672246669D+13 Y= 4.675000005909D+13 Z= 8.102423830386D+13
I= 8 X= -3.097651145894D+13 Y= 3.151200698768D+13 Z= -1.730566420536D+12
I= 9 X= -2.794540998361D+13 Y= -9.240305745524D+11 Z= -5.420867283882D+12
I= 10 X= 9.654818125675D+13 Y= 5.766808797387D+13 Z= -2.265494750411D+13
I= 11 X= 8.873845910170D+13 Y= -3.250705612859D+12 Z= -1.339056132869D+13
I= 12 X= 1.565925782022D+13 Y= 5.665581439916D+13 Z= -8.835244700469D+13

I= 13 X= 1.915676146014D+13 Y= 7.185948232118D+12 Z= -3.928145014041D+12
I= 14 X= -1.113178016118D+13 Y= -9.614325121685D+13 Z= 4.116207509462D+13
I= 15 X= -8.807214161049D+13 Y= -1.651037103658D+13 Z= -2.694239623279D+13
I= 16 X= 4.841262665237D+13 Y= -7.264308954207D+13 Z= -7.029833167148D+12
I= 17 X= -4.895316006607D+12 Y= 1.296154464139D+13 Z= 6.008870527896D+12
I= 18 X= 9.253186517308D+13 Y= -1.048368852046D+14 Z= 3.850818829579D+13
I= 19 X= 6.896153498195D+13 Y= 6.192007753480D+13 Z= -2.243072807258D+13
I= 20 X= -1.722038059861D+13 Y= 1.053564686214D+13 Z= 7.734551789510D+13
I= 21 X= 2.491435294051D+12 Y= -6.433753735165D+12 Z= 1.946313014751D+13
I= 22 X= -1.433467439473D+14 Y= 4.250043362884D+13 Z= -7.173003862835D+13
I= 23 X= -6.513420614034D+13 Y= -5.040057793618D+13 Z= -6.072563170041D+13
I= 24 X= 5.406314679318D+13 Y= 9.779976302638D+12 Z= -1.850053842499D+13
I= 25 X= -2.172779857554D+12 Y= -1.724926045213D+13 Z= -1.165290669952D+13
I= 26 X= -6.166554366507D+13 Y= 3.757978233477D+13 Z= 2.091410083802D+12
I= 27 X= -5.237832424641D+13 Y= 7.778460220009D+12 Z= 4.069337019613D+13
I= 28 X= 1.148583153932D+14 Y= -8.561505697646D+13 Z= -6.711664407309D+13
I= 29 X= 1.391651683435D+13 Y= -2.218649050043D+12 Z= -4.137168594549D+12
I= 30 X= 2.366562451198D+13 Y= 5.741161033728D+12 Z= -1.231336292362D+13
I= 31 X= -8.880462687850D+11 Y= -1.087762086858D+13 Z= -9.568402342125D+13
I= 32 X= -8.115541955227D+11 Y= 1.581791379489D+13 Z= 6.536364350830D+13
I= 33 X= -2.127732217174D+13 Y= -6.783975957013D+12 Z= -1.157289899331D+13
I= 34 X= -1.632534448685D+14 Y= -2.932425706237D+13 Z= 7.599478409848D+13
I= 35 X= -3.679325385251D+12 Y= 4.871651468710D+12 Z= 2.825570525233D+11
I= 36 X= 2.635871808520D+12 Y= -1.622288082883D+13 Z= -2.879241056606D+13
I= 37 X= 1.989575322004D+13 Y= 4.060496208809D+13 Z= 5.867795955250D+13
I= 38 X= -1.425979493286D+13 Y= 5.384669384590D+13 Z= 5.060142437272D+13

Seed: 43070838607

CM Start Point Coordinates: bohr

I= 0 X= -2.276549102336D+00 Y= 2.372393744585D+00 Z= -6.243969510162D-01

I= 1 X= -2.785648719940D+00 Y= 2.036841614448D-01 Z= -1.947475281793D+00
I= 2 X= -2.116404704428D+00 Y= 1.681272851225D+00 Z= 2.092040720523D+00
I= 3 X= -2.448694381967D+00 Y= -2.067852785693D+00 Z= -1.918172806969D-01
I= 4 X= -2.059047824592D+00 Y= -1.141812016585D+00 Z= 2.322912957278D+00
I= 5 X= 3.838527239878D+00 Y= 2.677313680579D+00 Z= -1.615799745267D+00
I= 6 X= 1.885015172759D+00 Y= 2.742351285918D-01 Z= -3.128189193745D+00
I= 7 X= 5.811427709578D+00 Y= 2.273604653848D+00 Z= -3.091318913030D+00
I= 8 X= 2.796045645761D+00 Y= 4.162365516749D+00 Z= -2.707912174828D+00
I= 9 X= -2.066803663092D+00 Y= -2.620971113725D+00 Z= 4.753395639647D+00
I= 10 X= -4.171442575685D+00 Y= -3.383358123041D+00 Z= 4.905167829972D+00
I= 11 X= -5.441080792242D-01 Y= -4.275371384183D+00 Z= 4.513694016231D+00
I= 12 X= -2.172112641637D+00 Y= -1.064356549540D+00 Z= 6.528219899717D+00
I= 13 X= -1.980126261225D+00 Y= 3.710990328327D+00 Z= 4.226725972126D+00
I= 14 X= -4.071576012858D+00 Y= 3.724087798948D+00 Z= 5.082440379832D+00
I= 15 X= -6.161520644502D-01 Y= 3.086428363900D+00 Z= 5.442728398476D+00
I= 16 X= -1.637736098414D+00 Y= 5.491816194848D+00 Z= 3.339258752926D+00
I= 17 X= -1.989785517682D+00 Y= 4.969030322076D+00 Z= -1.804318860662D+00
I= 18 X= -3.860465003415D+00 Y= 5.647471816178D+00 Z= -1.709317638465D+00
I= 19 X= -7.348639559741D-01 Y= 6.426815419607D+00 Z= -1.061727451827D+00
I= 20 X= -1.244825211774D+00 Y= 4.847766715105D+00 Z= -3.564035356812D+00
I= 21 X= -3.580653297390D+00 Y= 1.091562012681D-01 Z= -4.660900855321D+00
I= 22 X= -5.888848073579D+00 Y= 2.332788852094D-01 Z= -4.556032538267D+00
I= 23 X= -2.652929686088D+00 Y= 1.414734294432D+00 Z= -5.741074715857D+00
I= 24 X= -3.177474556052D+00 Y= -1.862168601960D+00 Z= -5.411139576761D+00
I= 25 X= -2.842231743879D+00 Y= -4.789400605676D+00 Z= -8.607768843899D-01
I= 26 X= -2.124139025034D+00 Y= -5.091852341919D+00 Z= -2.674127645897D+00
I= 27 X= -1.690415478194D+00 Y= -5.706602559274D+00 Z= 7.335490695627D-01
I= 28 X= -4.823969835803D+00 Y= -5.268776289455D+00 Z= -1.031938946557D+00
I= 29 X= 3.046674765345D+00 Y= -3.890517799183D+00 Z= -1.382479740246D+00
I= 30 X= 3.838914106388D+00 Y= -3.465655057561D+00 Z= 1.050782532480D+00

I= 31 X= 1.390429836678D+00 Y= -4.740821444890D+00 Z= -2.046882668755D+00
I= 32 X= 4.206962522800D+00 Y= -3.620596539725D+00 Z= -2.956379385845D+00
I= 33 X= 5.854818845927D+00 Y= -3.019946382910D+00 Z= 1.399755446410D+00
I= 34 X= 2.832072876132D+00 Y= -4.356042904456D+00 Z= 2.917863075613D+00
I= 35 X= 1.143774540248D+00 Y= -2.600432955953D-02 Z= -2.830780210898D-01
I= 36 X= 4.096529664003D+00 Y= 2.391448287289D+00 Z= 1.131520545392D+00
I= 37 X= 5.688400270416D+00 Y= 1.859727229021D+00 Z= 1.943459808714D+00
I= 38 X= 3.194592479879D+00 Y= 3.946750364023D+00 Z= 2.136841278261D+00

Forward Direction:

Total Energy: -656.4360007 Hartrees

Potential Energy: -656.6116855 Hartress

Kinetic Energy: 0.1756848 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.817329994645D+12 Y= -1.183171366697D+13 Z= -5.325530359674D+12
I= 1 X= 6.998637530926D+12 Y= -1.099558099020D+13 Z= -3.316151223197D+12
I= 2 X= -1.195985741331D+13 Y= 7.062309746598D+12 Z= 3.834554702120D+12
I= 3 X= 1.582761110960D+13 Y= 2.570308906861D+13 Z= -4.908869334894D+12
I= 4 X= -2.191266026175D+13 Y= -1.125897547722D+13 Z= 8.890398173733D+12
I= 5 X= 3.000229906684D+12 Y= 3.179145678677D+12 Z= 4.983252370963D+12
I= 6 X= -6.774113351181D+13 Y= -9.275969883328D+13 Z= 5.571181620350D+13
I= 7 X= -3.802066351321D+13 Y= 3.873479534526D+11 Z= 7.052916538789D+13
I= 8 X= -2.893964877292D+13 Y= 3.916007473592D+13 Z= 4.256533101148D+13
I= 9 X= 5.675093929490D+12 Y= 5.762501751622D+12 Z= 1.709349579602D+13
I= 10 X= -1.996314549941D+13 Y= 1.358126559691D+13 Z= -2.398634680126D+13
I= 11 X= -6.160534485435D+13 Y= 7.146805925457D+13 Z= -3.845862276825D+13
I= 12 X= -1.181176033338D+13 Y= -3.793496156948D+13 Z= -9.186846701366D+13
I= 13 X= 5.197556585749D+12 Y= -5.641135512942D+12 Z= -6.514551454185D+12
I= 14 X= -3.868282719484D+13 Y= -8.422944236750D+13 Z= 2.640745223689D+12
I= 15 X= -8.542427757068D+13 Y= -6.653990942829D+13 Z= -7.562696287629D+12
I= 16 X= 5.560488237164D+13 Y= 1.505253880829D+14 Z= 2.199727723238D+13

I= 17 X= 1.105420792601D+13 Y= -1.091224877298D+13 Z= -9.817866464257D+12
I= 18 X= 1.890841632589D+13 Y= 8.078265443049D+13 Z= 1.057190489065D+14
I= 19 X= -1.637287628816D+14 Y= -2.648960216760D+13 Z= -4.621813004236D+13
I= 20 X= 8.213955782461D+12 Y= -2.546238826820D+13 Z= 1.749902330909D+13
I= 21 X= -6.200748852753D+12 Y= -1.641326102645D+13 Z= 5.032632863769D+11
I= 22 X= -4.563037990529D+13 Y= -8.177206937085D+13 Z= -4.969189116024D+13
I= 23 X= 5.874634406364D+13 Y= 1.437569207271D+14 Z= 2.011413148004D+13
I= 24 X= 2.838743692840D+13 Y= -4.657156161619D+13 Z= 5.049246684989D+13
I= 25 X= 4.846207367453D+12 Y= -2.214067155968D+12 Z= -1.048474079995D+13
I= 26 X= 2.540887476347D+13 Y= -2.688578240143D+13 Z= -1.334376796376D+14
I= 27 X= -3.335220414260D+13 Y= -6.124338398175D+12 Z= 7.101638364845D+13
I= 28 X= 6.329979825627D+13 Y= 2.433438168143D+13 Z= 6.408573562828D+13
I= 29 X= 1.582120498441D+13 Y= 1.038663915773D+13 Z= -4.369261584617D+12
I= 30 X= -9.776180990899D+12 Y= 1.699190000079D+13 Z= 3.240111478986D+12
I= 31 X= -5.537782710456D+13 Y= -1.261765877606D+14 Z= -5.959456064968D+12
I= 32 X= -7.764820058962D+13 Y= -4.386870852881D+13 Z= -1.418278725901D+13
I= 33 X= 4.317264835885D+13 Y= 2.301738073014D+12 Z= 5.197096102770D+13
I= 34 X= -2.615040494917D+13 Y= -4.194383895252D+13 Z= 6.788379688954D+13
I= 35 X= 3.115033746146D+12 Y= 2.613663258394D+12 Z= -1.217503402828D+12
I= 36 X= -3.925544869766D+12 Y= -2.764750901041D+12 Z= 1.729810886130D+12
I= 37 X= -9.093343057128D+12 Y= 1.230298743672D+13 Z= 3.575346010521D+13
I= 38 X= -5.265865724226D+13 Y= -6.363287326455D+13 Z= -8.916980899945D+13

Backward Direction:

Total Energy: -656.4359995 Hartrees

Potential Energy: -656.6116855 Hartress

Kinetic Energy: 0.1756860 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.252127302037D+12 Y= -1.256978641764D+13 Z= -5.036702915216D+12

I= 1 X= 6.126881626413D+12 Y= -1.289353173684D+13 Z= -4.455496363169D+12

I= 2 X= -1.277122749456D+13 Y= 7.808138407393D+12 Z= 2.633738990116D+12

I= 3 X= 1.416515574060D+13 Y= 2.574196199896D+13 Z= -7.317596266060D+12
I= 4 X= -1.906921470345D+13 Y= -1.151266250010D+13 Z= 7.000882873776D+12
I= 5 X= -1.692601088719D+12 Y= -3.494572995134D+12 Z= -8.340927731773D+12
I= 6 X= 3.737749536913D+13 Y= 2.724583847623D+13 Z= 1.030083342994D+14
I= 7 X= -1.882074264745D+13 Y= 1.856558890542D+13 Z= 7.170381233604D+13
I= 8 X= -4.690941091922D+12 Y= 5.876076858758D+13 Z= 4.482125560325D+13
I= 9 X= 6.578824149650D+12 Y= 6.186910448911D+12 Z= 1.607198323224D+13
I= 10 X= -1.979786048105D+13 Y= 1.568164776512D+13 Z= -2.642112504323D+13
I= 11 X= -6.186636003778D+13 Y= 7.144509876842D+13 Z= -3.850937834386D+13
I= 12 X= -1.128211092411D+13 Y= -3.779310129631D+13 Z= -9.237142301253D+13
I= 13 X= 5.376707916158D+12 Y= -5.728303694658D+12 Z= -6.891610087704D+12
I= 14 X= -3.837825720455D+13 Y= -8.476645412296D+13 Z= 2.720455686346D+12
I= 15 X= -8.486417153711D+13 Y= -6.705362343267D+13 Z= -8.490190747241D+12
I= 16 X= 5.556586555936D+13 Y= 1.506904962374D+14 Z= 2.212785933045D+13
I= 17 X= 1.132855798622D+13 Y= -1.151769853390D+13 Z= -9.877823591434D+12
I= 18 X= 1.896626164921D+13 Y= 7.981740689085D+13 Z= 1.049272174059D+14
I= 19 X= -1.643087333877D+14 Y= -2.668280464952D+13 Z= -4.562008993725D+13
I= 20 X= 8.616704612177D+12 Y= -2.600337844551D+13 Z= 1.742993800722D+13
I= 21 X= -6.545968507870D+12 Y= -1.663013572439D+13 Z= -3.394704852352D+11
I= 22 X= -4.569207345892D+13 Y= -8.080015860652D+13 Z= -5.306926336594D+13
I= 23 X= 6.000118094144D+13 Y= 1.432107036846D+14 Z= 1.972250880762D+13
I= 24 X= 2.778249941183D+13 Y= -4.691131947491D+13 Z= 4.949603015126D+13
I= 25 X= 4.471022882133D+12 Y= -2.593081946464D+12 Z= -1.067834627383D+13
I= 26 X= 2.448087909162D+13 Y= -2.790093796080D+13 Z= -1.335509074022D+14
I= 27 X= -3.257878970036D+13 Y= -5.473186238505D+12 Z= 7.079192361539D+13
I= 28 X= 6.333812299387D+13 Y= 2.318567564635D+13 Z= 6.489883837995D+13
I= 29 X= 1.408368000129D+13 Y= 1.087469638813D+13 Z= -4.978674506279D+12
I= 30 X= -9.673859707365D+12 Y= 1.665564504713D+13 Z= 2.485398061036D+12
I= 31 X= -5.657909844254D+13 Y= -1.265319778217D+14 Z= -5.921920580553D+12
I= 32 X= -8.116379876774D+13 Y= -4.094921797051D+13 Z= -1.627586781717D+13

I= 33 X= 4.328107002693D+13 Y= 1.876797007995D+12 Z= 5.136982904032D+13
I= 34 X= -2.501774097463D+13 Y= -4.273242917788D+13 Z= 6.766701450026D+13
I= 35 X= 3.096131413695D+12 Y= 3.055163223953D+12 Z= 1.583541889949D+12
I= 36 X= -1.003418737404D+13 Y= -1.048046972727D+13 Z= -1.085849858609D+12
I= 37 X= -3.643868554958D+12 Y= 1.506949312931D+13 Z= 2.895709328744D+13
I= 38 X= -4.967431359317D+13 Y= -6.394384732532D+13 Z= -9.424550161636D+13

Seed: 4485029639

CM Start Point Coordinates: bohr

I= 0 X= -2.288734466288D+00 Y= 2.423259145152D+00 Z= -6.356435769751D-01
I= 1 X= -2.888682588286D+00 Y= 1.395592191014D-01 Z= -1.992088047318D+00
I= 2 X= -1.863863985812D+00 Y= 1.630101007172D+00 Z= 2.072432638692D+00
I= 3 X= -2.696858004736D+00 Y= -1.870475079169D+00 Z= -1.703861726996D-01
I= 4 X= -2.211309021477D+00 Y= -1.025648151340D+00 Z= 2.311149119803D+00
I= 5 X= 4.131946774134D+00 Y= 2.554454240661D+00 Z= -1.793932110158D+00
I= 6 X= 2.808652934472D+00 Y= -2.529385912613D-01 Z= -3.073969999746D+00
I= 7 X= 5.790193377702D+00 Y= 1.769452081498D+00 Z= -2.633477543177D+00
I= 8 X= 3.167474512759D+00 Y= 3.497421893404D+00 Z= -3.227399881870D+00
I= 9 X= -2.158198831774D+00 Y= -2.693240741407D+00 Z= 4.434256673407D+00
I= 10 X= -3.862682474715D+00 Y= -2.506754440894D+00 Z= 5.295701487630D+00
I= 11 X= -1.168153320897D+00 Y= -4.227948001965D+00 Z= 4.129950353012D+00
I= 12 X= -1.121176660465D+00 Y= -1.671947918818D+00 Z= 6.011412687187D+00
I= 13 X= -1.561106332234D+00 Y= 3.477423261591D+00 Z= 4.207854011134D+00
I= 14 X= -3.499653332516D+00 Y= 4.446803172488D+00 Z= 5.111236710830D+00
I= 15 X= -3.183983166726D-01 Y= 2.814720676406D+00 Z= 5.754557422976D+00
I= 16 X= -2.334954011264D-01 Y= 5.132496054543D+00 Z= 4.091040338995D+00
I= 17 X= -2.257894418313D+00 Y= 5.156865769099D+00 Z= -1.179056763441D+00
I= 18 X= -3.940141617242D+00 Y= 5.932377337105D+00 Z= -2.038816939011D-01
I= 19 X= -7.548705493279D-01 Y= 6.279275785776D+00 Z= -3.628750314145D-01
I= 20 X= -2.630938100177D+00 Y= 5.588599401806D+00 Z= -3.389897594081D+00

I= 21 X= -3.310143892387D+00 Y= 1.762979430046D-02 Z= -4.835407851856D+00
I= 22 X= -5.134346741364D+00 Y= 9.923693580096D-02 Z= -5.289650025534D+00
I= 23 X= -2.079007481865D+00 Y= 1.554494863741D+00 Z= -5.977682154904D+00
I= 24 X= -2.598589178466D+00 Y= -1.764864944875D+00 Z= -5.480824113718D+00
I= 25 X= -2.656194031553D+00 Y= -4.732232025474D+00 Z= -8.317387868788D-01
I= 26 X= -2.398702019373D+00 Y= -4.852501973396D+00 Z= -2.842925378307D+00
I= 27 X= -1.326543992283D+00 Y= -5.538311886226D+00 Z= 6.823096526271D-01
I= 28 X= -4.451025873750D+00 Y= -5.317616765013D+00 Z= -6.004374946303D-01
I= 29 X= 3.248255144963D+00 Y= -3.716759248299D+00 Z= -1.060952373275D+00
I= 30 X= 3.425773250779D+00 Y= -3.272165748313D+00 Z= 1.421571590188D+00
I= 31 X= 1.839968883017D+00 Y= -5.109118105172D+00 Z= -1.769263372472D+00
I= 32 X= 4.842148065798D+00 Y= -3.327583573515D+00 Z= -2.547419350501D+00
I= 33 X= 4.949580004642D+00 Y= -1.844420877045D+00 Z= 2.177500909957D+00
I= 34 X= 2.423512777497D+00 Y= -4.614235642026D+00 Z= 2.632586439982D+00
I= 35 X= 1.098709147816D+00 Y= -1.487909730155D-01 Z= -3.256829875926D-01
I= 36 X= 3.834246222887D+00 Y= 2.926509207065D+00 Z= 7.083804011829D-01
I= 37 X= 4.977688636754D+00 Y= 2.277976606670D+00 Z= 1.891233687708D+00
I= 38 X= 2.704986776013D+00 Y= 4.739039242745D+00 Z= 1.246540891824D+00

Forward Direction:

Total Energy: -656.4356851 Hartrees

Potential Energy: -656.6119570 Hartress

Kinetic Energy: 0.1762719 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.638540256853D+12 Y= 1.499988785926D+13 Z= -4.632700802375D+12
I= 1 X= -4.209230672263D+12 Y= 1.459130455150D+13 Z= -9.372081494502D+12
I= 2 X= 1.318536617419D+12 Y= -1.699260217725D+13 Z= -6.612459031636D+12
I= 3 X= 1.934148370611D+13 Y= -2.112968647479D+13 Z= -3.622256582238D+12
I= 4 X= -1.200682378214D+13 Y= -3.357797055477D+12 Z= 5.226886574749D+12
I= 5 X= -7.223384088410D+12 Y= -9.866669701562D+12 Z= 3.338415810361D+12
I= 6 X= -3.553883661872D+12 Y= -1.134956348292D+13 Z= -8.116859779849D+13

I= 7 X= 4.922015007428D+13 Y= -9.140630942123D+12 Z= -8.131137071905D+13
I= 8 X= 5.207451620760D+13 Y= 8.432398297782D+12 Z= -4.863703349654D+13
I= 9 X= -1.768727285009D+13 Y= 4.471371618369D+12 Z= 4.571345252683D+12
I= 10 X= 1.548622053545D+14 Y= 1.521528866901D+13 Z= -7.011615845175D+13
I= 11 X= 2.755886789198D+13 Y= 4.983197313447D+12 Z= -6.575198635998D+13
I= 12 X= 3.704590764623D+13 Y= 2.449633073385D+13 Z= 2.662581651913D+13
I= 13 X= 5.375502077274D+12 Y= -1.969138417989D+13 Z= -9.802238358499D+11
I= 14 X= -2.002577187847D+13 Y= 1.328203394104D+13 Z= 8.677354966320D+12
I= 15 X= -7.209833212018D+13 Y= 2.373512980883D+13 Z= -7.339970835878D+12
I= 16 X= 1.475397840887D+12 Y= 4.881449080154D+13 Z= -8.485215298570D+13
I= 17 X= 4.801878981821D+12 Y= -8.935458396892D+12 Z= 3.569342411067D+12
I= 18 X= -9.705712944279D+13 Y= 1.390874470240D+14 Z= 1.653200847643D+13
I= 19 X= 3.984845660055D+13 Y= -1.618705894646D+13 Z= 2.033954755807D+13
I= 20 X= -6.630343059691D+13 Y= -8.050556039026D+13 Z= 5.546433689013D+13
I= 21 X= 2.109186524058D+13 Y= 1.699818849313D+13 Z= 1.244961604449D+13
I= 22 X= 5.555215412273D+13 Y= -4.465240308077D+13 Z= -5.559213324760D+13
I= 23 X= -6.470581597902D+13 Y= -1.030797027468D+14 Z= 5.611351632400D+13
I= 24 X= -5.600283798299D+13 Y= 1.752864027470D+13 Z= 8.064548354748D+12
I= 25 X= -1.173720167382D+13 Y= 1.461634870779D+13 Z= 8.101036091262D+12
I= 26 X= 1.052662874281D+13 Y= 5.866617498096D+13 Z= 9.234225624804D+13
I= 27 X= 2.934633896022D+13 Y= -2.449535924506D+13 Z= -6.376580534982D+13
I= 28 X= -2.016570278784D+13 Y= -3.937286084231D+12 Z= 3.902761977848D+13
I= 29 X= 1.010781540615D+13 Y= 7.822688592731D+12 Z= 6.222231241879D+12
I= 30 X= 3.193168497000D+11 Y= 1.311760482991D+12 Z= -6.082463223378D+12
I= 31 X= 1.033757613058D+14 Y= -4.354723421641D+13 Z= -1.273362840364D+13
I= 32 X= 6.592757050749D+13 Y= -3.992283156566D+13 Z= -7.582112685108D+13
I= 33 X= -1.020800962180D+14 Y= -9.821572537460D+13 Z= -9.508103074660D+13
I= 34 X= 9.866017374115D+13 Y= 3.813701470790D+12 Z= 3.840105517830D+13
I= 35 X= -3.905696201873D+12 Y= -6.884493783490D+11 Z= 8.621341847752D+11
I= 36 X= 7.852503755820D+12 Y= 2.694327092828D+13 Z= 1.135683174859D+13

I= 37 X= 4.793368768518D+13 Y= -1.185515414281D+14 Z= -2.326382718094D+12

I= 38 X= -9.865414603357D+13 Y= 4.647945878048D+13 Z= 1.467080930464D+13

Backward Direction:

Total Energy: -656.4356938 Hartrees

Potential Energy: -656.6119570 Hartress

Kinetic Energy: 0.1762632 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.371026967010D+12 Y= 1.465055429551D+13 Z= -4.495997312637D+12

I= 1 X= -4.621837147675D+12 Y= 1.369299486981D+13 Z= -9.911339308775D+12

I= 2 X= 9.345110575709D+11 Y= -1.663959770277D+13 Z= -7.180811178159D+12

I= 3 X= 1.855463517871D+13 Y= -2.111128771958D+13 Z= -4.762319214139D+12

I= 4 X= -1.066100662753D+13 Y= -3.477868405029D+12 Z= 4.332569432581D+12

I= 5 X= -9.444524719203D+12 Y= -1.302537448319D+13 Z= -2.967985979968D+12

I= 6 X= 4.619929471924D+13 Y= 4.544966390788D+13 Z= -5.878291671861D+13

I= 7 X= 5.830756966772D+13 Y= -5.367776133767D+11 Z= -8.075540438366D+13

I= 8 X= 6.355155212434D+13 Y= 1.770950577103D+13 Z= -4.756929298632D+13

I= 9 X= -1.725953277073D+13 Y= 4.672246400108D+12 Z= 4.087858193873D+12

I= 10 X= 1.549404355867D+14 Y= 1.620941015975D+13 Z= -7.126855130123D+13

I= 11 X= 2.743532808655D+13 Y= 4.972329997335D+12 Z= -6.577600923621D+13

I= 12 X= 3.729659338696D+13 Y= 2.456347391401D+13 Z= 2.638776490209D+13

I= 13 X= 5.460295308072D+12 Y= -1.973264132250D+13 Z= -1.158687592818D+12

I= 14 X= -1.988161736146D+13 Y= 1.302786356194D+13 Z= 8.715082336082D+12

I= 15 X= -7.183323109829D+13 Y= 2.349198637615D+13 Z= -7.778958654239D+12

I= 16 X= 1.456930983014D+12 Y= 4.889263732452D+13 Z= -8.479034782173D+13

I= 17 X= 4.931730253157D+12 Y= -9.222020829316D+12 Z= 3.540964396531D+12

I= 18 X= -9.702975095789D+13 Y= 1.386305904892D+14 Z= 1.615723062384D+13

I= 19 X= 3.957395363893D+13 Y= -1.627850265500D+13 Z= 2.062260296465D+13

I= 20 X= -6.611280753304D+13 Y= -8.076161377980D+13 Z= 5.543163847654D+13

I= 21 X= 2.092847103004D+13 Y= 1.689554060092D+13 Z= 1.205074589193D+13

I= 22 X= 5.552295424947D+13 Y= -4.419239280232D+13 Z= -5.719066058489D+13

I= 23 X= -6.411189534624D+13 Y= -1.033382300322D+14 Z= 5.592815933660D+13
I= 24 X= -5.628915797178D+13 Y= 1.736783116349D+13 Z= 7.592929826250D+12
I= 25 X= -1.191477839117D+13 Y= 1.443695909160D+13 Z= 8.009401641670D+12
I= 26 X= 1.008740370924D+13 Y= 5.818569672224D+13 Z= 9.228866497272D+13
I= 27 X= 2.971239993071D+13 Y= -2.418716562768D+13 Z= -6.387204341852D+13
I= 28 X= -2.014756349308D+13 Y= -4.480974467183D+12 Z= 3.941246542378D+13
I= 29 X= 9.285436051480D+12 Y= 8.053688547806D+12 Z= 5.933793025316D+12
I= 30 X= 3.677460317581D+11 Y= 1.152609314066D+12 Z= -6.439672899218D+12
I= 31 X= 1.028071935119D+14 Y= -4.371544212574D+13 Z= -1.271586266945D+13
I= 32 X= 6.426362011958D+13 Y= -3.854102192445D+13 Z= -7.681179245783D+13
I= 33 X= -1.020287796930D+14 Y= -9.841685212536D+13 Z= -9.536554955306D+13
I= 34 X= 9.919626932620D+13 Y= 3.440457729001D+12 Z= 3.829845097923D+13
I= 35 X= -3.914642771623D+12 Y= -4.794852129293D+11 Z= 2.187883080207D+12
I= 36 X= 4.961252381375D+12 Y= 2.329138220837D+13 Z= 1.002416528657D+13
I= 37 X= 5.051295151117D+13 Y= -1.172421403020D+14 Z= -5.543137488316D+12
I= 38 X= -9.724164110171D+13 Y= 4.633227318623D+13 Z= 1.226845833034D+13

Seed: 53753451982

CM Start Point Coordinates: bohr

I= 0 X= -2.382179422291D+00 Y= 2.372437424338D+00 Z= -3.773330720838D-01
I= 1 X= -2.857708950415D+00 Y= 1.614338852718D-01 Z= -1.874466606284D+00
I= 2 X= -2.046246178684D+00 Y= 1.549758473919D+00 Z= 2.292799235050D+00
I= 3 X= -2.705511024052D+00 Y= -1.998643185646D+00 Z= -1.396486802027D-01
I= 4 X= -2.351136320108D+00 Y= -1.135582703117D+00 Z= 2.377151394918D+00
I= 5 X= 4.631128177446D+00 Y= 2.149426598276D+00 Z= -1.712714875373D+00
I= 6 X= 2.216820000919D+00 Y= 4.225288969548D-01 Z= -3.329512877571D+00
I= 7 X= 6.062926512113D+00 Y= 6.233614275815D-01 Z= -2.119809358572D+00
I= 8 X= 4.736138999229D+00 Y= 3.739225391119D+00 Z= -3.063776983671D+00
I= 9 X= -2.233165702556D+00 Y= -2.681302038433D+00 Z= 4.707266020715D+00
I= 10 X= -3.962072140935D+00 Y= -2.484408758858D+00 Z= 5.541841634702D+00

I= 11 X= -1.984780960225D+00 Y= -4.564200105146D+00 Z= 3.787994312262D+00
I= 12 X= -8.962022786328D-01 Y= -2.107482934647D+00 Z= 6.094541878450D+00
I= 13 X= -1.655892152941D+00 Y= 3.394037006003D+00 Z= 4.295419747082D+00
I= 14 X= -3.601027283950D+00 Y= 3.749941423058D+00 Z= 4.831409497964D+00
I= 15 X= -4.939547286148D-01 Y= 2.710753167325D+00 Z= 6.133513496848D+00
I= 16 X= -5.034723462535D-01 Y= 5.032693519543D+00 Z= 3.781363035878D+00
I= 17 X= -2.862657416550D+00 Y= 4.980474452172D+00 Z= -1.629517608481D+00
I= 18 X= -4.993906675261D+00 Y= 5.062761758593D+00 Z= -2.520142492962D+00
I= 19 X= -2.274506668506D+00 Y= 6.483414997070D+00 Z= -2.849935262326D-01
I= 20 X= -1.021205778881D+00 Y= 4.885727947647D+00 Z= -3.494286509017D+00
I= 21 X= -3.144466186795D+00 Y= -9.226308983080D-03 Z= -4.668505304886D+00
I= 22 X= -5.088113029447D+00 Y= 2.550086568535D-01 Z= -5.249091508396D+00
I= 23 X= -2.472370419828D+00 Y= 1.498670632856D+00 Z= -5.459189312323D+00
I= 24 X= -2.515553835188D+00 Y= -1.833308169300D+00 Z= -5.409537318919D+00
I= 25 X= -3.243531941432D+00 Y= -4.741789705380D+00 Z= -9.425974618839D-01
I= 26 X= -2.592748009378D+00 Y= -5.037561978910D+00 Z= -2.849552090159D+00
I= 27 X= -2.024776104436D+00 Y= -6.092244563771D+00 Z= 3.052004296702D-01
I= 28 X= -5.140885138463D+00 Y= -4.729008327826D+00 Z= -6.573197662410D-01
I= 29 X= 3.110219024747D+00 Y= -3.614907457699D+00 Z= -1.203305411968D+00
I= 30 X= 3.760285745779D+00 Y= -2.986740815607D+00 Z= 1.290684257814D+00
I= 31 X= 1.658298547793D+00 Y= -5.174016020729D+00 Z= -1.472235261339D+00
I= 32 X= 4.338864032435D+00 Y= -2.947093154428D+00 Z= -2.592921613189D+00
I= 33 X= 5.695718309348D+00 Y= -1.824999051547D+00 Z= 1.406488615198D+00
I= 34 X= 3.139675181712D+00 Y= -3.907231966075D+00 Z= 3.136948784471D+00
I= 35 X= 1.166760580305D+00 Y= -1.887326859004D-02 Z= -3.839088644211D-01
I= 36 X= 4.216366108029D+00 Y= 2.695535325729D+00 Z= 8.282603664435D-01
I= 37 X= 5.421548945036D+00 Y= 1.969889371171D+00 Z= 2.661533628158D+00
I= 38 X= 3.426724521544D+00 Y= 4.588286801458D+00 Z= 1.401158616646D+00

Forward Direction:

Total Energy: -656.4407729 Hartrees

Potential Energy: -656.6278933 Hartress

Kinetic Energy: 0.1871203 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.495567745255D+12 Y= -1.067660137809D+12 Z= -2.707464953544D+11
I= 1 X= 8.628316289070D+12 Y= -1.110272952861D+13 Z= -8.989670117719D+12
I= 2 X= -1.721459809817D+12 Y= 1.139055440115D+13 Z= -2.250436341855D+12
I= 3 X= 9.426791983860D+12 Y= -1.194457479423D+13 Z= 9.302129486957D+11
I= 4 X= -1.440107508367D+13 Y= 2.774730628718D+13 Z= -3.603749900421D+13
I= 5 X= -4.227791384354D+12 Y= 1.920990296910D+13 Z= 4.392842626952D+12
I= 6 X= -4.239796269854D+13 Y= -4.125530593843D+13 Z= 5.134254130808D+13
I= 7 X= 2.361965066755D+13 Y= 2.948812316585D+13 Z= 9.169993825118D+13
I= 8 X= 2.361858232088D+13 Y= -8.218536229451D+13 Z= 5.270042972362D+13
I= 9 X= 1.369490671118D+13 Y= 7.373128621989D+12 Z= -1.488035350689D+12
I= 10 X= 9.995485834283D+13 Y= 8.889997715084D+13 Z= -5.617452020371D+13
I= 11 X= 2.999012307116D+13 Y= -1.173541367638D+14 Z= -3.773147256990D+13
I= 12 X= -2.701290698491D+13 Y= -1.718917755991D+13 Z= 1.246773768623D+13
I= 13 X= 4.992850421198D+11 Y= -1.364226864321D+13 Z= -4.822064089715D+12
I= 14 X= 5.281605409011D+13 Y= -1.735401354711D+13 Z= 3.822082350583D+13
I= 15 X= -9.967246457117D+13 Y= 9.284196182595D+13 Z= -4.460110411407D+13
I= 16 X= 2.244256210081D+13 Y= -3.756964158645D+13 Z= 1.513558544231D+13
I= 17 X= -1.933279759197D+13 Y= 1.433512774138D+13 Z= 5.077437575856D+12
I= 18 X= -4.146526658480D+13 Y= -3.167418376806D+13 Z= 1.742261917395D+13
I= 19 X= 1.161311106789D+14 Y= 6.240328205318D+13 Z= 4.788803107919D+13
I= 20 X= 1.262862563454D+13 Y= -7.812259573013D+13 Z= -7.630766453565D+13
I= 21 X= -1.284573211794D+12 Y= -5.910065514138D+12 Z= -8.393190957368D+11
I= 22 X= -6.842370245715D+13 Y= -8.656573418497D+13 Z= -1.074137707758D+13
I= 23 X= 5.379387167936D+13 Y= -2.069609837163D+13 Z= 9.676581945477D+13
I= 24 X= -6.579201452345D+13 Y= 5.285382593505D+13 Z= 1.656295448752D+13
I= 25 X= -1.206526856630D+13 Y= 2.226636713512D+13 Z= 1.103133775274D+13
I= 26 X= 1.809736034253D+13 Y= 9.908126842072D+12 Z= 3.651413988364D+13

I= 27 X= 3.737500539580D+13 Y= -6.349701608148D+13 Z= 3.929335850422D+12
I= 28 X= -1.075370937973D+14 Y= 3.103595805963D+13 Z= 3.272232680388D+13
I= 29 X= 3.610536461656D+11 Y= -3.057600742446D+12 Z= 7.270038841841D+12
I= 30 X= -1.190618483255D+13 Y= 7.055573752406D+11 Z= 1.094870666202D+13
I= 31 X= 8.785288282950D+13 Y= 8.051128701567D+13 Z= -2.525876309737D+13
I= 32 X= -1.191442145893D+14 Y= -9.539298449463D+13 Z= 2.412495262316D+13
I= 33 X= 8.636854675916D+13 Y= 7.333403382406D+12 Z= 5.376686786414D+13
I= 34 X= 8.089576383717D+13 Y= 1.759398238624D+13 Z= 3.261307833425D+12
I= 35 X= 1.279418148203D+12 Y= -3.220876280156D+12 Z= -1.026053208307D+12
I= 36 X= 1.235156223161D+13 Y= -3.020023734274D+13 Z= -3.418405526312D+12
I= 37 X= 3.909601308655D+13 Y= 1.023267073306D+14 Z= -3.428351082439D+13
I= 38 X= -4.057112961117D+13 Y= 1.317281636119D+14 Z= 1.520573386088D+13

Backward Direction:

Total Energy: -656.4407905 Hartrees

Potential Energy: -656.6278933 Hartress

Kinetic Energy: 0.1871028 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.693638599562D+12 Y= -1.326311951782D+12 Z= -1.695291798049D+11
I= 1 X= 8.322816262249D+12 Y= -1.176785149801D+13 Z= -9.388944696704D+12
I= 2 X= -2.005798098794D+12 Y= 1.165192421093D+13 Z= -2.671252801566D+12
I= 3 X= 8.844197524396D+12 Y= -1.193095208081D+13 Z= 8.609346719769D+10
I= 4 X= -1.340461186509D+13 Y= 2.765840365742D+13 Z= -3.669966483858D+13
I= 5 X= -5.872357241152D+12 Y= 1.687115054439D+13 Z= -2.765119024647D+11
I= 6 X= -5.559962751286D+12 Y= 7.996944395569D+11 Z= 6.791723553432D+13
I= 7 X= 3.034811251326D+13 Y= 3.585854529401D+13 Z= 9.211158406493D+13
I= 8 X= 3.211635195792D+13 Y= -7.531645269694D+13 Z= 5.349100081773D+13
I= 9 X= 1.401161189031D+13 Y= 7.521859324681D+12 Z= -1.846016425116D+12
I= 10 X= 1.000127811804D+14 Y= 8.963603962259D+13 Z= -5.702776917054D+13
I= 11 X= 2.989865235493D+13 Y= -1.173621830826D+14 Z= -3.774925945847D+13
I= 12 X= -2.682729550074D+13 Y= -1.713946373277D+13 Z= 1.229148070038D+13

I= 13 X= 5.620672190450D+11 Y= -1.367281604938D+13 Z= -4.954201335246D+12
I= 14 X= 5.292278825046D+13 Y= -1.754220511692D+13 Z= 3.824875741738D+13
I= 15 X= -9.947617979688D+13 Y= 9.266193478281D+13 Z= -4.492613728521D+13
I= 16 X= 2.242888894925D+13 Y= -3.751178072135D+13 Z= 1.518134691731D+13
I= 17 X= -1.923665376055D+13 Y= 1.412295261643D+13 Z= 5.056426071415D+12
I= 18 X= -4.144499514299D+13 Y= -3.201244720405D+13 Z= 1.714512802851D+13
I= 19 X= 1.159278645571D+14 Y= 6.233557575242D+13 Z= 4.809760954650D+13
I= 20 X= 1.276976581838D+13 Y= -7.831218150070D+13 Z= -7.633187494579D+13
I= 21 X= -1.405552737495D+12 Y= -5.986067550842D+12 Z= -1.134648543449D+12
I= 22 X= -6.844532248229D+13 Y= -8.622513566702D+13 Z= -1.192495070571D+13
I= 23 X= 5.423361943030D+13 Y= -2.088751585231D+13 Z= 9.662857835812D+13
I= 24 X= -6.600401014184D+13 Y= 5.273476045671D+13 Z= 1.621376105298D+13
I= 25 X= -1.219674902982D+13 Y= 2.213354437029D+13 Z= 1.096349023169D+13
I= 26 X= 1.777215152689D+13 Y= 9.552373529372D+12 Z= 3.647446009998D+13
I= 27 X= 3.764604242231D+13 Y= -6.326882490995D+13 Z= 3.850675587854D+12
I= 28 X= -1.075236631973D+14 Y= 3.063340303000D+13 Z= 3.300727229933D+13
I= 29 X= -2.478483719206D+11 Y= -2.886564907794D+12 Z= 7.056474857322D+12
I= 30 X= -1.187032714256D+13 Y= 5.877194614756D+11 Z= 1.068422325805D+13
I= 31 X= 8.743190670053D+13 Y= 8.038674335545D+13 Z= -2.524560907996D+13
I= 32 X= -1.203762284254D+14 Y= -9.436987189743D+13 Z= 2.339144894351D+13
I= 33 X= 8.640654228188D+13 Y= 7.184486115123D+12 Z= 5.355620587368D+13
I= 34 X= 8.129269705279D+13 Y= 1.731762711775D+13 Z= 3.185338145066D+12
I= 35 X= 1.272793974172D+12 Y= -3.066156076462D+12 Z= -4.444882990330D+10
I= 36 X= 1.021083632440D+13 Y= -3.290415055695D+13 Z= -4.405131774989D+12
I= 37 X= 4.100573873517D+13 Y= 1.032962075718D+14 Z= -3.666524433545D+13
I= 38 X= -3.952528976259D+13 Y= 1.316191851895D+14 Z= 1.342699714280D+13

Seed: 5613632441

CM Start Point Coordinates: bohr

I= 0 X= -2.105176107363D+00 Y= 2.394915104702D+00 Z= -5.586884719969D-01

I= 1 X= -2.881145852386D+00 Y= 8.593460517055D-02 Z= -1.954207166320D+00
I= 2 X= -1.768342124132D+00 Y= 1.660305472174D+00 Z= 2.157897967596D+00
I= 3 X= -2.778149431091D+00 Y= -1.947760814019D+00 Z= -3.003993011241D-01
I= 4 X= -2.173548735651D+00 Y= -9.019331570021D-01 Z= 2.226227176046D+00
I= 5 X= 4.240274762411D+00 Y= 2.176231466227D+00 Z= -1.506326000843D+00
I= 6 X= 2.180766151166D+00 Y= 2.241713622343D-01 Z= -3.014866765314D+00
I= 7 X= 6.089919691188D+00 Y= 1.220963169611D+00 Z= -2.020017628163D+00
I= 8 X= 3.950701697937D+00 Y= 3.165470175509D+00 Z= -3.279718147707D+00
I= 9 X= -1.941032403819D+00 Y= -2.826040921527D+00 Z= 4.479405578515D+00
I= 10 X= -4.035745611061D+00 Y= -3.686612796365D+00 Z= 5.251493610576D+00
I= 11 X= -1.130254007840D+00 Y= -4.632424500366D+00 Z= 4.006990298739D+00
I= 12 X= -5.260241269300D-01 Y= -2.011336881783D+00 Z= 5.860600978127D+00
I= 13 X= -1.725751993189D+00 Y= 3.409000657302D+00 Z= 4.268281737743D+00
I= 14 X= -3.825879467135D+00 Y= 2.908926846920D+00 Z= 5.285429846389D+00
I= 15 X= -2.899143762405D-02 Y= 2.959877501572D+00 Z= 5.737413923287D+00
I= 16 X= -1.761156783762D+00 Y= 5.625841740348D+00 Z= 3.400563960918D+00
I= 17 X= -2.177479147850D+00 Y= 4.949408311057D+00 Z= -1.811963041391D+00
I= 18 X= -4.068826278248D+00 Y= 5.858582400180D+00 Z= -2.041987119400D+00
I= 19 X= -7.664722420078D-01 Y= 6.312078010335D+00 Z= -4.199850983546D-01
I= 20 X= -1.326958861809D+00 Y= 4.926436316744D+00 Z= -3.685358837259D+00
I= 21 X= -3.622735159126D+00 Y= -1.847366624533D-02 Z= -4.681226905055D+00
I= 22 X= -5.900378919121D+00 Y= 1.983250876131D-01 Z= -4.698144335343D+00
I= 23 X= -3.061244630992D+00 Y= 1.884231924775D+00 Z= -5.717481674039D+00
I= 24 X= -3.042721508209D+00 Y= -1.416250790999D+00 Z= -6.065888946367D+00
I= 25 X= -3.535508657143D+00 Y= -4.619159929415D+00 Z= -9.358218023643D-01
I= 26 X= -3.779368999632D+00 Y= -4.922685485327D+00 Z= -3.185289794385D+00
I= 27 X= -2.612862084903D+00 Y= -6.152411268053D+00 Z= 6.088918978787D-02
I= 28 X= -5.666651929698D+00 Y= -4.607590294128D+00 Z= 1.001960535008D-01
I= 29 X= 3.438943781833D+00 Y= -3.686510520641D+00 Z= -1.198877237187D+00
I= 30 X= 4.079179336091D+00 Y= -2.671794052967D+00 Z= 1.205213774353D+00

I= 31 X= 2.024454113428D+00 Y= -5.240255224580D+00 Z= -8.131772844278D-01
I= 32 X= 4.329904987731D+00 Y= -3.310427706231D+00 Z= -2.973451844336D+00
I= 33 X= 6.023013196240D+00 Y= -1.155362241992D+00 Z= 1.291154990075D+00
I= 34 X= 3.354197346135D+00 Y= -3.640327868228D+00 Z= 2.724800003906D+00
I= 35 X= 1.142587836065D+00 Y= -1.178661353930D-01 Z= -2.818350662782D-01
I= 36 X= 3.695032468663D+00 Y= 2.896802032878D+00 Z= 1.043547979509D+00
I= 37 X= 4.697283945544D+00 Y= 2.184273496649D+00 Z= 2.714172016022D+00
I= 38 X= 2.421359053755D+00 Y= 4.614170547194D+00 Z= 1.288583136300D+00

Forward Direction:

Total Energy: -656.4362225 Hartrees

Potential Energy: -656.6041947 Hartress

Kinetic Energy: 0.1679722 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.746727084378D+12 Y= -1.728163987339D+13 Z= -2.467148525038D+13
I= 1 X= 3.577815889953D+12 Y= -1.384203948408D+13 Z= 1.199350736508D+13
I= 2 X= 1.052311537708D+13 Y= -3.049876795627D+13 Z= 3.893051862863D+12
I= 3 X= -9.930378245704D+12 Y= 3.833091347996D+12 Z= 1.395982274813D+13
I= 4 X= 2.153980404257D+13 Y= 2.313718468229D+13 Z= -9.096438433342D+12
I= 5 X= -2.241664101551D+12 Y= -5.885613580373D+11 Z= 2.452451605109D+13
I= 6 X= -3.093830205935D+13 Y= 3.366575506576D+13 Z= -8.889224050108D+13
I= 7 X= 3.625769694800D+13 Y= -6.902977773023D+13 Z= 4.452836209622D+13
I= 8 X= -8.127525639293D+13 Y= 2.030655988733D+13 Z= -6.964469282855D+13
I= 9 X= 9.892739729780D+12 Y= 4.207148821687D+12 Z= -1.842492161860D+13
I= 10 X= -8.904984309880D+13 Y= -7.001389636627D+13 Z= 9.866661745217D+12
I= 11 X= -9.913577281242D+13 Y= 4.084179090379D+13 Z= 5.661977403790D+13
I= 12 X= -2.181953862584D+13 Y= 5.589562688507D+13 Z= 4.413004400244D+13
I= 13 X= -1.055520816190D+13 Y= -1.060899821861D+12 Z= 4.699347005925D+12
I= 14 X= 3.781180196930D+13 Y= 3.274799940377D+13 Z= 3.696843857829D+13
I= 15 X= -3.293578608781D+13 Y= 2.868804180273D+13 Z= 2.237278622137D+13
I= 16 X= 1.162411736209D+14 Y= 4.387851680711D+13 Z= -6.928559801724D+13

I= 17 X= 1.268703531280D+13 Y= -5.914018715197D+12 Z= 1.748603560685D+13
I= 18 X= 5.536999893912D+12 Y= 2.699546049459D+13 Z= 1.401514246656D+13
I= 19 X= -1.522547675163D+13 Y= 1.982615398892D+12 Z= -6.863780364441D+13
I= 20 X= 5.590028081166D+13 Y= 1.307654856576D+13 Z= 9.672095506033D+13
I= 21 X= -1.944169437470D+13 Y= -1.227946945033D+12 Z= -1.462548325404D+13
I= 22 X= -4.121795502383D+12 Y= -3.520886900339D+13 Z= -3.700692237127D+13
I= 23 X= 6.664041233030D+13 Y= 2.386960228410D+13 Z= -9.515784414538D+13
I= 24 X= 1.361477664076D+13 Y= -2.650945992071D+13 Z= -6.401810260580D+13
I= 25 X= -1.163610081779D+12 Y= 3.110898030553D+12 Z= 7.265553468266D+12
I= 26 X= -3.303419073414D+13 Y= -4.818821022681D+13 Z= -9.863554393372D+11
I= 27 X= -1.147122804642D+14 Y= -1.299637874614D+13 Z= -8.660310076850D+13
I= 28 X= -8.874368937087D+13 Y= -6.814382170610D+13 Z= 2.336676292040D+12
I= 29 X= -7.051879252145D+12 Y= -4.036844114836D+12 Z= -9.047651410841D+12
I= 30 X= 1.230313100826D+13 Y= 5.196908762327D+12 Z= -2.391365320430D+12
I= 31 X= -4.089271674063D+13 Y= 8.705395328306D+13 Z= 2.242672748051D+13
I= 32 X= 4.751680843826D+12 Y= -1.986006203458D+13 Z= 7.793326768554D+13
I= 33 X= -1.096538285868D+14 Y= -1.822983801809D+13 Z= -5.561852164330D+11
I= 34 X= 8.945633737962D+13 Y= 1.131387129623D+13 Z= 3.030658128348D+13
I= 35 X= -1.627017935593D+12 Y= 3.130059180559D+12 Z= 1.204502121132D+11
I= 36 X= 2.145970665598D+13 Y= 6.848325183016D+11 Z= 1.603572019775D+12
I= 37 X= 5.014149238172D+12 Y= -5.050636807593D+13 Z= -5.049580523356D+12
I= 38 X= -1.149225815757D+14 Y= 8.694695972448D+13 Z= 2.996546964890D+13

Backward Direction:

Total Energy: -656.4362368 Hartrees

Potential Energy: -656.6041947 Hartress

Kinetic Energy: 0.1679579 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.409967369214D+12 Y= -1.772139922480D+13 Z= -2.449939575201D+13

I= 1 X= 3.058405287376D+12 Y= -1.497287866950D+13 Z= 1.131466143800D+13

I= 2 X= 1.003968392712D+13 Y= -3.005438747085D+13 Z= 3.177580469398D+12

I= 3 X= -1.092090430535D+13 Y= 3.856252662317D+12 Z= 1.252465230851D+13
I= 4 X= 2.323398903095D+13 Y= 2.298603258910D+13 Z= -1.022225160327D+13
I= 5 X= -5.037752040870D+12 Y= -4.564904062259D+12 Z= 1.658568780255D+13
I= 6 X= 3.169359980055D+13 Y= 1.051675917551D+14 Z= -6.071197491629D+13
I= 7 X= 4.769741578820D+13 Y= -5.819879738215D+13 Z= 4.522824158198D+13
I= 8 X= -6.682736360961D+13 Y= 3.198506774654D+13 Z= -6.830056525501D+13
I= 9 X= 1.043120130448D+13 Y= 4.460020495553D+12 Z= -1.903356040427D+13
I= 10 X= -8.895136279069D+13 Y= -6.876244426617D+13 Z= 8.415969375601D+12
I= 11 X= -9.929129116530D+13 Y= 4.082811056455D+13 Z= 5.658953279663D+13
I= 12 X= -2.150396231416D+13 Y= 5.598015024445D+13 Z= 4.383037219079D+13
I= 13 X= -1.044846600796D+13 Y= -1.112836467867D+12 Z= 4.474687497315D+12
I= 14 X= 3.799327121305D+13 Y= 3.242803644448D+13 Z= 3.701593175781D+13
I= 15 X= -3.260206306489D+13 Y= 2.838196013734D+13 Z= 2.182016541043D+13
I= 16 X= 1.162179265829D+14 Y= 4.397689173764D+13 Z= -6.920779444214D+13
I= 17 X= 1.285049887905D+13 Y= -6.274758485566D+12 Z= 1.745031188251D+13
I= 18 X= 5.571465358613D+12 Y= 2.642034560065D+13 Z= 1.354335251009D+13
I= 19 X= -1.557103544691D+13 Y= 1.867501272902D+12 Z= -6.828147870552D+13
I= 20 X= 5.614024708548D+13 Y= 1.275421517426D+13 Z= 9.667979257143D+13
I= 21 X= -1.964738354744D+13 Y= -1.357165476702D+12 Z= -1.512760185694D+13
I= 22 X= -4.158553828343D+12 Y= -3.462978401815D+13 Z= -3.901923215226D+13
I= 23 X= 6.738807067412D+13 Y= 2.354415461898D+13 Z= -9.539118121732D+13
I= 24 X= 1.325434207937D+13 Y= -2.671189483689D+13 Z= -6.461180066038D+13
I= 25 X= -1.387152932946D+12 Y= 2.885073006093D+12 Z= 7.150199234869D+12
I= 26 X= -3.358711016898D+13 Y= -4.879306137395D+13 Z= -1.053818931645D+12
I= 27 X= -1.142514637842D+14 Y= -1.260840851185D+13 Z= -8.673683879706D+13
I= 28 X= -8.872085468350D+13 Y= -6.882824506084D+13 Z= 2.821140101347D+12
I= 29 X= -8.087133376927D+12 Y= -3.746049294531D+12 Z= -9.410752516484D+12
I= 30 X= 1.236409619089D+13 Y= 4.996560952099D+12 Z= -2.841039533655D+12
I= 31 X= -4.160845960440D+13 Y= 8.684220437248D+13 Z= 2.244909191558D+13
I= 32 X= 2.657013112991D+12 Y= -1.812056781995D+13 Z= 7.668616603182D+13

I= 33 X= -1.095892286675D+14 Y= -1.848302688996D+13 Z= -9.143523598454D+11
I= 34 X= 9.013120252615D+13 Y= 1.084401256708D+13 Z= 3.017741775275D+13
I= 35 X= -1.638280345102D+12 Y= 3.393114195464D+12 Z= 1.789372227001D+12
I= 36 X= 1.782004828307D+13 Y= -3.912355911457D+12 Z= -7.405818887382D+10
I= 37 X= 8.261061378619D+12 Y= -4.885802549019D+13 Z= -9.098999587548D+12
I= 38 X= -1.131444465252D+14 Y= 8.676167480216D+13 Z= 2.694126466091D+13

Seed: 5687982974

CM Start Point Coordinates: bohr

I= 0 X= -2.266015522546D+00 Y= 2.301422211246D+00 Z= -4.237964786905D-01
I= 1 X= -2.844239917749D+00 Y= 2.235256667550D-01 Z= -1.993630326871D+00
I= 2 X= -1.976362491065D+00 Y= 1.484648087273D+00 Z= 2.036940072054D+00
I= 3 X= -2.807346442904D+00 Y= -1.991621433180D+00 Z= -4.084937844098D-01
I= 4 X= -2.163952573246D+00 Y= -1.309061386588D+00 Z= 2.021959069509D+00
I= 5 X= 4.075431337272D+00 Y= 2.563462417922D+00 Z= -1.949255903147D+00
I= 6 X= 2.212708101106D+00 Y= -2.299545230835D-01 Z= -2.928524473705D+00
I= 7 X= 5.654131926461D+00 Y= 1.293465643301D+00 Z= -2.846865607265D+00
I= 8 X= 2.766110843525D+00 Y= 3.877192007828D+00 Z= -3.222753622074D+00
I= 9 X= -1.995598833934D+00 Y= -2.743917081421D+00 Z= 4.501488747140D+00
I= 10 X= -3.772791818595D+00 Y= -2.259936890997D+00 Z= 5.507165361729D+00
I= 11 X= -1.892051693726D+00 Y= -4.622570926680D+00 Z= 4.181877380309D+00
I= 12 X= -3.960229316636D-01 Y= -2.281743895121D+00 Z= 5.889854848974D+00
I= 13 X= -1.554429801329D+00 Y= 3.482349169668D+00 Z= 4.009540102136D+00
I= 14 X= -3.315583084637D+00 Y= 4.692303938872D+00 Z= 4.861675172775D+00
I= 15 X= -5.811126714460D-01 Y= 2.986493963319D+00 Z= 5.683270564431D+00
I= 16 X= -5.945800264032D-01 Y= 4.739030751953D+00 Z= 2.979832385121D+00
I= 17 X= -2.338636804655D+00 Y= 4.982969545772D+00 Z= -1.357464653543D+00
I= 18 X= -4.181400802682D+00 Y= 5.732200934499D+00 Z= -9.751952654926D-01
I= 19 X= -7.364255234233D-01 Y= 6.097557327276D+00 Z= -2.863603842090D-01
I= 20 X= -2.314446367434D+00 Y= 5.213626062957D+00 Z= -3.545370954751D+00

I= 21 X= -3.837056273692D+00 Y= 2.104539167821D-01 Z= -4.714391674499D+00
I= 22 X= -5.763813067816D+00 Y= 1.693203822041D+00 Z= -4.887770272680D+00
I= 23 X= -1.969899902730D+00 Y= 1.257348761328D+00 Z= -6.237232685897D+00
I= 24 X= -4.074805085366D+00 Y= -1.849760879427D+00 Z= -5.643063349563D+00
I= 25 X= -3.285526613157D+00 Y= -4.640294816840D+00 Z= -1.077963259167D+00
I= 26 X= -2.806711014509D+00 Y= -5.066530204949D+00 Z= -2.913308216247D+00
I= 27 X= -2.520436472027D+00 Y= -6.345242120323D+00 Z= 4.745580777492D-02
I= 28 X= -5.511086420851D+00 Y= -5.057983687100D+00 Z= -8.496373274347D-01
I= 29 X= 3.631092596796D+00 Y= -3.579862064418D+00 Z= -8.343737513786D-01
I= 30 X= 3.674975650988D+00 Y= -3.132006928585D+00 Z= 1.802714268374D+00
I= 31 X= 2.584681750299D+00 Y= -4.977649209701D+00 Z= -1.485287284003D+00
I= 32 X= 5.564324739346D+00 Y= -3.055601654804D+00 Z= -1.896995630009D+00
I= 33 X= 5.561501588730D+00 Y= -2.270141414214D+00 Z= 2.245408438726D+00
I= 34 X= 2.340608462036D+00 Y= -4.014511515182D+00 Z= 3.133174538516D+00
I= 35 X= 1.187150569445D+00 Y= -9.619092080173D-02 Z= -2.650968980654D-01
I= 36 X= 3.916781169664D+00 Y= 2.799851564213D+00 Z= 6.518870483569D-01
I= 37 X= 5.730622889901D+00 Y= 1.928796472763D+00 Z= 1.629945142431D+00
I= 38 X= 3.141743861919D+00 Y= 4.579773660691D+00 Z= 1.655775421993D+00

Forward Direction:

Total Energy: -656.4303792 Hartrees

Potential Energy: -656.5984849 Hartress

Kinetic Energy: 0.1681057 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.081456586498D+13 Y= 2.974833522937D+12 Z= -8.696811658222D+12
I= 1 X= 2.443854919830D+13 Y= -3.762810688929D+12 Z= 1.407279388992D+13
I= 2 X= -2.092689749643D+13 Y= -1.180873646800D+13 Z= 1.427579268100D+12
I= 3 X= -2.532869058839D+12 Y= -1.442159532859D+13 Z= -1.620927379982D+13
I= 4 X= 1.477796774696D+12 Y= 2.035444253273D+13 Z= 2.273990665264D+13
I= 5 X= -1.613535596533D+13 Y= -3.731855846116D+11 Z= -1.574393456822D+13
I= 6 X= -1.030500948637D+14 Y= 3.770388466544D+13 Z= -1.217862322102D+13

I= 7 X= 7.979415966333D+13 Y= -5.867605456118D+13 Z= -8.383108106117D+12
I= 8 X= 2.488943755512D+13 Y= -3.692610736172D+13 Z= -3.236122070217D+13
I= 9 X= 8.411906364787D+12 Y= 1.859445983949D+13 Z= -1.080229196106D+12
I= 10 X= -2.285875223149D+13 Y= 3.377955661753D+13 Z= -2.045494896201D+13
I= 11 X= 6.822322872187D+13 Y= -1.939293799121D+13 Z= 3.545841636718D+11
I= 12 X= 5.804301021124D+13 Y= -1.465226275482D+13 Z= 2.271534019568D+13
I= 13 X= 3.827377264211D+12 Y= 1.169362959424D+13 Z= -1.395613793513D+13
I= 14 X= 8.595349461312D+13 Y= 9.300358782814D+13 Z= 1.013787946331D+13
I= 15 X= 7.095154004282D+13 Y= 1.380744388276D+13 Z= 1.426555995867D+13
I= 16 X= -4.046507062884D+13 Y= -2.739673834382D+13 Z= 7.566586391909D+13
I= 17 X= 1.963321798815D+13 Y= -2.489481775315D+13 Z= -1.842999901719D+12
I= 18 X= -7.597106539161D+13 Y= 4.529306552867D+13 Z= 5.474645665401D+13
I= 19 X= -3.031974425871D+13 Y= 3.021255065687D+13 Z= 2.783532897995D+13
I= 20 X= 2.007713493623D+13 Y= 1.138754343991D+13 Z= -6.657079448967D+13
I= 21 X= 1.067190158939D+13 Y= 5.446119615278D+12 Z= -2.019369576616D+13
I= 22 X= -3.836926303524D+13 Y= 4.621738200018D+13 Z= 4.057086507605D+13
I= 23 X= 4.884666393926D+13 Y= 1.106710312370D+14 Z= -3.454489223506D+13
I= 24 X= 5.481006682023D+13 Y= -5.324140052668D+13 Z= 4.148548593209D+13
I= 25 X= -1.650171689660D+12 Y= 1.939454824022D+13 Z= 1.756441969418D+13
I= 26 X= 3.093244266477D+13 Y= -3.058340884414D+13 Z= -1.179349094059D+14
I= 27 X= -3.770073979805D+13 Y= 1.224514500309D+14 Z= 2.635047574444D+13
I= 28 X= -1.181659934051D+14 Y= -6.872360102261D+13 Z= -1.527510283739D+12
I= 29 X= 1.783819326301D+13 Y= -1.407713440139D+12 Z= 7.781942720636D+12
I= 30 X= -8.534333526260D+12 Y= 6.291402041023D+12 Z= -1.944699461952D+12
I= 31 X= -7.297440329213D+13 Y= 1.165469766764D+13 Z= -2.506974363475D+13
I= 32 X= 2.319394411032D+13 Y= 4.243984985171D+13 Z= -1.033566510274D+14
I= 33 X= -1.735933429348D+12 Y= -1.988564290480D+13 Z= -3.764574803680D+13
I= 34 X= -8.239323628242D+13 Y= -5.351504343059D+13 Z= 1.711168566767D+13
I= 35 X= -2.666345924918D+12 Y= -5.424610906966D+12 Z= 2.223474609578D+12
I= 36 X= 1.612488686243D+13 Y= -6.373604681381D+12 Z= 1.726127584846D+13

I= 37 X= -8.561501577313D+12 Y= 1.680081499723D+13 Z= -1.126057579908D+14

I= 38 X= -3.988991036227D+13 Y= 6.299348545413D+13 Z= 3.130135286704D+11

Backward Direction:

Total Energy: -656.4303713 Hartrees

Potential Energy: -656.5984849 Hartress

Kinetic Energy: 0.1681137 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.091589791933D+13 Y= 2.842508553098D+12 Z= -8.645029388363D+12

I= 1 X= 2.428225691648D+13 Y= -4.103083751955D+12 Z= 1.386852701723D+13

I= 2 X= -2.107236353672D+13 Y= -1.167502098385D+13 Z= 1.212291676823D+12

I= 3 X= -2.830921460892D+12 Y= -1.441462601549D+13 Z= -1.664112109451D+13

I= 4 X= 1.987582362757D+12 Y= 2.030896039322D+13 Z= 2.240114593185D+13

I= 5 X= -1.697670761112D+13 Y= -1.569679596063D+12 Z= -1.813275292933D+13

I= 6 X= -8.420395883123D+13 Y= 5.921901194853D+13 Z= -3.699092776549D+12

I= 7 X= 8.323640699974D+13 Y= -5.541697855001D+13 Z= -8.172512168660D+12

I= 8 X= 2.923685387847D+13 Y= -3.341200765592D+13 Z= -3.195676848883D+13

I= 9 X= 8.573931143223D+12 Y= 1.867054972034D+13 Z= -1.263370520188D+12

I= 10 X= -2.282911919579D+13 Y= 3.415612246954D+13 Z= -2.089146684203D+13

I= 11 X= 6.817643277475D+13 Y= -1.939705444325D+13 Z= 3.454844697115D+11

I= 12 X= 5.813796811884D+13 Y= -1.462682940881D+13 Z= 2.262516799557D+13

I= 13 X= 3.859496309947D+12 Y= 1.167800169375D+13 Z= -1.402373868646D+13

I= 14 X= 8.600809927853D+13 Y= 9.290730998321D+13 Z= 1.015217031869D+13

I= 15 X= 7.105195834787D+13 Y= 1.371534293703D+13 Z= 1.409927461606D+13

I= 16 X= -4.047206572655D+13 Y= -2.736713702585D+13 Z= 7.568927525467D+13

I= 17 X= 1.968240468949D+13 Y= -2.500336548390D+13 Z= -1.853749284672D+12

I= 18 X= -7.596069462562D+13 Y= 4.512001165323D+13 Z= 5.460449356710D+13

I= 19 X= -3.042372395105D+13 Y= 3.017791246318D+13 Z= 2.794254828255D+13

I= 20 X= 2.014934154439D+13 Y= 1.129055230989D+13 Z= -6.658318039782D+13

I= 21 X= 1.061000906732D+13 Y= 5.407237352702D+12 Z= -2.034478483054D+13

I= 22 X= -3.838032373547D+13 Y= 4.639163048650D+13 Z= 3.996535474880D+13

I= 23 X= 4.907163667465D+13 Y= 1.105731030132D+14 Z= -3.461510409515D+13
I= 24 X= 5.470161092802D+13 Y= -5.330231382738D+13 Z= 4.130684032223D+13
I= 25 X= -1.717436435413D+12 Y= 1.932659678213D+13 Z= 1.752970924345D+13
I= 26 X= 3.076606748414D+13 Y= -3.076541045446D+13 Z= -1.179552093814D+14
I= 27 X= -3.756207861640D+13 Y= 1.225681914974D+14 Z= 2.631023355817D+13
I= 28 X= -1.181591223769D+14 Y= -6.892954616403D+13 Z= -1.381733613222D+12
I= 29 X= 1.752668204375D+13 Y= -1.320212365117D+12 Z= 7.672684459151D+12
I= 30 X= -8.515988910895D+12 Y= 6.231116756115D+12 Z= -2.080007844057D+12
I= 31 X= -7.318977256908D+13 Y= 1.159098175484D+13 Z= -2.506301410438D+13
I= 32 X= 2.256365200751D+13 Y= 4.296326912554D+13 Z= -1.037319078323D+14
I= 33 X= -1.716495109012D+12 Y= -1.996182823399D+13 Z= -3.775352165528D+13
I= 34 X= -8.219016724013D+13 Y= -5.365642539669D+13 Z= 1.707281995662D+13
I= 35 X= -2.669734819649D+12 Y= -5.345456826584D+12 Z= 2.725658487127D+12
I= 36 X= 1.502970222564D+13 Y= -7.756913123348D+12 Z= 1.675647164805D+13
I= 37 X= -7.584495513824D+12 Y= 1.729680646032D+13 Z= -1.138242409064D+14
I= 38 X= -3.935486393955D+13 Y= 6.293773263352D+13 Z= -5.969792489383D+11

Seed: 6056085138

CM Start Point Coordinates: bohr

I= 0 X= -2.259726346305D+00 Y= 2.287627697564D+00 Z= -6.042141276671D-01
I= 1 X= -2.838236027796D+00 Y= 2.184421046624D-02 Z= -1.965554099769D+00
I= 2 X= -2.134545163523D+00 Y= 1.608610204715D+00 Z= 2.099791023678D+00
I= 3 X= -2.645275939811D+00 Y= -2.022342592751D+00 Z= -1.860779136244D-01
I= 4 X= -2.188635259836D+00 Y= -9.755954203511D-01 Z= 2.257352217094D+00
I= 5 X= 4.307340906241D+00 Y= 2.475736974092D+00 Z= -1.277461055785D+00
I= 6 X= 2.440104664242D+00 Y= 6.425856416503D-01 Z= -3.180651948820D+00
I= 7 X= 5.619166055738D+00 Y= 1.272296968986D+00 Z= -2.221065043572D+00
I= 8 X= 3.829348403245D+00 Y= 3.995979513054D+00 Z= -2.624512059386D+00
I= 9 X= -2.176108681062D+00 Y= -2.643736783475D+00 Z= 4.759515733760D+00
I= 10 X= -3.922874279592D+00 Y= -2.827863252941D+00 Z= 5.564180161705D+00

I= 11 X= -1.352014190583D+00 Y= -4.567721050526D+00 Z= 4.337417473781D+00
I= 12 X= -8.048101394225D-01 Y= -2.022047761783D+00 Z= 5.996045767961D+00
I= 13 X= -1.605253736114D+00 Y= 3.394184409659D+00 Z= 4.112156812857D+00
I= 14 X= -3.484592419878D+00 Y= 4.197779676752D+00 Z= 5.091602468804D+00
I= 15 X= -5.877130972866D-01 Y= 2.078694681775D+00 Z= 5.721632215109D+00
I= 16 X= -8.078414844755D-01 Y= 5.218579439667D+00 Z= 3.974368416179D+00
I= 17 X= -2.100750893295D+00 Y= 4.933064137454D+00 Z= -1.810705524051D+00
I= 18 X= -4.155018174286D+00 Y= 5.831708364268D+00 Z= -2.009931659656D+00
I= 19 X= -1.184996682561D+00 Y= 6.316925906744D+00 Z= -4.188780359490D-01
I= 20 X= -1.142806385136D+00 Y= 4.898725299318D+00 Z= -3.816351029815D+00
I= 21 X= -3.495997896820D+00 Y= -1.821471254087D-01 Z= -4.638412397944D+00
I= 22 X= -5.419544148127D+00 Y= -1.239315872966D+00 Z= -4.757980389259D+00
I= 23 X= -3.530153172493D+00 Y= 1.717319650320D+00 Z= -5.502364614257D+00
I= 24 X= -2.575991973462D+00 Y= -1.863329463729D+00 Z= -5.653152030276D+00
I= 25 X= -3.228527946673D+00 Y= -4.693069782647D+00 Z= -6.488271146128D-01
I= 26 X= -2.316036772562D+00 Y= -5.710469862398D+00 Z= -2.651569611860D+00
I= 27 X= -2.933941302589D+00 Y= -6.184181982386D+00 Z= 1.162026497571D+00
I= 28 X= -5.260819531794D+00 Y= -4.636432333911D+00 Z= -1.080899817873D+00
I= 29 X= 3.003942176544D+00 Y= -3.592131026587D+00 Z= -1.442525616733D+00
I= 30 X= 3.974581546973D+00 Y= -3.023470430019D+00 Z= 1.031452891977D+00
I= 31 X= 1.619051087832D+00 Y= -4.824954913831D+00 Z= -1.945566446600D+00
I= 32 X= 4.081058848373D+00 Y= -2.884084887491D+00 Z= -3.073992480332D+00
I= 33 X= 6.046002942147D+00 Y= -2.557461957445D+00 Z= 1.000302835662D+00
I= 34 X= 3.435874500082D+00 Y= -4.288253049372D+00 Z= 2.994528012844D+00
I= 35 X= 1.137059749437D+00 Y= -2.941064420496D-03 Z= -3.666820087672D-01
I= 36 X= 3.988547043032D+00 Y= 2.583858379138D+00 Z= 1.307847300747D+00
I= 37 X= 5.438513176743D+00 Y= 1.689742110025D+00 Z= 2.532365242960D+00
I= 38 X= 2.777687857633D+00 Y= 3.992950508851D+00 Z= 2.349741637847D+00

Forward Direction:

Total Energy: -656.4479769 Hartrees

Potential Energy: -656.6379384 Hartress

Kinetic Energy: 0.1899615 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.250096061875D+12 Y= -3.616898294788D+13 Z= 1.119384117286D+13
I= 1 X= 1.026436153601D+13 Y= 1.503623340442D+13 Z= -1.567671723285D+13
I= 2 X= -5.457157034334D+12 Y= 2.824241591253D+12 Z= -2.610564441827D+12
I= 3 X= 3.372259651061D+12 Y= 5.590250310035D+12 Z= -1.696428146347D+13
I= 4 X= 6.879526154609D+12 Y= -4.783540978816D+12 Z= -1.322626409487D+13
I= 5 X= 1.602085124606D+13 Y= -8.732088301180D+12 Z= 9.088639055052D+12
I= 6 X= 2.655598378546D+13 Y= -2.897646994055D+13 Z= -5.606578546732D+13
I= 7 X= 4.367252934695D+13 Y= 7.448391667277D+13 Z= -3.124432513148D+13
I= 8 X= -3.871988088870D+13 Y= 1.047452119386D+14 Z= -1.609999941653D+14
I= 9 X= 3.954850517356D+12 Y= -8.678134276671D+12 Z= 6.054937138909D+12
I= 10 X= -1.947813126873D+14 Y= 2.622939614996D+13 Z= 4.214241961133D+13
I= 11 X= 1.106064309570D+13 Y= 5.408935752075D+13 Z= -1.267544993068D+14
I= 12 X= 4.993547434011D+13 Y= 3.012160927318D+13 Z= -1.614869877884D+13
I= 13 X= 1.224812365099D+12 Y= 8.256765827971D+12 Z= -8.020324399289D+12
I= 14 X= 6.268660026381D+13 Y= 6.563947795975D+13 Z= -3.197761055799D+13
I= 15 X= -3.697105897664D+13 Y= -6.987528066040D+13 Z= 1.915963346795D+13
I= 16 X= -1.841919861353D+13 Y= 1.072350978345D+13 Z= 2.500108454727D+13
I= 17 X= -2.323991462565D+13 Y= 2.306932991167D+12 Z= 6.398081792514D+12
I= 18 X= 6.102512354844D+12 Y= -4.300364183117D+13 Z= -1.021441516148D+14
I= 19 X= 9.436430413097D+13 Y= 2.910077865522D+13 Z= 2.215307511530D+13
I= 20 X= 2.677803126588D+13 Y= -5.831586725328D+12 Z= -2.347450820732D+13
I= 21 X= -2.314303437735D+13 Y= 7.953727110231D+11 Z= 1.660813915071D+13
I= 22 X= 8.553898325677D+13 Y= 7.913581851904D+12 Z= 4.680445842188D+13
I= 23 X= 1.024588511586D+14 Y= 4.255852193008D+13 Z= 2.750908984251D+13
I= 24 X= 5.472970376591D+13 Y= 8.630498267068D+12 Z= 3.887345364302D+13
I= 25 X= 3.663932696478D+11 Y= 3.683801649597D+12 Z= 2.495452470118D+12
I= 26 X= -8.691092862261D+12 Y= -4.591540729115D+13 Z= 1.084350175301D+14

I= 27 X= 8.229719602042D+13 Y= -3.400047757368D+13 Z= 3.038844411676D+13
I= 28 X= -8.815854249592D+13 Y= -9.327393292045D+10 Z= -2.096268413481D+13
I= 29 X= 1.541602363402D+13 Y= -3.447775854132D+12 Z= -2.523526914996D+13
I= 30 X= -1.292185146214D+13 Y= -1.640281893364D+13 Z= 2.371637558286D+13
I= 31 X= 3.717200533529D+13 Y= 1.125711464028D+14 Z= 6.040955523733D+13
I= 32 X= -3.956227488464D+13 Y= -2.240303888623D+13 Z= 8.309803135549D+12
I= 33 X= 2.442793879670D+12 Y= 5.155446469898D+13 Z= 1.246485482897D+13
I= 34 X= -1.490955239257D+13 Y= 1.127414837590D+13 Z= -1.439508536871D+13
I= 35 X= -2.904693811688D+12 Y= 1.269800014238D+12 Z= 2.807592236297D+11
I= 36 X= 1.802690914282D+13 Y= -1.177090933996D+13 Z= 1.812110188704D+13
I= 37 X= 1.527306361852D+13 Y= 8.373663792042D+12 Z= -5.234858218513D+12
I= 38 X= -1.311334211290D+14 Y= 9.552629509648D+13 Z= -2.312084893792D+13

Backward Direction:

Total Energy: -656.4479729 Hartrees

Potential Energy: -656.6379384 Hartress

Kinetic Energy: 0.1899655 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.170864525593D+12 Y= -3.627244784393D+13 Z= 1.123432972966D+13
I= 1 X= 1.014215659752D+13 Y= 1.477017388990D+13 Z= -1.583643350233D+13
I= 2 X= -5.570896933531D+12 Y= 2.928793729848D+12 Z= -2.778897812075D+12
I= 3 X= 3.139212468775D+12 Y= 5.595699613511D+12 Z= -1.730194287191D+13
I= 4 X= 7.278127515623D+12 Y= -4.819103463636D+12 Z= -1.349114110716D+13
I= 5 X= 1.536299837980D+13 Y= -9.667626991672D+12 Z= 7.220821935269D+12
I= 6 X= 4.129177789792D+13 Y= -1.215379151536D+13 Z= -4.943564045530D+13
I= 7 X= 4.636402260376D+13 Y= 7.703218826382D+13 Z= -3.107966016199D+13
I= 8 X= -3.532063597938D+13 Y= 1.074928865630D+14 Z= -1.606837529740D+14
I= 9 X= 4.081537693065D+12 Y= -8.618639597608D+12 Z= 5.911738934567D+12
I= 10 X= -1.947581426167D+14 Y= 2.652383300599D+13 Z= 4.180110627032D+13
I= 11 X= 1.102405334126D+13 Y= 5.408613886994D+13 Z= -1.267616143576D+14
I= 12 X= 5.000972192916D+13 Y= 3.014149560375D+13 Z= -1.621920441641D+13

I= 13 X= 1.249926248601D+12 Y= 8.244546372606D+12 Z= -8.073181428573D+12
I= 14 X= 6.272929565526D+13 Y= 6.556419830896D+13 Z= -3.196643653709D+13
I= 15 X= -3.689254190101D+13 Y= -6.994729438547D+13 Z= 1.902961495324D+13
I= 16 X= -1.842466808148D+13 Y= 1.074665505657D+13 Z= 2.501938986783D+13
I= 17 X= -2.320145554178D+13 Y= 2.222059519346D+12 Z= 6.389676854312D+12
I= 18 X= 6.110621261141D+12 Y= -4.313895265869D+13 Z= -1.022551525515D+14
I= 19 X= 9.428300240049D+13 Y= 2.907369503361D+13 Z= 2.223690987529D+13
I= 20 X= 2.683448960745D+13 Y= -5.907424089528D+12 Z= -2.348419278024D+13
I= 21 X= -2.319142813969D+13 Y= 7.649706693457D+11 Z= 1.649000260738D+13
I= 22 X= 8.553033489626D+13 Y= 8.049826750427D+12 Z= 4.633100988883D+13
I= 23 X= 1.026347573463D+14 Y= 4.248195184954D+13 Z= 2.745419118682D+13
I= 24 X= 5.464490210476D+13 Y= 8.582870156165D+12 Z= 3.873377063709D+13
I= 25 X= 3.137989659531D+11 Y= 3.630670403143D+12 Z= 2.468312367555D+12
I= 26 X= -8.821181652849D+12 Y= -4.605771435360D+13 Z= 1.084191449802D+14
I= 27 X= 8.240561521007D+13 Y= -3.390919742638D+13 Z= 3.035697874195D+13
I= 28 X= -8.815317003506D+13 Y= -2.543024379543D+11 Z= -2.084870134103D+13
I= 29 X= 1.517245300802D+13 Y= -3.379358762415D+12 Z= -2.532069818771D+13
I= 30 X= -1.290750780671D+13 Y= -1.644995599937D+13 Z= 2.361057795536D+13
I= 31 X= 3.700360809422D+13 Y= 1.125213269274D+14 Z= 6.041481705825D+13
I= 32 X= -4.005510028663D+13 Y= -2.199377734431D+13 Z= 8.016389834143D+12
I= 33 X= 2.457992700040D+12 Y= 5.149489538856D+13 Z= 1.238058663737D+13
I= 34 X= -1.475077270073D+13 Y= 1.116360181346D+13 Z= -1.442547446844D+13
I= 35 X= -2.907343588561D+12 Y= 1.331690591300D+12 Z= 6.734168064317D+11
I= 36 X= 1.717058425297D+13 Y= -1.285251823510D+13 Z= 1.772639547386D+13
I= 37 X= 1.603698467389D+13 Y= 8.761479527122D+12 Z= -6.187590029987D+12
I= 38 X= -1.307150683239D+14 Y= 9.548270196855D+13 Z= -2.383237231008D+13

Seed: 7377033437

CM Start Point Coordinates: bohr

I= 0 X= -2.281336793531D+00 Y= 2.341856611260D+00 Z= -5.492765950894D-01

I= 1 X= -2.779961720082D+00 Y= -1.017431380799D-02 Z= -1.833524904920D+00
I= 2 X= -2.064592696752D+00 Y= 1.733989885396D+00 Z= 2.003592921907D+00
I= 3 X= -2.553216988765D+00 Y= -2.079544744344D+00 Z= -2.185966714437D-01
I= 4 X= -2.121440293752D+00 Y= -9.701348525138D-01 Z= 2.328212690596D+00
I= 5 X= 4.373962364475D+00 Y= 2.736565075490D+00 Z= -1.221749487075D+00
I= 6 X= 2.266211886396D+00 Y= 7.972644016125D-01 Z= -2.914697517064D+00
I= 7 X= 6.127896882871D+00 Y= 1.671203331229D+00 Z= -2.057073924164D+00
I= 8 X= 3.988856247308D+00 Y= 4.672805664107D+00 Z= -2.187254409459D+00
I= 9 X= -2.163456543617D+00 Y= -2.457132410835D+00 Z= 4.723301741305D+00
I= 10 X= -4.312514726667D+00 Y= -2.509527582596D+00 Z= 5.198273419410D+00
I= 11 X= -1.525089831209D+00 Y= -4.499164915159D+00 Z= 4.579653104708D+00
I= 12 X= -1.190835574035D+00 Y= -1.365754101073D+00 Z= 6.436461371487D+00
I= 13 X= -1.763023025040D+00 Y= 3.652672762697D+00 Z= 4.079438367857D+00
I= 14 X= -3.551537273401D+00 Y= 4.126408753949D+00 Z= 5.408216700932D+00
I= 15 X= -2.849612421147D-01 Y= 2.996037336125D+00 Z= 5.637230337962D+00
I= 16 X= -6.746196543118D-01 Y= 5.269679555272D+00 Z= 3.307894097991D+00
I= 17 X= -2.385600832419D+00 Y= 4.940192856161D+00 Z= -1.689664270737D+00
I= 18 X= -4.194764311400D+00 Y= 5.848314354002D+00 Z= -3.876391138304D-01
I= 19 X= -5.961147863180D-01 Y= 6.211128315965D+00 Z= -1.050034796294D+00
I= 20 X= -3.026155281040D+00 Y= 4.752467397201D+00 Z= -4.016425062058D+00
I= 21 X= -3.495227178700D+00 Y= -3.779113890075D-01 Z= -4.561222429619D+00
I= 22 X= -5.581346616693D+00 Y= -1.227586060698D+00 Z= -5.019513523258D+00
I= 23 X= -3.399321931609D+00 Y= 1.380239863490D+00 Z= -5.926556653759D+00
I= 24 X= -2.212543580830D+00 Y= -2.071381618139D+00 Z= -5.238856474522D+00
I= 25 X= -3.265664411655D+00 Y= -4.778648956655D+00 Z= -8.186182230931D-01
I= 26 X= -2.843200505375D+00 Y= -5.015321455585D+00 Z= -2.694553874149D+00
I= 27 X= -2.099777468593D+00 Y= -6.068110117450D+00 Z= 8.633240409767D-01
I= 28 X= -5.307964247019D+00 Y= -5.313553316480D+00 Z= -5.406644193715D-01
I= 29 X= 3.149259642292D+00 Y= -3.549565318430D+00 Z= -1.603496923745D+00
I= 30 X= 3.724165288692D+00 Y= -3.281388660029D+00 Z= 9.761298343039D-01

I= 31 X= 1.810999683936D+00 Y= -4.993680037121D+00 Z= -2.136009289926D+00
I= 32 X= 4.541614214914D+00 Y= -2.828374384692D+00 Z= -2.815640321025D+00
I= 33 X= 5.520081793598D+00 Y= -2.654088256506D+00 Z= 1.696242757765D+00
I= 34 X= 2.319231783850D+00 Y= -4.576034712908D+00 Z= 2.019174841873D+00
I= 35 X= 1.146494956252D+00 Y= -2.723278796496D-02 Z= -3.867067310614D-01
I= 36 X= 4.244271923362D+00 Y= 2.385493676697D+00 Z= 1.408551376722D+00
I= 37 X= 5.401881230185D+00 Y= 1.149005097483D+00 Z= 2.562259338119D+00
I= 38 X= 3.468382019313D+00 Y= 3.620078110002D+00 Z= 2.765931699693D+00

Forward Direction:

Total Energy: -656.4474475 Hartrees

Potential Energy: -656.6299845 Hartress

Kinetic Energy: 0.1825370 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.406142083388D+12 Y= 4.758837797698D+12 Z= 1.052473722160D+13
I= 1 X= -1.525238880868D+13 Y= 1.332658366443D+13 Z= -4.985904289980D+12
I= 2 X= 1.309388887049D+13 Y= -1.192464944101D+12 Z= -7.097197170423D+12
I= 3 X= -3.040524734821D+12 Y= -2.613923449333D+12 Z= 8.231058947366D+12
I= 4 X= 7.128788577430D+12 Y= -1.828873934539D+13 Z= 3.598767745451D+12
I= 5 X= 1.917371099353D+12 Y= -1.853316407752D+13 Z= -8.559930471144D+12
I= 6 X= -3.804323935647D+13 Y= -7.375857247878D+12 Z= 1.803275361842D+13
I= 7 X= -1.001519061378D+14 Y= 2.905457162922D+13 Z= -6.931117630818D+13
I= 8 X= 3.034663319150D+13 Y= 6.238364811460D+13 Z= -1.117934500353D+13
I= 9 X= -1.320737855809D+13 Y= 1.245803339234D+13 Z= -1.005141393618D+13
I= 10 X= 9.677933981409D+13 Y= 1.515074834498D+13 Z= -1.229794919562D+13
I= 11 X= -1.154755873125D+13 Y= -1.276450718813D+14 Z= -3.906469563434D+13
I= 12 X= -9.256181883105D+12 Y= -8.740390276463D+12 Z= 6.948578747369D+13
I= 13 X= 5.149029486054D+12 Y= 1.242148609150D+13 Z= 8.465720515881D+12
I= 14 X= 4.085654077821D+13 Y= -7.734086485380D+12 Z= -1.205415721554D+13
I= 15 X= -7.114034980678D+13 Y= 6.485895087902D+13 Z= -8.073962272020D+13
I= 16 X= 3.508456485918D+13 Y= 2.577404721424D+13 Z= 8.093039412042D+13

I= 17 X= -1.413912424796D+13 Y= 1.712801115603D+13 Z= -1.248755190225D+13
I= 18 X= 8.740978235164D+13 Y= 2.634163479458D+13 Z= -3.184398110936D+13
I= 19 X= 2.651440748954D+13 Y= 8.631763857695D+12 Z= 6.054934006127D+13
I= 20 X= 1.927757099804D+13 Y= 3.949980309798D+13 Z= -3.232112388868D+13
I= 21 X= 9.377988064747D+12 Y= -1.292088993895D+12 Z= 5.367359705608D+12
I= 22 X= -1.661655040527D+14 Y= -7.271932210103D+12 Z= 7.200434689151D+13
I= 23 X= 1.795604095340D+13 Y= -9.686441775873D+13 Z= 2.092567639684D+13
I= 24 X= 5.268164803303D+13 Y= 2.220290683764D+12 Z= -8.878346913530D+13
I= 25 X= 1.335337730690D+13 Y= -5.489735454134D+12 Z= -8.490012123823D+12
I= 26 X= 2.010108885396D+13 Y= -4.145315254037D+13 Z= -3.496964177954D+13
I= 27 X= 3.793284340529D+13 Y= 4.336649387830D+13 Z= 4.148707213267D+12
I= 28 X= -5.518311814023D+13 Y= 1.050420584582D+14 Z= 1.125596811930D+14
I= 29 X= -1.508325783916D+13 Y= -9.018196325225D+12 Z= -5.833917047830D+12
I= 30 X= -8.220902734290D+12 Y= -5.227413958240D+12 Z= -3.309512765018D+12
I= 31 X= 2.209329372307D+13 Y= 3.466208098277D+13 Z= 9.141635074397D+13
I= 32 X= 1.510455507049D+14 Y= 7.814164534726D+13 Z= -6.305137959514D+13
I= 33 X= 6.709289185535D+13 Y= 4.333968368381D+13 Z= 6.258540538950D+13
I= 34 X= 2.550408140659D+13 Y= -1.289834193782D+14 Z= 1.048224191768D+14
I= 35 X= -1.387198366064D+12 Y= -1.014001491370D+12 Z= -2.119119660765D+12
I= 36 X= 2.069666717887D+12 Y= 8.199484525548D+12 Z= 2.659947907179D+13
I= 37 X= 2.802781367222D+13 Y= -2.650337901010D+13 Z= 3.297357555220D+13
I= 38 X= -5.460218943149D+12 Y= -1.013824318069D+14 Z= -6.191994698127D+13

Backward Direction:

Total Energy: -656.4474347 Hartrees

Potential Energy: -656.6299845 Hartress

Kinetic Energy: 0.1825498 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.298947509318D+12 Y= 4.618857230030D+12 Z= 1.057951533072D+13

I= 1 X= -1.541772330476D+13 Y= 1.296662426623D+13 Z= -5.201988923753D+12

I= 2 X= 1.294000696045D+13 Y= -1.051013414830D+12 Z= -7.324940119707D+12

I= 3 X= -3.355820815446D+12 Y= -2.606550930425D+12 Z= 7.774227336730D+12
I= 4 X= 7.668067561829D+12 Y= -1.833685283229D+13 Z= 3.240408187711D+12
I= 5 X= 1.027343460286D+12 Y= -1.979888067344D+13 Z= -1.108695276714D+13
I= 6 X= -1.810676919904D+13 Y= 1.538401736574D+13 Z= 2.700286321334D+13
I= 7 X= -9.651050923770D+13 Y= 3.250219991653D+13 Z= -6.908839644615D+13
I= 8 X= 3.494556719770D+13 Y= 6.610105436437D+13 Z= -1.075149340626D+13
I= 9 X= -1.303597991302D+13 Y= 1.253852541772D+13 Z= -1.024515081145D+13
I= 10 X= 9.681068725230D+13 Y= 1.554910025366D+13 Z= -1.275972161943D+13
I= 11 X= -1.159706205454D+13 Y= -1.276494264951D+14 Z= -3.907432177552D+13
I= 12 X= -9.155730234301D+12 Y= -8.713485502377D+12 Z= 6.939039841361D+13
I= 13 X= 5.183006768590D+12 Y= 1.240495404702D+13 Z= 8.394208756110D+12
I= 14 X= 4.091430456767D+13 Y= -7.835934454893D+12 Z= -1.203903958150D+13
I= 15 X= -7.103412185198D+13 Y= 6.476152148769D+13 Z= -8.091552841529D+13
I= 16 X= 3.507716505175D+13 Y= 2.580536110990D+13 Z= 8.095515991279D+13
I= 17 X= -1.408709187588D+13 Y= 1.701318344955D+13 Z= -1.249892318388D+13
I= 18 X= 8.742075311143D+13 Y= 2.615856896950D+13 Z= -3.199415739254D+13
I= 19 X= 2.640441209688D+13 Y= 8.595121681768D+12 Z= 6.066276247644D+13
I= 20 X= 1.935395507877D+13 Y= 3.939720059293D+13 Z= -3.233422639173D+13
I= 21 X= 9.312514785823D+12 Y= -1.333220771082D+12 Z= 5.207529455899D+12
I= 22 X= -1.661772046585D+14 Y= -7.087602658902D+12 Z= 7.136380504735D+13
I= 23 X= 1.819402938794D+13 Y= -9.696801157287D+13 Z= 2.085140246836D+13
I= 24 X= 5.256691747878D+13 Y= 2.155853271322D+12 Z= -8.897245020155D+13
I= 25 X= 1.328222099017D+13 Y= -5.561618212823D+12 Z= -8.526730732636D+12
I= 26 X= 1.992508810251D+13 Y= -4.164568376552D+13 Z= -3.499111620040D+13
I= 27 X= 3.807952677181D+13 Y= 4.348998936040D+13 Z= 4.106136823191D+12
I= 28 X= -5.517584959147D+13 Y= 1.048241984635D+14 Z= 1.127138917168D+14
I= 29 X= -1.541279138910D+13 Y= -8.925632919763D+12 Z= -5.949496394978D+12
I= 30 X= -8.201496799551D+12 Y= -5.291187021446D+12 Z= -3.452649349845D+12
I= 31 X= 2.186546435886D+13 Y= 3.459467881556D+13 Z= 9.142346960637D+13
I= 32 X= 1.503787933590D+14 Y= 7.869534678713D+13 Z= -6.344834670275D+13

I= 33 X= 6.711345476742D+13 Y= 4.325909069084D+13 Z= 6.247139657794D+13
I= 34 X= 2.571889891179D+13 Y= -1.291329809314D+14 Z= 1.047813049073D+14
I= 35 X= -1.390783323362D+12 Y= -9.302679894744D+11 Z= -1.587882177313D+12
I= 36 X= 9.111206995222D+11 Y= 6.736145441319D+12 Z= 2.606546966777D+13
I= 37 X= 2.906134395273D+13 Y= -2.597869220016D+13 Z= 3.168459789122D+13
I= 38 X= -4.894217666837D+12 Y= -1.014414101739D+14 Z= -6.288258695793D+13

Seed: 8789762236

CM Start Point Coordinates: bohr

I= 0 X= -2.113504561814D+00 Y= 2.307224257787D+00 Z= -4.746620725803D-01
I= 1 X= -2.630993060472D+00 Y= 1.946839037496D-01 Z= -1.958083499831D+00
I= 2 X= -1.896164614005D+00 Y= 1.574016940787D+00 Z= 2.029821058751D+00
I= 3 X= -2.763078473208D+00 Y= -1.928628960906D+00 Z= -3.610117606544D-01
I= 4 X= -2.157917306208D+00 Y= -1.097595548421D+00 Z= 2.173691557228D+00
I= 5 X= 3.835436296930D+00 Y= 2.499340868395D+00 Z= -1.987117694787D+00
I= 6 X= 2.414296657230D+00 Y= -3.534534240041D-01 Z= -2.944791975230D+00
I= 7 X= 5.623595753753D+00 Y= 1.765453672572D+00 Z= -2.759273343798D+00
I= 8 X= 2.829978802279D+00 Y= 3.867200537277D+00 Z= -3.376301668807D+00
I= 9 X= -1.959574994370D+00 Y= -2.705058197963D+00 Z= 4.445330645129D+00
I= 10 X= -3.745906842330D+00 Y= -3.084970302433D+00 Z= 5.542386214312D+00
I= 11 X= -7.548002531231D-01 Y= -4.495087201207D+00 Z= 4.093106228805D+00
I= 12 X= -7.509509994462D-01 Y= -1.678411680795D+00 Z= 5.576803805069D+00
I= 13 X= -1.630807134017D+00 Y= 3.123942129692D+00 Z= 4.402155106722D+00
I= 14 X= -3.336650447547D+00 Y= 2.641831080068D+00 Z= 5.817465402773D+00
I= 15 X= 2.431016507342D-01 Y= 2.325313492057D+00 Z= 5.357625991863D+00
I= 16 X= -1.348475267168D+00 Y= 5.212406857106D+00 Z= 4.057219680027D+00
I= 17 X= -1.894282225602D+00 Y= 4.928658551514D+00 Z= -1.457060931634D+00
I= 18 X= -3.453386280501D+00 Y= 6.486350419952D+00 Z= -8.460987545922D-01
I= 19 X= 2.570583792457D-01 Y= 5.993568509375D+00 Z= -8.913938626684D-01
I= 20 X= -1.710283091264D+00 Y= 5.117711372164D+00 Z= -3.466466715342D+00

I= 21 X= -3.419267873561D+00 Y= 2.340397394355D-01 Z= -4.705343780590D+00
I= 22 X= -5.458953306615D+00 Y= 1.729680084218D+00 Z= -5.156031700313D+00
I= 23 X= -1.712022487545D+00 Y= 1.482620554795D+00 Z= -5.559846789680D+00
I= 24 X= -3.779528047058D+00 Y= -2.100723999402D+00 Z= -5.690890079784D+00
I= 25 X= -3.298398070253D+00 Y= -4.678512197035D+00 Z= -9.731180362358D-01
I= 26 X= -2.808635200399D+00 Y= -4.979623112038D+00 Z= -3.007473131090D+00
I= 27 X= -2.344084068152D+00 Y= -6.307569355250D+00 Z= 2.560085474157D-01
I= 28 X= -5.310047320046D+00 Y= -5.135056446979D+00 Z= -4.959217565625D-01
I= 29 X= 3.452312258069D+00 Y= -3.903720324229D+00 Z= -7.606221328254D-01
I= 30 X= 3.826422432984D+00 Y= -2.992159900812D+00 Z= 1.786924800721D+00
I= 31 X= 2.094978184925D+00 Y= -5.526268196364D+00 Z= -9.761806124047D-01
I= 32 X= 4.708464076123D+00 Y= -3.206595836412D+00 Z= -2.133220998368D+00
I= 33 X= 5.440884107435D+00 Y= -1.557641820432D+00 Z= 2.299460059005D+00
I= 34 X= 2.855028387686D+00 Y= -3.456704671461D+00 Z= 3.457407209671D+00
I= 35 X= 1.068277656212D+00 Y= -9.582891368893D-02 Z= -3.450436286791D-01
I= 36 X= 3.687015734907D+00 Y= 3.100714862482D+00 Z= 6.195428186876D-01
I= 37 X= 5.157358871900D+00 Y= 2.648619332803D+00 Z= 2.113089096594D+00
I= 38 X= 2.530157136716D+00 Y= 4.573894853010D+00 Z= 8.579862179945D-01

Forward Direction:

Total Energy: -656.4257811 Hartrees

Potential Energy: -656.6004934 Hartress

Kinetic Energy: 0.1747123 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.371379414413D+13 Y= 6.130348144802D+12 Z= 1.200537421420D+13
I= 1 X= 2.050646925615D+13 Y= 2.888561725221D+12 Z= 3.410847319888D+13
I= 2 X= 7.429679723116D+12 Y= 5.481647848763D+12 Z= -1.506217994960D+13
I= 3 X= -3.317495427574D+12 Y= 2.181407445585D+12 Z= -5.298881329938D+11
I= 4 X= 1.021715239517D+13 Y= 3.132897703438D+12 Z= -1.468403007863D+13
I= 5 X= 2.012251017840D+13 Y= -4.457880917862D+12 Z= 1.523053190099D+12
I= 6 X= -3.280222691245D+13 Y= 5.936481996860D+12 Z= -4.653475114597D+13

I= 7 X= 2.442807919645D+11 Y= -5.539867200016D+13 Z= 2.580650760911D+13
I= 8 X= -9.345380726546D+13 Y= 1.037690738383D+14 Z= -2.274749014689D+13
I= 9 X= 3.133094977843D+12 Y= -4.904323420779D+12 Z= 6.685408961582D+12
I= 10 X= -2.412307993124D+14 Y= 7.677169148341D+13 Z= 4.349358354389D+13
I= 11 X= 4.672483819319D+13 Y= 3.154256948910D+13 Z= -5.613802765388D+12
I= 12 X= 1.358452789040D+13 Y= -1.957116793725D+13 Z= -5.242825230389D+13
I= 13 X= -1.541026087738D+13 Y= 2.616817085210D+13 Z= 3.233908225568D+12
I= 14 X= 6.826208604841D+13 Y= 5.809649189133D+13 Z= -4.641726340712D+13
I= 15 X= 7.887194957166D+12 Y= -6.229744701158D+13 Z= 2.182052374540D+13
I= 16 X= -6.645933914892D+13 Y= -6.788597982335D+13 Z= 3.875923632759D+13
I= 17 X= 1.018933255489D+13 Y= 3.899527937212D+12 Z= 2.152905444261D+12
I= 18 X= -4.111811568030D+13 Y= -9.310825867690D+13 Z= 8.094720856277D+12
I= 19 X= -1.462333229649D+12 Y= -1.705259317049D+14 Z= -6.271439498761D+13
I= 20 X= -4.610438576406D+13 Y= -1.584765550555D+13 Z= 3.736001409269D+13
I= 21 X= -1.668039138848D+12 Y= 1.752555575478D+12 Z= 1.080480616462D+13
I= 22 X= 5.999771768353D+13 Y= 1.323687021421D+13 Z= 2.399673920925D+12
I= 23 X= 4.116132167898D+13 Y= 4.961126373484D+13 Z= -2.868405968050D+13
I= 24 X= 3.078539756614D+13 Y= -3.620195357569D+13 Z= 1.826639370726D+12
I= 25 X= -3.321067906053D+12 Y= -2.581161336929D+12 Z= -1.275954916907D+13
I= 26 X= -1.544117505761D+13 Y= -3.186651307328D+13 Z= -1.100172792800D+14
I= 27 X= 9.945611333374D+11 Y= 1.222097364402D+13 Z= 5.422103995429D+13
I= 28 X= -8.098743455373D+12 Y= 1.350980144201D+12 Z= -4.262605464484D+13
I= 29 X= -1.341216244299D+13 Y= 2.544454045465D+11 Z= -3.247481504273D+12
I= 30 X= -1.613580100525D+13 Y= -2.059942076978D+13 Z= -8.038690368581D+12
I= 31 X= 4.308671692733D+13 Y= 6.109156867550D+12 Z= 3.855314022615D+13
I= 32 X= 1.914219150378D+13 Y= 6.716719764166D+13 Z= -1.085630215238D+13
I= 33 X= 1.183777549082D+14 Y= 3.621657172537D+13 Z= 6.934157382045D+13
I= 34 X= -7.258612870871D+13 Y= -7.780062577212D+13 Z= -1.907343540831D+13
I= 35 X= 8.180520822757D+11 Y= -2.159134900060D+12 Z= 6.901563070557D+11
I= 36 X= -1.141353269139D+11 Y= 1.390670751839D+13 Z= -6.177333003388D+12

I= 37 X= 1.455929158346D+12 Y= -3.823540939292D+13 Z= -1.084067554735D+14

I= 38 X= 2.987864713733D+13 Y= 3.122699562976D+13 Z= 2.472997775932D+13

Backward Direction:

Total Energy: -656.4258264 Hartrees

Potential Energy: -656.6004934 Hartress

Kinetic Energy: 0.1746670 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.393225339634D+13 Y= 5.845072042962D+12 Z= 1.211701032023D+13

I= 1 X= 2.016952262535D+13 Y= 2.154975517160D+12 Z= 3.366809934643D+13

I= 2 X= 7.116073113844D+12 Y= 5.769921725424D+12 Z= -1.552631309311D+13

I= 3 X= -3.960059165486D+12 Y= 2.196432411870D+12 Z= -1.460896938039D+12

I= 4 X= 1.131618641842D+13 Y= 3.034843893867D+12 Z= -1.541435586142D+13

I= 5 X= 1.830866116235D+13 Y= -7.037372502281D+12 Z= -3.626940704934D+12

I= 6 X= 7.827687493237D+12 Y= 5.232040805166D+13 Z= -2.825394305004D+13

I= 7 X= 7.665335933765D+12 Y= -4.837251135197D+13 Z= 2.626052613730D+13

I= 8 X= -8.408132088359D+13 Y= 1.113450337025D+14 Z= -2.187554171990D+13

I= 9 X= 3.482400156630D+12 Y= -4.740283144850D+12 Z= 6.290579153360D+12

I= 10 X= -2.411669141957D+14 Y= 7.758352044410D+13 Z= 4.255250551303D+13

I= 11 X= 4.662395194151D+13 Y= 3.153369492139D+13 Z= -5.633420549384D+12

I= 12 X= 1.378924526556D+13 Y= -1.951633682617D+13 Z= -5.262265227735D+13

I= 13 X= -1.534101621902D+13 Y= 2.613447905336D+13 Z= 3.088169452274D+12

I= 14 X= 6.837980688259D+13 Y= 5.788892886337D+13 Z= -4.638645412716D+13

I= 15 X= 8.103684274288D+12 Y= -6.249600512337D+13 Z= 2.146203333444D+13

I= 16 X= -6.647441972539D+13 Y= -6.782216306355D+13 Z= 3.880970825114D+13

I= 17 X= 1.029537293428D+13 Y= 3.665512595338D+12 Z= 2.129731123410D+12

I= 18 X= -4.109575760171D+13 Y= -9.348134121387D+13 Z= 7.788666198808D+12

I= 19 X= -1.686500470201D+12 Y= -1.706006073444D+14 Z= -6.248324358930D+13

I= 20 X= -4.594871734396D+13 Y= -1.605675626115D+13 Z= 3.733331158688D+13

I= 21 X= -1.801471676400D+12 Y= 1.668730276245D+12 Z= 1.047907702062D+13

I= 22 X= 5.997387220321D+13 Y= 1.361252818204D+13 Z= 1.094269302659D+12

I= 23 X= 4.164633480021D+13 Y= 4.940014271753D+13 Z= -2.883542767353D+13
I= 24 X= 3.055158021531D+13 Y= -3.633327504312D+13 Z= 1.441501755848D+12
I= 25 X= -3.466082296704D+12 Y= -2.727656193214D+12 Z= -1.283438056652D+13
I= 26 X= -1.579985919107D+13 Y= -3.225888580086D+13 Z= -1.100610434923D+14
I= 27 X= 1.293497331920D+12 Y= 1.247265364657D+13 Z= 5.413428280888D+13
I= 28 X= -8.083930373661D+12 Y= 9.069881581655D+11 Z= -4.231177833242D+13
I= 29 X= -1.408374170288D+13 Y= 4.430867878174D+11 Z= -3.483028666630D+12
I= 30 X= -1.609625230718D+13 Y= -2.072938831361D+13 Z= -8.330398334474D+12
I= 31 X= 4.262240768271D+13 Y= 5.971793319499D+12 Z= 3.856764824726D+13
I= 32 X= 1.778336049517D+13 Y= 6.829562419139D+13 Z= -1.166530893433D+13
I= 33 X= 1.184196614926D+14 Y= 3.605232567951D+13 Z= 6.910922736603D+13
I= 34 X= -7.214833722760D+13 Y= -7.810542762998D+13 Z= -1.915722502921D+13
I= 35 X= 8.107460494645D+11 Y= -1.988488592910D+12 Z= 1.772801996708D+12
I= 36 X= -2.475216562017D+12 Y= 1.092446736853D+13 Z= -7.265627782268D+12
I= 37 X= 3.562232149160D+12 Y= -3.716611377282D+13 Z= -1.110336523878D+14
I= 38 X= 3.103214036929D+13 Y= 3.110679952765D+13 Z= 2.276814702845D+13

Seed: 9339681929

CM Start Point Coordinates: bohr

I= 0 X= -2.269640480657D+00 Y= 2.335385827948D+00 Z= -4.515508349735D-01
I= 1 X= -2.674712430158D+00 Y= -5.304525251958D-02 Z= -1.886979643548D+00
I= 2 X= -2.082346705336D+00 Y= 1.727815481082D+00 Z= 2.146740081640D+00
I= 3 X= -2.657283511768D+00 Y= -2.051999956054D+00 Z= -1.305938502524D-01
I= 4 X= -2.321546595037D+00 Y= -1.057666259948D+00 Z= 2.331411778185D+00
I= 5 X= 4.580210116549D+00 Y= 2.273358581096D+00 Z= -1.388730569582D+00
I= 6 X= 2.363533939172D+00 Y= 5.358243491488D-01 Z= -3.102730245406D+00
I= 7 X= 6.289282098962D+00 Y= 1.240712698812D+00 Z= -1.679955738943D+00
I= 8 X= 4.310266391737D+00 Y= 3.814875774535D+00 Z= -2.698827021215D+00
I= 9 X= -2.060247355394D+00 Y= -2.487960448629D+00 Z= 4.731258335579D+00
I= 10 X= -3.835871091046D+00 Y= -3.368139169177D+00 Z= 5.619419013523D+00

I= 11 X= -7.996379259735D-01 Y= -4.427450391855D+00 Z= 4.194387261759D+00
I= 12 X= -1.211910884044D+00 Y= -1.050245447238D+00 Z= 6.375803331967D+00
I= 13 X= -1.869610399891D+00 Y= 3.499281573772D+00 Z= 4.305607856193D+00
I= 14 X= -3.483930877965D+00 Y= 4.387305922397D+00 Z= 5.391657370032D+00
I= 15 X= -8.234851032317D-01 Y= 2.687268623698D+00 Z= 5.891449302923D+00
I= 16 X= -9.177884016266D-01 Y= 5.063571839469D+00 Z= 3.723790183231D+00
I= 17 X= -2.268977896580D+00 Y= 4.907979263328D+00 Z= -1.644042717918D+00
I= 18 X= -4.365132691731D+00 Y= 5.644957186076D+00 Z= -1.802522674646D+00
I= 19 X= -1.127298094283D+00 Y= 6.211853636856D+00 Z= -6.777010643008D-01
I= 20 X= -1.532625900630D+00 Y= 4.444958607381D+00 Z= -3.747043469960D+00
I= 21 X= -3.293356438634D+00 Y= -1.514373579199D-01 Z= -4.644938394915D+00
I= 22 X= -5.293898475091D+00 Y= -1.035237140632D+00 Z= -5.236658401345D+00
I= 23 X= -3.349195593003D+00 Y= 1.887303664755D+00 Z= -5.690466747207D+00
I= 24 X= -1.617382042710D+00 Y= -1.630873002062D+00 Z= -5.773780952946D+00
I= 25 X= -3.417651173362D+00 Y= -4.814407093062D+00 Z= -6.346401599243D-01
I= 26 X= -4.156286202141D+00 Y= -5.166448494950D+00 Z= -2.687320270575D+00
I= 27 X= -1.706570922514D+00 Y= -6.272449327355D+00 Z= -1.202388424354D-01
I= 28 X= -5.377250362833D+00 Y= -5.302103199715D+00 Z= 7.867920656092D-01
I= 29 X= 3.437380695138D+00 Y= -3.590913485734D+00 Z= -1.616836938283D+00
I= 30 X= 3.677648566712D+00 Y= -3.095823355798D+00 Z= 9.449361278525D-01
I= 31 X= 1.868918302899D+00 Y= -4.749185015596D+00 Z= -2.406612876001D+00
I= 32 X= 4.993614857111D+00 Y= -3.214790750357D+00 Z= -2.999813270168D+00
I= 33 X= 5.463324879263D+00 Y= -2.257664771080D+00 Z= 1.500241064458D+00
I= 34 X= 2.837687598459D+00 Y= -3.868762772222D+00 Z= 2.676861425665D+00
I= 35 X= 1.114361123561D+00 Y= 8.263402648239D-03 Z= -4.059865978599D-01
I= 36 X= 3.952820055090D+00 Y= 2.540968680994D+00 Z= 1.193106639964D+00
I= 37 X= 4.860622009125D+00 Y= 1.479449204043D+00 Z= 3.042901005115D+00
I= 38 X= 3.172574504278D+00 Y= 4.321371806175D+00 Z= 2.120240099177D+00

Forward Direction:

Total Energy: -656.4387555 Hartrees

Potential Energy: -656.6235648 Hartress

Kinetic Energy: 0.1848093 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.354789029292D+12 Y= 2.098775920670D+12 Z= 5.105687902992D+12
I= 1 X= 1.381974188006D+13 Y= 1.549657945059D+13 Z= -2.275064154163D+13
I= 2 X= 1.933575416808D+13 Y= 1.301567010103D+13 Z= -2.118421279094D+13
I= 3 X= 7.134749875387D+12 Y= 6.769016286041D+12 Z= 3.205037202149D+13
I= 4 X= -4.583841127146D+12 Y= -3.848249824895D+12 Z= 1.799689341476D+13
I= 5 X= -7.039050709435D+12 Y= -3.400547099300D+12 Z= 1.368849615909D+13
I= 6 X= -1.343772963728D+13 Y= -1.895139656639D+13 Z= -1.098730111876D+14
I= 7 X= -2.938719656666D+12 Y= 1.699160450112D+13 Z= 1.836363773025D+13
I= 8 X= -3.670195383407D+12 Y= 1.283961229884D+14 Z= -4.461328685568D+13
I= 9 X= -9.619696045251D+12 Y= 9.697099291325D+12 Z= 8.835383980224D+12
I= 10 X= 8.015325602220D+13 Y= 1.955575172112D+13 Z= -1.234028315910D+14
I= 11 X= 2.737738099350D+13 Y= -7.158484226474D+12 Z= 3.903367267517D+13
I= 12 X= 4.171700222427D+13 Y= -5.704767231742D+13 Z= -1.050957765416D+13
I= 13 X= 7.881525036844D+12 Y= -2.315364749861D+13 Z= -3.875756982328D+12
I= 14 X= 8.552598336803D+13 Y= 3.547757728673D+13 Z= 2.786290888833D+13
I= 15 X= -9.552966889942D+13 Y= 1.093815314123D+13 Z= -4.930054193073D+12
I= 16 X= 1.860186301344D+13 Y= -6.120455105552D+12 Z= -7.414511275965D+13
I= 17 X= -8.126634472628D+12 Y= -4.045975663598D+12 Z= -6.604599826282D+11
I= 18 X= 3.429632601525D+12 Y= 5.181743720854D+13 Z= 2.689716350279D+13
I= 19 X= -9.736733710253D+13 Y= -1.052916462352D+14 Z= -8.960338313287D+13
I= 20 X= -8.029625283031D+12 Y= -1.488732670617D+13 Z= 2.539259957056D+13
I= 21 X= 8.853186156328D+12 Y= 1.693993927293D+13 Z= 2.016525861258D+13
I= 22 X= -4.975705370234D+13 Y= 5.496028337990D+13 Z= -1.581820107589D+13
I= 23 X= -9.156444778739D+13 Y= 2.927776821070D+13 Z= -1.137309478283D+13
I= 24 X= 3.312623879411D+13 Y= -1.299850784858D+14 Z= -3.779825369959D+13
I= 25 X= -2.742661815268D+12 Y= 5.122086498840D+12 Z= -3.936042133538D+12
I= 26 X= -1.479112539487D+13 Y= -7.494365666290D+13 Z= -1.220163261816D+14

I= 27 X= -6.649538877693D+13 Y= 6.283498291898D+12 Z= -9.374815800242D+12
I= 28 X= -2.589966543713D+13 Y= -1.319324650043D+13 Z= -2.164959729805D+13
I= 29 X= -9.476447869327D+12 Y= 8.200142956951D+12 Z= -1.155396136051D+13
I= 30 X= -2.884687797232D+11 Y= -1.087663384062D+13 Z= 2.558397064233D+13
I= 31 X= -2.544839381924D+13 Y= 6.962052485449D+13 Z= 5.339068541807D+13
I= 32 X= 2.234859825023D+13 Y= -6.075079056801D+13 Z= 1.001914511289D+13
I= 33 X= 4.546532591446D+13 Y= 3.589290460732D+13 Z= 5.125056960519D+13
I= 34 X= 1.228711349088D+14 Y= 1.006794272378D+14 Z= -1.022699990895D+14
I= 35 X= 1.981088402506D+11 Y= -3.869943727320D+12 Z= 5.629761018027D+11
I= 36 X= -1.491488807769D+13 Y= -6.851465045268D+12 Z= -1.759211060711D+13
I= 37 X= 5.022785998588D+13 Y= 7.825159269323D+12 Z= 8.335872219806D+13
I= 38 X= -1.897557709734D+13 Y= 1.614827345506D+13 Z= -1.142478693779D+14

Backward Direction:

Total Energy: -656.4387575 Hartrees

Potential Energy: -656.6235648 Hartress

Kinetic Energy: 0.1848073 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.577631757466D+12 Y= 1.807775631293D+12 Z= 5.219564034678D+12
I= 1 X= 1.347603427209D+13 Y= 1.474827352169D+13 Z= -2.319985168344D+13
I= 2 X= 1.901585490662D+13 Y= 1.330972831543D+13 Z= -2.165765896386D+13
I= 3 X= 6.479292820550D+12 Y= 6.784342734439D+12 Z= 3.110068212667D+13
I= 4 X= -3.462754517297D+12 Y= -3.948271126200D+12 Z= 1.725191333346D+13
I= 5 X= -8.889295383914D+12 Y= -6.031797283766D+12 Z= 8.435165433143D+12
I= 6 X= 2.800744137817D+13 Y= 2.836324280800D+13 Z= -9.122539085760D+13
I= 7 X= 4.631242127773D+12 Y= 2.415874807289D+13 Z= 1.882676632821D+13
I= 8 X= 5.890353946533D+12 Y= 1.361240977295D+14 Z= -4.372384241291D+13
I= 9 X= -9.263381910008D+12 Y= 9.864431107704D+12 Z= 8.432631744915D+12
I= 10 X= 8.021842302252D+13 Y= 2.038387038292D+13 Z= -1.243627927459D+14
I= 11 X= 2.727447041608D+13 Y= -7.167536873496D+12 Z= 3.901366125051D+13
I= 12 X= 4.192582734273D+13 Y= -5.699174100373D+13 Z= -1.070787835764D+13

I= 13 X= 7.952159115399D+12 Y= -2.318801533901D+13 Z= -4.024420066829D+12
I= 14 X= 8.564606632133D+13 Y= 3.526584940674D+13 Z= 2.789433637062D+13
I= 15 X= -9.530883563132D+13 Y= 1.073561088181D+13 Z= -5.295737868885D+12
I= 16 X= 1.858647983539D+13 Y= -6.055357835689D+12 Z= -7.409362809306D+13
I= 17 X= -8.018466345439D+12 Y= -4.284686624925D+12 Z= -6.840993081167D+11
I= 18 X= 3.452439304313D+12 Y= 5.143686861239D+13 Z= 2.658496772121D+13
I= 19 X= -9.759600234165D+13 Y= -1.053678202700D+14 Z= -8.936759357956D+13
I= 20 X= -7.870833305294D+12 Y= -1.510062316016D+13 Z= 2.536536127839D+13
I= 21 X= 8.717076239170D+12 Y= 1.685443198525D+13 Z= 1.983299357421D+13
I= 22 X= -4.978137765045D+13 Y= 5.534347909402D+13 Z= -1.714979920006D+13
I= 23 X= -9.106970266573D+13 Y= 2.906241096641D+13 Z= -1.152750003348D+13
I= 24 X= 3.288772979368D+13 Y= -1.301190349738D+14 Z= -3.819111926344D+13
I= 25 X= -2.890585982238D+12 Y= 4.972652160669D+12 Z= -4.012375053105D+12
I= 26 X= -1.515700667529D+13 Y= -7.534390252049D+13 Z= -1.220609685492D+14
I= 27 X= -6.619045430061D+13 Y= 6.540228367382D+12 Z= -9.463313762110D+12
I= 28 X= -2.588455512290D+13 Y= -1.364614737592D+13 Z= -2.132901489740D+13
I= 29 X= -1.016150265589D+13 Y= 8.392569509341D+12 Z= -1.179423487864D+13
I= 30 X= -2.481265172014D+11 Y= -1.100920923818D+13 Z= 2.528640942914D+13
I= 31 X= -2.592201962756D+13 Y= 6.948040504845D+13 Z= 5.340548455368D+13
I= 32 X= 2.096250171124D+13 Y= -5.959972165723D+13 Z= 9.193905262168D+12
I= 33 X= 4.550807337942D+13 Y= 3.572536289708D+13 Z= 5.101356101658D+13
I= 34 X= 1.233177108676D+14 Y= 1.003685094002D+14 Z= -1.023554699811D+14
I= 35 X= 1.906562089029D+11 Y= -3.695873329498D+12 Z= 1.667345540559D+12
I= 36 X= -1.732334541814D+13 Y= -9.893545118460D+12 Z= -1.870224248677D+13
I= 37 X= 5.237642684828D+13 Y= 8.915910763567D+12 Z= 8.067911546848D+13
I= 38 X= -1.779893853281D+13 Y= 1.602566556813D+13 Z= -1.162490650841D+14

Seed: 9370370777

CM Start Point Coordinates: bohr

I= 0 X= -2.279331195446D+00 Y= 2.236807745734D+00 Z= -6.650357972417D-01

I= 1 X= -2.898767705031D+00 Y= -6.792149509468D-02 Z= -2.014984950057D+00
I= 2 X= -1.918430698696D+00 Y= 1.543570661491D+00 Z= 2.081325639432D+00
I= 3 X= -2.804410720864D+00 Y= -2.078236367581D+00 Z= -2.130767773925D-01
I= 4 X= -2.132821852869D+00 Y= -1.012287427296D+00 Z= 2.293864205592D+00
I= 5 X= 4.383490281198D+00 Y= 2.439284310238D+00 Z= -1.562218875134D+00
I= 6 X= 2.201695326259D+00 Y= 5.370678185941D-01 Z= -3.288624138053D+00
I= 7 X= 5.690428613978D+00 Y= 1.097691987283D+00 Z= -2.459780472491D+00
I= 8 X= 3.894814082917D+00 Y= 3.905060167291D+00 Z= -2.720268381989D+00
I= 9 X= -2.083758018069D+00 Y= -2.415706826346D+00 Z= 4.699542676409D+00
I= 10 X= -3.777799021285D+00 Y= -2.240291243410D+00 Z= 6.177349030076D+00
I= 11 X= -2.120115494949D+00 Y= -4.434090966300D+00 Z= 4.260914815440D+00
I= 12 X= -2.301549299103D-01 Y= -2.371031577020D+00 Z= 5.745352621259D+00
I= 13 X= -1.784931569246D+00 Y= 3.471877188963D+00 Z= 4.271784873180D+00
I= 14 X= -3.495283220115D+00 Y= 3.287942784601D+00 Z= 5.083463526420D+00
I= 15 X= -5.715198396983D-01 Y= 2.944835338593D+00 Z= 5.848923125731D+00
I= 16 X= -1.285256571477D+00 Y= 5.218148711160D+00 Z= 3.716279685364D+00
I= 17 X= -2.087307939802D+00 Y= 4.811377187928D+00 Z= -1.740503820963D+00
I= 18 X= -3.531327465260D+00 Y= 6.160666022740D+00 Z= -1.130636137481D+00
I= 19 X= -6.487543464229D-01 Y= 6.097633539778D+00 Z= -1.116331937514D+00
I= 20 X= -2.200205315499D+00 Y= 4.431994844878D+00 Z= -3.911242008746D+00
I= 21 X= -3.878028840811D+00 Y= -1.520846034473D-01 Z= -4.759680435958D+00
I= 22 X= -5.953160127774D+00 Y= 4.116182534243D-01 Z= -4.716894958321D+00
I= 23 X= -2.858458249625D+00 Y= 1.463220170127D+00 Z= -5.343477964021D+00
I= 24 X= -3.209536217312D+00 Y= -1.861867646323D+00 Z= -5.510589008927D+00
I= 25 X= -3.285233127972D+00 Y= -4.770098547961D+00 Z= -8.587378458246D-01
I= 26 X= -2.592356806820D+00 Y= -5.296183995544D+00 Z= -2.710794696355D+00
I= 27 X= -2.351010734034D+00 Y= -6.121135178721D+00 Z= 4.608605863393D-01
I= 28 X= -5.400558048526D+00 Y= -5.467124841629D+00 Z= -5.888302864559D-01
I= 29 X= 3.631310807659D+00 Y= -3.224041263523D+00 Z= -1.491226980257D+00
I= 30 X= 3.422780690815D+00 Y= -3.324972224533D+00 Z= 1.244562551649D+00

I= 31 X= 1.998035709800D+00 Y= -4.467392285703D+00 Z= -2.829458776772D+00
I= 32 X= 5.547677850589D+00 Y= -1.791974060377D+00 Z= -2.061962041559D+00
I= 33 X= 4.885091951591D+00 Y= -2.311756738528D+00 Z= 2.455114263904D+00
I= 34 X= 2.421362144782D+00 Y= -5.040866571025D+00 Z= 2.101640727426D+00
I= 35 X= 1.165197887154D+00 Y= -1.404963894198D-02 Z= -3.025835465107D-01
I= 36 X= 4.148765423841D+00 Y= 2.677387059560D+00 Z= 1.145514557097D+00
I= 37 X= 5.073646553406D+00 Y= 1.429069371785D+00 Z= 2.712429170844D+00
I= 38 X= 3.448013902533D+00 Y= 4.246425176194D+00 Z= 1.775067230786D+00

Forward Direction:

Total Energy: -656.4416215 Hartrees

Potential Energy: -656.6103943 Hartress

Kinetic Energy: 0.1687727 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.364355474438D+12 Y= 9.348892579793D+12 Z= -1.306687983259D+13
I= 1 X= 1.908393982248D+13 Y= -1.327813988503D+13 Z= 1.034058540274D+13
I= 2 X= -5.534376481259D+12 Y= -1.204619561253D+13 Z= 7.717729108197D+12
I= 3 X= 1.086723787999D+13 Y= 2.702575949081D+13 Z= 1.576338235850D+12
I= 4 X= -3.539814301257D+12 Y= -2.288069687882D+13 Z= -2.041909107925D+13
I= 5 X= 2.445222758129D+13 Y= -7.667536022883D+12 Z= 2.415199671737D+13
I= 6 X= 1.814431142045D+12 Y= -2.708087382971D+13 Z= 4.725807932450D+13
I= 7 X= -1.124773025041D+14 Y= 9.255858903942D+13 Z= 1.361421673199D+13
I= 8 X= -3.927360865439D+13 Y= -8.149586311852D+13 Z= -6.836381376705D+13
I= 9 X= -4.442778296918D+12 Y= 2.022244314399D+13 Z= -8.477997892590D+12
I= 10 X= -1.630191968962D+13 Y= 4.507252745703D+13 Z= 6.866936015094D+12
I= 11 X= 5.906453550720D+13 Y= 2.216816495945D+13 Z= -3.561196233664D+13
I= 12 X= -6.359199355213D+13 Y= -3.938784354106D+13 Z= -2.690911226317D+13
I= 13 X= 5.377911067756D+12 Y= 1.274809844378D+13 Z= 2.916809517048D+12
I= 14 X= 6.017386401793D+13 Y= -3.357853264926D+13 Z= -4.321299660776D+13
I= 15 X= 1.043706505558D+14 Y= 5.428049383657D+12 Z= 2.806240035369D+13
I= 16 X= 6.004069957534D+13 Y= -2.689472956096D+13 Z= 6.077609688366D+13

I= 17 X= -4.845252216034D+12 Y= 3.500393656195D+12 Z= -4.065959557373D+13
I= 18 X= -5.553287270213D+13 Y= 7.781584153332D+13 Z= 4.871406113834D+13
I= 19 X= 1.271593702804D+13 Y= -2.129373534998D+13 Z= 6.269411333466D+13
I= 20 X= 3.104071373795D+13 Y= -8.159037538430D+13 Z= 1.455994004976D+14
I= 21 X= 7.837122767859D+12 Y= 9.859878583100D+12 Z= 1.062888949490D+13
I= 22 X= -1.297991651786D+14 Y= 2.259511891848D+13 Z= -2.969065552147D+13
I= 23 X= -3.290553593714D+13 Y= -4.060619707119D+13 Z= 3.516765313875D+13
I= 24 X= 2.427142903588D+13 Y= -2.644770102805D+13 Z= 1.338460938850D+12
I= 25 X= -9.139845259786D+12 Y= 1.287796027066D+11 Z= -6.767078223605D+12
I= 26 X= 2.290174974829D+13 Y= -1.346009431754D+13 Z= 5.929194890487D+13
I= 27 X= 2.556550404490D+13 Y= 4.878279753453D+12 Z= 1.568063987256D+13
I= 28 X= -1.881819996112D+14 Y= -5.041299164114D+13 Z= 1.037871494730D+12
I= 29 X= 8.572634547928D+10 Y= 9.041068608687D+12 Z= 5.606893869559D+12
I= 30 X= -1.210994152423D+12 Y= 1.041801845164D+13 Z= -9.315494403522D+12
I= 31 X= -3.909963555236D+13 Y= -7.275319204512D+12 Z= -3.910704854770D+13
I= 32 X= 6.006322288787D+12 Y= 6.597145429129D+13 Z= 1.254788305604D+13
I= 33 X= 3.424519530865D+13 Y= 3.087899498697D+13 Z= 1.584109399087D+13
I= 34 X= -6.553646098659D+13 Y= -3.968570777636D+13 Z= 4.211173963045D+13
I= 35 X= -1.900891183478D+12 Y= -5.603382599804D+12 Z= -1.261881016389D+12
I= 36 X= -4.226309951750D+12 Y= 1.225978436358D+13 Z= 5.841959621896D+12
I= 37 X= 5.445594373558D+13 Y= -1.715239639364D+13 Z= 3.328898760078D+13
I= 38 X= -1.387168978652D+13 Y= 1.243407061912D+13 Z= 9.816047290111D+13

Backward Direction:

Total Energy: -656.4416079 Hartrees

Potential Energy: -656.6103943 Hartress

Kinetic Energy: 0.1687863 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.024026597595D+12 Y= 8.904472419348D+12 Z= -1.289296643556D+13

I= 1 X= 1.855902422452D+13 Y= -1.442096432096D+13 Z= 9.654544697758D+12

I= 2 X= -6.022931598882D+12 Y= -1.159710533980D+13 Z= 6.994674759843D+12

I= 3 X= 9.866213686762D+12 Y= 2.704916628094D+13 Z= 1.259570797760D+11
I= 4 X= -1.827673415935D+12 Y= -2.303345096325D+13 Z= -2.155683623011D+13
I= 5 X= 2.162650517874D+13 Y= -1.168602217126D+13 Z= 1.612902844520D+13
I= 6 X= 6.511013998819D+13 Y= 4.517877824331D+13 Z= 7.573701470191D+13
I= 7 X= -1.009163392988D+14 Y= 1.035043620113D+14 Z= 1.432151392148D+13
I= 8 X= -2.467258923551D+13 Y= -6.969358007485D+13 Z= -6.700544040001D+13
I= 9 X= -3.898609814929D+12 Y= 2.047799489075D+13 Z= -9.093087364254D+12
I= 10 X= -1.620239562816D+13 Y= 4.633724312503D+13 Z= 5.400868432853D+12
I= 11 X= 5.890736888371D+13 Y= 2.215433963010D+13 Z= -3.564252410186D+13
I= 12 X= -6.327307258036D+13 Y= -3.930242436202D+13 Z= -2.721196017010D+13
I= 13 X= 5.485784529364D+12 Y= 1.269561134522D+13 Z= 2.689768946888D+12
I= 14 X= 6.035725657492D+13 Y= -3.390188673873D+13 Z= -4.316500005773D+13
I= 15 X= 1.047079105605D+14 Y= 5.118723695118D+12 Z= 2.750392255946D+13
I= 16 X= 6.001720616198D+13 Y= -2.679531200428D+13 Z= 6.085472506429D+13
I= 17 X= -4.680056172294D+12 Y= 3.135830570181D+12 Z= -4.069569791724D+13
I= 18 X= -5.549804195064D+13 Y= 7.723463126182D+13 Z= 4.823727089311D+13
I= 19 X= 1.236671591652D+13 Y= -2.141006952177D+13 Z= 6.305421479612D+13
I= 20 X= 3.128322331258D+13 Y= -8.191612504073D+13 Z= 1.455578017442D+14
I= 21 X= 7.629253592103D+12 Y= 9.729290522867D+12 Z= 1.012144916739D+13
I= 22 X= -1.298363130869D+14 Y= 2.318034135128D+13 Z= -3.172429285584D+13
I= 23 X= -3.214995350770D+13 Y= -4.093509400254D+13 Z= 3.493184303847D+13
I= 24 X= 2.390717440137D+13 Y= -2.665228145709D+13 Z= 7.384705475002D+11
I= 25 X= -9.365757341851D+12 Y= -9.943883970160D+10 Z= -6.883655046452D+12
I= 26 X= 2.234297017253D+13 Y= -1.407135599847D+13 Z= 5.922377039510D+13
I= 27 X= 2.603120471700D+13 Y= 5.270361905970D+12 Z= 1.554548440735D+13
I= 28 X= -1.881589229065D+14 Y= -5.110466889886D+13 Z= 1.527469917015D+12
I= 29 X= -9.604999658991D+11 Y= 9.334945428245D+12 Z= 5.239944422303D+12
I= 30 X= -1.149382825458D+12 Y= 1.021554724515D+13 Z= -9.769934508464D+12
I= 31 X= -3.982296424844D+13 Y= -7.489312349157D+12 Z= -3.908444708172D+13
I= 32 X= 3.889454127824D+12 Y= 6.772938460751D+13 Z= 1.128756393872D+13

I= 33 X= 3.431047989414D+13 Y= 3.062312268153D+13 Z= 1.547913079352D+13
I= 34 X= -6.485444324956D+13 Y= -4.016054632329D+13 Z= 4.198120715430D+13
I= 35 X= -1.912272959107D+12 Y= -5.337539584357D+12 Z= 4.247291422336D+11
I= 36 X= -7.904543406637D+12 Y= 7.613872429802D+12 Z= 4.146548974268D+12
I= 37 X= 5.773726841789D+13 Y= -1.548658377298D+13 Z= 2.919665058925D+13
I= 38 X= -1.207470909725D+13 Y= 1.224682194736D+13 Z= 9.510421573853D+13

Cobalt:

Seed: 10237587652

CM Start Point Coordinates: bohr

I= 0 X= -2.243061721481D+00 Y= -1.982695049738D+00 Z= -7.004289238439D-02
I= 1 X= 1.079903052682D-02 Y= -2.780222252360D+00 Z= -1.525619876072D+00
I= 2 X= -1.343857110796D+00 Y= -1.128907578502D+00 Z= 2.422517664742D+00
I= 3 X= 2.174413352669D+00 Y= -2.051394769374D+00 Z= -6.069807890396D-02
I= 4 X= 1.320667405128D+00 Y= -1.258081422353D+00 Z= 2.374034282857D+00
I= 5 X= -2.823103744933D+00 Y= 2.943406799326D+00 Z= -2.304528334381D+00
I= 6 X= 3.084010083901D-02 Y= 2.317499116063D+00 Z= -3.276443515044D+00
I= 7 X= -2.442699135610D+00 Y= 4.735725265054D+00 Z= -3.521823024862D+00
I= 8 X= -4.099064427812D+00 Y= 2.053167595198D+00 Z= -3.439213841483D+00
I= 9 X= 2.947116100133D+00 Y= -5.086884927773D-01 Z= 4.480213131157D+00
I= 10 X= 3.672842115059D+00 Y= -2.461606116119D+00 Z= 5.398125167720D+00
I= 11 X= 4.949504808415D+00 Y= 6.377762141036D-01 Z= 4.168484663961D+00
I= 12 X= 1.148310485743D+00 Y= 5.158261272794D-01 Z= 6.068628263530D+00
I= 13 X= -3.004704475632D+00 Y= -5.679053736911D-01 Z= 4.744697158795D+00
I= 14 X= -2.622613714303D+00 Y= -1.902747698535D+00 Z= 6.291464053223D+00
I= 15 X= -2.520148072395D+00 Y= 1.248781843163D+00 Z= 5.469117667323D+00
I= 16 X= -4.996344450741D+00 Y= -4.317655788405D-01 Z= 3.800317208378D+00
I= 17 X= -4.784255577106D+00 Y= -2.255214059224D+00 Z= -9.654702296825D-01
I= 18 X= -5.803020034721D+00 Y= -3.928062346792D+00 Z= -1.335673929821D-01

I= 19 X= -5.842153129430D+00 Y= -8.154151916394D-01 Z= -5.484104945473D-01
I= 20 X= -5.025235238598D+00 Y= -2.414632054556D+00 Z= -2.861707861361D+00
I= 21 X= -2.947952707377D-02 Y= -3.749325808843D+00 Z= -4.183485180998D+00
I= 22 X= -8.603848402458D-01 Y= -6.010165930358D+00 Z= -4.181135810835D+00
I= 23 X= -1.267083477315D+00 Y= -2.412343996021D+00 Z= -5.686472400622D+00
I= 24 X= 1.908660203017D+00 Y= -3.854776398512D+00 Z= -4.995277361713D+00
I= 25 X= 4.819629488852D+00 Y= -2.618878419408D+00 Z= -8.867852225410D-01
I= 26 X= 5.052396471510D+00 Y= -2.741122263448D+00 Z= -3.155865319098D+00
I= 27 X= 6.376437523597D+00 Y= -1.370904215868D+00 Z= -2.539240879730D-01
I= 28 X= 5.860768851020D+00 Y= -4.362672617320D+00 Z= -1.977678461824D-01
I= 29 X= 2.823210424617D+00 Y= 3.301693865421D+00 Z= -2.410110516431D+00
I= 30 X= 2.525428338475D+00 Y= 3.801625946657D+00 Z= 1.787092471508D-01
I= 31 X= 4.181038579097D+00 Y= 1.839718501241D+00 Z= -2.797242529201D+00
I= 32 X= 2.368198263206D+00 Y= 4.775305989548D+00 Z= -3.572826879438D+00
I= 33 X= 1.850034201395D+00 Y= 5.765100109286D+00 Z= 7.535987305988D-01
I= 34 X= 4.091724052485D+00 Y= 3.023252843368D+00 Z= 1.597453271871D+00
I= 35 X= 6.929885148789D-02 Y= 1.068620971530D+00 Z= -3.770815768185D-01
I= 36 X= -2.709363346336D+00 Y= 3.431962002060D+00 Z= 2.788693333310D-01
I= 37 X= -2.055414211212D+00 Y= 5.171564486883D+00 Z= 1.001088555622D+00
I= 38 X= -4.239646599710D+00 Y= 2.700480280697D+00 Z= 1.448954486202D+00

Forward Direction:

Total Energy: -691.9853800 Hartrees

Potential Energy: -692.1731457 Hartress

Kinetic Energy: 0.1877658 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.548353480821D+13 Y= 1.513803355910D+13 Z= 2.767984503238D+12
I= 1 X= -1.195882972113D+13 Y= 1.252131922266D+13 Z= 1.297401809663D+12
I= 2 X= -2.371110998808D+13 Y= 9.279882659294D+12 Z= 3.546483555085D+12
I= 3 X= -2.322787104203D+13 Y= 8.866875389344D+12 Z= -4.956845637453D+12
I= 4 X= -4.864351998690D+12 Y= -3.551986494297D+12 Z= -2.174911679500D+12

I= 5 X= 1.235310775838D+13 Y= 1.228897081093D+13 Z= -8.550554616242D+12
I= 6 X= 7.269208600583D+13 Y= 1.210684562777D+13 Z= -4.775099459137D+13
I= 7 X= 2.992110239335D+13 Y= -1.401899424482D+14 Z= 9.406243374774D+13
I= 8 X= 1.630456451774D+12 Y= -3.485585651415D+13 Z= -3.946120414885D+13
I= 9 X= 2.717615699449D+13 Y= -2.529860656446D+12 Z= 5.506988218283D+12
I= 10 X= 3.958303450096D+13 Y= 2.528961768363D+13 Z= -2.624808171302D+13
I= 11 X= -1.270147134620D+14 Y= -2.233275411931D+13 Z= 6.670085016843D+13
I= 12 X= -3.941215183117D+12 Y= 5.623420866191D+13 Z= -2.118904851304D+13
I= 13 X= -6.681669667806D+12 Y= -3.425540925911D+13 Z= 1.310308911603D+13
I= 14 X= 1.491643169620D+12 Y= 7.201639231807D+13 Z= -1.012375472672D+14
I= 15 X= 8.409983864544D+13 Y= 1.791948357724D+13 Z= -4.030632956010D+13
I= 16 X= -1.254345360995D+13 Y= 3.380809074928D+13 Z= -7.422691716448D+13
I= 17 X= 1.243556630022D+13 Y= 1.610770544198D+13 Z= -1.064957846684D+13
I= 18 X= -3.621180748433D+13 Y= -1.571454213788D+13 Z= 2.000156338946D+13
I= 19 X= -6.196398080908D+13 Y= 1.599527838516D+13 Z= 5.992005632560D+13
I= 20 X= 6.127836268139D+13 Y= -6.447080831079D+13 Z= -8.430284710066D+12
I= 21 X= 2.872379644561D+12 Y= -8.183113669581D+12 Z= 1.377753391987D+13
I= 22 X= 4.775082909311D+13 Y= 9.553835968673D+13 Z= -7.040796027619D+13
I= 23 X= -3.116628639035D+13 Y= -1.752543293729D+13 Z= 1.922573888668D+13
I= 24 X= -1.798956849810D+13 Y= -2.137182687455D+13 Z= 1.024623542352D+14
I= 25 X= 4.771655142348D+12 Y= -1.632114883770D+13 Z= -7.324785174499D+12
I= 26 X= -7.522812537200D+12 Y= 6.441438834731D+13 Z= -1.168328172039D+13
I= 27 X= 4.550853888853D+13 Y= 8.206583649439D+13 Z= 3.616254376542D+13
I= 28 X= -6.900512175269D+11 Y= -2.056343981839D+12 Z= 4.989080697952D+13
I= 29 X= -1.069877167868D+13 Y= 1.532490248200D+13 Z= -1.142686414920D+13
I= 30 X= 1.386442118368D+13 Y= -3.004877578779D+12 Z= -1.042678819341D+13
I= 31 X= 4.032126631630D+13 Y= 2.512817259297D+13 Z= -1.088060585493D+14
I= 32 X= -2.795565599790D+13 Y= 6.440976155362D+13 Z= 9.217736912999D+12
I= 33 X= 8.292264463425D+13 Y= -4.690368811619D+13 Z= -2.756420549618D+13
I= 34 X= -9.062124410053D+13 Y= -3.448099936888D+13 Z= -4.666383577204D+13

I= 35 X= -7.439304611038D+12 Y= -6.138807887301D+12 Z= -1.835352044374D+12

I= 36 X= 5.850628236809D+12 Y= 1.321645903827D+12 Z= 3.339164140706D+13

I= 37 X= -1.367711067752D+14 Y= -5.241020416243D+13 Z= 6.349947368501D+12

I= 38 X= -3.769976630357D+13 Y= -2.753546785579D+13 Z= 5.440151640281D+13

Backward Direction:

Total Energy: -691.9852557 Hartrees

Potential Energy: -692.1731457 Hartress

Kinetic Energy: 0.1878901 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.566381472787D+13 Y= 1.716538616576D+13 Z= 5.746397986551D+12

I= 1 X= -1.059563460278D+13 Y= 1.252170585854D+13 Z= 1.297202359357D+12

I= 2 X= -2.298049726452D+13 Y= 8.163242172221D+12 Z= 5.172016541786D+12

I= 3 X= -2.304736611444D+13 Y= 6.839326006960D+12 Z= -7.935663563024D+12

I= 4 X= -4.133586276838D+12 Y= -2.435160762044D+12 Z= -3.800438699269D+12

I= 5 X= 1.597409199308D+13 Y= -2.129719138136D+10 Z= -2.323407907674D+13

I= 6 X= -6.063280581422D+13 Y= 1.212656302936D+13 Z= -4.775096884678D+13

I= 7 X= 1.049829689625D+13 Y= -1.424732782533D+14 Z= 7.652396581488D+13

I= 8 X= -8.153257017941D+12 Y= -3.964610388545D+13 Z= -4.356878213834D+13

I= 9 X= 2.923109063771D+13 Y= -6.270560662316D+12 Z= 4.303175455972D+12

I= 10 X= 3.822432992748D+13 Y= 2.047304475011D+13 Z= -2.890625706806D+13

I= 11 X= -1.243345134973D+14 Y= -2.974923707337D+13 Z= 6.596465763758D+13

I= 12 X= 1.272972538651D+12 Y= 5.277811527857D+13 Z= -2.079677629134D+13

I= 13 X= -4.626945958270D+12 Y= -3.051467052193D+13 Z= 1.430746819104D+13

I= 14 X= 1.345021371339D+11 Y= 7.683350048443D+13 Z= -9.857852756030D+13

I= 15 X= 8.931296194926D+13 Y= 2.137716384118D+13 Z= -4.069883706436D+13

I= 16 X= -9.864238008436D+12 Y= 4.122240865978D+13 Z= -7.348927050262D+13

I= 17 X= 1.227424698015D+13 Y= 1.632180382417D+13 Z= -6.658063879628D+12

I= 18 X= -3.540815234714D+13 Y= -1.401990232931D+13 Z= 2.808996975712D+13

I= 19 X= -6.239866733368D+13 Y= 1.709535723154D+13 Z= 6.159036010150D+13

I= 20 X= 6.010270267427D+13 Y= -6.910253429128D+13 Z= -4.026420333912D+12

I= 21 X= -6.072025950642D+11 Y= -8.181305023036D+12 Z= 1.377631857838D+13
I= 22 X= 3.875712620968D+13 Y= 9.554024704924D+13 Z= -7.041137098327D+13
I= 23 X= -3.347746199641D+13 Y= -1.331602271516D+13 Z= 1.960022214429D+13
I= 24 X= -2.030128538845D+13 Y= -2.557611232390D+13 Z= 1.020860029668D+14
I= 25 X= 4.610713653320D+12 Y= -1.653597496152D+13 Z= -1.131639506785D+13
I= 26 X= -8.697628188494D+12 Y= 6.904473471534D+13 Z= -1.608748074651D+13
I= 27 X= 4.507441565474D+13 Y= 8.096420981951D+13 Z= 3.449267443128D+13
I= 28 X= 1.135939892950D+11 Y= -3.752108443752D+12 Z= 4.180291780144D+13
I= 29 X= -7.078422633746D+12 Y= 2.763120160915D+13 Z= 3.253296804771D+12
I= 30 X= 1.948639685293D+13 Y= -1.518218097947D+12 Z= 4.125123412682D+11
I= 31 X= 3.054339987832D+13 Y= 2.991820919350D+13 Z= -1.047010900688D+14
I= 32 X= -4.737613832175D+13 Y= 6.669280852743D+13 Z= 2.674993107435D+13
I= 33 X= 8.089630847082D+13 Y= -5.402543042046D+13 Z= -4.394644566864D+12
I= 34 X= -8.986747040208D+13 Y= -4.233659851419D+13 Z= -3.736399893592D+13
I= 35 X= -8.555390742075D+12 Y= -6.138395565293D+12 Z= -1.834018551560D+12
I= 36 X= 1.147303062226D+13 Y= -1.665995756900D+11 Z= 2.255169582660D+13
I= 37 X= -1.388011256328D+14 Y= -4.528388486906D+13 Z= -1.682259110294D+13
I= 38 X= -3.694469890471D+13 Y= -1.968234809735D+13 Z= 4.510184756860D+13

Seed: 11324992302

CM Start Point Coordinates: bohr

I= 0 X= -2.091141532692D+00 Y= -1.970910379039D+00 Z= -8.761879850698D-02
I= 1 X= 1.126285684136D-02 Y= -2.745420412357D+00 Z= -1.517109991710D+00
I= 2 X= -1.312030167462D+00 Y= -1.304036087527D+00 Z= 2.413921791811D+00
I= 3 X= 2.224449192807D+00 Y= -2.097958039527D+00 Z= 2.293797082591D-02
I= 4 X= 1.399263462458D+00 Y= -1.379512240190D+00 Z= 2.430499888593D+00
I= 5 X= -2.697439907596D+00 Y= 3.236757425759D+00 Z= -2.467394510709D+00
I= 6 X= -8.407834363602D-02 Y= 1.324292415486D+00 Z= -3.380707852507D+00
I= 7 X= -1.296768733086D+00 Y= 4.114733564960D+00 Z= -3.694725861432D+00
I= 8 X= -4.093597871334D+00 Y= 2.057892687085D+00 Z= -3.569628615187D+00

I= 9 X= 2.909067793506D+00 Y= -9.314950841219D-01 Z= 4.709219081487D+00
I= 10 X= 1.733809764444D+00 Y= -2.173318918624D+00 Z= 6.427908729753D+00
I= 11 X= 5.199974236192D+00 Y= -1.683089529157D+00 Z= 4.733331919591D+00
I= 12 X= 2.650152504622D+00 Y= 1.343850743643D+00 Z= 5.187952803940D+00
I= 13 X= -2.864985058468D+00 Y= -7.806328508593D-01 Z= 4.481832829626D+00
I= 14 X= -2.615586597636D+00 Y= -2.342583838587D+00 Z= 5.975134173444D+00
I= 15 X= -2.868057345476D+00 Y= 1.007689556483D+00 Z= 5.254275940280D+00
I= 16 X= -4.916366732324D+00 Y= -9.742370619987D-01 Z= 3.734529000307D+00
I= 17 X= -4.819145736189D+00 Y= -2.456661084690D+00 Z= -6.681065768157D-01
I= 18 X= -4.918370024419D+00 Y= -4.482550701690D+00 Z= 1.085994152020D-01
I= 19 X= -6.434362893254D+00 Y= -1.256033795779D+00 Z= 6.882692844953D-01
I= 20 X= -4.850814639180D+00 Y= -2.370536076950D+00 Z= -2.922863250896D+00
I= 21 X= -5.342662335069D-02 Y= -3.735900115967D+00 Z= -4.065581197360D+00
I= 22 X= -1.026902601445D-01 Y= -5.686249120768D+00 Z= -4.176245256478D+00
I= 23 X= -1.699964489217D+00 Y= -3.599819210195D+00 Z= -5.064860433326D+00
I= 24 X= 1.736190131998D+00 Y= -3.269073089500D+00 Z= -5.396268684424D+00
I= 25 X= 4.866221252862D+00 Y= -2.132630709510D+00 Z= -7.376407442722D-01
I= 26 X= 5.118713880595D+00 Y= -1.904039121946D+00 Z= -2.756275399891D+00
I= 27 X= 6.170416612805D+00 Y= -7.198070743378D-01 Z= 3.944447552855D-01
I= 28 X= 5.643546027173D+00 Y= -4.274887954594D+00 Z= -8.366589933060D-01
I= 29 X= 2.657328329401D+00 Y= 3.089568237830D+00 Z= -2.509749404060D+00
I= 30 X= 2.971675960032D+00 Y= 3.692050637578D+00 Z= 4.601394381637D-02
I= 31 X= 4.133631782499D+00 Y= 1.955574813142D+00 Z= -3.348109874756D+00
I= 32 X= 1.685868044534D+00 Y= 4.527530308885D+00 Z= -3.827280861898D+00
I= 33 X= 2.262534137444D+00 Y= 5.573540667816D+00 Z= 9.456320305783D-01
I= 34 X= 3.712111289451D+00 Y= 2.776566260525D+00 Z= 1.718750791069D+00
I= 35 X= -8.203085024044D-02 Y= 1.145311120887D+00 Z= -4.211903327173D-01
I= 36 X= -2.789387990805D+00 Y= 3.963280162972D+00 Z= 1.310055549519D-01
I= 37 X= -1.863206529354D+00 Y= 5.864865674364D+00 Z= 9.207968958223D-01
I= 38 X= -4.408461026407D+00 Y= 3.341485668671D+00 Z= 1.529930123434D+00

Forward Direction:

Total Energy: -691.9926979 Hartrees

Potential Energy: -692.1505561 Hartress

Kinetic Energy: 0.1578582 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.380142820367D+12 Y= -7.453210633519D+12 Z= -1.145237125884D+13
I= 1 X= -1.014705333789D+13 Y= 1.268881990252D+13 Z= 8.574272856902D+12
I= 2 X= 1.733549214248D+13 Y= 1.481325402100D+13 Z= 1.576266759656D+12
I= 3 X= -1.980401677216D+13 Y= -9.571657826432D+12 Z= 2.117951176131D+13
I= 4 X= -1.895975001825D+13 Y= -1.481545741489D+13 Z= -1.034212069094D+13
I= 5 X= -9.754226771668D+12 Y= -3.419617594261D+12 Z= -2.450139674518D+12
I= 6 X= 6.908752091662D+13 Y= -3.333053611861D+12 Z= 1.908906196188D+13
I= 7 X= 6.261088000361D+13 Y= 7.770493209270D+13 Z= -4.942798335712D+13
I= 8 X= -6.662881757372D+13 Y= 2.507640737495D+13 Z= -6.169245773536D+13
I= 9 X= -4.900054763933D+12 Y= 1.619963500957D+13 Z= -1.813944761542D+12
I= 10 X= 1.828626092071D+13 Y= 1.588508216128D+12 Z= 3.472644150523D+13
I= 11 X= 3.515450721557D+13 Y= 3.706751470921D+13 Z= 7.436599775811D+13
I= 12 X= 8.180939839549D+13 Y= -3.579557835266D+13 Z= -8.635636410634D+13
I= 13 X= -1.089716463836D+13 Y= -6.689422290533D+12 Z= 1.489580870751D+13
I= 14 X= -9.810278295790D+12 Y= 1.072666323557D+14 Z= 2.943239821599D+13
I= 15 X= -4.640448779834D+13 Y= -9.296987527757D+13 Z= -8.842041374437D+13
I= 16 X= 2.014312974385D+13 Y= 1.110230839549D+13 Z= 4.964903796015D+12
I= 17 X= -6.070046424515D+12 Y= 2.573096893645D+13 Z= -2.950806893493D+12
I= 18 X= 2.864223502619D+13 Y= -2.323927178198D+13 Z= -5.802993536701D+13
I= 19 X= 1.006244428961D+14 Y= -8.335607319326D+13 Z= -2.989982647313D+13
I= 20 X= 6.208882247978D+13 Y= -8.279813073701D+13 Z= -1.834003011792D+13
I= 21 X= 3.234408914702D+11 Y= 1.529854506495D+13 Z= 4.306442385058D+12
I= 22 X= 6.872475977389D+12 Y= -1.304824132808D+14 Z= 1.535186940115D+13
I= 23 X= 5.602258804694D+12 Y= 1.195622954163D+13 Z= 4.518903451854D+12
I= 24 X= -3.994947717467D+12 Y= 8.561171491030D+13 Z= -1.573218118596D+12

I= 25 X= 2.961314968556D+13 Y= -1.251013207599D+13 Z= 4.690760018635D+12
I= 26 X= 4.837088111493D+13 Y= -1.480393146173D+12 Z= -1.273657591959D+14
I= 27 X= 3.958735592448D+13 Y= 1.608828777907D+13 Z= 6.551906853394D+13
I= 28 X= 1.826369181640D+13 Y= -1.624472712443D+13 Z= -2.016420206575D+13
I= 29 X= 6.915164971511D+10 Y= -1.586666917282D+13 Z= 1.703285141118D+13
I= 30 X= -6.295546964007D+12 Y= -1.453253331284D+13 Z= -2.820710253252D+13
I= 31 X= -2.644993781699D+13 Y= 4.356798110908D+13 Z= 6.196606392326D+13
I= 32 X= -1.796309295709D+13 Y= 6.331756298840D+13 Z= -6.467838408008D+13
I= 33 X= 4.128045182760D+13 Y= -4.137424214429D+13 Z= 1.960639410031D+13
I= 34 X= 6.092929831988D+13 Y= 4.195453711804D+13 Z= -3.706811259641D+12
I= 35 X= -4.774125943146D+12 Y= 4.818058905509D+11 Z= 2.039690788356D+12
I= 36 X= 2.369553249726D+12 Y= -7.292127017166D+12 Z= 4.909114072895D+12
I= 37 X= -6.850491741611D+11 Y= -3.656433324882D+12 Z= -7.362187858960D+12
I= 38 X= 8.201185614868D+13 Y= 5.259763345210D+13 Z= -6.931959338021D+13

Backward Direction:

Total Energy: -691.9926762 Hartrees

Potential Energy: -692.1505561 Hartress

Kinetic Energy: 0.1578800 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.550628370819D+12 Y= -5.923394823404D+12 Z= -9.305416353658D+12
I= 1 X= -8.907384080003D+12 Y= 1.268908445646D+13 Z= 8.574146544676D+12
I= 2 X= 1.774597175080D+13 Y= 1.378358405886D+13 Z= 2.781075317872D+12
I= 3 X= -1.963338197639D+13 Y= -1.110162916572D+13 Z= 1.903226092901D+13
I= 4 X= -1.854916683952D+13 Y= -1.378565550836D+13 Z= -1.154695461821D+13
I= 5 X= -6.675696942318D+12 Y= -1.185536765467D+13 Z= -1.284683310085D+13
I= 6 X= -3.734696919934D+13 Y= -3.318265192046D+12 Z= 1.908885780719D+13
I= 7 X= 4.803081979961D+13 Y= 7.782431941362D+13 Z= -6.113197167381D+13
I= 8 X= -7.444460232398D+13 Y= 2.343659585984D+13 Z= -6.463590526436D+13
I= 9 X= -3.588350956950D+12 Y= 1.379611116797D+13 Z= -2.677108560063D+12
I= 10 X= 1.726519746952D+13 Y= -1.600146538659D+12 Z= 3.281127183027D+13

I= 11 X= 3.689843010731D+13 Y= 3.218961243887D+13 Z= 7.386146882676D+13
I= 12 X= 8.525167943691D+13 Y= -3.804936391293D+13 Z= -8.606571236981D+13
I= 13 X= -9.585612547090D+12 Y= -4.285872748747D+12 Z= 1.575932809762D+13
I= 14 X= -1.083035653100D+13 Y= 1.104556158278D+14 Z= 3.134807360485D+13
I= 15 X= -4.296291340704D+13 Y= -9.071504545007D+13 Z= -8.871121738168D+13
I= 16 X= 2.188639373009D+13 Y= 1.597878960536D+13 Z= 5.470382271837D+12
I= 17 X= -6.097777157557D+12 Y= 2.593558345771D+13 Z= -3.337892972508D+11
I= 18 X= 2.934550351933D+13 Y= -2.215391767520D+13 Z= -5.284135712149D+13
I= 19 X= 1.002821143465D+14 Y= -8.270930189059D+13 Z= -2.874513587112D+13
I= 20 X= 6.145007192645D+13 Y= -8.571275348892D+13 Z= -1.546550245740D+13
I= 21 X= -1.888273772908D+12 Y= 1.529975297501D+13 Z= 4.305630206190D+12
I= 22 X= 1.129472472351D+12 Y= -1.304811606739D+14 Z= 1.534957815407D+13
I= 23 X= 4.069389862642D+12 Y= 1.462216585936D+13 Z= 4.852539029015D+12
I= 24 X= -5.528205289186D+12 Y= 8.294924669530D+13 Z= -1.908175541428D+12
I= 25 X= 2.958564430148D+13 Y= -1.271520272899D+13 Z= 2.073691266248D+12
I= 26 X= 4.773269402477D+13 Y= 1.433234347523D+12 Z= -1.302404722904D+14
I= 27 X= 3.924535515031D+13 Y= 1.544055442417D+13 Z= 6.436462310020D+13
I= 28 X= 1.896688610649D+13 Y= -1.733075492401D+13 Z= -2.535231050025D+13
I= 29 X= 3.147286595022D+12 Y= -7.433715172817D+12 Z= 2.742729733115D+13
I= 30 X= -1.866653490515D+12 Y= -1.306845704942D+13 Z= -2.115996371905D+13
I= 31 X= -3.426088442188D+13 Y= 4.520843958075D+13 Z= 6.490793474806D+13
I= 32 X= -3.254182728002D+13 Y= 6.319769245360D+13 Z= -5.297879551326D+13
I= 33 X= 3.988560684601D+13 Y= -4.606751932775D+13 Z= 3.505327680066D+13
I= 34 X= 6.115323695101D+13 Y= 3.663346307120D+13 Z= 2.932765735301D+12
I= 35 X= -5.749291917370D+12 Y= 4.820729169939D+11 Z= 2.040597434653D+12
I= 36 X= 6.798869153830D+12 Y= -8.757313231348D+12 Z= -2.138432295301D+12
I= 37 X= -2.082206881027D+12 Y= 1.040008840691D+12 Z= -2.281134113563D+13
I= 38 X= 8.223696637908D+13 Y= 5.791731590992D+13 Z= -7.595896714025D+13

Seed: 12095833256

CM Start Point Coordinates: bohr

I= 0 X= -2.196880664087D+00 Y= -2.049580056087D+00 Z= -3.278116404390D-02
I= 1 X= -8.770221627476D-02 Y= -2.658195136761D+00 Z= -1.401000215790D+00
I= 2 X= -1.409135756182D+00 Y= -1.263148683263D+00 Z= 2.547998902063D+00
I= 3 X= 2.111545028613D+00 Y= -2.112477217715D+00 Z= -1.316440240620D-01
I= 4 X= 1.316940399337D+00 Y= -1.257400460598D+00 Z= 2.487988558539D+00
I= 5 X= -2.637522290147D+00 Y= 3.321241449086D+00 Z= -2.412595916664D+00
I= 6 X= 1.100116382660D-01 Y= 1.181112432091D+00 Z= -3.212347398460D+00
I= 7 X= -1.294612699623D+00 Y= 4.601275496792D+00 Z= -3.365824197297D+00
I= 8 X= -4.250483769617D+00 Y= 2.578207534025D+00 Z= -3.658267678521D+00
I= 9 X= 3.235534864010D+00 Y= -9.118109928902D-01 Z= 4.594798632530D+00
I= 10 X= 3.496288739383D+00 Y= -2.803543120570D+00 Z= 5.822569169338D+00
I= 11 X= 5.140618828746D+00 Y= -3.080687392526D-01 Z= 3.964234624554D+00
I= 12 X= 3.039071009693D+00 Y= 5.573700318240D-01 Z= 6.258014244324D+00
I= 13 X= -3.034399599159D+00 Y= -7.338697892406D-01 Z= 4.696225256590D+00
I= 14 X= -2.900803814135D+00 Y= -1.868344494278D+00 Z= 6.598832746814D+00
I= 15 X= -2.374562960018D+00 Y= 1.257965921106D+00 Z= 5.507923805454D+00
I= 16 X= -5.146316201553D+00 Y= -5.782317517079D-01 Z= 3.966258726208D+00
I= 17 X= -4.848444793658D+00 Y= -2.622108996180D+00 Z= -7.792409253439D-01
I= 18 X= -5.263571936148D+00 Y= -4.241755542984D+00 Z= 1.610393651569D-01
I= 19 X= -6.269889389250D+00 Y= -1.045105254918D+00 Z= 5.326200559856D-02
I= 20 X= -5.404828308238D+00 Y= -2.468197368477D+00 Z= -2.639468282994D+00
I= 21 X= -3.712537339546D-03 Y= -3.800878540359D+00 Z= -4.097339171271D+00
I= 22 X= -9.258662786796D-01 Y= -5.787373879305D+00 Z= -3.826621411609D+00
I= 23 X= -1.489264631943D+00 Y= -2.798324973178D+00 Z= -5.509751095113D+00
I= 24 X= 2.034254697213D+00 Y= -3.857481011123D+00 Z= -4.847246693380D+00
I= 25 X= 4.950887529138D+00 Y= -2.398760295657D+00 Z= -6.729694447414D-01
I= 26 X= 5.093612231660D+00 Y= -3.011560217200D+00 Z= -2.782064969792D+00
I= 27 X= 6.113540636675D+00 Y= -4.407674002057D-01 Z= -5.143031483985D-01
I= 28 X= 5.448533136752D+00 Y= -3.960017418414D+00 Z= 9.294242770688D-01

I= 29 X= 2.938217817709D+00 Y= 3.238785017418D+00 Z= -2.330805308485D+00
I= 30 X= 2.654581242397D+00 Y= 3.882473796566D+00 Z= 2.448615317053D-01
I= 31 X= 4.529522219329D+00 Y= 2.278967389095D+00 Z= -3.362497139497D+00
I= 32 X= 1.970142220310D+00 Y= 4.931045095153D+00 Z= -3.531954087786D+00
I= 33 X= 2.079899729119D+00 Y= 5.380183373052D+00 Z= 1.026593493427D+00
I= 34 X= 3.538232007530D+00 Y= 2.597498950788D+00 Z= 1.937949315128D+00
I= 35 X= -4.277416508627D-02 Y= 1.163584290229D+00 Z= -6.272347505460D-01
I= 36 X= -2.860526208042D+00 Y= 3.656194083886D+00 Z= 2.677915715390D-01
I= 37 X= -1.825681843593D+00 Y= 5.050170872880D+00 Z= 1.224788088797D+00
I= 38 X= -4.487138293445D+00 Y= 2.696121328215D+00 Z= 9.797109345382D-01

Forward Direction:

Total Energy: -691.9881613 Hartrees

Potential Energy: -692.1715909 Hartress

Kinetic Energy: 0.1834296 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.579466065734D+13 Y= -1.823173021640D+13 Z= -1.273325767984D+13
I= 1 X= 9.392891733872D+12 Y= 4.887922690658D+12 Z= -3.184133725906D+12
I= 2 X= -1.137537391889D+13 Y= -8.702380090703D+11 Z= 1.353929121810D+13
I= 3 X= 1.049340521127D+13 Y= 6.024851475545D+12 Z= -1.045555877927D+13
I= 4 X= -2.638566249682D+13 Y= -9.081595364568D+11 Z= 5.294121775678D+12
I= 5 X= 5.077235585767D+12 Y= -2.095059510511D+12 Z= -4.701143027878D+11
I= 6 X= -2.482335672071D+12 Y= -1.747991395884D+13 Z= 5.881541410135D+13
I= 7 X= -6.531774935739D+13 Y= -7.372924779704D+13 Z= 1.558699150619D+13
I= 8 X= 7.583314505892D+13 Y= 7.019295906557D+13 Z= 3.298676363231D+13
I= 9 X= -8.132786568372D+12 Y= 1.117397399822D+13 Z= -1.379439080963D+13
I= 10 X= -1.535869603351D+13 Y= -1.130491023840D+13 Z= 6.054660334075D+13
I= 11 X= 1.062084388636D+13 Y= -3.088382999643D+13 Z= 4.384138496787D+13
I= 12 X= -3.815904525948D+13 Y= -1.314577125261D+13 Z= 3.555203162399D+13
I= 13 X= -7.651543747236D+12 Y= 3.959395332567D+12 Z= 1.935921726324D+12
I= 14 X= 3.937043330314D+13 Y= -3.202947640079D+13 Z= -7.636168750044D+12

I= 15 X= -1.050120751715D+13 Y= -1.889115204773D+14 Z= -1.235559430527D+14
I= 16 X= -6.868373591858D+13 Y= 1.278844585511D+14 Z= 2.570358825490D+13
I= 17 X= 1.473810053442D+13 Y= -7.225382999840D+10 Z= 1.184129377214D+13
I= 18 X= -4.530404578586D+13 Y= 1.108459614229D+14 Z= -2.939913171107D+13
I= 19 X= 2.694302453364D+13 Y= -1.805994391857D+14 Z= -9.844677157392D+12
I= 20 X= -1.108048651621D+13 Y= -2.836034557263D+13 Z= 3.346016242677D+13
I= 21 X= 5.093352304883D+12 Y= 5.166634603956D+12 Z= -9.465522601106D+12
I= 22 X= 1.719903516997D+13 Y= 1.536731092711D+14 Z= 1.736310006161D+13
I= 23 X= 1.090107731262D+13 Y= 6.354602694771D+13 Z= -8.309857887613D+13
I= 24 X= -5.859807063087D+13 Y= -4.510452130381D+13 Z= -5.472541107692D+13
I= 25 X= -6.599784846220D+12 Y= -7.114722624642D+12 Z= 7.959823329180D+12
I= 26 X= 4.545679616764D+13 Y= 6.556217622934D+13 Z= -2.869198008385D+13
I= 27 X= -8.378083414288D+12 Y= 5.726940113698D+13 Z= -5.094449928672D+13
I= 28 X= -1.804222097325D+13 Y= 3.961058125159D+13 Z= -6.849835283938D+13
I= 29 X= 1.079432146156D+13 Y= -2.258300717284D+13 Z= -2.194796120153D+13
I= 30 X= -3.777551864281D+13 Y= -4.443274939662D+12 Z= 1.036073852253D+13
I= 31 X= -1.417730826058D+13 Y= 5.932371578721D+13 Z= 4.409769135200D+13
I= 32 X= 4.870770628096D+13 Y= 8.266375681182D+13 Z= 1.195141062075D+12
I= 33 X= -1.030506825438D+12 Y= 7.849586477359D+13 Z= 2.588548431117D+13
I= 34 X= 6.773423623744D+13 Y= 5.022625628743D+13 Z= 3.163793373624D+13
I= 35 X= 3.050317700841D+12 Y= 4.529010387606D+10 Z= 4.443528934436D+12
I= 36 X= 5.807891740757D+12 Y= 4.218449344584D+12 Z= 4.037630632899D+12
I= 37 X= -3.993941032043D+13 Y= -7.527357788618D+13 Z= -7.728802969120D+12
I= 38 X= 3.663487765588D+12 Y= -1.641955066596D+13 Z= -1.899301818913D+13

Backward Direction:

Total Energy: -691.9881981 Hartrees

Potential Energy: -692.1715909 Hartress

Kinetic Energy: 0.1833928 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.587710701120D+13 Y= -1.735351272309D+13 Z= -1.145575424446D+13

I= 1 X= 1.001006472372D+13 Y= 4.888086736291D+12 Z= -3.184217072818D+12
I= 2 X= -1.107667530317D+13 Y= -1.377581485607D+12 Z= 1.424069283180D+13
I= 3 X= 1.057594643393D+13 Y= 5.146547857501D+12 Z= -1.173323624892D+13
I= 4 X= -2.608689910866D+13 Y= -4.007368005269D+11 Z= 4.592718972757D+12
I= 5 X= 6.689522453571D+12 Y= -7.319860920762D+12 Z= -6.744463816266D+12
I= 6 X= -6.097299602870D+13 Y= -1.747138405868D+13 Z= 5.881539700978D+13
I= 7 X= -7.372178473710D+13 Y= -7.448560578428D+13 Z= 8.182928646176D+12
I= 8 X= 7.154027771444D+13 Y= 6.836738325873D+13 Z= 3.122714287068D+13
I= 9 X= -7.272804901842D+12 Y= 9.606514409949D+12 Z= -1.431015117459D+13
I= 10 X= -1.594673524078D+13 Y= -1.333504696810D+13 Z= 5.940657614347D+13
I= 11 X= 1.174667850345D+13 Y= -3.400576766551D+13 Z= 4.352891987260D+13
I= 12 X= -3.596253093332D+13 Y= -1.459815808254D+13 Z= 3.572128167121D+13
I= 13 X= -6.791652176198D+12 Y= 5.526871270339D+12 Z= 2.451918343037D+12
I= 14 X= 3.878304683280D+13 Y= -2.999911739652D+13 Z= -6.495792307968D+12
I= 15 X= -8.305142114237D+12 Y= -1.874584656637D+14 Z= -1.237252918433D+14
I= 16 X= -6.755831703118D+13 Y= 1.310054852100D+14 Z= 2.601666462331D+13
I= 17 X= 1.468009447095D+13 Y= 2.592988668504D+10 Z= 1.352046358828D+13
I= 18 X= -4.494368118414D+13 Y= 1.115556201846D+14 Z= -2.601093217981D+13
I= 19 X= 2.675291634039D+13 Y= -1.801460632572D+14 Z= -9.134480970901D+12
I= 20 X= -1.155838496367D+13 Y= -3.029341176208D+13 Z= 3.531117892762D+13
I= 21 X= 3.638344495942D+12 Y= 5.167398263327D+12 Z= -9.466035822028D+12
I= 22 X= 1.343493428735D+13 Y= 1.536739051712D+14 Z= 1.736165826629D+13
I= 23 X= 9.926582621422D+12 Y= 6.530499420829D+13 Z= -8.292990876718D+13
I= 24 X= -5.957279729772D+13 Y= -4.686131899510D+13 Z= -5.489487930998D+13
I= 25 X= -6.657634778475D+12 Y= -7.213209771702D+12 Z= 6.280614845614D+12
I= 26 X= 4.497925415557D+13 Y= 6.749465061718D+13 Z= -3.054313286550D+13
I= 27 X= -8.567960248444D+12 Y= 5.681538031178D+13 Z= -5.165451789625D+13
I= 28 X= -1.768186890454D+13 Y= 3.890045691177D+13 Z= -7.188631805337D+13
I= 29 X= 1.240634384200D+13 Y= -1.735989990257D+13 Z= -1.567503200095D+13
I= 30 X= -3.531659092153D+13 Y= -3.756039170968D+12 Z= 1.491313936945D+13

I= 31 X= -1.846758895689D+13 Y= 6.114930213095D+13 Z= 4.585623130042D+13
I= 32 X= 4.030462331737D+13 Y= 8.341995615976D+13 Z= 8.596528477696D+12
I= 33 X= -1.891329931279D+12 Y= 7.549683105542D+13 Z= 3.566489244235D+13
I= 34 X= 6.801719407311D+13 Y= 4.689997404563D+13 Z= 3.561872886722D+13
I= 35 X= 2.550047042316D+12 Y= 4.546314372218D+10 Z= 4.444094000475D+12
I= 36 X= 8.267016999021D+12 Y= 3.530537511234D+12 Z= -5.150396325013D+11
I= 37 X= -4.080176981530D+13 Y= -7.227259796795D+13 Z= -1.750950392500D+13
I= 38 X= 3.947030692791D+12 Y= -1.309428191286D+13 Z= -2.297373087751D+13

Seed: 12310538170

CM Start Point Coordinates: bohr

I= 0 X= -2.145797740700D+00 Y= -2.243183445012D+00 Z= -1.147184222662D-01
I= 1 X= -6.798603994277D-02 Y= -2.931311527827D+00 Z= -1.494957809678D+00
I= 2 X= -1.338756853761D+00 Y= -1.395197762051D+00 Z= 2.554085518687D+00
I= 3 X= 1.991559453899D+00 Y= -2.072143256114D+00 Z= -3.416179332605D-02
I= 4 X= 1.267408362388D+00 Y= -1.178848911364D+00 Z= 2.419445557023D+00
I= 5 X= -2.677131106626D+00 Y= 3.298567868147D+00 Z= -2.401453004487D+00
I= 6 X= 2.559623812781D-01 Y= 1.355282755393D+00 Z= -3.375007811204D+00
I= 7 X= -1.888459075116D+00 Y= 4.750166552545D+00 Z= -3.387402591986D+00
I= 8 X= -3.676395447989D+00 Y= 2.035915376465D+00 Z= -3.659576852634D+00
I= 9 X= 2.859678515398D+00 Y= -5.849817375278D-01 Z= 4.577278864402D+00
I= 10 X= 3.942647756926D+00 Y= -2.520746063587D+00 Z= 5.482328781214D+00
I= 11 X= 4.933097382849D+00 Y= 3.054145360481D-01 Z= 4.113672629147D+00
I= 12 X= 1.630649122900D+00 Y= 3.367304897881D-01 Z= 6.277848927890D+00
I= 13 X= -2.916562140949D+00 Y= -6.339476947700D-01 Z= 4.700990800440D+00
I= 14 X= -2.184021287621D+00 Y= -1.966245522251D+00 Z= 6.163277909078D+00
I= 15 X= -2.350051383717D+00 Y= 1.391212767857D+00 Z= 5.282433969531D+00
I= 16 X= -5.060891046387D+00 Y= -1.129896491993D+00 Z= 4.467043390503D+00
I= 17 X= -4.784390324923D+00 Y= -2.240451903890D+00 Z= -7.287328002059D-01
I= 18 X= -5.667163936097D+00 Y= -4.412572903363D+00 Z= -2.841219284066D-01

I= 19 X= -5.608844063810D+00 Y= -1.017121306714D+00 Z= 5.903779428061D-01
I= 20 X= -4.883590626533D+00 Y= -1.746212146735D+00 Z= -3.111210355366D+00
I= 21 X= -5.335465866519D-02 Y= -3.815068156196D+00 Z= -4.115659793332D+00
I= 22 X= -8.724156076776D-01 Y= -5.765923443307D+00 Z= -3.991269361641D+00
I= 23 X= -1.343563464782D+00 Y= -2.621344950053D+00 Z= -5.423156783350D+00
I= 24 X= 1.715552975030D+00 Y= -4.049393594364D+00 Z= -5.007675841883D+00
I= 25 X= 4.886728220965D+00 Y= -2.134105739830D+00 Z= -8.618964778760D-01
I= 26 X= 5.052823424495D+00 Y= -2.111683203394D+00 Z= -2.898872998633D+00
I= 27 X= 5.795066224832D+00 Y= -2.828860318421D-01 Z= -1.764816733901D-01
I= 28 X= 6.161132731431D+00 Y= -3.855471895913D+00 Z= -2.940437059714D-01
I= 29 X= 3.025094044498D+00 Y= 3.226798374327D+00 Z= -2.247018390634D+00
I= 30 X= 2.895645717836D+00 Y= 3.763126796232D+00 Z= 2.464507827631D-01
I= 31 X= 4.061876085547D+00 Y= 1.683814939329D+00 Z= -2.864843500934D+00
I= 32 X= 2.133552992972D+00 Y= 4.524630131717D+00 Z= -3.820237974934D+00
I= 33 X= 2.354251779585D+00 Y= 5.529152693247D+00 Z= 1.545951556157D+00
I= 34 X= 4.008029774863D+00 Y= 2.837900434357D+00 Z= 1.746594859030D+00
I= 35 X= -4.935401195052D-02 Y= 1.029283387347D+00 Z= -5.528564154415D-01
I= 36 X= -2.894754039153D+00 Y= 3.775881808317D+00 Z= 1.914160908754D-01
I= 37 X= -1.786154986900D+00 Y= 5.266301703882D+00 Z= 1.304032788858D+00
I= 38 X= -4.401247398366D+00 Y= 2.772152801455D+00 Z= 1.606863575386D+00

Forward Direction:

Total Energy: -692.0032491 Hartrees

Potential Energy: -692.1728918 Hartress

Kinetic Energy: 0.1696427 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.156864421220D+13 Y= 1.139049369551D+13 Z= -3.692437519679D+12

I= 1 X= -2.280760238876D+13 Y= 1.559541217536D+13 Z= 1.132917709414D+13

I= 2 X= 2.099414041203D+13 Y= -3.772511228245D+12 Z= -8.763762079812D+12

I= 3 X= 1.059434494413D+12 Y= -2.146959190104D+13 Z= 4.028806013868D+12

I= 4 X= -7.408596704295D+11 Y= 1.089400094346D+13 Z= -1.755168755766D+13

I= 5 X= 1.499589398980D+13 Y= -2.934810892188D+12 Z= -2.377306025807D+13
I= 6 X= 6.719030459868D+13 Y= 1.391137504142D+13 Z= -8.210285113644D+13
I= 7 X= -2.288707955222D+13 Y= -7.013083129182D+13 Z= 2.152372981415D+13
I= 8 X= 7.863197007694D+13 Y= 1.077953868611D+13 Z= 1.047015619653D+14
I= 9 X= -6.185891672427D+12 Y= -1.382354072678D+13 Z= 6.364471389467D+12
I= 10 X= 2.607690331799D+13 Y= 1.397855718894D+14 Z= -9.043390721392D+13
I= 11 X= -7.108639754805D+13 Y= -6.093259704096D+13 Z= 3.008447321545D+13
I= 12 X= -2.289279229476D+13 Y= 4.181415627712D+13 Z= 3.702058193774D+13
I= 13 X= -1.108471384247D+13 Y= 9.734221971733D+12 Z= -1.196143727748D+12
I= 14 X= 4.798059112777D+13 Y= 3.390420503417D+12 Z= -1.341007863586D+13
I= 15 X= -6.718533634961D+13 Y= 1.158823206010D+13 Z= 4.815802774541D+13
I= 16 X= 5.143221839293D+13 Y= 5.511339891074D+13 Z= 6.446009626357D+13
I= 17 X= 4.225984912322D+12 Y= -2.387127920481D+12 Z= -1.953489855805D+13
I= 18 X= -5.923039243860D+13 Y= -7.972031024485D+12 Z= 6.097647368381D+12
I= 19 X= 4.859294763659D+13 Y= 9.960085595958D+12 Z= 8.096391953596D+13
I= 20 X= -1.750928909699D+13 Y= -1.002880071621D+14 Z= -7.440406789807D+13
I= 21 X= -1.006283965269D+13 Y= 1.316047511965D+13 Z= -1.024405201392D+13
I= 22 X= 6.420825548643D+13 Y= -8.877243798450D+13 Z= -3.348063663160D+13
I= 23 X= 1.886106631150D+13 Y= -4.134498892176D+13 Z= -2.613575280067D+13
I= 24 X= -5.958203622837D+13 Y= -9.910470694581D+11 Z= 1.546714086093D+13
I= 25 X= 9.493129042020D+12 Y= -2.290920381211D+12 Z= 7.723277266451D+12
I= 26 X= 8.194595347617D+12 Y= 1.280376031753D+13 Z= 4.913561964996D+13
I= 27 X= -6.032728395053D+13 Y= -1.456711534202D+14 Z= 2.771812202433D+13
I= 28 X= 6.811509789731D+12 Y= 3.526693037497D+13 Z= -2.697054023550D+13
I= 29 X= -7.200530884571D+12 Y= -4.536885644717D+12 Z= 4.887002102905D+12
I= 30 X= -1.143459581138D+13 Y= -6.094965956321D+12 Z= -3.106337693419D+12
I= 31 X= -1.122858750694D+14 Y= 5.341609447268D+13 Z= 5.771401101016D+13
I= 32 X= 5.147974880786D+13 Y= 8.995103580606D+13 Z= -8.654831150262D+13
I= 33 X= -2.697424134007D+13 Y= 7.468099666005D+13 Z= -8.956771508807D+12
I= 34 X= 1.506943830473D+13 Y= -7.262584188544D+12 Z= -3.747118003872D+13

I= 35 X= 1.674940846012D+12 Y= -3.229271770079D+12 Z= 2.568133814257D+12
I= 36 X= -1.602283541789D+13 Y= 7.478484108319D+12 Z= 3.654665246234D+13
I= 37 X= 1.682233203491D+13 Y= -2.026157538550D+13 Z= 2.280110581264D+13
I= 38 X= 7.786723070845D+13 Y= 4.970608747777D+13 Z= -3.389157845536D+13

Backward Direction:

Total Energy: -692.0032492 Hartrees

Potential Energy: -692.1728918 Hartress

Kinetic Energy: 0.1696426 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.190124126771D+13 Y= 1.307188802611D+13 Z= -1.756502737891D+12
I= 1 X= -2.055554398104D+13 Y= 1.559558832614D+13 Z= 1.132914033666D+13
I= 2 X= 2.085160791799D+13 Y= -5.692791606477D+12 Z= -7.531472342760D+12
I= 3 X= 1.392109008858D+12 Y= -2.315118687580D+13 Z= 2.092585172123D+12
I= 4 X= -8.833283922001D+11 Y= 1.281439320797D+13 Z= -1.878413091947D+13
I= 5 X= 1.983878637095D+13 Y= -8.608726457293D+12 Z= -3.231933319375D+13
I= 6 X= -7.436301475777D+13 Y= 1.392724855158D+13 Z= -8.210401807995D+13
I= 7 X= -3.859074116746D+13 Y= -6.223303864478D+13 Z= 1.511124612377D+13
I= 8 X= 6.821596826707D+13 Y= 1.730232867936D+13 Z= 1.021244370323D+14
I= 9 X= -5.751417182425D+12 Y= -1.469821025114D+13 Z= 5.606404925284D+12
I= 10 X= 2.497236952185D+13 Y= 1.381605750210D+14 Z= -9.215666681712D+13
I= 11 X= -7.034381127744D+13 Y= -6.326500314947D+13 Z= 2.974491797110D+13
I= 12 X= -2.118467853676D+13 Y= 4.082995643147D+13 Z= 3.731747016767D+13
I= 13 X= -1.065037798259D+13 Y= 1.060890488059D+13 Z= -4.379887422969D+11
I= 14 X= 4.687631948798D+13 Y= 5.015461992023D+12 Z= -1.168731714507D+13
I= 15 X= -6.547759239808D+13 Y= 1.257293410377D+13 Z= 4.786108083303D+13
I= 16 X= 5.217443392804D+13 Y= 5.744513964904D+13 Z= 6.480007233607D+13
I= 17 X= 4.591763337810D+12 Y= -1.980724674951D+12 Z= -1.832343022215D+13
I= 18 X= -5.804920820331D+13 Y= -7.594426016696D+12 Z= 7.943792059398D+12
I= 19 X= 4.815633607812D+13 Y= 9.898084172032D+12 Z= 8.178743486640D+13
I= 20 X= -1.716423612752D+13 Y= -1.010446238424D+14 Z= -7.313571409051D+13

I= 21 X= -1.074873020260D+13 Y= 1.316114150668D+13 Z= -1.024450237860D+13
I= 22 X= 6.229529439253D+13 Y= -8.877178444762D+13 Z= -3.348196429662D+13
I= 23 X= 1.806628703705D+13 Y= -4.056666159456D+13 Z= -2.555383473760D+13
I= 24 X= -6.037715912146D+13 Y= -1.767244349288D+12 Z= 1.488413995387D+13
I= 25 X= 9.858903066137D+12 Y= -2.697433088163D+12 Z= 6.511839894681D+12
I= 26 X= 8.539956386588D+12 Y= 1.355947574555D+13 Z= 4.786734421393D+13
I= 27 X= -6.076394478731D+13 Y= -1.456093409706D+14 Z= 2.689452716317D+13
I= 28 X= 7.992330966516D+12 Y= 3.488932294424D+13 Z= -2.881583389276D+13
I= 29 X= -2.357716545052D+12 Y= 1.134795004352D+12 Z= 1.343202966790D+13
I= 30 X= -5.780175928169D+12 Y= -3.043007627650D+12 Z= -1.332280123000D+11
I= 31 X= -1.226947632476D+14 Y= 4.689741338102D+13 Z= 6.029105713720D+13
I= 32 X= 3.577574356653D+13 Y= 8.205159376016D+13 Z= -8.013925403711D+13
I= 33 X= -2.794154902637D+13 Y= 7.239223423945D+13 Z= -5.647014634271D+11
I= 34 X= 1.386183442670D+13 Y= -1.055345527880D+13 Z= -3.176707516883D+13
I= 35 X= 4.256561168848D+10 Y= -3.229164249921D+12 Z= 2.568710450986D+12
I= 36 X= -1.036752796409D+13 Y= 4.425672005918D+12 Z= 3.357342860625D+13
I= 37 X= 1.585444773050D+13 Y= -1.797055158982D+13 Z= 1.440644002472D+13
I= 38 X= 7.666173811397D+13 Y= 5.299744983177D+13 Z= -3.959513768415D+13

Seed: 12336245867

CM Start Point Coordinates: bohr

I= 0 X= -2.102460045531D+00 Y= -1.860939212842D+00 Z= -7.017922342623D-02
I= 1 X= 2.774017535750D-02 Y= -2.817310477428D+00 Z= -1.618897015798D+00
I= 2 X= -1.291519865200D+00 Y= -1.159612002414D+00 Z= 2.463253468398D+00
I= 3 X= 2.160128699631D+00 Y= -2.101191785104D+00 Z= -1.122859662999D-01
I= 4 X= 1.384285152304D+00 Y= -9.387741606578D-01 Z= 2.199680642895D+00
I= 5 X= -2.894900443500D+00 Y= 3.196730723865D+00 Z= -2.383190221823D+00
I= 6 X= 2.472481988208D-01 Y= 1.039349394276D+00 Z= -3.587366822393D+00
I= 7 X= -1.405053700628D+00 Y= 4.592200918881D+00 Z= -3.002585105733D+00
I= 8 X= -4.207976830709D+00 Y= 2.043934224581D+00 Z= -3.815410268302D+00

I= 9 X= 3.029731013598D+00 Y= -3.824231405134D-01 Z= 4.639075431806D+00
I= 10 X= 3.730727586518D+00 Y= -2.464841163540D+00 Z= 5.498503878667D+00
I= 11 X= 4.749931402080D+00 Y= 9.042405207845D-01 Z= 3.778563683169D+00
I= 12 X= 1.604114896698D+00 Y= 9.954408977268D-01 Z= 5.741492882974D+00
I= 13 X= -2.983425588413D+00 Y= -8.225428979680D-01 Z= 4.644749946031D+00
I= 14 X= -3.581888173330D+00 Y= -2.636110631726D+00 Z= 5.191437770752D+00
I= 15 X= -2.173741046771D+00 Y= 4.348629103728D-01 Z= 6.375693624075D+00
I= 16 X= -4.741558729234D+00 Y= 1.776868114523D-01 Z= 4.022225100549D+00
I= 17 X= -4.901150169981D+00 Y= -2.093223368303D+00 Z= -6.338956575240D-01
I= 18 X= -5.739844855574D+00 Y= -4.213406059492D+00 Z= -3.714496926602D-01
I= 19 X= -5.987821353423D+00 Y= -6.620048500522D-01 Z= 4.785804650661D-01
I= 20 X= -5.231316499161D+00 Y= -1.743856296948D+00 Z= -2.836982074192D+00
I= 21 X= -5.322023276546D-02 Y= -3.970956199344D+00 Z= -4.027583793731D+00
I= 22 X= 5.237990228067D-01 Y= -5.793755628676D+00 Z= -3.783326684546D+00
I= 23 X= -1.986138809559D+00 Y= -3.624426849443D+00 Z= -4.896354441059D+00
I= 24 X= 1.270760920562D+00 Y= -2.769606925923D+00 Z= -5.215861187258D+00
I= 25 X= 4.986494623994D+00 Y= -2.749733169695D+00 Z= -8.718296115270D-01
I= 26 X= 5.296281817516D+00 Y= -2.901838993431D+00 Z= -2.965380113044D+00
I= 27 X= 6.020976119945D+00 Y= -1.285573032957D+00 Z= -1.704373494627D-01
I= 28 X= 5.526153967540D+00 Y= -4.754139311526D+00 Z= 2.325176395377D-01
I= 29 X= 2.921621881264D+00 Y= 3.282874260708D+00 Z= -2.100390666254D+00
I= 30 X= 2.731276640155D+00 Y= 3.748997399951D+00 Z= 5.473126500125D-01
I= 31 X= 4.446122649084D+00 Y= 1.839101829440D+00 Z= -2.936182037926D+00
I= 32 X= 2.332450729580D+00 Y= 4.788551812404D+00 Z= -3.570395105400D+00
I= 33 X= 1.840784333045D+00 Y= 5.329600755196D+00 Z= 1.209404095724D+00
I= 34 X= 4.201467466029D+00 Y= 3.099704189654D+00 Z= 2.044178604004D+00
I= 35 X= -1.282703007101D-02 Y= 1.085968518172D+00 Z= -6.163086897939D-01
I= 36 X= -2.987220514176D+00 Y= 3.377698650484D+00 Z= 3.806404133706D-01
I= 37 X= -1.852928388068D+00 Y= 4.787332792239D+00 Z= 1.328837011217D+00
I= 38 X= -4.458506902852D+00 Y= 2.306816283105D+00 Z= 8.965811271195D-01

Forward Direction:

Total Energy: -691.9837403 Hartrees

Potential Energy: -692.1608266 Hartress

Kinetic Energy: 0.1770863 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.164214525899D+13 Y= 2.647638989692D+12 Z= -1.776357410477D+13
I= 1 X= 2.364030052203D+12 Y= -2.447351841483D+12 Z= -2.554157157488D+13
I= 2 X= 1.797015321237D+13 Y= -5.336340785119D+12 Z= 1.952899926479D+13
I= 3 X= 1.157979132716D+13 Y= 1.518628341150D+13 Z= -7.008331053873D+12
I= 4 X= 1.401444080239D+13 Y= 1.824107890139D+13 Z= 1.675244051990D+13
I= 5 X= 4.464087378406D+12 Y= 1.440381311219D+13 Z= -1.931225899380D+13
I= 6 X= 4.781514734616D+13 Y= -4.768107913412D+13 Z= 6.318904254633D+13
I= 7 X= -4.542800170046D+13 Y= 1.266873518508D+13 Z= 3.055666996004D+13
I= 8 X= 5.577429501828D+13 Y= 5.091708066710D+13 Z= 7.205647175181D+12
I= 9 X= -1.253220941161D+13 Y= 7.005795560711D+12 Z= -7.582574112690D+12
I= 10 X= 7.108961484649D+13 Y= -2.814080491620D+13 Z= 3.127994323498D+13
I= 11 X= 7.806264794186D+13 Y= -3.131172389033D+13 Z= -1.084395716101D+14
I= 12 X= 3.133348323626D+13 Y= -5.564658356490D+13 Z= -5.285617292640D+13
I= 13 X= -5.293735370171D+12 Y= -1.581235083923D+13 Z= 4.920552422995D+12
I= 14 X= -2.758382461511D+13 Y= -6.558534083399D+13 Z= -1.630385215696D+13
I= 15 X= -1.566766857556D+12 Y= 3.301990880599D+13 Z= 1.397339967262D+13
I= 16 X= -3.483064920783D+13 Y= 7.717408924389D+13 Z= -3.424675828949D+13
I= 17 X= -1.296912260453D+13 Y= 4.829678731498D+12 Z= 2.487862852963D+13
I= 18 X= 2.558162072646D+12 Y= 7.260436915085D+13 Z= -2.715551456997D+13
I= 19 X= 6.490360142104D+11 Y= -4.132228778074D+13 Z= 1.932344636130D+13
I= 20 X= -4.926912959082D+13 Y= -3.555734003288D+12 Z= 2.872974484723D+13
I= 21 X= 1.632383538597D+13 Y= -1.790585481798D+13 Z= 5.311648149138D+12
I= 22 X= -2.309168704061D+13 Y= 8.199783515216D+13 Z= -7.558564455342D+13
I= 23 X= -3.112596066329D+13 Y= -3.680817590038D+13 Z= -5.190000021449D+13
I= 24 X= -7.615341599776D+13 Y= 2.155248489841D+13 Z= 1.845354226971D+13

I= 25 X= -3.158899426972D+12 Y= 2.348370618085D+13 Z= -1.163608522099D+13
I= 26 X= -1.145103750433D+14 Y= -1.168847391429D+14 Z= 1.378931974552D+14
I= 27 X= 4.167202175817D+13 Y= 2.468530426936D+13 Z= 1.333510817333D+14
I= 28 X= -3.037079159813D+12 Y= -1.078572555215D+14 Z= 2.147119698488D+13
I= 29 X= 1.503241882033D+13 Y= -1.277474085364D+13 Z= -2.462135472640D+13
I= 30 X= 2.531752556664D+13 Y= -3.281677232819D+11 Z= -3.316813248304D+12
I= 31 X= -8.823869687490D+13 Y= -4.104763030687D+12 Z= 6.369597746199D+13
I= 32 X= 2.381301178605D+13 Y= 3.779307921658D+13 Z= -5.535357213848D+13
I= 33 X= -5.742459360930D+13 Y= -2.638156465923D+13 Z= 5.855976263826D+13
I= 34 X= -2.891459035516D+13 Y= -3.672336080711D+13 Z= -4.315021076570D+13
I= 35 X= -2.882927119335D+12 Y= 4.813037726734D+11 Z= 7.595089671228D+12
I= 36 X= -2.963770341847D+13 Y= -1.955872551663D+13 Z= 1.893660841688D+12
I= 37 X= 4.217759021858D+13 Y= 1.982689341766D+13 Z= -2.110924137120D+13
I= 38 X= -2.421300756657D+13 Y= 3.089543534086D+12 Z= -6.780276211364D+13

Backward Direction:

Total Energy: -691.9837559 Hartrees

Potential Energy: -692.1608266 Hartress

Kinetic Energy: 0.1770707 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.165252831846D+13 Y= 3.632832253210D+12 Z= -1.603027922220D+13
I= 1 X= 2.426224475584D+12 Y= -2.447086618230D+12 Z= -2.554173737382D+13
I= 2 X= 1.872579691144D+13 Y= -5.346854704181D+12 Z= 2.038093615277D+13
I= 3 X= 1.156957603385D+13 Y= 1.420101456432D+13 Z= -8.741848924732D+12
I= 4 X= 1.477019262875D+13 Y= 1.825170520120D+13 Z= 1.590059136166D+13
I= 5 X= 5.238987541763D+12 Y= 5.994016011394D+12 Z= -2.839144911815D+13
I= 6 X= -3.929579507345D+11 Y= -4.767124087758D+13 Z= 6.318969107678D+13
I= 7 X= -5.508315052384D+13 Y= 6.318466054084D+12 Z= 1.768076170878D+13
I= 8 X= 5.225189960705D+13 Y= 4.297171344900D+13 Z= 4.765587792888D+12
I= 9 X= -1.085398335014D+13 Y= 3.995673499849D+12 Z= -8.296194488312D+12
I= 10 X= 7.041740837530D+13 Y= -3.174972528962D+13 Z= 2.973032260958D+13

I= 11 X= 8.015736439021D+13 Y= -3.695953133204D+13 Z= -1.089423769104D+14
I= 12 X= 3.526763719441D+13 Y= -5.833344195350D+13 Z= -5.265032375201D+13
I= 13 X= -3.615630290505D+12 Y= -1.280219991911D+13 Z= 5.634651973970D+12
I= 14 X= -2.825471748249D+13 Y= -6.197594670455D+13 Z= -1.475344741842D+13
I= 15 X= 2.366595301326D+12 Y= 3.570797392100D+13 Z= 1.376736306214D+13
I= 16 X= -3.273664958915D+13 Y= 8.282023963582D+13 Z= -3.374282609833D+13
I= 17 X= -1.331489949003D+13 Y= 4.811238469096D+12 Z= 2.794170489110D+13
I= 18 X= 2.673233241018D+12 Y= 7.397801578480D+13 Z= -2.062266188067D+13
I= 19 X= 4.785319905268D+11 Y= -4.026620066457D+13 Z= 2.043580053195D+13
I= 20 X= -5.054699282554D+13 Y= -7.457557090036D+12 Z= 3.214579583167D+13
I= 21 X= 1.345547241359D+13 Y= -1.790452974314D+13 Z= 5.310759108264D+12
I= 22 X= -3.043056269293D+13 Y= 8.199924029964D+13 Z= -7.558810537646D+13
I= 23 X= -3.284960669998D+13 Y= -3.331066118790D+13 Z= -5.186324792492D+13
I= 24 X= -7.787738143052D+13 Y= 1.805859532459D+13 Z= 1.841563256779D+13
I= 25 X= -3.504322591418D+12 Y= 2.350152840897D+13 Z= -1.469926672218D+13
I= 26 X= -1.157876179208D+14 Y= -1.129837164206D+14 Z= 1.344767935135D+14
I= 27 X= 4.150206770470D+13 Y= 2.362787890062D+13 Z= 1.322391741521D+14
I= 28 X= -2.921822782040D+12 Y= -1.092319468371D+14 Z= 1.493836988122D+13
I= 29 X= 1.580677010827D+13 Y= -4.367438023098D+12 Z= -1.554462558002D+13
I= 30 X= 2.751868446256D+13 Y= -5.792995887663D+11 Z= 5.170760110032D+12
I= 31 X= -9.175946289609D+13 Y= 3.838208988733D+12 Z= 6.613365259156D+13
I= 32 X= 1.416020710974D+13 Y= 4.414396259225D+13 Z= -4.248166368917D+13
I= 33 X= -5.879104104309D+13 Y= -3.177866836587D+13 Z= 7.561218209766D+13
I= 34 X= -2.756735421203D+13 Y= -4.226648052942D+13 Z= -3.755580519527D+13
I= 35 X= -3.047020527301D+12 Y= 4.816296254001D+11 Z= 7.596020984497D+12
I= 36 X= -2.743662277405D+13 Y= -1.930861145054D+13 Z= -6.594451185900D+12
I= 37 X= 4.080802707305D+13 Y= 2.522704264678D+13 Z= -3.816304015972D+13
I= 38 X= -2.286569848999D+13 Y= 8.630094844026D+12 Z= -7.339730350099D+13

Seed: 13240811936

CM Start Point Coordinates: bohr

I= 0 X= -2.133966286039D+00 Y= -2.013471243976D+00 Z= 1.282063638930D-03
I= 1 X= 4.356509065408D-02 Y= -2.660036033071D+00 Z= -1.407872384542D+00
I= 2 X= -1.273719418090D+00 Y= -1.121209002399D+00 Z= 2.395064210544D+00
I= 3 X= 2.062778892854D+00 Y= -2.068614723375D+00 Z= 5.157541633404D-02
I= 4 X= 1.340668324039D+00 Y= -1.336584392434D+00 Z= 2.619954402687D+00
I= 5 X= -3.144158845812D+00 Y= 3.043161714022D+00 Z= -2.295339277605D+00
I= 6 X= -2.716063196623D-01 Y= 2.180019572718D+00 Z= -3.162320213309D+00
I= 7 X= -2.761264986435D+00 Y= 4.628866987028D+00 Z= -3.871416189680D+00
I= 8 X= -4.489107811815D+00 Y= 1.260166225773D+00 Z= -2.681701152777D+00
I= 9 X= 3.167648571545D+00 Y= -9.671142369246D-01 Z= 4.692022458050D+00
I= 10 X= 3.368867073806D+00 Y= -2.920044104843D+00 Z= 5.555918296235D+00
I= 11 X= 4.899901222775D+00 Y= -3.678871945947D-02 Z= 4.329924335148D+00
I= 12 X= 2.333831517709D+00 Y= 2.440858730204D-01 Z= 6.372392121354D+00
I= 13 X= -3.267643036797D+00 Y= -6.834501458088D-01 Z= 4.530821727426D+00
I= 14 X= -3.935629159928D+00 Y= -2.773139132318D+00 Z= 5.340633135136D+00
I= 15 X= -2.287038310304D+00 Y= 4.964362232410D-01 Z= 6.098459797095D+00
I= 16 X= -5.209230718393D+00 Y= 3.278299880415D-01 Z= 3.950333437855D+00
I= 17 X= -4.814815241216D+00 Y= -2.649298592300D+00 Z= -9.699313368745D-01
I= 18 X= -5.624112668930D+00 Y= -4.268935321711D+00 Z= 3.120723618607D-01
I= 19 X= -6.246072885839D+00 Y= -9.074343044055D-01 Z= -5.033099819990D-01
I= 20 X= -5.265259867952D+00 Y= -3.433180714085D+00 Z= -3.064898562336D+00
I= 21 X= 1.943234620206D-01 Y= -3.764608278939D+00 Z= -4.134025179560D+00
I= 22 X= -2.377204999859D-02 Y= -5.652118918375D+00 Z= -4.015754697731D+00
I= 23 X= -1.429697709441D+00 Y= -3.387449145822D+00 Z= -5.298576008699D+00
I= 24 X= 2.150407089779D+00 Y= -3.110332615422D+00 Z= -4.879837977677D+00
I= 25 X= 4.824656016828D+00 Y= -2.612649289825D+00 Z= -7.776333269423D-01
I= 26 X= 4.702478605896D+00 Y= -3.189058594667D+00 Z= -3.032507612785D+00
I= 27 X= 6.319507188039D+00 Y= -1.197645717900D+00 Z= -2.535142193533D-01
I= 28 X= 5.053624737545D+00 Y= -4.590695505524D+00 Z= -3.691818084265D-01

I= 29 X= 2.800589889890D+00 Y= 3.479848293118D+00 Z= -2.638512852494D+00
I= 30 X= 3.043257994708D+00 Y= 3.693471120843D+00 Z= -4.001310462167D-02
I= 31 X= 3.972217065884D+00 Y= 1.641772844957D+00 Z= -3.617950380965D+00
I= 32 X= 1.906579240158D+00 Y= 4.915785478987D+00 Z= -3.565519144729D+00
I= 33 X= 2.727134081744D+00 Y= 5.824775322769D+00 Z= 2.000932009734D-01
I= 34 X= 4.593330912587D+00 Y= 2.674827515069D+00 Z= 1.207212703625D+00
I= 35 X= 3.675174920002D-02 Y= 1.207930842939D+00 Z= -4.197706940505D-01
I= 36 X= -2.881665476333D+00 Y= 3.910761674901D+00 Z= 2.484178675512D-01
I= 37 X= -2.070867139723D+00 Y= 5.828539072818D+00 Z= 5.804083258305D-01
I= 38 X= -4.105125069899D+00 Y= 3.271009550058D+00 Z= 1.817705662804D+00

Forward Direction:

Total Energy: -691.9949096 Hartrees

Potential Energy: -692.1719240 Hartress

Kinetic Energy: 0.1770145 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.570187764909D+12 Y= 5.075613517925D+12 Z= -9.811296966225D+12
I= 1 X= 2.211014543358D+13 Y= 5.497601198458D+12 Z= -1.394848200789D+13
I= 2 X= -5.738982776050D+12 Y= -1.397217345927D+13 Z= 1.064082175882D+13
I= 3 X= -5.604314549263D+12 Y= -1.118260873752D+13 Z= 5.428630136402D+12
I= 4 X= 2.126452809971D+12 Y= 7.484742875600D+12 Z= 1.250774802797D+13
I= 5 X= 3.510643574112D+12 Y= -2.016580818000D+13 Z= 1.895792962360D+13
I= 6 X= 6.992933545056D+13 Y= -4.241373573764D+13 Z= 8.393072671207D+13
I= 7 X= -3.081814198145D+13 Y= 7.251437121576D+13 Z= -2.645336606312D+13
I= 8 X= -6.878996400925D+12 Y= 7.121593251969D+13 Z= -4.822337087902D+13
I= 9 X= 3.653064178805D+12 Y= 2.527124055523D+13 Z= 1.099060570872D+13
I= 10 X= 1.730951939727D+13 Y= -1.479336143762D+14 Z= 1.329987820857D+14
I= 11 X= 4.336610201035D+13 Y= 5.853695578292D+12 Z= -4.265349822930D+13
I= 12 X= -1.513768598475D+13 Y= 1.094226423585D+13 Z= -7.023004518825D+13
I= 13 X= 1.270491576404D+13 Y= 4.975053747251D+12 Z= 1.879210164040D+13
I= 14 X= 1.388878034174D+13 Y= -2.456002899312D+13 Z= -2.922761284043D+13

I= 15 X= -7.088462945319D+13 Y= -2.588012643451D+13 Z= -1.399159385101D+13
I= 16 X= -9.134038055371D+13 Y= -3.663767052095D+12 Z= 3.545606749394D+13
I= 17 X= -9.649123256141D+12 Y= -1.142221166348D+13 Z= -1.195034029878D+13
I= 18 X= -3.705800982958D+13 Y= -5.690168625354D+12 Z= 6.585799898534D+13
I= 19 X= 8.450746690390D+13 Y= -1.166130074348D+14 Z= 2.436809313834D+12
I= 20 X= 1.365672503691D+13 Y= 8.221810118353D+13 Z= -1.387192459907D+14
I= 21 X= -9.236366399385D+12 Y= -1.324721152849D+13 Z= 2.511688425922D+11
I= 22 X= 2.045634834567D+13 Y= 8.824344467978D+12 Z= 8.248099884300D+12
I= 23 X= 4.023886863898D+13 Y= 1.393129234963D+13 Z= 2.501111994235D+12
I= 24 X= -1.130031390378D+14 Y= -2.164737481102D+13 Z= 8.400695577398D+13
I= 25 X= 1.275742248776D+12 Y= -1.316539543407D+13 Z= 1.709611844769D+13
I= 26 X= -5.994177518543D+13 Y= -3.739629102973D+13 Z= 4.250482271160D+13
I= 27 X= -9.449675927084D+13 Y= 8.389054646672D+13 Z= 5.210360755744D+13
I= 28 X= -7.131127404849D+13 Y= 9.074902713872D+13 Z= -1.137649958762D+13
I= 29 X= 6.201397744277D+12 Y= 4.315298834942D+11 Z= -5.365775439283D+12
I= 30 X= 5.149311955015D+12 Y= 6.276136658853D+12 Z= -1.963116014162D+13
I= 31 X= -6.440600343964D+13 Y= 1.495330761773D+13 Z= 7.555460672099D+13
I= 32 X= 4.100416515009D+13 Y= -3.642182467822D+13 Z= 1.803262002221D+13
I= 33 X= 4.014476569981D+11 Y= 3.788658134059D+13 Z= -4.882092234719D+13
I= 34 X= 3.426667657550D+12 Y= 4.621095465759D+13 Z= -2.021461839060D+13
I= 35 X= -2.409895600426D+12 Y= 3.587377923386D+12 Z= -4.832122858319D+12
I= 36 X= 5.635430098975D+12 Y= -4.513580838297D+12 Z= -3.248936176852D+13
I= 37 X= 7.944768990416D+13 Y= 8.804675882886D+13 Z= 5.048951621068D+13
I= 38 X= -4.470438860698D+13 Y= 1.405075203038D+13 Z= 6.086279743965D+13

Backward Direction:

Total Energy: -691.9949878 Hartrees

Potential Energy: -692.1719240 Hartress

Kinetic Energy: 0.1769362 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.535234316690D+12 Y= 6.354112000642D+12 Z= -7.499301181255D+12

I= 1 X= 2.205928233551D+13 Y= 5.497962335761D+12 Z= -1.394871228277D+13
I= 2 X= -4.670562796328D+12 Y= -1.386917842228D+13 Z= 1.175998366049D+13
I= 3 X= -5.639037476284D+12 Y= -1.246120090346D+13 Z= 3.116339146682D+12
I= 4 X= 3.195020509127D+12 Y= 7.381898592776D+12 Z= 1.138871852780D+13
I= 5 X= 4.300393679536D+12 Y= -3.161144185473D+13 Z= 6.749683765265D+12
I= 6 X= 1.100359474732D+13 Y= -4.240091219583D+13 Z= 8.393170773594D+13
I= 7 X= -4.339524134640D+13 Y= 6.312479704531D+13 Z= -4.411678917001D+13
I= 8 X= -1.118000315450D+13 Y= 5.967377074594D+13 Z= -5.148718780537D+13
I= 9 X= 5.979893832964D+12 Y= 2.110360967379D+13 Z= 1.003633632360D+13
I= 10 X= 1.643457011797D+13 Y= -1.528949678817D+14 Z= 1.309312922521D+14
I= 11 X= 4.625810766250D+13 Y= -1.923527756851D+12 Z= -4.333779040328D+13
I= 12 X= -9.725335779397D+12 Y= 7.234679481529D+12 Z= -6.995957479039D+13
I= 13 X= 1.503158428750D+13 Y= 9.142724256909D+12 Z= 1.974703754634D+13
I= 14 X= 1.301565716997D+13 Y= -1.959801386883D+13 Z= -2.715902357682D+13
I= 15 X= -6.547336690356D+13 Y= -2.217088023922D+13 Z= -1.426232349235D+13
I= 16 X= -8.844935741162D+13 Y= 4.111173320331D+12 Z= 3.614191417175D+13
I= 17 X= -1.015645243318D+13 Y= -1.147298950011D+13 Z= -7.729098974033D+12
I= 18 X= -3.696906181168D+13 Y= -3.786980465511D+12 Z= 7.490618444560D+13
I= 19 X= 8.429512990281D+13 Y= -1.151281966703D+14 Z= 3.946232339951D+12
I= 20 X= 1.184355049996D+13 Y= 7.679275066475D+13 Z= -1.340064967987D+14
I= 21 X= -1.321677539266D+13 Y= -1.324539418149D+13 Z= 2.499496921651D+11
I= 22 X= 1.028192922384D+13 Y= 8.826274892523D+12 Z= 8.244730353591D+12
I= 23 X= 3.787043563311D+13 Y= 1.878832784698D+13 Z= 2.516972247468D+12
I= 24 X= -1.153719988753D+14 Y= -2.649945723926D+13 Z= 8.398953877377D+13
I= 25 X= 7.689094200066D+11 Y= -1.311547758865D+13 Z= 1.287472788421D+13
I= 26 X= -6.175409848198D+13 Y= -3.197200757191D+13 Z= 3.779157381554D+13
I= 27 X= -9.470832197292D+13 Y= 8.240387066771D+13 Z= 5.059481592956D+13
I= 28 X= -7.122204406511D+13 Y= 8.884437425602D+13 Z= -2.042470130704D+13
I= 29 X= 6.990382906100D+12 Y= 1.187380270855D+13 Z= 6.839095616981D+12
I= 30 X= 7.889425576333D+12 Y= 5.736834094887D+12 Z= -7.910860452924D+12

I= 31 X= -6.870516137819D+13 Y= 2.649185850761D+13 Z= 7.881508491991D+13
I= 32 X= 2.843037422770D+13 Y= -2.703128797965D+13 Z= 3.569064405736D+13
I= 33 X= -1.455487762244D+12 Y= 3.045825771257D+13 Z= -2.542192303163D+13
I= 34 X= 5.390013620056D+12 Y= 3.863930759057D+13 Z= -1.271901436498D+13
I= 35 X= -2.539926055797D+12 Y= 3.587828302413D+12 Z= -4.830852183776D+12
I= 36 X= 8.375379585079D+12 Y= -3.975653267998D+12 Z= -4.421040984863D+13
I= 37 X= 7.758642050276D+13 Y= 9.547921469934D+13 Z= 2.708874173868D+13
I= 38 X= -4.274106979323D+13 Y= 2.161876712543D+13 Z= 5.336696950970D+13

Seed: 13731475592

CM Start Point Coordinates: bohr

I= 0 X= -2.166799697984D+00 Y= -2.080912253623D+00 Z= -1.572794184769D-02
I= 1 X= -8.873153551691D-02 Y= -2.598128205583D+00 Z= -1.509718175450D+00
I= 2 X= -1.276413203340D+00 Y= -1.255174659390D+00 Z= 2.355918229083D+00
I= 3 X= 2.189009292544D+00 Y= -2.201253303396D+00 Z= 4.217379323335D-02
I= 4 X= 1.391499994113D+00 Y= -1.184898048146D+00 Z= 2.357336754583D+00
I= 5 X= -2.576513925496D+00 Y= 3.331333004841D+00 Z= -2.492694831982D+00
I= 6 X= -2.661171562424D-02 Y= 1.927525971427D+00 Z= -3.320250562459D+00
I= 7 X= -1.325304511840D+00 Y= 4.944694056852D+00 Z= -3.366971486213D+00
I= 8 X= -3.591304685997D+00 Y= 2.081302425574D+00 Z= -3.894833538873D+00
I= 9 X= 2.995984985009D+00 Y= -7.867706624674D-01 Z= 4.531513974869D+00
I= 10 X= 3.987486093872D+00 Y= -2.662031573323D+00 Z= 5.444291892368D+00
I= 11 X= 5.016065219798D+00 Y= 1.609661360992D-01 Z= 3.849357469745D+00
I= 12 X= 2.225262677660D+00 Y= 3.300505047403D-01 Z= 6.251912032205D+00
I= 13 X= -2.831272922012D+00 Y= -4.461588473667D-01 Z= 4.521952653823D+00
I= 14 X= -2.866804798100D+00 Y= -1.900557241697D+00 Z= 6.155244991923D+00
I= 15 X= -1.859828883169D+00 Y= 1.620777097696D+00 Z= 5.204816500259D+00
I= 16 X= -4.974649956220D+00 Y= 1.142846400485D-01 Z= 4.181015882269D+00
I= 17 X= -4.882102749217D+00 Y= -2.568335328804D+00 Z= -7.047666614832D-01
I= 18 X= -5.591288964446D+00 Y= -4.001432298062D+00 Z= 5.498638671092D-01

I= 19 X= -6.064513803517D+00 Y= -1.073176476304D+00 Z= -3.728252678805D-01
I= 20 X= -5.398379311148D+00 Y= -3.016381669382D+00 Z= -2.786526879540D+00
I= 21 X= -7.254134873938D-02 Y= -3.687244663832D+00 Z= -4.204669010062D+00
I= 22 X= -3.941402892945D-01 Y= -5.916834079842D+00 Z= -4.026538494878D+00
I= 23 X= -1.502813402380D+00 Y= -2.171078884368D+00 Z= -5.246927283466D+00
I= 24 X= 1.820067036046D+00 Y= -3.338286263420D+00 Z= -5.232855452309D+00
I= 25 X= 4.911343209581D+00 Y= -2.741873996778D+00 Z= -8.237100202940D-01
I= 26 X= 5.220400417018D+00 Y= -3.702657226995D+00 Z= -2.854887268752D+00
I= 27 X= 5.900895533097D+00 Y= -6.493228923811D-01 Z= -7.684124445165D-01
I= 28 X= 5.612488676508D+00 Y= -4.145633414352D+00 Z= 4.319869429454D-01
I= 29 X= 2.730599676427D+00 Y= 3.107682595341D+00 Z= -2.197549667403D+00
I= 30 X= 2.397716909465D+00 Y= 4.104395492624D+00 Z= 3.846150527787D-01
I= 31 X= 4.201113590357D+00 Y= 1.575619153169D+00 Z= -2.302236225021D+00
I= 32 X= 2.469711495719D+00 Y= 4.318051280858D+00 Z= -3.575629132255D+00
I= 33 X= 1.569772681983D+00 Y= 6.099165404545D+00 Z= 5.873615136768D-01
I= 34 X= 3.491720028374D+00 Y= 3.311183240883D+00 Z= 2.016707182692D+00
I= 35 X= 5.198082937561D-02 Y= 1.091946784741D+00 Z= -5.147800770647D-01
I= 36 X= -3.041271254993D+00 Y= 3.498882136905D+00 Z= 3.294149767779D-01
I= 37 X= -2.238173141041D+00 Y= 5.076922808793D+00 Z= 1.132990571315D+00
I= 38 X= -4.916638135181D+00 Y= 2.752830208489D+00 Z= 1.396193259402D+00

Forward Direction:

Total Energy: -691.9952183 Hartrees

Potential Energy: -692.1773766 Hartress

Kinetic Energy: 0.1821583 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.683275934211D+13 Y= 1.549900529824D+13 Z= 2.405487734144D+12

I= 1 X= 7.423842021996D+11 Y= -1.405114657629D+13 Z= -5.049870935682D+12

I= 2 X= -5.672852100344D+12 Y= -7.817649284433D+12 Z= -2.800522926843D+11

I= 3 X= 3.081754433902D+12 Y= 1.762546255315D+13 Z= 9.386798506090D+12

I= 4 X= 4.950645412583D+12 Y= 1.057084420142D+12 Z= 1.506134154844D+13

I= 5 X= 1.438191149175D+12 Y= 3.979946119071D+12 Z= -2.424775994167D+13
I= 6 X= 4.886559019932D+13 Y= -2.925813806893D+13 Z= 6.749198312972D+13
I= 7 X= 2.844871733685D+13 Y= 6.999395945844D+13 Z= 2.204456464067D+12
I= 8 X= 2.464800893736D+13 Y= 1.097223724840D+13 Z= -1.317434368124D+13
I= 9 X= -1.437110596598D+13 Y= 8.473478511079D+12 Z= -2.568052926099D+13
I= 10 X= 2.255453504648D+13 Y= -1.329452296766D+14 Z= 5.087473287156D+13
I= 11 X= -9.197290440586D+13 Y= 8.977801293727D+13 Z= -4.287603951799D+13
I= 12 X= 1.888541732098D+13 Y= -2.939666842683D+13 Z= -2.632467914928D+13
I= 13 X= 1.032718300692D+13 Y= -1.173591717668D+13 Z= 6.693757015009D+12
I= 14 X= -8.948889958365D+13 Y= 2.632374834107D+13 Z= 8.345803681222D+12
I= 15 X= 2.103739891344D+12 Y= 6.160667942564D+13 Z= -3.811797084415D+12
I= 16 X= 1.023361998729D+14 Y= -3.858461895666D+13 Z= 1.884723542108D+13
I= 17 X= 2.061927040557D+13 Y= 1.887674748521D+12 Z= 2.576707586385D+13
I= 18 X= -1.109677464532D+14 Y= -2.508046424491D+13 Z= -2.372168582839D+13
I= 19 X= 1.333222096543D+12 Y= 3.457213435380D+13 Z= 1.010407562950D+14
I= 20 X= 3.128972632351D+12 Y= 4.481773859122D+13 Z= -1.785595608461D+13
I= 21 X= 1.909196717805D+13 Y= -4.050782542723D+11 Z= -1.875596739037D+12
I= 22 X= -7.533971684649D+13 Y= 8.526850917276D+13 Z= 9.448777816830D+12
I= 23 X= -1.200251277300D+14 Y= 8.095640178120D+13 Z= -6.544273616869D+13
I= 24 X= -4.735411302861D+13 Y= -3.833468967289D+13 Z= -1.517982765262D+13
I= 25 X= 2.789784772080D+12 Y= 1.839391875716D+13 Z= 4.917943475890D+12
I= 26 X= 2.928282498938D+13 Y= 5.876720593347D+12 Z= -3.572830250347D+13
I= 27 X= -7.714100682873D+13 Y= -4.504287193622D+13 Z= -1.077544988956D+13
I= 28 X= -2.519103611286D+13 Y= -4.942930298477D+13 Z= 5.936338484887D+13
I= 29 X= 1.269852523161D+13 Y= -6.978728858134D+12 Z= -1.744894991429D+13
I= 30 X= 2.521625036154D+12 Y= -1.822140159522D+13 Z= 8.147659042556D+12
I= 31 X= -4.606555398007D+13 Y= 1.388682200783D+13 Z= 9.534509336761D+13
I= 32 X= -2.907208281750D+13 Y= 1.672387090751D+13 Z= -1.375704324077D+13
I= 33 X= 2.207733602252D+13 Y= 1.382332994831D+14 Z= -3.471462162078D+13
I= 34 X= 1.013060484321D+14 Y= -6.195290612174D+13 Z= 8.315524489337D+13

I= 35 X= -3.152438767624D+11 Y= -2.589422617507D+12 Z= -4.886124696317D+12

I= 36 X= 5.449803204433D+12 Y= -2.795849898666D+12 Z= -3.370785417511D+12

I= 37 X= -9.154005467160D+13 Y= -1.055214990031D+14 Z= 3.479365519411D+13

I= 38 X= -2.095937421507D+13 Y= -3.051768145566D+13 Z= 1.245330352842D+14

Backward Direction:

Total Energy: -691.9952095 Hartrees

Potential Energy: -692.1773766 Hartress

Kinetic Energy: 0.1821671 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.673024398480D+13 Y= 1.633938703532D+13 Z= 3.559027709130D+12

I= 1 X= 1.477661227052D+12 Y= -1.405100824109D+13 Z= -5.049934092311D+12

I= 2 X= -5.483589148460D+12 Y= -8.431404774762D+12 Z= 3.761838727453D+11

I= 3 X= 3.184346499196D+12 Y= 1.678499356461D+13 Z= 8.233098358302D+12

I= 4 X= 5.139962204122D+12 Y= 1.670910369366D+12 Z= 1.440508377174D+13

I= 5 X= 3.218388020752D+12 Y= -4.345701738941D+11 Z= -2.978325178951D+13

I= 6 X= -1.110212841912D+13 Y= -2.925003746459D+13 Z= 6.749181346604D+13

I= 7 X= 2.045896661443D+13 Y= 7.053347795883D+13 Z= -3.831291194104D+12

I= 8 X= 2.024310788532D+13 Y= 1.057944698638D+13 Z= -1.475113240079D+13

I= 9 X= -1.371200237053D+13 Y= 7.260964820584D+12 Z= -2.614306332727D+13

I= 10 X= 2.199470895906D+13 Y= -1.345821725235D+14 Z= 4.984598364314D+13

I= 11 X= -9.108655426075D+13 Y= 8.728323465468D+13 Z= -4.314007740452D+13

I= 12 X= 2.064974762076D+13 Y= -3.054365214344D+13 Z= -2.616639069426D+13

I= 13 X= 1.098620497330D+13 Y= -1.052339027372D+13 Z= 7.156467967268D+12

I= 14 X= -9.004823454562D+13 Y= 2.796085245828D+13 Z= 9.374796895809D+12

I= 15 X= 3.867706841291D+12 Y= 6.275419741437D+13 Z= -3.970162375849D+12

I= 16 X= 1.032222096203D+14 Y= -3.609056658702D+13 Z= 1.911175690852D+13

I= 17 X= 2.062821746700D+13 Y= 2.011153198653D+12 Z= 2.710310274605D+13

I= 18 X= -1.105565048886D+14 Y= -2.453399181117D+13 Z= -2.110675168978D+13

I= 19 X= 1.141485400785D+12 Y= 3.488026713089D+13 Z= 1.016478779273D+14

I= 20 X= 2.841980496368D+12 Y= 4.336594286490D+13 Z= -1.639226942098D+13

I= 21 X= 1.798347639630D+13 Y= -4.044550540391D+11 Z= -1.876015902922D+12
I= 22 X= -7.822610908990D+13 Y= 8.526915314531D+13 Z= 9.447591817358D+12
I= 23 X= -1.208128785233D+14 Y= 8.228958924109D+13 Z= -6.524632485315D+13
I= 24 X= -4.814207221616D+13 Y= -3.966607459997D+13 Z= -1.537694252047D+13
I= 25 X= 2.798840246998D+12 Y= 1.827021364037D+13 Z= 3.581893806711D+12
I= 26 X= 2.899612338436D+13 Y= 7.327981349145D+12 Z= -3.719207384455D+13
I= 27 X= -7.733258841693D+13 Y= -4.535148014468D+13 Z= -1.138245813413D+13
I= 28 X= -2.477985246515D+13 Y= -4.997610040331D+13 Z= 5.674872917906D+13
I= 29 X= 1.447852689597D+13 Y= -2.565697391807D+12 Z= -1.191461795961D+13
I= 30 X= 5.002578523489D+12 Y= -1.732908879900D+13 Z= 1.172768495620D+13
I= 31 X= -5.046768766942D+13 Y= 1.428017501257D+13 Z= 9.692111687727D+13
I= 32 X= -3.706121508340D+13 Y= 1.618401872062D+13 Z= -7.723626515272D+12
I= 33 X= 2.134562145740D+13 Y= 1.358302229187D+14 Z= -2.675300194943D+13
I= 34 X= 1.013403557042D+14 Y= -6.471989919237D+13 Z= 8.670536912957D+13
I= 35 X= -8.851452611690D+11 Y= -2.589287279361D+12 Z= -4.885652260404D+12
I= 36 X= 7.931014578972D+12 Y= -3.688750088294D+12 Z= -6.951014847823D+12
I= 37 X= -9.227291977369D+13 Y= -1.031167580819D+14 Z= 2.683078210007D+13
I= 38 X= -2.092437308551D+13 Y= -2.775132952729D+13 Z= 1.209830423505D+14

Seed: 144341594

CM Start Point Coordinates: bohr

I= 0 X= -2.149086712168D+00 Y= -2.326015070131D+00 Z= -1.725012835355D-02
I= 1 X= -7.850816594117D-02 Y= -2.902479941626D+00 Z= -1.658854512434D+00
I= 2 X= -1.326067981551D+00 Y= -1.383080629766D+00 Z= 2.471885205624D+00
I= 3 X= 2.239433461190D+00 Y= -2.093734719728D+00 Z= -1.941725641033D-01
I= 4 X= 1.213019436813D+00 Y= -1.217382074326D+00 Z= 2.370209043396D+00
I= 5 X= -2.736695203834D+00 Y= 3.616984442488D+00 Z= -2.380408304513D+00
I= 6 X= 4.320599359012D-02 Y= 1.985299909720D+00 Z= -3.037696173320D+00
I= 7 X= -2.064611569384D+00 Y= 5.534682058862D+00 Z= -3.206477536007D+00
I= 8 X= -3.960366946751D+00 Y= 2.390024956601D+00 Z= -3.754766947844D+00

I= 9 X= 2.893936022737D+00 Y= -8.419690396458D-01 Z= 4.511996702193D+00
I= 10 X= 2.332969799263D+00 Y= -2.115341109519D+00 Z= 6.142215728922D+00
I= 11 X= 5.115882479544D+00 Y= -1.262742049232D+00 Z= 4.271173825449D+00
I= 12 X= 2.626941105203D+00 Y= 1.166455241334D+00 Z= 5.306042371626D+00
I= 13 X= -2.827070037528D+00 Y= -2.864838686109D-01 Z= 4.769851491432D+00
I= 14 X= -2.773432384577D+00 Y= -1.967464465852D+00 Z= 6.040997650060D+00
I= 15 X= -1.798377803658D+00 Y= 1.474923372595D+00 Z= 5.476400774402D+00
I= 16 X= -4.423840301569D+00 Y= 4.392185143282D-01 Z= 4.274987185079D+00
I= 17 X= -4.917160091332D+00 Y= -2.635934303509D+00 Z= -9.253554830090D-01
I= 18 X= -5.136220058928D+00 Y= -4.476149356837D+00 Z= -3.949654724784D-01
I= 19 X= -6.121021291948D+00 Y= -1.115275102335D+00 Z= 2.494339740667D-01
I= 20 X= -5.218243625251D+00 Y= -2.722511300655D+00 Z= -2.952439675665D+00
I= 21 X= 4.134492243831D-02 Y= -4.215203522951D+00 Z= -4.143341010726D+00
I= 22 X= 3.939590390711D-01 Y= -6.175006282467D+00 Z= -3.711227024779D+00
I= 23 X= -1.452793929655D+00 Y= -3.843308451520D+00 Z= -5.736284249475D+00
I= 24 X= 1.635733138183D+00 Y= -3.016292841216D+00 Z= -5.261015190790D+00
I= 25 X= 4.900761912909D+00 Y= -2.287534888465D+00 Z= -8.398807431206D-01
I= 26 X= 5.448687340337D+00 Y= -2.459864218593D+00 Z= -2.994738349601D+00
I= 27 X= 5.705025266242D+00 Y= -4.260620954671D-01 Z= 7.260162819642D-02
I= 28 X= 5.941128672430D+00 Y= -4.015530186104D+00 Z= 8.273759038996D-02
I= 29 X= 2.778630602352D+00 Y= 3.312113527727D+00 Z= -2.279273311751D+00
I= 30 X= 2.770615301172D+00 Y= 3.644632697947D+00 Z= 2.746329705401D-01
I= 31 X= 3.935566289655D+00 Y= 2.124077998938D+00 Z= -3.118464742608D+00
I= 32 X= 2.078865038299D+00 Y= 4.636024041203D+00 Z= -3.443201535312D+00
I= 33 X= 1.932148367563D+00 Y= 5.326800507745D+00 Z= 1.108242032277D+00
I= 34 X= 3.914458169177D+00 Y= 2.812124326893D+00 Z= 1.625063756286D+00
I= 35 X= -8.473661466005D-03 Y= 1.118538550340D+00 Z= -4.425803512113D-01
I= 36 X= -2.873255707097D+00 Y= 3.871605064170D+00 Z= 2.846339467766D-01
I= 37 X= -2.506831021526D+00 Y= 5.921851072396D+00 Z= 1.076438071881D+00
I= 38 X= -4.318633768492D+00 Y= 2.775392497443D+00 Z= 1.038164136698D+00

Forward Direction:

Total Energy: -691.9985711 Hartrees

Potential Energy: -692.1855464 Hartress

Kinetic Energy: 0.1869753 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.841003289915D+12 Y= -1.866225572010D+13 Z= 1.030280327958D+13
I= 1 X= 9.447873035199D+12 Y= -1.140389726742D+13 Z= -9.782527135797D+12
I= 2 X= 2.563799320644D+11 Y= 8.524104856275D+12 Z= 3.859241987914D+12
I= 3 X= -2.850218676622D+12 Y= -1.098980086134D+13 Z= -1.285520670704D+13
I= 4 X= 8.197850686127D+12 Y= 2.396837821221D+13 Z= 3.532579754477D+12
I= 5 X= -5.063380786593D+12 Y= 2.314594374469D+13 Z= -1.205179738778D+13
I= 6 X= 4.630558627195D+13 Y= -1.984666439419D+13 Z= -7.109697172409D+13
I= 7 X= -3.045785222503D+13 Y= -1.406844507357D+14 Z= 6.940020578625D+13
I= 8 X= -1.215678543652D+14 Y= 1.587084619811D+13 Z= -7.788766159998D+13
I= 9 X= -9.073418291695D+12 Y= -3.142594968508D+13 Z= 1.859956697122D+13
I= 10 X= 1.684368422160D+13 Y= 5.943244443095D+13 Z= -1.384787867913D+14
I= 11 X= -2.150734524506D+13 Y= -5.596639396081D+13 Z= 5.948015878422D+13
I= 12 X= -1.743147608415D+13 Y= 7.589782288258D+13 Z= -5.846026673291D+13
I= 13 X= -1.479457750283D+12 Y= -4.273695494198D+12 Z= -4.576087616214D+12
I= 14 X= 3.172891195053D+13 Y= 4.161140715317D+13 Z= -4.054425782308D+13
I= 15 X= -1.736680394085D+13 Y= 6.339863697689D+13 Z= -3.532334646174D+13
I= 16 X= 6.670218576784D+13 Y= 1.229774500513D+13 Z= -6.864325622982D+12
I= 17 X= -9.527794289715D+12 Y= -1.164378063338D+13 Z= -2.788203930282D+13
I= 18 X= 7.730668671597D+13 Y= 2.968834913911D+13 Z= 3.944635103730D+13
I= 19 X= -3.849536035258D+13 Y= 6.386631886155D+13 Z= -2.930953875857D+13
I= 20 X= -6.115627457805D+13 Y= 4.686225716203D+13 Z= -2.618023396446D+13
I= 21 X= -2.400365823787D+12 Y= 1.006597575828D+13 Z= 1.291384957108D+13
I= 22 X= -1.935518094556D+13 Y= -1.290569175888D+14 Z= 1.102642275270D+14
I= 23 X= 6.904309848469D+13 Y= -2.237201055182D+13 Z= 4.369971036071D+12
I= 24 X= 4.566336959538D+13 Y= 3.082322980983D+13 Z= -1.079276099100D+14

I= 25 X= -3.794429969823D+12 Y= 8.445765646190D+12 Z= -1.174175344773D+13
I= 26 X= 5.244986797158D+12 Y= -1.616448855442D+13 Z= 1.873865484417D+14
I= 27 X= -5.918247596606D+11 Y= -2.622758641641D+13 Z= 3.551631655841D+13
I= 28 X= 3.256825398723D+13 Y= 9.168625923795D+13 Z= -1.516427909588D+13
I= 29 X= -2.481389810176D+12 Y= 9.988681567119D+11 Z= -5.256037320334D+12
I= 30 X= 7.315912922707D+12 Y= -4.846521882903D+12 Z= -1.010528973413D+13
I= 31 X= -1.221162249381D+12 Y= 4.416887996383D+12 Z= 5.376657182756D+13
I= 32 X= -3.960644346991D+13 Y= -5.675434458098D+13 Z= -2.124822892422D+13
I= 33 X= -7.577620286004D+13 Y= 8.035305393969D+13 Z= 6.511895824102D+13
I= 34 X= 5.774354587394D+13 Y= -1.635739057243D+13 Z= 6.448721473961D+13
I= 35 X= -4.070424354223D+11 Y= -1.606255392820D+12 Z= 5.111972093143D+12
I= 36 X= 2.841884501886D+12 Y= 1.991424016198D+13 Z= 5.227909299877D+12
I= 37 X= -2.405650153992D+13 Y= -4.047215775287D+13 Z= 1.723039600562D+13
I= 38 X= 4.049811692264D+13 Y= -2.001524005682D+13 Z= 9.716068497011D+13

Backward Direction:

Total Energy: -691.9985633 Hartrees

Potential Energy: -692.1855464 Hartress

Kinetic Energy: 0.1869831 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.939474602594D+12 Y= -1.774740440715D+13 Z= 1.159687115111D+13
I= 1 X= 1.016788672127D+13 Y= -1.140373631176D+13 Z= -9.782605114277D+12
I= 2 X= 5.160851985451D+11 Y= 7.927253034867D+12 Z= 4.581937457268D+12
I= 3 X= -2.751656031976D+12 Y= -1.190474446785D+13 Z= -1.414945248460D+13
I= 4 X= 8.457619090845D+12 Y= 2.456530973168D+13 Z= 2.809872128024D+12
I= 5 X= -3.257362186444D+12 Y= 1.801499779569D+13 Z= -1.833822308647D+13
I= 6 X= -1.675462930348D+13 Y= -1.983781160240D+13 Z= -7.109707121598D+13
I= 7 X= -3.918462904353D+13 Y= -1.407992480420D+14 Z= 6.224639900710D+13
I= 8 X= -1.261980321568D+14 Y= 1.469063400758D+13 Z= -7.966365834948D+13
I= 9 X= -8.264854902737D+12 Y= -3.290565203626D+13 Z= 1.807881299932D+13
I= 10 X= 1.623264967279D+13 Y= 5.748052349562D+13 Z= -1.396332471448D+14

I= 11 X= -2.043630678993D+13 Y= -5.895605940259D+13 Z= 5.917328989209D+13
I= 12 X= -1.532319284807D+13 Y= 7.451423745087D+13 Z= -5.828591204316D+13
I= 13 X= -6.709857649609D+11 Y= -2.793977422850D+12 Z= -4.055113750330D+12
I= 14 X= 3.111848623259D+13 Y= 4.356353230449D+13 Z= -3.938948180900D+13
I= 15 X= -1.525895302061D+13 Y= 6.478286241378D+13 Z= -3.549779456379D+13
I= 16 X= 6.777282167976D+13 Y= 1.528653915716D+13 Z= -6.556873974280D+12
I= 17 X= -9.553877353188D+12 Y= -1.152576986078D+13 Z= -2.627711366886D+13
I= 18 X= 7.771746430400D+13 Y= 3.035695146768D+13 Z= 4.264164847692D+13
I= 19 X= -3.869863049235D+13 Y= 6.427162526052D+13 Z= -2.860833536910D+13
I= 20 X= -6.156335890800D+13 Y= 4.506061340043D+13 Z= -2.441589232974D+13
I= 21 X= -3.764835326546D+12 Y= 1.006671396242D+13 Z= 1.291335327818D+13
I= 22 X= -2.289503915994D+13 Y= -1.290561511697D+14 Z= 1.102628287909D+14
I= 23 X= 6.810508556261D+13 Y= -2.072615792449D+13 Z= 4.564330094921D+12
I= 24 X= 4.472512226478D+13 Y= 2.917949148492D+13 Z= -1.081227683121D+14
I= 25 X= -3.820372231801D+12 Y= 8.327472648414D+12 Z= -1.334671175841D+13
I= 26 X= 4.838246875685D+12 Y= -1.436344459259D+13 Z= 1.856220890423D+14
I= 27 X= -7.948889195577D+11 Y= -2.663348876632D+13 Z= 3.481526822232D+13
I= 28 X= 3.297899390350D+13 Y= 9.101723655985D+13 Z= -1.835930373957D+13
I= 29 X= -6.756158895019D+11 Y= 6.128121933391D+12 Z= 1.029014975853D+12
I= 30 X= 9.945593370132D+12 Y= -4.005573219301D+12 Z= -5.776593265362D+12
I= 31 X= -5.848489814952D+12 Y= 5.597405616868D+12 Z= 5.554158602468D+13
I= 32 X= -4.833238422694D+13 Y= -5.663980942250D+13 Z= -1.409708705385D+13
I= 33 X= -7.662390258742D+13 Y= 7.747761526426D+13 Z= 7.456223192529D+13
I= 34 X= 5.791231544696D+13 Y= -1.960077823266D+13 Z= 6.849597298022D+13
I= 35 X= -9.767660902682D+11 Y= -1.606091248938D+12 Z= 5.112524345546D+12
I= 36 X= 5.471807418856D+12 Y= 1.907261895741D+13 Z= 8.989611071351D+11
I= 37 X= -2.490563142528D+13 Y= -3.759479719326D+13 Z= 7.785766890454D+12
I= 38 X= 4.066756738573D+13 Y= -1.677273302705D+13 Z= 9.315204053787D+13

Seed: 17492730888

CM Start Point Coordinates: bohr

I= 0 X= -2.284987197085D+00 Y= -2.237847559684D+00 Z= -1.463593499779D-01
I= 1 X= -3.726522354795D-02 Y= -2.930062928628D+00 Z= -1.506115903141D+00
I= 2 X= -1.332100019961D+00 Y= -1.199408280459D+00 Z= 2.333893343062D+00
I= 3 X= 2.295566265401D+00 Y= -1.967984723172D+00 Z= -6.995073685453D-02
I= 4 X= 1.278503976478D+00 Y= -1.037356853781D+00 Z= 2.419587109412D+00
I= 5 X= -2.548032256706D+00 Y= 3.301831871112D+00 Z= -2.395149184637D+00
I= 6 X= 1.228671910303D-01 Y= 1.697008933911D+00 Z= -3.449593646407D+00
I= 7 X= -1.666895822019D+00 Y= 4.924783905838D+00 Z= -3.285207955907D+00
I= 8 X= -3.941127330704D+00 Y= 2.136644801878D+00 Z= -3.630647876879D+00
I= 9 X= 2.971443979780D+00 Y= -7.487468848999D-01 Z= 4.611445211572D+00
I= 10 X= 3.223028737275D+00 Y= -2.818434040489D+00 Z= 5.511390380178D+00
I= 11 X= 4.662369396497D+00 Y= 1.919700273117D-01 Z= 3.884261798779D+00
I= 12 X= 2.051448773635D+00 Y= 7.176666198718D-01 Z= 5.809183511001D+00
I= 13 X= -2.808790139785D+00 Y= -6.623610148957D-01 Z= 4.775619881629D+00
I= 14 X= -3.306740975993D+00 Y= -2.677723736083D+00 Z= 5.934572330932D+00
I= 15 X= -1.772208406247D+00 Y= 6.588595848210D-01 Z= 6.254515016294D+00
I= 16 X= -4.899099999243D+00 Y= -6.090111866470D-02 Z= 4.139686919576D+00
I= 17 X= -5.006136645380D+00 Y= -2.682305323704D+00 Z= -7.403955995871D-01
I= 18 X= -5.686725632420D+00 Y= -4.073625514981D+00 Z= 3.860334706871D-01
I= 19 X= -5.927974035803D+00 Y= -6.054951368632D-01 Z= -4.531942638865D-01
I= 20 X= -4.952169259208D+00 Y= -3.206680612200D+00 Z= -2.936646246153D+00
I= 21 X= -5.962204805935D-03 Y= -3.851355840618D+00 Z= -4.189411514594D+00
I= 22 X= -7.968154249964D-01 Y= -6.011452177867D+00 Z= -3.994752083188D+00
I= 23 X= -1.302172274521D+00 Y= -2.754960643488D+00 Z= -5.447944785537D+00
I= 24 X= 2.082606321785D+00 Y= -4.015959210675D+00 Z= -4.884596498181D+00
I= 25 X= 4.793152957475D+00 Y= -2.367757817195D+00 Z= -8.000302521278D-01
I= 26 X= 4.952351891615D+00 Y= -1.907090822066D+00 Z= -3.004544875342D+00
I= 27 X= 6.151822308573D+00 Y= -1.339685247610D+00 Z= 5.833111284664D-01
I= 28 X= 5.478009839037D+00 Y= -4.487662246362D+00 Z= -6.217678753488D-01

I= 29 X= 2.799604371201D+00 Y= 3.117672825875D+00 Z= -2.365699829513D+00
I= 30 X= 2.730946504965D+00 Y= 3.943611001819D+00 Z= 3.181183680080D-01
I= 31 X= 4.495883711676D+00 Y= 1.619668485264D+00 Z= -3.134178974956D+00
I= 32 X= 2.284773219947D+00 Y= 4.590024810109D+00 Z= -3.837028044194D+00
I= 33 X= 1.865433899541D+00 Y= 5.853030730986D+00 Z= 1.090482811379D+00
I= 34 X= 3.657068279925D+00 Y= 2.633761713266D+00 Z= 1.824358819939D+00
I= 35 X= -4.769297423262D-02 Y= 1.157813358729D+00 Z= -4.850110208827D-01
I= 36 X= -2.661102104329D+00 Y= 3.703503650720D+00 Z= 1.813065251967D-01
I= 37 X= -1.923327595131D+00 Y= 5.241674655661D+00 Z= 1.197405056068D+00
I= 38 X= -4.264415547963D+00 Y= 2.890042588712D+00 Z= 1.530040797951D+00

Forward Direction:

Total Energy: -692.0040928 Hartrees

Potential Energy: -692.1748513 Hartress

Kinetic Energy: 0.1707585 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.977113525289D+12 Y= -7.918173997146D+12 Z= -1.421755199466D+13
I= 1 X= 2.177689194817D+12 Y= -2.424751142783D+13 Z= -1.562095734675D+13
I= 2 X= 8.995154625037D+12 Y= 2.262259778520D+13 Z= -1.718726671481D+13
I= 3 X= 3.896103596051D+11 Y= 8.507509987624D+12 Z= -3.009273982648D+12
I= 4 X= 1.416732330653D+13 Y= -2.143483663418D+13 Z= -5.946752182072D+12
I= 5 X= 1.264064856611D+12 Y= 8.920703328826D+12 Z= 7.989069862131D+12
I= 6 X= 5.993488599126D+13 Y= 7.710854518620D+11 Z= -1.167789892637D+13
I= 7 X= -1.133074507942D+14 Y= -3.862509693678D+13 Z= -6.128447499945D+12
I= 8 X= -4.899997195471D+13 Y= 2.345448050789D+13 Z= -4.018532747026D+12
I= 9 X= -4.522925562788D+12 Y= 8.921499696467D+12 Z= 1.962704246308D+13
I= 10 X= -3.000030016613D+13 Y= 2.414214337022D+13 Z= -3.626179712494D+13
I= 11 X= -4.452620681963D+13 Y= 1.615093276089D+13 Z= -6.659936468137D+13
I= 12 X= 3.498268550080D+13 Y= -3.472958845317D+13 Z= 4.210694447934D+13
I= 13 X= 9.245915784190D+12 Y= 2.158695114226D+13 Z= 4.034381168107D+12
I= 14 X= -9.645798100758D+12 Y= -2.210803597531D+13 Z= 2.045556865185D+14

I= 15 X= -5.013417168299D+13 Y= -1.073862962682D+14 Z= -2.550743705586D+13
I= 16 X= -9.401401351183D+13 Y= 3.038369519983D+13 Z= -2.658949543456D+13
I= 17 X= 9.708032528499D+12 Y= -2.623734259782D+11 Z= -2.432984534123D+13
I= 18 X= -3.668783337557D+13 Y= -3.310673964512D+13 Z= 2.389477029252D+13
I= 19 X= -9.051589519229D+13 Y= -3.828590215993D+13 Z= 6.303050399484D+13
I= 20 X= 4.775240531266D+13 Y= -3.631826979251D+13 Z= 6.558010201991D+13
I= 21 X= 1.405897422220D+13 Y= -8.358966545963D+12 Z= 1.497306452653D+13
I= 22 X= -8.024302378160D+11 Y= 1.470914897470D+14 Z= 1.542184507779D+11
I= 23 X= -4.400662991912D+12 Y= 2.427061617299D+13 Z= -7.636614231737D+13
I= 24 X= -1.196580402307D+14 Y= -4.228687082721D+13 Z= -2.075593312810D+12
I= 25 X= -1.650962989519D+13 Y= 2.843613919109D+12 Z= 8.421204287651D+11
I= 26 X= 4.259054031344D+12 Y= -2.387179796582D+13 Z= -3.425645318215D+13
I= 27 X= -1.743939835516D+13 Y= -4.500412168623D+11 Z= 2.145749553736D+13
I= 28 X= 1.339505513336D+12 Y= -9.922581021682D+13 Z= 8.533101876378D+13
I= 29 X= 1.515451179911D+13 Y= 1.916540501589D+12 Z= 5.802773053634D+12
I= 30 X= -6.519205703076D+11 Y= -3.072400488951D+13 Z= -2.154809028033D+13
I= 31 X= -1.454291169012D+13 Y= 1.386001935340D+12 Z= 3.080783828002D+13
I= 32 X= -4.216875233444D+13 Y= 1.507009944865D+13 Z= -9.261223737107D+13
I= 33 X= -2.581652083312D+13 Y= 7.029215405184D+13 Z= 4.865536221478D+13
I= 34 X= 4.236550957038D+13 Y= 8.228185693151D+13 Z= 5.288314759777D+13
I= 35 X= 1.648030547699D+12 Y= 4.610297251025D+12 Z= 4.092056905033D+12
I= 36 X= -1.605264704348D+13 Y= 2.990819375398D+11 Z= 6.700915545618D+12
I= 37 X= 2.003126281993D+13 Y= -2.028819390912D+13 Z= 4.019194771310D+13
I= 38 X= 3.737726082667D+13 Y= -1.887911522847D+12 Z= -3.705975057323D+13

Backward Direction:

Total Energy: -692.0041094 Hartrees

Potential Energy: -692.1748513 Hartress

Kinetic Energy: 0.1707419 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.836509210944D+12 Y= -6.315014091985D+12 Z= -1.185662231021D+13

I= 1 X= 3.243682334984D+12 Y= -2.424720415200D+13 Z= -1.562111645479D+13
I= 2 X= 9.580889147109D+12 Y= 2.175021231158D+13 Z= -1.590061482546D+13
I= 3 X= 5.303937631477D+11 Y= 6.904194877330D+12 Z= -5.370524035957D+12
I= 4 X= 1.475317948354D+13 Y= -2.056230421381D+13 Z= -7.233397690735D+12
I= 5 X= 4.107769540844D+12 Y= -8.622556444057D+11 Z= -3.660924787205D+12
I= 6 X= -4.516302944579D+13 Y= 7.866824716185D+11 Z= -1.167786587488D+13
I= 7 X= -1.286706509865D+14 Y= -4.053522324544D+13 Z= -2.008409520248D+13
I= 8 X= -5.671201547400D+13 Y= 1.955445787570D+13 Z= -7.275519227218D+12
I= 9 X= -2.884397924635D+12 Y= 5.939699124630D+12 Z= 1.867254326102D+13
I= 10 X= -3.107495470200D+13 Y= 2.030806427559D+13 Z= -3.836893406252D+13
I= 11 X= -4.239099330875D+13 Y= 1.024546602395D+13 Z= -6.718441375370D+13
I= 12 X= 3.913381799067D+13 Y= -3.748264235985D+13 Z= 4.241744339090D+13
I= 13 X= 1.088427705557D+13 Y= 2.456878252986D+13 Z= 4.989332241734D+12
I= 14 X= -1.071920515608D+13 Y= -1.827352940272D+13 Z= 2.066634985583D+14
I= 15 X= -4.598388633848D+13 Y= -1.046319788411D+14 Z= -2.581812347864D+13
I= 16 X= -9.187958313641D+13 Y= 3.628743782171D+13 Z= -2.600328809169D+13
I= 17 X= 9.575132896188D+12 Y= -9.551520970049D+10 Z= -2.115108436940D+13
I= 18 X= -3.605782597206D+13 Y= -3.175570303511D+13 Z= 3.034271238387D+13
I= 19 X= -9.085881765792D+13 Y= -3.740559486950D+13 Z= 6.435732001227D+13
I= 20 X= 4.680863962077D+13 Y= -4.001381322594D+13 Z= 6.908797885736D+13
I= 21 X= 1.128395310102D+13 Y= -8.357527447818D+12 Z= 1.497209751327D+13
I= 22 X= -7.973552323819D+12 Y= 1.470929919245D+14 Z= 1.515053565432D+11
I= 23 X= -6.240239940712D+12 Y= 2.762823550218D+13 Z= -7.607291107372D+13
I= 24 X= -1.214980463286D+14 Y= -4.564041507196D+13 Z= -2.370306716533D+12
I= 25 X= -1.664222733145D+13 Y= 2.676174984950D+12 Z= -2.336717019906D+12
I= 26 X= 3.315960335776D+12 Y= -2.017734802399D+13 Z= -3.776459836593D+13
I= 27 X= -1.778186989395D+13 Y= -1.331584150070D+12 Z= 2.013102789623D+13
I= 28 X= 1.969508843518D+12 Y= -1.005777460679D+14 Z= 7.888348121257D+13
I= 29 X= 1.799770939561D+13 Y= 1.169634972505D+13 Z= 1.745009147398D+13
I= 30 X= 3.783152655513D+12 Y= -2.956782766946D+13 Z= -1.291251015999D+13

I= 31 X= -2.225035576438D+13 Y= 5.285812135642D+12 Z= 3.406273899428D+13
I= 32 X= -5.753009116849D+13 Y= 1.698001242559D+13 Z= -7.866156971494D+13
I= 33 X= -2.742649226887D+13 Y= 6.462190193407D+13 Z= 6.709260976742D+13
I= 34 X= 4.298113587286D+13 Y= 7.603549755307D+13 Z= 6.025858253704D+13
I= 35 X= 7.730143798041D+11 Y= 4.610625810179D+12 Z= 4.093117036684D+12
I= 36 X= -1.161724206517D+13 Y= -8.583543853166D+11 Z= -1.935179139397D+12
I= 37 X= 1.841835278234D+13 Y= -1.461430609319D+13 Z= 2.175234697287D+13
I= 38 X= 3.799389907352D+13 Y= 4.356460027896D+12 Z= -4.443505699156D+13

Seed: 17974054075

CM Start Point Coordinates: bohr

I= 0 X= -2.214751529449D+00 Y= -1.972645959883D+00 Z= -8.322151954207D-02
I= 1 X= -9.937822026695D-02 Y= -2.585509504262D+00 Z= -1.619144708726D+00
I= 2 X= -1.229540439964D+00 Y= -1.275838979740D+00 Z= 2.372084869802D+00
I= 3 X= 2.139198333396D+00 Y= -2.030418246923D+00 Z= -3.321449913715D-02
I= 4 X= 1.282695916928D+00 Y= -1.277189150982D+00 Z= 2.470324251494D+00
I= 5 X= -2.715419796161D+00 Y= 3.195443195204D+00 Z= -2.390166411824D+00
I= 6 X= 3.635383244187D-02 Y= 1.643147107815D+00 Z= -3.503768164027D+00
I= 7 X= -2.124236424021D+00 Y= 4.826922286102D+00 Z= -3.705508291494D+00
I= 8 X= -4.206266814365D+00 Y= 2.061508769554D+00 Z= -3.204789805071D+00
I= 9 X= 2.934981560669D+00 Y= -7.816933419165D-01 Z= 4.756082915150D+00
I= 10 X= 2.014468468573D+00 Y= -1.871305767548D+00 Z= 6.610349413722D+00
I= 11 X= 5.080754256183D+00 Y= -1.309465721050D+00 Z= 4.261918149270D+00
I= 12 X= 2.985381885182D+00 Y= 1.598869303790D+00 Z= 5.163482840947D+00
I= 13 X= -2.836237203290D+00 Y= -7.174808566298D-01 Z= 4.641114092615D+00
I= 14 X= -2.869193918723D+00 Y= -2.500119911797D+00 Z= 5.557314774798D+00
I= 15 X= -1.610225845211D+00 Y= 4.126883272497D-01 Z= 6.225757818854D+00
I= 16 X= -5.062156203633D+00 Y= 3.921255562923D-01 Z= 4.575894053639D+00
I= 17 X= -4.885519706253D+00 Y= -2.677899886435D+00 Z= -7.027958082026D-01
I= 18 X= -5.556741457198D+00 Y= -4.285572183889D+00 Z= 2.616642963111D-01

I= 19 X= -6.536004565120D+00 Y= -1.310180559404D+00 Z= -2.323770181696D-01
I= 20 X= -5.042631364277D+00 Y= -3.071671539991D+00 Z= -2.682825911108D+00
I= 21 X= -2.580670003984D-01 Y= -3.784572760391D+00 Z= -4.182638359222D+00
I= 22 X= -1.309507543080D-01 Y= -6.020791963551D+00 Z= -4.138108405559D+00
I= 23 X= -1.907409583501D+00 Y= -3.384920963681D+00 Z= -5.055604551859D+00
I= 24 X= 1.354488533554D+00 Y= -3.309471438270D+00 Z= -5.532991953650D+00
I= 25 X= 4.872936451933D+00 Y= -2.285256890030D+00 Z= -6.656865455156D-01
I= 26 X= 5.352664402281D+00 Y= -1.496330514745D+00 Z= -2.734338074010D+00
I= 27 X= 5.895304370178D+00 Y= -8.424186299980D-01 Z= 3.430340826347D-01
I= 28 X= 5.572404535970D+00 Y= -4.323682861963D+00 Z= -4.049957434503D-01
I= 29 X= 3.031625005671D+00 Y= 3.048325222195D+00 Z= -2.186273150386D+00
I= 30 X= 2.511661824866D+00 Y= 3.890506721825D+00 Z= 2.351945093073D-01
I= 31 X= 4.597869683443D+00 Y= 1.726008412458D+00 Z= -2.818110180403D+00
I= 32 X= 2.498908451646D+00 Y= 4.252095234438D+00 Z= -3.967650700718D+00
I= 33 X= 1.540487878182D+00 Y= 5.547614353401D+00 Z= 4.720066719272D-01
I= 34 X= 3.779886347353D+00 Y= 3.139537929869D+00 Z= 1.643519194421D+00
I= 35 X= 4.342059501862D-02 Y= 1.125564751166D+00 Z= -5.821397332379D-01
I= 36 X= -2.726292603683D+00 Y= 3.750141207318D+00 Z= 2.622559690740D-01
I= 37 X= -2.082485979787D+00 Y= 5.493734750377D+00 Z= 1.162381304659D+00
I= 38 X= -3.832326156860D+00 Y= 2.349826191803D+00 Z= 1.525509693108D+00

Forward Direction:

Total Energy: -691.9983969 Hartrees

Potential Energy: -692.2073940 Hartress

Kinetic Energy: 0.2089970 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.210681541333D+13 Y= 1.592449538556D+13 Z= 2.588269069921D+13
I= 1 X= -1.415917932309D+13 Y= -5.825330913413D+12 Z= -7.623825561510D+12
I= 2 X= -1.931143628100D+13 Y= -1.361379290113D+13 Z= -1.059804492838D+13
I= 3 X= 6.699342002174D+12 Y= 1.357823591818D+13 Z= -3.861564849704D+12
I= 4 X= 7.105138198303D+12 Y= 6.452839271573D+12 Z= -1.040384974652D+13

I= 5 X= -1.747436930370D+13 Y= 1.008255040515D+13 Z= 4.585489679729D+12
I= 6 X= 3.518221137249D+13 Y= 2.737459473332D+13 Z= 1.851445983830D+13
I= 7 X= 1.253143159998D+14 Y= -1.817064971069D+13 Z= 9.651439505631D+12
I= 8 X= -3.113429862975D+12 Y= -3.029930409690D+13 Z= 8.579555411511D+12
I= 9 X= -6.292767827538D+12 Y= -2.877428685969D+12 Z= 4.567697353297D+12
I= 10 X= 3.938840614232D+13 Y= 2.774080362717D+13 Z= -1.356423035439D+14
I= 11 X= -8.485910927185D+13 Y= 3.263063104242D+12 Z= -7.590282167729D+13
I= 12 X= 6.740304137722D+13 Y= 4.500479335712D+13 Z= -1.075467826025D+14
I= 13 X= -1.077413667505D+13 Y= -9.772239114446D+12 Z= 4.029365437954D+12
I= 14 X= 1.180520006126D+13 Y= -2.072082036787D+13 Z= 8.911434900341D+13
I= 15 X= -5.191779561513D+13 Y= -6.988710090942D+13 Z= 1.207215691843D+13
I= 16 X= 1.244627050992D+14 Y= 5.855335417743D+13 Z= -2.446810420897D+13
I= 17 X= 7.206669526744D+11 Y= 1.659017596703D+13 Z= 2.164883871043D+12
I= 18 X= -2.688169370867D+13 Y= -5.491307754137D+13 Z= 5.687563563702D+13
I= 19 X= 7.175422973752D+13 Y= -1.019707377157D+14 Z= -8.523726184466D+11
I= 20 X= 2.732302062217D+13 Y= -1.154735453761D+14 Z= -1.138800482239D+14
I= 21 X= -1.523803829214D+13 Y= 3.271333688349D+12 Z= -1.654490436907D+12
I= 22 X= -5.672913949984D+13 Y= -9.857959778547D+13 Z= -1.951388401760D+13
I= 23 X= -1.751271667138D+13 Y= -8.684639293542D+12 Z= 1.231758529946D+13
I= 24 X= 6.405352443592D+13 Y= 1.372292543463D+14 Z= -1.931143275467D+13
I= 25 X= -2.034316593028D+12 Y= -1.001330141743D+12 Z= 4.126060784095D+12
I= 26 X= -3.005596767028D+13 Y= 1.655814130795D+12 Z= 7.247136879013D+13
I= 27 X= -9.282279068295D+13 Y= -5.925289861816D+13 Z= -2.897513097538D+13
I= 28 X= -2.516763501785D+12 Y= 9.011133867598D+13 Z= -6.937920280094D+13
I= 29 X= -8.122725499285D+12 Y= 9.169195531045D+12 Z= -8.180722632879D+12
I= 30 X= 2.241459446954D+13 Y= -1.059065502835D+13 Z= -7.457403079507D+12
I= 31 X= 4.062587955356D+13 Y= 3.062967848046D+13 Z= 7.876808296361D+13
I= 32 X= 2.656693607876D+13 Y= -1.732355748614D+14 Z= 2.976677741575D+13
I= 33 X= -1.247103110842D+14 Y= 9.144422786051D+13 Z= 4.679227253522D+13
I= 34 X= -8.057790999874D+13 Y= 2.489859350680D+13 Z= -5.978850154780D+13

I= 35 X= 4.009233208681D+12 Y= -2.175280971051D+12 Z= 4.904911413203D+12
I= 36 X= 1.831480720173D+13 Y= -1.977866244545D+12 Z= -3.460110957799D+12
I= 37 X= 9.030306344339D+13 Y= 6.250817556662D+13 Z= 2.194839545589D+12
I= 38 X= -7.680675769776D+13 Y= -7.220684385342D+13 Z= 2.519565280785D+13

Backward Direction:

Total Energy: -691.9983885 Hartrees

Potential Energy: -692.2073940 Hartress

Kinetic Energy: 0.2090055 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.220615518001D+13 Y= 1.686256511462D+13 Z= 2.721435963882D+13
I= 1 X= -1.343088115400D+13 Y= -5.825164588295D+12 Z= -7.623906673444D+12
I= 2 X= -1.903847321567D+13 Y= -1.421693724291D+13 Z= -9.855975954939D+12
I= 3 X= 6.798776386432D+12 Y= 1.264007187873D+13 Z= -5.193416657297D+12
I= 4 X= 7.378166564602D+12 Y= 7.056065709310D+12 Z= -1.114592978500D+13
I= 5 X= -1.563890214742D+13 Y= 4.780984793916D+12 Z= -1.892828426601D+12
I= 6 X= -2.920250149673D+13 Y= 2.738367650360D+13 Z= 1.851436841106D+13
I= 7 X= 1.163624534822D+14 Y= -1.837557319078D+13 Z= 2.243631411059D+12
I= 8 X= -7.840616588132D+12 Y= -3.160295366557D+13 Z= 6.751096379496D+12
I= 9 X= -5.452373511516D+12 Y= -4.414527127080D+12 Z= 4.031586407676D+12
I= 10 X= 3.876166507825D+13 Y= 2.571823757617D+13 Z= -1.368303549458D+14
I= 11 X= -8.374770387736D+13 Y= 1.635103516294D+11 Z= -7.621989256253D+13
I= 12 X= 6.958813500228D+13 Y= 4.356932921087D+13 Z= -1.073677495139D+14
I= 13 X= -9.933836387742D+12 Y= -8.235124379961D+12 Z= 4.565705247046D+12
I= 14 X= 1.117909252648D+13 Y= -1.869804134402D+13 Z= 9.030273029982D+13
I= 15 X= -4.973314984842D+13 Y= -6.845097324570D+13 Z= 1.189302680970D+13
I= 16 X= 1.255736937691D+14 Y= 6.165200344285D+13 Z= -2.415042877699D+13
I= 17 X= 6.894722504809D+11 Y= 1.670914353414D+13 Z= 3.829236645324D+12
I= 18 X= -2.646507496546D+13 Y= -5.421835134432D+13 Z= 6.019533385592D+13
I= 19 X= 7.154647858106D+13 Y= -1.015464662552D+14 Z= -1.283694472158D+11
I= 20 X= 2.689384664162D+13 Y= -1.173483894397D+14 Z= -1.120496941649D+14

I= 21 X= -1.665673190725D+13 Y= 3.272098046591D+12 Z= -1.655004298769D+12
I= 22 X= -6.040823558758D+13 Y= -9.857880380214D+13 Z= -1.951533162890D+13
I= 23 X= -1.848452952119D+13 Y= -6.972853259558D+12 Z= 1.251446025970D+13
I= 24 X= 6.308147029681D+13 Y= 1.355196551447D+14 Z= -1.950913151083D+13
I= 25 X= -2.065364080652D+12 Y= -1.120591470121D+12 Z= 2.461673537425D+12
I= 26 X= -3.048478495145D+13 Y= 3.530041028398D+12 Z= 7.064089085042D+13
I= 27 X= -9.303032602134D+13 Y= -5.967779089989D+13 Z= -2.969897118702D+13
I= 28 X= -2.100180278481D+12 Y= 8.941617321582D+13 Z= -7.269862504915D+13
I= 29 X= -6.287513239516D+12 Y= 1.446901659885D+13 Z= -1.703826538498D+12
I= 30 X= 2.510218070771D+13 Y= -9.744565296809D+12 Z= -2.965257655547D+12
I= 31 X= 3.590159521833D+13 Y= 3.193360306069D+13 Z= 8.059551593635D+13
I= 32 X= 1.761595106637D+13 Y= -1.730309076204D+14 Z= 3.717183715016D+13
I= 33 X= -1.255858778168D+14 Y= 8.846358943222D+13 Z= 5.657161797082D+13
I= 34 X= -8.038853286872D+13 Y= 2.154417248787D+13 Z= -5.566011126111D+13
I= 35 X= 3.431345245142D+12 Y= -2.175110572678D+12 Z= 4.905482398621D+12
I= 36 X= 2.100263731665D+13 Y= -2.824649713303D+12 Z= -7.952518237872D+12
I= 37 X= 8.942600818273D+13 Y= 6.549079831313D+13 Z= -7.585894588726D+12
I= 38 X= -7.661669164204D+13 Y= -6.885334851488D+13 Z= 2.106737560009D+13

Seed: 18114500697

CM Start Point Coordinates: bohr

I= 0 X= -2.240133302593D+00 Y= -2.142232240616D+00 Z= 6.215637780566D-02
I= 1 X= -1.009909592551D-01 Y= -2.450824839941D+00 Z= -1.614769699832D+00
I= 2 X= -1.359864512399D+00 Y= -1.171396766947D+00 Z= 2.384541307863D+00
I= 3 X= 2.277231584911D+00 Y= -2.025571661658D+00 Z= -1.192813350217D-02
I= 4 X= 1.370479013257D+00 Y= -1.205471777992D+00 Z= 2.462868060546D+00
I= 5 X= -2.790576649762D+00 Y= 3.122559496975D+00 Z= -2.327532321916D+00
I= 6 X= 2.230204424676D-02 Y= 1.101885084811D+00 Z= -3.497575001166D+00
I= 7 X= -2.306425876415D+00 Y= 4.717569061307D+00 Z= -3.737066614622D+00
I= 8 X= -4.381850016297D+00 Y= 1.570058093982D+00 Z= -2.999755562902D+00

I= 9 X= 2.848794934999D+00 Y= -2.942801107381D-01 Z= 4.597270697866D+00
I= 10 X= 2.769613290791D+00 Y= -1.709867536676D+00 Z= 6.338084993367D+00
I= 11 X= 5.024813933653D+00 Y= -4.010372063594D-01 Z= 4.243782051779D+00
I= 12 X= 2.469876458154D+00 Y= 1.822903355261D+00 Z= 5.176655498094D+00
I= 13 X= -3.054262980909D+00 Y= -7.970160649241D-01 Z= 4.602666243668D+00
I= 14 X= -3.514523423612D+00 Y= -2.763167529773D+00 Z= 5.224469705897D+00
I= 15 X= -2.177539611669D+00 Y= 5.858993069073D-01 Z= 5.978046461361D+00
I= 16 X= -5.232532261250D+00 Y= -1.322303336975D-01 Z= 3.902775953051D+00
I= 17 X= -4.816299701570D+00 Y= -2.860680569238D+00 Z= -7.685440555025D-01
I= 18 X= -5.994088658482D+00 Y= -4.283929563558D+00 Z= 5.521789364465D-01
I= 19 X= -6.271133890064D+00 Y= -1.310132194526D+00 Z= -5.514583544781D-01
I= 20 X= -4.782201007287D+00 Y= -3.337225300000D+00 Z= -2.895916117383D+00
I= 21 X= -1.052900081929D-01 Y= -3.217529407012D+00 Z= -4.191814726834D+00
I= 22 X= 1.093480175784D-01 Y= -5.534137012026D+00 Z= -4.315294659016D+00
I= 23 X= -1.801255032732D+00 Y= -3.211737179541D+00 Z= -5.059683880181D+00
I= 24 X= 1.523389442354D+00 Y= -2.754223327970D+00 Z= -5.658477468281D+00
I= 25 X= 4.791916458346D+00 Y= -2.667612578827D+00 Z= -8.500736081003D-01
I= 26 X= 5.204897385693D+00 Y= -2.441772291334D+00 Z= -2.818615287885D+00
I= 27 X= 6.114047168498D+00 Y= -1.500753400776D+00 Z= 8.223883448805D-01
I= 28 X= 4.704723605114D+00 Y= -4.835901009629D+00 Z= -6.032914057206D-01
I= 29 X= 2.789721010681D+00 Y= 3.099533353945D+00 Z= -2.455778869557D+00
I= 30 X= 2.986077743777D+00 Y= 3.647162943170D+00 Z= 2.606236803524D-01
I= 31 X= 4.264145291279D+00 Y= 1.779872596661D+00 Z= -3.226106227741D+00
I= 32 X= 2.056360711038D+00 Y= 4.483576495852D+00 Z= -3.653258741307D+00
I= 33 X= 2.181418382101D+00 Y= 5.474504753401D+00 Z= 1.104106477876D+00
I= 34 X= 4.498068787703D+00 Y= 2.576175965028D+00 Z= 1.024334321997D+00
I= 35 X= 3.774155581492D-02 Y= 1.104530437653D+00 Z= -4.335010615551D-01
I= 36 X= -2.645113382536D+00 Y= 3.661804426586D+00 Z= 2.193869748551D-01
I= 37 X= -2.203301234530D+00 Y= 5.702151015451D+00 Z= 2.665066136671D-01
I= 38 X= -3.909886692477D+00 Y= 2.938128047235D+00 Z= 1.524281544505D+00

Forward Direction:

Total Energy: -692.0038809 Hartrees

Potential Energy: -692.1827102 Hartress

Kinetic Energy: 0.1788293 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.741693025791D+13 Y= -3.411265436492D+12 Z= -2.978861658782D+12
I= 1 X= 5.049783366069D+12 Y= 6.859375965449D+12 Z= 4.342646987094D+12
I= 2 X= -2.392674472577D+13 Y= 2.783345386767D+13 Z= -5.521003764192D+12
I= 3 X= 1.253040047519D+13 Y= -1.966685683748D+13 Z= -3.651115621331D+12
I= 4 X= 7.380051731172D+12 Y= -2.256038042602D+12 Z= 6.004474002175D+12
I= 5 X= 9.274468473947D+12 Y= 3.797291372120D+12 Z= -1.182543003599D+13
I= 6 X= 2.716115546738D+13 Y= 4.262118924981D+13 Z= -1.938606398766D+13
I= 7 X= 2.714860194341D+13 Y= 8.551349928647D+13 Z= -3.995866728540D+13
I= 8 X= 1.240903564180D+13 Y= -4.079629963499D+12 Z= 1.248315372295D+14
I= 9 X= -1.609267119306D+13 Y= -1.207004096763D+12 Z= 1.129599249013D+13
I= 10 X= -1.650392089458D+13 Y= 1.035432330340D+14 Z= 5.872251642084D+13
I= 11 X= 9.113883429915D+13 Y= 4.511567729263D+13 Z= -2.116453100532D+13
I= 12 X= 1.410856963645D+13 Y= 6.796900249188D+12 Z= 8.808721780522D+13
I= 13 X= -1.075050748432D+13 Y= -2.678609278215D+12 Z= -2.316189047302D+12
I= 14 X= -6.028327881118D+13 Y= 1.453583666367D+14 Z= -5.942432669143D+13
I= 15 X= 3.689586688585D+13 Y= -3.675228110395D+13 Z= -6.598754831782D+13
I= 16 X= 1.900936765914D+13 Y= 4.919393372608D+13 Z= 1.091286771018D+14
I= 17 X= 6.433625380056D+12 Y= -8.381815609054D+12 Z= -2.171562675680D+13
I= 18 X= 2.058682537612D+13 Y= -4.959364130660D+12 Z= 5.843401805500D+13
I= 19 X= -8.817382074161D+13 Y= 1.086273100184D+14 Z= 9.266251294510D+13
I= 20 X= 3.255433603228D+12 Y= -3.161608877704D+13 Z= -2.520825838678D+13
I= 21 X= -7.662207303551D+12 Y= 2.759297588153D+12 Z= -1.859068686477D+12
I= 22 X= 7.078984683931D+13 Y= -5.387172054191D+13 Z= -2.846792544137D+13
I= 23 X= -2.471834818461D+13 Y= 6.327099877770D+13 Z= -6.047766106345D+13
I= 24 X= 5.181797833857D+13 Y= -2.848950359329D+13 Z= 1.412629645791D+13

I= 25 X= -4.019872324962D+12 Y= 1.276795030383D+13 Z= 4.660573096714D+12
I= 26 X= -8.866652362894D+12 Y= 1.302555346229D+13 Z= 4.703319527550D+13
I= 27 X= 2.084914325998D+13 Y= 6.094074966334D+13 Z= 2.205129479993D+12
I= 28 X= -5.260036280276D+13 Y= -9.628823810455D+13 Z= 5.729364012787D+12
I= 29 X= 4.944968140711D+12 Y= 6.596089404856D+12 Z= 1.077516687088D+12
I= 30 X= 5.277857109837D+12 Y= -9.595208808314D+12 Z= -2.589851819037D+13
I= 31 X= 9.026511205430D+13 Y= -1.302613935991D+14 Z= 2.890994458536D+13
I= 32 X= -4.462343740914D+13 Y= -5.634301964629D+13 Z= 8.036917648830D+12
I= 33 X= 9.099819518983D+12 Y= 2.568105899480D+13 Z= 2.589824215663D+13
I= 34 X= -3.049621796899D+13 Y= 2.035834333291D+13 Z= -2.818253354647D+13
I= 35 X= 6.413249520984D+12 Y= -8.367168939710D+12 Z= 2.423584453353D+12
I= 36 X= -2.783108000066D+13 Y= -6.528537422163D+12 Z= 1.947589937047D+13
I= 37 X= 5.254854393141D+13 Y= -3.708131230648D+13 Z= -1.770196511456D+13
I= 38 X= 8.057648180149D+13 Y= 1.169554621309D+14 Z= -9.535563209002D+13

Backward Direction:

Total Energy: -692.0038591 Hartrees

Potential Energy: -692.1827102 Hartress

Kinetic Energy: 0.1788511 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.756543150228D+13 Y= -2.526611967268D+12 Z= -1.016333450561D+12
I= 1 X= 4.253079794635D+12 Y= 6.859723974020D+12 Z= 4.342400304029D+12
I= 2 X= -2.267923042705D+13 Y= 2.857979318163D+13 Z= -4.667936109292D+12
I= 3 X= 1.238213285349D+13 Y= -2.055154971448D+13 Z= -5.613881588629D+12
I= 4 X= 8.627711106610D+12 Y= -3.002244706193D+12 Z= 5.151605670635D+12
I= 5 X= 8.571668798371D+12 Y= -7.202278270997D+12 Z= -2.273879661189D+13
I= 6 X= 7.423416908308D+12 Y= 4.263038780618D+13 Z= -1.938457830114D+13
I= 7 X= 1.817109234738D+13 Y= 7.236781588347D+13 Z= -5.770336071242D+13
I= 8 X= 1.099595163529D+13 Y= -1.919289769648D+13 Z= 1.220098934685D+14
I= 9 X= -1.362041503447D+13 Y= -5.603430729920D+12 Z= 1.047250602051D+13
I= 10 X= -1.712449125482D+13 Y= 9.850120375665D+13 Z= 5.696476466072D+13

I= 11 X= 9.414506560408D+13 Y= 3.714142785254D+13 Z= -2.182204539529D+13
I= 12 X= 1.963014244942D+13 Y= 2.953449545071D+12 Z= 8.829368340048D+13
I= 13 X= -8.278386933745D+12 Y= 1.717857503133D+12 Z= -1.491982551667D+12
I= 14 X= -6.090188317413D+13 Y= 1.504011248788D+14 Z= -5.766533998791D+13
I= 15 X= 4.241633876796D+13 Y= -3.290712808450D+13 Z= -6.619428590095D+13
I= 16 X= 2.201461647111D+13 Y= 5.716583605943D+13 Z= 1.097878002424D+14
I= 17 X= 5.743363929234D+12 Y= -8.572337453919D+12 Z= -1.736955160341D+13
I= 18 X= 2.029890328073D+13 Y= -2.944528430750D+12 Z= 6.799627762091D+13
I= 19 X= -8.826907196154D+13 Y= 1.103163262381D+14 Z= 9.408839806233D+13
I= 20 X= 1.104446714183D+12 Y= -3.746472924653D+13 Z= -2.032849861316D+13
I= 21 X= -1.191022300087D+13 Y= 2.761121152296D+12 Z= -1.860290872274D+12
I= 22 X= 5.998384796996D+13 Y= -5.386976568404D+13 Z= -2.847127620599D+13
I= 23 X= -2.711904011607D+13 Y= 6.847382757902D+13 Z= -6.065093030804D+13
I= 24 X= 4.941691956606D+13 Y= -3.368746543277D+13 Z= 1.429817185119D+13
I= 25 X= -4.709574594838D+12 Y= 1.295754155137D+13 Z= 3.143199141608D+11
I= 26 X= -1.101678403974D+13 Y= 1.887329054284D+13 Z= 4.215284794161D+13
I= 27 X= 2.075477862069D+13 Y= 5.924969972573D+13 Z= 7.799798103716D+11
I= 28 X= -5.288784896787D+13 Y= -9.830471880281D+13 Z= -3.833193571465D+12
I= 29 X= 4.241334460564D+12 Y= 1.759261602951D+13 Z= 1.198749955532D+13
I= 30 X= 6.500415844402D+12 Y= -1.120350436142D+13 Z= -1.370336933974D+13
I= 31 X= 8.885176980006D+13 Y= -1.151535331023D+14 Z= 3.172786208730D+13
I= 32 X= -5.359711615532D+13 Y= -4.319571290350D+13 Z= 2.577666861296D+13
I= 33 X= 7.330613153745D+12 Y= 1.808457705509D+13 Z= 4.943860773715D+13
I= 34 X= -2.789321672757D+13 Y= 1.292986976686D+13 Z= -2.163198881494D+13
I= 35 X= 6.803167002435D+12 Y= -8.366698119282D+12 Z= 2.424823099755D+12
I= 36 X= -2.660899722432D+13 Y= -4.921506695175D+12 Z= 7.279946932335D+12
I= 37 X= 5.077465632044D+13 Y= -2.948092906435D+13 Z= -4.124347324746D+13
I= 38 X= 8.317875919104D+13 Y= 1.243796927529D+14 Z= -1.019066076546D+14

Seed: 18408551020

CM Start Point Coordinates: bohr

I= 0 X= -2.326438287270D+00 Y= -2.204154577443D+00 Z= -9.917178664581D-02
I= 1 X= 6.849635256612D-02 Y= -2.689246189073D+00 Z= -1.520046509449D+00
I= 2 X= -1.304500910424D+00 Y= -1.271112458763D+00 Z= 2.225907134335D+00
I= 3 X= 2.103483526981D+00 Y= -2.294167268350D+00 Z= 1.859480686853D-02
I= 4 X= 1.341133464855D+00 Y= -1.202500066669D+00 Z= 2.438787396531D+00
I= 5 X= -2.763320133989D+00 Y= 3.361424202275D+00 Z= -2.296619743242D+00
I= 6 X= -4.419560076263D-02 Y= 1.525524350872D+00 Z= -3.294677857849D+00
I= 7 X= -2.421433728430D+00 Y= 4.535963723063D+00 Z= -3.901085066234D+00
I= 8 X= -3.831961996621D+00 Y= 1.683073135737D+00 Z= -2.933330199913D+00
I= 9 X= 2.997153802557D+00 Y= -4.584447393508D-01 Z= 4.613227230953D+00
I= 10 X= 3.079330558400D+00 Y= -2.007257922719D+00 Z= 5.873247030256D+00
I= 11 X= 5.081025905993D+00 Y= 3.374530121153D-01 Z= 4.328926956923D+00
I= 12 X= 2.083488693281D+00 Y= 1.150320982357D+00 Z= 5.522384500944D+00
I= 13 X= -2.786010830903D+00 Y= -5.870550982756D-01 Z= 4.706024012108D+00
I= 14 X= -2.462901616751D+00 Y= -1.822670422678D+00 Z= 6.428481117615D+00
I= 15 X= -2.388536014084D+00 Y= 1.143459936206D+00 Z= 5.530420864703D+00
I= 16 X= -4.705039301724D+00 Y= -7.286664635036D-01 Z= 4.665751710894D+00
I= 17 X= -5.017694886691D+00 Y= -2.308509770223D+00 Z= -8.899637505590D-01
I= 18 X= -5.837687203327D+00 Y= -4.035482537670D+00 Z= 5.610108036149D-01
I= 19 X= -6.277414619985D+00 Y= -8.537375614860D-01 Z= -4.118052112041D-01
I= 20 X= -5.248644046078D+00 Y= -2.578154751581D+00 Z= -2.938634814928D+00
I= 21 X= 2.300888424736D-01 Y= -3.750359080062D+00 Z= -4.245612449118D+00
I= 22 X= 5.763922422036D-01 Y= -5.906598842476D+00 Z= -4.187207008109D+00
I= 23 X= -1.661650976629D+00 Y= -3.333958636145D+00 Z= -5.273247816036D+00
I= 24 X= 1.549013932669D+00 Y= -2.881315505505D+00 Z= -5.599406974557D+00
I= 25 X= 4.820994747071D+00 Y= -2.527080154972D+00 Z= -7.563468082372D-01
I= 26 X= 5.107977566574D+00 Y= -2.487786237481D+00 Z= -3.090166496830D+00
I= 27 X= 5.737818795180D+00 Y= -1.005388168622D+00 Z= 3.501188203970D-01
I= 28 X= 5.491112595796D+00 Y= -4.277572723886D+00 Z= 3.083930202209D-01

I= 29 X= 2.825332618549D+00 Y= 3.485498842808D+00 Z= -2.343898705057D+00
I= 30 X= 2.728128890718D+00 Y= 3.660568888076D+00 Z= 2.414537128158D-01
I= 31 X= 4.384413400058D+00 Y= 2.257579612996D+00 Z= -2.809410958285D+00
I= 32 X= 2.223886149653D+00 Y= 4.713744423355D+00 Z= -3.529159357943D+00
I= 33 X= 2.034729279881D+00 Y= 5.273291404425D+00 Z= 1.582787545325D+00
I= 34 X= 4.132028425910D+00 Y= 3.032056885673D+00 Z= 1.205593637497D+00
I= 35 X= -5.793762239540D-02 Y= 9.699976839602D-01 Z= -5.141827532212D-01
I= 36 X= -2.718904604623D+00 Y= 3.821957563236D+00 Z= 3.468363297639D-01
I= 37 X= -1.781695964973D+00 Y= 5.702204229159D+00 Z= 8.182884698408D-01
I= 38 X= -3.788986379653D+00 Y= 2.938430933909D+00 Z= 1.817095016378D+00

Forward Direction:

Total Energy: -692.0071834 Hartrees

Potential Energy: -692.1944070 Hartress

Kinetic Energy: 0.1872237 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.343858265905D+13 Y= -5.517334816894D+11 Z= 4.747218147592D+12
I= 1 X= -9.870646650932D+12 Y= -5.165475602195D+11 Z= 8.839341666192D+12
I= 2 X= 1.819222132134D+12 Y= 1.313513671971D+13 Z= -1.762690027994D+13
I= 3 X= 1.179699471154D+13 Y= -1.009311124469D+13 Z= 6.439575563967D+12
I= 4 X= 1.832454173169D+13 Y= 1.140002718852D+13 Z= -7.900622217698D+12
I= 5 X= -3.470690635425D+12 Y= 7.946340149601D+12 Z= 3.197676436694D+13
I= 6 X= -2.544756556720D+12 Y= -7.087836513022D+12 Z= -8.864169909628D+13
I= 7 X= -1.851389133888D+13 Y= 3.116694410644D+12 Z= 1.839784309614D+13
I= 8 X= -8.707642058782D+13 Y= 1.894618930753D+12 Z= -6.852625767210D+13
I= 9 X= -6.511827599258D+12 Y= -8.314908899583D+12 Z= -1.357180102724D+13
I= 10 X= -9.014373739788D+11 Y= 8.527835374906D+13 Z= -7.330396139909D+13
I= 11 X= -2.643913263956D+12 Y= -5.926311783540D+13 Z= -3.205570549945D+13
I= 12 X= -9.447237788144D+13 Y= 6.792143060398D+13 Z= 2.033728197371D+13
I= 13 X= -1.790808447317D+13 Y= -2.930601347925D+13 Z= -1.737161038902D+13
I= 14 X= -1.966716382464D+12 Y= 4.228516569202D+13 Z= -3.997366402029D+13

I= 15 X= 4.742171561348D+13 Y= 1.514933700467D+13 Z= -1.723066726233D+13
I= 16 X= 1.089606501196D+14 Y= 6.464620195586D+13 Z= 3.135276837083D+13
I= 17 X= -1.392053239692D+13 Y= -3.075520413389D+12 Z= -3.604789784140D+12
I= 18 X= 2.577881320403D+13 Y= 1.012391347250D+14 Z= -8.525345378170D+13
I= 19 X= -1.777366200864D+13 Y= -8.097779643473D+13 Z= 5.425673606805D+13
I= 20 X= 2.040457684111D+13 Y= -3.378654657125D+13 Z= 7.366010362027D+13
I= 21 X= 2.187423568079D+13 Y= -1.540723032365D+13 Z= -6.836983135493D+11
I= 22 X= 1.204826225402D+13 Y= 1.299494544981D+14 Z= -8.747915463268D+13
I= 23 X= -8.478403682790D+13 Y= 2.238661333840D+13 Z= -4.130370328963D+13
I= 24 X= -7.622351530066D+13 Y= 7.932349690141D+11 Z= 3.164372418738D+13
I= 25 X= -8.302921870835D+12 Y= 1.644979639828D+13 Z= -9.666044786513D+11
I= 26 X= 4.615613152014D+13 Y= -8.985928748230D+13 Z= 2.230167168760D+13
I= 27 X= -1.776311240565D+13 Y= 6.395620331792D+11 Z= 9.841186075032D+13
I= 28 X= 9.496676987521D+13 Y= -5.225250249643D+13 Z= -6.201293544062D+13
I= 29 X= 3.428232598816D+12 Y= 3.117092584082D+12 Z= -1.057649844113D+13
I= 30 X= 4.424999531310D+12 Y= -4.357155278823D+11 Z= 2.524158245740D+13
I= 31 X= -8.812902552147D+13 Y= 4.427581791745D+13 Z= -3.739313890565D+13
I= 32 X= 3.614011705781D+13 Y= -1.008100829637D+14 Z= -6.478710704657D+13
I= 33 X= 1.996836223320D+13 Y= -1.139429974817D+14 Z= -2.300892419735D+13
I= 34 X= -5.881532301922D+13 Y= -9.379955714801D+12 Z= 9.367972007738D+12
I= 35 X= 9.732313202113D+11 Y= 2.580153507934D+12 Z= 3.530717009051D+12
I= 36 X= -1.905945761004D+13 Y= -8.211742789078D+12 Z= 4.835392500699D+10
I= 37 X= 8.367100452903D+12 Y= 5.877227031445D+13 Z= 1.066673579162D+14
I= 38 X= 1.213667584481D+14 Y= 4.228226156245D+13 Z= -1.130660747621D+13

Backward Direction:

Total Energy: -692.0071895 Hartrees

Potential Energy: -692.1944070 Hartress

Kinetic Energy: 0.1872175 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.325560182487D+13 Y= 2.626350396575D+11 Z= 6.688863045336D+12

I= 1 X= -1.088753393213D+13 Y= -5.161906718158D+11 Z= 8.839082071973D+12
I= 2 X= 3.156815219515D+12 Y= 1.407348399483D+13 Z= -1.681232346907D+13
I= 3 X= 1.161425652886D+13 Y= -1.090750657082D+13 Z= 4.497699333247D+12
I= 4 X= 1.966228432391D+13 Y= 1.046181257116D+13 Z= -8.714975431261D+12
I= 5 X= -4.582707870653D+12 Y= -3.325815020360D+12 Z= 2.101249178584D+13
I= 6 X= -1.288352562755D+13 Y= -7.079247689450D+12 Z= -8.864003108119D+13
I= 7 X= -2.688045094216D+13 Y= -1.145959698006D+13 Z= 7.117584851562D+09
I= 8 X= -8.779539557067D+13 Y= -1.467091526079D+13 Z= -7.133340281616D+13
I= 9 X= -3.915020677109D+12 Y= -1.292514441757D+13 Z= -1.439060882962D+13
I= 10 X= -1.478344403113D+12 Y= 8.003792634090D+13 Z= -7.504384983615D+13
I= 11 X= 4.976424351664D+11 Y= -6.756902985465D+13 Z= -3.272948466651D+13
I= 12 X= -8.872816069692D+13 Y= 6.390758825833D+13 Z= 2.053453411037D+13
I= 13 X= -1.531141136900D+13 Y= -2.469573626992D+13 Z= -1.655204340596D+13
I= 14 X= -2.541552116336D+12 Y= 4.752636509398D+13 Z= -3.823246220405D+13
I= 15 X= 5.316478965066D+13 Y= 1.916495215164D+13 Z= -1.742820425799D+13
I= 16 X= 1.121011887242D+14 Y= 7.294966765527D+13 Z= 3.202822694281D+13
I= 17 X= -1.468223067475D+13 Y= -3.308749908313D+12 Z= 9.265414281412D+11
I= 18 X= 2.538367191774D+13 Y= 1.033537065588D+14 Z= -7.522192320167D+13
I= 19 X= -1.784210897504D+13 Y= -7.917668020243D+13 Z= 5.571133318962D+13
I= 20 X= 1.809080073863D+13 Y= -3.995025241238D+13 Z= 7.875478386897D+13
I= 21 X= 1.740764207776D+13 Y= -1.540534091027D+13 Z= -6.849643308995D+11
I= 22 X= 6.989109292829D+11 Y= 1.299514845207D+14 Z= -8.748261859716D+13
I= 23 X= -8.727760810234D+13 Y= 2.786179538708D+13 Z= -4.153179344978D+13
I= 24 X= -7.871745088575D+13 Y= -4.676930828224D+12 Z= 3.187041336174D+13
I= 25 X= -9.064025088566D+12 Y= 1.668204431052D+13 Z= -5.498127422492D+12
I= 26 X= 4.384324171946D+13 Y= -8.369647467445D+13 Z= 1.720636056299D+13
I= 27 X= -1.783061269324D+13 Y= -1.163703048163D+12 Z= 9.695805171527D+13
I= 28 X= 9.457211960656D+13 Y= -5.436882373984D+13 Z= -7.204484715117D+13
I= 29 X= 2.315334197155D+12 Y= 1.438617941394D+13 Z= 3.842689365103D+11
I= 30 X= 5.299724965448D+12 Y= -2.376024561596D+12 Z= 3.798864817331D+13

I= 31 X= -8.884881060098D+13 Y= 6.083529169161D+13 Z= -3.458995111074D+13
I= 32 X= 2.777765781378D+13 Y= -8.623194083960D+13 Z= -4.640138049811D+13
I= 33 X= 1.815942922392D+13 Y= -1.218503983373D+14 Z= 1.397119325760D+12
I= 34 X= -5.595585884819D+13 Y= -1.703323502730D+13 Z= 1.590584092341D+13
I= 35 X= 1.510815805176D+12 Y= 2.580646177565D+12 Z= 3.531991038277D+12
I= 36 X= -1.818530522998D+13 Y= -6.272714751652D+12 Z= -1.269955791016D+13
I= 37 X= 6.553231839973D+12 Y= 6.668365042216D+13 Z= 8.226029453592D+13
I= 38 X= 1.242252938022D+14 Y= 4.993099108648D+13 Z= -1.784497570944D+13

Seed: 18445319666

CM Start Point Coordinates: bohr

I= 0 X= -2.182142446933D+00 Y= -2.144629491414D+00 Z= -1.491642632787D-01
I= 1 X= 3.756037991896D-02 Y= -2.714709552570D+00 Z= -1.470525964159D+00
I= 2 X= -1.377005340466D+00 Y= -1.466514877091D+00 Z= 2.382830073233D+00
I= 3 X= 2.184840371439D+00 Y= -2.103322228035D+00 Z= -3.113532432224D-02
I= 4 X= 1.353973931945D+00 Y= -1.161668695211D+00 Z= 2.375024392475D+00
I= 5 X= -2.865098572564D+00 Y= 3.327615817094D+00 Z= -2.375875375613D+00
I= 6 X= 3.572492938327D-01 Y= 1.276053413706D+00 Z= -3.467479328633D+00
I= 7 X= -1.912909816954D+00 Y= 4.644905148336D+00 Z= -3.716809230888D+00
I= 8 X= -4.361196188345D+00 Y= 2.231630931274D+00 Z= -3.259752791009D+00
I= 9 X= 2.921416118842D+00 Y= -2.960733816149D-01 Z= 4.401457676057D+00
I= 10 X= 2.708461141972D+00 Y= -1.511489062119D+00 Z= 6.205353172866D+00
I= 11 X= 4.913641408753D+00 Y= -1.156057422383D+00 Z= 3.902155417446D+00
I= 12 X= 2.733426795367D+00 Y= 1.932850645153D+00 Z= 5.256421565392D+00
I= 13 X= -2.909593774662D+00 Y= -4.968094826526D-01 Z= 4.690715020688D+00
I= 14 X= -3.173483515557D+00 Y= -1.993275668459D+00 Z= 6.119409531048D+00
I= 15 X= -2.025789262809D+00 Y= 9.288394610294D-01 Z= 5.574145779009D+00
I= 16 X= -4.653289839980D+00 Y= -9.356432110418D-02 Z= 3.853730916122D+00
I= 17 X= -4.919439515927D+00 Y= -2.453548114954D+00 Z= -7.725657368330D-01
I= 18 X= -5.781489355821D+00 Y= -4.464502650131D+00 Z= -1.637662552614D-01

I= 19 X= -6.002052896432D+00 Y= -1.067005732373D+00 Z= 1.765221916084D-01
I= 20 X= -5.315996398554D+00 Y= -2.762706771852D+00 Z= -2.899939631060D+00
I= 21 X= -6.389136953950D-02 Y= -3.856947929339D+00 Z= -4.249328500007D+00
I= 22 X= 9.321266728120D-01 Y= -6.020408928165D+00 Z= -4.435308653859D+00
I= 23 X= -2.156190091053D+00 Y= -3.905665747641D+00 Z= -5.137450223304D+00
I= 24 X= 1.403038524213D+00 Y= -2.349036092497D+00 Z= -5.282883718780D+00
I= 25 X= 4.948624419920D+00 Y= -2.565058916764D+00 Z= -9.955598784525D-01
I= 26 X= 5.260910742680D+00 Y= -2.384942887048D+00 Z= -2.964268290355D+00
I= 27 X= 6.565918068807D+00 Y= -1.481526065244D+00 Z= 1.720563575950D-01
I= 28 X= 5.291843393288D+00 Y= -4.885151194772D+00 Z= -6.577438493539D-01
I= 29 X= 3.134190914141D+00 Y= 3.127173938352D+00 Z= -2.078000958805D+00
I= 30 X= 2.581115799779D+00 Y= 3.831240264618D+00 Z= 4.556732829928D-01
I= 31 X= 4.600179591578D+00 Y= 1.647919074952D+00 Z= -2.488750631759D+00
I= 32 X= 2.125564148837D+00 Y= 4.069111783427D+00 Z= -3.802509492379D+00
I= 33 X= 1.619276938957D+00 Y= 5.422263369349D+00 Z= 1.119567364138D+00
I= 34 X= 4.010066022870D+00 Y= 3.125693952223D+00 Z= 1.937851909654D+00
I= 35 X= -4.001488145711D-02 Y= 1.093677603896D+00 Z= -4.872595869716D-01
I= 36 X= -2.753346996262D+00 Y= 3.677405247724D+00 Z= 3.321319075801D-01
I= 37 X= -2.051972577340D+00 Y= 5.288712821616D+00 Z= 9.413866347121D-01
I= 38 X= -3.833387084487D+00 Y= 2.610619172296D+00 Z= 1.557142401424D+00

Forward Direction:

Total Energy: -691.9926994 Hartrees

Potential Energy: -692.1761245 Hartress

Kinetic Energy: 0.1834251 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.691054932297D+13 Y= 9.319616043663D+12 Z= 3.648423002031D+13

I= 1 X= -1.217925906323D+13 Y= -1.468072420450D+13 Z= 4.827816802123D+12

I= 2 X= -1.199511239452D+13 Y= -4.829369473839D+12 Z= -9.666142930678D+12

I= 3 X= 9.314465436017D+12 Y= 5.945466892082D+12 Z= 7.583750039918D+12

I= 4 X= -1.034520167366D+13 Y= 4.642278237463D+12 Z= 5.478980587466D+12

I= 5 X= 2.226424337537D+13 Y= 1.486103460443D+13 Z= 2.788730994206D+12
I= 6 X= 6.223208434627D+13 Y= 7.230047384554D+12 Z= -2.590825388584D+13
I= 7 X= 1.868472850010D+13 Y= 1.661798445184D+13 Z= 1.318404890520D+13
I= 8 X= -1.769362364484D+14 Y= -1.773808365739D+14 Z= -3.200386315609D+13
I= 9 X= 9.913961404286D+12 Y= 2.757168504365D+13 Z= 5.202064205387D+12
I= 10 X= -8.225237968076D+13 Y= 1.914160774756D+13 Z= -3.788915830687D+13
I= 11 X= -8.481286028873D+13 Y= -4.543778565563D+13 Z= -1.278839219415D+13
I= 12 X= 5.715622034845D+12 Y= -1.235197613182D+13 Z= -2.002224556031D+13
I= 13 X= -1.860979859342D+12 Y= 1.454854451049D+13 Z= 1.559983418630D+13
I= 14 X= -3.198215012188D+13 Y= -5.639237679193D+13 Z= -2.115284947687D+13
I= 15 X= 5.418110462948D+12 Y= -5.736231327661D+13 Z= -7.506040976356D+13
I= 16 X= 5.134797217693D+13 Y= -5.438078363753D+13 Z= 5.207360125554D+13
I= 17 X= 1.495696082147D+13 Y= -2.427462098503D+13 Z= -1.720678142973D+13
I= 18 X= -4.606061745686D+12 Y= 3.679996079946D+13 Z= -3.646257968226D+12
I= 19 X= -1.303225781070D+14 Y= 1.086296256439D+13 Z= 5.038619976388D+13
I= 20 X= -7.018991740775D+12 Y= -5.202961904663D+12 Z= 2.053945799045D+13
I= 21 X= -1.207477542826D+13 Y= -2.127822436266D+13 Z= 9.666162289369D+12
I= 22 X= 2.210652360651D+13 Y= 1.028953129696D+14 Z= -1.431376465890D+13
I= 23 X= 5.604398674789D+13 Y= -8.252469147267D+13 Z= -3.487379946697D+13
I= 24 X= 5.265310042410D+13 Y= 2.077011080839D+13 Z= -7.075607494676D+13
I= 25 X= -3.125039211367D+12 Y= -4.104379197809D+11 Z= -1.260560726237D+13
I= 26 X= 2.748263124336D+13 Y= 7.637395471446D+12 Z= 1.277858261898D+14
I= 27 X= -7.162457722409D+13 Y= 9.788383026551D+12 Z= -1.079845782804D+14
I= 28 X= -5.314522028191D+13 Y= 2.932354236119D+13 Z= -2.333061861543D+13
I= 29 X= 1.112512958707D+13 Y= 7.612580908399D+12 Z= -2.001158178295D+13
I= 30 X= -1.504711383969D+13 Y= 1.026302308633D+13 Z= -1.630247392563D+13
I= 31 X= 2.580413339005D+12 Y= 3.848383276856D+13 Z= -4.770097526803D+13
I= 32 X= 6.195144851293D+13 Y= 4.506547454423D+13 Z= -1.800711733382D+13
I= 33 X= 2.395715484300D+13 Y= 4.150597040739D+13 Z= 8.827692308785D+13
I= 34 X= 8.619510883862D+11 Y= 6.593270620265D+12 Z= 1.919042037799D+13

I= 35 X= -4.446707768865D+11 Y= -4.158250707023D+12 Z= -1.705948032827D+12

I= 36 X= 3.335261745764D+12 Y= 1.471411899640D+13 Z= 3.433507659324D+12

I= 37 X= 2.645373640263D+13 Y= -6.972446955401D+13 Z= 4.698519210179D+13

I= 38 X= -1.128500317877D+12 Y= -1.127610094412D+14 Z= 4.492615013404D+13

Backward Direction:

Total Energy: -691.9925784 Hartrees

Potential Energy: -692.1761245 Hartress

Kinetic Energy: 0.1835461 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.706113507389D+13 Y= 1.118667240236D+13 Z= 3.927220347464D+13

I= 1 X= -1.101842706479D+13 Y= -1.468035595767D+13 Z= 4.827622259048D+12

I= 2 X= -1.125914529460D+13 Y= -5.773876609724D+12 Z= -8.159365196146D+12

I= 3 X= 9.465267607577D+12 Y= 4.078232474000D+12 Z= 4.795399936649D+12

I= 4 X= -9.609088352759D+12 Y= 5.586959505382D+12 Z= 3.972221690441D+12

I= 5 X= 2.544376895210D+13 Y= 3.141588341099D+12 Z= -1.104008056671D+13

I= 6 X= -5.793858892693D+13 Y= 7.248246278108D+12 Z= -2.590812995483D+13

I= 7 X= 7.634889064023D+11 Y= 1.368942727227D+13 Z= -3.653609581651D+12

I= 8 X= -1.857522598549D+14 Y= -1.826774729734D+14 Z= -3.585662456550D+13

I= 9 X= 1.191350516069D+13 Y= 2.393887904966D+13 Z= 4.073165700520D+12

I= 10 X= -8.350553769147D+13 Y= 1.450602311054D+13 Z= -4.037779342543D+13

I= 11 X= -8.221973941573D+13 Y= -5.258990039940D+13 Z= -1.348923178011D+13

I= 12 X= 1.073818410203D+13 Y= -1.569353508475D+13 Z= -1.965859023030D+13

I= 13 X= 1.383675868907D+11 Y= 1.818138775937D+13 Z= 1.672928634958D+13

I= 14 X= -3.323378092671D+13 Y= -5.175626564670D+13 Z= -1.866337785000D+13

I= 15 X= 1.043964901391D+13 Y= -5.401922434755D+13 Z= -7.542429333332D+13

I= 16 X= 5.394014899459D+13 Y= -4.723075807859D+13 Z= 5.277584623349D+13

I= 17 X= 1.476626568583D+13 Y= -2.409674967607D+13 Z= -1.335385291281D+13

I= 18 X= -3.909353346948D+12 Y= 3.844729381054D+13 Z= 4.212658223272D+12

I= 19 X= -1.307164772188D+14 Y= 1.195823316409D+13 Z= 5.197181338832D+13

I= 20 X= -8.213025025313D+12 Y= -9.728620222453D+12 Z= 2.479617678823D+13

I= 21 X= -1.546476658742D+13 Y= -2.127648843103D+13 Z= 9.664996009417D+12
I= 22 X= 1.335620567422D+13 Y= 1.028971279822D+14 Z= -1.431703227885D+13
I= 23 X= 5.382092492538D+13 Y= -7.841932679704D+13 Z= -3.455180852092D+13
I= 24 X= 5.042953123747D+13 Y= 1.666964447551D+13 Z= -7.107982555544D+13
I= 25 X= -3.315359554462D+12 Y= -5.890210218988D+11 Z= -1.645863278553D+13
I= 26 X= 2.628940872480D+13 Y= 1.216176285009D+13 Z= 1.235287693864D+14
I= 27 X= -7.201791428613D+13 Y= 8.691594407642D+12 Z= -1.095697547353D+14
I= 28 X= -5.244849095201D+13 Y= 2.767509485952D+13 Z= -3.118909390141D+13
I= 29 X= 1.430403233859D+13 Y= 1.932828296982D+13 Z= -6.185998013364D+12
I= 30 X= -9.953293045254D+12 Y= 1.147873407121D+13 Z= -5.812803996248D+12
I= 31 X= -6.230416331682D+12 Y= 4.377991379494D+13 Z= -4.385079290114D+13
I= 32 X= 4.403253991010D+13 Y= 4.799388463604D+13 Z= -1.175386415714D+12
I= 33 X= 2.203088373284D+13 Y= 3.464222651425D+13 Z= 1.105273506950D+14
I= 34 X= 1.710689824572D+12 Y= -9.131225035445D+11 Z= 2.792435606975D+13
I= 35 X= -1.412908869608D+12 Y= -4.157851210420D+12 Z= -1.704675334363D+12
I= 36 X= 8.429430529497D+12 Y= 1.349690846120D+13 Z= -7.056791794865D+12
I= 37 X= 2.452386482554D+13 Y= -6.285638115514D+13 Z= 2.473203303484D+13
I= 38 X= -2.786577279148D+11 Y= -1.052571145341D+14 Z= 3.619233490709D+13

Seed: 18501431564

CM Start Point Coordinates: bohr

I= 0 X= -2.115246924063D+00 Y= -2.007889192476D+00 Z= -5.885899786456D-02
I= 1 X= 6.591578005449D-03 Y= -2.677459653236D+00 Z= -1.441423013917D+00
I= 2 X= -1.214642327130D+00 Y= -1.271865891307D+00 Z= 2.358480825944D+00
I= 3 X= 2.190995360414D+00 Y= -2.181790298623D+00 Z= -8.443960877779D-02
I= 4 X= 1.357152098193D+00 Y= -1.215643935292D+00 Z= 2.436585830154D+00
I= 5 X= -3.031651746141D+00 Y= 3.223878176626D+00 Z= -2.273319534991D+00
I= 6 X= -4.081526987997D-01 Y= 1.896255863511D+00 Z= -3.493918924253D+00
I= 7 X= -2.302036134740D+00 Y= 4.587495389467D+00 Z= -4.026523827623D+00
I= 8 X= -4.217824462977D+00 Y= 1.596103805965D+00 Z= -2.751632800635D+00

I= 9 X= 2.762586691485D+00 Y= -5.748629444799D-01 Z= 4.733938473592D+00
I= 10 X= 2.753883770950D+00 Y= -2.076679484462D+00 Z= 6.201450532843D+00
I= 11 X= 4.896448428120D+00 Y= -3.820410803818D-01 Z= 4.550247901332D+00
I= 12 X= 1.841456322786D+00 Y= 1.357529633683D+00 Z= 5.538911867685D+00
I= 13 X= -3.085391106086D+00 Y= -8.358258045385D-01 Z= 4.612878326394D+00
I= 14 X= -3.268498083749D+00 Y= -3.105661852690D+00 Z= 5.131609745849D+00
I= 15 X= -2.232753471871D+00 Y= 3.155612226947D-01 Z= 6.107503158728D+00
I= 16 X= -4.986255689885D+00 Y= -6.913214496687D-02 Z= 3.829529940184D+00
I= 17 X= -4.925327323243D+00 Y= -2.591332774347D+00 Z= -5.497896862229D-01
I= 18 X= -6.048233767943D+00 Y= -3.885926851123D+00 Z= 1.107173052786D+00
I= 19 X= -6.227155446024D+00 Y= -5.765776607682D-01 Z= -8.577031997191D-01
I= 20 X= -5.109782872160D+00 Y= -3.767471284734D+00 Z= -2.497532260946D+00
I= 21 X= 9.108106510196D-02 Y= -3.550697086668D+00 Z= -4.118747995849D+00
I= 22 X= -5.514288042646D-01 Y= -5.764041783204D+00 Z= -4.097778740284D+00
I= 23 X= -1.128487106280D+00 Y= -2.485117360592D+00 Z= -5.642940213923D+00
I= 24 X= 2.130453657500D+00 Y= -3.435906901751D+00 Z= -5.142665876820D+00
I= 25 X= 4.793637969140D+00 Y= -2.426388210268D+00 Z= -7.345022107673D-01
I= 26 X= 5.237347457353D+00 Y= -1.994428005145D+00 Z= -2.523640248896D+00
I= 27 X= 5.822915623368D+00 Y= -1.201329499071D+00 Z= 3.873600783986D-01
I= 28 X= 5.343875152611D+00 Y= -4.586280093224D+00 Z= -3.306748453142D-01
I= 29 X= 2.734378703128D+00 Y= 3.233222919136D+00 Z= -2.474706482770D+00
I= 30 X= 2.736744114206D+00 Y= 3.472129160229D+00 Z= 1.724322768635D-01
I= 31 X= 4.246184912195D+00 Y= 2.094387221078D+00 Z= -3.413596060855D+00
I= 32 X= 1.840042990175D+00 Y= 4.649706732260D+00 Z= -3.822781924095D+00
I= 33 X= 2.139930424919D+00 Y= 5.243554734956D+00 Z= 9.626711272294D-01
I= 34 X= 3.976177702219D+00 Y= 2.615789097860D+00 Z= 1.539882645024D+00
I= 35 X= 8.816057569519D-02 Y= 1.122606798235D+00 Z= -5.860314756544D-01
I= 36 X= -2.622871661634D+00 Y= 3.901177032079D+00 Z= 3.365279305838D-01
I= 37 X= -1.257600385701D+00 Y= 5.736691416533D+00 Z= 9.499032428760D-01
I= 38 X= -3.812187862324D+00 Y= 3.119813479252D+00 Z= 1.854627980647D+00

Forward Direction:

Total Energy: -691.9957366 Hartrees

Potential Energy: -692.1824562 Hartress

Kinetic Energy: 0.1867196 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.433358891609D+12 Y= 2.162614286392D+12 Z= 2.688684749893D+13
I= 1 X= -7.743117063525D+12 Y= -1.029741151951D+13 Z= 5.281878872099D+12
I= 2 X= -3.662800241093D+12 Y= -1.628287420213D+12 Z= -9.188895262039D+12
I= 3 X= -2.953400673391D+12 Y= 1.842912092542D+12 Z= 1.984703898135D+13
I= 4 X= -1.228629954919D+13 Y= 7.580999605014D+12 Z= -3.980217274355D+13
I= 5 X= -9.146346866679D+12 Y= -3.407756024410D+12 Z= 1.199837403607D+13
I= 6 X= 4.812268202545D+13 Y= 7.801965919451D+12 Z= -1.667343307614D+12
I= 7 X= 7.835514979081D+13 Y= 3.206324151116D+13 Z= -5.494409831719D+13
I= 8 X= -9.027828329146D+13 Y= 1.889797646615D+13 Z= -5.680185735658D+13
I= 9 X= 1.385028113831D+13 Y= -2.805002377154D+12 Z= 6.691980793310D+12
I= 10 X= 1.074332026390D+13 Y= -9.899230020836D+12 Z= 2.065121139066D+13
I= 11 X= 8.911769624187D+13 Y= 8.660335245019D+13 Z= -4.526349799755D+13
I= 12 X= -2.130289483129D+13 Y= 1.570060150309D+14 Z= 5.362207456835D+13
I= 13 X= -2.503960315102D+13 Y= -1.448290456089D+13 Z= -1.708922168956D+13
I= 14 X= -2.520446211315D+12 Y= 3.368414431960D+13 Z= 4.612909258758D+13
I= 15 X= 8.242422650582D+13 Y= 1.074772611796D+13 Z= 7.868079915482D+13
I= 16 X= 7.719497304733D+13 Y= 1.929248656012D+13 Z= 7.789264128458D+13
I= 17 X= 2.978879882432D+12 Y= 3.688174070813D+11 Z= -7.251827887963D+12
I= 18 X= -1.700878086259D+13 Y= 1.038150053541D+14 Z= -5.317047466155D+13
I= 19 X= 5.652352281616D+13 Y= -3.345588453579D+13 Z= -3.890906594489D+13
I= 20 X= -5.378927730782D+13 Y= -2.543969381057D+13 Z= 8.840762365980D+12
I= 21 X= 3.600198962279D+12 Y= -7.547833909609D+12 Z= -6.806712705523D+12
I= 22 X= 7.800747720925D+13 Y= 9.634749366318D+13 Z= -3.184165113069D+12
I= 23 X= 4.352251271383D+12 Y= -6.156177049229D+13 Z= 3.491352043137D+13
I= 24 X= 1.242573910529D+14 Y= -1.241999885598D+13 Z= -6.041370129746D+13

I= 25 X= -2.321907597839D+13 Y= -8.158917035424D+12 Z= 1.767443830549D+13
I= 26 X= 5.800286672116D+13 Y= 7.834096585805D+13 Z= 1.050867217190D+14
I= 27 X= -9.122321090282D+13 Y= 7.642025893546D+13 Z= -9.383442388525D+13
I= 28 X= -2.986991053368D+13 Y= 3.099311575395D+12 Z= 5.188013093891D+13
I= 29 X= -9.276398939578D+12 Y= 1.192114155860D+13 Z= 1.451846687102D+13
I= 30 X= 6.086167740305D+12 Y= -1.970985121433D+13 Z= -1.859523496720D+13
I= 31 X= 7.640904675669D+13 Y= -2.727002943710D+13 Z= 6.337928015531D+13
I= 32 X= 4.256120886913D+13 Y= -1.183686285533D+14 Z= 7.729558340380D+13
I= 33 X= -5.479777965067D+12 Y= 1.931004269831D+13 Z= 5.680440240182D+13
I= 34 X= 1.755859803596D+13 Y= -4.657256900455D+13 Z= 8.926865887360D+12
I= 35 X= 5.330492319593D+12 Y= 4.623720566451D+12 Z= -7.698525916310D+12
I= 36 X= -5.111249864263D+12 Y= -8.725231160355D+12 Z= 6.097527876180D+12
I= 37 X= 2.929187323636D+13 Y= 1.033299308944D+12 Z= 4.354134174364D+13
I= 38 X= -3.384829218633D+13 Y= -5.013743005050D+13 Z= 8.526620125063D+12

Backward Direction:

Total Energy: -691.9957700 Hartrees

Potential Energy: -692.1824562 Hartress

Kinetic Energy: 0.1866862 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.446354365534D+12 Y= 3.416274453774D+12 Z= 2.901599420346D+13
I= 1 X= -7.503434679238D+12 Y= -1.029709470896D+13 Z= 5.281686294711D+12
I= 2 X= -2.808385087274D+12 Y= -1.783983802311D+12 Z= -8.121388453261D+12
I= 3 X= -2.940207342617D+12 Y= 5.891503915113D+11 Z= 1.771761556319D+13
I= 4 X= -1.143175584063D+13 Y= 7.736833027211D+12 Z= -4.086959064643D+13
I= 5 X= -7.896917411292D+12 Y= -1.345996114680D+13 Z= 9.649459000934D+11
I= 6 X= -1.765693588526D+13 Y= 7.814416576171D+12 Z= -1.666688150014D+12
I= 7 X= 6.612689306071D+13 Y= 2.538415654827D+13 Z= -7.016446367326D+13
I= 8 X= -9.509004328677D+13 Y= 1.028992002531D+13 Z= -5.978809295309D+13
I= 9 X= 1.580405668526D+13 Y= -6.316494890857D+12 Z= 5.818299450413D+12
I= 10 X= 9.891130546382D+12 Y= -1.415237399147D+13 Z= 1.874828718299D+13

I= 11 X= 9.157133001319D+13 Y= 7.996312117428D+13 Z= -4.586452371505D+13
I= 12 X= -1.667119795587D+13 Y= 1.538564080253D+14 Z= 5.387994628091D+13
I= 13 X= -2.308597645359D+13 Y= -1.097137803377D+13 Z= -1.621498517950D+13
I= 14 X= -3.371112442577D+12 Y= 3.793783403392D+13 Z= 4.803291449522D+13
I= 15 X= 8.705498932454D+13 Y= 1.389875222266D+13 Z= 7.842270851293D+13
I= 16 X= 7.964775840899D+13 Y= 2.593077104760D+13 Z= 7.849498856799D+13
I= 17 X= 2.610391136816D+12 Y= 3.781103770710D+11 Z= -3.654515429288D+12
I= 18 X= -1.678867808250D+13 Y= 1.054158371158D+14 Z= -4.555340141392D+13
I= 19 X= 5.629566209318D+13 Y= -3.225149001005D+13 Z= -3.757400836091D+13
I= 20 X= -5.522639051184D+13 Y= -2.996319423893D+13 Z= 1.284642389674D+13
I= 21 X= 2.651184426150D+11 Y= -7.546267097074D+12 Z= -6.807764200049D+12
I= 22 X= 6.946265165391D+13 Y= 9.634915118152D+13 Z= -3.187081630976D+12
I= 23 X= 2.319522815028D+12 Y= -5.749950722954D+13 Z= 3.499912966759D+13
I= 24 X= 1.222242712506D+14 Y= -1.647795267908D+13 Z= -6.050071659486D+13
I= 25 X= -2.358716007371D+13 Y= -8.168925771675D+12 Z= 1.407700789123D+13
I= 26 X= 5.656648691699D+13 Y= 8.286348265561D+13 Z= 1.010806619226D+14
I= 27 X= -9.145044548148D+13 Y= 7.521431853425D+13 Z= -9.516897584975D+13
I= 28 X= -2.964962299681D+13 Y= 1.497284090978D+12 Z= 4.426315052874D+13
I= 29 X= -8.027603703112D+12 Y= 2.197032396209D+13 Z= 2.554898445827D+13
I= 30 X= 9.029122821302D+12 Y= -1.976902996697D+13 Z= -8.656042197659D+12
I= 31 X= 7.159968430839D+13 Y= -1.866440771406D+13 Z= 6.636278031563D+13
I= 32 X= 3.033561009739D+13 Y= -1.116889637732D+14 Z= 9.251111337742D+13
I= 33 X= -7.116484482528D+12 Y= 1.296008783129D+13 Z= 7.695423026063D+13
I= 34 X= 1.901060172764D+13 Y= -5.316465601337D+13 Z= 1.575820470672D+13
I= 35 X= 5.020513324787D+12 Y= 4.624101661581D+12 Z= -7.697416587503D+12
I= 36 X= -2.168317947161D+12 Y= -8.667281505858D+12 Z= -3.842290105967D+12
I= 37 X= 2.765155663544D+13 Y= 7.386909926401D+12 Z= 2.338974060957D+13
I= 38 X= -3.239604702659D+13 Y= -4.354824668255D+13 Z= 1.695166645421D+12

Seed: 18981160378

CM Start Point Coordinates: bohr

I= 0 X= -2.123390028439D+00 Y= -1.917503349389D+00 Z= -2.334234230090D-02
I= 1 X= 9.423509606378D-02 Y= -2.678095730494D+00 Z= -1.640741089088D+00
I= 2 X= -1.232468152443D+00 Y= -1.110173910125D+00 Z= 2.394798343033D+00
I= 3 X= 2.116574049118D+00 Y= -2.224967956337D+00 Z= 3.303986657199D-02
I= 4 X= 1.381988506162D+00 Y= -1.211181543035D+00 Z= 2.429579312835D+00
I= 5 X= -3.028444013604D+00 Y= 3.185021262537D+00 Z= -2.101958196535D+00
I= 6 X= -5.711974067704D-02 Y= 1.019840139562D+00 Z= -3.386194378655D+00
I= 7 X= -2.031507305580D+00 Y= 4.517300902324D+00 Z= -3.184574870324D+00
I= 8 X= -4.331241838338D+00 Y= 1.841335123277D+00 Z= -2.949947655005D+00
I= 9 X= 3.009767715672D+00 Y= -5.271675201564D-01 Z= 4.622724274142D+00
I= 10 X= 3.331196046827D+00 Y= -2.177090723249D+00 Z= 5.545632574560D+00
I= 11 X= 4.877600636595D+00 Y= 1.530227716694D-01 Z= 3.974597452760D+00
I= 12 X= 1.968745131595D+00 Y= 6.347637394087D-01 Z= 6.391792514391D+00
I= 13 X= -2.907457133828D+00 Y= -7.319429555743D-01 Z= 4.736732484831D+00
I= 14 X= -2.262801395872D+00 Y= -2.243815550812D+00 Z= 6.324106026011D+00
I= 15 X= -2.385281145959D+00 Y= 9.847307294122D-01 Z= 5.804553111523D+00
I= 16 X= -5.201603868802D+00 Y= -9.415678174100D-01 Z= 4.584683551707D+00
I= 17 X= -4.724884254556D+00 Y= -2.244400738259D+00 Z= -1.029754005699D+00
I= 18 X= -5.364900259478D+00 Y= -4.151234226013D+00 Z= -3.850613349904D-01
I= 19 X= -6.071690055371D+00 Y= -7.979075858236D-01 Z= -4.325182624521D-01
I= 20 X= -4.497298685245D+00 Y= -2.332186392151D+00 Z= -3.135088570570D+00
I= 21 X= -5.548335660762D-02 Y= -3.962569193537D+00 Z= -3.966511929898D+00
I= 22 X= -1.034557583726D+00 Y= -6.030309688765D+00 Z= -3.708476624907D+00
I= 23 X= -1.639583927097D+00 Y= -2.512140214458D+00 Z= -5.267655063132D+00
I= 24 X= 1.777402691686D+00 Y= -4.138513482773D+00 Z= -5.212573072635D+00
I= 25 X= 4.831265169868D+00 Y= -2.830102500772D+00 Z= -6.004703631700D-01
I= 26 X= 4.879399703599D+00 Y= -3.026172795471D+00 Z= -2.841207987562D+00
I= 27 X= 6.169500133399D+00 Y= -1.617792025185D+00 Z= 5.255394923617D-02
I= 28 X= 5.399253862540D+00 Y= -4.721823255734D+00 Z= 7.951351920676D-01

I= 29 X= 2.728621034269D+00 Y= 3.425710631704D+00 Z= -2.155071809597D+00
I= 30 X= 2.886302102494D+00 Y= 3.960074801274D+00 Z= 3.730915229486D-01
I= 31 X= 4.428960281373D+00 Y= 2.394898427306D+00 Z= -3.218185943824D+00
I= 32 X= 1.833776231703D+00 Y= 4.920455407810D+00 Z= -3.146817367875D+00
I= 33 X= 1.625497178941D+00 Y= 5.331662306399D+00 Z= 1.289237167052D+00
I= 34 X= 4.219631548952D+00 Y= 2.646046605453D+00 Z= 1.456016687836D+00
I= 35 X= 7.921590086642D-03 Y= 1.109209316763D+00 Z= -7.567316908439D-01
I= 36 X= -2.960075183203D+00 Y= 3.613500238648D+00 Z= 4.713785189320D-01
I= 37 X= -2.055499458986D+00 Y= 5.508623802252D+00 Z= 8.152997714890D-01
I= 38 X= -4.238174585336D+00 Y= 2.432244930013D+00 Z= 1.893268082117D+00

Forward Direction:

Total Energy: -692.0041611 Hartrees

Potential Energy: -692.1825624 Hartress

Kinetic Energy: 0.1784013 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.224643833310D+12 Y= -4.529117991892D+12 Z= -1.272246133131D+12
I= 1 X= -7.062647917352D+12 Y= 3.428362566467D+12 Z= 2.693011317059D+13
I= 2 X= -1.424050491776D+13 Y= 1.407985026374D+13 Z= -2.701108350992D+13
I= 3 X= -1.942830297216D+13 Y= -8.127582412274D+12 Z= -1.226315519793D+13
I= 4 X= 1.768297661812D+12 Y= -6.649031392591D+12 Z= 4.861112677913D+12
I= 5 X= 1.380795459199D+13 Y= 4.430145774006D+12 Z= 4.942506885304D+12
I= 6 X= 4.156894770639D+13 Y= 1.495811485564D+13 Z= 8.161174853066D+13
I= 7 X= 3.259388430316D+13 Y= -2.500630197011D+12 Z= 5.925910017492D+12
I= 8 X= -1.360269813606D+14 Y= -1.186179967407D+14 Z= -1.651307672071D+14
I= 9 X= 1.986224863091D+13 Y= 2.720422193802D+12 Z= 2.563114555377D+12
I= 10 X= -3.659196871336D+11 Y= -6.146649178666D+13 Z= 6.011373053180D+13
I= 11 X= -1.013716389702D+14 Y= -3.487445555946D+13 Z= 4.441668046184D+13
I= 12 X= -3.443522092080D+13 Y= 6.669907534434D+13 Z= 1.774782463949D+12
I= 13 X= 1.849345975466D+13 Y= -8.041367102483D+11 Z= -8.503085439129D+12
I= 14 X= -6.211412513926D+12 Y= -5.927066611700D+13 Z= 6.103442657753D+13

I= 15 X= 3.900994307182D+13 Y= 8.997552964727D+13 Z= -2.428094934276D+12
I= 16 X= -5.095674001587D+13 Y= 4.514619480972D+13 Z= 5.240399393453D+13
I= 17 X= 6.557413778339D+12 Y= -2.030583873495D+13 Z= 9.664538876523D+12
I= 18 X= -2.716730123107D+13 Y= 1.685533914728D+12 Z= -4.455232791185D+12
I= 19 X= 6.176828740714D+13 Y= 8.831484365073D+13 Z= 3.537325192958D+13
I= 20 X= -1.166538773034D+13 Y= 6.278591390043D+12 Z= -1.058008458034D+14
I= 21 X= -2.196205428943D+12 Y= -1.348736188867D+13 Z= 2.089748660836D+13
I= 22 X= -6.411080117235D+13 Y= 1.907474467471D+13 Z= -2.987768120204D+13
I= 23 X= 2.386958681073D+13 Y= -1.064639200356D+13 Z= -1.584047047004D+13
I= 24 X= 4.866662703422D+13 Y= 9.891647680623D+13 Z= -3.599900670405D+13
I= 25 X= -1.751391504154D+13 Y= 9.554049910879D+12 Z= 6.219396797394D+12
I= 26 X= 3.080575025186D+12 Y= 2.156464337041D+13 Z= -4.726442954462D+13
I= 27 X= 1.027976043377D+14 Y= -8.580214451313D+13 Z= 2.099016848325D+12
I= 28 X= 9.428543119386D+13 Y= 1.928724715648D+13 Z= 1.710628169495D+11
I= 29 X= 8.357101718120D+12 Y= -1.750694301228D+13 Z= 9.638287696609D+11
I= 30 X= 2.267527554083D+12 Y= 1.282310002404D+13 Z= -3.457671500005D+13
I= 31 X= 3.265269393509D+12 Y= 4.280909830940D+12 Z= -1.314134315367D+13
I= 32 X= -7.370710679263D+13 Y= 7.478525236700D+12 Z= 2.635876210369D+13
I= 33 X= -2.837706148396D+13 Y= 1.140381851983D+14 Z= 5.302755091861D+13
I= 34 X= 9.327176067115D+13 Y= 9.832819893364D+12 Z= -2.542605940558D+13
I= 35 X= -3.544622038836D+12 Y= 1.775745305272D+12 Z= -2.107783604718D+12
I= 36 X= 4.391715184385D+12 Y= 5.510582464848D+12 Z= 2.421240616426D+13
I= 37 X= 1.246093464178D+12 Y= -3.286123510443D+13 Z= -6.363422039666D+13
I= 38 X= -2.151589918971D+13 Y= -8.072478911867D+13 Z= -1.954989519956D+12

Backward Direction:

Total Energy: -692.0043214 Hartrees

Potential Energy: -692.1825624 Hartress

Kinetic Energy: 0.1782410 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.193676949953D+12 Y= -3.435213402254D+12 Z= 7.090294720252D+11

I= 1 X= -7.112661287001D+12 Y= 3.428672398880D+12 Z= 2.692991543193D+13
I= 2 X= -1.332201290600D+13 Y= 1.417373145703D+13 Z= -2.605283904613D+13
I= 3 X= -1.945907199597D+13 Y= -9.221566941840D+12 Z= -1.424468361426D+13
I= 4 X= 2.686916435769D+12 Y= -6.742783383909D+12 Z= 3.902982507735D+12
I= 5 X= 1.447302431428D+13 Y= -5.389193103365D+12 Z= -5.524100526267D+12
I= 6 X= -8.669506493714D+12 Y= 1.496908951963D+13 Z= 8.161259477885D+13
I= 7 X= 2.183036506482D+13 Y= -1.059120468808D+13 Z= -9.234304512733D+12
I= 8 X= -1.396936654013D+14 Y= -1.285544382410D+14 Z= -1.679281467026D+14
I= 9 X= 2.186047569991D+13 Y= -8.583718519857D+11 Z= 1.745234219494D+12
I= 10 X= -1.114670023249D+12 Y= -6.572523010982D+13 Z= 5.834196189761D+13
I= 11 X= -9.888861924688D+13 Y= -4.155088860498D+13 Z= 4.382961940863D+13
I= 12 X= -2.978917407026D+13 Y= 6.351590548306D+13 Z= 2.006366179133D+12
I= 13 X= 2.049154869694D+13 Y= 2.774691362090D+12 Z= -7.684632556738D+12
I= 14 X= -6.958594518948D+12 Y= -5.501135935698D+13 Z= 6.280714002344D+13
I= 15 X= 4.365505626800D+13 Y= 9.316012580738D+13 Z= -2.659901199017D+12
I= 16 X= -4.847456356297D+13 Y= 5.182066798177D+13 Z= 5.299238958916D+13
I= 17 X= 6.120441728088D+12 Y= -2.035061022326D+13 Z= 1.328845713031D+13
I= 18 X= -2.709417603226D+13 Y= 3.319885285989D+12 Z= 3.314699196352D+12
I= 19 X= 6.158704899978D+13 Y= 8.959091458563D+13 Z= 3.666799219690D+13
I= 20 X= -1.322441403497D+13 Y= 1.618708730874D+12 Z= -1.017547343648D+14
I= 21 X= -5.614648453262D+12 Y= -1.348580207599D+13 Z= 2.089644027588D+13
I= 22 X= -7.284831825729D+13 Y= 1.907640168813D+13 Z= -2.988057293669D+13
I= 23 X= 2.183661904095D+13 Y= -6.474922975502D+12 Z= -1.582847135369D+13
I= 24 X= 4.663329344555D+13 Y= 9.474925808422D+13 Z= -3.601234044515D+13
I= 25 X= -1.795046064046D+13 Y= 9.598082670176D+12 Z= 2.595350060874D+12
I= 26 X= 1.522279017899D+12 Y= 2.622361149814D+13 Z= -5.131097076129D+13
I= 27 X= 1.026170314551D+14 Y= -8.707981755544D+13 Z= 8.048190029039D+11
I= 28 X= 9.435879968106D+13 Y= 1.765163715237D+13 Z= -7.598885700156D+12
I= 29 X= 9.021514373061D+12 Y= -7.690485802127D+12 Z= 1.142753969241D+13
I= 30 X= 4.606271253770D+12 Y= 1.235113076493D+13 Z= -2.451379227798D+13

I= 31 X= -3.998458549986D+11 Y= 1.421423704505D+13 Z= -1.034683241918D+13
I= 32 X= -8.446778219794D+13 Y= 1.556993143331D+13 Z= 4.151434679023D+13
I= 33 X= -2.997001645494D+13 Y= 1.076614392770D+14 Z= 7.311080002233D+13
I= 34 X= 9.496224487835D+13 Y= 3.335722549043D+12 Z= -1.900106390864D+13
I= 35 X= -3.651785799569D+12 Y= 1.776131998773D+12 Z= -2.106693331374D+12
I= 36 X= 6.730315317780D+12 Y= 5.981372636555D+12 Z= 1.414884063980D+13
I= 37 X= -3.505840750008D+11 Y= -2.648094465879D+13 Z= -8.371898763351D+13
I= 38 X= -1.982544425591D+13 Y= -7.423081405328D+13 Z= -8.380178970415D+12

Seed: 19497515402

CM Start Point Coordinates: bohr

I= 0 X= -2.226698474818D+00 Y= -1.924569466882D+00 Z= -2.314780949218D-02
I= 1 X= 8.734570078523D-02 Y= -2.791830930132D+00 Z= -1.500577875358D+00
I= 2 X= -1.268175245572D+00 Y= -1.181353059582D+00 Z= 2.380083161858D+00
I= 3 X= 2.357700783688D+00 Y= -2.183890134343D+00 Z= -1.031997235617D-01
I= 4 X= 1.348699738286D+00 Y= -1.376761202071D+00 Z= 2.424275942189D+00
I= 5 X= -2.635639248740D+00 Y= 3.425444913747D+00 Z= -2.478345251668D+00
I= 6 X= -1.035942143310D-01 Y= 1.202425255255D+00 Z= -3.107527401737D+00
I= 7 X= -1.969785906454D+00 Y= 4.878935593343D+00 Z= -3.567113140072D+00
I= 8 X= -3.838732272007D+00 Y= 2.098061273826D+00 Z= -3.338029930047D+00
I= 9 X= 2.941010206072D+00 Y= -9.033077354557D-01 Z= 4.665333437168D+00
I= 10 X= 3.836073651120D+00 Y= -3.164207747169D+00 Z= 5.361349251869D+00
I= 11 X= 4.709890949997D+00 Y= 6.948031565034D-01 Z= 3.778158656675D+00
I= 12 X= 2.151360859903D+00 Y= -3.681519631634D-02 Z= 6.296881194673D+00
I= 13 X= -2.850887510881D+00 Y= -6.438165686708D-01 Z= 4.614267813287D+00
I= 14 X= -3.541505530028D+00 Y= -2.146732856481D+00 Z= 6.014731420344D+00
I= 15 X= -2.115336892486D+00 Y= 6.820809250070D-01 Z= 6.027144955449D+00
I= 16 X= -4.625667660310D+00 Y= -1.018440160176D-01 Z= 4.041589942909D+00
I= 17 X= -5.004157726395D+00 Y= -2.383231923671D+00 Z= -7.398115248590D-01
I= 18 X= -5.462543081763D+00 Y= -4.555878500742D+00 Z= -5.814281447782D-01

I= 19 X= -6.185818252484D+00 Y= -1.171712340507D+00 Z= 2.034332014192D-01
I= 20 X= -5.310683878428D+00 Y= -1.934627292128D+00 Z= -2.949880381537D+00
I= 21 X= -1.747325944925D-01 Y= -4.173683391442D+00 Z= -3.986160459350D+00
I= 22 X= -1.189393892799D+00 Y= -6.041772536398D+00 Z= -3.856954042046D+00
I= 23 X= -1.396594213711D+00 Y= -3.057268719418D+00 Z= -5.349732324641D+00
I= 24 X= 1.992746761900D+00 Y= -4.303744271111D+00 Z= -4.981929505979D+00
I= 25 X= 4.963529860273D+00 Y= -2.246691697590D+00 Z= -8.822925185286D-01
I= 26 X= 5.299329113964D+00 Y= -2.509008190494D+00 Z= -2.964415928288D+00
I= 27 X= 6.001607767435D+00 Y= -6.737317089344D-01 Z= -4.012875957611D-02
I= 28 X= 5.615194984415D+00 Y= -4.095539081238D+00 Z= -6.974647904761D-02
I= 29 X= 2.926613453775D+00 Y= 3.155074736267D+00 Z= -2.281094946097D+00
I= 30 X= 2.443015156704D+00 Y= 3.887939667917D+00 Z= 2.958548980508D-01
I= 31 X= 4.690948218422D+00 Y= 1.960548166243D+00 Z= -2.856155056804D+00
I= 32 X= 2.286547011496D+00 Y= 4.529565720356D+00 Z= -3.626678966166D+00
I= 33 X= 1.741701827477D+00 Y= 5.855997324008D+00 Z= 4.695824496039D-01
I= 34 X= 3.468109431421D+00 Y= 3.436104589822D+00 Z= 2.024737307602D+00
I= 35 X= 2.982325848931D-02 Y= 1.164101020810D+00 Z= -5.284568450407D-01
I= 36 X= -3.014680200110D+00 Y= 3.647020935162D+00 Z= 2.209793661190D-01
I= 37 X= -2.397140289455D+00 Y= 5.563887910905D+00 Z= 1.445320309322D+00
I= 38 X= -4.125949486592D+00 Y= 2.612323629607D+00 Z= 1.497480890600D+00

Forward Direction:

Total Energy: -692.0032706 Hartrees

Potential Energy: -692.1851276 Hartress

Kinetic Energy: 0.1818570 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.125313169281D+11 Y= -1.360893500191D+12 Z= -9.929315013529D+12

I= 1 X= -1.682544698830D+13 Y= -1.831868643385D+13 Z= -7.074628131122D+12

I= 2 X= -2.697038083571D+13 Y= -2.803463095728D+12 Z= -4.653593180261D+12

I= 3 X= 1.384168973560D+13 Y= 7.468435176937D+12 Z= 6.103493574063D+12

I= 4 X= 1.002430900690D+13 Y= -7.439574423959D+12 Z= 3.486420973235D+12

I= 5 X= 8.817453575437D+12 Y= 1.698401395803D+13 Z= -1.003212627591D+13
I= 6 X= 2.905580225960D+13 Y= 4.606440935276D+13 Z= 9.148135847122D+12
I= 7 X= -6.074485885981D+13 Y= -2.750807413111D+13 Z= 8.951028096099D+13
I= 8 X= 2.694655093055D+13 Y= -7.738824315679D+13 Z= -3.602457950760D+13
I= 9 X= -2.322751286592D+13 Y= -7.291520731316D+12 Z= -7.330696433512D+11
I= 10 X= -2.430283697173D+13 Y= 4.166664060983D+13 Z= 1.551213952750D+13
I= 11 X= 4.483214460948D+13 Y= 8.318896491476D+13 Z= -7.858818899579D+13
I= 12 X= -7.247365967775D+13 Y= 1.769723750986D+13 Z= 1.532175730904D+13
I= 13 X= -8.470128142228D+12 Y= -7.510921113228D+12 Z= 2.362561034300D+13
I= 14 X= 5.653193809976D+13 Y= 6.309351267423D+13 Z= -1.153078240381D+13
I= 15 X= -7.683640645937D+13 Y= -1.545973252629D+14 Z= -3.697503929232D+13
I= 16 X= 2.509595058916D+13 Y= -3.344670952231D+13 Z= -3.063323894498D+13
I= 17 X= -1.105425495016D+13 Y= 1.032884443134D+13 Z= 8.724732965420D+12
I= 18 X= 1.665071490572D+13 Y= 2.620874260504D+13 Z= 5.790501685012D+13
I= 19 X= 1.099904448698D+13 Y= -5.487278967571D+12 Z= 3.526708467393D+13
I= 20 X= 1.711749026106D+14 Y= 5.163382020648D+13 Z= 1.577560907263D+13
I= 21 X= 6.126325221856D+12 Y= 1.473434768971D+13 Z= 7.483158496744D+12
I= 22 X= 6.122010301406D+13 Y= -5.372505840732D+13 Z= 4.755181149384D+13
I= 23 X= -1.001209526649D+14 Y= 4.232683604358D+13 Z= -3.872110414171D+13
I= 24 X= 4.448952255063D+13 Y= -1.984000470743D+13 Z= 3.208724932212D+13
I= 25 X= 1.362347353520D+13 Y= -8.855716350626D+12 Z= 8.668212829424D+12
I= 26 X= -1.579307076992D+13 Y= -4.175912576150D+13 Z= -4.391792972607D+13
I= 27 X= -3.563735882400D+13 Y= -8.451386755007D+12 Z= 6.507121562217D+13
I= 28 X= 7.735106010511D+12 Y= 1.639208932170D+14 Z= -1.103366031142D+14
I= 29 X= 5.468385234915D+12 Y= 2.133117565888D+13 Z= -2.605124814691D+13
I= 30 X= -2.293346930145D+12 Y= 1.218752847436D+13 Z= -1.441814335678D+13
I= 31 X= -4.882644061956D+13 Y= 6.085733772578D+13 Z= -1.338985822288D+13
I= 32 X= -7.412494519137D+12 Y= -6.374888789175D+13 Z= -4.004992897604D+10
I= 33 X= 1.358235378116D+13 Y= -6.308015826020D+13 Z= 3.642537021666D+13
I= 34 X= 1.334662546299D+13 Y= -1.782251780636D+13 Z= 1.256453411203D+14

I= 35 X= 4.275921544010D+12 Y= -5.354937192889D+12 Z= 8.665092325497D+11
I= 36 X= -2.374464877652D+12 Y= -9.113784357815D+12 Z= -1.739989950401D+12
I= 37 X= 1.012206721143D+14 Y= 1.088828948832D+14 Z= -1.915981493979D+13
I= 38 X= -2.562365414925D+13 Y= -6.773556475088D+13 Z= 2.037122374956D+13

Backward Direction:

Total Energy: -692.0032895 Hartrees

Potential Energy: -692.1851276 Hartress

Kinetic Energy: 0.1818381 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.933590285417D+11 Y= -5.669333946111D+11 Z= -8.612826038133D+12
I= 1 X= -1.660662577235D+13 Y= -1.831849442930D+13 Z= -7.074742385231D+12
I= 2 X= -2.647400131402D+13 Y= -2.961486778832D+12 Z= -3.984450655487D+12
I= 3 X= 1.386098080643D+13 Y= 6.674408521414D+12 Z= 4.786832332909D+12
I= 4 X= 1.052076617610D+13 Y= -7.281466459629D+12 Z= 2.817325315303D+12
I= 5 X= 9.718693096858D+12 Y= 1.088889493972D+13 Z= -1.680270112614D+13
I= 6 X= -1.445487060568D+13 Y= 4.607226581432D+13 Z= 9.148479741824D+12
I= 7 X= -6.846499149777D+13 Y= -3.115282880244D+13 Z= 8.035710256201D+13
I= 8 X= 2.376162548323D+13 Y= -8.221255941463D+13 Z= -3.78622633267D+13
I= 9 X= -2.206605102176D+13 Y= -9.382255658706D+12 Z= -1.272020854967D+12
I= 10 X= -2.484120667651D+13 Y= 3.911469173490D+13 Z= 1.433578764992D+13
I= 11 X= 4.629759533966D+13 Y= 7.921183271650D+13 Z= -7.895262959079D+13
I= 12 X= -6.969670917838D+13 Y= 1.581503620066D+13 Z= 1.548337097768D+13
I= 13 X= -7.308758473348D+12 Y= -5.420165763849D+12 Z= 2.416489039355D+13
I= 14 X= 5.599447132128D+13 Y= 6.564578343939D+13 Z= -1.035390379931D+13
I= 15 X= -7.406001685259D+13 Y= -1.527142737590D+14 Z= -3.713678337095D+13
I= 16 X= 2.656089055392D+13 Y= -2.947074265450D+13 Z= -3.026800834890D+13
I= 17 X= -1.125776645908D+13 Y= 1.034840661213D+13 Z= 1.087751578921D+13
I= 18 X= 1.682086913195D+13 Y= 2.716114087789D+13 Z= 6.243842853054D+13
I= 19 X= 1.085018845890D+13 Y= -4.782752769264D+12 Z= 3.607902072638D+13
I= 20 X= 1.703436562781D+14 Y= 4.895338823771D+13 Z= 1.816996543888D+13

I= 21 X= 4.145654093780D+12 Y= 1.473529016707D+13 Z= 7.482525906503D+12
I= 22 X= 5.614001269425D+13 Y= -5.372406315795D+13 Z= 4.755005412657D+13
I= 23 X= -1.013412492757D+14 Y= 4.473739084326D+13 Z= -3.865066972249D+13
I= 24 X= 4.326898438840D+13 Y= -2.224795694545D+13 Z= 3.201595232160D+13
I= 25 X= 1.342019925288D+13 Y= -8.875702409989D+12 Z= 6.515361814079D+12
I= 26 X= -1.662387620978D+13 Y= -3.907930233506D+13 Z= -4.631251732268D+13
I= 27 X= -3.578584880102D+13 Y= -9.156826157335D+12 Z= 6.425957351756D+13
I= 28 X= 7.905355788761D+12 Y= 1.629677938309D+14 Z= -1.148699311122D+14
I= 29 X= 6.369249927852D+12 Y= 2.742444352879D+13 Z= -1.928242429716D+13
I= 30 X= -3.702565511069D+11 Y= 1.225876411389D+13 Z= -8.483101666873D+12
I= 31 X= -5.200971230431D+13 Y= 6.568036807488D+13 Z= -1.154981917416D+13
I= 32 X= -1.513107957435D+13 Y= -6.010385026128D+13 Z= 9.110172333754D+12
I= 33 X= 1.258843312061D+13 Y= -6.688545558239D+13 Z= 4.853963810095D+13
I= 34 X= 1.415666257287D+13 Y= -2.180467762572D+13 Z= 1.298516652543D+14
I= 35 X= 4.037368133533D+12 Y= -5.354709860076D+12 Z= 8.671801521898D+11
I= 36 X= -4.513572920984D+11 Y= -9.185770789454D+12 Z= -7.675402454833D+12
I= 37 X= 1.002246132218D+14 Y= 1.126904157323D+14 Z= -3.127521341369D+13
I= 38 X= -2.481340206948D+13 Y= -6.375509156113D+13 Z= 1.616485126418D+13

Seed: 20174731796

CM Start Point Coordinates: bohr

I= 0 X= -2.168324813609D+00 Y= -2.041649494363D+00 Z= -7.009223516568D-02
I= 1 X= 8.152271519496D-02 Y= -2.647735746731D+00 Z= -1.497838558762D+00
I= 2 X= -1.275340449663D+00 Y= -1.238824411257D+00 Z= 2.475896315601D+00
I= 3 X= 2.145945522645D+00 Y= -2.029917762066D+00 Z= -1.580004763360D-02
I= 4 X= 1.323247960975D+00 Y= -1.275108644818D+00 Z= 2.430359683430D+00
I= 5 X= -2.911300600462D+00 Y= 3.350493342651D+00 Z= -2.334829785667D+00
I= 6 X= -7.591233429867D-02 Y= 1.243059456475D+00 Z= -3.219883521103D+00
I= 7 X= -1.971036206943D+00 Y= 4.524172807930D+00 Z= -4.233870348006D+00
I= 8 X= -4.556679467795D+00 Y= 2.102409053187D+00 Z= -2.939968964747D+00

I= 9 X= 2.975607850967D+00 Y= -7.372793575267D-01 Z= 4.602362939815D+00
I= 10 X= 3.697223454941D+00 Y= -2.056912413837D+00 Z= 6.073977154312D+00
I= 11 X= 4.978645336106D+00 Y= -2.673005262482D-01 Z= 3.923880196226D+00
I= 12 X= 2.763564453600D+00 Y= 7.866872918215D-01 Z= 5.638586983359D+00
I= 13 X= -3.235644140922D+00 Y= -7.184195659082D-01 Z= 4.663853512095D+00
I= 14 X= -3.661433062493D+00 Y= -2.893759576421D+00 Z= 5.436028615477D+00
I= 15 X= -2.354684778106D+00 Y= 4.636657919565D-01 Z= 5.977158883866D+00
I= 16 X= -5.132346493473D+00 Y= 1.350640945231D-01 Z= 4.227375149752D+00
I= 17 X= -4.812241851991D+00 Y= -2.650120916952D+00 Z= -7.429912321438D-01
I= 18 X= -5.406406058483D+00 Y= -4.074125591034D+00 Z= 4.531048071501D-01
I= 19 X= -6.203131801038D+00 Y= -1.317409431982D+00 Z= -2.828142278544D-01
I= 20 X= -5.020760654034D+00 Y= -2.575335293337D+00 Z= -2.946450656457D+00
I= 21 X= -2.575417809608D-02 Y= -3.835017545425D+00 Z= -4.087004597097D+00
I= 22 X= -3.148112348620D-01 Y= -5.891919066406D+00 Z= -3.788234771352D+00
I= 23 X= -1.401819075365D+00 Y= -2.738991990084D+00 Z= -5.479794048123D+00
I= 24 X= 2.099692471072D+00 Y= -3.584988349887D+00 Z= -5.223912230492D+00
I= 25 X= 4.927584933986D+00 Y= -2.435759754869D+00 Z= -8.944264567373D-01
I= 26 X= 5.253642232922D+00 Y= -3.109993977833D+00 Z= -2.991512733334D+00
I= 27 X= 6.215837565006D+00 Y= -5.783861818558D-01 Z= -7.224584143015D-01
I= 28 X= 5.653242126243D+00 Y= -3.715968037029D+00 Z= 3.568438587208D-01
I= 29 X= 2.725004231349D+00 Y= 3.106754409628D+00 Z= -2.240338457746D+00
I= 30 X= 2.692068722549D+00 Y= 3.720066756793D+00 Z= 2.443967855398D-01
I= 31 X= 4.246176926245D+00 Y= 2.020997165989D+00 Z= -2.891458325152D+00
I= 32 X= 2.202313170953D+00 Y= 4.566397223459D+00 Z= -3.710316689356D+00
I= 33 X= 1.573708897716D+00 Y= 5.269660158864D+00 Z= 8.796755307619D-01
I= 34 X= 4.183794354401D+00 Y= 3.224643339394D+00 Z= 1.664878244612D+00
I= 35 X= -4.046023327031D-03 Y= 1.096112662909D+00 Z= -5.457137032165D-01
I= 36 X= -2.513359927775D+00 Y= 3.996064013140D+00 Z= 2.434535753112D-01
I= 37 X= -1.634901284488D+00 Y= 5.945963833840D+00 Z= 1.225727563286D+00
I= 38 X= -4.052130180470D+00 Y= 3.157432590097D+00 Z= 1.419106949250D+00

Forward Direction:

Total Energy: -692.0058009 Hartrees

Potential Energy: -692.1833603 Hartress

Kinetic Energy: 0.1775595 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.406982763924D+12 Y= 1.973789104289D+13 Z= -1.656312981034D+13
I= 1 X= 1.845173977157D+13 Y= -1.551596215212D+13 Z= -4.535306413173D+12
I= 2 X= -1.351952795690D+13 Y= 1.535199710891D+13 Z= 1.655801215526D+13
I= 3 X= 1.055718333370D+13 Y= 1.007671273535D+13 Z= 1.763349991855D+12
I= 4 X= -1.890852349502D+13 Y= 7.802460235044D+11 Z= 3.425924963631D+13
I= 5 X= -8.088687140620D+11 Y= 7.998416378647D+12 Z= 6.589538313971D+11
I= 6 X= 7.897629117682D+13 Y= 1.798406010624D+13 Z= 8.734997546069D+13
I= 7 X= 2.524577626451D+13 Y= 9.739688821823D+12 Z= -1.702919684828D+13
I= 8 X= -1.008042105899D+14 Y= 1.482249195393D+13 Z= -1.038516644000D+14
I= 9 X= -9.401155466781D+12 Y= -5.946476793934D+12 Z= -8.727702368519D+12
I= 10 X= -9.647813868933D+13 Y= -5.577730094547D+13 Z= 3.211790907920D+13
I= 11 X= 4.350028393928D+13 Y= 4.492828519098D+12 Z= 6.467988597488D+13
I= 12 X= -5.837773466074D+13 Y= 1.203739747392D+14 Z= 6.753338164245D+13
I= 13 X= 1.108088001060D+13 Y= 1.438245494642D+12 Z= -4.813971074314D+12
I= 14 X= 8.386850494239D+13 Y= -2.975982930086D+13 Z= -6.665042111461D+12
I= 15 X= 2.693844883281D+13 Y= -1.691718217808D+14 Z= -3.871286014210D+13
I= 16 X= -7.197163229842D+12 Y= 4.164562281401D+13 Z= -6.474763230191D+09
I= 17 X= 8.146127067500D+12 Y= 2.123109611147D+11 Z= -9.973186925651D+12
I= 18 X= -8.348699229014D+13 Y= -3.795517014786D+13 Z= 1.006393555881D+14
I= 19 X= -2.087000258046D+13 Y= 1.190168584375D+13 Z= 2.965171291053D+13
I= 20 X= 4.538670297295D+13 Y= 3.148018049436D+13 Z= -1.222971156555D+13
I= 21 X= -1.103486093184D+12 Y= 1.371104348589D+11 Z= -1.294271808926D+13
I= 22 X= -2.041883767095D+13 Y= -2.932063574129D+11 Z= 3.457687900787D+13
I= 23 X= -8.182233421313D+13 Y= -4.465585247995D+13 Z= -1.184473491809D+14
I= 24 X= 2.310851690911D+13 Y= 6.448032417794D+13 Z= 6.281403855383D+13

I= 25 X= 1.919475410007D+13 Y= -1.429141251279D+13 Z= 1.119491944787D+13
I= 26 X= -6.415860518789D+13 Y= 6.245550078239D+12 Z= -7.571054908981D+13
I= 27 X= 3.534856116688D+13 Y= -1.145908322870D+12 Z= 2.862031633553D+13
I= 28 X= -3.416650407723D+13 Y= 4.955558783391D+13 Z= 4.524929003500D+13
I= 29 X= 8.625435437941D+12 Y= -2.292267516116D+13 Z= 4.455559829061D+12
I= 30 X= -9.330492594347D+12 Y= 6.830234319126D+12 Z= -5.315266393751D+12
I= 31 X= -7.425240289102D+13 Y= 5.858527981202D+13 Z= -2.407267527500D+13
I= 32 X= 1.375104404978D+13 Y= 5.185808524596D+13 Z= -6.985787354275D+13
I= 33 X= 1.326840266472D+14 Y= -4.287494338680D+13 Z= 7.361410332821D+13
I= 34 X= 1.642799735945D+13 Y= 4.606826715217D+13 Z= -7.442379124027D+12
I= 35 X= -4.039947224431D+12 Y= -6.130368876970D+12 Z= -2.666926473081D+12
I= 36 X= 8.698577000683D+12 Y= 2.060587462076D+13 Z= 1.517875067009D+12
I= 37 X= -5.291750392454D+13 Y= -6.624746309846D+13 Z= -4.730817150405D+13
I= 38 X= -3.566710049721D+13 Y= -1.450313602160D+13 Z= -3.930017861562D+13

Backward Direction:

Total Energy: -692.0058041 Hartrees

Potential Energy: -692.1833603 Hartress

Kinetic Energy: 0.1775563 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.643673653808D+12 Y= 2.137456604405D+13 Z= -1.442464454473D+13
I= 1 X= 2.011060274008D+13 Y= -1.551572197381D+13 Z= -4.535403382069D+12
I= 2 X= -1.330235112711D+13 Y= 1.395555478586D+13 Z= 1.781261886998D+13
I= 3 X= 1.079400152428D+13 Y= 8.439860237441D+12 Z= -3.754372156407D+11
I= 4 X= -1.869125457800D+13 Y= 2.176817118968D+12 Z= 3.300456877059D+13
I= 5 X= 3.030336572113D+12 Y= 3.185716944083D+11 Z= -9.386934854329D+12
I= 6 X= -4.408047169082D+13 Y= 1.799973935367D+13 Z= 8.734940462562D+13
I= 7 X= 9.767316437161D+12 Y= 1.277129785120D+13 Z= -2.713866208118D+13
I= 8 X= -1.098485955225D+14 Y= 1.618084153274D+13 Z= -1.067547040171D+14
I= 9 X= -8.374413413214D+12 Y= -7.857216254821D+12 Z= -9.579886418309D+12
I= 10 X= -9.756390670149D+13 Y= -5.848591418915D+13 Z= 3.021185442739D+13

I= 11 X= 4.492702074734D+13 Y= 4.066571099545D+11 Z= 6.422048907370D+13
I= 12 X= -5.547092762967D+13 Y= 1.185209465052D+14 Z= 6.783589987058D+13
I= 13 X= 1.210747026307D+13 Y= 3.349006882243D+12 Z= -3.961519615155D+12
I= 14 X= 8.278348411650D+13 Y= -2.705098269091D+13 Z= -4.758653589303D+12
I= 15 X= 2.984465199966D+13 Y= -1.673179176143D+14 Z= -3.901550035444D+13
I= 16 X= -5.770999256595D+12 Y= 4.573060908962D+13 Z= 4.537051416493D+11
I= 17 X= 8.264617681229D+12 Y= 4.990854764179D+11 Z= -7.795847029202D+12
I= 18 X= -8.258196314930D+13 Y= -3.709883506384D+13 Z= 1.047484236929D+14
I= 19 X= -2.125881311060D+13 Y= 1.230466789058D+13 Z= 3.072045791809D+13
I= 20 X= 4.509483756000D+13 Y= 2.927681237877D+13 Z= -9.861426723231D+12
I= 21 X= -2.817257150622D+12 Y= 1.381555023139D+11 Z= -1.294342163103D+13
I= 22 X= -2.491820435905D+13 Y= -2.921366446726D+11 Z= 3.457487287158D+13
I= 23 X= -8.312952018862D+13 Y= -4.260822873291D+13 Z= -1.180099373427D+14
I= 24 X= 2.180094638674D+13 Y= 6.243578202765D+13 Z= 6.237535086751D+13
I= 25 X= 1.931339153481D+13 Y= -1.457852857654D+13 Z= 9.017557432181D+12
I= 26 X= -6.444998415262D+13 Y= 8.447925418318D+12 Z= -7.807892698271D+13
I= 27 X= 3.495994845783D+13 Y= -1.549594602048D+12 Z= 2.755170328314D+13
I= 28 X= -3.326165973577D+13 Y= 4.869880835869D+13 Z= 4.114084947436D+13
I= 29 X= 1.246435135376D+13 Y= -1.524550844962D+13 Z= 1.449950197429D+13
I= 30 X= -4.298093746556D+12 Y= 8.936039641514D+12 Z= 4.397916731237D+11
I= 31 X= -8.329094015565D+13 Y= 5.722889280689D+13 Z= -2.117070404226D+13
I= 32 X= -1.726670633958D+12 Y= 4.882554113337D+13 Z= -5.975258840938D+13
I= 33 X= 1.314032785075D+14 Y= -4.682314541455D+13 Z= 8.692995484945D+13
I= 34 X= 1.612403587487D+13 Y= 4.133172049406D+13 Z= -9.347625925432D+11
I= 35 X= -5.292830108055D+12 Y= -6.130152729994D+12 Z= -2.666113474553D+12
I= 36 X= 1.373158604502D+13 Y= 1.849901872060D+13 Z= -4.237494233137D+12
I= 37 X= -5.419999154350D+13 Y= -6.229633012199D+13 Z= -6.062648966081D+13
I= 38 X= -3.596950060276D+13 Y= -9.767322611115D+12 Z= -4.580745722822D+13

Seed: 20322869887

CM Start Point Coordinates: bohr

I= 0 X= -2.112556852302D+00 Y= -2.222868034873D+00 Z= 3.460053347423D-02
I= 1 X= -4.226953316994D-02 Y= -2.944512872710D+00 Z= -1.395826804070D+00
I= 2 X= -1.319494915994D+00 Y= -1.281159399250D+00 Z= 2.283085525340D+00
I= 3 X= 2.093396897747D+00 Y= -2.017142403527D+00 Z= -1.764383135259D-02
I= 4 X= 1.290697225399D+00 Y= -1.184115474622D+00 Z= 2.347062142844D+00
I= 5 X= -2.542957059010D+00 Y= 3.518247214385D+00 Z= -2.211856008225D+00
I= 6 X= 2.194232491915D-01 Y= 1.678550295321D+00 Z= -3.051570795859D+00
I= 7 X= -1.744375042572D+00 Y= 4.905091619186D+00 Z= -3.580513311040D+00
I= 8 X= -4.139816901414D+00 Y= 2.347330920217D+00 Z= -3.163648090598D+00
I= 9 X= 2.818709386445D+00 Y= -6.757993860653D-01 Z= 4.633088135151D+00
I= 10 X= 2.038931829357D+00 Y= -1.826620661137D+00 Z= 6.215725671345D+00
I= 11 X= 4.980298959927D+00 Y= -1.173230242270D+00 Z= 4.490406576089D+00
I= 12 X= 2.205771041434D+00 Y= 1.608723069422D+00 Z= 5.077555034907D+00
I= 13 X= -2.853709270721D+00 Y= -3.753860778174D-01 Z= 4.516994223883D+00
I= 14 X= -3.282123580896D+00 Y= -2.182102335416D+00 Z= 5.355550688459D+00
I= 15 X= -1.902869382277D+00 Y= 8.697313699495D-01 Z= 5.822653706684D+00
I= 16 X= -4.723515536402D+00 Y= 1.052485959189D+00 Z= 4.011667094343D+00
I= 17 X= -4.829551936348D+00 Y= -2.652868588953D+00 Z= -9.797091955842D-01
I= 18 X= -5.651292399522D+00 Y= -4.397889594221D+00 Z= -9.785264627216D-02
I= 19 X= -6.525942889818D+00 Y= -1.028125410343D+00 Z= -5.247381028788D-01
I= 20 X= -4.769692162878D+00 Y= -3.315223573426D+00 Z= -2.997221145502D+00
I= 21 X= -7.296102449313D-02 Y= -4.180401075472D+00 Z= -3.966436530403D+00
I= 22 X= -4.349535519585D-01 Y= -6.271544586654D+00 Z= -4.199077394134D+00
I= 23 X= -1.578800067393D+00 Y= -3.130398823925D+00 Z= -5.460204182921D+00
I= 24 X= 2.158315172078D+00 Y= -4.065284353312D+00 Z= -4.524550673255D+00
I= 25 X= 4.787538054512D+00 Y= -2.126377123442D+00 Z= -1.073512885692D+00
I= 26 X= 4.860461208880D+00 Y= -2.060471958973D+00 Z= -3.103772945407D+00
I= 27 X= 6.131650769868D+00 Y= -5.959280595629D-01 Z= -4.971031169964D-01
I= 28 X= 5.734292812008D+00 Y= -4.064146613802D+00 Z= -3.432179459847D-01

I= 29 X= 2.721529370004D+00 Y= 3.498729264066D+00 Z= -2.305285099849D+00
I= 30 X= 2.945579426451D+00 Y= 3.838090764626D+00 Z= 3.931674579551D-01
I= 31 X= 4.018845184733D+00 Y= 1.872952380033D+00 Z= -3.225638499560D+00
I= 32 X= 1.734236379435D+00 Y= 4.844927214080D+00 Z= -3.372418252346D+00
I= 33 X= 2.017018649701D+00 Y= 5.683231559956D+00 Z= 1.398615976079D+00
I= 34 X= 4.144204708579D+00 Y= 2.375148435743D+00 Z= 1.429365293132D+00
I= 35 X= -2.976383444597D-02 Y= 1.017644222893D+00 Z= -5.507438789905D-01
I= 36 X= -2.656740623719D+00 Y= 3.695762706834D+00 Z= 5.428523548419D-01
I= 37 X= -1.901430953597D+00 Y= 5.218604111173D+00 Z= 1.652896166054D+00
I= 38 X= -4.553519057474D+00 Y= 2.988327164524D+00 Z= 1.546156487539D+00

Forward Direction:

Total Energy: -691.9974894 Hartrees

Potential Energy: -692.1655482 Hartress

Kinetic Energy: 0.1680589 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.432672940831D+13 Y= 2.356158018510D+12 Z= -9.981265124083D+12
I= 1 X= 2.553649937305D+12 Y= 7.059151307589D+12 Z= 2.153632239425D+13
I= 2 X= 1.372880520937D+13 Y= 1.606984324270D+12 Z= -1.598546571266D+13
I= 3 X= 1.174800824430D+13 Y= -2.772407628000D+12 Z= 1.139739530362D+13
I= 4 X= -1.187036986664D+13 Y= 1.152692152952D+13 Z= 4.909978831517D+12
I= 5 X= 7.790225390921D+12 Y= 1.100363620552D+13 Z= 3.280655565960D+12
I= 6 X= 7.472029401966D+13 Y= -4.651296312172D+13 Z= -1.510242228682D+13
I= 7 X= -2.964840011659D+12 Y= -3.777083147048D+13 Z= 1.481433960086D+13
I= 8 X= -2.600372767529D+13 Y= -2.943270473878D+13 Z= 2.871191911026D+13
I= 9 X= 7.865744237474D+12 Y= -4.783262166787D+12 Z= -3.523781689740D+12
I= 10 X= -3.419835593956D+13 Y= -6.311013461447D+13 Z= 5.160471282681D+13
I= 11 X= -4.612179744243D+12 Y= 2.405754774259D+13 Z= -7.984953740899D+12
I= 12 X= -6.113797875554D+13 Y= 1.543275035130D+14 Z= 6.521511220751D+13
I= 13 X= -1.937774262889D+13 Y= 5.127105004152D+12 Z= 2.810885489751D+12
I= 14 X= 6.030685613271D+13 Y= 1.640520442324D+13 Z= 4.899336220901D+13

I= 15 X= 6.677882623045D+13 Y= -2.286643867884D+13 Z= -7.606561784294D+13
I= 16 X= 8.957431870112D+13 Y= 4.581342673020D+13 Z= -5.191768739159D+13
I= 17 X= 2.901519219774D+13 Y= 8.207603859110D+11 Z= 3.069451437428D+12
I= 18 X= 1.742831412586D+13 Y= -9.061362679506D+12 Z= -5.388887726987D+13
I= 19 X= -4.698445355452D+13 Y= 7.896523234785D+13 Z= 4.460785927424D+13
I= 20 X= -5.455654125056D+13 Y= -3.572075870052D+13 Z= 4.557124190649D+13
I= 21 X= -5.673718818353D+12 Y= 1.395097436557D+13 Z= -5.741591975060D+12
I= 22 X= 2.778453087296D+13 Y= -7.858436766848D+13 Z= 5.216351756441D+13
I= 23 X= 4.435143374990D+13 Y= -4.019652508049D+13 Z= 1.653943130961D+13
I= 24 X= 5.381251530809D+12 Y= 1.771189979649D+13 Z= -6.947982623787D+13
I= 25 X= 2.156660104450D+13 Y= -2.351967433993D+13 Z= 9.050748642933D+12
I= 26 X= 8.003553661101D+12 Y= 4.315215640651D+13 Z= -9.093522876268D+13
I= 27 X= -5.374751038822D+13 Y= 2.532161068118D+13 Z= -2.777989538477D+13
I= 28 X= -1.341253082088D+13 Y= 9.146977442324D+13 Z= 6.508270568119D+12
I= 29 X= -6.331501052258D+12 Y= -9.585779113082D+12 Z= 1.988491867383D+13
I= 30 X= -9.372177802163D+12 Y= -4.166146335815D+12 Z= -5.581393161130D+12
I= 31 X= 1.102447505508D+13 Y= -9.809113302636D+13 Z= -4.293446536304D+13
I= 32 X= -7.353698013233D+12 Y= 6.761069502862D+13 Z= -1.079196749996D+14
I= 33 X= 2.993841925521D+13 Y= 6.134228253143D+13 Z= -3.715043273339D+12
I= 34 X= 1.182351180281D+14 Y= -2.614103860463D+13 Z= 2.703103105150D+13
I= 35 X= -7.362996245466D+12 Y= -4.484767989603D+12 Z= -8.045365618980D+12
I= 36 X= 1.071456049106D+13 Y= 4.519998271771D+12 Z= 9.734129432676D+12
I= 37 X= -6.022084422190D+13 Y= -4.683963222880D+13 Z= -6.735967244322D+13
I= 38 X= 2.753443284054D+13 Y= 1.389180884836D+13 Z= 1.496282438909D+14

Backward Direction:

Total Energy: -691.9974753 Hartrees

Potential Energy: -692.1655482 Hartress

Kinetic Energy: 0.1680729 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.414075656550D+13 Y= 3.998206687415D+12 Z= -7.685496925941D+12

I= 1 X= 3.902519308914D+12 Y= 7.059432918042D+12 Z= 2.153618891582D+13
I= 2 X= 1.415721690446D+13 Y= 4.855924600303D+11 Z= -1.469415365867D+13
I= 3 X= 1.193413950815D+13 Y= -4.414623848266D+12 Z= 9.101310280738D+12
I= 4 X= -1.144184802866D+13 Y= 1.264845433401D+13 Z= 3.618636973047D+12
I= 5 X= 1.112455241289D+13 Y= 2.022831869915D+12 Z= -7.819669113203D+12
I= 6 X= -4.002684775853D+13 Y= -4.649709758224D+13 Z= -1.510266076048D+13
I= 7 X= -1.860795904916D+13 Y= -3.748331786322D+13 Z= 2.384079969673D+12
I= 8 X= -3.443037181525D+13 Y= -3.102199089183D+13 Z= 2.556603084278D+13
I= 9 X= 9.253012068554D+12 Y= -7.326858962172D+12 Z= -4.446358820227D+12
I= 10 X= -3.529396512679D+13 Y= -6.649415192383D+13 Z= 4.955688133261D+13
I= 11 X= -2.764409046757D+12 Y= 1.888393504057D+13 Z= -8.522085764610D+12
I= 12 X= -5.748574265252D+13 Y= 1.519390058138D+14 Z= 6.552662426186D+13
I= 13 X= -1.799063707263D+13 Y= 7.670729080163D+12 Z= 3.733838099639D+12
I= 14 X= 5.921228758565D+13 Y= 1.978956807359D+13 Z= 5.104172515146D+13
I= 15 X= 7.043031218175D+13 Y= -2.047683333126D+13 Z= -7.637729071504D+13
I= 16 X= 9.142138939613D+13 Y= 5.098553251031D+13 Z= -5.137954894698D+13
I= 17 X= 2.899355809557D+13 Y= 1.044110823177D+12 Z= 5.844300761819D+12
I= 18 X= 1.819155369668D+13 Y= -7.913112696375D+12 Z= -4.839878075383D+13
I= 19 X= -4.735313511296D+13 Y= 7.964359424024D+13 Z= 4.583811882459D+13
I= 20 X= -5.522066684874D+13 Y= -3.879900134759D+13 Z= 4.861785293086D+13
I= 21 X= -8.011886769547D+12 Y= 1.395225732896D+13 Z= -5.742454659131D+12
I= 22 X= 2.171046731070D+13 Y= -7.858303799925D+13 Z= 5.216108265566D+13
I= 23 X= 4.272436987708D+13 Y= -3.737915932053D+13 Z= 1.690195996011D+13
I= 24 X= 3.753772228231D+12 Y= 1.489822208146D+13 Z= -6.984376610470D+13
I= 25 X= 2.154520364217D+13 Y= -2.374350634514D+13 Z= 6.275846180467D+12
I= 26 X= 7.340026455342D+12 Y= 4.622933471144D+13 Z= -9.398203309097D+13
I= 27 X= -5.411584847125D+13 Y= 2.464223402034D+13 Z= -2.900989896184D+13
I= 28 X= -1.264937667787D+13 Y= 9.032081649309D+13 Z= 1.018685159212D+12
I= 29 X= -2.997590573709D+12 Y= -6.079587654357D+11 Z= 3.098285609264D+13
I= 30 X= -4.602221766448D+12 Y= -2.565053962911D+12 Z= 1.884823793712D+12

I= 31 X= 2.603060868511D+12 Y= -9.650108273005D+13 Z= -3.979023552846D+13
I= 32 X= -2.299543085500D+13 Y= 6.732263980454D+13 Z= -9.549410898337D+13
I= 33 X= 2.845285221704D+13 Y= 5.636357143042D+13 Z= 1.268891073932D+13
I= 34 X= 1.184456555237D+14 Y= -3.180000838160D+13 Z= 3.412501676417D+13
I= 35 X= -8.421207009973D+12 Y= -4.484485189672D+12 Z= -8.044401071722D+12
I= 36 X= 1.548497862989D+13 Y= 2.917722040551D+12 Z= 2.267481868350D+12
I= 37 X= -6.170885332832D+13 Y= -4.185754891760D+13 Z= -8.376606567534D+13
I= 38 X= 2.774624478874D+13 Y= 1.954932641677D+13 Z= 1.425344829349D+14

Seed: 20399373177

CM Start Point Coordinates: bohr

I= 0 X= -2.205536532425D+00 Y= -2.174543592546D+00 Z= -3.414297990478D-02
I= 1 X= -1.001898991525D-03 Y= -2.511480408030D+00 Z= -1.550819032230D+00
I= 2 X= -1.212102010364D+00 Y= -1.245848979232D+00 Z= 2.462671797427D+00
I= 3 X= 2.226092245969D+00 Y= -1.960312043814D+00 Z= -1.407366304408D-01
I= 4 X= 1.347538835513D+00 Y= -1.296107692351D+00 Z= 2.531631819237D+00
I= 5 X= -3.070999854978D+00 Y= 3.290980252313D+00 Z= -2.378298210120D+00
I= 6 X= 6.822557701365D-02 Y= 1.006070114143D+00 Z= -3.589039477292D+00
I= 7 X= -2.180685343046D+00 Y= 4.645617314520D+00 Z= -3.446153684678D+00
I= 8 X= -4.324026493138D+00 Y= 1.860175005889D+00 Z= -3.456151271359D+00
I= 9 X= 3.039547642782D+00 Y= -8.790934587435D-01 Z= 4.556565670167D+00
I= 10 X= 2.511477205453D+00 Y= -1.910293069643D+00 Z= 6.413498505969D+00
I= 11 X= 4.881094363802D+00 Y= -1.266151892968D+00 Z= 3.873766806578D+00
I= 12 X= 2.899365712780D+00 Y= 1.009502851210D+00 Z= 5.163150805176D+00
I= 13 X= -2.806940373181D+00 Y= -4.783772910366D-01 Z= 4.768194581071D+00
I= 14 X= -2.414702630160D+00 Y= -1.567468030405D+00 Z= 6.679046603481D+00
I= 15 X= -2.189874718918D+00 Y= 1.651958119922D+00 Z= 5.330875710737D+00
I= 16 X= -4.769360415554D+00 Y= -7.514436063713D-01 Z= 4.358067374809D+00
I= 17 X= -4.824211584999D+00 Y= -2.743800936386D+00 Z= -6.832842537387D-01
I= 18 X= -5.254707803493D+00 Y= -4.705370928111D+00 Z= 2.084454889721D-01

I= 19 X= -6.317419077299D+00 Y= -1.763461857270D+00 Z= -1.342669689300D-01
I= 20 X= -5.522347177274D+00 Y= -3.099848582675D+00 Z= -2.683177570707D+00
I= 21 X= -1.410184104384D-02 Y= -3.303176959022D+00 Z= -4.332108060323D+00
I= 22 X= 6.909331336698D-01 Y= -5.627992327963D+00 Z= -4.470840880553D+00
I= 23 X= -2.186980440708D+00 Y= -3.002438238269D+00 Z= -4.948101807820D+00
I= 24 X= 1.382092452915D+00 Y= -1.785917451872D+00 Z= -5.124738354632D+00
I= 25 X= 4.902725587360D+00 Y= -2.893692062417D+00 Z= -5.889342920741D-01
I= 26 X= 5.416125533736D+00 Y= -4.049543156533D+00 Z= -2.562168449162D+00
I= 27 X= 6.222329614564D+00 Y= -1.183561710730D+00 Z= -2.407626030547D-01
I= 28 X= 5.532882274920D+00 Y= -4.276673948920D+00 Z= 1.303572019942D+00
I= 29 X= 3.334102503416D+00 Y= 3.144352740761D+00 Z= -2.237387008089D+00
I= 30 X= 2.703003933553D+00 Y= 3.811967118644D+00 Z= 2.487195537554D-01
I= 31 X= 4.689855857168D+00 Y= 1.807673424905D+00 Z= -2.702696789421D+00
I= 32 X= 2.775853188439D+00 Y= 4.138303098207D+00 Z= -3.801734953484D+00
I= 33 X= 1.959459838177D+00 Y= 5.540236685964D+00 Z= 8.790440000680D-01
I= 34 X= 3.708959080470D+00 Y= 3.146843372118D+00 Z= 1.986709018149D+00
I= 35 X= -8.492208389154D-02 Y= 1.158097890233D+00 Z= -5.781378489283D-01
I= 36 X= -3.065942357453D+00 Y= 3.707909745793D+00 Z= 1.228092581866D-01
I= 37 X= -2.525812421484D+00 Y= 5.869010359378D+00 Z= 8.349558436373D-01
I= 38 X= -4.280144454068D+00 Y= 2.453608900748D+00 Z= 1.252829931699D+00

Forward Direction:

Total Energy: -691.9920494 Hartrees

Potential Energy: -692.1681987 Hartress

Kinetic Energy: 0.1761493 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.871725426739D+12 Y= -2.256859121715D+10 Z= 2.028408654124D+12

I= 1 X= -2.096713540073D+13 Y= 1.448952981437D+13 Z= -6.951690440609D+12

I= 2 X= 1.668416899303D+13 Y= -1.839805553407D+13 Z= 1.779140027595D+12

I= 3 X= -4.321031111782D+12 Y= -2.970303007852D+12 Z= 7.256897268938D+12

I= 4 X= -1.924646141541D+13 Y= 3.537966017540D+12 Z= -1.484393864737D+13

I= 5 X= 9.038668945610D+12 Y= 1.056453429672D+13 Z= -5.006220790223D+12
I= 6 X= 7.461920035264D+13 Y= 2.031948099949D+13 Z= 2.221916654875D+13
I= 7 X= 2.031486142423D+13 Y= 7.410469034979D+13 Z= -1.524360445646D+13
I= 8 X= -8.791168884362D+13 Y= -1.046128157928D+14 Z= 9.548049556379D+13
I= 9 X= 2.208558788734D+12 Y= -1.965355068445D+13 Z= -4.827585267402D+12
I= 10 X= 4.891634358679D+13 Y= 1.371285489262D+14 Z= -6.299423062081D+13
I= 11 X= 2.210488945272D+13 Y= 2.945333458907D+13 Z= -1.488714731902D+13
I= 12 X= -4.949988538510D+13 Y= -4.269778453190D+13 Z= 4.803815999173D+13
I= 13 X= 1.266659093180D+13 Y= 9.756969285244D+12 Z= 1.198006486800D+13
I= 14 X= -5.341241426005D+13 Y= -1.805093171917D+13 Z= -1.783091932981D+13
I= 15 X= -2.545981879031D+13 Y= 2.461845291030D+13 Z= -4.445788052508D+13
I= 16 X= -1.096571777039D+14 Y= -5.949436570556D+13 Z= 1.084299286778D+13
I= 17 X= 2.158892848560D+13 Y= 2.763367565758D+13 Z= 2.358619599590D+13
I= 18 X= 5.221183136800D+13 Y= 2.881464212260D+13 Z= -6.951457202216D+13
I= 19 X= -5.463030879376D+13 Y= -1.769544164968D+13 Z= -8.323264585443D+13
I= 20 X= -5.214744751953D+13 Y= 6.781924423466D+13 Z= 7.843860440320D+13
I= 21 X= -1.626889003330D+13 Y= -1.050090486563D+13 Z= 3.769755057290D+12
I= 22 X= -1.219841412048D+13 Y= 3.273974865547D+13 Z= -3.900118718828D+13
I= 23 X= 5.432077087159D+13 Y= -1.897344495662D+13 Z= -2.641371855369D+13
I= 24 X= 1.754198794166D+13 Y= 4.634283533634D+13 Z= 2.129906674105D+13
I= 25 X= 3.586650114516D+12 Y= 8.426210277141D+12 Z= 5.194546529508D+12
I= 26 X= -2.347028209318D+13 Y= -1.112741374388D+13 Z= -8.617400698680D+13
I= 27 X= -6.225065532512D+13 Y= -1.509344988368D+14 Z= -7.542116373697D+13
I= 28 X= -2.046369776600D+12 Y= 6.181933166433D+13 Z= -1.091596252548D+13
I= 29 X= 2.637673836968D+12 Y= -1.118880274441D+13 Z= 6.001147621240D+12
I= 30 X= -2.654287978355D+12 Y= 2.008947123312D+12 Z= -2.262920605722D+13
I= 31 X= 1.608996689176D+13 Y= 2.991179121731D+13 Z= 4.140288931172D+13
I= 32 X= -2.523668137911D+13 Y= -6.505214128498D+13 Z= -2.580069350039D+13
I= 33 X= 5.335648572641D+12 Y= 6.475128467923D+13 Z= 1.666832728074D+13
I= 34 X= 8.457972509480D+13 Y= -2.058184242061D+13 Z= -2.514784685236D+13

I= 35 X= 3.993877422958D+12 Y= -2.756770120505D+12 Z= 4.580486805432D+12
I= 36 X= -1.671604000820D+13 Y= -2.932936261382D+13 Z= -1.129310328925D+13
I= 37 X= 7.043837196062D+13 Y= 1.292972542259D+14 Z= 1.666720829099D+13
I= 38 X= 2.024471842029D+13 Y= 1.095947474294D+14 Z= 2.523035887127D+13

Backward Direction:

Total Energy: -691.9920392 Hartrees

Potential Energy: -692.1681987 Hartrees

Kinetic Energy: 0.1761595 Hartrees

CM Start Point Velocity: bohr/s

I= 0 X= -1.595918269800D+12 Y= 1.146372876052D+12 Z= 3.244233011100D+12
I= 1 X= -1.912838464136D+13 Y= 1.448961708933D+13 Z= -6.951684692266D+12
I= 2 X= 1.640283205959D+13 Y= -1.997515147565D+13 Z= 2.607645031942D+12
I= 3 X= -4.045196675236D+12 Y= -4.139393093635D+12 Z= 6.040886016244D+12
I= 4 X= -1.952776938421D+13 Y= 5.115129597958D+12 Z= -1.567258913009D+13
I= 5 X= 1.285352877664D+13 Y= 7.724297448016D+12 Z= -1.006351866047D+13
I= 6 X= -3.133497450625D+13 Y= 2.033040003312D+13 Z= 2.221806594032D+13
I= 7 X= 9.495886980662D+12 Y= 8.197954074495D+13 Z= -1.772136111445D+13
I= 8 X= -9.571359193048D+13 Y= -9.752245115220D+13 Z= 9.389080178629D+13
I= 9 X= 2.201431783036D+12 Y= -1.971921635224D+13 Z= -5.296093391041D+12
I= 10 X= 4.815388117333D+13 Y= 1.365758037376D+14 Z= -6.407461380636D+13
I= 11 X= 2.226072440007D+13 Y= 2.876156181544D+13 Z= -1.505722510562D+13
I= 12 X= -4.894941181987D+13 Y= -4.292374112673D+13 Z= 4.823763709768D+13
I= 13 X= 1.265937621931D+13 Y= 9.822639695272D+12 Z= 1.244854168082D+13
I= 14 X= -5.417494627737D+13 Y= -1.749825274546D+13 Z= -1.675070496260D+13
I= 15 X= -2.490947735710D+13 Y= 2.484456046266D+13 Z= -4.465736522596D+13
I= 16 X= -1.095014919725D+14 Y= -5.880278029600D+13 Z= 1.101317203407D+13
I= 17 X= 2.196486593529D+13 Y= 2.797193629435D+13 Z= 2.391736935824D+13
I= 18 X= 5.315833315655D+13 Y= 2.882688892590D+13 Z= -6.941494689415D+13
I= 19 X= -5.495238072619D+13 Y= -1.797579303000D+13 Z= -8.279690307239D+13
I= 20 X= -5.158612941987D+13 Y= 6.804433011979D+13 Z= 7.873990687460D+13

I= 21 X= -1.621007671683D+13 Y= -1.050064458511D+13 Z= 3.769577709222D+12
I= 22 X= -1.217794494446D+13 Y= 3.273998098154D+13 Z= -3.900174470883D+13
I= 23 X= 5.404142093225D+13 Y= -1.909286824775D+13 Z= -2.594308822446D+13
I= 24 X= 1.726242475273D+13 Y= 4.646322315378D+13 Z= 2.082779713244D+13
I= 25 X= 3.962507182263D+12 Y= 8.087993883081D+12 Z= 4.863421577946D+12
I= 26 X= -2.290884509293D+13 Y= -1.135306696972D+13 Z= -8.647516824651D+13
I= 27 X= -6.257288722527D+13 Y= -1.506540122023D+14 Z= -7.585706864391D+13
I= 28 X= -1.100206801788D+12 Y= 6.180730975965D+13 Z= -1.101489312248D+13
I= 29 X= 6.452588649271D+12 Y= -8.349862400324D+12 Z= 1.105795568262D+13
I= 30 X= 1.518282162743D+12 Y= 4.573641153793D+12 Z= -2.202720105787D+13
I= 31 X= 8.293560684776D+12 Y= 2.282532617670D+13 Z= 4.299303608315D+13
I= 32 X= -3.605644749172D+13 Y= -7.292848164657D+13 Z= -2.332488614537D+13
I= 33 X= 4.836823595262D+12 Y= 6.404096079250D+13 Z= 1.986720232247D+13
I= 34 X= 8.329391560864D+13 Y= -2.208466274008D+13 Z= -2.167134427721D+13
I= 35 X= 2.686929559214D+12 Y= -2.756752444350D+12 Z= 4.580758821047D+12
I= 36 X= -1.254272283412D+13 Y= -3.189453785533D+13 Z= -1.189508518251D+13
I= 37 X= 6.993974938425D+13 Y= 1.300087765961D+14 Z= 1.346649788841D+13
I= 38 X= 1.896062959145D+13 Y= 1.110985295587D+14 Z= 2.175433458083D+13

Seed: 2072860618

CM Start Point Coordinates: bohr

I= 0 X= -2.133146837334D+00 Y= -2.223875736280D+00 Z= -5.787351947337D-02
I= 1 X= 6.155047539833D-02 Y= -2.733664351652D+00 Z= -1.505024034405D+00
I= 2 X= -1.388729889207D+00 Y= -1.250143384885D+00 Z= 2.443751685296D+00
I= 3 X= 2.226238595420D+00 Y= -2.089162072569D+00 Z= -2.198389253862D-02
I= 4 X= 1.296903024544D+00 Y= -1.321652955337D+00 Z= 2.419257668252D+00
I= 5 X= -2.931163577911D+00 Y= 3.230242185956D+00 Z= -2.214978469288D+00
I= 6 X= 4.691447211026D-03 Y= 1.275663442975D+00 Z= -3.638086145957D+00
I= 7 X= -2.272122651736D+00 Y= 4.764363583520D+00 Z= -3.558207918652D+00
I= 8 X= -4.029831410215D+00 Y= 1.823954391577D+00 Z= -3.056333490415D+00

I= 9 X= 2.852128191562D+00 Y= -8.086938094677D-01 Z= 4.697632436175D+00
I= 10 X= 2.509631537636D+00 Y= -2.457717123734D+00 Z= 5.940185274904D+00
I= 11 X= 4.724326642189D+00 Y= -4.634303713604D-01 Z= 3.984736820766D+00
I= 12 X= 2.509278377441D+00 Y= 6.620792959220D-01 Z= 6.249358811360D+00
I= 13 X= -2.678474680525D+00 Y= -5.134782652219D-01 Z= 4.832440126951D+00
I= 14 X= -2.789494503705D+00 Y= -2.230777807142D+00 Z= 6.428108046946D+00
I= 15 X= -1.733916785679D+00 Y= 1.120689249831D+00 Z= 5.866075491584D+00
I= 16 X= -4.493330723969D+00 Y= 1.127385936716D-01 Z= 4.590884110731D+00
I= 17 X= -4.767121636119D+00 Y= -2.361549490209D+00 Z= -9.435232705887D-01
I= 18 X= -5.881165871063D+00 Y= -4.562750414036D+00 Z= -1.037819587199D+00
I= 19 X= -6.073609284398D+00 Y= -1.136641133346D+00 Z= 4.184608675771D-01
I= 20 X= -5.168628853753D+00 Y= -1.521734438392D+00 Z= -3.215783827541D+00
I= 21 X= -1.113115611889D-01 Y= -3.803742088359D+00 Z= -3.986825929357D+00
I= 22 X= -4.777899061972D-01 Y= -5.985055533930D+00 Z= -3.687472898217D+00
I= 23 X= -1.539769178746D+00 Y= -3.172294475188D+00 Z= -5.157466420545D+00
I= 24 X= 1.896802364720D+00 Y= -3.835845173428D+00 Z= -4.981485355494D+00
I= 25 X= 4.955382369079D+00 Y= -2.540294864382D+00 Z= -6.976608781265D-01
I= 26 X= 4.867058778224D+00 Y= -1.974046211531D+00 Z= -2.911049703759D+00
I= 27 X= 6.341058790483D+00 Y= -1.306154421623D+00 Z= 6.527235729879D-01
I= 28 X= 5.603082391898D+00 Y= -4.596231625375D+00 Z= -7.460654063154D-01
I= 29 X= 3.080049576938D+00 Y= 3.335172357239D+00 Z= -2.256793240526D+00
I= 30 X= 2.748512637675D+00 Y= 3.956784153213D+00 Z= 2.271410045579D-01
I= 31 X= 4.285707910957D+00 Y= 2.107574211832D+00 Z= -3.080205696177D+00
I= 32 X= 2.459273275258D+00 Y= 4.745336777714D+00 Z= -3.532636059935D+00
I= 33 X= 2.116521418381D+00 Y= 5.686819457402D+00 Z= 8.149289122906D-01
I= 34 X= 4.061940269518D+00 Y= 3.164370422586D+00 Z= 1.784878380453D+00
I= 35 X= -4.229128975399D-02 Y= 1.111316165280D+00 Z= -6.700433998232D-01
I= 36 X= -3.043169361753D+00 Y= 3.666883562553D+00 Z= 3.377556549337D-01
I= 37 X= -2.093542651674D+00 Y= 5.274255663741D+00 Z= 9.418039877602D-01
I= 38 X= -4.349309816837D+00 Y= 2.497572185479D+00 Z= 1.136869251246D+00

Forward Direction:

Total Energy: -692.0024268 Hartrees

Potential Energy: -692.1960255 Hartress

Kinetic Energy: 0.1935987 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.341385470812D+12 Y= -3.655176786297D+12 Z= 8.936127939705D+12
I= 1 X= -1.642568336535D+13 Y= -1.162556799362D+13 Z= -5.894908888679D+12
I= 2 X= -3.074366372872D+13 Y= -1.062602559160D+13 Z= -2.260281629557D+13
I= 3 X= 1.639837858344D+13 Y= -9.471129472437D+12 Z= 1.232848284864D+13
I= 4 X= 5.826928661228D+12 Y= 8.584500354323D+12 Z= 2.364517600690D+13
I= 5 X= 7.327242333462D+12 Y= 1.271591684956D+13 Z= -1.566775197369D+12
I= 6 X= 3.346798748275D+13 Y= -5.799943192092D+13 Z= 3.168966148217D+13
I= 7 X= -3.124215026906D+13 Y= -1.576969759747D+14 Z= 6.011990835679D+13
I= 8 X= 1.176425649481D+14 Y= -3.762577597511D+13 Z= -2.580652229052D+13
I= 9 X= 7.550573050803D+12 Y= 2.631528028399D+12 Z= -3.349590561988D+12
I= 10 X= 3.458521078650D+13 Y= -2.495496038812D+13 Z= -1.330586687808D+13
I= 11 X= -1.350003432790D+13 Y= -8.668816179159D+13 Z= 1.193795913499D+12
I= 12 X= -1.280828955888D+14 Y= 9.876324862654D+13 Z= 1.663429556091D+13
I= 13 X= 1.981581058083D+12 Y= 2.346664969942D+13 Z= -8.044651651978D+12
I= 14 X= 1.229153451909D+13 Y= -9.781589091209D+13 Z= 1.160564763213D+13
I= 15 X= -8.394922144327D+13 Y= 2.067226497750D+13 Z= -1.812098663566D+11
I= 16 X= -6.796641710871D+13 Y= -2.812140407907D+13 Z= 1.169647641617D+13
I= 17 X= 2.544620009387D+13 Y= 6.712155471917D+11 Z= -7.647321040075D+12
I= 18 X= 1.463583529170D+13 Y= -4.778765276551D+13 Z= -3.591897535281D+13
I= 19 X= 2.297819941952D+13 Y= 1.118318746103D+14 Z= -1.477064993960D+13
I= 20 X= 4.467540630640D+13 Y= 1.222475047878D+13 Z= -7.039438990396D+13
I= 21 X= 9.738114653335D+12 Y= 3.560315956859D+12 Z= -5.317207213065D+12
I= 22 X= -3.488374798698D+13 Y= 1.792374811358D+13 Z= 2.936873074162D+13
I= 23 X= -8.643986847092D+12 Y= -5.426688800210D+13 Z= 9.593777502950D+13
I= 24 X= -1.046069172234D+14 Y= 4.220499227771D+12 Z= 1.065643997871D+14

I= 25 X= -1.343979903064D+13 Y= -4.337783619153D+12 Z= 1.604993845883D+13
I= 26 X= 1.067615513418D+14 Y= 2.524748657389D+13 Z= -9.428794900633D+13
I= 27 X= 6.916555810346D+12 Y= -3.543700490185D+13 Z= -1.338701179569D+13
I= 28 X= -7.328713282587D+13 Y= 1.404902266651D+14 Z= -3.790941461916D+13
I= 29 X= 6.622477826518D+12 Y= 9.679121761362D+12 Z= 2.613787745037D+12
I= 30 X= 1.366875057614D+12 Y= 5.387430849112D+11 Z= -1.328831705163D+13
I= 31 X= -2.465263429551D+13 Y= 5.207632704886D+13 Z= -1.718575760484D+13
I= 32 X= 6.251842083262D+13 Y= -1.167579785776D+13 Z= -1.354621962769D+14
I= 33 X= -2.367016004546D+13 Y= 9.273856184935D+13 Z= 6.523121680473D+13
I= 34 X= -6.514806126684D+12 Y= -6.523288496574D+13 Z= 2.091463409996D+13
I= 35 X= 1.460327550689D+11 Y= -3.112995691421D+12 Z= -6.078415216784D+11
I= 36 X= -1.285908403203D+13 Y= -3.545476991243D+12 Z= 5.289588775264D+12
I= 37 X= 9.511869859017D+13 Y= 2.728036965190D+13 Z= 7.150402271854D+13
I= 38 X= 4.743235382059D+13 Y= 6.255762754583D+13 Z= -4.201758716663D+13

Backward Direction:

Total Energy: -692.0024333 Hartrees

Potential Energy: -692.1960255 Hartress

Kinetic Energy: 0.1935922 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.213814466004D+12 Y= -2.193793080780D+12 Z= 1.109001531648D+13
I= 1 X= -1.545763053578D+13 Y= -1.162528741898D+13 Z= -5.895054338517D+12
I= 2 X= -3.020728043524D+13 Y= -1.141800896050D+13 Z= -2.142957107303D+13
I= 3 X= 1.652611319556D+13 Y= -1.093265453456D+13 Z= 1.017430328683D+13
I= 4 X= 6.363423058209D+12 Y= 9.376617804617D+12 Z= 2.247193713970D+13
I= 5 X= 9.913444075619D+12 Y= 3.783280971742D+12 Z= -1.219837706003D+13
I= 6 X= -6.223420061591D+13 Y= -5.798521269559D+13 Z= 3.168969549574D+13
I= 7 X= -4.524802262337D+13 Y= -1.594702102195D+14 Z= 4.737182905236D+13
I= 8 X= 1.106200695966D+14 Y= -4.121523248159D+13 Z= -2.877818923046D+13
I= 9 X= 9.048350594875D+12 Y= -9.386305812880D+10 Z= -4.220464314814D+12
I= 10 X= 3.360552081087D+13 Y= -2.845772271000D+13 Z= -1.522823428550D+13

I= 11 X= -1.154880708303D+13 Y= -9.208386719910D+13 Z= 6.595994209058D+11
I= 12 X= -1.242903117886D+14 Y= 9.624750534633D+13 Z= 1.691742841658D+13
I= 13 X= 3.479206821245D+12 Y= 2.619206894689D+13 Z= -7.173364732770D+12
I= 14 X= 1.131298507584D+13 Y= -9.431273760214D+13 Z= 1.352863275444D+13
I= 15 X= -8.015741157109D+13 Y= 2.318916270265D+13 Z= -4.645141096405D+11
I= 16 X= -6.601590520915D+13 Y= -2.272727401303D+13 Z= 1.223173131227D+13
I= 17 X= 2.532341927209D+13 Y= 8.225689996413D+11 Z= -4.742809119699D+12
I= 18 X= 1.520844400224D+13 Y= -4.655273342117D+13 Z= -3.002535492253D+13
I= 19 X= 2.266585250848D+13 Y= 1.126375188495D+14 Z= -1.355933388042D+13
I= 20 X= 4.381078458286D+13 Y= 8.845933137291D+12 Z= -6.718893496396D+13
I= 21 X= 7.201307256310D+12 Y= 3.561630525674D+12 Z= -5.318090525013D+12
I= 22 X= -4.143883117164D+13 Y= 1.792512043993D+13 Z= 2.936625267071D+13
I= 23 X= -1.032455033426D+13 Y= -5.119732701879D+13 Z= 9.620418661084D+13
I= 24 X= -1.062878722534D+14 Y= 1.154659915433D+12 Z= 1.062966356187D+14
I= 25 X= -1.356230335387D+13 Y= -4.489668055228D+12 Z= 1.314535642559D+13
I= 26 X= 1.058975433987D+14 Y= 2.862530631323D+13 Z= -9.749364976532D+13
I= 27 X= 6.604621603932D+12 Y= -3.624377914340D+13 Z= -1.459800896601D+13
I= 28 X= -7.271452661420D+13 Y= 1.392544844779D+14 Z= -4.380266768892D+13
I= 29 X= 9.208215864161D+12 Y= 1.860888299425D+13 Z= 1.324294499866D+13
I= 30 X= 5.406485995479D+12 Y= 1.586722771564D+12 Z= -5.396746715796D+12
I= 31 X= -3.167094435998D+13 Y= 5.566557591399D+13 Z= -1.421599879872D+13
I= 32 X= 4.851425263894D+13 Y= -9.902753469042D+12 Z= -1.227186624198D+14
I= 33 X= -2.514008613805D+13 Y= 8.755792661239D+13 Z= 8.207336527517D+13
I= 34 X= -5.947627561506D+12 Y= -7.093739195224D+13 Z= 2.764439022599D+13
I= 35 X= -6.492889798990D+11 Y= -3.112695425947D+12 Z= -6.068734112610D+11
I= 36 X= -8.819172435395D+12 Y= -4.594605931495D+12 Z= -2.602452002387D+12
I= 37 X= 9.364608566845D+13 Y= 3.246432408793D+13 Z= 5.465972957715D+13
I= 38 X= 4.800045143083D+13 Y= 6.826031417156D+13 Z= -4.874722747094D+13

Seed: 21165468539

CM Start Point Coordinates: bohr

I= 0 X= -2.095664730915D+00 Y= -2.101458354397D+00 Z= 2.023837567619D-02
I= 1 X= 8.081213428588D-03 Y= -2.832835747864D+00 Z= -1.490403525032D+00
I= 2 X= -1.342022908515D+00 Y= -1.352371080161D+00 Z= 2.399895819877D+00
I= 3 X= 2.233229608769D+00 Y= -1.974360776025D+00 Z= -2.553303736769D-02
I= 4 X= 1.245031899207D+00 Y= -1.204963679175D+00 Z= 2.522268247044D+00
I= 5 X= -3.024167396962D+00 Y= 3.144007636646D+00 Z= -2.225218245955D+00
I= 6 X= 5.738637195785D-02 Y= 1.866926571089D+00 Z= -3.311750075031D+00
I= 7 X= -2.485593535173D+00 Y= 4.514358318274D+00 Z= -3.696170700390D+00
I= 8 X= -4.804069349841D+00 Y= 1.752948093130D+00 Z= -2.915137945466D+00
I= 9 X= 3.077180106726D+00 Y= -5.238286198323D-01 Z= 4.576615129161D+00
I= 10 X= 3.760339768550D+00 Y= -2.602579796499D+00 Z= 5.548592265753D+00
I= 11 X= 4.974757343904D+00 Y= 8.894473876365D-01 Z= 3.544812692965D+00
I= 12 X= 2.015265084812D+00 Y= 6.298780803530D-01 Z= 5.982554132188D+00
I= 13 X= -3.239207475141D+00 Y= -8.938451092576D-01 Z= 4.648264757887D+00
I= 14 X= -3.492347365850D+00 Y= -2.498084432467D+00 Z= 5.967514161747D+00
I= 15 X= -2.561552617445D+00 Y= 5.884948898462D-01 Z= 5.939843543651D+00
I= 16 X= -5.090971012202D+00 Y= 1.812442669670D-01 Z= 3.898946919572D+00
I= 17 X= -4.826966714027D+00 Y= -2.149898381578D+00 Z= -7.738152881812D-01
I= 18 X= -5.951520289365D+00 Y= -3.834968343869D+00 Z= 3.012391933679D-01
I= 19 X= -5.848795530195D+00 Y= -2.712308136297D-01 Z= -9.654163742420D-01
I= 20 X= -4.546148321075D+00 Y= -3.078240988965D+00 Z= -2.730553606307D+00
I= 21 X= -1.595016476401D-02 Y= -3.764121415564D+00 Z= -4.077076413511D+00
I= 22 X= -8.243527563348D-02 Y= -5.959511086519D+00 Z= -4.648402337925D+00
I= 23 X= -1.703976975541D+00 Y= -2.799415310126D+00 Z= -5.356686250013D+00
I= 24 X= 1.646437785841D+00 Y= -3.184139168541D+00 Z= -5.092582294538D+00
I= 25 X= 4.866403827648D+00 Y= -2.282152518511D+00 Z= -8.550614750932D-01
I= 26 X= 4.962894585878D+00 Y= -2.753127426852D+00 Z= -2.757244951438D+00
I= 27 X= 6.069960230713D+00 Y= -5.994486277499D-01 Z= -4.632840136935D-01
I= 28 X= 5.930795722533D+00 Y= -3.665103413495D+00 Z= 3.273269085041D-01

I= 29 X= 2.866926999210D+00 Y= 3.064327608897D+00 Z= -2.254869258552D+00
I= 30 X= 2.912139106540D+00 Y= 3.649854162442D+00 Z= 2.782096669220D-01
I= 31 X= 4.162987940433D+00 Y= 1.709373838072D+00 Z= -3.032043792779D+00
I= 32 X= 2.306449411996D+00 Y= 4.465904484156D+00 Z= -3.727021447005D+00
I= 33 X= 1.997629333202D+00 Y= 5.218796460924D+00 Z= 1.263678159282D+00
I= 34 X= 4.785087197592D+00 Y= 2.914351323107D+00 Z= 1.289506309954D+00
I= 35 X= -8.937407337503D-03 Y= 1.054702195727D+00 Z= -5.553331223783D-01
I= 36 X= -2.648769954772D+00 Y= 3.867704494726D+00 Z= 2.101269670744D-01
I= 37 X= -1.948379839857D+00 Y= 5.644103720622D+00 Z= 4.409013726840D-01
I= 38 X= -3.824987771067D+00 Y= 2.944120313257D+00 Z= 1.496323140794D+00

Forward Direction:

Total Energy: -692.0080090 Hartrees

Potential Energy: -692.1835817 Hartress

Kinetic Energy: 0.1755727 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.843014007749D+12 Y= -1.140897793913D+12 Z= 2.276799730590D+13
I= 1 X= 1.064091593321D+13 Y= -7.588285849363D+12 Z= -1.495936060512D+13
I= 2 X= -1.315492310306D+13 Y= -2.433938626669D+13 Z= 5.102648659125D+12
I= 3 X= 1.174983425496D+13 Y= -1.513781823573D+13 Z= -6.077033869113D+12
I= 4 X= 1.576486847461D+13 Y= 4.166549532198D+12 Z= -1.019614153028D+13
I= 5 X= 7.759705257376D+12 Y= -1.657192546807D+11 Z= 8.856848118047D+12
I= 6 X= 7.032993356553D+12 Y= -2.721689379398D+13 Z= 8.435289036616D+13
I= 7 X= -2.743936678054D+13 Y= -2.719833321104D+13 Z= -6.425431309120D+13
I= 8 X= 1.063225597752D+14 Y= 2.044640563738D+13 Z= -5.696512915706D+12
I= 9 X= -4.394084902870D+12 Y= -1.083216648712D+13 Z= 3.178628537744D+12
I= 10 X= -1.398844641916D+13 Y= 1.482993143460D+14 Z= -1.279501199771D+14
I= 11 X= 3.123115154297D+13 Y= -4.425936940048D+13 Z= -4.228958415405D+13
I= 12 X= -3.506529643543D+13 Y= 1.289259924168D+12 Z= 1.373434428182D+13
I= 13 X= -6.089491017655D+11 Y= 1.938188190578D+12 Z= -3.569529025671D+10
I= 14 X= 7.144632445002D+12 Y= -4.897636196525D+13 Z= -9.485463232024D+13

I= 15 X= -4.639112203840D+13 Y= 4.676995753244D+13 Z= 1.777458502433D+13
I= 16 X= 6.269654684086D+13 Y= 7.251967225168D+13 Z= -1.060983350479D+12
I= 17 X= -2.414121892329D+12 Y= -2.996313466840D+12 Z= -4.098068007517D+12
I= 18 X= 4.445628297276D+13 Y= -1.008478245304D+13 Z= 7.502234945179D+13
I= 19 X= -8.536018416362D+12 Y= 4.210741015894D+12 Z= 2.877056910360D+13
I= 20 X= 1.227215595074D+14 Y= 5.393969438475D+13 Z= -4.337363169389D+13
I= 21 X= -7.796561220131D+12 Y= 6.774792546774D+12 Z= 1.456241230855D+13
I= 22 X= -6.762719545197D+13 Y= 3.798028718761D+13 Z= -4.721510996315D+13
I= 23 X= -2.061653228521D+13 Y= -9.537377005426D+12 Z= -4.045761341345D+13
I= 24 X= 7.682710094761D+13 Y= 1.006606960223D+14 Z= -1.042703312817D+14
I= 25 X= -4.814330025133D+12 Y= 8.383187672845D+12 Z= 6.877781237230D+12
I= 26 X= -2.583443119350D+13 Y= 1.903800713140D+13 Z= 1.879619033474D+14
I= 27 X= 3.856189331969D+13 Y= 1.115825746030D+13 Z= -3.895336165244D+13
I= 28 X= -7.918909747707D+13 Y= 1.035228849397D+14 Z= 2.074201009787D+13
I= 29 X= 1.239685041649D+13 Y= -1.879968214620D+13 Z= 1.250764655033D+12
I= 30 X= 7.792476823679D+12 Y= 1.815456788359D+12 Z= -4.697849727886D+12
I= 31 X= -5.836620979758D+13 Y= 5.615172024983D+13 Z= 2.396871130442D+13
I= 32 X= 3.840012123342D+13 Y= 7.914444874639D+13 Z= -1.883060210247D+12
I= 33 X= -2.323007869061D+13 Y= 3.130569493876D+13 Z= 4.396253998199D+12
I= 34 X= -4.430699962360D+13 Y= 7.980162684938D+13 Z= -8.552796977837D+13
I= 35 X= -3.366946133413D+12 Y= -1.322156185321D+12 Z= -2.258457164341D+12
I= 36 X= -1.523507371102D+13 Y= 1.043295442311D+13 Z= 2.790497340249D+12
I= 37 X= -2.113167772125D+13 Y= -1.228851035001D+14 Z= 2.509795259651D+13
I= 38 X= 3.981958611364D+13 Y= 6.667851619213D+13 Z= 4.650861503989D+13

Backward Direction:

Total Energy: -692.0080158 Hartrees

Potential Energy: -692.1835817 Hartress

Kinetic Energy: 0.1755659 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.899563833283D+12 Y= -5.265575357925D+11 Z= 2.399495215049D+13

I= 1 X= 1.037295658717D+13 Y= -7.588080939639D+12 Z= -1.495949917729D+13
I= 2 X= -1.247900696068D+13 Y= -2.407401779091D+13 Z= 5.665581381139D+12
I= 3 X= 1.169341889469D+13 Y= -1.575219537964D+13 Z= -7.304141256502D+12
I= 4 X= 1.644086930801D+13 Y= 3.901262549128D+12 Z= -1.075897615782D+13
I= 5 X= 7.739698010365D+12 Y= -6.650411570826D+12 Z= 2.202020310911D+12
I= 6 X= -1.455491585397D+13 Y= -2.721062787538D+13 Z= 8.435361978411D+13
I= 7 X= -3.357076022792D+13 Y= -3.383630037370D+13 Z= -7.450790985837D+13
I= 8 X= 1.047556714697D+14 Y= 1.262119223709D+13 Z= -7.444952562783D+12
I= 9 X= -3.000281393354D+12 Y= -1.331850471850D+13 Z= 2.667902682329D+12
I= 10 X= -1.441371967632D+13 Y= 1.454007553551D+14 Z= -1.290482039933D+14
I= 11 X= 3.294222994702D+13 Y= -4.882560149412D+13 Z= -4.267724500914D+13
I= 12 X= -3.189646911479D+13 Y= -9.009814357538D+11 Z= 1.387048634266D+13
I= 13 X= 7.847692527042D+11 Y= 4.424549537836D+12 Z= 4.754336281098D+11
I= 14 X= 6.720461262822D+12 Y= -4.607739833393D+13 Z= -9.375586833581D+13
I= 15 X= -4.322292877159D+13 Y= 4.896117399326D+13 Z= 1.763828878329D+13
I= 16 X= 6.440705634265D+13 Y= 7.708456192891D+13 Z= -6.724050493107D+11
I= 17 X= -2.766378327363D+12 Y= -3.070403201632D+12 Z= -1.613933274318D+12
I= 18 X= 4.438726911552D+13 Y= -8.947081002299D+12 Z= 8.042589058592D+13
I= 19 X= -8.621525174573D+12 Y= 5.135789041900D+12 Z= 2.961785239202D+13
I= 20 X= 1.215636544737D+14 Y= 5.066290565004D+13 Z= -4.059141294194D+13
I= 21 X= -1.018690397147D+13 Y= 6.775846840423D+12 Z= 1.456170542177D+13
I= 22 X= -7.372043336535D+13 Y= 3.798141278168D+13 Z= -4.721705502135D+13
I= 23 X= -2.199823603292D+13 Y= -6.614440511110D+12 Z= -4.050891056120D+13
I= 24 X= 7.544516923585D+13 Y= 9.774059998906D+13 Z= -1.042198834231D+14
I= 25 X= -5.166278992622D+12 Y= 8.456756857077D+12 Z= 4.393550836556D+12
I= 26 X= -2.699184216723D+13 Y= 2.231423031097D+13 Z= 1.851793670943D+14
I= 27 X= 3.847687080058D+13 Y= 1.023207556540D+13 Z= -3.980024619524D+13
I= 28 X= -7.925789882409D+13 Y= 1.023842776864D+14 Z= 1.533836940721D+13
I= 29 X= 1.237637817160D+13 Y= -1.231683420022D+13 Z= 7.903635507777D+12
I= 30 X= 8.893787460113D+12 Y= 1.161338400120D+12 Z= 2.240375529010D+12

I= 31 X= -5.993270138490D+13 Y= 6.397426842081D+13 Z= 2.571509380891D+13
I= 32 X= 3.227081049746D+13 Y= 8.578318455149D+13 Z= 8.367556360302D+12
I= 33 X= -2.427724097972D+13 Y= 2.695071683803D+13 Z= 1.799012488626D+13
I= 34 X= -4.296561647409D+13 Y= 7.546321962645D+13 Z= -8.149002420106D+13
I= 35 X= -3.275966058199D+12 Y= -1.321888871869D+12 Z= -2.257731652235D+12
I= 36 X= -1.413395784310D+13 Y= 1.108631189958D+13 Z= -4.148178916594D+12
I= 37 X= -2.218146055482D+13 Y= -1.185278065628D+14 Z= 1.150325614128D+13
I= 38 X= 4.116073073847D+13 Y= 7.101462504167D+13 Z= 4.247047363940D+13

Seed: 21461384799

CM Start Point Coordinates: bohr

I= 0 X= -2.171436463895D+00 Y= -2.238231195880D+00 Z= -7.267328139707D-02
I= 1 X= 1.136629359756D-01 Y= -2.803190483196D+00 Z= -1.504339863017D+00
I= 2 X= -1.213680885519D+00 Y= -1.157275370584D+00 Z= 2.350596897203D+00
I= 3 X= 2.175861370101D+00 Y= -2.337492351190D+00 Z= -1.401673675233D-01
I= 4 X= 1.391539771051D+00 Y= -1.372304923300D+00 Z= 2.396806668577D+00
I= 5 X= -2.698359321334D+00 Y= 3.231566187190D+00 Z= -2.172381198885D+00
I= 6 X= -4.270825928542D-02 Y= 1.550536953569D+00 Z= -3.137376098402D+00
I= 7 X= -2.033993896698D+00 Y= 4.644712176022D+00 Z= -3.446585347620D+00
I= 8 X= -4.286097272197D+00 Y= 1.925502348765D+00 Z= -3.198990598325D+00
I= 9 X= 2.828479758118D+00 Y= -7.265082143330D-01 Z= 4.684008399016D+00
I= 10 X= 2.716273759548D+00 Y= -2.733656244751D+00 Z= 5.784385253101D+00
I= 11 X= 4.943231785111D+00 Y= 8.550540881049D-02 Z= 4.652388682198D+00
I= 12 X= 1.677483820408D+00 Y= 5.459867665852D-01 Z= 5.719321644321D+00
I= 13 X= -2.969411909188D+00 Y= -5.823535485246D-01 Z= 4.501002912478D+00
I= 14 X= -2.803098067804D+00 Y= -2.161022754754D+00 Z= 5.513736557785D+00
I= 15 X= -2.332962823077D+00 Y= 8.293104380540D-01 Z= 5.649318480145D+00
I= 16 X= -4.835281151817D+00 Y= -3.352138279430D-02 Z= 3.696016159948D+00
I= 17 X= -4.819344910915D+00 Y= -2.210593561843D+00 Z= -6.585804874743D-01
I= 18 X= -6.061171025066D+00 Y= -3.387209761079D+00 Z= 8.985269187397D-01

I= 19 X= -6.091471991301D+00 Y= -6.480239577773D-02 Z= -6.226687303204D-01
I= 20 X= -4.828430793800D+00 Y= -3.143188809131D+00 Z= -2.799332406066D+00
I= 21 X= 1.401035319114D-02 Y= -3.842842731871D+00 Z= -4.065213132444D+00
I= 22 X= 4.223081199336D-01 Y= -5.828927183331D+00 Z= -3.672448770941D+00
I= 23 X= -2.086097542666D+00 Y= -3.525151795633D+00 Z= -4.797686043582D+00
I= 24 X= 1.098820677169D+00 Y= -2.919733276475D+00 Z= -5.655883382026D+00
I= 25 X= 4.999819146991D+00 Y= -2.423230223395D+00 Z= -7.085302524247D-01
I= 26 X= 5.247472719350D+00 Y= -1.961564155841D+00 Z= -2.971778066947D+00
I= 27 X= 6.163091220057D+00 Y= -1.176119023860D+00 Z= 4.612984141788D-01
I= 28 X= 5.501970672056D+00 Y= -4.439371616027D+00 Z= -2.622959213032D-01
I= 29 X= 2.701922617589D+00 Y= 3.447668591559D+00 Z= -2.313275852683D+00
I= 30 X= 2.590666644486D+00 Y= 3.985137088081D+00 Z= 1.684934173554D-01
I= 31 X= 4.016127677404D+00 Y= 1.973691800785D+00 Z= -3.243230326060D+00
I= 32 X= 1.819297863463D+00 Y= 4.679456155249D+00 Z= -3.689551079807D+00
I= 33 X= 1.898621256017D+00 Y= 5.515702254853D+00 Z= 1.310526484813D+00
I= 34 X= 3.991984209881D+00 Y= 3.078546271770D+00 Z= 1.319228801330D+00
I= 35 X= -2.958960654559D-03 Y= 1.015335396208D+00 Z= -5.832526625859D-01
I= 36 X= -2.764294523575D+00 Y= 3.861036408047D+00 Z= 3.639327604479D-01
I= 37 X= -1.832429408359D+00 Y= 5.473679397969D+00 Z= 1.072655153721D+00
I= 38 X= -4.226411308198D+00 Y= 3.241072736066D+00 Z= 1.833977254133D+00

Forward Direction:

Total Energy: -692.0008858 Hartrees

Potential Energy: -692.1881688 Hartress

Kinetic Energy: 0.1872831 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.906004076605D+13 Y= 1.046030898717D+13 Z= -2.070003502238D+13

I= 1 X= -5.523670683451D+12 Y= 1.242471241833D+13 Z= -8.137881896536D+12

I= 2 X= -2.661447971637D+12 Y= 1.705512006705D+11 Z= 1.203924666750D+13

I= 3 X= 1.928283980707D+13 Y= -2.608312920074D+13 Z= -1.071316362515D+13

I= 4 X= 3.889031189026D+11 Y= 4.880702211404D+12 Z= -7.431093290097D+12

I= 5 X= 8.948758842564D+12 Y= 2.271385487780D+13 Z= 3.624411061105D+13
I= 6 X= 1.276107098201D+13 Y= -3.771718137932D+13 Z= 6.498795408211D+13
I= 7 X= -2.155428302553D+13 Y= 1.035887916328D+14 Z= 2.409522035346D+13
I= 8 X= -1.088069868255D+13 Y= -9.402790959309D+13 Z= -6.983790136551D+13
I= 9 X= 4.115483901240D+12 Y= 1.880358077909D+13 Z= -1.025975178110D+13
I= 10 X= -2.951096987461D+13 Y= 1.220517488363D+14 Z= 3.158479438117D+13
I= 11 X= -7.402909141478D+13 Y= -1.360898794550D+14 Z= 1.366047512733D+13
I= 12 X= 7.696865360500D+12 Y= -4.684449263476D+13 Z= 9.830396461399D+13
I= 13 X= 6.886622636176D+12 Y= 3.000670725728D+12 Z= 6.076220840911D+12
I= 14 X= -2.501843429595D+13 Y= -4.159564076203D+13 Z= -1.808166991505D+13
I= 15 X= -4.330275333411D+13 Y= -1.067300204944D+14 Z= -9.020926595678D+13
I= 16 X= -4.960440221647D+13 Y= 3.275583359145D+12 Z= 1.947547388152D+13
I= 17 X= 1.290022460726D+13 Y= -8.649661813368D+12 Z= 1.652608306910D+13
I= 18 X= -1.653882375809D+13 Y= 4.885176989660D+13 Z= -6.803411977724D+13
I= 19 X= 1.234953952237D+12 Y= -2.465126651566D+13 Z= 4.999548931218D+13
I= 20 X= -1.118711133087D+14 Y= -1.679040761472D+13 Z= -8.917346044914D+13
I= 21 X= 1.673705763208D+13 Y= 1.406346457787D+13 Z= 1.060773791071D+12
I= 22 X= -1.712045884466D+13 Y= -1.571644290477D+14 Z= -1.752380883966D+13
I= 23 X= -1.391414422713D+13 Y= 2.257161690412D+13 Z= -4.809292025757D+13
I= 24 X= -4.508092570683D+13 Y= -3.600657014891D+13 Z= -3.189565473263D+13
I= 25 X= -1.140831473944D+12 Y= 8.987190688156D+11 Z= 1.078876893767D+13
I= 26 X= 4.618750870574D+12 Y= -5.492339919129D+12 Z= 1.578984757842D+13
I= 27 X= 7.336256586379D+12 Y= -4.685332589714D+12 Z= -5.032342924823D+13
I= 28 X= -1.100506724062D+14 Y= 6.465601910900D+13 Z= 7.929491986372D+12
I= 29 X= -8.208375952163D+12 Y= -7.481726198353D+12 Z= 5.476006248331D+11
I= 30 X= 2.330894293332D+11 Y= -2.371258170610D+13 Z= -8.353934015901D+12
I= 31 X= -8.325380482834D+13 Y= 5.886746063540D+13 Z= 7.658227497965D+13
I= 32 X= -1.326991991130D+13 Y= 8.672260891898D+13 Z= -4.017110220451D+13
I= 33 X= -1.310079736612D+14 Y= 8.841096764516D+13 Z= 5.514927919100D+13
I= 34 X= -2.212735995632D+13 Y= -4.745074530171D+13 Z= 9.089512773159D+13

I= 35 X= -2.553425724586D+12 Y= -9.936388602505D+11 Z= 1.867552366543D+11
I= 36 X= 9.354471584037D+12 Y= -3.908048970681D+12 Z= -1.953895151762D+13
I= 37 X= -2.041213315165D+13 Y= -1.274626244715D+13 Z= -1.773648048864D+13
I= 38 X= -2.776289418699D+12 Y= 1.776064452265D+13 Z= 3.761316318698D+12

Backward Direction:

Total Energy: -692.0008533 Hartrees

Potential Energy: -692.1881688 Hartress

Kinetic Energy: 0.1873156 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.905807826683D+13 Y= 1.118732212944D+13 Z= -1.943759936801D+13
I= 1 X= -5.442861388227D+12 Y= 1.242490363481D+13 Z= -8.138000270141D+12
I= 2 X= -2.127129574374D+12 Y= 1.318419332564D+11 Z= 1.266431792130D+13
I= 3 X= 1.928099771016D+13 Y= -2.681019928348D+13 Z= -1.197576234168D+13
I= 4 X= 9.232993378851D+11 Y= 4.919493132251D+12 Z= -8.056104804083D+12
I= 5 X= 9.577864579715D+12 Y= 1.664913451304D+13 Z= 2.965727307406D+13
I= 6 X= -2.377804544701D+13 Y= -3.770993614304D+13 Z= 6.498839567794D+13
I= 7 X= -2.866659994276D+13 Y= 9.920750049734D+13 Z= 1.484677424745D+13
I= 8 X= -1.355167339943D+13 Y= -9.956436662662D+13 Z= -7.161269379065D+13
I= 9 X= 5.314382756575D+12 Y= 1.665164408726D+13 Z= -1.077887901699D+13
I= 10 X= -3.000632296425D+13 Y= 1.194623543437D+14 Z= 3.045626735304D+13
I= 11 X= -7.252939961422D+13 Y= -1.401387449191D+14 Z= 1.329787203339D+13
I= 12 X= 1.051858410612D+13 Y= -4.876863839793D+13 Z= 9.845498332412D+13
I= 13 X= 8.085433358221D+12 Y= 5.152628118915D+12 Z= 6.595689771355D+12
I= 14 X= -2.551285017955D+13 Y= -3.900590911769D+13 Z= -1.695258608703D+13
I= 15 X= -4.048160284457D+13 Y= -1.048050096040D+14 Z= -9.036041874673D+13
I= 16 X= -4.810522550206D+13 Y= 7.323261225812D+12 Z= 1.983888411322D+13
I= 17 X= 1.266061447069D+13 Y= -8.656145508703D+12 Z= 1.872110610771D+13
I= 18 X= -1.643788571478D+13 Y= 4.983343966677D+13 Z= -6.336463091092D+13
I= 19 X= 1.106762998086D+12 Y= -2.390227113634D+13 Z= 5.079885118757D+13
I= 20 X= -1.127730028014D+14 Y= -1.957368518930D+13 Z= -8.672683905941D+13

I= 21 X= 1.468886573767D+13 Y= 1.406441642179D+13 Z= 1.060135072672D+12
I= 22 X= -2.236345015469D+13 Y= -1.571634205476D+14 Z= -1.752557804188D+13
I= 23 X= -1.515116122689D+13 Y= 2.506811889806D+13 Z= -4.805735211315D+13
I= 24 X= -4.631817511270D+13 Y= -3.850046310474D+13 Z= -3.193206250136D+13
I= 25 X= -1.380190425779D+12 Y= 9.047620983446D+11 Z= 8.593671858075D+12
I= 26 X= 3.717307184149D+12 Y= -2.709645307880D+12 Z= 1.334297691976D+13
I= 27 X= 7.208455419173D+12 Y= -5.435281350485D+12 Z= -5.112647496407D+13
I= 28 X= -1.099496087691D+14 Y= 6.367360751122D+13 Z= 3.260035228756D+12
I= 29 X= -7.579661306633D+12 Y= -1.418813597021D+12 Z= 7.132670189361D+12
I= 30 X= 1.888288295670D+12 Y= -2.384127390573D+13 Z= -2.277920704227D+12
I= 31 X= -8.592350668065D+13 Y= 6.440228347326D+13 Z= 7.835537291225D+13
I= 32 X= -2.038057761917D+13 Y= 9.110430945534D+13 Z= -3.092555237343D+13
I= 33 X= -1.319941249758D+14 Y= 8.454085516597D+13 Z= 6.739597629736D+13
I= 34 X= -2.119023733690D+13 Y= -5.144085845819D+13 Z= 9.496092552388D+13
I= 35 X= -2.696518772358D+12 Y= -9.934056871205D+11 Z= 1.874260138547D+11
I= 36 X= 1.100962935265D+13 Y= -3.780093516521D+12 Z= -2.561534921307D+13
I= 37 X= -2.140050654777D+13 Y= -8.873950349153D+12 Z= -2.998419937714D+13
I= 38 X= -1.839080624404D+12 Y= 2.174894162606D+13 Z= -3.045690279061D+11

Seed: 22402754432

CM Start Point Coordinates: bohr

I= 0 X= -2.193210503245D+00 Y= -2.116009821750D+00 Z= -1.509710134236D-01
I= 1 X= -1.129302337507D-01 Y= -2.684672697946D+00 Z= -1.550355166001D+00
I= 2 X= -1.323511877867D+00 Y= -1.365918784543D+00 Z= 2.319394148968D+00
I= 3 X= 2.185608644875D+00 Y= -2.298585339745D+00 Z= -4.361939759680D-02
I= 4 X= 1.326890869540D+00 Y= -1.314765070717D+00 Z= 2.334106857134D+00
I= 5 X= -2.611460658094D+00 Y= 3.537802306706D+00 Z= -2.546848821752D+00
I= 6 X= 1.720383088582D-01 Y= 1.437482793476D+00 Z= -3.111501265287D+00
I= 7 X= -1.747320544762D+00 Y= 5.207630346442D+00 Z= -3.589009980788D+00
I= 8 X= -3.784555301493D+00 Y= 2.132026338259D+00 Z= -4.032315587910D+00

I= 9 X= 3.063313158362D+00 Y= -6.534366538458D-01 Z= 4.581826697850D+00
I= 10 X= 3.245134626516D+00 Y= -2.359666702999D+00 Z= 5.294287485871D+00
I= 11 X= 4.877385619013D+00 Y= -1.673731236883D-01 Z= 3.508958577000D+00
I= 12 X= 2.084622878306D+00 Y= 6.628441722701D-01 Z= 6.132088739772D+00
I= 13 X= -2.708506749545D+00 Y= -7.027411377137D-01 Z= 4.671547792114D+00
I= 14 X= -2.559726515103D+00 Y= -2.125581192335D+00 Z= 6.172472975054D+00
I= 15 X= -2.076974165429D+00 Y= 9.906455417708D-01 Z= 5.466517941025D+00
I= 16 X= -4.912193237561D+00 Y= -6.822409194514D-01 Z= 4.170227384030D+00
I= 17 X= -4.937404005454D+00 Y= -2.294969860720D+00 Z= -7.614131562171D-01
I= 18 X= -5.253767030033D+00 Y= -4.598341897636D+00 Z= -6.144479978436D-01
I= 19 X= -6.261285654680D+00 Y= -1.115407901581D+00 Z= 7.378349014873D-01
I= 20 X= -5.247024027660D+00 Y= -1.832193828261D+00 Z= -2.776105990875D+00
I= 21 X= -1.746008714230D-01 Y= -4.091109602621D+00 Z= -4.051847566645D+00
I= 22 X= 1.127517603870D-01 Y= -6.381389201181D+00 Z= -3.696860657694D+00
I= 23 X= -2.110056453264D+00 Y= -3.746033052427D+00 Z= -4.917362945045D+00
I= 24 X= 1.356741362376D+00 Y= -3.329396840432D+00 Z= -5.276725930485D+00
I= 25 X= 4.913766692315D+00 Y= -2.515878765271D+00 Z= -6.908779150096D-01
I= 26 X= 5.097322234967D+00 Y= -2.979988887032D+00 Z= -2.550036676082D+00
I= 27 X= 6.097308697982D+00 Y= -8.781886215425D-01 Z= -1.310172568996D-01
I= 28 X= 5.854266480196D+00 Y= -3.940519708798D+00 Z= 3.678729006946D-01
I= 29 X= 2.755736930084D+00 Y= 3.399833040922D+00 Z= -2.140816316956D+00
I= 30 X= 2.749772651996D+00 Y= 4.074944118195D+00 Z= 3.203753773992D-01
I= 31 X= 4.370929677588D+00 Y= 1.991704820538D+00 Z= -2.609045028590D+00
I= 32 X= 2.179262611347D+00 Y= 4.340323753641D+00 Z= -3.793155353510D+00
I= 33 X= 2.036013139079D+00 Y= 5.654280775162D+00 Z= 9.530937474482D-01
I= 34 X= 4.065039579552D+00 Y= 3.544160335459D+00 Z= 1.879055073720D+00
I= 35 X= 4.140664356296D-02 Y= 1.096577856906D+00 Z= -5.036679187100D-01
I= 36 X= -3.192132303678D+00 Y= 3.650889318845D+00 Z= 1.703888041489D-01
I= 37 X= -2.192261060005D+00 Y= 5.283270585141D+00 Z= 1.342155751205D+00
I= 38 X= -4.745013707623D+00 Y= 2.763544867351D+00 Z= 1.223915614311D+00

Forward Direction:

Total Energy: -692.0021985 Hartrees

Potential Energy: -692.1971016 Hartress

Kinetic Energy: 0.1949031 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.352702273734D+12 Y= 1.082249204641D+13 Z= 3.559238569176D+12
I= 1 X= 4.690807647489D+12 Y= 2.242649922869D+12 Z= -2.773637027162D+13
I= 2 X= 1.147543504460D+13 Y= -3.284390311711D+12 Z= -9.691994731446D+12
I= 3 X= -2.880822040382D+13 Y= -1.622925437621D+13 Z= 2.509414889507D+12
I= 4 X= 1.488884950213D+13 Y= 1.777895471849D+12 Z= 1.217258073972D+13
I= 5 X= -2.540365761389D+12 Y= 4.148845011328D+12 Z= 2.313503258038D+12
I= 6 X= 2.579008032655D+13 Y= -2.376006356348D+13 Z= 7.655195308126D+13
I= 7 X= 2.152339580715D+13 Y= -7.017003507467D+13 Z= -2.285699784913D+13
I= 8 X= 1.646781704570D+14 Y= 6.711594792763D+13 Z= 1.140157615823D+14
I= 9 X= -1.071744672612D+13 Y= -1.295285537825D+13 Z= 4.018643179463D+12
I= 10 X= 2.574117578971D+12 Y= -9.066424401712D+13 Z= -7.146766386419D+13
I= 11 X= -1.278069927554D+13 Y= -6.076108558038D+12 Z= -5.781787641173D+13
I= 12 X= -3.371182352430D+12 Y= 7.204714499294D+13 Z= -3.637477205235D+13
I= 13 X= -1.127140809444D+13 Y= 5.416078829628D+12 Z= 9.793519697958D+09
I= 14 X= 6.224901428253D+13 Y= -8.416931161882D+13 Z= -9.677238559819D+12
I= 15 X= -8.913576964637D+13 Y= -2.000480744677D+13 Z= 8.279103107344D+12
I= 16 X= -1.576271480649D+14 Y= 5.328761223093D+13 Z= 1.597368244693D+13
I= 17 X= 2.582391661031D+13 Y= 1.616030135160D+12 Z= 9.620449326666D+12
I= 18 X= -1.915263713970D+13 Y= 3.119662656556D+13 Z= -4.118233837491D+13
I= 19 X= 6.042197462940D+13 Y= -4.797048124765D+13 Z= 2.451378839614D+13
I= 20 X= -5.699757661128D+13 Y= -1.417529343869D+13 Z= -9.541659603465D+13
I= 21 X= -1.689669627401D+13 Y= -2.443309249793D+12 Z= 1.155007725068D+12
I= 22 X= 5.525328691355D+13 Y= 7.703592933422D+13 Z= 1.188002511208D+14
I= 23 X= -6.393828014000D+13 Y= 5.066539421446D+13 Z= -4.173845174995D+13
I= 24 X= 2.456145743193D+13 Y= -1.886271258249D+13 Z= 5.671712604427D+13

I= 25 X= 4.086824890129D+12 Y= 3.179373769735D+12 Z= -1.223943216019D+13
I= 26 X= -8.783336260736D+13 Y= -2.709106860183D+13 Z= 1.104063791317D+13
I= 27 X= 5.956070513453D+12 Y= -3.737028643203D+13 Z= 6.244605845394D+13
I= 28 X= 7.079769745412D+13 Y= -1.882767958989D+14 Z= 7.294854997124D+13
I= 29 X= -1.240466523704D+13 Y= -4.076727914168D+12 Z= 2.696856642577D+12
I= 30 X= 1.103313272992D+13 Y= -1.059611743542D+12 Z= 4.152909763624D+12
I= 31 X= -3.520687322182D+13 Y= 1.247750577396D+13 Z= -8.505546708486D+13
I= 32 X= 9.122976855916D+13 Y= -5.747264655015D+13 Z= -7.412343273897D+13
I= 33 X= -5.453158745119D+13 Y= -1.139367579392D+13 Z= 1.764606783620D+13
I= 34 X= -8.780587872767D+13 Y= 4.972466100173D+13 Z= -8.063884044548D+13
I= 35 X= 2.863937943475D+12 Y= 5.867081391176D+12 Z= 6.235637988738D+11
I= 36 X= -6.436943111797D+12 Y= 8.626142105651D+12 Z= 6.372107002393D+12
I= 37 X= -5.374024487984D+13 Y= -1.900107521046D+13 Z= 3.061007352950D+13
I= 38 X= 7.349173685335D+13 Y= -1.378028808741D+13 Z= -1.671045445814D+13

Backward Direction:

Total Energy: -692.0021566 Hartrees

Potential Energy: -692.1971016 Hartress

Kinetic Energy: 0.1949450 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.493564379390D+12 Y= 1.214763263784D+13 Z= 5.438834013301D+12
I= 1 X= 5.722880264428D+12 Y= 2.242884459043D+12 Z= -2.773648446464D+13
I= 2 X= 1.185885339924D+13 Y= -4.139297435620D+12 Z= -8.644066478377D+12
I= 3 X= -2.866722496547D+13 Y= -1.755452829653D+13 Z= 6.295612935001D+11
I= 4 X= 1.527235991844D+13 Y= 2.632918433082D+12 Z= 1.112463644563D+13
I= 5 X= 5.780965963924D+10 Y= -3.327091472126D+12 Z= -6.827371521149D+12
I= 6 X= -6.525143213579D+13 Y= -2.374723590744D+13 Z= 7.655182046353D+13
I= 7 X= 8.878949257584D+12 Y= -7.043104790329D+13 Z= -3.329780573197D+13
I= 8 X= 1.579937369041D+14 Y= 6.530489448521D+13 Z= 1.114352466326D+14
I= 9 X= -9.533976556353D+12 Y= -1.511772212365D+13 Z= 3.262018268812D+12
I= 10 X= 1.688832498719D+12 Y= -9.351448172031D+13 Z= -7.314453391715D+13

I= 11 X= -1.121500403997D+13 Y= -1.044351207242D+13 Z= -5.826499067591D+13
I= 12 X= -2.920712891771D+11 Y= 7.002484462541D+13 Z= -3.612194815676D+13
I= 13 X= -1.008807068163D+13 Y= 7.580968541231D+12 Z= 7.667406540392D+11
I= 14 X= 6.136462107634D+13 Y= -8.131877432692D+13 Z= -7.999904412750D+12
I= 15 X= -8.605728981655D+13 Y= -1.798157224338D+13 Z= 8.026142558761D+12
I= 16 X= -1.560620401624D+14 Y= 5.765374274644D+13 Z= 1.642164844339D+13
I= 17 X= 2.578130263743D+13 Y= 1.784752002058D+12 Z= 1.196545309234D+13
I= 18 X= -1.856261488916D+13 Y= 3.217502555399D+13 Z= -3.650698572274D+13
I= 19 X= 6.012827901468D+13 Y= -4.737397775665D+13 Z= 2.553489990391D+13
I= 20 X= -5.760000040227D+13 Y= -1.681477639456D+13 Z= -9.283792357488D+13
I= 21 X= -1.889438219131D+13 Y= -2.442231910232D+12 Z= 1.154283458737D+12
I= 22 X= 5.007222854673D+13 Y= 7.703704829829D+13 Z= 1.187982105463D+14
I= 23 X= -6.530782503676D+13 Y= 5.307561877008D+13 Z= -4.145955241780D+13
I= 24 X= 2.319157197796D+13 Y= -2.126985408512D+13 Z= 5.643706437037D+13
I= 25 X= 4.044417916816D+12 Y= 3.010238414816D+12 Z= -1.458448438561D+13
I= 26 X= -8.843528382309D+13 Y= -2.445245683386D+13 Z= 8.461791566341D+12
I= 27 X= 5.662677966454D+12 Y= -3.796766414540D+13 Z= 6.142517551474D+13
I= 28 X= 7.138766865667D+13 Y= -1.892558132113D+14 Z= 6.827358857172D+13
I= 29 X= -9.806848559744D+12 Y= 3.396747283924D+12 Z= 1.183572713487D+13
I= 30 X= 1.483256730858D+13 Y= 1.408840570822D+11 Z= 1.048113386090D+13
I= 31 X= -4.188720019840D+13 Y= 1.428896020092D+13 Z= -8.247639550882D+13
I= 32 X= 7.858655498044D+13 Y= -5.721199982008D+13 Z= -6.368650209940D+13
I= 33 X= -5.576636112477D+13 Y= -1.559368178257D+13 Z= 3.142914578273D+13
I= 34 X= -8.754368830911D+13 Y= 4.499549645845D+13 Z= -7.481281396835D+13
I= 35 X= 2.045544313300D+12 Y= 5.867321412823D+12 Z= 6.243688432928D+11
I= 36 X= -2.637162495013D+12 Y= 7.424667694299D+12 Z= 4.351420521360D+10
I= 37 X= -5.497711406853D+13 Y= -1.479827055984D+13 Z= 1.682503348278D+13
I= 38 X= 7.375490346463D+13 Y= -9.052423753084D+12 Z= -2.253632002005D+13

Seed: 22676000783

CM Start Point Coordinates: bohr

I= 0 X= -2.228740995005D+00 Y= -2.159295191020D+00 Z= -6.579114749954D-02
I= 1 X= 1.707681005027D-03 Y= -2.861260606149D+00 Z= -1.489315357587D+00
I= 2 X= -1.362994525152D+00 Y= -1.120172680773D+00 Z= 2.334265035481D+00
I= 3 X= 2.218501234794D+00 Y= -1.901096173678D+00 Z= -7.754736116832D-02
I= 4 X= 1.371567278461D+00 Y= -1.347260837987D+00 Z= 2.374316865456D+00
I= 5 X= -2.765172418546D+00 Y= 3.274425668372D+00 Z= -2.390955493904D+00
I= 6 X= -1.540462714598D-01 Y= 1.978687339567D+00 Z= -2.956850756247D+00
I= 7 X= -2.100557946548D+00 Y= 4.830156512038D+00 Z= -3.673088981326D+00
I= 8 X= -3.887071759983D+00 Y= 1.714385606010D+00 Z= -3.149120998816D+00
I= 9 X= 3.163507186560D+00 Y= -1.046963018213D+00 Z= 4.680671513281D+00
I= 10 X= 2.818491663349D+00 Y= -2.875188700940D+00 Z= 5.500753577472D+00
I= 11 X= 5.373984256536D+00 Y= -8.722795655039D-01 Z= 4.139295788721D+00
I= 12 X= 2.918859134281D+00 Y= 5.179722113450D-01 Z= 6.032202740456D+00
I= 13 X= -2.959850908731D+00 Y= -3.376572903693D-01 Z= 4.529136009604D+00
I= 14 X= -2.955334407148D+00 Y= -2.032978719549D+00 Z= 6.029677284347D+00
I= 15 X= -2.388218724626D+00 Y= 1.859292110290D+00 Z= 5.064949896870D+00
I= 16 X= -5.101004730359D+00 Y= -2.526845637143D-02 Z= 4.197102033368D+00
I= 17 X= -4.974759017813D+00 Y= -2.370168665584D+00 Z= -8.361250687588D-01
I= 18 X= -5.704262540117D+00 Y= -3.891162755781D+00 Z= -1.514888431370D-01
I= 19 X= -6.356972046749D+00 Y= -7.836156721541D-01 Z= -6.858836984849D-01
I= 20 X= -4.943570276628D+00 Y= -2.962763941176D+00 Z= -2.892394814078D+00
I= 21 X= 1.761713139580D-01 Y= -3.833339435284D+00 Z= -3.923695849958D+00
I= 22 X= 1.056702845218D+00 Y= -5.871229960488D+00 Z= -4.131212272688D+00
I= 23 X= -1.953159254179D+00 Y= -4.467135979169D+00 Z= -4.948268791453D+00
I= 24 X= 1.356004279550D+00 Y= -2.395936636725D+00 Z= -5.199517667272D+00
I= 25 X= 4.879790900736D+00 Y= -2.352099102765D+00 Z= -9.529679284642D-01
I= 26 X= 5.166515615842D+00 Y= -1.851307734611D+00 Z= -2.843350681076D+00
I= 27 X= 6.210809082677D+00 Y= -1.117173645490D+00 Z= 3.536472097211D-01
I= 28 X= 5.267693755831D+00 Y= -4.367734933721D+00 Z= -4.795402143581D-01

I= 29 X= 2.842198248864D+00 Y= 3.189882841817D+00 Z= -2.460933409945D+00
I= 30 X= 2.600857630629D+00 Y= 3.671217215805D+00 Z= 2.155626858123D-01
I= 31 X= 4.179054227703D+00 Y= 1.744298546139D+00 Z= -3.193919554341D+00
I= 32 X= 2.468149377462D+00 Y= 4.567654297926D+00 Z= -3.440575104650D+00
I= 33 X= 1.928887498328D+00 Y= 5.602842013881D+00 Z= 4.546130922568D-01
I= 34 X= 3.957319940555D+00 Y= 3.107953825018D+00 Z= 1.663915148500D+00
I= 35 X= -4.150300046848D-02 Y= 1.166065271957D+00 Z= -4.063949429585D-01
I= 36 X= -2.826346059888D+00 Y= 3.454655501140D+00 Z= 2.358805937392D-01
I= 37 X= -2.147097423818D+00 Y= 5.469780082550D+00 Z= 9.674526487474D-01
I= 38 X= -4.208800974853D+00 Y= 2.269218395099D+00 Z= 1.238202667786D+00

Forward Direction:

Total Energy: -692.0036577 Hartrees

Potential Energy: -692.1777554 Hartress

Kinetic Energy: 0.1740977 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.643472361854D+13 Y= -1.716549022705D+13 Z= -2.071679359176D+13
I= 1 X= -1.803530347779D+12 Y= -1.062847369478D+13 Z= -1.213169397924D+13
I= 2 X= 4.249097314272D+11 Y= -1.003434654111D+13 Z= -2.443414238626D+12
I= 3 X= 2.291152785742D+13 Y= -1.651493481225D+13 Z= 1.603190024290D+13
I= 4 X= -7.403475140053D+12 Y= 6.540410673825D+12 Z= 5.550077893813D+11
I= 5 X= 8.156704510834D+12 Y= -1.126900427583D+12 Z= 2.987555379052D+12
I= 6 X= 1.233412694406D+13 Y= -1.768179056045D+13 Z= 3.059475483425D+13
I= 7 X= -7.069453208387D+13 Y= 5.618019069044D+13 Z= -8.736902017916D+13
I= 8 X= 1.337348235193D+13 Y= -2.645350584050D+13 Z= 1.128083857059D+13
I= 9 X= 1.086779733216D+13 Y= -6.648847387707D+12 Z= -2.127620685008D+12
I= 10 X= 3.456661607541D+13 Y= -3.711554865295D+13 Z= -1.054299212301D+13
I= 11 X= 8.946430310466D+13 Y= -2.559577068286D+13 Z= 6.436030879807D+13
I= 12 X= 5.619404487168D+12 Y= -1.850836322826D+13 Z= 1.614125163902D+13
I= 13 X= -6.286124052205D+12 Y= 2.675843593653D+13 Z= 3.511731073798D+12
I= 14 X= 2.359976983454D+13 Y= -1.973400473873D+13 Z= 8.395860574381D+13

I= 15 X= -7.675222321389D+13 Y= -1.331666695123D+14 Z= 3.548638754124D+13
I= 16 X= -9.313126254862D+12 Y= 2.130703139751D+13 Z= -2.405913958460D+13
I= 17 X= 9.224872057067D+12 Y= -8.073289870295D+12 Z= 9.819438214178D+11
I= 18 X= 7.065115748930D+13 Y= 2.866804918676D+13 Z= -2.704146033024D+13
I= 19 X= 2.235255700797D+13 Y= -2.909733755879D+13 Z= -8.781180072309D+13
I= 20 X= -5.535331814749D+13 Y= 6.742629331695D+12 Z= 5.259796239783D+13
I= 21 X= 2.630817150840D+13 Y= 2.613846790351D+12 Z= 8.474379668084D+12
I= 22 X= -9.665045112797D+12 Y= 1.589375972113D+14 Z= -6.688089773788D+12
I= 23 X= -4.393107095843D+13 Y= -1.199471047598D+13 Z= -3.916362190915D+13
I= 24 X= -4.572551081437D+13 Y= -3.054719072976D+13 Z= -6.218244316450D+12
I= 25 X= -4.842223327231D+12 Y= -5.571227401445D+12 Z= -1.416804081919D+13
I= 26 X= -1.033907474989D+14 Y= 2.842820279599D+13 Z= 6.110744963143D+13
I= 27 X= 1.036773379292D+14 Y= 9.311314654496D+13 Z= 9.398295702539D+13
I= 28 X= -3.882987837948D+13 Y= 6.544802261620D+13 Z= 1.977736200449D+13
I= 29 X= 4.376912958515D+12 Y= -1.256986873128D+13 Z= 1.051660226794D+13
I= 30 X= -2.097404386726D+13 Y= 1.253957067639D+13 Z= -9.720627872952D+12
I= 31 X= -1.095210138421D+13 Y= 7.868519052989D+13 Z= -7.426552358270D+13
I= 32 X= -1.198914905513D+13 Y= 2.190466211240D+13 Z= -5.539528160538D+13
I= 33 X= 3.182419258895D+13 Y= 5.308366761597D+13 Z= 6.041751362813D+13
I= 34 X= -3.718270235584D+13 Y= 5.000072565424D+13 Z= -1.206397868950D+14
I= 35 X= 2.331145072359D+12 Y= -6.226062990711D+10 Z= -1.103682092093D+12
I= 36 X= -7.154847221221D+12 Y= 9.199786532190D+12 Z= 3.122994190287D+13
I= 37 X= -6.467461273812D+13 Y= -1.948673642034D+12 Z= -9.548701370904D+12
I= 38 X= 6.596790610072D+13 Y= 5.830249937499D+13 Z= -7.098423643509D+13

Backward Direction:

Total Energy: -692.0036470 Hartrees

Potential Energy: -692.1777554 Hartress

Kinetic Energy: 0.1741083 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.644607304809D+13 Y= -1.652380315872D+13 Z= -1.957446102006D+13

I= 1 X= -1.791117051444D+12 Y= -1.062829733065D+13 Z= -1.213180520394D+13
I= 2 X= 9.358349238516D+11 Y= -1.001628780468D+13 Z= -1.885618803067D+12
I= 3 X= 2.290029042924D+13 Y= -1.715667016953D+13 Z= 1.488942117642D+13
I= 4 X= -6.892477942035D+12 Y= 6.522426189408D+12 Z= -2.726552149794D+09
I= 5 X= 8.615329530589D+12 Y= -6.718092298079D+12 Z= -3.016983525776D+12
I= 6 X= -1.828919987043D+13 Y= -1.767537054699D+13 Z= 3.059520701789D+13
I= 7 X= -7.699337083669D+13 Y= 5.179876281720D+13 Z= -9.595925428142D+13
I= 8 X= 1.113690280776D+13 Y= -3.189151058155D+13 Z= 9.670770608092D+12
I= 9 X= 1.199268958253D+13 Y= -8.665242723794D+12 Z= -2.598444507265D+12
I= 10 X= 3.412822806643D+13 Y= -3.952551622438D+13 Z= -1.156437884892D+13
I= 11 X= 9.086574094044D+13 Y= -2.937002571963D+13 Z= 6.402602656971D+13
I= 12 X= 8.247385914620D+12 Y= -2.030554950969D+13 Z= 1.627604022390D+13
I= 13 X= -5.161311478075D+12 Y= 2.877485052964D+13 Z= 3.982876530845D+12
I= 14 X= 2.316226333615D+13 Y= -1.732371855421D+13 Z= 8.498052061417D+13
I= 15 X= -7.412477031625D+13 Y= -1.313686768359D+14 Z= 3.535147348015D+13
I= 16 X= -7.912166503977D+12 Y= 2.508017885576D+13 Z= -2.372410371772D+13
I= 17 X= 8.987141406770D+12 Y= -8.091033597236D+12 Z= 3.029603586363D+12
I= 18 X= 7.071321333272D+13 Y= 2.958849836169D+13 Z= -2.266460510406D+13
I= 19 X= 2.224340882132D+13 Y= -2.838506503295D+13 Z= -8.707321634178D+13
I= 20 X= -5.621870171406D+13 Y= 4.123970729132D+12 Z= 5.488266783879D+13
I= 21 X= 2.438480424364D+13 Y= 2.614730724533D+12 Z= 8.473786630535D+12
I= 22 X= -1.458402397284D+13 Y= 1.589385352555D+14 Z= -6.689730187973D+12
I= 23 X= -4.508184420068D+13 Y= -9.648709047547D+12 Z= -3.914648166967D+13
I= 24 X= -4.687649472024D+13 Y= -3.289077791103D+13 Z= -6.236150118156D+12
I= 25 X= -5.079715617886D+12 Y= -5.553898620004D+12 Z= -1.621577176901D+13
I= 26 X= -1.042557170978D+14 Y= 3.104633403922D+13 Z= 5.882250533828D+13
I= 27 X= 1.035685610350D+14 Y= 9.239997516659D+13 Z= 9.324467472270D+13
I= 28 X= -3.876769310493D+13 Y= 6.452686998403D+13 Z= 1.540051278925D+13
I= 29 X= 4.835169224633D+12 Y= -6.980327943968D+12 Z= 1.651949958050D+13
I= 30 X= -1.956520761834D+13 Y= 1.233043068987D+13 Z= -4.041679096726D+12

I= 31 X= -1.318767638172D+13 Y= 8.412152786067D+13 Z= -7.265706079838D+13
I= 32 X= -1.828640409947D+13 Y= 2.628652539781D+13 Z= -4.680769721531D+13
I= 33 X= 3.091631438262D+13 Y= 4.947773425432D+13 Z= 7.179544511728D+13
I= 34 X= -3.625929080168D+13 Y= 4.630954513494D+13 Z= -1.169456521448D+14
I= 35 X= 2.241971520447D+12 Y= -6.204251496953D+10 Z= -1.103062236623D+12
I= 36 X= -5.746075296433D+12 Y= 9.408252014588D+12 Z= 2.555063174133D+13
I= 37 X= -6.558458237713D+13 Y= 1.659281799344D+12 Z= -2.092752809157D+13
I= 38 X= 6.689133915954D+13 Y= 6.199194317676D+13 Z= -7.467846982124D+13

Seed: 23239193623

CM Start Point Coordinates: bohr

I= 0 X= -2.163545092509D+00 Y= -1.933995483224D+00 Z= -9.600403314526D-02
I= 1 X= 4.753971621801D-02 Y= -2.619878849255D+00 Z= -1.469581147657D+00
I= 2 X= -1.315743908972D+00 Y= -1.322679342973D+00 Z= 2.552826575427D+00
I= 3 X= 2.177130358801D+00 Y= -2.060460184135D+00 Z= -1.165490129368D-01
I= 4 X= 1.367069202020D+00 Y= -1.479042476398D+00 Z= 2.394524212465D+00
I= 5 X= -2.666597657736D+00 Y= 3.410017321083D+00 Z= -2.502636609716D+00
I= 6 X= 1.153864679317D-01 Y= 1.911441108828D+00 Z= -2.964165814206D+00
I= 7 X= -2.043790345025D+00 Y= 4.976737278398D+00 Z= -3.728449378580D+00
I= 8 X= -3.908059151396D+00 Y= 2.041196804814D+00 Z= -3.556061040669D+00
I= 9 X= 2.877112976480D+00 Y= -6.341124642394D-01 Z= 4.692795307023D+00
I= 10 X= 3.507279171780D+00 Y= -2.563745023816D+00 Z= 6.051221861225D+00
I= 11 X= 4.577924089790D+00 Y= 5.805872825103D-01 Z= 4.125205532663D+00
I= 12 X= 1.500460233427D+00 Y= 3.377897416724D-01 Z= 6.491655511641D+00
I= 13 X= -3.017529612695D+00 Y= -7.318929290981D-01 Z= 4.838725308246D+00
I= 14 X= -2.640100149258D+00 Y= -2.260497177310D+00 Z= 6.396546145752D+00
I= 15 X= -2.887820650345D+00 Y= 1.009932012518D+00 Z= 5.929076543566D+00
I= 16 X= -5.134492023225D+00 Y= -1.305428591957D+00 Z= 4.232878167097D+00
I= 17 X= -4.758463211767D+00 Y= -2.210462465408D+00 Z= -9.694433358184D-01
I= 18 X= -5.389325760777D+00 Y= -4.283235497657D+00 Z= -4.342822182110D-01

I= 19 X= -5.766809380114D+00 Y= -8.776298997690D-01 Z= -1.434570648230D-01
I= 20 X= -4.828214961907D+00 Y= -2.027026021876D+00 Z= -3.034580490152D+00
I= 21 X= -1.572596137457D-01 Y= -4.118609223375D+00 Z= -3.924977534924D+00
I= 22 X= 2.085357450765D-01 Y= -6.420048478132D+00 Z= -3.489702606520D+00
I= 23 X= -1.762678869823D+00 Y= -3.575156425334D+00 Z= -4.879023656086D+00
I= 24 X= 1.477629439279D+00 Y= -3.504039142594D+00 Z= -5.225851313644D+00
I= 25 X= 4.740241106669D+00 Y= -2.392211575847D+00 Z= -1.031490232263D+00
I= 26 X= 4.897294007158D+00 Y= -2.182374451767D+00 Z= -3.361020041696D+00
I= 27 X= 6.097026262195D+00 Y= -1.079818220936D+00 Z= 1.185710983522D-01
I= 28 X= 5.253522625965D+00 Y= -4.565880172102D+00 Z= -6.350048689221D-01
I= 29 X= 2.717428538477D+00 Y= 3.414727553364D+00 Z= -2.374806805965D+00
I= 30 X= 2.863597134943D+00 Y= 3.812204598512D+00 Z= 8.038529857204D-02
I= 31 X= 4.184403039674D+00 Y= 2.217908245051D+00 Z= -3.466932135339D+00
I= 32 X= 1.524006894240D+00 Y= 4.940305710103D+00 Z= -3.589157981838D+00
I= 33 X= 1.524855676431D+00 Y= 5.343263638484D+00 Z= 8.853077643887D-01
I= 34 X= 4.092795128310D+00 Y= 2.943682155267D+00 Z= 1.760382923483D+00
I= 35 X= 8.478730119788D-02 Y= 1.078799933511D+00 Z= -4.460779824450D-01
I= 36 X= -2.963487018143D+00 Y= 3.589652862416D+00 Z= 1.760682119115D-01
I= 37 X= -2.125563348859D+00 Y= 5.475315255109D+00 Z= 8.636275515430D-01
I= 38 X= -4.425695923503D+00 Y= 2.612491253541D+00 Z= 9.494897501375D-01

Forward Direction:

Total Energy: -691.9947739 Hartrees

Potential Energy: -692.1636023 Hartress

Kinetic Energy: 0.1688284 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.138031184510D+12 Y= 8.078312947460D+12 Z= -1.331843918491D+13

I= 1 X= -7.146383751714D+10 Y= -1.482296145302D+13 Z= -1.244053160019D+13

I= 2 X= -4.720609296267D+13 Y= 2.605328224196D+12 Z= 1.553108143108D+13

I= 3 X= 1.539675277487D+13 Y= 4.234894234821D+12 Z= -1.376942429544D+13

I= 4 X= -3.777735057987D+12 Y= -4.616928604768D+12 Z= 4.358192480964D+12

I= 5 X= -1.750099623468D+13 Y= 1.230051335663D+13 Z= 9.463730621677D+12
I= 6 X= 2.343113470165D+13 Y= -3.403394617968D+13 Z= 3.205685350834D+13
I= 7 X= 6.808495558015D+12 Y= 9.766069568648D+13 Z= -8.244107349877D+13
I= 8 X= 8.609885878050D+13 Y= 1.493544054450D+13 Z= -4.905140723127D+13
I= 9 X= 8.784798460758D+12 Y= 5.351899323789D+12 Z= 9.460514452057D+11
I= 10 X= -1.143641357735D+13 Y= -5.547919157169D+13 Z= 9.949161295202D+13
I= 11 X= -8.962309423201D+13 Y= -1.186610340984D+13 Z= -2.718798079940D+13
I= 12 X= -7.701764757940D+13 Y= -3.923040039900D+13 Z= -8.605386627913D+12
I= 13 X= 8.011320212931D+12 Y= -6.883605880841D+12 Z= -1.397092281266D+13
I= 14 X= 7.721003392436D+13 Y= -1.314084929227D+13 Z= 6.069583901071D+13
I= 15 X= -3.319546769281D+13 Y= 8.280645953997D+13 Z= 1.176611053440D+14
I= 16 X= 2.661992281378D+13 Y= 3.374758589664D+13 Z= -2.292472818259D+13
I= 17 X= -3.465333326016D+12 Y= 6.520239589825D+12 Z= -5.882102449772D+12
I= 18 X= -3.633730702161D+13 Y= -7.162518748482D+13 Z= 4.236001828203D+13
I= 19 X= -1.305634443332D+13 Y= 3.354430108320D+13 Z= 3.552598886162D+13
I= 20 X= 4.355959552636D+13 Y= -4.449645687497D+13 Z= -4.492928891926D+13
I= 21 X= 7.551155834497D+12 Y= 1.370913824303D+11 Z= -1.475380046893D+13
I= 22 X= -2.093809948637D+12 Y= 2.890414647604D+13 Z= -1.412212652030D+12
I= 23 X= -1.193215691257D+14 Y= 3.699983254180D+13 Z= 2.849833650001D+13
I= 24 X= -9.328217189610D+13 Y= 3.364841713784D+13 Z= 3.946645563844D+13
I= 25 X= -1.156461839463D+13 Y= -1.466174499542D+13 Z= 8.143919924663D+12
I= 26 X= 6.252608007218D+13 Y= -4.459461799985D+13 Z= -8.659834957842D+13
I= 27 X= -3.614970712253D+13 Y= -7.093847763630D+13 Z= -3.321339932692D+12
I= 28 X= 1.145709617554D+14 Y= 5.574207750637D+13 Z= -1.144052079849D+13
I= 29 X= 9.020186368969D+12 Y= 1.417588856229D+13 Z= -4.545323410528D+12
I= 30 X= 2.859115428862D+13 Y= -2.210233082721D+12 Z= 9.773516635386D+12
I= 31 X= 8.335713856972D+12 Y= 7.487032831010D+12 Z= 1.308249524007D+14
I= 32 X= 8.199097711713D+13 Y= 1.808812732296D+13 Z= 3.631399548753D+13
I= 33 X= 5.227246016775D+13 Y= -7.796721855351D+13 Z= -9.730957721028D+13
I= 34 X= -2.264890235256D+12 Y= 2.418705313587D+12 Z= 6.344178984937D+12

I= 35 X= -8.223156235925D+10 Y= -1.502830617158D+12 Z= 1.111096892338D+12
I= 36 X= 8.139172151554D+12 Y= 9.590583110218D+12 Z= 7.978477954796D+12
I= 37 X= -2.992147903792D+13 Y= -1.027852546411D+14 Z= -3.162800331868D+13
I= 38 X= -8.366766683454D+12 Y= -2.769275466588D+13 Z= 4.037032074129D+13

Backward Direction:

Total Energy: -691.9947439 Hartrees

Potential Energy: -692.1636023 Hartress

Kinetic Energy: 0.1688583 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.121017945777D+12 Y= 8.735339157683D+12 Z= -1.223235313788D+13
I= 1 X= 1.166471857117D+11 Y= -1.482280347377D+13 Z= -1.244062537796D+13
I= 2 X= -4.680001542723D+13 Y= 2.468326945368D+12 Z= 1.608409103611D+13
I= 3 X= 1.541386362213D+13 Y= 3.577812740255D+12 Z= -1.485565264787D+13
I= 4 X= -3.371593669655D+12 Y= -4.479857813681D+12 Z= 3.805220592805D+12
I= 5 X= -1.674366052184D+13 Y= 7.285047373526D+12 Z= 3.883637305295D+12
I= 6 X= -1.276946405620D+13 Y= -3.402744759081D+13 Z= 3.205713065262D+13
I= 7 X= 4.223873269303D+11 Y= 9.470592605444D+13 Z= -8.996462681031D+13
I= 8 X= 8.344880729551D+13 Y= 1.100896133568D+13 Z= -5.057022646048D+13
I= 9 X= 9.737984095083D+12 Y= 3.635716297245D+12 Z= 5.015592287721D+11
I= 10 X= -1.188179109647D+13 Y= -5.757615346413D+13 Z= 9.852116599405D+13
I= 11 X= -8.841966774097D+13 Y= -1.513336618108D+13 Z= -2.748786780669D+13
I= 12 X= -7.473603604598D+13 Y= -4.077618168114D+13 Z= -8.471824743492D+12
I= 13 X= 8.964429838344D+12 Y= -5.167406076464D+12 Z= -1.352616090114D+13
I= 14 X= 7.676539725057D+13 Y= -1.104362367323D+13 Z= 6.166671750889D+13
I= 15 X= -3.091431706636D+13 Y= 8.435293916196D+13 Z= 1.175274362899D+14
I= 16 X= 2.782292953017D+13 Y= 3.701389136735D+13 Z= -2.262419229797D+13
I= 17 X= -3.630613902218D+12 Y= 6.537862380618D+12 Z= -4.113765628215D+12
I= 18 X= -3.619327335958D+13 Y= -7.084349229197D+13 Z= 4.608107837182D+13
I= 19 X= -1.318000406596D+13 Y= 3.412121007228D+13 Z= 3.619436931490D+13
I= 20 X= 4.287998850724D+13 Y= -4.669526002366D+13 Z= -4.296282951383D+13

I= 21 X= 5.925879808968D+12 Y= 1.378660530881D+11 Z= -1.475432048908D+13
I= 22 X= -6.262975501496D+12 Y= 2.890496433003D+13 Z= -1.413657511105D+12
I= 23 X= -1.203243687518D+14 Y= 3.897763561197D+13 Z= 2.855832394084D+13
I= 24 X= -9.428517074965D+13 Y= 3.167275438226D+13 Z= 3.940575724838D+13
I= 25 X= -1.172970458074D+13 Y= -1.467971534733D+13 Z= 6.375527497171D+12
I= 26 X= 6.184683569085D+13 Y= -4.239631673286D+13 Z= -8.856499772851D+13
I= 27 X= -3.627306748970D+13 Y= -7.151613583148D+13 Z= -3.989479756168D+12
I= 28 X= 1.147150725536D+14 Y= 5.495980738755D+13 Z= -1.516150857959D+13
I= 29 X= 9.777214693464D+12 Y= 1.918982923638D+13 Z= 1.033330584172D+12
I= 30 X= 3.018878717371D+13 Y= -2.139881446266D+12 Z= 1.464723127775D+13
I= 31 X= 5.687045069521D+12 Y= 1.141247472503D+13 Z= 1.323424542503D+14
I= 32 X= 7.560613540773D+13 Y= 2.104312226928D+13 Z= 4.383511366687D+13
I= 33 X= 5.145443135444D+13 Y= -8.109354136051D+13 Z= -8.735249745498D+13
I= 34 X= -1.606048055830D+12 Y= -8.564430716597D+11 Z= 9.812448970543D+12
I= 35 X= -2.840718646975D+11 Y= -1.502643947405D+12 Z= 1.111648779670D+12
I= 36 X= 9.736822656218D+12 Y= 9.519613016883D+12 Z= 3.104459112352D+12
I= 37 X= -3.074126177530D+13 Y= -9.965710143219D+13 Z= -4.158601946436D+13
I= 38 X= -7.707740072288D+12 Y= -2.441898610082D+13 Z= 3.690201332055D+13

Seed: 23251358091

CM Start Point Coordinates: bohr

I= 0 X= -2.179659478716D+00 Y= -2.156123638950D+00 Z= -5.322649674831D-02
I= 1 X= -9.105717116635D-02 Y= -2.777527895975D+00 Z= -1.458443388771D+00
I= 2 X= -1.292059114982D+00 Y= -1.234698982349D+00 Z= 2.514205212865D+00
I= 3 X= 2.112810498994D+00 Y= -1.917454031049D+00 Z= -9.058545793963D-03
I= 4 X= 1.260174961524D+00 Y= -1.121066413335D+00 Z= 2.345588183156D+00
I= 5 X= -2.754730234219D+00 Y= 3.510571694859D+00 Z= -2.212127382598D+00
I= 6 X= -1.779165074514D-02 Y= 2.065164203624D+00 Z= -3.197796198523D+00
I= 7 X= -2.106531136633D+00 Y= 5.289092146386D+00 Z= -3.276943445815D+00
I= 8 X= -4.169811528130D+00 Y= 2.241339361841D+00 Z= -2.814174439496D+00

I= 9 X= 2.973695062635D+00 Y= -7.372045962148D-01 Z= 4.524045029815D+00
I= 10 X= 2.842086138441D+00 Y= -1.943680086824D+00 Z= 6.144015661726D+00
I= 11 X= 4.966382978388D+00 Y= -8.913627191851D-01 Z= 3.996604496535D+00
I= 12 X= 2.834324425573D+00 Y= 1.351740695810D+00 Z= 5.135974862193D+00
I= 13 X= -2.844756359824D+00 Y= -6.411973220867D-01 Z= 4.717751589580D+00
I= 14 X= -2.812451932460D+00 Y= -2.212335835693D+00 Z= 5.842360115028D+00
I= 15 X= -2.500016541555D+00 Y= 1.133305209260D+00 Z= 5.867880700181D+00
I= 16 X= -4.729886252399D+00 Y= -3.328088558717D-01 Z= 3.963602037522D+00
I= 17 X= -4.906044896915D+00 Y= -2.603122978301D+00 Z= -9.140791980359D-01
I= 18 X= -5.491342936497D+00 Y= -4.626563834474D+00 Z= -7.040510530221D-01
I= 19 X= -6.096559043516D+00 Y= -1.299607490099D+00 Z= -2.557069035281D-02
I= 20 X= -5.306501048918D+00 Y= -2.515555883555D+00 Z= -3.174940600423D+00
I= 21 X= 1.252056606987D-01 Y= -4.170823445427D+00 Z= -3.958119911035D+00
I= 22 X= 7.050415650363D-01 Y= -6.138146891796D+00 Z= -3.842607706284D+00
I= 23 X= -2.045718505498D+00 Y= -3.979153226090D+00 Z= -4.783438592090D+00
I= 24 X= 1.532469917625D+00 Y= -3.195385728213D+00 Z= -5.311497511096D+00
I= 25 X= 4.865707980264D+00 Y= -2.522742868725D+00 Z= -7.224087990845D-01
I= 26 X= 5.572476622807D+00 Y= -3.254077249674D+00 Z= -2.736463236308D+00
I= 27 X= 6.318916412569D+00 Y= -9.829153460042D-01 Z= 9.050976680528D-02
I= 28 X= 5.696851486665D+00 Y= -4.461705997599D+00 Z= 2.546668676374D-01
I= 29 X= 2.809966082314D+00 Y= 3.625733891943D+00 Z= -2.356505599220D+00
I= 30 X= 2.778795229802D+00 Y= 3.635757854880D+00 Z= 4.761003938254D-01
I= 31 X= 3.842692468824D+00 Y= 2.148576455208D+00 Z= -3.227108809043D+00
I= 32 X= 2.210487208207D+00 Y= 5.343101368426D+00 Z= -3.302804894710D+00
I= 33 X= 1.983239955824D+00 Y= 5.179189075989D+00 Z= 1.557247030549D+00
I= 34 X= 4.500316888956D+00 Y= 2.142172119714D+00 Z= 1.365781815365D+00
I= 35 X= -6.846654719314D-02 Y= 1.071709843136D+00 Z= -6.672073941692D-01
I= 36 X= -2.710580008068D+00 Y= 3.914868004758D+00 Z= 3.188385709994D-01
I= 37 X= -1.651657975712D+00 Y= 5.415563365475D+00 Z= 1.389895898757D+00
I= 38 X= -3.829272186888D+00 Y= 2.711494006228D+00 Z= 1.552829247729D+00

Forward Direction:

Total Energy: -691.9992997 Hartrees

Potential Energy: -692.2040322 Hartress

Kinetic Energy: 0.2047325 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.168763565624D+11 Y= -1.210434524984D+13 Z= -9.072731143404D+12
I= 1 X= -2.436608009644D+12 Y= 7.659548509643D+12 Z= 1.950242521138D+13
I= 2 X= 1.302347111103D+13 Y= -1.202672006716D+13 Z= -1.856501795908D+13
I= 3 X= 1.632181385198D+13 Y= -6.129492662054D+12 Z= -1.171877259969D+13
I= 4 X= -1.406824646129D+13 Y= 5.336068093233D+12 Z= 2.288367651041D+13
I= 5 X= 7.904404220942D+12 Y= 2.075514016645D+13 Z= 2.658430192098D+13
I= 6 X= 2.946701741010D+13 Y= 2.660027545083D+13 Z= 7.051292045187D+13
I= 7 X= -1.557899334740D+13 Y= -7.551184395406D+13 Z= 7.283021150193D+13
I= 8 X= -1.100417209733D+14 Y= -6.333236359886D+13 Z= -1.578592267829D+13
I= 9 X= -1.356186228204D+13 Y= -1.437612464261D+13 Z= -1.260971825052D+12
I= 10 X= -2.701214033104D+13 Y= -4.969096961044D+13 Z= 4.474253716934D+13
I= 11 X= 1.830253134864D+14 Y= 5.430589301932D+13 Z= -4.534028803254D+13
I= 12 X= 6.681798968574D+12 Y= -2.666412817039D+13 Z= -2.180493986921D+13
I= 13 X= 1.185860710920D+13 Y= 1.520648226258D+13 Z= 1.340527696937D+13
I= 14 X= -1.662384689457D+13 Y= -7.579076103608D+13 Z= 1.836361538042D+13
I= 15 X= 9.928259603151D+12 Y= -1.648673733110D+13 Z= -1.185631363913D+14
I= 16 X= 8.059546222155D+13 Y= -5.802215919941D+12 Z= -3.762977475579D+12
I= 17 X= -5.847251972884D+12 Y= -2.779309899212D+13 Z= 4.642613392606D+12
I= 18 X= 1.046075045886D+14 Y= 5.369776143968D+13 Z= -1.125844639151D+14
I= 19 X= -9.726693912383D+13 Y= 8.761894468098D+13 Z= -7.777396235549D+12
I= 20 X= 4.029962509945D+13 Y= 6.030602367269D+13 Z= 2.669917518274D+13
I= 21 X= 6.605989233429D+12 Y= 1.422499144716D+12 Z= -2.198046863061D+13
I= 22 X= 2.051151769244D+13 Y= -1.205289028960D+14 Z= 1.421726111716D+13
I= 23 X= 2.905616631769D+13 Y= 2.896440188197D+13 Z= 1.338322547465D+13
I= 24 X= 3.515856902225D+13 Y= 7.662319606674D+13 Z= -9.027491513139D+13

I= 25 X= -3.767032655053D+13 Y= -1.215142466780D+13 Z= 2.767332751487D+12
I= 26 X= -5.163990260183D+13 Y= 2.745134012527D+13 Z= 6.341259685071D+13
I= 27 X= -4.368553849866D+13 Y= 4.465283054699D+13 Z= 1.204781848301D+13
I= 28 X= 4.220318117788D+13 Y= 6.940372518412D+12 Z= 8.444901784914D+12
I= 29 X= 1.642881450094D+13 Y= -3.146185734079D+12 Z= 1.978017218157D+13
I= 30 X= 3.567226143963D+11 Y= 2.421879083429D+13 Z= 2.519150905310D+11
I= 31 X= 2.798959456589D+13 Y= -4.763124719598D+13 Z= -1.255124785026D+14
I= 32 X= -5.465089708042D+13 Y= 5.472385425172D+13 Z= -3.200561309948D+13
I= 33 X= -5.593190136545D+13 Y= -5.102858759443D+13 Z= -4.538697295299D+13
I= 34 X= -5.505967460513D+12 Y= -5.745347326856D+13 Z= 6.612375898189D+12
I= 35 X= 8.543356900195D+11 Y= 1.707988249598D+12 Z= -2.870147664075D+12
I= 36 X= -8.835844336484D+12 Y= 1.128008972814D+13 Z= -2.178455492786D+13
I= 37 X= -4.454134722026D+13 Y= 8.326872544819D+13 Z= 4.069388771757D+13
I= 38 X= -1.630080403923D+13 Y= -9.309504042921D+13 Z= 9.181972150418D+13

Backward Direction:

Total Energy: -691.9993097 Hartrees

Potential Energy: -692.2040322 Hartress

Kinetic Energy: 0.2047225 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.459176366220D+11 Y= -1.128183978630D+13 Z= -7.858010592802D+12
I= 1 X= -1.896917477524D+12 Y= 7.659707086254D+12 Z= 1.950234273029D+13
I= 2 X= 1.332880234723D+13 Y= -1.246789920651D+13 Z= -1.790415195679D+13
I= 3 X= 1.639286516765D+13 Y= -6.952077508887D+12 Z= -1.293365788091D+13
I= 4 X= -1.376285240522D+13 Y= 5.777322912646D+12 Z= 2.222281473339D+13
I= 5 X= 9.351529907438D+12 Y= 1.570676665460D+13 Z= 2.058386129152D+13
I= 6 X= -2.425430241655D+13 Y= 2.660828074442D+13 Z= 7.051294507526D+13
I= 7 X= -2.346372977996D+13 Y= -7.655487636489D+13 Z= 6.561786873273D+13
I= 8 X= -1.139835863409D+14 Y= -6.540085070143D+13 Z= -1.746226860175D+13
I= 9 X= -1.271303644877D+13 Y= -1.592028715047D+13 Z= -1.752227419509D+12
I= 10 X= -2.756363835612D+13 Y= -5.167330971504D+13 Z= 4.365836294408D+13

I= 11 X= 1.841303202877D+14 Y= 5.125149436055D+13 Z= -4.564219385753D+13
I= 12 X= 8.828392138927D+12 Y= -2.808870677308D+13 Z= -2.164545443876D+13
I= 13 X= 1.270734739909D+13 Y= 1.675066068931D+13 Z= 1.389676680364D+13
I= 14 X= -1.717469818117D+13 Y= -7.380819896883D+13 Z= 1.944814032379D+13
I= 15 X= 1.207441494176D+13 Y= -1.506150516398D+13 Z= -1.187227188956D+14
I= 16 X= 8.170006432723D+13 Y= -2.748709073849D+12 Z= -3.460472361665D+12
I= 17 X= -5.918652726691D+12 Y= -2.770896521332D+13 Z= 6.286997844586D+12
I= 18 X= 1.049274180422D+14 Y= 5.439753154284D+13 Z= -1.092450286866D+14
I= 19 X= -9.744238643890D+13 Y= 8.807686148724D+13 Z= -7.093053203113D+12
I= 20 X= 3.980692487556D+13 Y= 5.839015599394D+13 Z= 2.851424886814D+13
I= 21 X= 5.168094305431D+12 Y= 1.423242822123D+12 Z= -2.198096836278D+13
I= 22 X= 1.679664958672D+13 Y= -1.205281263520D+14 Z= 1.421585950503D+13
I= 23 X= 2.810514303079D+13 Y= 3.070450196220D+13 Z= 1.353192166778D+13
I= 24 X= 3.420732488971D+13 Y= 7.488520029617D+13 Z= -9.042437479016D+13
I= 25 X= -3.774157016986D+13 Y= -1.223585961326D+13 Z= 1.122908479283D+12
I= 26 X= -5.213225530174D+13 Y= 2.936664531345D+13 Z= 6.159738314251D+13
I= 27 X= -4.386075087212D+13 Y= 4.419427314340D+13 Z= 1.136365744428D+13
I= 28 X= 4.252309470592D+13 Y= 6.240135535600D+12 Z= 5.105671275816D+12
I= 29 X= 1.787567710659D+13 Y= 1.900564950845D+12 Z= 2.577922983457D+13
I= 30 X= 2.625763538910D+12 Y= 2.480026007652D+13 Z= 4.721156428729D+12
I= 31 X= 2.405007437092D+13 Y= -4.556289671144D+13 Z= -1.238372161094D+14
I= 32 X= -6.253466388130D+13 Y= 5.576678631533D+13 Z= -2.479583678667D+13
I= 33 X= -5.676249330234D+13 Y= -5.396101599981D+13 Z= -3.585801159056D+13
I= 34 X= -5.178319612478D+12 Y= -6.067894182172D+13 Z= 1.040929468447D+13
I= 35 X= 4.099562979627D+11 Y= 1.708158337171D+12 Z= -2.869600347785D+12
I= 36 X= -6.566636609453D+12 Y= 1.069797148482D+13 Z= -2.625406294798D+13
I= 37 X= -4.537346277392D+13 Y= 8.620302901481D+13 Z= 3.116371987772D+13
I= 38 X= -1.597264366562D+13 Y= -8.987060816984D+13 Z= 8.802286605331D+13

Seed: 23568097734

CM Start Point Coordinates: bohr

I= 0 X= -2.313097431394D+00 Y= -2.052451720476D+00 Z= -3.172267866721D-02
I= 1 X= -1.001267262518D-01 Y= -2.688499031060D+00 Z= -1.531713173082D+00
I= 2 X= -1.382520625187D+00 Y= -1.257191518194D+00 Z= 2.447647404816D+00
I= 3 X= 2.143609866435D+00 Y= -2.038668977684D+00 Z= 3.471811829043D-03
I= 4 X= 1.284776517581D+00 Y= -1.438163231112D+00 Z= 2.525933879506D+00
I= 5 X= -2.899947390650D+00 Y= 3.149743182111D+00 Z= -2.170105560182D+00
I= 6 X= -2.921220319029D-01 Y= 1.467644741117D+00 Z= -3.165648759648D+00
I= 7 X= -2.492001050485D+00 Y= 4.553180670275D+00 Z= -3.794152618042D+00
I= 8 X= -4.307661477324D+00 Y= 1.609938039851D+00 Z= -2.867216304939D+00
I= 9 X= 2.989110841166D+00 Y= -7.927453268233D-01 Z= 4.765057112725D+00
I= 10 X= 3.738235472015D+00 Y= -2.923741322503D+00 Z= 5.468429726410D+00
I= 11 X= 4.874945952754D+00 Y= 2.008428888092D-01 Z= 3.563611121081D+00
I= 12 X= 2.089256427929D+00 Y= 2.872176861531D-01 Z= 6.910025415243D+00
I= 13 X= -2.864214937686D+00 Y= -7.737469811421D-01 Z= 4.715391955671D+00
I= 14 X= -2.660404806544D+00 Y= -2.187463305108D+00 Z= 6.360690038153D+00
I= 15 X= -2.615209696135D+00 Y= 1.038014988400D+00 Z= 5.801755644165D+00
I= 16 X= -5.044316445634D+00 Y= -6.918481216531D-01 Z= 4.459861536533D+00
I= 17 X= -4.913027998146D+00 Y= -2.248386842186D+00 Z= -8.959905058982D-01
I= 18 X= -5.340935872680D+00 Y= -4.228500959279D+00 Z= -7.380564065356D-01
I= 19 X= -6.176836886892D+00 Y= -1.137014121360D+00 Z= 1.678369566994D-01
I= 20 X= -5.075196035451D+00 Y= -2.107114582260D+00 Z= -3.021659632722D+00
I= 21 X= 4.143246930710D-02 Y= -4.079633425120D+00 Z= -4.076437798735D+00
I= 22 X= 3.924367972327D-01 Y= -5.893433372526D+00 Z= -3.495845902508D+00
I= 23 X= -1.689223971355D+00 Y= -4.134122492681D+00 Z= -5.117684738414D+00
I= 24 X= 1.741895530193D+00 Y= -3.512284133438D+00 Z= -5.319053349110D+00
I= 25 X= 4.772045174765D+00 Y= -2.532548169509D+00 Z= -7.412672542629D-01
I= 26 X= 4.971715792048D+00 Y= -2.729719556366D+00 Z= -2.772709643704D+00
I= 27 X= 6.190332503473D+00 Y= -1.204902781284D+00 Z= -3.843028726965D-01
I= 28 X= 5.553341796212D+00 Y= -4.402476414781D+00 Z= 3.058453815198D-01

I= 29 X= 2.866626403976D+00 Y= 3.371079468260D+00 Z= -2.266010319500D+00
I= 30 X= 2.524439578230D+00 Y= 3.937189342767D+00 Z= 2.231713144424D-01
I= 31 X= 4.486758775911D+00 Y= 2.279821905019D+00 Z= -3.571043548789D+00
I= 32 X= 2.046655874186D+00 Y= 4.690615372837D+00 Z= -3.538285366258D+00
I= 33 X= 1.475098591144D+00 Y= 5.866384758192D+00 Z= 7.036566840680D-01
I= 34 X= 3.955977507157D+00 Y= 2.907071495797D+00 Z= 1.580787121675D+00
I= 35 X= 1.303648647760D-01 Y= 1.185543097612D+00 Z= -6.547971995599D-01
I= 36 X= -2.805172028178D+00 Y= 3.784572061076D+00 Z= 2.315588150419D-01
I= 37 X= -2.025556675340D+00 Y= 5.640871704706D+00 Z= 8.593359104087D-01
I= 38 X= -3.608684035500D+00 Y= 2.671759827625D+00 Z= 1.803732151757D+00

Forward Direction:

Total Energy: -691.9977724 Hartrees

Potential Energy: -692.1814916 Hartress

Kinetic Energy: 0.1837192 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.751552715877D+13 Y= -1.028966879244D+13 Z= -1.548475753653D+13
I= 1 X= 5.599251240102D+12 Y= -5.182171232026D+12 Z= -2.563755191016D+12
I= 2 X= 2.074127795957D+13 Y= -1.095688314957D+13 Z= 1.341727914809D+13
I= 3 X= 8.634434765587D+11 Y= 1.154888707513D+13 Z= -1.873354249010D+13
I= 4 X= -2.666042085286D+13 Y= 9.438411962892D+12 Z= -1.162918217570D+13
I= 5 X= -1.763815575074D+12 Y= -1.846345019805D+13 Z= 7.630462411651D+12
I= 6 X= 6.229883011535D+13 Y= -1.946025372927D+13 Z= -1.546138507317D+13
I= 7 X= -4.734519652500D+13 Y= 3.845738172537D+13 Z= 2.111521154914D+13
I= 8 X= -8.780895088478D+13 Y= -5.829698119756D+13 Z= -7.209081181725D+13
I= 9 X= -3.442981346133D+12 Y= 2.579880547355D+12 Z= 1.943188886132D+13
I= 10 X= -7.291989172008D+13 Y= 8.537676913334D+13 Z= -1.188590437260D+14
I= 11 X= 1.021944189521D+14 Y= 8.934612883708D+13 Z= -1.732053029243D+13
I= 12 X= 9.127807278461D+13 Y= -7.645184270797D+13 Z= 2.543656730300D+13
I= 13 X= 7.230595193297D+11 Y= -1.356807883054D+13 Z= -3.665777183912D+12
I= 14 X= -8.343801855232D+12 Y= -1.107746739776D+14 Z= -1.004808103031D+13

I= 15 X= -2.838509569408D+13 Y= 5.338416232392D+13 Z= -2.506414802195D+13
I= 16 X= -3.066192796045D+13 Y= -3.990312739704D+13 Z= 2.118362371969D+13
I= 17 X= -1.203728808248D+13 Y= 3.474782621676D+12 Z= -7.974796164916D+12
I= 18 X= 3.752563111982D+13 Y= -7.299764793602D+13 Z= 1.022699968276D+14
I= 19 X= 3.885225165854D+13 Y= 7.630009649365D+12 Z= 4.267179340956D+12
I= 20 X= 6.062364477304D+11 Y= 1.170627450288D+14 Z= -7.181092967266D+12
I= 21 X= -1.048598540951D+13 Y= 6.733852114476D+12 Z= 2.316212452875D+12
I= 22 X= -5.656781214413D+13 Y= -4.200296262426D+13 Z= 2.155626900183D+12
I= 23 X= 1.033752870103D+13 Y= -2.981888238852D+13 Z= 1.109366728786D+14
I= 24 X= 7.692414674933D+12 Y= 3.113118076974D+13 Z= 3.670546872371D+13
I= 25 X= 4.484033088517D+12 Y= 6.979185658909D+12 Z= 1.292030409433D+13
I= 26 X= -2.462900153110D+13 Y= 2.701664983058D+13 Z= 8.163211101289D+13
I= 27 X= 6.078387187624D+13 Y= 7.495987590475D+13 Z= -3.161817527044D+13
I= 28 X= 4.060995314270D+13 Y= -1.434871105109D+14 Z= 4.848665682360D+13
I= 29 X= 2.563382231194D+13 Y= -1.099018697431D+13 Z= -8.084474085186D+12
I= 30 X= 8.049052145530D+11 Y= -1.088515234168D+13 Z= -8.181689009723D+12
I= 31 X= -5.227995262895D+13 Y= 1.100060545227D+14 Z= 2.339581254240D+13
I= 32 X= 1.428444020738D+13 Y= 1.011817147064D+13 Z= -1.575204785301D+13
I= 33 X= -1.089556771042D+14 Y= 7.633664195083D+13 Z= 2.111763465489D+13
I= 34 X= -7.267869712960D+13 Y= -5.166094661581D+13 Z= -5.676998391536D+13
I= 35 X= 6.197715768089D+12 Y= 5.633254552992D+12 Z= -9.873737702570D+10
I= 36 X= 5.149224663506D+11 Y= -3.517522715595D+12 Z= 3.285158379434D+12
I= 37 X= 1.918890010956D+13 Y= -1.817288778001D+13 Z= 4.387145544377D+13
I= 38 X= 1.090359279713D+13 Y= 1.259553317593D+14 Z= 3.955161603542D+13

Backward Direction:

Total Energy: -691.9977675 Hartrees

Potential Energy: -692.1814916 Hartress

Kinetic Energy: 0.1837241 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.736830940412D+13 Y= -9.050944421036D+12 Z= -1.377308618508D+13

I= 1 X= 6.659221980546D+12 Y= -5.181964257200D+12 Z= -2.563851016914D+12
I= 2 X= 2.103615518564D+13 Y= -1.184043569684D+13 Z= 1.438703421548D+13
I= 3 X= 1.010776611398D+12 Y= 1.031003489086D+13 Z= -2.044545097734D+13
I= 4 X= -2.636546292423D+13 Y= 1.032206925081D+13 Z= -1.259896571941D+13
I= 5 X= 8.211063643594D+11 Y= -2.506682871301D+13 Z= -6.060265089525D+11
I= 6 X= -2.543545927273D+13 Y= -1.944830325679D+13 Z= -1.546160991321D+13
I= 7 X= -5.913070482625D+13 Y= 3.904458607008D+13 Z= 1.204569678418D+13
I= 8 X= -9.425287514068D+13 Y= -5.909896274339D+13 Z= -7.443262684862D+13
I= 9 X= -2.444481029517D+12 Y= 7.452993898927D+11 Z= 1.874500638521D+13
I= 10 X= -7.374555055988D+13 Y= 8.291356233940D+13 Z= -1.203856595908D+14
I= 11 X= 1.035323528245D+14 Y= 8.558768632449D+13 Z= -1.771548111024D+13
I= 12 X= 9.393428969421D+13 Y= -7.818248997474D+13 Z= 2.567048916373D+13
I= 13 X= 1.721438758083D+12 Y= -1.173347779819D+13 Z= -2.978625867220D+12
I= 14 X= -9.168714800616D+12 Y= -1.083112209989D+14 Z= -8.521090670158D+12
I= 15 X= -2.572942527443D+13 Y= 5.511561440714D+13 Z= -2.529818603379D+13
I= 16 X= -2.932450530638D+13 Y= -3.614577891514D+13 Z= 2.157930405724D+13
I= 17 X= -1.203471481998D+13 Y= 3.651927713078D+12 Z= -5.960892754067D+12
I= 18 X= 3.812086652339D+13 Y= -7.217030679732D+13 Z= 1.062277216732D+14
I= 19 X= 3.857124823194D+13 Y= 8.104900931550D+12 Z= 5.174013866846D+12
I= 20 X= 1.551605482851D+11 Y= 1.148572516271D+14 Z= -4.972961147082D+12
I= 21 X= -1.216664634926D+13 Y= 6.734788427421D+12 Z= 2.315582752753D+12
I= 22 X= -6.094020022941D+13 Y= -4.200199403395D+13 Z= 2.153846826758D+12
I= 23 X= 9.152542321714D+12 Y= -2.779612127428D+13 Z= 1.112204182278D+14
I= 24 X= 6.507118888593D+12 Y= 2.911112165081D+13 Z= 3.642067642463D+13
I= 25 X= 4.486772892494D+12 Y= 6.801695965802D+12 Z= 1.090636474913D+13
I= 26 X= -2.507964086948D+13 Y= 2.922134950583D+13 Z= 7.942384681477D+13
I= 27 X= 6.050310803285D+13 Y= 7.448426052711D+13 Z= -3.252483334483D+13
I= 28 X= 4.120511066582D+13 Y= -1.443149504749D+14 Z= 4.452933347464D+13
I= 29 X= 2.821844698652D+13 Y= -4.389019546486D+12 Z= 1.502723398981D+11
I= 30 X= 4.440761995505D+12 Y= -9.608530900403D+12 Z= -2.776886267053D+12

I= 31 X= -5.871984589045D+13 Y= 1.108087745285D+14 Z= 2.573645535078D+13
I= 32 X= 2.499891741900D+12 Y= 9.530505226680D+12 Z= -6.686006637516D+12
I= 33 X= -1.100493806458D+14 Y= 7.271763457554D+13 Z= 3.308305754073D+13
I= 34 X= -7.258918632529D+13 Y= -5.580800706588D+13 Z= -5.149441207495D+13
I= 35 X= 5.372696700398D+12 Y= 5.633459022862D+12 Z= -9.802976207048D+10
I= 36 X= 4.151148027816D+12 Y= -4.795019777649D+12 Z= -2.119953290568D+12
I= 37 X= 1.809344802620D+13 Y= -1.455139452952D+13 Z= 3.190418769789D+13
I= 38 X= 1.099410428354D+13 Y= 1.301013930430D+14 Z= 3.427622910842D+13

Seed: 24369831866

CM Start Point Coordinates: bohr

I= 0 X= -2.175061624079D+00 Y= -2.160012797770D+00 Z= -3.607213726790D-02
I= 1 X= -5.352856559206D-02 Y= -2.711297357952D+00 Z= -1.616142027069D+00
I= 2 X= -1.353107649008D+00 Y= -1.175818305031D+00 Z= 2.430120857898D+00
I= 3 X= 2.172625312547D+00 Y= -2.071986819039D+00 Z= -2.255420756039D-01
I= 4 X= 1.355486586912D+00 Y= -1.108584741698D+00 Z= 2.283400449051D+00
I= 5 X= -2.573942037705D+00 Y= 3.502429532177D+00 Z= -2.317887842699D+00
I= 6 X= 3.479607188728D-01 Y= 1.445661727732D+00 Z= -3.286945385584D+00
I= 7 X= -1.676978639624D+00 Y= 5.450717253977D+00 Z= -3.242134066893D+00
I= 8 X= -3.822934745903D+00 Y= 2.305522293341D+00 Z= -3.271846848057D+00
I= 9 X= 2.844127764804D+00 Y= -6.992710196902D-01 Z= 4.600518462101D+00
I= 10 X= 3.133217442662D+00 Y= -2.556319797318D+00 Z= 5.458990781370D+00
I= 11 X= 5.007474849790D+00 Y= -8.803883567892D-03 Z= 4.246770113472D+00
I= 12 X= 2.007741276133D+00 Y= 7.343758788421D-01 Z= 6.101073898914D+00
I= 13 X= -2.893309967935D+00 Y= -5.484515620757D-01 Z= 4.651615769176D+00
I= 14 X= -2.076933456444D+00 Y= -1.788341953449D+00 Z= 6.609262429512D+00
I= 15 X= -2.656678160603D+00 Y= 1.948953482204D+00 Z= 4.848231352272D+00
I= 16 X= -5.069376528310D+00 Y= -1.759156768487D+00 Z= 4.240972164650D+00
I= 17 X= -5.020851245992D+00 Y= -2.470824282027D+00 Z= -6.539674447478D-01
I= 18 X= -5.838047883953D+00 Y= -4.288047519525D+00 Z= 2.826282637944D-01

I= 19 X= -6.116213165204D+00 Y= -8.476737414307D-01 Z= -3.752356389795D-03
I= 20 X= -5.256454418722D+00 Y= -2.612355386401D+00 Z= -2.587615577246D+00
I= 21 X= 1.326702322438D-01 Y= -4.125608583173D+00 Z= -3.960351725190D+00
I= 22 X= 4.981886493365D-01 Y= -6.372789183552D+00 Z= -3.562455537838D+00
I= 23 X= -1.850825482437D+00 Y= -4.252384491029D+00 Z= -4.757385571793D+00
I= 24 X= 1.382796541301D+00 Y= -3.480267573090D+00 Z= -5.701644747765D+00
I= 25 X= 4.811971783471D+00 Y= -2.504846499729D+00 Z= -8.634570162158D-01
I= 26 X= 5.170855843063D+00 Y= -2.377546442578D+00 Z= -2.974994802461D+00
I= 27 X= 6.097714876608D+00 Y= -1.275529229709D+00 Z= 1.899235079208D-01
I= 28 X= 5.454232204487D+00 Y= -4.365996328359D+00 Z= -4.797633645723D-01
I= 29 X= 2.920120958170D+00 Y= 3.552326826443D+00 Z= -2.155626675579D+00
I= 30 X= 2.666343179216D+00 Y= 3.753508294061D+00 Z= 4.255629028612D-01
I= 31 X= 4.149061705706D+00 Y= 2.226351294093D+00 Z= -2.778337238891D+00
I= 32 X= 2.479241298724D+00 Y= 4.677853232556D+00 Z= -3.831718966391D+00
I= 33 X= 1.877865940386D+00 Y= 5.610259029569D+00 Z= 1.288819123397D+00
I= 34 X= 3.930109629209D+00 Y= 2.994239175260D+00 Z= 1.915310891259D+00
I= 35 X= -3.460869032626D-02 Y= 1.091750489957D+00 Z= -6.204679739824D-01
I= 36 X= -2.707771799486D+00 Y= 3.456575294787D+00 Z= 3.492645589691D-01
I= 37 X= -2.269535823051D+00 Y= 5.336646430092D+00 Z= 1.521823433394D+00
I= 38 X= -4.376274607794D+00 Y= 2.661272242544D+00 Z= 1.391070210838D+00

Forward Direction:

Total Energy: -691.9910062 Hartrees

Potential Energy: -692.1747952 Hartress

Kinetic Energy: 0.1837890 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.414473880561D+13 Y= -8.753312115412D+12 Z= 2.796180357579D+13
I= 1 X= 6.892347313324D+12 Y= -4.356187778936D+12 Z= 1.830997170568D+13
I= 2 X= -7.214337018339D+12 Y= -4.741196270950D+12 Z= -2.615249218528D+13
I= 3 X= -1.938295148071D+12 Y= 9.612656123959D+12 Z= 2.152482486125D+13
I= 4 X= -1.576580134750D+13 Y= 6.265204016735D+12 Z= 2.582443770516D+11

I= 5 X= -3.692770398876D+12 Y= 2.249472749177D+13 Z= 1.354186762545D+12
I= 6 X= 5.777082522838D+13 Y= -3.213796118128D+13 Z= 7.163691189414D+13
I= 7 X= -4.707773171619D+13 Y= -1.282458372297D+14 Z= 1.107095690419D+14
I= 8 X= -5.191953755241D+13 Y= 4.962536682477D+13 Z= -3.483434923755D+13
I= 9 X= -1.761126978323D+13 Y= 3.830927904003D+12 Z= -1.974261106621D+13
I= 10 X= -2.254308601057D+13 Y= -6.743463310621D+13 Z= -1.316510868094D+13
I= 11 X= 1.257194576482D+14 Y= -9.828166742183D+12 Z= 7.815492281741D+11
I= 12 X= 4.435509823263D+13 Y= -2.369850614742D+13 Z= -7.716928614404D+13
I= 13 X= -4.301280269614D+12 Y= 1.594349657750D+13 Z= 5.945340041511D+12
I= 14 X= -2.530221766548D+13 Y= 6.256020359433D+13 Z= -4.328237000289D+13
I= 15 X= -1.472810411881D+13 Y= -1.062475357997D+14 Z= 1.294139276151D+13
I= 16 X= 6.095279702933D+11 Y= -6.798502161093D+13 Z= 9.182596419751D+13
I= 17 X= 5.059477700904D+12 Y= 2.034384312525D+12 Z= -6.325210699353D+12
I= 18 X= 7.686004995590D+13 Y= 8.066699933890D+13 Z= 2.830771022292D+13
I= 19 X= -1.613835124828D+13 Y= -9.830890223980D+13 Z= 3.870767238893D+13
I= 20 X= -6.590846932483D+13 Y= 2.554192201685D+13 Z= -1.239147461918D+14
I= 21 X= -2.852231940513D+12 Y= 1.415394407526D+12 Z= -2.311918677649D+13
I= 22 X= -2.925556821299D+13 Y= -5.080562746522D+13 Z= 5.016856212951D+13
I= 23 X= -3.302418670275D+13 Y= 2.735505868205D+13 Z= -8.384282405142D+13
I= 24 X= 6.903199174150D+13 Y= 2.664239016504D+13 Z= -2.438763279686D+13
I= 25 X= 1.965021507093D+12 Y= -1.207564427799D+13 Z= 2.056529467660D+13
I= 26 X= -5.672889156938D+13 Y= 2.681380747780D+13 Z= 2.069442557902D+13
I= 27 X= 2.427458309900D+13 Y= -5.778137009944D+12 Z= 2.744754612383D+13
I= 28 X= -5.645024641485D+13 Y= 1.415091830797D+14 Z= -5.610712456264D+13
I= 29 X= 8.827935390416D+12 Y= -3.585852378052D+12 Z= 1.157016444088D+11
I= 30 X= 9.436568065323D+12 Y= -2.219361407115D+13 Z= -1.470563446834D+13
I= 31 X= -2.124655895193D+13 Y= -4.167908958270D+12 Z= 1.202436874595D+14
I= 32 X= -1.996063339718D+13 Y= -7.204777486297D+12 Z= -4.520056697590D+12
I= 33 X= 3.344467179139D+12 Y= 9.751415413520D+13 Z= 3.294204234365D+13
I= 34 X= 6.996279539359D+13 Y= -3.812475956832D+13 Z= 3.926270674412D+12

I= 35 X= -4.542911644919D+12 Y= -1.344952483974D+12 Z= -4.436476931239D+12

I= 36 X= 1.675635643540D+13 Y= 1.617574013539D+13 Z= 5.692705391929D+12

I= 37 X= 5.288756641888D+13 Y= -7.883453297199D+13 Z= -1.612222860134D+13

I= 38 X= -3.352462115716D+13 Y= -3.524544117559D+12 Z= -1.266855941221D+13

Backward Direction:

Total Energy: -691.9909946 Hartrees

Potential Energy: -692.1747952 Hartress

Kinetic Energy: 0.1838007 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.415610243697D+13 Y= -7.365656514538D+12 Z= 3.032733543147D+13

I= 1 X= 7.139143225197D+12 Y= -4.355834719954D+12 Z= 1.830975643645D+13

I= 2 X= -6.256249337826D+12 Y= -4.897129883515D+12 Z= -2.496897503439D+13

I= 3 X= -1.926710709948D+12 Y= 8.224888751688D+12 Z= 1.915898592497D+13

I= 4 X= -1.480757032649D+13 Y= 6.421289993037D+12 Z= -9.251717197715D+11

I= 5 X= -2.340154627645D+12 Y= 1.129327021247D+13 Z= -1.091845253828D+13

I= 6 X= -1.452837526607D+13 Y= -3.212417190488D+13 Z= 7.163765667742D+13

I= 7 X= -6.061966395224D+13 Y= -1.358003650533D+14 Z= 9.372820287314D+13

I= 8 X= -5.720761444807D+13 Y= 3.992407461711D+13 Z= -3.815345078259D+13

I= 9 X= -1.542771647007D+13 Y= -9.264183656803D+10 Z= -2.071363973140D+13

I= 10 X= -2.348672880306D+13 Y= -7.218146677177D+13 Z= -1.527937372035D+13

I= 11 X= 1.284597682215D+14 Y= -1.724113349636D+13 Z= 1.118121584354D+11

I= 12 X= 4.952501549178D+13 Y= -2.721580895086D+13 Z= -7.688338291707D+13

I= 13 X= -2.117892319363D+12 Y= 1.986710428818D+13 Z= 6.916989522525D+12

I= 14 X= -2.624415709628D+13 Y= 6.730764788425D+13 Z= -4.116709972519D+13

I= 15 X= -9.559229264974D+12 Y= -1.027286488298D+14 Z= 1.265524494048D+13

I= 16 X= 3.348892113299D+12 Y= -6.057422837461D+13 Z= 9.249717704202D+13

I= 17 X= 4.643360746114D+12 Y= 2.040894687880D+12 Z= -2.308773272559D+12

I= 18 X= 7.709518603659D+13 Y= 8.245589292825D+13 Z= 3.681914528308D+13

I= 19 X= -1.638931079047D+13 Y= -9.695970112549D+13 Z= 4.019469437372D+13

I= 20 X= -6.752096752267D+13 Y= 2.048403647805D+13 Z= -1.194416097968D+14

I= 21 X= -6.580075805935D+12 Y= 1.417142454045D+12 Z= -2.312035985035D+13
I= 22 X= -3.880520282731D+13 Y= -5.080377772772D+13 Z= 5.016530911029D+13
I= 23 X= -3.529269315347D+13 Y= 3.189627107681D+13 Z= -8.375254168216D+13
I= 24 X= 6.676305037207D+13 Y= 2.210598283671D+13 Z= -2.447947918871D+13
I= 25 X= 1.549357672721D+12 Y= -1.208295505761D+13 Z= 1.654872480533D+13
I= 26 X= -5.834057162671D+13 Y= 3.187060020542D+13 Z= 1.622084249882D+13
I= 27 X= 2.402432501406D+13 Y= -7.129067473375D+12 Z= 2.596109085026D+13
I= 28 X= -5.621489989612D+13 Y= 1.397189503704D+14 Z= -6.461846377760D+13
I= 29 X= 1.017984176659D+13 Y= 7.612241683480D+12 Z= 1.238509382499D+13
I= 30 X= 1.267771130136D+13 Y= -2.228913139915D+13 Z= -3.604834607208D+12
I= 31 X= -2.653201939672D+13 Y= 5.530617638864D+12 Z= 1.235597267875D+14
I= 32 X= -3.349958614230D+13 Y= 3.504153838493D+11 Z= 1.245592793295D+13
I= 33 X= 1.521055408078D+12 Y= 9.042580273443D+13 Z= 5.542414333869D+13
I= 34 X= 7.160023455032D+13 Y= -4.547463056729D+13 Z= 1.152091061765D+13
I= 35 X= -4.874360957276D+12 Y= -1.344526792964D+12 Z= -4.435240301935D+12
I= 36 X= 1.999746521266D+13 Y= 1.626988940227D+13 Z= -5.408793459350D+12
I= 37 X= 5.106011782997D+13 Y= -7.174210974932D+13 Z= -3.860629033181D+13
I= 38 X= -3.188693186594D+13 Y= 3.822070873371D+12 Z= -2.026333297440D+13

Seed: 25612201332

CM Start Point Coordinates: bohr

I= 0 X= -2.177593453249D+00 Y= -2.099940130023D+00 Z= -1.122117038965D-01
I= 1 X= 3.038031203014D-02 Y= -2.698919209463D+00 Z= -1.506813561182D+00
I= 2 X= -1.558400265707D+00 Y= -1.231027902734D+00 Z= 2.356612002906D+00
I= 3 X= 2.058850430079D+00 Y= -1.924202251741D+00 Z= 7.115419365652D-03
I= 4 X= 1.169885824084D+00 Y= -1.167329706575D+00 Z= 2.605333390000D+00
I= 5 X= -2.930955724101D+00 Y= 3.082262220736D+00 Z= -2.058552666939D+00
I= 6 X= -3.014436023416D-02 Y= 5.764628655470D-01 Z= -3.349467814405D+00
I= 7 X= -2.666753454079D+00 Y= 4.373044073612D+00 Z= -3.855452784086D+00
I= 8 X= -4.360331503004D+00 Y= 1.667344774905D+00 Z= -2.455356994561D+00

I= 9 X= 2.731091647203D+00 Y= -7.708346015773D-01 Z= 4.838998786777D+00
I= 10 X= 2.775784674431D+00 Y= -2.626561187320D+00 Z= 5.986529193837D+00
I= 11 X= 4.628277504080D+00 Y= -1.224487214014D-01 Z= 4.359039965248D+00
I= 12 X= 1.723090010495D+00 Y= 6.917221830638D-01 Z= 6.064527383991D+00
I= 13 X= -2.906788099246D+00 Y= -8.045885496845D-01 Z= 4.779195639233D+00
I= 14 X= -2.243742697797D+00 Y= -2.265522184459D+00 Z= 6.469322309870D+00
I= 15 X= -2.692844974824D+00 Y= 1.152474543329D+00 Z= 5.302677322245D+00
I= 16 X= -5.140049202141D+00 Y= -8.217880287363D-01 Z= 4.347777140387D+00
I= 17 X= -4.850962426187D+00 Y= -2.698838926844D+00 Z= -5.939520724526D-01
I= 18 X= -5.534415653757D+00 Y= -4.092890497434D+00 Z= 7.095804710931D-01
I= 19 X= -6.074007593100D+00 Y= -1.067285715891D+00 Z= -1.477312690277D-01
I= 20 X= -5.481556382618D+00 Y= -2.775488775895D+00 Z= -2.387299789905D+00
I= 21 X= 2.705638412260D-01 Y= -3.465563960035D+00 Z= -4.222157314057D+00
I= 22 X= 5.079914729812D-01 Y= -5.405295834486D+00 Z= -4.287185822732D+00
I= 23 X= -1.273622825120D+00 Y= -3.288409475123D+00 Z= -5.482431927122D+00
I= 24 X= 1.792312467669D+00 Y= -2.498457989323D+00 Z= -5.203119236977D+00
I= 25 X= 4.818269820339D+00 Y= -2.641882773849D+00 Z= -5.199366855290D-01
I= 26 X= 5.369600346479D+00 Y= -3.498177730885D+00 Z= -2.309463376299D+00
I= 27 X= 6.481916599129D+00 Y= -1.656738558564D+00 Z= 2.068935876991D-01
I= 28 X= 5.384190215539D+00 Y= -4.357735746335D+00 Z= 8.512579000730D-01
I= 29 X= 2.620748877637D+00 Y= 3.777950233351D+00 Z= -2.588384888512D+00
I= 30 X= 3.138461724516D+00 Y= 3.458338812155D+00 Z= 2.793195866756D-02
I= 31 X= 3.654527543201D+00 Y= 2.352819989210D+00 Z= -3.949250972093D+00
I= 32 X= 1.332543301602D+00 Y= 5.196026720325D+00 Z= -3.064412992918D+00
I= 33 X= 2.132076512967D+00 Y= 4.886404209104D+00 Z= 1.364360130085D+00
I= 34 X= 4.527587616270D+00 Y= 2.058170075265D+00 Z= 8.810733575710D-01
I= 35 X= 1.531000183438D-03 Y= 1.121323573667D+00 Z= -7.468840757096D-01
I= 36 X= -2.449095865082D+00 Y= 3.874758304203D+00 Z= 4.185750157839D-01
I= 37 X= -1.138013312232D+00 Y= 6.006654944922D+00 Z= 4.074672108479D-01
I= 38 X= -3.340733842727D+00 Y= 3.168678747624D+00 Z= 2.353880631966D+00

Forward Direction:

Total Energy: -691.9968695 Hartrees

Potential Energy: -692.1891663 Hartress

Kinetic Energy: 0.1922968 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.241082982243D+12 Y= -4.114198477467D+12 Z= 3.729708104534D+11
I= 1 X= 7.809722007428D+12 Y= -1.682791778236D+13 Z= -2.783613569844D+13
I= 2 X= -9.333805592935D+12 Y= 9.494488506356D+12 Z= -1.394784321707D+13
I= 3 X= -1.152212252088D+13 Y= 1.784352921386D+13 Z= 3.321999744515D+13
I= 4 X= -4.880871816922D+12 Y= 2.282830809208D+13 Z= -3.038029500127D+13
I= 5 X= 2.291931949599D+13 Y= 4.378226035031D+12 Z= 2.367343805366D+13
I= 6 X= 3.031725727652D+13 Y= -1.927889142335D+13 Z= 4.477522249839D+13
I= 7 X= 2.535291204507D+13 Y= -3.015528652933D+12 Z= -9.593825921373D+13
I= 8 X= -1.322288716364D+14 Y= -1.142549386708D+13 Z= 2.326783265478D+13
I= 9 X= 7.531674486339D+12 Y= -9.373656675758D+12 Z= 8.954747520147D+12
I= 10 X= -2.085859531420D+13 Y= -6.600961369729D+13 Z= -1.481651207950D+13
I= 11 X= 5.279068932232D+13 Y= 1.136455867709D+13 Z= -1.058397325195D+14
I= 12 X= -1.191375226047D+14 Y= 1.667814889069D+14 Z= 4.077154652091D+13
I= 13 X= -1.526691120599D+13 Y= -2.039815864367D+12 Z= 9.430119891641D+12
I= 14 X= 2.590324890475D+13 Y= -7.577813704020D+12 Z= -1.490162608837D+13
I= 15 X= -3.310048641714D+13 Y= -1.250293466493D+13 Z= 6.588246729839D+13
I= 16 X= 7.952349215960D+13 Y= 8.864537448272D+13 Z= 6.032560524377D+13
I= 17 X= -6.284597284528D+12 Y= -8.678004316289D+12 Z= 2.838050560432D+12
I= 18 X= -3.983151438544D+13 Y= -1.294758665265D+13 Z= -3.221490787101D+13
I= 19 X= -2.186533790265D+13 Y= -4.031750041167D+13 Z= -5.369765596131D+13
I= 20 X= -1.693406758538D+13 Y= 6.751583738025D+13 Z= -7.858374594252D+12
I= 21 X= -2.355252945322D+13 Y= 1.760772631827D+13 Z= -2.617024604853D+12
I= 22 X= 1.524537394531D+13 Y= -8.631892752412D+13 Z= 2.931405538901D+13
I= 23 X= 1.415418158854D+14 Y= -5.577134592129D+13 Z= -6.612734291356D+12
I= 24 X= 2.188796033166D+13 Y= 4.550166206562D+13 Z= -1.373682970852D+13

I= 25 X= 3.686818428890D+13 Y= -3.677136027587D+12 Z= 3.492605482684D+12
I= 26 X= -3.228344597785D+13 Y= 5.652772260876D+13 Z= 1.509647275735D+14
I= 27 X= -1.511328821504D+13 Y= -4.273544488969D+13 Z= -7.910800311205D+13
I= 28 X= 2.732576740255D+13 Y= -5.579493064610D+13 Z= 4.737817933671D+13
I= 29 X= 3.216263933870D+12 Y= 6.503178263316D+12 Z= -4.694872592830D+12
I= 30 X= -5.477398013699D+12 Y= 1.746873623765D+12 Z= -5.123675369603D+12
I= 31 X= -2.815839845301D+13 Y= -5.292276860740D+13 Z= 1.830124777418D+13
I= 32 X= 1.099074852948D+13 Y= 3.340854909278D+13 Z= 3.019185109838D+13
I= 33 X= -4.819602160821D+13 Y= 9.318165572280D+13 Z= 1.526177399072D+13
I= 34 X= 1.073452455557D+13 Y= -8.072894448519D+12 Z= 4.636195093197D+13
I= 35 X= 3.582758293650D+12 Y= -6.488882434926D+12 Z= 9.925651270822D+11
I= 36 X= -1.216884059592D+13 Y= -2.257742020718D+13 Z= -9.846190980645D+12
I= 37 X= -1.552711092063D+13 Y= 7.097371000833D+13 Z= 3.388414969113D+12
I= 38 X= 4.337270383961D+13 Y= 6.408426265103D+13 Z= -6.109311052791D+13

Backward Direction:

Total Energy: -691.9969067 Hartrees

Potential Energy: -692.1891663 Hartress

Kinetic Energy: 0.1922596 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.225097327843D+12 Y= -3.508662248272D+12 Z= 1.373050242582D+12
I= 1 X= 7.984963702771D+12 Y= -1.682777241767D+13 Z= -2.783622187618D+13
I= 2 X= -8.960801355950D+12 Y= 9.366563725070D+12 Z= -1.343836540475D+13
I= 3 X= -1.150604708194D+13 Y= 1.723794195669D+13 Z= 3.221978700070D+13
I= 4 X= -4.507808827496D+12 Y= 2.295629683761D+13 Z= -3.088973824948D+13
I= 5 X= 2.362037612687D+13 Y= -2.366134307088D+11 Z= 1.853671045964D+13
I= 6 X= -3.098092843761D+12 Y= -1.927290304822D+13 Z= 4.477547592768D+13
I= 7 X= 1.946794757056D+13 Y= -5.722389085613D+12 Z= -1.028586249235D+14
I= 8 X= -1.346750867703D+14 Y= -1.502673700644D+13 Z= 2.186942562912D+13
I= 9 X= 8.408040445809D+12 Y= -1.095162583171D+13 Z= 8.545490696322D+12
I= 10 X= -2.126903210251D+13 Y= -6.793828372403D+13 Z= -1.571010227758D+13

I= 11 X= 5.389733380259D+13 Y= 8.359721341503D+12 Z= -1.061156653311D+14
I= 12 X= -1.170390854512D+14 Y= 1.653599904083D+14 Z= 4.089459394100D+13
I= 13 X= -1.439061528302D+13 Y= -4.618312662243D+11 Z= 9.839624680932D+12
I= 14 X= 2.549349307389D+13 Y= -5.648901257269D+12 Z= -1.400763927485D+13
I= 15 X= -3.100247326819D+13 Y= -1.108079388833D+13 Z= 6.575932138132D+13
I= 16 X= 8.062975047287D+13 Y= 9.164933142323D+13 Z= 6.060213474961D+13
I= 17 X= -6.436090934134D+12 Y= -8.661380479359D+12 Z= 4.464301326296D+12
I= 18 X= -3.969790899292D+13 Y= -1.222886773651D+13 Z= -2.879357891860D+13
I= 19 X= -2.197943360855D+13 Y= -3.978742968029D+13 Z= -5.308259334539D+13
I= 20 X= -1.755821072779D+13 Y= 6.549450117857D+13 Z= -6.050003812245D+12
I= 21 X= -2.504676220351D+13 Y= 1.760843891970D+13 Z= -2.617502915148D+12
I= 22 X= 1.141219878815D+13 Y= -8.631817525455D+13 Z= 2.931272626257D+13
I= 23 X= 1.406194773623D+14 Y= -5.395306927148D+13 Z= -6.556994873142D+12
I= 24 X= 2.096543836243D+13 Y= 4.368535454731D+13 Z= -1.379322352406D+13
I= 25 X= 3.671686921223D+13 Y= -3.694079394298D+12 Z= 1.866303511543D+12
I= 26 X= -3.290725579634D+13 Y= 5.854859653798D+13 Z= 1.491561832644D+14
I= 27 X= -1.522710892132D+13 Y= -4.326620434671D+13 Z= -7.972284500156D+13
I= 28 X= 2.745944324418D+13 Y= -5.651417788018D+13 Z= 4.395691758593D+13
I= 29 X= 3.917038039427D+12 Y= 1.111661376745D+13 Z= 4.405310436539D+11
I= 30 X= -4.003312715461D+12 Y= 1.814749167846D+12 Z= -6.419510366467D+11
I= 31 X= -3.060333545375D+13 Y= -4.932247428640D+13 Z= 1.969844412080D+13
I= 32 X= 5.106947463910D+12 Y= 3.611561481392D+13 Z= 3.710997546590D+13
I= 33 X= -4.894875204690D+13 Y= 9.030637783641D+13 Z= 2.442046244272D+13
I= 34 X= 1.133867424790D+13 Y= -1.108599171677D+13 Z= 4.955506468444D+13
I= 35 X= 3.395555778816D+12 Y= -6.488710798668D+12 Z= 9.930728791165D+11
I= 36 X= -1.069473820312D+13 Y= -2.264586492305D+13 Z= -1.432819499754D+13
I= 37 X= -1.628145369014D+13 Y= 7.385067230781D+13 Z= -5.771136704240D+12
I= 38 X= 4.397702521040D+13 Y= 6.709609253031D+13 Z= -6.428625812504D+13

Seed: 25704926461

CM Start Point Coordinates: bohr

I= 0 X= -2.159263180590D+00 Y= -2.296715695224D+00 Z= -9.653803983266D-02
I= 1 X= 1.230241164910D-02 Y= -2.829080579376D+00 Z= -1.581811892274D+00
I= 2 X= -1.324764213633D+00 Y= -1.155165321113D+00 Z= 2.405017368552D+00
I= 3 X= 2.219170610078D+00 Y= -2.088793470096D+00 Z= 3.517086731198D-02
I= 4 X= 1.363934050114D+00 Y= -1.188968317906D+00 Z= 2.318773296920D+00
I= 5 X= -2.867927662459D+00 Y= 3.525009256556D+00 Z= -2.305616133093D+00
I= 6 X= -1.217775818720D-01 Y= 1.547061832861D+00 Z= -3.224275073237D+00
I= 7 X= -2.354112799916D+00 Y= 5.292863746220D+00 Z= -3.467776844005D+00
I= 8 X= -4.194689528017D+00 Y= 2.108597429629D+00 Z= -2.797682219516D+00
I= 9 X= 3.245070433775D+00 Y= -9.094133892340D-01 Z= 4.622512279189D+00
I= 10 X= 3.021314737253D+00 Y= -2.629209877548D+00 Z= 5.860220802895D+00
I= 11 X= 5.040355528646D+00 Y= -5.872568430661D-01 Z= 3.869521478251D+00
I= 12 X= 2.642848574017D+00 Y= 1.111714341761D+00 Z= 5.519473394727D+00
I= 13 X= -3.044567776970D+00 Y= -4.581557723122D-01 Z= 4.496304775093D+00
I= 14 X= -3.413501785074D+00 Y= -2.249178296528D+00 Z= 5.920408697550D+00
I= 15 X= -2.311088779204D+00 Y= 1.015086458812D+00 Z= 5.638576339030D+00
I= 16 X= -4.831399120697D+00 Y= 3.139677701473D-01 Z= 3.834110639015D+00
I= 17 X= -4.666267309638D+00 Y= -2.698802355570D+00 Z= -7.990863692420D-01
I= 18 X= -5.370984176178D+00 Y= -4.126916866174D+00 Z= 3.885267882331D-01
I= 19 X= -5.770601344900D+00 Y= -7.494129508426D-01 Z= -1.020805011479D-01
I= 20 X= -5.300855191282D+00 Y= -2.748680969530D+00 Z= -2.974995962433D+00
I= 21 X= -6.838598908018D-02 Y= -3.958338318341D+00 Z= -4.130289395966D+00
I= 22 X= -1.044848635992D+00 Y= -6.084697982328D+00 Z= -4.078954659895D+00
I= 23 X= -1.257717251153D+00 Y= -3.116049971671D+00 Z= -5.242337573920D+00
I= 24 X= 1.908744631973D+00 Y= -4.167362414740D+00 Z= -5.205452936253D+00
I= 25 X= 4.877169098959D+00 Y= -2.738571116153D+00 Z= -7.041336310881D-01
I= 26 X= 4.607374218815D+00 Y= -2.758597774104D+00 Z= -2.720738184777D+00
I= 27 X= 5.937532331789D+00 Y= -1.013343671716D+00 Z= -3.230734549164D-01
I= 28 X= 5.449450038821D+00 Y= -4.304127422842D+00 Z= 3.494998461904D-01

I= 29 X= 2.798853001486D+00 Y= 3.269828476316D+00 Z= -2.185124893170D+00
I= 30 X= 2.602183832354D+00 Y= 4.112225823068D+00 Z= 3.524477094192D-01
I= 31 X= 4.046272519080D+00 Y= 1.579765564259D+00 Z= -3.065375350617D+00
I= 32 X= 2.405765808615D+00 Y= 5.035446502736D+00 Z= -3.524456696733D+00
I= 33 X= 1.746458888209D+00 Y= 6.045743069953D+00 Z= 8.392929846627D-01
I= 34 X= 3.654373922972D+00 Y= 3.283260351883D+00 Z= 1.934445036858D+00
I= 35 X= 2.371246943799D-02 Y= 1.125430353639D+00 Z= -5.623533909297D-01
I= 36 X= -2.957326203616D+00 Y= 3.822615037196D+00 Z= 3.161696316199D-01
I= 37 X= -1.952889259958D+00 Y= 5.328038004319D+00 Z= 1.147186250394D+00
I= 38 X= -4.281988404428D+00 Y= 2.649912136466D+00 Z= 1.639998898805D+00

Forward Direction:

Total Energy: -691.9949422 Hartrees

Potential Energy: -692.1920302 Hartress

Kinetic Energy: 0.1970880 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.134889072539D+13 Y= 8.511244436966D+12 Z= 1.266956924347D+13
I= 1 X= -2.313775475726D+13 Y= -1.665292907455D+13 Z= -1.471038752967D+13
I= 2 X= -1.207167230077D+13 Y= -8.970282659752D+12 Z= 1.042865774774D+13
I= 3 X= 1.156105047268D+13 Y= 5.033991978490D+12 Z= -4.242613904628D+12
I= 4 X= 1.472954252254D+13 Y= 2.089700435755D+13 Z= 3.256696699297D+13
I= 5 X= 2.206084502376D+12 Y= -2.015135839703D+13 Z= -1.997128549885D+13
I= 6 X= 4.201390067598D+13 Y= 1.173820642296D+13 Z= -8.144937473425D+13
I= 7 X= 4.510883095487D+13 Y= 5.447024840070D+13 Z= -7.303033112454D+13
I= 8 X= 7.742878546686D+13 Y= 5.011596307785D+13 Z= 1.184153508406D+14
I= 9 X= -1.390209773059D+13 Y= 6.910646667015D+12 Z= 8.303748193515D+12
I= 10 X= -2.749455938283D+13 Y= 9.722139826789D+12 Z= -7.791237422381D+13
I= 11 X= -5.753182290857D+13 Y= 7.020728781902D+13 Z= -1.690204209294D+13
I= 12 X= 9.569024039752D+13 Y= -1.017698555721D+14 Z= -5.306823142249D+13
I= 13 X= 7.445226465744D+12 Y= -1.307494683554D+13 Z= -9.067483109836D+12
I= 14 X= -3.508053156284D+13 Y= -1.315854556714D+13 Z= 1.742044943324D+13

I= 15 X= -9.030890791777D+13 Y= -1.117609637826D+13 Z= 1.874069218961D+13
I= 16 X= 1.590540344301D+13 Y= 1.298782202461D+13 Z= 7.327803730904D+13
I= 17 X= 2.949398415961D+12 Y= -1.748649479108D+12 Z= -1.783550822666D+13
I= 18 X= 7.593296660204D+13 Y= -3.416731459807D+13 Z= -4.745337606266D+13
I= 19 X= -2.205483934677D+13 Y= 7.347441073452D+13 Z= 2.114410023385D+13
I= 20 X= -5.370950845302D+13 Y= 3.507068229846D+13 Z= 9.354204880695D+13
I= 21 X= 3.912990289813D+12 Y= 4.008027132064D+13 Z= 1.681150335915D+12
I= 22 X= 2.750623698546D+12 Y= -9.471808333273D+13 Z= -2.986182376317D+13
I= 23 X= -8.714631260085D+13 Y= -3.307834021964D+12 Z= -6.632626236272D+13
I= 24 X= -6.070848998860D+13 Y= -3.652454384319D+13 Z= -3.450944886272D+13
I= 25 X= 1.697000955115D+13 Y= -1.217883228892D+13 Z= -1.335975347107D+12
I= 26 X= -4.318483777210D+13 Y= -6.374456627705D+13 Z= 1.082291631086D+14
I= 27 X= -2.295496544473D+13 Y= -7.298851189821D+13 Z= -3.741439522917D+13
I= 28 X= 1.206800237240D+14 Y= 5.886040078537D+13 Z= -3.894561350211D+13
I= 29 X= -3.457987769417D+12 Y= -9.489569900990D+12 Z= -1.685120997936D+13
I= 30 X= 3.540397160281D+12 Y= 5.137172239692D+12 Z= -2.198069994684D+13
I= 31 X= -5.749098062287D+13 Y= -3.648010314789D+12 Z= 7.393284725026D+13
I= 32 X= -4.130424185028D+11 Y= -4.379445291649D+13 Z= -1.769835922504D+13
I= 33 X= -7.348241747175D+13 Y= 7.125908236149D+13 Z= 8.188725007812D+13
I= 34 X= 1.791090652123D+13 Y= -6.331631011884D+13 Z= 9.130340114184D+13
I= 35 X= -3.411657000254D+11 Y= -2.690977047868D+11 Z= -5.348010039116D+11
I= 36 X= -1.186053340894D+13 Y= -8.439505752149D+12 Z= 3.160194297952D+13
I= 37 X= 3.933319345802D+13 Y= 5.283185494911D+13 Z= 1.002625572169D+13
I= 38 X= -3.092838189342D+12 Y= 1.065552700660D+14 Z= 2.027786186435D+12

Backward Direction:

Total Energy: -691.9949427 Hartrees

Potential Energy: -692.1920302 Hartress

Kinetic Energy: 0.1970874 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.120404769278D+13 Y= 9.456966092779D+12 Z= 1.472698489760D+13

I= 1 X= -2.390425189222D+13 Y= -1.665256801684D+13 Z= -1.471064146738D+13
I= 2 X= -1.079490523768D+13 Y= -8.247955242190D+12 Z= 1.133181137307D+13
I= 3 X= 1.141644889985D+13 Y= 4.088225351254D+12 Z= -6.300279979794D+12
I= 4 X= 1.600645988150D+13 Y= 2.017481557704D+13 Z= 3.166401439917D+13
I= 5 X= 1.594547316068D+12 Y= -3.156564450399D+13 Z= -3.136210459565D+13
I= 6 X= 1.856001355939D+13 Y= 1.174800354940D+13 Z= -8.144787677125D+13
I= 7 X= 3.554234722987D+13 Y= 4.116100505479D+13 Z= -9.138204878679D+13
I= 8 X= 7.574327673594D+13 Y= 3.475680607447D+13 Z= 1.154619484239D+14
I= 9 X= -1.135565106755D+13 Y= 2.379978194135D+12 Z= 7.441674036692D+12
I= 10 X= -2.815627286826D+13 Y= 4.512086997581D+12 Z= -7.975485977310D+13
I= 11 X= -5.443052954553D+13 Y= 6.197267533400D+13 Z= -1.758435547351D+13
I= 12 X= 1.013942012499D+14 Y= -1.057356300820D+14 Z= -5.284967439927D+13
I= 13 X= 9.991530861303D+12 Y= -8.544236871593D+12 Z= -8.204668182113D+12
I= 14 X= -3.574022190512D+13 Y= -7.947743809716D+12 Z= 1.926420213976D+13
I= 15 X= -8.460608502983D+13 Y= -7.208563893577D+12 Z= 1.852185474621D+13
I= 16 X= 1.900568037234D+13 Y= 2.122001121858D+13 Z= 7.396201085627D+13
I= 17 X= 2.249441881502D+12 Y= -1.934937374607D+12 Z= -1.334888276040D+13
I= 18 X= 7.566427034842D+13 Y= -3.209148315411D+13 Z= -3.760041245211D+13
I= 19 X= -2.216244759951D+13 Y= 7.520599543944D+13 Z= 2.262573633381D+13
I= 20 X= -5.590868717157D+13 Y= 2.905266443811D+13 Z= 9.857753946620D+13
I= 21 X= -4.611329033245D+11 Y= 4.008215743704D+13 Z= 1.679886146771D+12
I= 22 X= -8.379969726962D+12 Y= -9.471606279396D+13 Z= -2.986529178945D+13
I= 23 X= -8.962748299496D+13 Y= 2.048050626028D+12 Z= -6.649087791306D+13
I= 24 X= -6.319004454386D+13 Y= -4.187538664121D+13 Z= -3.434628793447D+13
I= 25 X= 1.627062667086D+13 Y= -1.199350168097D+13 Z= -5.822782768689D+12
I= 26 X= -4.538313202283D+13 Y= -5.772749568097D+13 Z= 1.031930714139D+14
I= 27 X= -2.306166521592D+13 Y= -7.472218762992D+13 Z= -3.889527854653D+13
I= 28 X= 1.204117666056D+14 Y= 5.678288131995D+13 Z= -4.879886357975D+13
I= 29 X= -4.070382433107D+12 Y= 1.921543405107D+12 Z= -5.463890853751D+12
I= 30 X= 4.922701144090D+12 Y= 3.556050318871D+12 Z= -9.400808743811D+12

I= 31 X= -5.917659339490D+13 Y= 1.170569163517D+13 Z= 7.688242462841D+13
I= 32 X= -9.975603329771D+12 Y= -3.048358128840D+13 Z= 6.482098004729D+11
I= 33 X= -7.531956556431D+13 Y= 6.341305935155D+13 Z= 1.062303051457D+14
I= 34 X= 2.055435393055D+13 Y= -7.101262121728D+13 Z= 9.815352146235D+13
I= 35 X= 2.197412264234D+10 Y= -2.686121932062D+11 Z= -5.335170685197D+11
I= 36 X= -1.047869769511D+13 Y= -6.859700900940D+12 Z= 1.902122468426D+13
I= 37 X= 3.749122920225D+13 Y= 6.068193198516D+13 Z= -1.431803036428D+13
I= 38 X= -4.500857092238D+11 Y= 1.142472388748D+14 Z= -4.822763831834D+12

Seed: 26124319993

CM Start Point Coordinates: bohr

I= 0 X= -2.183390601340D+00 Y= -1.947144078589D+00 Z= -1.089444078568D-01
I= 1 X= -1.097307236687D-01 Y= -2.778025057976D+00 Z= -1.560757215742D+00
I= 2 X= -1.275255712553D+00 Y= -1.187218072172D+00 Z= 2.316333199829D+00
I= 3 X= 2.189596805491D+00 Y= -2.066485166504D+00 Z= -9.343604441187D-02
I= 4 X= 1.279443598274D+00 Y= -1.093178854630D+00 Z= 2.287064956072D+00
I= 5 X= -3.084311662440D+00 Y= 2.810874694676D+00 Z= -1.982667310504D+00
I= 6 X= -2.454053216862D-01 Y= 1.216405226456D+00 Z= -3.172131384042D+00
I= 7 X= -3.033703624539D+00 Y= 4.102088789217D+00 Z= -3.801385275699D+00
I= 8 X= -4.344054863909D+00 Y= 1.336678210020D+00 Z= -2.377388582613D+00
I= 9 X= 2.764222614259D+00 Y= -7.250818118222D-01 Z= 4.820858575823D+00
I= 10 X= 2.227580283385D+00 Y= -2.265038111967D+00 Z= 6.472303559867D+00
I= 11 X= 5.090275947378D+00 Y= -1.152820059371D+00 Z= 4.602889337999D+00
I= 12 X= 2.331296068614D+00 Y= 1.144442187072D+00 Z= 5.784222025903D+00
I= 13 X= -2.883799337385D+00 Y= -8.323410949902D-01 Z= 4.785823129102D+00
I= 14 X= -2.889467877682D+00 Y= -2.534595737693D+00 Z= 6.208594025059D+00
I= 15 X= -2.452187880856D+00 Y= 8.011565202668D-01 Z= 5.781565820793D+00
I= 16 X= -4.645106327214D+00 Y= -1.037227946143D+00 Z= 4.334099544922D+00
I= 17 X= -4.959290841013D+00 Y= -2.362190268489D+00 Z= -8.478205286754D-01
I= 18 X= -5.614379354027D+00 Y= -3.922310728188D+00 Z= 7.973730855833D-01

I= 19 X= -5.666067711569D+00 Y= -2.383856729896D-01 Z= -8.074051037682D-01
I= 20 X= -5.194211579032D+00 Y= -3.366637386870D+00 Z= -2.778460341455D+00
I= 21 X= 2.441009132270D-01 Y= -3.732117932186D+00 Z= -4.206423995826D+00
I= 22 X= -2.950455228576D-01 Y= -5.658875146714D+00 Z= -4.447947871533D+00
I= 23 X= -1.118052752398D+00 Y= -3.022050846912D+00 Z= -5.595565203958D+00
I= 24 X= 2.302281147385D+00 Y= -3.635068754670D+00 Z= -5.080139059358D+00
I= 25 X= 4.904915831130D+00 Y= -2.361308275424D+00 Z= -5.236705421123D-01
I= 26 X= 5.500650982522D+00 Y= -2.404475867067D+00 Z= -2.668831700674D+00
I= 27 X= 6.159217680230D+00 Y= -1.419868268934D+00 Z= 7.358792629148D-01
I= 28 X= 5.144754202922D+00 Y= -4.358998350260D+00 Z= -7.887934496328D-02
I= 29 X= 2.783118471523D+00 Y= 3.228329607274D+00 Z= -2.548033283145D+00
I= 30 X= 2.984286587174D+00 Y= 3.615262185473D+00 Z= 1.784828317419D-01
I= 31 X= 3.938226465406D+00 Y= 1.830398723778D+00 Z= -3.712778964794D+00
I= 32 X= 2.116114752409D+00 Y= 4.764778466684D+00 Z= -3.371998971655D+00
I= 33 X= 2.591624073216D+00 Y= 5.693841363580D+00 Z= 1.249587816919D+00
I= 34 X= 4.609882507365D+00 Y= 2.643143472830D+00 Z= 1.303949984143D+00
I= 35 X= -2.813804450595D-02 Y= 1.147992466739D+00 Z= -6.302583188619D-01
I= 36 X= -2.629882096243D+00 Y= 3.953916454451D+00 Z= 4.157686832675D-01
I= 37 X= -1.674054779499D+00 Y= 6.122728591655D+00 Z= 2.976057565700D-01
I= 38 X= -3.480824630765D+00 Y= 3.441335293856D+00 Z= 2.261885741477D+00

Forward Direction:

Total Energy: -691.9956910 Hartrees

Potential Energy: -692.1492488 Hartress

Kinetic Energy: 0.1535578 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.594063338437D+12 Y= -1.095115092307D+13 Z= 5.348072813510D+12

I= 1 X= -5.551858602778D+12 Y= 9.429845326254D+12 Z= 3.204624926220D+12

I= 2 X= 1.425710881627D+13 Y= 4.891820877793D+12 Z= 1.683414132881D+12

I= 3 X= 1.948786773458D+13 Y= -1.030692123614D+13 Z= -1.898878995456D+13

I= 4 X= -8.379378520503D+12 Y= 6.650524000580D+12 Z= -7.850625496024D+12

I= 5 X= 1.802282898871D+13 Y= 2.226608126556D+13 Z= 1.614164161012D+13
I= 6 X= 5.440162276338D+13 Y= 5.875370013822D+13 Z= 3.303148236603D+13
I= 7 X= -2.667715620409D+13 Y= 2.948267493398D+13 Z= -4.066552087022D+13
I= 8 X= -8.963439037329D+13 Y= -3.239852253267D+13 Z= -6.288538730297D+13
I= 9 X= -2.184397705727D+13 Y= 1.947792612246D+13 Z= -9.470880480347D+12
I= 10 X= -7.238577433100D+12 Y= -1.175485966883D+14 Z= -1.223345798888D+13
I= 11 X= 5.372678249199D+12 Y= 5.719934592103D+12 Z= -2.910168273152D+13
I= 12 X= 2.751108783524D+13 Y= -3.582861554004D+13 Z= 7.803737132827D+13
I= 13 X= 4.645866541871D+12 Y= -2.257007131411D+12 Z= 1.504779331709D+13
I= 14 X= 2.171114051636D+13 Y= -4.395204212156D+13 Z= -6.732666566861D+11
I= 15 X= -3.909349066843D+12 Y= -1.713945318832D+13 Z= -3.359185694414D+13
I= 16 X= -1.180843963703D+14 Y= 2.431684175357D+13 Z= -7.849297817512D+13
I= 17 X= 8.097176890405D+11 Y= -7.007995611983D+12 Z= 1.345632336535D+13
I= 18 X= 2.367624616293D+13 Y= 1.095822595270D+13 Z= -7.241403041453D+12
I= 19 X= 1.689130473041D+12 Y= 1.361855565598D+13 Z= 9.109844889498D+12
I= 20 X= -7.644504767658D+13 Y= -3.844650484911D+13 Z= -7.774020522209D+13
I= 21 X= 1.055675485028D+12 Y= -2.433630303465D+13 Z= -8.172382716858D+12
I= 22 X= -8.504350843891D+13 Y= 1.116569796671D+14 Z= -6.828798206900D+13
I= 23 X= -3.061517291428D+13 Y= -3.527875466581D+13 Z= 6.900519114954D+13
I= 24 X= 3.170802906975D+13 Y= -7.606968145585D+12 Z= 3.622194908447D+13
I= 25 X= -1.442588124817D+13 Y= 4.623094114187D+11 Z= 7.774093166931D+12
I= 26 X= -1.099968977806D+14 Y= 6.249779011213D+13 Z= -5.452584347553D+13
I= 27 X= 2.602028781253D+13 Y= -2.519390111879D+13 Z= -2.349913725955D+13
I= 28 X= 1.612568132042D+13 Y= -7.553741148528D+13 Z= 8.539187676107D+13
I= 29 X= -5.880013691285D+12 Y= 1.092174243321D+13 Z= 4.139084268028D+12
I= 30 X= 1.715557625546D+13 Y= 6.297251404925D+12 Z= -1.070522184863D+13
I= 31 X= 2.595391694183D+13 Y= 5.330856823565D+13 Z= -1.362013151521D+13
I= 32 X= -5.655417702519D+13 Y= -1.175202506342D+14 Z= 2.767696908158D+13
I= 33 X= 2.228987673472D+13 Y= -1.236834549464D+14 Z= -4.782016773257D+13
I= 34 X= -3.772636095108D+13 Y= -5.041955038085D+12 Z= 2.968455199539D+13

I= 35 X= 5.370752591675D+12 Y= -7.526612484073D+11 Z= -7.350090364620D+11
I= 36 X= -1.399699388397D+13 Y= 5.322480590048D+12 Z= 1.659726499237D+13
I= 37 X= 3.813164945987D+12 Y= 3.076335087166D+13 Z= -6.124670573200D+12
I= 38 X= -3.897921936019D+13 Y= -4.933977198137D+13 Z= -1.045005344430D+14

Backward Direction:

Total Energy: -691.9956949 Hartrees

Potential Energy: -692.1492488 Hartress

Kinetic Energy: 0.1535539 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.611109521927D+12 Y= -1.006385817098D+13 Z= 6.832099822693D+12
I= 1 X= -5.334143721471D+12 Y= 9.430063363092D+12 Z= 3.204494167880D+12
I= 2 X= 1.482974516233D+13 Y= 4.739005141944D+12 Z= 2.433988170967D+12
I= 3 X= 1.950504927434D+13 Y= -1.119428746247D+13 Z= -2.047301065083D+13
I= 4 X= -7.806653889008D+12 Y= 6.803434919187D+12 Z= -8.601143350028D+12
I= 5 X= 1.898599805996D+13 Y= 1.534595339937D+13 Z= 8.488284424110D+12
I= 6 X= 6.517258509294D+12 Y= 5.876249158279D+13 Z= 3.303189510819D+13
I= 7 X= -3.531449852347D+13 Y= 2.517522386213D+13 Z= -5.108925585499D+13
I= 8 X= -9.313864720707D+13 Y= -3.804104120308D+13 Z= -6.496337040622D+13
I= 9 X= -2.051560402834D+13 Y= 1.708812480130D+13 Z= -1.007893642433D+13
I= 10 X= -7.840768136742D+12 Y= -1.204572252343D+14 Z= -1.355962028419D+13
I= 11 X= 7.045809801166D+12 Y= 1.183926959795D+12 Z= -2.951544789378D+13
I= 12 X= 3.067706819528D+13 Y= -3.797710235953D+13 Z= 7.821866367856D+13
I= 13 X= 5.974135705104D+12 Y= 1.328174773529D+11 Z= 1.565622588462D+13
I= 14 X= 2.110998365588D+13 Y= -4.104304447415D+13 Z= 6.535011634255D+11
I= 15 X= -7.440078823115D+11 Y= -1.498999692118D+13 Z= -3.377329839488D+13
I= 16 X= -1.164118461681D+14 Y= 2.885151997331D+13 Z= -7.807831131532D+13
I= 17 X= 5.703314365108D+11 Y= -6.991608290277D+12 Z= 1.591238556983D+13
I= 18 X= 2.385408975353D+13 Y= 1.204717046542D+13 Z= -2.058758667420D+12
I= 19 X= 1.524597018640D+12 Y= 1.442921038245D+13 Z= 1.003066550401D+13
I= 20 X= -7.740559052855D+13 Y= -4.151582687016D+13 Z= -7.500735096614D+13

I= 21 X= -1.210459082730D+12 Y= -2.433522981409D+13 Z= -8.173103003800D+12
I= 22 X= -9.085345830341D+13 Y= 1.116581137371D+14 Z= -6.828998193152D+13
I= 23 X= -3.200576133251D+13 Y= -3.251993317153D+13 Z= 6.907741410007D+13
I= 24 X= 3.031716817528D+13 Y= -1.036283039778D+13 Z= 3.614875101302D+13
I= 25 X= -1.466499476610D+13 Y= 4.454366941653D+11 Z= 5.317952075271D+12
I= 26 X= -1.109569385842D+14 Y= 6.556642627331D+13 Z= -5.725896435113D+13
I= 27 X= 2.585617521816D+13 Y= -2.600560330446D+13 Z= -2.441961922154D+13
I= 28 X= 1.630364055218D+13 Y= -7.662716275949D+13 Z= 8.020931624259D+13
I= 29 X= -4.917274231076D+12 Y= 1.783977626924D+13 Z= 1.179044766921D+13
I= 30 X= 1.928100509392D+13 Y= 6.333345023640D+12 Z= -3.928562252828D+12
I= 31 X= 2.245145408454D+13 Y= 5.894954738620D+13 Z= -1.154399505468D+13
I= 32 X= -6.518973551866D+13 Y= -1.132124496427D+14 Z= 3.809735793119D+13
I= 33 X= 2.116205435720D+13 Y= -1.280226241284D+14 Z= -3.402289000903D+13
I= 34 X= -3.677725612404D+13 Y= -9.569364178747D+12 Z= 3.443339933832D+13
I= 35 X= 5.121063989431D+12 Y= -7.524015844113D+11 Z= -7.342465905798D+11
I= 36 X= -1.187155859077D+13 Y= 5.285536889583D+12 Z= 9.820180914535D+12
I= 37 X= 2.682893709950D+12 Y= 3.510504168674D+13 Z= -1.992320877660D+13
I= 38 X= -3.802989914367D+13 Y= -4.481430868435D+13 Z= -1.092494455277D+14

Seed: 2820608934

CM Start Point Coordinates: bohr

I= 0 X= -2.136692599906D+00 Y= -1.911542581835D+00 Z= -3.001060952735D-01
I= 1 X= 8.499101452643D-02 Y= -2.754632389486D+00 Z= -1.534663019274D+00
I= 2 X= -1.307650473955D+00 Y= -1.066029427358D+00 Z= 2.220401928580D+00
I= 3 X= 2.198043600848D+00 Y= -2.141459661686D+00 Z= -1.353276204420D-01
I= 4 X= 1.412123324668D+00 Y= -1.168829426935D+00 Z= 2.214451663067D+00
I= 5 X= -3.175277287381D+00 Y= 3.111903573675D+00 Z= -2.126106067944D+00
I= 6 X= -1.021766405962D-01 Y= 9.711596414778D-01 Z= -3.509367195728D+00
I= 7 X= -2.675238845231D+00 Y= 4.211466756875D+00 Z= -3.716006149041D+00
I= 8 X= -4.784035077863D+00 Y= 1.602449420703D+00 Z= -2.048162808988D+00

I= 9 X= 2.627361552560D+00 Y= -3.173386087975D-01 Z= 4.546718186167D+00
I= 10 X= 1.675876291657D+00 Y= -1.465898786263D+00 Z= 6.518636948660D+00
I= 11 X= 4.606707317304D+00 Y= -6.356852654577D-01 Z= 4.576226307362D+00
I= 12 X= 2.055147365471D+00 Y= 1.737903958100D+00 Z= 4.667363363601D+00
I= 13 X= -2.910956314986D+00 Y= -9.222332841738D-01 Z= 4.752287731710D+00
I= 14 X= -2.752966733471D+00 Y= -2.628883323362D+00 Z= 5.804262743749D+00
I= 15 X= -1.763772356546D+00 Y= 4.080015006213D-01 Z= 5.936041659484D+00
I= 16 X= -4.580209258992D+00 Y= -1.418865094954D-01 Z= 4.047720443910D+00
I= 17 X= -4.678920737748D+00 Y= -2.330231914070D+00 Z= -8.596013129369D-01
I= 18 X= -5.621924898786D+00 Y= -4.033947203507D+00 Z= -7.627846163052D-03
I= 19 X= -5.990696455528D+00 Y= -6.680643971277D-01 Z= -2.555713268352D-01
I= 20 X= -4.907894240207D+00 Y= -2.640538326083D+00 Z= -2.764753389214D+00
I= 21 X= 2.699621863159D-02 Y= -3.916702349043D+00 Z= -4.081299781094D+00
I= 22 X= -5.456325892025D-01 Y= -5.804009601210D+00 Z= -4.403749548885D+00
I= 23 X= -1.567726689290D+00 Y= -2.833224506880D+00 Z= -5.255878746063D+00
I= 24 X= 1.776115243611D+00 Y= -3.721536510281D+00 Z= -5.014879735306D+00
I= 25 X= 4.923355337933D+00 Y= -2.325517396171D+00 Z= -7.471356337770D-01
I= 26 X= 5.071755222171D+00 Y= -2.709284049524D+00 Z= -2.588389544595D+00
I= 27 X= 5.728920512520D+00 Y= -6.314962966947D-01 Z= -3.065079566426D-01
I= 28 X= 5.945362466839D+00 Y= -3.823366354355D+00 Z= 2.194929211710D-01
I= 29 X= 2.780148715805D+00 Y= 3.088066704283D+00 Z= -2.154332841458D+00
I= 30 X= 3.006873190059D+00 Y= 3.428657981805D+00 Z= 3.432437413962D-01
I= 31 X= 4.244270497441D+00 Y= 1.877306472747D+00 Z= -2.955139328611D+00
I= 32 X= 1.870820588585D+00 Y= 4.257762640458D+00 Z= -3.712239323423D+00
I= 33 X= 1.943331705675D+00 Y= 4.988072339402D+00 Z= 1.257195478024D+00
I= 34 X= 4.666002385430D+00 Y= 2.474180438491D+00 Z= 1.146195317233D+00
I= 35 X= -1.138861507825D-02 Y= 1.033912710516D+00 Z= -5.287070188373D-01
I= 36 X= -2.668425372869D+00 Y= 4.080995684944D+00 Z= 4.668539371907D-01
I= 37 X= -1.925256994560D+00 Y= 6.087354220654D+00 Z= 2.294347525085D-01
I= 38 X= -3.867510052148D+00 Y= 3.922833332912D+00 Z= 2.030305233378D+00

Forward Direction:

Total Energy: -691.9867788 Hartrees

Potential Energy: -692.1930706 Hartress

Kinetic Energy: 0.2062918 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.358018317430D+13 Y= 2.316214520368D+13 Z= -2.109739512964D+13
I= 1 X= -1.312409189502D+13 Y= -4.663106773202D+11 Z= 1.032087156648D+13
I= 2 X= -5.220200156127D+12 Y= -1.039245889180D+12 Z= -7.411677894230D+11
I= 3 X= -1.427344055465D+13 Y= -8.902895797021D+12 Z= -5.597900170154D+12
I= 4 X= 2.149805847323D+13 Y= 2.649308840135D+13 Z= 3.317189447217D+13
I= 5 X= 5.784024919697D+12 Y= -8.230100511132D+12 Z= 1.756387781347D+13
I= 6 X= 5.670364043669D+13 Y= -5.849429404124D+13 Z= -6.644608481383D+13
I= 7 X= 4.861635537804D+13 Y= 1.782560665065D+14 Z= -1.128819456182D+14
I= 8 X= 2.527143818627D+13 Y= 2.382755268348D+13 Z= -1.834980048986D+13
I= 9 X= 1.784086290598D+11 Y= -5.064011307246D+12 Z= -5.241633563940D+12
I= 10 X= 2.823102707058D+13 Y= -9.400128947494D+13 Z= -5.012154429426D+13
I= 11 X= 3.243419825255D+13 Y= 1.515054517586D+13 Z= 9.498418855048D+12
I= 12 X= -7.394582087820D+13 Y= 9.004971352967D+13 Z= -2.457841592363D+13
I= 13 X= 2.337987478298D+12 Y= 1.105729815597D+13 Z= 1.034622672889D+13
I= 14 X= -1.053397308339D+14 Y= 2.291633046228D+13 Z= 4.181753472073D+13
I= 15 X= 1.807242482647D+13 Y= -1.535008089263D+14 Z= -7.284524911858D+13
I= 16 X= -9.254563019187D+13 Y= -1.054555420669D+14 Z= -4.193633798721D+13
I= 17 X= -3.422919643008D+12 Y= -1.266358167907D+13 Z= 1.617887002271D+13
I= 18 X= 3.445812497376D+13 Y= 1.519358824727D+14 Z= -8.509497111839D+13
I= 19 X= -3.528890668755D+13 Y= -3.903961929831D+13 Z= -4.213465671617D+13
I= 20 X= -8.801402945199D+13 Y= 4.417009581977D+13 Z= -6.136372990022D+13
I= 21 X= -7.996040437318D+12 Y= -2.387961657675D+13 Z= -8.903632906527D+12
I= 22 X= 1.063460188276D+14 Y= 8.202646541562D+13 Z= 5.961332723549D+12
I= 23 X= -3.996638910960D+13 Y= -1.783202628741D+13 Z= -3.174482743738D+13
I= 24 X= 2.153244008761D+13 Y= -6.614034250689D+13 Z= 5.746012819198D+13

I= 25 X= 3.901037214534D+12 Y= -6.038332526088D+12 Z= -1.603762117102D+13
I= 26 X= 5.660792105106D+13 Y= 2.225051631376D+13 Z= 1.170243510577D+13
I= 27 X= 1.528863547540D+13 Y= 2.634469847085D+11 Z= -3.549390273500D+13
I= 28 X= -1.567101069457D+13 Y= 2.371952352511D+13 Z= 4.132947204062D+13
I= 29 X= -4.898449377126D+11 Y= 1.527904767230D+13 Z= -1.013951589210D+13
I= 30 X= -3.247457127328D+13 Y= 1.379681689310D+13 Z= -3.143377026357D+12
I= 31 X= 6.075159371340D+13 Y= 2.378717501176D+13 Z= -3.449436961005D+13
I= 32 X= -6.405535441798D+13 Y= -6.497102639692D+13 Z= -2.082434983537D+13
I= 33 X= 8.236197522229D+13 Y= -2.765919099723D+13 Z= -3.950730787766D+13
I= 34 X= 1.260213903392D+13 Y= -4.376474802815D+13 Z= 1.181562222274D+14
I= 35 X= 2.785464472470D+12 Y= -3.899858535778D+12 Z= 2.092004151556D+12
I= 36 X= -2.227171927645D+12 Y= 3.123550421459D+12 Z= 1.191420829161D+13
I= 37 X= 1.644696341217D+13 Y= -7.042703727789D+13 Z= -1.178790456607D+13
I= 38 X= -2.441804731603D+12 Y= -2.607399553413D+13 Z= 8.882581231393D+11

Backward Direction:

Total Energy: -691.9867779 Hartrees

Potential Energy: -692.1930706 Hartress

Kinetic Energy: 0.2062927 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.363997727855D+13 Y= 2.460266925770D+13 Z= -1.878179424653D+13
I= 1 X= -1.257387840427D+13 Y= -4.659820510679D+11 Z= 1.032068182784D+13
I= 2 X= -4.421832988798D+12 Y= -1.461762485439D+12 Z= 4.570675154862D+11
I= 3 X= -1.421344585228D+13 Y= -1.034354569953D+13 Z= -7.913806880769D+12
I= 4 X= 2.229655789573D+13 Y= 2.691575221830D+13 Z= 3.197372251566D+13
I= 5 X= 7.670509247217D+12 Y= -1.866922964872D+13 Z= 5.775735473109D+12
I= 6 X= -2.647190071607D+13 Y= -5.848010506178D+13 Z= -6.644562318672D+13
I= 7 X= 3.466459438509D+13 Y= 1.729807071121D+14 Z= -1.283780625512D+14
I= 8 X= 1.917842915646D+13 Y= 1.650823396066D+13 Z= -2.157788700610D+13
I= 9 X= 2.112257272979D+12 Y= -8.553040406324D+12 Z= -6.186653626285D+12
I= 10 X= 2.725728232640D+13 Y= -9.830773299374D+13 Z= -5.219004689416D+13

I= 11 X= 3.489084190523D+13 Y= 8.456226490749D+12 Z= 8.874214732094D+12
I= 12 X= -6.926483690832D+13 Y= 8.689183323614D+13 Z= -2.428907721187D+13
I= 13 X= 4.271673749799D+12 Y= 1.454636176468D+13 Z= 1.129179134457D+13
I= 14 X= -1.063119785793D+14 Y= 2.722330320134D+13 Z= 4.388689778755D+13
I= 15 X= 2.275246114184D+13 Y= -1.503414974882D+14 Z= -7.313480596174D+13
I= 16 X= -9.008985219887D+13 Y= -9.876318340150D+13 Z= -4.131080770568D+13
I= 17 X= -3.723920477529D+12 Y= -1.259682940055D+13 Z= 1.979806784849D+13
I= 18 X= 3.483714798701D+13 Y= 1.535234640243D+14 Z= -7.753390940354D+13
I= 19 X= -3.556937895578D+13 Y= -3.789445746174D+13 Z= -4.073825424100D+13
I= 20 X= -8.934187993354D+13 Y= 3.972821793963D+13 Z= -5.734517631065D+13
I= 21 X= -1.128916970027D+13 Y= -2.387802047323D+13 Z= -8.904704494661D+12
I= 22 X= 9.788652300712D+13 Y= 8.202814659974D+13 Z= 5.958349273998D+12
I= 23 X= -4.202717275723D+13 Y= -1.382899122868D+13 Z= -3.157996979330D+13
I= 24 X= 1.947123255947D+13 Y= -7.013894526103D+13 Z= 5.729376921649D+13
I= 25 X= 3.600423441320D+12 Y= -6.105786174248D+12 Z= -1.965692767350D+13
I= 26 X= 5.528081701050D+13 Y= 2.669132338639D+13 Z= 7.683511105614D+12
I= 27 X= 1.500875598971D+13 Y= -8.832231393548D+11 Z= -3.688983229247D+13
I= 28 X= -1.529186228405D+13 Y= 2.213079568124D+13 Z= 3.376862048789D+13
I= 29 X= 1.396020619898D+12 Y= 2.571496249286D+13 Z= 1.645660441151D+12
I= 30 X= -2.884992556960D+13 Y= 1.417453676369D+13 Z= 6.803031555947D+12
I= 31 X= 5.466189446007D+13 Y= 3.110474579962D+13 Z= -3.126891525617D+13
I= 32 X= -7.800461763899D+13 Y= -5.969534622597D+13 Z= -5.333353617222D+12
I= 33 X= 8.065608086878D+13 Y= -3.406916979599D+13 Z= -1.900626173989D+13
I= 34 X= 1.382147965172D+13 Y= -5.054936720950D+13 Z= 1.255135843775D+14
I= 35 X= 2.256103413618D+12 Y= -3.899478090408D+12 Z= 2.093149130404D+12
I= 36 X= 1.397577906612D+12 Y= 2.744531387290D+12 Z= 1.967184402429D+12
I= 37 X= 1.473752799345D+13 Y= -6.401323383315D+13 Z= -3.229101925133D+13
I= 38 X= -1.221932240777D+12 Y= -1.929208852167D+13 Z= -6.469136221848D+12

Seed: 28766904189

CM Start Point Coordinates: bohr

I= 0 X= -2.104901339182D+00 Y= -1.999556343648D+00 Z= 2.716428652915D-02
I= 1 X= 4.426075730912D-02 Y= -2.629479292261D+00 Z= -1.665825995627D+00
I= 2 X= -1.390952242928D+00 Y= -1.302587203057D+00 Z= 2.409257674419D+00
I= 3 X= 2.059399515456D+00 Y= -2.128046185003D+00 Z= -3.284097726660D-02
I= 4 X= 1.290423922098D+00 Y= -1.285422857212D+00 Z= 2.343722764325D+00
I= 5 X= -2.843100423357D+00 Y= 2.996137674199D+00 Z= -2.366488802793D+00
I= 6 X= 2.671107169901D-01 Y= 1.381870167476D+00 Z= -2.984862640261D+00
I= 7 X= -2.248961791126D+00 Y= 4.225152442891D+00 Z= -3.603828679766D+00
I= 8 X= -4.555396601340D+00 Y= 2.009547803660D+00 Z= -3.133000844027D+00
I= 9 X= 3.156520370799D+00 Y= -6.249816476307D-01 Z= 4.486170979129D+00
I= 10 X= 2.823428247518D+00 Y= -1.754614346228D+00 Z= 6.449888832188D+00
I= 11 X= 5.003709472680D+00 Y= -7.082380737365D-01 Z= 3.970650835251D+00
I= 12 X= 2.803321031340D+00 Y= 1.480261437581D+00 Z= 4.712169920105D+00
I= 13 X= -3.168136869170D+00 Y= -9.820423261348D-01 Z= 4.744984175479D+00
I= 14 X= -3.014451821304D+00 Y= -2.727759748918D+00 Z= 5.693666897471D+00
I= 15 X= -2.289580299887D+00 Y= 7.372243717306D-01 Z= 5.601566608510D+00
I= 16 X= -5.071512350830D+00 Y= -1.086930054358D+00 Z= 4.172879578935D+00
I= 17 X= -4.675658728764D+00 Y= -2.313543902377D+00 Z= -8.754601069380D-01
I= 18 X= -5.258245064127D+00 Y= -4.179732000893D+00 Z= -1.474925995188D-01
I= 19 X= -5.899148728560D+00 Y= -6.103524317789D-01 Z= 3.198674631109D-02
I= 20 X= -4.652911033982D+00 Y= -2.593693025701D+00 Z= -2.828836053232D+00
I= 21 X= -1.983044846698D-02 Y= -3.877495200705D+00 Z= -4.088120353512D+00
I= 22 X= 4.430935679750D-02 Y= -5.968953826240D+00 Z= -4.202575685825D+00
I= 23 X= -1.987462858022D+00 Y= -3.560124193257D+00 Z= -5.327525771076D+00
I= 24 X= 1.798216982912D+00 Y= -3.086279327999D+00 Z= -5.105332090131D+00
I= 25 X= 4.869968967336D+00 Y= -2.623796002894D+00 Z= -6.892127338840D-01
I= 26 X= 5.433215245022D+00 Y= -2.567138842093D+00 Z= -2.548181465455D+00
I= 27 X= 5.947399963494D+00 Y= -1.012298184833D+00 Z= 2.972125155646D-01
I= 28 X= 5.468610097997D+00 Y= -3.961001110537D+00 Z= 4.337938655896D-01

I= 29 X= 2.761968666522D+00 Y= 3.212073955271D+00 Z= -2.362736381418D+00
I= 30 X= 2.857188026564D+00 Y= 3.845370944515D+00 Z= 2.180070447439D-01
I= 31 X= 3.929234737376D+00 Y= 2.081839765331D+00 Z= -3.301604493351D+00
I= 32 X= 1.781964005880D+00 Y= 4.767876441095D+00 Z= -3.456597513422D+00
I= 33 X= 2.089253713770D+00 Y= 5.637314746578D+00 Z= 5.485763990284D-01
I= 34 X= 4.208875748868D+00 Y= 2.846181156040D+00 Z= 1.397512597319D+00
I= 35 X= -7.652701427566D-02 Y= 1.169925731481D+00 Z= -4.543712285493D-01
I= 36 X= -2.577008325377D+00 Y= 3.969651794755D+00 Z= 1.194040190520D-01
I= 37 X= -1.339011098944D+00 Y= 5.382728259672D+00 Z= 9.390916697563D-01
I= 38 X= -3.904467181553D+00 Y= 3.244430669736D+00 Z= 1.955490387448D+00

Forward Direction:

Total Energy: -692.0021305 Hartrees

Potential Energy: -692.1761484 Hartress

Kinetic Energy: 0.1740179 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.117427983637D+13 Y= 2.761960294961D+13 Z= 2.459445224187D+12
I= 1 X= -1.505106082626D+12 Y= -6.969126043978D+12 Z= -2.178021323967D+13
I= 2 X= 1.181237410079D+12 Y= -1.086407863214D+13 Z= -1.963597379414D+13
I= 3 X= -4.052375998259D+12 Y= -9.190323674596D+12 Z= -4.170779796791D+12
I= 4 X= 1.435861885037D+13 Y= 6.704477392817D+12 Z= 1.760524904179D+13
I= 5 X= -1.181402063960D+13 Y= 7.380706361486D+12 Z= 7.116845561117D+12
I= 6 X= 5.765537807144D+13 Y= 9.186070623656D+13 Z= 3.594538101603D+13
I= 7 X= 5.558777796970D+13 Y= 5.428293126863D+13 Z= 1.794873704320D+13
I= 8 X= -8.833286331988D+13 Y= -4.449759451984D+13 Z= 1.390606634433D+13
I= 9 X= 5.492075879907D+12 Y= -1.000168348966D+13 Z= -8.475083146919D+12
I= 10 X= -3.532094533943D+13 Y= 2.469836236719D+13 Z= -2.678131656394D+13
I= 11 X= -6.178850663857D+12 Y= 5.764220498500D+13 Z= -5.781431664559D+13
I= 12 X= -2.312764781414D+13 Y= -4.645884902754D+13 Z= 2.420919903216D+12
I= 13 X= -1.296301170014D+13 Y= -9.942842011703D+12 Z= -1.111384986018D+13
I= 14 X= -2.019530146431D+13 Y= -4.442088375313D+13 Z= 3.640596934467D+13

I= 15 X= 1.243812542223D+14 Y= 1.501711250551D+14 Z= 6.848817104353D+13
I= 16 X= 4.061132890077D+13 Y= 1.621776994097D+13 Z= 1.932539944667D+11
I= 17 X= 3.115660249544D+12 Y= 8.167291562908D+12 Z= 5.576257537517D+12
I= 18 X= -6.136845307626D+13 Y= -8.896229213043D+13 Z= 4.378957413105D+13
I= 19 X= 7.407681806042D+13 Y= -2.890693382900D+13 Z= -3.958146460813D+13
I= 20 X= 3.454780108269D+13 Y= 7.849541810645D+13 Z= -5.639185812110D+13
I= 21 X= -3.960122524847D+12 Y= 1.767340868816D+13 Z= 1.315339322055D+13
I= 22 X= -4.837159302019D+13 Y= 2.382906356976D+13 Z= 4.423732636265D+13
I= 23 X= -5.490497522769D+13 Y= -1.878503827582D+13 Z= 1.606772984812D+14
I= 24 X= 8.233434800266D+13 Y= 8.921254051751D+13 Z= -1.873305765716D+13
I= 25 X= -1.601345291307D+12 Y= -1.960486937037D+10 Z= 8.545119023361D+12
I= 26 X= 6.482919520558D+13 Y= -5.044261730819D+13 Z= 4.127147822044D+13
I= 27 X= 6.864445590586D+13 Y= 6.267707505407D+13 Z= 1.913438324785D+13
I= 28 X= 3.024204573729D+13 Y= -3.164041520896D+13 Z= -4.428601208528D+13
I= 29 X= -1.357003198972D+13 Y= -2.023658271377D+12 Z= -7.120244937467D+12
I= 30 X= -1.268154792976D+13 Y= -9.348348719668D+11 Z= -2.003473906215D+13
I= 31 X= 2.208771284618D+13 Y= -4.660868471296D+13 Z= -1.050926883032D+13
I= 32 X= -2.938371490689D+13 Y= -1.043051001342D+14 Z= 1.063067022128D+14
I= 33 X= -6.167462766515D+13 Y= 8.860322885803D+13 Z= -2.694256458220D+13
I= 34 X= 3.631267073043D+12 Y= -1.249036396532D+14 Z= 5.319291494558D+13
I= 35 X= 6.038133496882D+12 Y= -4.203884061284D+12 Z= 4.029117594029D+10
I= 36 X= 8.226669296147D+12 Y= -3.677092767685D+12 Z= 9.403952057976D+12
I= 37 X= 3.710709704302D+13 Y= 1.164193603250D+13 Z= 2.970222309366D+13
I= 38 X= -1.333702332927D+13 Y= -3.934532365369D+13 Z= -5.594177289294D+13

Backward Direction:

Total Energy: -692.0020946 Hartrees

Potential Energy: -692.1761484 Hartress

Kinetic Energy: 0.1740539 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.117587368390D+13 Y= 2.929606931198D+13 Z= 5.362022715651D+12

I= 1 X= -1.300805191645D+12 Y= -6.968687408281D+12 Z= -2.178048406311D+13
I= 2 X= 2.401371982879D+12 Y= -1.096926002587D+13 Z= -1.819643678974D+13
I= 3 X= -4.053693950535D+12 Y= -1.086692193111D+13 Z= -7.073732388988D+12
I= 4 X= 1.557893188357D+13 Y= 6.809846347527D+12 Z= 1.616584743440D+13
I= 5 X= -1.033386587324D+13 Y= -6.531696260905D+12 Z= -8.014017195727D+12
I= 6 X= -2.709857420987D+13 Y= 9.187740549381D+13 Z= 3.594638025357D+13
I= 7 X= 3.919350968876D+13 Y= 4.433661369703D+13 Z= -3.247620310919D+12
I= 8 X= -9.452889323380D+13 Y= -5.709640888149D+13 Z= 9.826740641992D+12
I= 9 X= 8.236361632163D+12 Y= -1.492830233803D+13 Z= -9.668323762295D+12
I= 10 X= -3.646285461672D+13 Y= 1.876525452388D+13 Z= -2.937594460463D+13
I= 11 X= -2.744316914098D+12 Y= 4.836680824159D+13 Z= -5.864612670836D+13
I= 12 X= -1.666275793772D+13 Y= -5.086572338434D+13 Z= 2.768708367554D+12
I= 13 X= -1.021892872246D+13 Y= -5.016175731506D+12 Z= -9.919827295280D+12
I= 14 X= -2.133506634290D+13 Y= -3.848700466941D+13 Z= 3.900187025642D+13
I= 15 X= 1.308448418138D+14 Y= 1.545799814970D+14 Z= 6.814007573846D+13
I= 16 X= 4.404468186895D+13 Y= 2.549044622728D+13 Z= 1.026912679880D+12
I= 17 X= 2.571127138567D+12 Y= 8.156004647094D+12 Z= 1.060429408566D+13
I= 18 X= -6.112745251120D+13 Y= -8.671505478562D+13 Z= 5.447939713897D+13
I= 19 X= 7.377999577369D+13 Y= -2.719537872694D+13 Z= -3.773793582105D+13
I= 20 X= 3.248921388304D+13 Y= 7.212667272083D+13 Z= -5.078820985453D+13
I= 21 X= -8.647954341465D+12 Y= 1.767559033975D+13 Z= 1.315192934064D+13
I= 22 X= -6.037294011541D+13 Y= 2.383137461397D+13 Z= 4.423327066896D+13
I= 23 X= -5.773952638139D+13 Y= -1.307163091922D+13 Z= 1.607636621221D+14
I= 24 X= 7.949926259956D+13 Y= 8.350511579754D+13 Z= -1.882134985007D+13
I= 25 X= -2.145304426118D+12 Y= -9.326408038428D+09 Z= 3.516913212067D+12
I= 26 X= 6.277162910753D+13 Y= -4.407521258810D+13 Z= 3.566726028045D+13
I= 27 X= 6.834852458283D+13 Y= 6.096333940024D+13 Z= 1.729157593717D+13
I= 28 X= 3.048333008857D+13 Y= -3.388934781380D+13 Z= -5.497575492193D+13
I= 29 X= -1.209077180735D+13 Y= 1.188459274536D+13 Z= 8.006565641636D+12
I= 30 X= -8.848837367888D+12 Y= -1.202468405208D+12 Z= -6.120006925406D+12

I= 31 X= 1.589465445690D+13 Y= -3.401357006179D+13 Z= -6.433817233589D+12
I= 32 X= -4.577419360878D+13 Y= -9.435786109633D+13 Z= 1.274964092430D+14
I= 33 X= -6.393723683814D+13 Y= 7.973681477898D+13 Z= 1.124570286674D+12
I= 34 X= 5.762891985896D+12 Y= -1.340530714981D+14 Z= 6.253633489202D+13
I= 35 X= 5.696849480622D+12 Y= -4.203350157903D+12 Z= 4.182948025352D+10
I= 36 X= 1.205929354151D+13 Y= -3.411150634824D+12 Z= -4.511659778120D+12
I= 37 X= 3.483940351510D+13 Y= 2.051339783580D+13 Z= 1.632729976891D+12
I= 38 X= -1.120518313680D+13 Y= -3.020003867484D+13 Z= -6.528538829523D+13

Seed: 28801055485

CM Start Point Coordinates: bohr

I= 0 X= -2.079406048920D+00 Y= -2.061071641628D+00 Z= -1.973564059297D-01
I= 1 X= 1.015237750181D-01 Y= -2.754278361003D+00 Z= -1.507031360970D+00
I= 2 X= -1.392668178372D+00 Y= -1.386978609852D+00 Z= 2.430695567461D+00
I= 3 X= 2.196917655644D+00 Y= -2.180601639506D+00 Z= 7.264405299371D-02
I= 4 X= 1.178522381737D+00 Y= -1.204295529185D+00 Z= 2.427962047263D+00
I= 5 X= -3.249736710036D+00 Y= 3.005195645523D+00 Z= -2.232388503025D+00
I= 6 X= -1.704922621576D-01 Y= 1.569631149720D+00 Z= -3.121007646215D+00
I= 7 X= -2.725859145444D+00 Y= 4.334560671378D+00 Z= -3.832470475780D+00
I= 8 X= -4.473807275189D+00 Y= 1.211975128976D+00 Z= -2.419514255583D+00
I= 9 X= 2.760831273130D+00 Y= -4.704158327192D-01 Z= 4.675990470041D+00
I= 10 X= 3.204166585469D+00 Y= -2.354186430056D+00 Z= 5.823561994821D+00
I= 11 X= 4.854256587604D+00 Y= 2.305873197815D-02 Z= 4.056072941016D+00
I= 12 X= 1.959575431951D+00 Y= 9.939959066241D-01 Z= 6.268098428081D+00
I= 13 X= -3.063524514931D+00 Y= -7.038792759601D-01 Z= 4.528775340001D+00
I= 14 X= -2.716063702824D+00 Y= -1.979189179290D+00 Z= 6.140512827694D+00
I= 15 X= -3.011113444441D+00 Y= 1.234292496636D+00 Z= 5.245932389365D+00
I= 16 X= -5.224400719613D+00 Y= -8.270044984866D-01 Z= 3.952654835694D+00
I= 17 X= -4.683810297661D+00 Y= -2.378803615569D+00 Z= -7.958338078667D-01
I= 18 X= -5.414255860438D+00 Y= -4.269561182508D+00 Z= -9.885765373139D-02

I= 19 X= -6.146295892640D+00 Y= -9.694542992887D-01 Z= 1.225798510271D-01
I= 20 X= -5.138448132122D+00 Y= -2.665235938190D+00 Z= -2.787423600092D+00
I= 21 X= 1.140430115119D-01 Y= -3.620863045020D+00 Z= -4.213149976684D+00
I= 22 X= 9.275237309312D-01 Y= -5.756564773063D+00 Z= -4.172324958758D+00
I= 23 X= -1.610911950036D+00 Y= -3.230551762436D+00 Z= -5.153016750481D+00
I= 24 X= 1.616127823430D+00 Y= -2.254074571220D+00 Z= -5.372081329322D+00
I= 25 X= 4.875999370916D+00 Y= -2.524810282667D+00 Z= -7.769031340718D-01
I= 26 X= 4.812363599906D+00 Y= -2.995250968315D+00 Z= -2.726447413502D+00
I= 27 X= 6.228735458217D+00 Y= -8.047641955007D-01 Z= -6.379714535569D-01
I= 28 X= 5.642293552769D+00 Y= -4.189343934973D+00 Z= 5.639330535002D-01
I= 29 X= 2.518742121943D+00 Y= 3.250985572651D+00 Z= -2.499644730483D+00
I= 30 X= 3.217051320927D+00 Y= 3.296782504618D+00 Z= 2.184625570089D-01
I= 31 X= 3.891965391365D+00 Y= 1.899965204841D+00 Z= -3.938896958523D+00
I= 32 X= 1.822341435354D+00 Y= 4.975252883551D+00 Z= -3.598431079042D+00
I= 33 X= 2.800250533685D+00 Y= 4.998854540570D+00 Z= 1.194975189753D+00
I= 34 X= 4.880362493231D+00 Y= 2.075992036846D+00 Z= 1.044964297272D+00
I= 35 X= -9.638112395149D-03 Y= 1.175578418454D+00 Z= -4.852383026421D-01
I= 36 X= -2.515914302260D+00 Y= 3.919610888551D+00 Z= 3.437439321627D-01
I= 37 X= -1.482570042359D+00 Y= 6.112691997218D+00 Z= 9.479424360901D-02
I= 38 X= -3.706996447649D+00 Y= 3.341663575338D+00 Z= 2.244072585215D+00

Forward Direction:

Total Energy: -692.0029168 Hartrees

Potential Energy: -692.1887692 Hartress

Kinetic Energy: 0.1858523 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.690334048767D+12 Y= 2.734792979555D+12 Z= -3.663433852693D+12

I= 1 X= -1.485161139999D+13 Y= 1.467043028721D+13 Z= 3.970415033000D+13

I= 2 X= -6.958613122387D+12 Y= -1.159634942437D+13 Z= -1.772858160689D+13

I= 3 X= -6.651170446364D+12 Y= 1.744356840578D+13 Z= 9.067495904193D+12

I= 4 X= 5.715936865743D+12 Y= 1.563242094433D+12 Z= 7.948082673965D+12

I= 5 X= 3.503732019494D+12 Y= 1.617510142025D+13 Z= 3.623068453099D+12
I= 6 X= 5.744513646252D+13 Y= -3.532874885620D+13 Z= -7.997821541540D+13
I= 7 X= -8.651165008150D+12 Y= 3.411176425636D+13 Z= 2.585999135516D+13
I= 8 X= 2.855456917002D+13 Y= -2.745908684207D+13 Z= -3.563074159979D+13
I= 9 X= -6.589120365102D+12 Y= 2.581581752133D+13 Z= -2.369131001337D+13
I= 10 X= -1.580468443633D+13 Y= -7.416586384464D+13 Z= 7.258937446270D+13
I= 11 X= 6.474578876071D+13 Y= 4.404715939338D+13 Z= -1.821843974902D+13
I= 12 X= 2.680633706810D+13 Y= -1.035763101514D+14 Z= -9.934008191776D+12
I= 13 X= -2.902411902194D+12 Y= -2.132313622626D+12 Z= 2.143993379915D+13
I= 14 X= 5.825888266444D+13 Y= 1.412667806708D+13 Z= 5.440798059381D+13
I= 15 X= 5.255194856814D+13 Y= 4.273860781041D+13 Z= 2.679715868798D+13
I= 16 X= 4.022192369342D+13 Y= 6.141139510596D+13 Z= -1.213133130827D+14
I= 17 X= 7.219034723591D+12 Y= -1.426701915999D+13 Z= 4.875796255521D+12
I= 18 X= 2.412979282478D+13 Y= 7.924157314114D+13 Z= -2.104732183875D+13
I= 19 X= -1.223481925393D+14 Y= 7.250882968153D+13 Z= 4.386633865334D+13
I= 20 X= 6.078957741444D+13 Y= 4.174751311157D+11 Z= 2.721333093218D+13
I= 21 X= 8.546973612957D+12 Y= -7.492898859013D+12 Z= -3.441018609860D+13
I= 22 X= -7.517389673113D+12 Y= -1.617233177167D+14 Z= 1.365434437950D+13
I= 23 X= 2.846062441734D+13 Y= 9.515894903666D+13 Z= 6.887221239590D+13
I= 24 X= 1.295027127675D+13 Y= 4.938302485150D+13 Z= -5.062488980811D+13
I= 25 X= -3.179930784794D+12 Y= -9.269015455076D+12 Z= -4.315749692176D+12
I= 26 X= 6.712615512934D+13 Y= 1.241162546740D+13 Z= -3.283773571784D+13
I= 27 X= -7.047024336638D+13 Y= -4.983010988749D+13 Z= -6.484529598485D+13
I= 28 X= -3.348306860901D+13 Y= 7.754653725368D+13 Z= -9.829565229299D+13
I= 29 X= -2.220285951802D+13 Y= 4.378084368290D+12 Z= 6.758460958063D+12
I= 30 X= -1.435024180650D+13 Y= 3.715618521641D+12 Z= -1.522007673623D+13
I= 31 X= 6.668557743025D+13 Y= -9.748801132009D+13 Z= 4.675943506511D+13
I= 32 X= 1.972003245162D+13 Y= -1.067143376328D+14 Z= 9.036669079182D+13
I= 33 X= -2.969325637794D+13 Y= -4.891891459321D+13 Z= -2.815519905857D+13
I= 34 X= 3.186302643759D+13 Y= -2.835947152010D+13 Z= -4.947058482805D+12

I= 35 X= 2.700060115854D+12 Y= -5.360705322089D+12 Z= 2.658607513502D+12
I= 36 X= 1.865673834131D+13 Y= -3.606851851576D+12 Z= 6.825593360768D+12
I= 37 X= -7.350836496093D+13 Y= -2.785842699403D+13 Z= -6.907521186610D+12
I= 38 X= 1.256983812268D+13 Y= 3.775591175752D+13 Z= -6.756108314235D+13

Backward Direction:

Total Energy: -692.0029590 Hartrees

Potential Energy: -692.1887692 Hartress

Kinetic Energy: 0.1858101 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.561325928538D+12 Y= 3.963366610300D+12 Z= -1.916173620963D+12
I= 1 X= -1.390448235866D+13 Y= 1.467064898798D+13 Z= 3.970404333646D+13
I= 2 X= -6.596639631067D+12 Y= -1.238032834058D+13 Z= -1.675601355022D+13
I= 3 X= -6.522037754372D+12 Y= 1.621487149257D+13 Z= 7.319995887195D+12
I= 4 X= 6.077996259118D+12 Y= 2.347328774790D+12 Z= 6.975501091594D+12
I= 5 X= 5.896602886067D+12 Y= 9.204593839066D+12 Z= -4.883201836331D+12
I= 6 X= -2.669303562060D+13 Y= -3.531685178905D+13 Z= -7.997832805057D+13
I= 7 X= -2.037768553557D+13 Y= 3.378479196116D+13 Z= 1.610944904866D+13
I= 8 X= 2.237722789799D+13 Y= -2.922925468699D+13 Z= -3.803040605216D+13
I= 9 X= -5.480872700114D+12 Y= 2.378937692708D+13 Z= -2.439488313423D+13
I= 10 X= -1.662564986935D+13 Y= -7.682896244533D+13 Z= 7.103052138061D+13
I= 11 X= 6.621023411524D+13 Y= 3.996488100518D+13 Z= -1.863532347931D+13
I= 12 X= 2.968377087028D+13 Y= -1.054675744669D+14 Z= -9.699361498507D+12
I= 13 X= -1.794287613738D+12 Y= -1.058515663113D+11 Z= 2.214380894481D+13
I= 14 X= 5.743875312115D+13 Y= 1.679005782349D+13 Z= 5.596727003310D+13
I= 15 X= 5.542879268665D+13 Y= 4.463074583225D+13 Z= 2.656238404809D+13
I= 16 X= 4.168582069993D+13 Y= 6.549248344666D+13 Z= -1.208956328655D+14
I= 17 X= 7.175190400640D+12 Y= -1.411257866458D+13 Z= 7.068129098050D+12
I= 18 X= 2.467235165762D+13 Y= 8.015759426313D+13 Z= -1.667047882100D+13
I= 19 X= -1.226198252789D+14 Y= 7.307032082975D+13 Z= 4.481791442793D+13
I= 20 X= 6.021959689826D+13 Y= -2.056433046126D+12 Z= 2.962477862185D+13

I= 21 X= 6.675771998697D+12 Y= -7.491892799483D+12 Z= -3.441086242170D+13
I= 22 X= -1.236902260891D+13 Y= -1.617222723879D+14 Z= 1.365243949985D+13
I= 23 X= 2.718114451127D+13 Y= 9.741707742065D+13 Z= 6.912843255418D+13
I= 24 X= 1.167047472509D+13 Y= 4.712777322210D+13 Z= -5.088219164279D+13
I= 25 X= -3.223580390087D+12 Y= -9.423843543801D+12 Z= -6.508128388255D+12
I= 26 X= 6.655664404326D+13 Y= 1.488472392635D+13 Z= -3.524934754003D+13
I= 27 X= -7.074159087620D+13 Y= -5.039242126659D+13 Z= -6.579665606992D+13
I= 28 X= -3.294055381688D+13 Y= 7.662993451475D+13 Z= -1.026721360839D+14
I= 29 X= -1.981032515853D+13 Y= 1.134630083745D+13 Z= 1.526285961613D+13
I= 30 X= -1.083629132688D+13 Y= 4.812843571058D+12 Z= -9.300791976116D+12
I= 31 X= 6.051202379992D+13 Y= -9.571750889393D+13 Z= 4.915774324127D+13
I= 32 X= 7.994674767565D+12 Y= -1.063876925255D+14 Z= 1.001136229954D+14
I= 33 X= -3.084423864227D+13 Y= -5.284425146462D+13 Z= -1.528259633099D+13
I= 34 X= 3.212201666750D+13 Y= -3.277199057427D+13 Z= 4.718420103769D+11
I= 35 X= 1.947439102831D+12 Y= -5.360480753165D+12 Z= 2.659358488274D+12
I= 36 X= 2.217100502154D+13 Y= -4.704988221199D+12 Z= 9.059631240926D+11
I= 37 X= -7.466131154266D+13 Y= -2.393048209613D+13 Z= -1.978194192954D+13
I= 38 X= 1.282972440034D+13 Y= 4.216720322202D+13 Z= -7.297983796516D+13

Seed: 29165319613

CM Start Point Coordinates: bohr

I= 0 X= -2.179701177960D+00 Y= -2.158701151265D+00 Z= 8.724426588029D-02
I= 1 X= -4.481750575539D-02 Y= -2.683347096154D+00 Z= -1.544196760109D+00
I= 2 X= -1.242979828561D+00 Y= -1.201679992921D+00 Z= 2.535777225912D+00
I= 3 X= 2.184341892819D+00 Y= -2.041633764713D+00 Z= -9.099078017387D-02
I= 4 X= 1.402033338896D+00 Y= -1.362562868635D+00 Z= 2.358183487878D+00
I= 5 X= -2.620253923913D+00 Y= 3.385914317397D+00 Z= -2.479411075411D+00
I= 6 X= 8.075095406332D-02 Y= 1.620226557967D+00 Z= -3.144406036231D+00
I= 7 X= -1.937571744441D+00 Y= 4.679640232214D+00 Z= -3.811531297855D+00
I= 8 X= -3.848281537922D+00 Y= 1.974640536434D+00 Z= -3.432445075809D+00

I= 9 X= 2.980973542091D+00 Y= -7.999666536137D-01 Z= 4.699327429684D+00
I= 10 X= 3.056605306740D+00 Y= -2.563711747622D+00 Z= 5.975885826690D+00
I= 11 X= 5.044692379340D+00 Y= -5.882657405917D-01 Z= 4.316770031551D+00
I= 12 X= 2.310023760582D+00 Y= 5.953163272330D-01 Z= 5.942638078703D+00
I= 13 X= -2.803673465082D+00 Y= -6.764142148853D-01 Z= 4.716248802895D+00
I= 14 X= -2.013834187959D+00 Y= -2.259140993043D+00 Z= 6.282078386975D+00
I= 15 X= -2.496410949088D+00 Y= 1.241179829613D+00 Z= 5.542663573910D+00
I= 16 X= -4.986586499842D+00 Y= -7.833027461598D-01 Z= 4.292220894899D+00
I= 17 X= -4.798596646866D+00 Y= -2.475776603393D+00 Z= -7.785629523725D-01
I= 18 X= -5.628628814010D+00 Y= -4.022867461497D+00 Z= 4.847181099217D-01
I= 19 X= -5.757854540134D+00 Y= -7.240511885350D-01 Z= -4.440895957807D-01
I= 20 X= -5.233620714441D+00 Y= -3.176729109362D+00 Z= -2.684173774507D+00
I= 21 X= -2.141467609572D-01 Y= -3.684944020805D+00 Z= -4.192304368653D+00
I= 22 X= -1.670900211165D+00 Y= -5.729326781847D+00 Z= -3.994964113837D+00
I= 23 X= -1.295290369653D+00 Y= -2.024404013666D+00 Z= -5.791891152176D+00
I= 24 X= 2.291510852261D+00 Y= -4.187974568061D+00 Z= -4.712161543075D+00
I= 25 X= 4.860526934574D+00 Y= -2.372897497206D+00 Z= -7.779307571359D-01
I= 26 X= 5.324122363488D+00 Y= -3.080789441316D+00 Z= -2.898608373875D+00
I= 27 X= 5.924803025047D+00 Y= -6.474942015909D-01 Z= -4.114106943442D-01
I= 28 X= 5.618357147297D+00 Y= -3.793612785365D+00 Z= 3.807970912729D-01
I= 29 X= 3.082882508242D+00 Y= 3.002040116173D+00 Z= -2.17767492534D+00
I= 30 X= 2.392439600827D+00 Y= 3.981711224211D+00 Z= 2.274186401263D-01
I= 31 X= 4.722464800864D+00 Y= 1.711870459049D+00 Z= -2.234348032447D+00
I= 32 X= 2.458472424054D+00 Y= 4.266661169312D+00 Z= -3.879170667157D+00
I= 33 X= 1.620121321862D+00 Y= 6.078539870259D+00 Z= 3.227813395756D-01
I= 34 X= 3.478541754389D+00 Y= 3.121826482436D+00 Z= 2.048142587363D+00
I= 35 X= -3.079575133504D-02 Y= 1.125325002030D+00 Z= -5.689707007455D-01
I= 36 X= -2.862488624078D+00 Y= 3.614603133697D+00 Z= 1.797243656736D-01
I= 37 X= -2.432246586962D+00 Y= 5.320314514632D+00 Z= 1.084682873182D+00
I= 38 X= -4.454196164863D+00 Y= 2.341246137026D+00 Z= 1.141028028117D+00

Forward Direction:

Total Energy: -692.0080060 Hartrees

Potential Energy: -692.1779470 Hartress

Kinetic Energy: 0.1699410 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.508647051098D+13 Y= -7.547687640470D+12 Z= -1.444320157293D+13
I= 1 X= -1.393091356907D+13 Y= -6.797384982266D+12 Z= 1.509895554429D+13
I= 2 X= -3.111104883061D+12 Y= -4.212459525274D+12 Z= 3.167461639652D+12
I= 3 X= 1.804157660908D+13 Y= 6.116622891676D+12 Z= -3.462953531832D+13
I= 4 X= -1.286237736596D+13 Y= 4.484328262608D+12 Z= 1.302950691920D+13
I= 5 X= 2.196801628574D+13 Y= 1.644109592030D+11 Z= 1.410214232007D+13
I= 6 X= 1.563059056423D+13 Y= -6.099224428953D+13 Z= 3.640567856209D+13
I= 7 X= 1.753035957310D+13 Y= 5.593438055256D+13 Z= -9.543527696664D+13
I= 8 X= -1.262912116735D+14 Y= -3.323194735903D+13 Z= -1.589546600443D+13
I= 9 X= -2.865111591239D+12 Y= -1.542059899581D+13 Z= -6.845134105885D+11
I= 10 X= 3.092892952621D+13 Y= 1.408994107281D+13 Z= -1.549448541185D+13
I= 11 X= 4.570866364022D+13 Y= -9.529904737199D+12 Z= 4.715724514958D+13
I= 12 X= -2.256886706512D+13 Y= 1.615651417296D+14 Z= 1.689086858093D+13
I= 13 X= 2.010146127948D+13 Y= 1.571189686770D+13 Z= 1.402129240155D+13
I= 14 X= -6.497139902832D+13 Y= 8.991305814639D+13 Z= 2.171744879406D+13
I= 15 X= -6.812612386687D+13 Y= -1.377762737449D+14 Z= 6.329218010621D+12
I= 16 X= -5.481588927275D+13 Y= -4.930229833164D+13 Z= 8.964204471985D+12
I= 17 X= 1.625723050280D+12 Y= 1.008851391087D+13 Z= -4.393219501559D+12
I= 18 X= -9.051237388198D+12 Y= 8.667918905805D+12 Z= 1.429867079504D+13
I= 19 X= -6.090731328815D+13 Y= 4.402587808787D+13 Z= 8.679515773303D+13
I= 20 X= -4.888176436030D+13 Y= -1.057491032196D+14 Z= -4.079586896919D+13
I= 21 X= 3.099766022812D+13 Y= -9.386684832900D+12 Z= -8.443362306209D+12
I= 22 X= -5.007380404184D+13 Y= 1.216126130530D+14 Z= -2.940352947511D+13
I= 23 X= -4.258347572196D+13 Y= -7.431535241318D+13 Z= -1.515952724147D+13
I= 24 X= -5.988658744723D+13 Y= -5.133600102560D+13 Z= -2.761477512634D+13

I= 25 X= -1.447297006326D+13 Y= -4.443263110074D+12 Z= 3.084105438662D+12
I= 26 X= -4.317299281604D+13 Y= -1.375772814145D+13 Z= 6.709679841753D+13
I= 27 X= 2.478480427186D+13 Y= 3.606268023742D+13 Z= 8.927799106820D+13
I= 28 X= 1.989588038104D+12 Y= 2.318633685320D+13 Z= -4.725057288341D+13
I= 29 X= -1.193071378076D+13 Y= -5.288594908724D+12 Z= 7.098448532511D+12
I= 30 X= 5.908421737346D+12 Y= -6.432647668767D+12 Z= -1.665246137031D+13
I= 31 X= 1.108934595186D+13 Y= -7.069266056341D+12 Z= -1.052730393194D+14
I= 32 X= 6.586035375721D+13 Y= -3.925236560255D+13 Z= 1.578952020168D+11
I= 33 X= -1.756551624241D+13 Y= -5.140029449774D+13 Z= 5.706038738204D+13
I= 34 X= -9.216954999102D+13 Y= 2.410839688284D+13 Z= -6.499515013952D+13
I= 35 X= 6.086277705732D+12 Y= 4.937872717051D+12 Z= 1.581996542729D+11
I= 36 X= -5.623076736405D+12 Y= 1.157838874252D+12 Z= 6.020591295215D+12
I= 37 X= 8.112440725550D+12 Y= -8.831080578276D+12 Z= 3.699149891243D+13
I= 38 X= -3.984177183194D+13 Y= 3.426917751970D+13 Z= 2.071644203365D+12

Backward Direction:

Total Energy: -692.0080056 Hartrees

Potential Energy: -692.1779470 Hartress

Kinetic Energy: 0.1699414 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.514240751934D+13 Y= -6.915456946724D+12 Z= -1.318710965555D+13
I= 1 X= -1.419283462663D+13 Y= -6.797175888253D+12 Z= 1.509881452331D+13
I= 2 X= -2.424742905682D+12 Y= -3.951633660362D+12 Z= 3.745357843589D+12
I= 3 X= 1.798577663714D+13 Y= 5.484353775819D+12 Z= -3.588578361756D+13
I= 4 X= -1.217592901211D+13 Y= 4.223585751735D+12 Z= 1.245170970291D+13
I= 5 X= 2.197013377921D+13 Y= -6.453144378180D+12 Z= 7.298338477011D+12
I= 6 X= -6.968346827299D+12 Y= -6.098580180073D+13 Z= 3.640641455671D+13
I= 7 X= 1.122540677741D+13 Y= 4.922395537565D+13 Z= -1.058870917442D+14
I= 8 X= -1.279321396766D+14 Y= -4.115550265607D+13 Z= -1.768458457647D+13
I= 9 X= -1.446390690560D+12 Y= -1.795184808563D+13 Z= -1.207146209314D+12
I= 10 X= 3.049154712548D+13 Y= 1.113621880768D+13 Z= -1.661860054885D+13

I= 11 X= 4.745130143061D+13 Y= -1.418198316130D+13 Z= 4.676163994059D+13
I= 12 X= -1.934005005624D+13 Y= 1.593343471505D+14 Z= 1.703062422191D+13
I= 13 X= 2.152009498838D+13 Y= 1.824316951275D+13 Z= 1.454433528944D+13
I= 14 X= -6.540766002032D+13 Y= 9.286719190332D+13 Z= 2.284225507118D+13
I= 15 X= -6.489795303751D+13 Y= -1.355444857254D+14 Z= 6.189305380016D+12
I= 16 X= -5.307383145109D+13 Y= -4.465158746172D+13 Z= 9.360744157459D+12
I= 17 X= 1.269374210117D+12 Y= 1.001509098273D+13 Z= -1.862648587200D+12
I= 18 X= -9.115908910711D+12 Y= 9.826065730257D+12 Z= 1.979956247973D+13
I= 19 X= -6.099624932804D+13 Y= 4.496583899368D+13 Z= 8.766018170802D+13
I= 20 X= -5.005709631640D+13 Y= -1.090832441498D+14 Z= -3.796205212347D+13
I= 21 X= 2.856485927237D+13 Y= -9.385610126694D+12 Z= -8.444082895159D+12
I= 22 X= -5.627603536888D+13 Y= 1.216137601708D+14 Z= -2.940551264373D+13
I= 23 X= -4.399156855240D+13 Y= -7.134077755319D+13 Z= -1.520896931028D+13
I= 24 X= -6.129491357888D+13 Y= -5.430767888098D+13 Z= -2.756620132180D+13
I= 25 X= -1.482900639153D+13 Y= -4.370369792304D+12 Z= 5.534374402839D+11
I= 26 X= -4.434782114669D+13 Y= -1.042416621463D+13 Z= 6.426265925437D+13
I= 27 X= 2.469636017511D+13 Y= 3.512156594715D+13 Z= 8.841337203880D+13
I= 28 X= 1.925130871498D+12 Y= 2.202726932581D+13 Z= -5.275156180994D+13
I= 29 X= -1.192906928983D+13 Y= 1.327075385994D+12 Z= 1.390025749110D+13
I= 30 X= 7.054045178670D+12 Y= -7.083364500507D+12 Z= -9.586442597374D+12
I= 31 X= 9.448854159016D+12 Y= 8.515992683600D+11 Z= -1.034860120543D+14
I= 32 X= 5.955751631548D+13 Y= -3.254116680631D+13 Z= 1.060666493230D+13
I= 33 X= -1.863437032955D+13 Y= -5.583744525430D+13 Z= 7.091654184365D+13
I= 34 X= -9.081172412263D+13 Y= 1.968344313558D+13 Z= -6.086440655995D+13
I= 35 X= 6.171184452245D+12 Y= 4.938144922966D+12 Z= 1.589397614544D+11
I= 36 X= -4.477647145827D+12 Y= 1.807778327979D+12 Z= -1.045886415715D+12
I= 37 X= 7.040920359531D+12 Y= -4.391562396587D+12 Z= 2.313449328126D+13
I= 38 X= -3.848417861628D+13 Y= 3.869179739833D+13 Z= -2.059295886746D+12

Seed: 29461475743

CM Start Point Coordinates: bohr

I= 0 X= -2.270175200537D+00 Y= -2.163872176212D+00 Z= -8.416039108552D-02
I= 1 X= -1.319717910355D-01 Y= -2.863446564070D+00 Z= -1.440021917588D+00
I= 2 X= -1.395189292719D+00 Y= -1.099256467244D+00 Z= 2.338211908288D+00
I= 3 X= 2.024385846889D+00 Y= -2.129404073573D+00 Z= -7.758765411359D-02
I= 4 X= 1.249707726969D+00 Y= -1.120897166038D+00 Z= 2.288083140363D+00
I= 5 X= -2.962387795668D+00 Y= 3.052715402921D+00 Z= -1.942274155747D+00
I= 6 X= -1.794442175030D-02 Y= 1.812779317910D+00 Z= -3.341749009143D+00
I= 7 X= -2.592485013986D+00 Y= 4.520157220386D+00 Z= -3.666610148934D+00
I= 8 X= -4.547357799538D+00 Y= 1.734084519062D+00 Z= -2.301071246339D+00
I= 9 X= 2.767824334781D+00 Y= -4.028640978877D-01 Z= 4.732406950870D+00
I= 10 X= 2.381489787749D+00 Y= -1.905100790446D+00 Z= 6.023480317047D+00
I= 11 X= 4.869153257835D+00 Y= -6.362222522902D-01 Z= 4.639972236889D+00
I= 12 X= 2.385991370430D+00 Y= 1.375398142890D+00 Z= 5.581712168432D+00
I= 13 X= -3.034017942722D+00 Y= -3.620200788501D-01 Z= 4.458840171424D+00
I= 14 X= -2.873560046929D+00 Y= -1.707489591624D+00 Z= 5.983875724361D+00
I= 15 X= -2.400232720713D+00 Y= 1.620819896994D+00 Z= 5.351829491622D+00
I= 16 X= -4.931270037317D+00 Y= -2.414562591799D-01 Z= 3.931069648847D+00
I= 17 X= -4.855901049291D+00 Y= -2.687282634978D+00 Z= -8.484107294164D-01
I= 18 X= -5.336154420408D+00 Y= -4.593391628621D+00 Z= 4.489797422021D-01
I= 19 X= -6.198973938743D+00 Y= -9.524871447699D-01 Z= -7.364157520267D-01
I= 20 X= -5.192104674330D+00 Y= -3.682385631688D+00 Z= -2.893077469279D+00
I= 21 X= 1.818349026485D-01 Y= -3.544066138798D+00 Z= -4.416096620590D+00
I= 22 X= 3.694178078076D-01 Y= -5.824546519853D+00 Z= -4.366501278882D+00
I= 23 X= -1.544735364588D+00 Y= -2.960745427199D+00 Z= -5.310356877480D+00
I= 24 X= 1.708037079755D+00 Y= -2.427462698191D+00 Z= -5.379579748166D+00
I= 25 X= 4.848013732409D+00 Y= -2.404560969684D+00 Z= -8.042908273608D-01
I= 26 X= 5.603814500397D+00 Y= -3.015397297928D+00 Z= -2.469750270609D+00
I= 27 X= 5.750690339530D+00 Y= -5.636835158169D-01 Z= -3.365115026032D-01
I= 28 X= 5.860793510600D+00 Y= -3.638487522398D+00 Z= 1.088277646572D+00

I= 29 X= 2.618301501995D+00 Y= 3.446174779180D+00 Z= -2.439574905852D+00
I= 30 X= 3.070399899466D+00 Y= 3.493980137331D+00 Z= 2.395750219243D-01
I= 31 X= 3.908750342705D+00 Y= 2.396732080214D+00 Z= -3.875543688667D+00
I= 32 X= 1.158713123775D+00 Y= 5.326386522695D+00 Z= -3.103215205996D+00
I= 33 X= 2.112228351545D+00 Y= 5.157665485104D+00 Z= 1.468360747533D+00
I= 34 X= 4.553116208688D+00 Y= 2.206315120163D+00 Z= 1.173482663529D+00
I= 35 X= 1.572026405133D-02 Y= 9.699792662837D-01 Z= -5.239616522226D-01
I= 36 X= -2.224645257369D+00 Y= 3.809311958274D+00 Z= 4.865627978287D-01
I= 37 X= -1.290716310054D+00 Y= 5.537303176444D+00 Z= 9.055819475697D-01
I= 38 X= -3.300673371870D+00 Y= 2.983356063172D+00 Z= 2.159705277282D+00

Forward Direction:

Total Energy: -691.9931476 Hartrees

Potential Energy: -692.1822752 Hartress

Kinetic Energy: 0.1891276 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.324269764681D+12 Y= 1.182250693601D+13 Z= 3.042935823321D+13
I= 1 X= -5.962341757579D+12 Y= -4.206199498619D+11 Z= 1.239248114076D+13
I= 2 X= 2.876606238470D+13 Y= -1.034482350906D+13 Z= -1.143549449076D+13
I= 3 X= 1.687293504013D+13 Y= 6.465537890842D+12 Z= -1.448663970169D+13
I= 4 X= -1.741301346903D+13 Y= -1.089591481031D+13 Z= -1.293483608622D+13
I= 5 X= 1.616016735107D+12 Y= -5.799825262203D+12 Z= 3.012549168289D+13
I= 6 X= 1.613324209057D+12 Y= 1.775852113312D+13 Z= 8.355648229328D+13
I= 7 X= 5.355321143252D+13 Y= 3.379567627758D+13 Z= -7.169482205579D+12
I= 8 X= 1.593501508088D+13 Y= -1.743235409978D+12 Z= -5.836609983513D+13
I= 9 X= -1.352256634636D+13 Y= 1.825623872051D+13 Z= 3.242202587000D+12
I= 10 X= -3.990464810490D+13 Y= -3.537594778860D+13 Z= 2.114229431348D+13
I= 11 X= 8.933114107694D+13 Y= 5.489524677696D+13 Z= 2.764201628386D+13
I= 12 X= -4.691744519461D+12 Y= -6.086011546917D+13 Z= 5.830908816900D+13
I= 13 X= 1.447789383640D+11 Y= -9.819511489027D+12 Z= 6.651688379012D+12
I= 14 X= 5.179792702232D+13 Y= 5.557212309809D+13 Z= 1.800669269611D+13

I= 15 X= 6.645715056172D+13 Y= 3.542206807312D+13 Z= 1.129671758295D+14
I= 16 X= -1.041390650105D+14 Y= 2.793567697355D+13 Z= -1.013256892301D+13
I= 17 X= -1.369578212635D+13 Y= -8.062161742311D+11 Z= 4.748382934784D+12
I= 18 X= 9.807274519201D+12 Y= -3.798998026248D+13 Z= 4.493954078985D+12
I= 19 X= 1.318041630126D+13 Y= 9.594152870813D+13 Z= 2.532185950976D+13
I= 20 X= -1.612012331565D+13 Y= -1.089366908968D+13 Z= 9.496121946053D+12
I= 21 X= 1.297566113331D+13 Y= 6.538622831338D+12 Z= -1.316902797799D+13
I= 22 X= 7.303093349386D+13 Y= 5.748993223040D+13 Z= -3.922235057209D+13
I= 23 X= -4.549553152699D+13 Y= -3.980794987711D+12 Z= -2.377779141924D+13
I= 24 X= -1.425012693827D+14 Y= -1.216486008115D+14 Z= 1.434703231690D+13
I= 25 X= -4.747551109874D+12 Y= 2.806549146848D+13 Z= -6.996863002963D+12
I= 26 X= 1.770415559160D+13 Y= 4.471025021945D+13 Z= -2.152237849020D+13
I= 27 X= 5.400382903965D+13 Y= -5.144511976999D+13 Z= -5.414766114128D+13
I= 28 X= 3.843932821187D+13 Y= -8.826560701959D+13 Z= 8.774852096892D+13
I= 29 X= -1.850063974826D+13 Y= 1.156135400237D+13 Z= -1.210448503663D+13
I= 30 X= -4.694813047086D+12 Y= -3.407813188895D+13 Z= -5.587729454600D+11
I= 31 X= 1.993687843819D+12 Y= 3.867756634337D+13 Z= -3.388976156078D+13
I= 32 X= 9.073033589996D+13 Y= -9.978391157138D+13 Z= -2.356327620604D+13
I= 33 X= -4.441939401508D+13 Y= 2.060647955051D+14 Z= 1.743172456601D+13
I= 34 X= -5.506154056261D+13 Y= 4.845140638395D+12 Z= 6.744098715681D+12
I= 35 X= 4.965709700619D+12 Y= -5.801938175894D+12 Z= -7.344892853906D+12
I= 36 X= -1.626527539622D+13 Y= 1.236273202324D+13 Z= 3.894115275061D+12
I= 37 X= 2.742035074061D+13 Y= -1.340756484719D+13 Z= -1.325729944758D+13
I= 38 X= 4.217503715707D+13 Y= -8.119699612821D+13 Z= -8.387842120872D+12

Backward Direction:

Total Energy: -691.9930252 Hartrees

Potential Energy: -692.1822752 Hartress

Kinetic Energy: 0.1892501 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.224715845860D+12 Y= 1.321191837398D+13 Z= 3.254058810416D+13

I= 1 X= -5.175101068780D+12 Y= -4.203360394381D+11 Z= 1.239232758203D+13
I= 2 X= 2.936488293826D+13 Y= -1.097977796543D+13 Z= -1.030627743722D+13
I= 3 X= 1.697265746522D+13 Y= 5.075996502809D+12 Z= -1.659815322769D+13
I= 4 X= -1.681407979143D+13 Y= -1.026082792086D+13 Z= -1.406402826928D+13
I= 5 X= 3.856438117774D+12 Y= -1.483098088906D+13 Z= 1.958637080825D+13
I= 6 X= -8.569786448755D+13 Y= 1.777209695991D+13 Z= 8.355665570011D+13
I= 7 X= 4.018907242729D+13 Y= 3.094738597991D+13 Z= -2.025524231026D+13
I= 8 X= 9.531633282010D+12 Y= -6.401888563946D+12 Z= -6.128988890215D+13
I= 9 X= -1.194781106448D+13 Y= 1.540061261133D+13 Z= 2.385689334534D+12
I= 10 X= -4.083873793646D+13 Y= -3.898751187695D+13 Z= 1.925740468764D+13
I= 11 X= 9.136199797356D+13 Y= 4.931196851939D+13 Z= 2.710195601247D+13
I= 12 X= -7.753520518513D+11 Y= -6.347539478725D+13 Z= 5.858165366479D+13
I= 13 X= 1.719385697759D+12 Y= -6.963856377468D+12 Z= 7.508639698015D+12
I= 14 X= 5.086504436545D+13 Y= 5.918410630255D+13 Z= 1.989225254280D+13
I= 15 X= 7.037274631331D+13 Y= 3.803854158445D+13 Z= 1.126944311715D+14
I= 16 X= -1.021089411219D+14 Y= 3.351732330716D+13 Z= -9.591409164025D+12
I= 17 X= -1.387182195088D+13 Y= -6.894832692143D+11 Z= 7.759019735694D+12
I= 18 X= 1.029058412940D+13 Y= -3.669385954738D+13 Z= 1.067450630687D+13
I= 19 X= 1.289248672160D+13 Y= 9.682316521938D+13 Z= 2.654020758184D+13
I= 20 X= -1.709887634605D+13 Y= -1.447228201645D+13 Z= 1.282672575071D+13
I= 21 X= 1.030262898047D+13 Y= 6.539971621294D+12 Z= -1.316993397850D+13
I= 22 X= 6.614029534271D+13 Y= 5.749134520916D+13 Z= -3.922488478921D+13
I= 23 X= -4.722652598935D+13 Y= -7.403646369188D+11 Z= -2.355671214318D+13
I= 24 X= -1.442326486072D+14 Y= -1.248852410781D+14 Z= 1.412461170165D+13
I= 25 X= -4.923290329561D+12 Y= 2.794819509022D+13 Z= -1.000757953378D+13
I= 26 X= 1.672603265595D+13 Y= 4.828788584087D+13 Z= -2.485325821862D+13
I= 27 X= 5.371635308333D+13 Y= -5.232796066008D+13 Z= -5.536565386567D+13
I= 28 X= 3.892267761706D+13 Y= -8.956262058708D+13 Z= 8.156826793552D+13
I= 29 X= -1.626071250876D+13 Y= 2.058965111598D+13 Z= -1.567871692225D+12
I= 30 X= -9.718920337244D+11 Y= -3.329770420614D+13 Z= 7.658386880182D+12

I= 31 X= -4.405983611493D+12 Y= 4.333551355182D+13 Z= -3.096803422085D+13
I= 32 X= 7.736808664675D+13 Y= -9.693563440997D+13 Z= -1.048204863425D+13
I= 33 X= -4.590159914305D+13 Y= 2.007098332230D+14 Z= 3.472933374859D+13
I= 34 X= -5.430472214278D+13 Y= -9.611813105077D+11 Z= 1.338088613318D+13
I= 35 X= 4.293457496348D+12 Y= -5.801624867376D+12 Z= -7.343909585947D+12
I= 36 X= -1.254213188653D+13 Y= 1.158115689005D+13 Z= -4.323541778712D+12
I= 37 X= 2.593529697958D+13 Y= -8.049264659094D+12 Z= -3.055693268504D+13
I= 38 X= 4.293260608889D+13 Y= -7.539270732601D+13 Z= -1.502456766223D+13

Seed: 30047930840

CM Start Point Coordinates: bohr

I= 0 X= -2.289876602925D+00 Y= -1.997663742669D+00 Z= -6.613734053597D-02
I= 1 X= 6.989743527496D-02 Y= -2.706686723914D+00 Z= -1.499832329564D+00
I= 2 X= -1.298185328003D+00 Y= -1.143878292418D+00 Z= 2.397160311451D+00
I= 3 X= 2.228915993977D+00 Y= -2.211912419341D+00 Z= 2.525300351172D-01
I= 4 X= 1.355186964481D+00 Y= -1.239083038804D+00 Z= 2.479802206685D+00
I= 5 X= -2.846532553169D+00 Y= 3.468663811988D+00 Z= -2.536314064059D+00
I= 6 X= -4.455164279012D-03 Y= 1.502021759669D+00 Z= -3.379671265425D+00
I= 7 X= -2.607013203447D+00 Y= 5.169981312030D+00 Z= -3.509143119340D+00
I= 8 X= -4.434541871147D+00 Y= 2.020723480823D+00 Z= -3.501413328024D+00
I= 9 X= 2.995022492073D+00 Y= -1.116844941163D+00 Z= 4.699548301328D+00
I= 10 X= 3.201324324463D+00 Y= -2.842147623852D+00 Z= 5.702252558506D+00
I= 11 X= 4.894581865660D+00 Y= -8.349645558637D-01 Z= 4.152460413876D+00
I= 12 X= 2.558756520801D+00 Y= 2.586272957100D-01 Z= 6.166324744765D+00
I= 13 X= -2.871039225349D+00 Y= -4.692270972918D-01 Z= 4.712539338824D+00
I= 14 X= -3.797357716002D+00 Y= -2.410949534567D+00 Z= 5.853934855108D+00
I= 15 X= -1.578174806487D+00 Y= 5.856873846059D-01 Z= 6.266356798727D+00
I= 16 X= -4.259526545398D+00 Y= 1.191349989567D+00 Z= 4.120746414907D+00
I= 17 X= -4.899821013998D+00 Y= -2.622039508352D+00 Z= -8.590898895728D-01
I= 18 X= -5.858787843500D+00 Y= -3.900357576082D+00 Z= -1.866943794979D-01

I= 19 X= -6.167802455588D+00 Y= -9.850838873408D-01 Z= -4.693616256124D-01
I= 20 X= -4.760984262061D+00 Y= -2.756459863738D+00 Z= -2.914698993003D+00
I= 21 X= 1.421723525075D-01 Y= -3.778912624417D+00 Z= -4.073211859167D+00
I= 22 X= -1.790593848186D-01 Y= -5.610129110982D+00 Z= -4.128072660621D+00
I= 23 X= -1.596588114249D+00 Y= -3.695337471115D+00 Z= -5.096588552472D+00
I= 24 X= 1.789452922149D+00 Y= -3.273964007399D+00 Z= -5.487490967181D+00
I= 25 X= 4.865836567452D+00 Y= -2.321650584879D+00 Z= -9.495436743974D-01
I= 26 X= 4.831057141586D+00 Y= -2.024957479047D+00 Z= -2.989777188707D+00
I= 27 X= 6.089262928050D+00 Y= -1.037501736068D+00 Z= 3.025790995202D-01
I= 28 X= 6.062475563357D+00 Y= -4.099562427770D+00 Z= -4.260814720938D-01
I= 29 X= 2.823688713686D+00 Y= 3.292478970641D+00 Z= -2.490336377478D+00
I= 30 X= 2.597677937355D+00 Y= 3.857924660745D+00 Z= 1.146122585878D-01
I= 31 X= 4.486609807271D+00 Y= 1.944992827109D+00 Z= -2.854765306367D+00
I= 32 X= 2.092178130350D+00 Y= 4.448140601163D+00 Z= -4.152742902322D+00
I= 33 X= 1.782116021191D+00 Y= 5.673693057698D+00 Z= 4.215999044045D-01
I= 34 X= 4.036669707993D+00 Y= 2.541764842534D+00 Z= 8.524789916696D-01
I= 35 X= -1.251547070057D-02 Y= 1.083184679416D+00 Z= -4.191648457520D-01
I= 36 X= -2.797302502188D+00 Y= 3.691798832571D+00 Z= 1.285326450471D-01
I= 37 X= -2.253838895383D+00 Y= 5.247120131331D+00 Z= 1.240794737531D+00
I= 38 X= -4.495151889769D+00 Y= 2.618273236180D+00 Z= 1.020034417146D+00

Forward Direction:

Total Energy: -691.9878481 Hartrees

Potential Energy: -692.1442545 Hartress

Kinetic Energy: 0.1564064 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.330962515028D+12 Y= 1.381831315842D+13 Z= 5.538448590669D+11
I= 1 X= -1.143848440959D+13 Y= -1.154810893429D+13 Z= -4.898715715463D+11
I= 2 X= -1.140334982455D+13 Y= 5.349963683243D+12 Z= 2.008530899264D+12
I= 3 X= 4.307438024938D+12 Y= 5.139199200905D+12 Z= 5.176141202706D+12
I= 4 X= 4.479219281731D+12 Y= -2.426777144132D+12 Z= -2.955651146455D+13

I= 5 X= 8.578155113696D+11 Y= 3.312822902279D+12 Z= 2.277247321200D+12
I= 6 X= 4.812403610194D+13 Y= 3.951682274920D+13 Z= -8.112474249569D+13
I= 7 X= 1.387338910058D+13 Y= -4.576582540262D+13 Z= -5.844849680398D+13
I= 8 X= -5.829049730430D+13 Y= 7.554314306365D+13 Z= -1.119612277391D+13
I= 9 X= 7.963289098753D+12 Y= -9.224220258191D+12 Z= 2.431197574715D+12
I= 10 X= -1.033878718765D+13 Y= -1.107107426706D+14 Z= 6.584146182753D+12
I= 11 X= 4.129265940514D+12 Y= -8.281079465417D+12 Z= -8.018337606601D+13
I= 12 X= 2.412689366052D+13 Y= 9.260751212129D+13 Z= 5.242734038836D+13
I= 13 X= 1.440048951420D+13 Y= 4.199398742198D+12 Z= 1.220107173724D+13
I= 14 X= -2.452507274239D+13 Y= -4.349976695675D+13 Z= -2.156239392488D+13
I= 15 X= -7.551888487720D+13 Y= -6.108152035510D+13 Z= 2.437702777650D+13
I= 16 X= 1.261963873383D+13 Y= -1.308333911229D+13 Z= 2.185915560351D+13
I= 17 X= -2.272402280212D+12 Y= 5.376771675341D+12 Z= 1.357562141555D+13
I= 18 X= 2.370444466361D+13 Y= -2.953308906523D+13 Z= -2.305517390462D+12
I= 19 X= 1.345936286775D+14 Y= 5.786022451109D+12 Z= -2.047248036015D+12
I= 20 X= -6.020016641384D+13 Y= 1.735741529008D+13 Z= -9.939722970651D+13
I= 21 X= -9.071965705937D+12 Y= 9.478108449699D+12 Z= -5.618781280328D+11
I= 22 X= 5.754417175782D+13 Y= 1.330292159406D+13 Z= 5.488711465979D+13
I= 23 X= -2.844631075826D+12 Y= 2.049801605072D+13 Z= 4.659297557855D+13
I= 24 X= 6.589442640702D+13 Y= 1.606198022798D+11 Z= -8.773183695707D+13
I= 25 X= 1.399821955185D+13 Y= 2.220416340197D+12 Z= 1.125385609095D+13
I= 26 X= 2.853174234988D+13 Y= -1.105317594982D+14 Z= -2.144549379367D+13
I= 27 X= 3.778916114881D+13 Y= -7.542075148201D+13 Z= 1.174566314339D+13
I= 28 X= 1.109673986599D+14 Y= -1.177384227722D+14 Z= -5.602983340577D+13
I= 29 X= -1.348069240417D+13 Y= -1.749333381967D+13 Z= 1.218862068690D+13
I= 30 X= -1.375883415423D+13 Y= 1.329646258434D+13 Z= -7.034211068660D+11
I= 31 X= 5.801347342644D+13 Y= -6.217165684912D+13 Z= 4.552589328013D+12
I= 32 X= -3.771412082758D+12 Y= 3.338648992916D+13 Z= -1.257518446424D+14
I= 33 X= 3.013248192327D+13 Y= 9.411513215003D+12 Z= 2.886693352025D+13
I= 34 X= -3.255043328460D+13 Y= 8.231815930292D+12 Z= -8.605645718213D+11

I= 35 X= -5.211332185745D+12 Y= 1.480569005328D+12 Z= -4.955360447051D+11
I= 36 X= 4.753371880163D+12 Y= -1.521104815548D+13 Z= -3.808896728559D+12
I= 37 X= 3.428850231728D+13 Y= 1.584864239455D+14 Z= 4.193836891021D+13
I= 38 X= -5.994167905910D+13 Y= 4.208227876677D+13 Z= 6.715681703068D+13

Backward Direction:

Total Energy: -691.9878461 Hartrees

Potential Energy: -692.1442545 Hartress

Kinetic Energy: 0.1564083 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.432777495966D+12 Y= 1.476929419502D+13 Z= 1.900609469312D+12
I= 1 X= -1.069337519401D+13 Y= -1.154794118869D+13 Z= -4.899530252169D+11
I= 2 X= -1.113115936972D+13 Y= 4.732501225933D+12 Z= 2.760112357189D+12
I= 3 X= 4.409348282293D+12 Y= 4.188122321302D+12 Z= 3.829191491659D+12
I= 4 X= 4.751475552777D+12 Y= -1.809231706899D+12 Z= -3.030810513365D+13
I= 5 X= 2.729679654858D+12 Y= -2.034263089559D+12 Z= -4.268258936868D+12
I= 6 X= -1.733433135819D+13 Y= 3.952602665277D+13 Z= -8.112484236993D+13
I= 7 X= 4.800765119291D+12 Y= -4.591431347535D+13 Z= -6.590904388574D+13
I= 8 X= -6.309667780472D+13 Y= 7.428506751609D+13 Z= -1.304472812171D+13
I= 9 X= 8.807565856917D+12 Y= -1.076899334360D+13 Z= 1.889162078191D+12
I= 10 X= -1.097401943410D+13 Y= -1.127468061703D+14 Z= 5.382658575567D+12
I= 11 X= 5.247010231902D+12 Y= -1.140018489370D+13 Z= -8.050317102601D+13
I= 12 X= 2.632622905910D+13 Y= 9.116368085816D+13 Z= 5.260866545766D+13
I= 13 X= 1.524467117628D+13 Y= 5.744188231520D+12 Z= 1.274333691252D+13
I= 14 X= -2.515966899352D+13 Y= -4.146349005554D+13 Z= -2.036057611455D+13
I= 15 X= -7.332000038278D+13 Y= -5.963702145020D+13 Z= 2.419560514897D+13
I= 16 X= 1.373696332090D+13 Y= -9.965142751103D+12 Z= 2.217955867890D+13
I= 17 X= -2.301003090132D+12 Y= 5.498761571915D+12 Z= 1.525017965164D+13
I= 18 X= 2.412991217919D+13 Y= -2.883502145969D+13 Z= 1.030448442570D+12
I= 19 X= 1.343825576077D+14 Y= 6.210236683834D+12 Z= -1.316679668997D+12
I= 20 X= -6.062725851935D+13 Y= 1.547543446209D+13 Z= -9.755611068589D+13

I= 21 X= -1.049687240438D+13 Y= 9.478878276366D+12 Z= -5.623956813380D+11
I= 22 X= 5.384800092279D+13 Y= 1.330372098436D+13 Z= 5.488565622979D+13
I= 23 X= -3.823029568180D+12 Y= 2.221694548640D+13 Z= 4.679420235878D+13
I= 24 X= 6.491578393717D+13 Y= -1.556105565201D+12 Z= -8.793389604294D+13
I= 25 X= 1.396976610740D+13 Y= 2.098131685408D+12 Z= 9.579263604710D+12
I= 26 X= 2.810500957821D+13 Y= -1.086504028221D+14 Z= -2.328673608913D+13
I= 27 X= 3.757830556371D+13 Y= -7.584558867318D+13 Z= 1.101525731294D+13
I= 28 X= 1.113928281681D+14 Y= -1.184369303776D+14 Z= -5.936551670643D+13
I= 29 X= -1.160908395381D+13 Y= -1.214801000256D+13 Z= 1.873269470886D+13
I= 30 X= -1.102825455342D+13 Y= 1.416520578398D+13 Z= 3.814142253548D+12
I= 31 X= 5.321024895360D+13 Y= -6.091327658531D+13 Z= 6.400167126063D+12
I= 32 X= -1.284316018961D+13 Y= 3.353470969552D+13 Z= -1.182940729867D+14
I= 33 X= 2.924918055257D+13 Y= 6.411743616404D+12 Z= 3.871537624852D+13
I= 34 X= -3.236954101069D+13 Y= 4.850737842560D+12 Z= 3.312491097820D+12
I= 35 X= -5.801451083480D+12 Y= 1.480740336056D+12 Z= -4.949604037890D+11
I= 36 X= 7.484201956978D+12 Y= -1.608049185733D+13 Z= -8.326722994467D+12
I= 37 X= 3.340370692544D+13 Y= 1.614881958880D+14 Z= 3.208851760243D+13
I= 38 X= -5.976008208629D+13 Y= 4.546243383697D+13 Z= 6.298387846899D+13

Seed: 30581075018

CM Start Point Coordinates: bohr

I= 0 X= -2.326005191684D+00 Y= -1.985440216755D+00 Z= 1.383501126316D-02
I= 1 X= -9.170572595813D-02 Y= -2.864372007932D+00 Z= -1.413074865659D+00
I= 2 X= -1.367893796502D+00 Y= -1.229614616193D+00 Z= 2.424912930506D+00
I= 3 X= 2.106152536982D+00 Y= -2.196626592307D+00 Z= 2.541402323604D-02
I= 4 X= 1.415630284749D+00 Y= -1.261393377489D+00 Z= 2.473624669634D+00
I= 5 X= -2.701463739801D+00 Y= 3.307780273169D+00 Z= -2.347507676146D+00
I= 6 X= -5.432750861660D-02 Y= 1.294632579204D+00 Z= -3.537422184117D+00
I= 7 X= -1.807292638930D+00 Y= 4.613755718221D+00 Z= -3.713673117103D+00
I= 8 X= -3.614568654162D+00 Y= 2.001985890183D+00 Z= -3.484021049554D+00

I= 9 X= 3.103784071084D+00 Y= -8.366606352667D-01 Z= 4.427586437235D+00
I= 10 X= 3.230125267851D+00 Y= -2.744918701509D+00 Z= 5.696882662819D+00
I= 11 X= 5.196340933068D+00 Y= -1.050856948097D+00 Z= 3.910022967627D+00
I= 12 X= 2.442417633610D+00 Y= 6.776729676281D-01 Z= 5.577513786238D+00
I= 13 X= -2.843769305444D+00 Y= -5.715401895006D-01 Z= 4.637326309687D+00
I= 14 X= -2.531707338579D+00 Y= -2.052675524690D+00 Z= 6.274144342337D+00
I= 15 X= -2.740344402069D+00 Y= 1.359124724916D+00 Z= 5.538705965638D+00
I= 16 X= -4.995143772110D+00 Y= -6.362645824408D-01 Z= 4.313818045997D+00
I= 17 X= -4.828974136187D+00 Y= -2.661427067912D+00 Z= -8.407804645640D-01
I= 18 X= -4.960164845151D+00 Y= -5.049438161263D+00 Z= -8.496802654413D-01
I= 19 X= -6.499755362387D+00 Y= -1.811075423749D+00 Z= 3.319112604410D-01
I= 20 X= -4.636366449900D+00 Y= -2.145618753478D+00 Z= -3.091392131982D+00
I= 21 X= -6.123220633013D-02 Y= -3.700650397494D+00 Z= -3.992938160323D+00
I= 22 X= -4.662285280635D-01 Y= -5.775956451939D+00 Z= -4.075860351456D+00
I= 23 X= -1.549202670383D+00 Y= -2.906024250563D+00 Z= -5.520523560519D+00
I= 24 X= 1.718080983223D+00 Y= -3.362216657132D+00 Z= -4.846292608718D+00
I= 25 X= 4.912854165189D+00 Y= -2.543402294369D+00 Z= -7.317510612235D-01
I= 26 X= 4.944218801725D+00 Y= -1.787661353409D+00 Z= -2.867740658951D+00
I= 27 X= 5.811283423718D+00 Y= -1.136239110368D+00 Z= 5.323115976267D-01
I= 28 X= 5.727695249950D+00 Y= -4.208627897422D+00 Z= -4.797393971595D-01
I= 29 X= 2.973453874242D+00 Y= 3.152417378409D+00 Z= -2.302500061464D+00
I= 30 X= 2.407516396429D+00 Y= 3.960725042668D+00 Z= 3.171052284097D-01
I= 31 X= 4.462099070810D+00 Y= 1.848829278029D+00 Z= -3.041268286563D+00
I= 32 X= 2.039829747684D+00 Y= 4.586559349058D+00 Z= -3.821444542820D+00
I= 33 X= 1.711474293805D+00 Y= 6.001297534112D+00 Z= 5.494829371798D-01
I= 34 X= 3.329718084089D+00 Y= 3.193101128938D+00 Z= 1.992861553964D+00
I= 35 X= 1.349789517594D-03 Y= 1.152347518071D+00 Z= -5.592157156215D-01
I= 36 X= -2.725161631076D+00 Y= 3.832829657319D+00 Z= 2.680114693315D-01
I= 37 X= -2.220716937498D+00 Y= 5.463842345517D+00 Z= 9.788568588934D-01
I= 38 X= -4.297119649047D+00 Y= 2.889517652177D+00 Z= 1.097587225718D+00

Forward Direction:

Total Energy: -692.0040141 Hartrees

Potential Energy: -692.1895787 Hartress

Kinetic Energy: 0.1855646 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.766357904981D+12 Y= -1.082166262612D+13 Z= 4.428486289202D+12
I= 1 X= 1.761293345150D+13 Y= -3.379095069348D+12 Z= 9.206288535750D+12
I= 2 X= -1.144297461412D+13 Y= -7.214312908267D+12 Z= 1.359662231017D+13
I= 3 X= 4.785328280189D+12 Y= 1.731474451295D+13 Z= 3.557760480004D+11
I= 4 X= 2.109760323123D+13 Y= 8.484658766281D+12 Z= -1.403233954441D+13
I= 5 X= -2.818598757520D+12 Y= -3.041338457790D+12 Z= -1.217681366088D+12
I= 6 X= 4.991229447769D+13 Y= 1.646003354863D+13 Z= -5.587701486624D+13
I= 7 X= -6.757368354180D+13 Y= 3.555297893712D+13 Z= 1.801487507726D+13
I= 8 X= -1.140669442920D+14 Y= -3.824690591810D+13 Z= -8.463689903666D+13
I= 9 X= -2.665091281388D+13 Y= -1.286704846702D+13 Z= -8.059922552687D+12
I= 10 X= 8.478518109686D+12 Y= 1.204686663060D+14 Z= -7.235098270265D+13
I= 11 X= 8.804633794503D+13 Y= 7.364097628583D+13 Z= 1.901026010428D+13
I= 12 X= 9.810450536357D+13 Y= -4.438471315598D+13 Z= -1.277817134530D+14
I= 13 X= 3.048467217389D+12 Y= 2.679310513457D+12 Z= -7.977299398322D+12
I= 14 X= 6.487514593455D+13 Y= -2.188410435829D+13 Z= 1.153721155599D+14
I= 15 X= -4.443428348516D+13 Y= -2.231995212553D+13 Z= 1.982181563670D+13
I= 16 X= 8.872831591433D+12 Y= -1.558660916291D+13 Z= 4.145179627125D+13
I= 17 X= 2.516753182205D+13 Y= 2.361465057837D+12 Z= 8.089479482498D+12
I= 18 X= -5.244747035717D+12 Y= 5.905407931589D+13 Z= -4.247635214092D+13
I= 19 X= -1.731482233222D+14 Y= 6.320281848282D+13 Z= -1.779401214660D+12
I= 20 X= -7.339174136733D+12 Y= -9.958971309209D+12 Z= -4.196219438022D+13
I= 21 X= -1.216074807410D+13 Y= 1.906525374682D+13 Z= -1.221862832332D+12
I= 22 X= -1.156141911450D+12 Y= -1.456501372899D+14 Z= -2.481953222674D+13
I= 23 X= -1.442799731736D+13 Y= 2.685307922525D+12 Z= -1.232833735533D+13
I= 24 X= -3.501196329031D+11 Y= -9.851403360026D+13 Z= -1.533838695562D+13

I= 25 X= -3.990873555561D+12 Y= 9.896316641384D+12 Z= 8.930150664305D+12
I= 26 X= -2.493377065629D+13 Y= 1.072252270210D+13 Z= -1.401123222013D+14
I= 27 X= -9.928330175079D+12 Y= -5.641857312015D+13 Z= 7.505996513948D+13
I= 28 X= -8.806523995001D+11 Y= 1.845910500185D+13 Z= 5.196866924954D+13
I= 29 X= 4.370957058433D+12 Y= -5.625660583305D+12 Z= 1.033686557345D+13
I= 30 X= 1.089085956947D+13 Y= -1.415128925152D+13 Z= -7.638536854813D+11
I= 31 X= -7.524535428927D+13 Y= -2.811677164241D+13 Z= -1.713342089429D+13
I= 32 X= 2.910419116327D+13 Y= 9.443653928016D+13 Z= -8.538408201789D+13
I= 33 X= -6.359163195652D+13 Y= 1.452652382534D+13 Z= 1.466153996071D+13
I= 34 X= -9.649829653602D+13 Y= 2.657369649713D+13 Z= -6.196204870524D+13
I= 35 X= -1.296462547960D+12 Y= -1.200798457552D+12 Z= -3.499645399723D+12
I= 36 X= 5.625559248557D+12 Y= -4.540528753991D+12 Z= 3.156143912416D+13
I= 37 X= 8.040194831117D+13 Y= 3.009858253776D+13 Z= 6.456976710606D+12
I= 38 X= -1.952348680241D+13 Y= 7.315262972648D+12 Z= -7.057448771778D+12

Backward Direction:

Total Energy: -692.0039751 Hartrees

Potential Energy: -692.1895787 Hartress

Kinetic Energy: 0.1856036 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.793917329502D+12 Y= -1.015222274356D+13 Z= 5.666092601696D+12
I= 1 X= 1.752959401123D+13 Y= -3.378898663534D+12 Z= 9.206161473557D+12
I= 2 X= -1.084568920647D+13 Y= -7.110113087880D+12 Z= 1.418848935154D+13
I= 3 X= 4.757895078278D+12 Y= 1.664525746249D+13 Z= -8.819873014603D+11
I= 4 X= 2.169496918289D+13 Y= 8.380539978366D+12 Z= -1.462412919627D+13
I= 5 X= -2.498102671087D+12 Y= -9.263775245062D+12 Z= -7.793718503651D+12
I= 6 X= 2.062440025432D+13 Y= 1.646677228989D+13 Z= -5.587644111029D+13
I= 7 X= -7.417969549677D+13 Y= 3.014136852166D+13 Z= 8.354813703838D+12
I= 8 X= -1.162026223972D+14 Y= -4.482124454429D+13 Z= -8.638782326810D+13
I= 9 X= -2.536834603853D+13 Y= -1.516192017666D+13 Z= -8.571743085560D+12
I= 10 X= 8.019254043914D+12 Y= 1.177510125187D+14 Z= -7.345791188181D+13

I= 11 X= 8.963548034857D+13 Y= 6.937563420716D+13 Z= 1.863825172051D+13
I= 12 X= 1.010707788620D+14 Y= -4.642122479547D+13 Z= -1.276386530368D+14
I= 13 X= 4.330947800993D+12 Y= 4.974203924058D+12 Z= -7.465110568081D+12
I= 14 X= 6.441689029284D+13 Y= -1.916608391263D+13 Z= 1.164796557333D+14
I= 15 X= -4.146860546097D+13 Y= -2.028252934774D+13 Z= 1.967861261425D+13
I= 16 X= 1.046143696799D+13 Y= -1.132251961119D+13 Z= 4.182465829555D+13
I= 17 X= 2.487662689241D+13 Y= 2.323306009336D+12 Z= 1.040591048545D+13
I= 18 X= -5.224196297487D+12 Y= 6.010258788166D+13 Z= -3.749275160829D+13
I= 19 X= -1.732555579567D+14 Y= 6.402955375519D+13 Z= -9.606412927442D+11
I= 20 X= -8.355327002281D+12 Y= -1.295573765386D+13 Z= -3.937398718627D+13
I= 21 X= -1.435618308118D+13 Y= 1.906624750422D+13 Z= -1.222529374537D+12
I= 22 X= -6.764039903271D+12 Y= -1.456490803746D+14 Z= -2.482137246189D+13
I= 23 X= -1.572487537346D+13 Y= 5.365688699220D+12 Z= -1.233375264519D+13
I= 24 X= -1.647226509438D+12 Y= -1.011917136233D+14 Z= -1.533381034692D+13
I= 25 X= -4.281502555376D+12 Y= 9.934000371410D+12 Z= 6.613635874531D+12
I= 26 X= -2.594945811374D+13 Y= 1.371871795014D+13 Z= -1.427008091731D+14
I= 27 X= -1.003523316631D+13 Y= -5.724634023762D+13 Z= 7.424155791008D+13
I= 28 X= -8.599361429589D+11 Y= 1.740978255384D+13 Z= 4.698503873076D+13
I= 29 X= 4.691029932645D+12 Y= 5.949630117204D+11 Z= 1.691105753246D+13
I= 30 X= 1.227547205172D+13 Y= -1.452565108058D+13 Z= 5.677279897278D+12
I= 31 X= -7.738017880837D+13 Y= -2.154454030247D+13 Z= -1.538435032171D+13
I= 32 X= 2.250002631072D+13 Y= 9.984872497550D+13 Z= -7.572693753422D+13
I= 33 X= -6.460001403923D+13 Y= 1.045402383948D+13 Z= 2.746087691950D+13
I= 34 X= -9.537758970269D+13 Y= 2.244604631046D+13 Z= -5.793567364062D+13
I= 35 X= -1.328812543494D+12 Y= -1.200550786861D+12 Z= -3.498953293249D+12
I= 36 X= 7.010058783426D+12 Y= -4.166910203319D+12 Z= 2.511989238128D+13
I= 37 X= 7.939117161748D+13 Y= 3.417332382856D+13 Z= -6.343283363092D+12
I= 38 X= -1.840284670390D+13 Y= 1.144088262125D+13 Z= -1.108396163411D+13

Seed: 31995162837

CM Start Point Coordinates: bohr

I= 0 X= -2.183456702134D+00 Y= -1.977281814853D+00 Z= 2.188289864301D-02
I= 1 X= 4.545569656562D-02 Y= -2.632933958719D+00 Z= -1.521839085659D+00
I= 2 X= -1.424891864960D+00 Y= -1.156933911372D+00 Z= 2.345961189089D+00
I= 3 X= 2.153848609907D+00 Y= -2.024000087850D+00 Z= -9.586156035958D-02
I= 4 X= 1.390202721598D+00 Y= -1.241645451221D+00 Z= 2.432821138346D+00
I= 5 X= -2.861377935763D+00 Y= 3.262694015694D+00 Z= -2.261038774177D+00
I= 6 X= -7.700888839614D-02 Y= 1.259743187854D+00 Z= -3.518805793761D+00
I= 7 X= -1.874175592982D+00 Y= 4.754823550440D+00 Z= -3.423672328043D+00
I= 8 X= -4.159021527599D+00 Y= 1.942459004497D+00 Z= -3.252830823474D+00
I= 9 X= 2.892476380683D+00 Y= -2.821226896689D-01 Z= 4.756989699960D+00
I= 10 X= 2.501531489989D+00 Y= -1.532312312761D+00 Z= 6.643018315814D+00
I= 11 X= 4.897575610221D+00 Y= -4.007434886612D-01 Z= 4.301346495734D+00
I= 12 X= 2.306715518524D+00 Y= 1.876879202958D+00 Z= 4.913764595034D+00
I= 13 X= -2.894344963433D+00 Y= -7.751925699220D-01 Z= 4.770435178800D+00
I= 14 X= -2.756958966420D+00 Y= -2.599991697996D+00 Z= 5.864386007353D+00
I= 15 X= -2.542618377103D+00 Y= 1.088165100741D+00 Z= 5.788649415970D+00
I= 16 X= -5.151996928061D+00 Y= -1.137807271630D+00 Z= 4.116044323986D+00
I= 17 X= -4.822735629426D+00 Y= -2.304575214852D+00 Z= -8.299414705781D-01
I= 18 X= -5.361518443134D+00 Y= -4.167051198203D+00 Z= -1.635852765118D-01
I= 19 X= -6.275409163799D+00 Y= -1.007956570473D+00 Z= -1.879795646025D-01
I= 20 X= -4.889254426524D+00 Y= -2.438861097744D+00 Z= -2.641301199648D+00
I= 21 X= -1.158746652758D-01 Y= -3.824053291576D+00 Z= -4.156672486425D+00
I= 22 X= -8.390684720735D-01 Y= -5.811650305051D+00 Z= -4.065568474580D+00
I= 23 X= -1.282485579594D+00 Y= -2.625962311058D+00 Z= -5.773582227449D+00
I= 24 X= 2.060886299446D+00 Y= -3.702697778194D+00 Z= -5.026522424758D+00
I= 25 X= 4.890503111776D+00 Y= -2.439755519654D+00 Z= -9.344021535925D-01
I= 26 X= 4.859406888119D+00 Y= -1.913308465187D+00 Z= -3.139186633086D+00
I= 27 X= 6.556330484202D+00 Y= -1.423564197772D+00 Z= 3.840039919642D-01
I= 28 X= 5.391443010727D+00 Y= -4.554513759712D+00 Z= -9.846138469545D-01

I= 29 X= 2.925914928639D+00 Y= 3.212445587038D+00 Z= -2.194157530952D+00
I= 30 X= 2.838397160174D+00 Y= 3.708699664521D+00 Z= 4.045685348936D-01
I= 31 X= 4.678093083573D+00 Y= 1.989728503471D+00 Z= -2.823170711499D+00
I= 32 X= 2.267146277633D+00 Y= 4.577997954129D+00 Z= -3.746313753429D+00
I= 33 X= 1.755990361537D+00 Y= 5.169811882678D+00 Z= 1.012654217095D+00
I= 34 X= 4.289737005267D+00 Y= 3.050523452539D+00 Z= 1.486889944384D+00
I= 35 X= 8.115404199140D-04 Y= 9.579640655166D-01 Z= -6.012405690292D-01
I= 36 X= -2.891250193109D+00 Y= 3.707998795880D+00 Z= 3.046175470203D-01
I= 37 X= -1.770301430381D+00 Y= 5.217879717116D+00 Z= 1.023317403196D+00
I= 38 X= -3.952216620717D+00 Y= 3.126623938293D+00 Z= 2.134172548443D+00

Forward Direction:

Total Energy: -692.0036239 Hartrees

Potential Energy: -692.1945490 Hartress

Kinetic Energy: 0.1909251 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.798632984836D+12 Y= 3.847218567054D+12 Z= -3.645561631799D+12
I= 1 X= -1.385860435021D+13 Y= 2.697804112610D+12 Z= -5.290192433314D+12
I= 2 X= 1.607150702414D+13 Y= -2.996921894022D+12 Z= -4.751369554022D+12
I= 3 X= -3.151154495480D+13 Y= 2.580145665771D+13 Z= -6.186548302659D+12
I= 4 X= -6.920274334885D+12 Y= -1.845492281791D+12 Z= -8.004107047322D+12
I= 5 X= 7.912601495949D+12 Y= -1.446705980605D+12 Z= -6.877051262846D+12
I= 6 X= 3.662233839869D+13 Y= -1.631965639077D+13 Z= 6.782397422045D+13
I= 7 X= -2.653605268444D+13 Y= -2.107657002224D+13 Z= 4.922745514743D+13
I= 8 X= -7.189326388079D+13 Y= -1.168963803166D+14 Z= -9.313026425265D+13
I= 9 X= -3.029986863662D+12 Y= 2.386961758815D+13 Z= 1.608334491060D+12
I= 10 X= 3.554295921193D+13 Y= -9.549445371653D+13 Z= 9.549874198638D+13
I= 11 X= 9.279382622125D+13 Y= -3.857992862095D+13 Z= 5.642055418773D+13
I= 12 X= 2.627579759182D+13 Y= 3.572739581346D+13 Z= 6.058714657243D+12
I= 13 X= -1.279905357044D+13 Y= 1.846406013168D+13 Z= 9.928619199690D+12
I= 14 X= 1.682174270890D+13 Y= -5.241702344682D+13 Z= 7.631796247835D+12

I= 15 X= -1.213066827563D+13 Y= -1.417891115078D+14 Z= -3.878837687385D+13
I= 16 X= -2.877261034534D+13 Y= -5.356733310938D+13 Z= -1.174779267141D+14
I= 17 X= 1.107271922106D+12 Y= 8.514675385996D+12 Z= -1.737643362001D+13
I= 18 X= -5.769502348155D+12 Y= -6.151607332952D+13 Z= 8.683037187961D+13
I= 19 X= 4.203752491002D+13 Y= -2.908814606644D+13 Z= 5.122203917368D+13
I= 20 X= 3.810461419081D+13 Y= 1.066796686176D+13 Z= 2.795739739896D+12
I= 21 X= -2.316632615622D+12 Y= -3.976145317356D+12 Z= 7.912165516832D+12
I= 22 X= 3.151919999072D+13 Y= 5.423122796597D+13 Z= -1.177438128560D+14
I= 23 X= 9.469473482331D+13 Y= -5.640653866384D+13 Z= 8.276665701736D+13
I= 24 X= 2.422008115798D+13 Y= -5.531294147505D+13 Z= 6.195064442729D+13
I= 25 X= 9.218560014390D+12 Y= -9.262564972907D+12 Z= 1.368436242722D+13
I= 26 X= 7.924414600868D+12 Y= 2.556492645565D+13 Z= -1.495479200354D+14
I= 27 X= -2.284896348581D+13 Y= -1.963171574788D+13 Z= -3.979685906694D+13
I= 28 X= 3.918914817975D+13 Y= -3.950203475179D+13 Z= -1.405560592529D+13
I= 29 X= -9.212343150245D+12 Y= 1.007359796563D+13 Z= 1.876563894612D+12
I= 30 X= -7.305771497985D+11 Y= 9.859224055149D+12 Z= -1.174062692108D+13
I= 31 X= -1.057058018452D+14 Y= -4.447399077306D+13 Z= -4.393163803511D+12
I= 32 X= 1.072748961274D+14 Y= -1.118781309342D+14 Z= -1.265934545180D+13
I= 33 X= 6.703963972883D+13 Y= -1.388996926307D+14 Z= -3.615187775162D+13
I= 34 X= 6.941537220588D+13 Y= 3.789495232361D+11 Z= 1.473545710894D+13
I= 35 X= -6.846010696541D+11 Y= 4.489420485887D+11 Z= 2.064594270799D+12
I= 36 X= 1.269685511539D+13 Y= -1.036373018945D+13 Z= 1.220324510234D+13
I= 37 X= 3.669847083438D+13 Y= 7.594798919288D+12 Z= 1.144797629316D+14
I= 38 X= -9.898430128042D+12 Y= 6.042267118147D+13 Z= 3.925902985120D+12

Backward Direction:

Total Energy: -692.0036200 Hartrees

Potential Energy: -692.1945490 Hartress

Kinetic Energy: 0.1909290 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.916577695079D+12 Y= 4.676242177915D+12 Z= -1.868358001494D+12

I= 1 X= -1.447523333000D+13 Y= 2.698113491897D+12 Z= -5.290408687792D+12
I= 2 X= 1.715382928800D+13 Y= -2.412736959885D+12 Z= -3.965372464100D+12
I= 3 X= -3.162928338756D+13 Y= 2.497239178872D+13 Z= -7.963969012720D+12
I= 4 X= -5.837823431769D+12 Y= -2.429557750366D+12 Z= -8.789935707669D+12
I= 5 X= 7.467222228061D+12 Y= -1.122892390639D+13 Z= -1.668326643946D+13
I= 6 X= 1.453536244568D+13 Y= -1.631109184105D+13 Z= 6.782522876124D+13
I= 7 X= -3.490212075277D+13 Y= -3.226082023390D+13 Z= 3.354119875013D+13
I= 8 X= -7.348426093082D+13 Y= -1.298428828514D+14 Z= -9.567833693595D+13
I= 9 X= -8.603577029093D+11 Y= 2.000783275464D+13 Z= 8.644836980956D+11
I= 10 X= 3.496399840550D+13 Y= -9.994479195139D+13 Z= 9.390736308437D+13
I= 11 X= 9.543946152151D+13 Y= -4.561018556924D+13 Z= 5.583579526955D+13
I= 12 X= 3.114693881485D+13 Y= 3.234376389528D+13 Z= 6.248900429566D+12
I= 13 X= -1.062954738903D+13 Y= 2.232588042338D+13 Z= 1.067310057649D+13
I= 14 X= 1.624450436418D+13 Y= -4.796604839918D+13 Z= 9.224251562672D+12
I= 15 X= -7.260499333977D+12 Y= -1.384039786926D+14 Z= -3.897880175224D+13
I= 16 X= -2.612784407033D+13 Y= -4.653914470364D+13 Z= -1.168917511845D+14
I= 17 X= 5.183142314995D+11 Y= 8.362655673842D+12 Z= -1.354690842715D+13
I= 18 X= -5.979671106943D+12 Y= -5.974706049989D+13 Z= 9.522783983804D+13
I= 19 X= 4.193944347559D+13 Y= -2.761826423796D+13 Z= 5.249315467588D+13
I= 20 X= 3.624188116506D+13 Y= 5.544614027708D+12 Z= 7.092348033038D+12
I= 21 X= -6.042558681729D+12 Y= -3.974533029499D+12 Z= 7.911084811492D+12
I= 22 X= 2.203547506231D+13 Y= 5.423295423736D+13 Z= -1.177467789511D+14
I= 23 X= 9.257504158390D+13 Y= -5.184527818011D+13 Z= 8.263573044761D+13
I= 24 X= 2.210005634815D+13 Y= -5.986988675469D+13 Z= 6.208031886221D+13
I= 25 X= 8.630089510341D+12 Y= -9.111360055908D+12 Z= 9.854683118581D+12
I= 26 X= 6.062437478029D+12 Y= 3.068746088554D+13 Z= -1.538450376346D+14
I= 27 X= -2.294627413502D+13 Y= -2.110337672606D+13 Z= -4.106733651091D+13
I= 28 X= 3.897934696662D+13 Y= -4.127248160227D+13 Z= -2.245330416506D+13
I= 29 X= -9.658451962463D+12 Y= 1.985308670264D+13 Z= 1.167978709999D+13
I= 30 X= 5.300493212455D+11 Y= 8.562876262598D+12 Z= -1.009635880794D+12

I= 31 X= -1.072967784763D+14 Y= -3.153205897518D+13 Z= -1.848341366705D+12
I= 32 X= 9.891215487554D+13 Y= -1.006925228725D+14 Z= 3.022485227116D+12
I= 33 X= 6.546434855536D+13 Y= -1.455992092312D+14 Z= -1.534622690977D+13
I= 34 X= 7.164228074443D+13 Y= -6.208726331537D+12 Z= 2.064127624570D+13
I= 35 X= -4.011113653820D+11 Y= 4.493560884194D+11 Z= 2.065693682642D+12
I= 36 X= 1.395709739963D+13 Y= -9.068514182199D+12 Z= 1.471549766955D+12
I= 37 X= 3.511907993460D+13 Y= 1.429779365097D+13 Z= 9.367302674831D+13
I= 38 X= -7.672079591409D+12 Y= 6.700666616118D+13 Z= -1.980272804869D+12

Seed: 32631781433

CM Start Point Coordinates: bohr

I= 0 X= -2.256620915306D+00 Y= -2.138975368254D+00 Z= 4.235754123595D-02
I= 1 X= 2.118760118509D-02 Y= -2.770028383947D+00 Z= -1.454102674683D+00
I= 2 X= -1.395012721522D+00 Y= -1.145797333803D+00 Z= 2.289822791871D+00
I= 3 X= 2.215722104558D+00 Y= -2.179298945682D+00 Z= 1.091878076393D-02
I= 4 X= 1.337975472661D+00 Y= -1.199263741549D+00 Z= 2.297952724983D+00
I= 5 X= -2.682174875823D+00 Y= 3.136463422126D+00 Z= -2.439747248996D+00
I= 6 X= 2.266247293928D-01 Y= 1.877117990321D+00 Z= -3.465302751309D+00
I= 7 X= -2.354511267482D+00 Y= 5.188875112692D+00 Z= -3.439347642316D+00
I= 8 X= -4.014844484779D+00 Y= 1.877181705909D+00 Z= -3.454150761813D+00
I= 9 X= 2.907979185906D+00 Y= -7.866530564361D-01 Z= 4.483961052199D+00
I= 10 X= 2.837241486283D+00 Y= -2.483763113093D+00 Z= 5.812027516008D+00
I= 11 X= 5.016337533124D+00 Y= -3.961334968876D-01 Z= 3.839726527730D+00
I= 12 X= 2.011753360325D+00 Y= 3.783874792689D-01 Z= 5.801810156605D+00
I= 13 X= -2.833280968675D+00 Y= -5.378389750171D-01 Z= 4.677550762533D+00
I= 14 X= -2.747776781292D+00 Y= -1.926621092919D+00 Z= 6.351368620050D+00
I= 15 X= -2.186782751348D+00 Y= 1.143680224906D+00 Z= 5.448003631727D+00
I= 16 X= -4.830217477814D+00 Y= -3.447637159297D-01 Z= 4.459115472450D+00
I= 17 X= -4.960376837214D+00 Y= -2.431185675507D+00 Z= -6.368019755607D-01
I= 18 X= -6.205496827760D+00 Y= -3.478112622175D+00 Z= 1.161891230657D+00

I= 19 X= -5.930201255195D+00 Y= -3.607063813872D-01 Z= -1.113852042028D+00
I= 20 X= -5.302369190300D+00 Y= -3.980393781338D+00 Z= -2.266460782091D+00
I= 21 X= 4.103710645442D-02 Y= -3.502184024557D+00 Z= -4.275538103962D+00
I= 22 X= 1.289763285688D+00 Y= -5.609939122674D+00 Z= -4.737653099460D+00
I= 23 X= -1.907955351948D+00 Y= -3.850571244168D+00 Z= -5.112640202971D+00
I= 24 X= 1.182911669272D+00 Y= -1.679303508116D+00 Z= -5.175573808406D+00
I= 25 X= 4.896700379230D+00 Y= -2.653409718039D+00 Z= -7.214181860733D-01
I= 26 X= 5.091482590221D+00 Y= -3.321014308887D+00 Z= -2.735207826665D+00
I= 27 X= 6.456630345922D+00 Y= -1.139307011095D+00 Z= -5.287904018574D-01
I= 28 X= 5.382395819413D+00 Y= -4.290042176580D+00 Z= 6.881925837528D-01
I= 29 X= 2.964027268944D+00 Y= 3.297893150864D+00 Z= -2.338141438520D+00
I= 30 X= 2.587675660130D+00 Y= 3.994857348359D+00 Z= 2.478817873643D-01
I= 31 X= 4.193635857500D+00 Y= 1.646142914972D+00 Z= -2.930836482668D+00
I= 32 X= 2.592225802842D+00 Y= 4.730447453967D+00 Z= -3.612976239572D+00
I= 33 X= 1.518857544292D+00 Y= 5.682112113051D+00 Z= 7.801266099978D-01
I= 34 X= 3.746606649440D+00 Y= 3.177239863884D+00 Z= 1.806842366416D+00
I= 35 X= 2.665456704922D-02 Y= 1.078291817651D+00 Z= -5.074356321079D-01
I= 36 X= -2.935260623787D+00 Y= 3.538530126589D+00 Z= 3.101400435157D-01
I= 37 X= -2.147109227711D+00 Y= 5.578091173226D+00 Z= 1.035645923644D+00
I= 38 X= -4.401203293650D+00 Y= 2.549330538412D+00 Z= 1.355073574318D+00

Forward Direction:

Total Energy: -692.0022587 Hartrees

Potential Energy: -692.1939372 Hartress

Kinetic Energy: 0.1916785 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.928128176811D+12 Y= 9.976015345592D+12 Z= -6.240523801284D+10

I= 1 X= -2.982044296535D+12 Y= -3.506349302881D+12 Z= 3.835379389974D+11

I= 2 X= 1.204030716741D+13 Y= 1.678809832444D+12 Z= 6.378222003821D+12

I= 3 X= 1.399634506267D+13 Y= -9.799659943513D+12 Z= -1.837755422991D+13

I= 4 X= -2.238270601360D+13 Y= 8.601475036866D+12 Z= -9.558753068583D+11

I= 5 X= -2.362223787948D+13 Y= -2.140910130609D+13 Z= -6.627633002052D+12
I= 6 X= 2.772124904313D+13 Y= -3.194537303684D+13 Z= 4.733206846528D+13
I= 7 X= 5.264611566436D+13 Y= 6.416312994904D+13 Z= 1.319286790674D+14
I= 8 X= -8.403914435439D+13 Y= -3.180560699027D+13 Z= 4.637324151417D+13
I= 9 X= 2.673527595443D+12 Y= 1.428097137961D+13 Z= -1.455441265114D+13
I= 10 X= -1.574569185354D+13 Y= 2.730589725753D+13 Z= 5.924124072938D+13
I= 11 X= 3.587785173299D+13 Y= -2.084659162090D+13 Z= -6.442315315393D+13
I= 12 X= -9.600813203130D+13 Y= -6.423542080347D+13 Z= 1.423092743714D+13
I= 13 X= 1.678990672958D+13 Y= -2.927798585273D+13 Z= -2.269251837223D+13
I= 14 X= -9.617112109164D+13 Y= -2.990923107745D+13 Z= -1.911994721419D+13
I= 15 X= 7.837953946005D+13 Y= 1.584491226167D+14 Z= 3.573751200690D+13
I= 16 X= -2.716806653304D+13 Y= 4.563894857766D+12 Z= 1.170618599253D+13
I= 17 X= -2.154884868291D+12 Y= 8.761146325597D+12 Z= -5.525334944311D+12
I= 18 X= 3.413883843553D+13 Y= -1.075647796510D+12 Z= 2.169547246569D+13
I= 19 X= 1.336181916131D+13 Y= -2.547962041383D+13 Z= -1.936783159385D+13
I= 20 X= 7.363873423149D+13 Y= 4.032583638864D+13 Z= 8.142824085186D+12
I= 21 X= -2.233533943094D+13 Y= -1.628099111977D+13 Z= 8.479156287310D+11
I= 22 X= -4.461888481142D+12 Y= 2.999594270771D+13 Z= -1.238478253390D+13
I= 23 X= 6.330499513968D+13 Y= 1.057092907286D+11 Z= 3.742787420447D+13
I= 24 X= 5.901619797736D+13 Y= 1.006292485377D+14 Z= 3.414541314953D+10
I= 25 X= 1.280832624826D+12 Y= -1.728834462535D+13 Z= -7.692192717543D+12
I= 26 X= 1.087352356481D+13 Y= 3.170997555399D+13 Z= 8.691997066146D+13
I= 27 X= 4.858209191244D+13 Y= 4.183520328359D+13 Z= 3.240645307543D+13
I= 28 X= -4.432342482577D+12 Y= 1.241966494941D+14 Z= -4.194831569277D+12
I= 29 X= 2.185191682614D+12 Y= 2.770407721419D+13 Z= -1.552526668678D+13
I= 30 X= 1.823351124518D+12 Y= -2.086356396512D+13 Z= -1.908290361640D+12
I= 31 X= 1.415104311640D+14 Y= -1.737190665268D+14 Z= -4.750770811310D+13
I= 32 X= 4.719977515530D+13 Y= 4.433227248945D+13 Z= -4.475735719737D+13
I= 33 X= 3.256041511889D+13 Y= 6.783306291369D+13 Z= 5.129826219143D+13
I= 34 X= 2.290704220427D+13 Y= -4.260676760351D+12 Z= 1.138002716381D+14

I= 35 X= -5.739042286100D+12 Y= 2.043741065698D+12 Z= 5.421359224892D+12
I= 36 X= 1.803947434608D+13 Y= 1.024755754655D+13 Z= 1.553957293837D+13
I= 37 X= -5.686468471746D+13 Y= -1.885802384003D+13 Z= -2.996282087434D+13
I= 38 X= -3.647244895095D+13 Y= -1.017213287376D+13 Z= 6.909881394348D+13

Backward Direction:

Total Energy: -692.0022251 Hartrees

Potential Energy: -692.1939372 Hartress

Kinetic Energy: 0.1917121 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.926536870729D+12 Y= 1.053212662217D+13 Z= 9.035277173640D+11
I= 1 X= -2.920783329560D+12 Y= -3.506202956768D+12 Z= 3.834473681722D+11
I= 2 X= 1.244938973017D+13 Y= 1.649689581212D+12 Z= 6.856412364948D+12
I= 3 X= 1.399484590827D+13 Y= -1.035581475542D+13 Z= -1.934361187579D+13
I= 4 X= -2.197356388688D+13 Y= 8.630657736457D+12 Z= -1.434019798074D+12
I= 5 X= -2.314192437956D+13 Y= -2.605039690136D+13 Z= -1.166786452103D+13
I= 6 X= -2.132193848281D+11 Y= -3.193983090861D+13 Z= 4.733240681595D+13
I= 7 X= 4.720552007533D+13 Y= 6.080694544189D+13 Z= 1.248502975015D+14
I= 8 X= -8.608110915564D+13 Y= -3.604575460249D+13 Z= 4.501524815987D+13
I= 9 X= 3.591221752662D+12 Y= 1.263380217302D+13 Z= -1.495162487679D+13
I= 10 X= -1.612461126426D+13 Y= 2.532403534242D+13 Z= 5.837776383395D+13
I= 11 X= 3.702573386529D+13 Y= -2.394555423819D+13 Z= -6.470065113381D+13
I= 12 X= -9.384843774927D+13 Y= -6.570817662175D+13 Z= 1.434645963098D+13
I= 13 X= 1.770753339732D+13 Y= -2.763080080719D+13 Z= -2.229504452829D+13
I= 14 X= -9.654932319692D+13 Y= -2.792711097711D+13 Z= -1.825604402504D+13
I= 15 X= 8.053879876230D+13 Y= 1.599225406812D+14 Z= 3.562187727162D+13
I= 16 X= -2.602057869771D+13 Y= 7.661948499044D+12 Z= 1.198430174228D+13
I= 17 X= -2.338414822195D+12 Y= 8.756074042309D+12 Z= -3.845271345769D+12
I= 18 X= 3.421579526579D+13 Y= -3.242367603585D+11 Z= 2.526967967168D+13
I= 19 X= 1.326379984670D+13 Y= -2.490621445476D+13 Z= -1.875304268615D+13
I= 20 X= 7.294820568058D+13 Y= 3.819531606882D+13 Z= 1.001548207391D+13

I= 21 X= -2.390313786194D+13 Y= -1.628026257545D+13 Z= 8.474268122112D+11
I= 22 X= -8.475119611670D+12 Y= 2.999671462661D+13 Z= -1.238613658345D+13
I= 23 X= 6.235821621456D+13 Y= 2.016684357922D+12 Z= 3.745494764487D+13
I= 24 X= 5.806924121889D+13 Y= 9.872027036198D+13 Z= 6.429562335362D+09
I= 25 X= 1.097494884971D+12 Y= -1.728360977693D+13 Z= -9.372313153233D+12
I= 26 X= 1.018333589964D+13 Y= 3.384004967515D+13 Z= 8.504712152260D+13
I= 27 X= 4.848437126637D+13 Y= 4.126106774125D+13 Z= 3.179190596934D+13
I= 28 X= -4.355289515750D+12 Y= 1.234446708407D+14 Z= -7.769014761430D+12
I= 29 X= 2.665205846040D+12 Y= 3.234398954232D+13 Z= -1.048638830462D+13
I= 30 X= 3.088967531487D+12 Y= -2.096289953144D+13 Z= 2.742372618431D+12
I= 31 X= 1.394694389384D+14 Y= -1.694801710088D+14 Z= -4.615101197505D+13
I= 32 X= 4.176044978327D+13 Y= 4.768877083708D+13 Z= -3.768119198503D+13
I= 33 X= 3.180573113599D+13 Y= 6.487093196982D+13 Z= 6.067140868070D+13
I= 34 X= 2.362477406611D+13 Y= -7.314405606242D+12 Z= 1.169112952096D+14
I= 35 X= -5.848149917031D+12 Y= 2.043919525500D+12 Z= 5.421872574613D+12
I= 36 X= 1.930505900532D+13 Y= 1.034632939258D+13 Z= 1.088861569396D+13
I= 37 X= -5.762106963987D+13 Y= -1.589420956666D+13 Z= -3.933674891212D+13
I= 38 X= -3.575465171568D+13 Y= -7.119794378445D+12 Z= 6.598772316547D+13

Seed: 3292668439

CM Start Point Coordinates: bohr

I= 0 X= -2.157272419594D+00 Y= -2.135041765151D+00 Z= -4.514808136234D-02
I= 1 X= -1.488843631670D-01 Y= -2.784761784498D+00 Z= -1.561932360780D+00
I= 2 X= -1.305344649336D+00 Y= -1.349922326910D+00 Z= 2.259675364946D+00
I= 3 X= 2.073902977544D+00 Y= -1.913345962793D+00 Z= -1.651161278550D-01
I= 4 X= 1.294678767877D+00 Y= -1.225620445100D+00 Z= 2.359935145764D+00
I= 5 X= -2.761589365610D+00 Y= 3.161392796353D+00 Z= -2.249071435931D+00
I= 6 X= 9.646418799585D-02 Y= 1.733875945980D+00 Z= -3.065420897616D+00
I= 7 X= -1.830558675351D+00 Y= 4.390966772533D+00 Z= -3.477466093458D+00
I= 8 X= -4.581819382290D+00 Y= 2.117249082210D+00 Z= -3.429868202713D+00

I= 9 X= 2.921715148009D+00 Y= -3.986552587052D-01 Z= 4.420658097858D+00
I= 10 X= 3.508410837178D+00 Y= -1.875712598905D+00 Z= 6.072658099813D+00
I= 11 X= 5.075218457027D+00 Y= 3.375873071249D-01 Z= 3.917096880295D+00
I= 12 X= 2.045004671693D+00 Y= 1.222235463781D+00 Z= 5.318305666519D+00
I= 13 X= -2.961950097670D+00 Y= -9.143033827116D-01 Z= 4.634197068731D+00
I= 14 X= -3.138062880784D+00 Y= -2.579643150256D+00 Z= 5.749267552066D+00
I= 15 X= -2.009936854129D+00 Y= 5.676759825089D-01 Z= 5.863405173407D+00
I= 16 X= -4.901354181467D+00 Y= -2.615209569894D-01 Z= 4.004351673310D+00
I= 17 X= -4.913692600489D+00 Y= -2.260969092136D+00 Z= -8.105361342541D-01
I= 18 X= -6.302599236244D+00 Y= -3.626196180813D+00 Z= 2.605384000317D-01
I= 19 X= -5.801156268843D+00 Y= -4.890442973622D-01 Z= -4.145380695755D-01
I= 20 X= -4.706439595327D+00 Y= -2.706017204152D+00 Z= -3.107029884464D+00
I= 21 X= 5.113731455286D-02 Y= -4.145631788475D+00 Z= -4.107447942864D+00
I= 22 X= -2.877223859338D-01 Y= -6.142581126449D+00 Z= -3.558665696987D+00
I= 23 X= -1.680023486203D+00 Y= -3.827618025303D+00 Z= -5.553944575950D+00
I= 24 X= 2.020640619688D+00 Y= -4.004468173441D+00 Z= -5.011075848479D+00
I= 25 X= 4.702370781570D+00 Y= -2.290945678076D+00 Z= -8.556837872673D-01
I= 26 X= 4.963887789242D+00 Y= -2.969628453074D+00 Z= -2.892121569997D+00
I= 27 X= 6.097160256779D+00 Y= -1.105618851930D+00 Z= -1.470220442153D-02
I= 28 X= 5.900362947370D+00 Y= -4.117595266608D+00 Z= 1.118276109259D-03
I= 29 X= 2.957208335299D+00 Y= 3.314366789452D+00 Z= -2.141321342678D+00
I= 30 X= 2.684699870561D+00 Y= 3.697597001474D+00 Z= 3.019158400229D-01
I= 31 X= 4.287658740177D+00 Y= 1.834812633836D+00 Z= -2.913267049768D+00
I= 32 X= 2.037891658375D+00 Y= 4.536608553265D+00 Z= -3.728709552184D+00
I= 33 X= 1.831305688905D+00 Y= 5.512105960204D+00 Z= 9.776016987387D-01
I= 34 X= 3.868843368151D+00 Y= 2.896099700793D+00 Z= 1.648797927613D+00
I= 35 X= 3.195870100102D-02 Y= 1.112183452416D+00 Z= -4.638078375941D-01
I= 36 X= -2.686151415445D+00 Y= 3.783945981427D+00 Z= 2.921552441713D-01
I= 37 X= -1.490350988135D+00 Y= 5.682666385846D+00 Z= 7.343527363232D-01
I= 38 X= -3.904785347794D+00 Y= 2.871985981905D+00 Z= 1.970715334273D+00

Forward Direction:

Total Energy: -692.0029821 Hartrees

Potential Energy: -692.1848374 Hartress

Kinetic Energy: 0.1818553 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.494322012825D+13 Y= -1.747004581169D+12 Z= -1.648720313869D+13
I= 1 X= -2.265760993296D+13 Y= -6.673951455500D+11 Z= 1.945137776125D+12
I= 2 X= -9.550423552046D+12 Y= -1.066558392755D+13 Z= -9.328310800387D+12
I= 3 X= 2.248762782611D+13 Y= 2.278260184271D+13 Z= -6.952378660715D+12
I= 4 X= -7.383601270226D+12 Y= -3.836273965174D+12 Z= -1.142916485402D+13
I= 5 X= -2.541093282657D+12 Y= -1.433852645093D+13 Z= -1.234697929153D+12
I= 6 X= 3.626210286978D+13 Y= 2.523869371657D+13 Z= 8.409690561351D+13
I= 7 X= -1.075716020541D+13 Y= 1.780153040243D+13 Z= 6.574120350440D+13
I= 8 X= 1.087619694960D+14 Y= 5.590155663517D+13 Z= 4.969052578347D+13
I= 9 X= -1.282570902724D+13 Y= -8.401161630258D+12 Z= 2.369287564541D+13
I= 10 X= -1.278105802762D+13 Y= 1.115732777231D+14 Z= -3.223791076169D+12
I= 11 X= 1.006753801536D+14 Y= -1.380975276752D+13 Z= -1.823219846934D+13
I= 12 X= -8.579474438528D+12 Y= -2.329644633772D+13 Z= 9.382772722777D+13
I= 13 X= -1.954560565706D+13 Y= 2.845108229493D+12 Z= -1.107097672883D+13
I= 14 X= 1.705804179156D+13 Y= -5.515261360350D+13 Z= 1.084569873687D+14
I= 15 X= 6.666518037938D+13 Y= 3.311603994440D+13 Z= 8.933164586976D+12
I= 16 X= -9.784812713428D+13 Y= 5.940189836954D+13 Z= -3.464333218938D+12
I= 17 X= 3.684428974090D+12 Y= -1.181621209259D+12 Z= 5.747849339954D+12
I= 18 X= 5.546910841463D+12 Y= 3.034440697499D+13 Z= -1.018558553432D+14
I= 19 X= 1.019208702814D+14 Y= 2.552838246714D+13 Z= -1.615270510319D+13
I= 20 X= 5.942053374915D+13 Y= 1.264505691197D+13 Z= 9.899606133524D+13
I= 21 X= 2.886300363446D+13 Y= 8.856788599306D+12 Z= -8.424775647923D+11
I= 22 X= -1.922163874061D+13 Y= -1.291541302977D+13 Z= 4.617730589475D+13
I= 23 X= -1.583320121114D+14 Y= 9.512359904414D+13 Z= -2.970472591977D+13
I= 24 X= -7.347640380029D+12 Y= 7.661840736006D+12 Z= -6.693024054703D+13

I= 25 X= 3.414103119459D+11 Y= 7.912144824234D+12 Z= -5.493888794067D+12
I= 26 X= -1.725927380644D+13 Y= 3.173403930120D+12 Z= 1.309813386337D+13
I= 27 X= 1.253518642046D+13 Y= -1.647948016951D+14 Z= -1.341101305188D+13
I= 28 X= -1.388406267719D+13 Y= -7.789490436447D+13 Z= 5.655564843463D+13
I= 29 X= 6.948351700860D+12 Y= 8.855265608052D+12 Z= -1.361824680954D+13
I= 30 X= -7.382595272175D+12 Y= 3.325631806482D+11 Z= -5.493160964504D+12
I= 31 X= -1.629415527078D+13 Y= -1.155789994852D+14 Z= 1.332331539764D+13
I= 32 X= -1.646161587501D+13 Y= 4.485975670492D+13 Z= -3.814684591542D+12
I= 33 X= -3.764471375783D+13 Y= 1.259577144255D+13 Z= 2.907895347447D+13
I= 34 X= -6.564980407443D+13 Y= 2.677899505468D+12 Z= 4.142248410881D+13
I= 35 X= 3.304218604127D+12 Y= -4.843435337069D+12 Z= 1.115730349293D+12
I= 36 X= 6.818115382918D+12 Y= 2.452719117360D+11 Z= 1.546011824591D+13
I= 37 X= 8.496785386099D+13 Y= 1.068058683983D+14 Z= -7.452672289303D+12
I= 38 X= 2.469387743128D+13 Y= -2.866511973664D+13 Z= -9.241565926129D+13

Backward Direction:

Total Energy: -692.0030088 Hartrees

Potential Energy: -692.1848374 Hartress

Kinetic Energy: 0.1818286 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.492350512273D+13 Y= -8.268421580509D+11 Z= -1.495414543790D+13
I= 1 X= -2.241934975179D+13 Y= -6.671706392510D+11 Z= 1.945003615473D+12
I= 2 X= -8.964903047587D+12 Y= -1.083512421199D+13 Z= -8.551221041824D+12
I= 3 X= 2.250748198451D+13 Y= 2.186236280312D+13 Z= -8.485636652160D+12
I= 4 X= -6.797989909789D+12 Y= -3.666635447723D+12 Z= -1.220619808259D+13
I= 5 X= -1.521769972573D+12 Y= -2.146453619560D+13 Z= -9.131160222209D+12
I= 6 X= -1.374088019606D+13 Y= 2.524780546272D+13 Z= 8.409732041838D+13
I= 7 X= -1.970996809810D+13 Y= 1.344347148530D+13 Z= 5.502182901326D+13
I= 8 X= 1.051022826296D+14 Y= 5.016680819815D+13 Z= 4.754479496168D+13
I= 9 X= -1.146225700823D+13 Y= -1.085470273088D+13 Z= 2.306496865957D+13
I= 10 X= -1.340530848670D+13 Y= 1.085832691793D+14 Z= -4.593719275307D+12

I= 11 X= 1.023940202558D+14 Y= -1.847130362071D+13 Z= -1.865827571229D+13
I= 12 X= -5.325325176724D+12 Y= -2.550357901619D+13 Z= 9.401541900853D+13
I= 13 X= -1.818226097247D+13 Y= 5.298673272584D+12 Z= -1.044268338774D+13
I= 14 X= 1.643485193674D+13 Y= -5.216222671309D+13 Z= 1.098275357728D+14
I= 15 X= 6.991867246513D+13 Y= 3.532416894861D+13 Z= 8.745319720656D+12
I= 16 X= -9.613008497709D+13 Y= 6.406208313282D+13 Z= -3.037329621391D+12
I= 17 X= 3.441733977156D+12 Y= -1.162080266220D+12 Z= 8.271539042381D+12
I= 18 X= 5.737069967962D+12 Y= 3.146225321756D+13 Z= -9.653532571475D+13
I= 19 X= 1.017493948081D+14 Y= 2.635822496112D+13 Z= -1.520402422605D+13
I= 20 X= 5.843909794396D+13 Y= 9.496359440770D+12 Z= 1.018036242163D+14
I= 21 X= 2.653740136129D+13 Y= 8.857892307994D+12 Z= -8.432183267930D+11
I= 22 X= -2.518510074673D+13 Y= -1.291424708669D+13 Z= 4.617524864369D+13
I= 23 X= -1.597616289017D+14 Y= 9.795443270450D+13 Z= -2.962680796991D+13
I= 24 X= -8.777538571995D+12 Y= 4.834052379488D+12 Z= -6.700916453821D+13
I= 25 X= 9.899458494287D+10 Y= 7.892105991210D+12 Z= -8.017659131603D+12
I= 26 X= -1.824019341201D+13 Y= 6.321392775191D+12 Z= 1.029029835204D+13
I= 27 X= 1.236414172376D+13 Y= -1.656257182442D+14 Z= -1.435934771462D+13
I= 28 X= -1.369378763689D+13 Y= -7.901357685184D+13 Z= 5.123521039733D+13
I= 29 X= 7.967234486312D+12 Y= 1.597911552350D+13 Z= -5.723834981601D+12
I= 30 X= -5.167393111192D+12 Y= 3.902359180489D+11 Z= 1.467586570996D+12
I= 31 X= -1.995195649539D+13 Y= -1.098457999160D+14 Z= 1.546715436425D+13
I= 32 X= -2.541259914905D+13 Y= 4.921816281250D+13 Z= 6.901239572945D+12
I= 33 X= -3.880637911265D+13 Y= 8.136116380096D+12 Z= 4.326690197497D+13
I= 34 X= -6.468593487555D+13 Y= -1.981347562074D+12 Z= 4.632489824853D+13
I= 35 X= 3.037415550660D+12 Y= -4.843168667148D+12 Z= 1.116515149799D+12
I= 36 X= 9.033330164055D+12 Y= 1.867227560512D+11 Z= 8.498935176182D+12
I= 37 X= 8.380367650499D+13 Y= 1.112681214387D+14 Z= -2.164192937626D+13
I= 38 X= 2.565798154197D+13 Y= -2.400786223102D+13 Z= -9.731813499500D+13

Seed: 33076722442

CM Start Point Coordinates: bohr

I= 0 X= -2.276842229464D+00 Y= -2.016733920884D+00 Z= -1.145071896504D-01
I= 1 X= -1.047877621205D-01 Y= -2.893522496970D+00 Z= -1.479253053194D+00
I= 2 X= -1.260016097058D+00 Y= -1.168891623931D+00 Z= 2.410145073235D+00
I= 3 X= 2.219564453077D+00 Y= -1.960014955157D+00 Z= -6.483791181128D-03
I= 4 X= 1.338934027496D+00 Y= -1.183967257842D+00 Z= 2.501422062781D+00
I= 5 X= -2.847747060827D+00 Y= 3.571303273771D+00 Z= -2.354197108205D+00
I= 6 X= -2.128349469077D-01 Y= 1.836646942213D+00 Z= -3.157166125418D+00
I= 7 X= -1.630782568298D+00 Y= 4.846934093769D+00 Z= -3.501533232017D+00
I= 8 X= -4.062512232298D+00 Y= 2.235283317029D+00 Z= -3.536799759926D+00
I= 9 X= 3.002302396398D+00 Y= -8.525813977937D-01 Z= 4.708711825349D+00
I= 10 X= 2.463327106513D+00 Y= -2.108033405438D+00 Z= 5.973052418869D+00
I= 11 X= 4.929178992408D+00 Y= -1.691619655126D+00 Z= 4.366900038158D+00
I= 12 X= 3.244983951525D+00 Y= 1.359077387073D+00 Z= 5.679818988802D+00
I= 13 X= -2.869797495786D+00 Y= -5.085263149312D-01 Z= 4.707365882940D+00
I= 14 X= -2.270957018955D+00 Y= -1.694432465793D+00 Z= 6.611977930615D+00
I= 15 X= -2.727405403808D+00 Y= 1.499231899954D+00 Z= 5.418018940084D+00
I= 16 X= -4.867875198905D+00 Y= -7.031022311311D-01 Z= 4.098964068437D+00
I= 17 X= -4.905232541915D+00 Y= -2.529260069627D+00 Z= -9.346064085546D-01
I= 18 X= -5.470038240157D+00 Y= -4.650897433351D+00 Z= -3.728662958736D-01
I= 19 X= -6.597617457521D+00 Y= -1.480455465047D+00 Z= 2.904888485907D-01
I= 20 X= -5.269201889619D+00 Y= -2.367713008563D+00 Z= -2.931304172159D+00
I= 21 X= 8.204988497578D-03 Y= -4.106309238116D+00 Z= -4.022220766975D+00
I= 22 X= 3.408564093012D-01 Y= -6.170957056420D+00 Z= -3.885512320225D+00
I= 23 X= -2.173415798588D+00 Y= -4.196978396810D+00 Z= -5.116724043732D+00
I= 24 X= 1.566278331371D+00 Y= -3.563393874476D+00 Z= -5.432530945769D+00
I= 25 X= 4.710780698621D+00 Y= -2.277948574001D+00 Z= -8.966606621861D-01
I= 26 X= 4.528279600497D+00 Y= -2.248055926843D+00 Z= -2.957740864777D+00
I= 27 X= 6.094844390937D+00 Y= -5.459991203694D-01 Z= -2.903687678989D-01
I= 28 X= 5.518917776418D+00 Y= -3.960441484899D+00 Z= -7.513143247969D-02

I= 29 X= 3.057419843664D+00 Y= 3.387258710761D+00 Z= -2.285943087063D+00
I= 30 X= 2.781280217669D+00 Y= 3.670494129298D+00 Z= 3.402217499470D-01
I= 31 X= 4.599808120927D+00 Y= 2.063741163039D+00 Z= -3.111982082437D+00
I= 32 X= 1.847736388187D+00 Y= 5.231381349569D+00 Z= -3.124852008950D+00
I= 33 X= 2.057906441485D+00 Y= 5.602168923504D+00 Z= 1.017911012180D+00
I= 34 X= 3.750874732699D+00 Y= 2.437433607196D+00 Z= 1.769882308407D+00
I= 35 X= 7.443462980712D-02 Y= 1.088373501624D+00 Z= -6.092913639200D-01
I= 36 X= -3.096520251879D+00 Y= 3.586609414339D+00 Z= 3.838691093805D-01
I= 37 X= -2.447439668397D+00 Y= 5.075502773457D+00 Z= 1.348885605701D+00
I= 38 X= -4.678631506113D+00 Y= 2.444302783316D+00 Z= 1.328529102731D+00

Forward Direction:

Total Energy: -691.9963254 Hartrees

Potential Energy: -692.1752726 Hartress

Kinetic Energy: 0.1789472 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.568203169887D+12 Y= 2.598574194231D+12 Z= 9.852825402871D+12
I= 1 X= -1.607557345295D+13 Y= 6.747484949665D+12 Z= 6.360688266662D+12
I= 2 X= 1.502219184237D+13 Y= -1.392167663471D+13 Z= -1.387800426203D+13
I= 3 X= -2.104497401196D+13 Y= 1.035188313684D+13 Z= -8.051560447456D+11
I= 4 X= 5.816756032053D+12 Y= -4.968174352155D+11 Z= -4.668824415970D+12
I= 5 X= -6.201619133775D+12 Y= -1.626878464013D+11 Z= 1.692336586468D+13
I= 6 X= 3.876771904897D+13 Y= 5.154875203607D+13 Z= -5.914647421447D+13
I= 7 X= -1.276169945806D+13 Y= 4.106276513275D+13 Z= 2.044292138007D+12
I= 8 X= 3.171020260225D+13 Y= -9.103224144341D+12 Z= -7.009647567336D+12
I= 9 X= -6.101240458072D+12 Y= 9.313356299857D+12 Z= 2.120867257114D+13
I= 10 X= 1.544190584130D+11 Y= -6.435506898630D+13 Z= -1.194768231659D+14
I= 11 X= 2.176296827005D+13 Y= -9.437433594686D+13 Z= 7.923139167733D+12
I= 12 X= -1.992936930940D+13 Y= 2.974650974125D+13 Z= 2.732509974650D+13
I= 13 X= 1.509003412239D+12 Y= -2.130344322683D+13 Z= 6.956820201608D+12
I= 14 X= 2.996505257359D+13 Y= 4.148116440657D+13 Z= -4.046774525276D+13

I= 15 X= -5.749247099192D+13 Y= 9.442256008939D+13 Z= 2.779927210272D+13
I= 16 X= 5.933932756839D+13 Y= -1.573199989442D+13 Z= -3.797525981735D+11
I= 17 X= 6.351201964935D+12 Y= 2.053373951271D+13 Z= -1.207751444262D+13
I= 18 X= 3.398729989735D+13 Y= -1.283810502515D+14 Z= 1.594567411367D+13
I= 19 X= 3.768243409643D+13 Y= -1.302622118415D+13 Z= -3.269381600068D+13
I= 20 X= -3.317860657132D+13 Y= 5.994797991426D+12 Z= 6.058680698271D+13
I= 21 X= 8.160611035979D+12 Y= -3.590861683170D+12 Z= -6.566719788785D+12
I= 22 X= 1.257991374010D+13 Y= -1.647700261409D+13 Z= 3.602329098131D+13
I= 23 X= -1.691405752594D+14 Y= 6.085981847434D+13 Z= 2.367014950313D+13
I= 24 X= 1.519957896271D+13 Y= -5.042337368175D+13 Z= 3.501221338354D+13
I= 25 X= 2.301764201099D+13 Y= -5.005520950606D+12 Z= 8.063075178027D+12
I= 26 X= 2.856599826400D+13 Y= 7.757641436407D+13 Z= 1.438024051141D+13
I= 27 X= -1.209763090780D+13 Y= -9.901388342288D+13 Z= -1.128190161198D+14
I= 28 X= -9.730077485838D+13 Y= 4.232838478517D+13 Z= 2.883374309974D+12
I= 29 X= -8.951114823412D+12 Y= 1.182000685337D+13 Z= -3.291934346279D+13
I= 30 X= 4.538714828570D+12 Y= -1.668793943934D+13 Z= 6.296324803250D+12
I= 31 X= 1.119313895664D+13 Y= -1.964109720934D+13 Z= -3.427402821021D+13
I= 32 X= 8.029650047006D+13 Y= -1.383065835076D+14 Z= 4.708240992782D+13
I= 33 X= 4.417508586656D+13 Y= 1.368558652045D+14 Z= -2.017322710200D+13
I= 34 X= -4.310641141956D+12 Y= 2.932093971262D+13 Z= -1.052760386358D+13
I= 35 X= -3.309543704572D+12 Y= 3.257003267530D+12 Z= 5.797451055009D+11
I= 36 X= -9.353507590118D+11 Y= -2.375990179106D+13 Z= -1.198090023594D+13
I= 37 X= 1.004602474383D+13 Y= 1.194200912026D+14 Z= 1.019173755752D+14
I= 38 X= 1.721487069967D+13 Y= 8.330656370144D+12 Z= 8.661605724588D+13

Backward Direction:

Total Energy: -691.9964186 Hartrees

Potential Energy: -692.1752726 Hartress

Kinetic Energy: 0.1788540 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.590047179977D+12 Y= 4.323916287651D+12 Z= 1.277149802614D+13

I= 1 X= -1.572146026963D+13 Y= 6.747917838945D+12 Z= 6.360426048976D+12
I= 2 X= 1.618189002358D+13 Y= -1.415745186588D+13 Z= -1.241135982990D+13
I= 3 X= -2.102286006537D+13 Y= 8.626400491491D+12 Z= -3.724208364282D+12
I= 4 X= 6.976629778399D+12 Y= -2.608545343781D+11 Z= -6.135349839071D+12
I= 5 X= -4.442314199991D+12 Y= -1.389889109888D+13 Z= 1.817209876815D+12
I= 6 X= -5.243100165412D+13 Y= 5.156587666265D+13 Z= -5.914559827103D+13
I= 7 X= -2.958201035587D+13 Y= 3.208245324730D+13 Z= -1.872676591813D+13
I= 8 X= 2.503827108361D+13 Y= -2.072304485077D+13 Z= -1.110149798545D+13
I= 9 X= -3.439827738559D+12 Y= 4.528859548220D+12 Z= 2.001147088143D+13
I= 10 X= -1.017919212972D+12 Y= -7.015718931353D+13 Z= -1.220852918521D+14
I= 11 X= 2.510775673268D+13 Y= -1.034303398632D+14 Z= 7.101841684408D+12
I= 12 X= -1.361160147494D+13 Y= 2.545258283640D+13 Z= 2.767937898202D+13
I= 13 X= 4.170211995051D+12 Y= -1.651890005021D+13 Z= 8.154777752203D+12
I= 14 X= 2.879478852965D+13 Y= 4.728402716422D+13 Z= -3.785805609569D+13
I= 15 X= -5.117597765790D+13 Y= 9.871842239500D+13 Z= 2.744469453478D+13
I= 16 X= 6.268295804547D+13 Y= -6.678650795718D+12 Z= 4.433466981123D+11
I= 17 X= 5.854874655171D+12 Y= 2.055147748266D+13 Z= -7.172123677508D+12
I= 18 X= 3.430134458347D+13 Y= -1.262001424323D+14 Z= 2.632348487439D+13
I= 19 X= 3.736719653099D+13 Y= -1.138975090382D+13 Z= -3.086859928693D+13
I= 20 X= -3.512787807411D+13 Y= -1.639355582262D+11 Z= 6.604802053245D+13
I= 21 X= 3.618299466610D+12 Y= -3.588723360191D+12 Z= -6.568154824809D+12
I= 22 X= 9.400807253196D+11 Y= -1.647474114941D+13 Z= 3.601930958498D+13
I= 23 X= -1.719138423084D+14 Y= 6.639182067065D+13 Z= 2.379383632842D+13
I= 24 X= 1.242577559336D+13 Y= -5.594949078322D+13 Z= 3.488660160662D+13
I= 25 X= 2.252186465896D+13 Y= -5.024233307523D+12 Z= 3.157524298295D+12
I= 26 X= 2.661772732760D+13 Y= 8.373379930096D+13 Z= 8.918486476523D+12
I= 27 X= -1.241201803019D+13 Y= -1.006524577861D+14 Z= -1.146435469193D+14
I= 28 X= -9.698648354963D+13 Y= 4.014585122418D+13 Z= -7.494299587041D+12
I= 29 X= -7.192672990204D+12 Y= 2.555207300621D+13 Z= -1.781715971696D+13
I= 30 X= 8.610386218381D+12 Y= -1.673004872952D+13 Z= 1.984497256213D+13

I= 31 X= 4.524556035388D+12 Y= -8.024534580622D+12 Z= -3.018589733855D+13
I= 32 X= 6.347979840359D+13 Y= -1.293255041504D+14 Z= 6.784685171751D+13
I= 33 X= 4.193800224115D+13 Y= 1.281950101891D+14 Z= 7.323790330387D+12
I= 34 X= -2.351962584497D+12 Y= 2.031834293365D+13 Z= -1.169454561914D+12
I= 35 X= -3.751433500109D+12 Y= 3.257522662855D+12 Z= 5.812603619687D+11
I= 36 X= 3.136300252363D+12 Y= -2.371947400353D+13 Z= -2.553039936621D+13
I= 37 X= 7.804026353266D+12 Y= 1.280859442599D+14 Z= 7.441791493749D+13
I= 38 X= 1.917390399383D+13 Y= 1.732931216318D+13 Z= 7.725775891249D+13

Seed: 34588604110

CM Start Point Coordinates: bohr

I= 0 X= -2.004370439519D+00 Y= -2.143487288309D+00 Z= 1.098021490706D-01
I= 1 X= -3.963113084620D-02 Y= -2.767563120037D+00 Z= -1.563434988227D+00
I= 2 X= -1.316485189185D+00 Y= -1.209477760002D+00 Z= 2.394122234648D+00
I= 3 X= 2.200046324173D+00 Y= -2.215433909735D+00 Z= -3.606109451868D-02
I= 4 X= 1.398460657770D+00 Y= -1.215064441284D+00 Z= 2.297961505001D+00
I= 5 X= -2.625616052094D+00 Y= 3.353492743093D+00 Z= -2.362872170074D+00
I= 6 X= 4.042603523743D-01 Y= 9.786179490060D-01 Z= -3.320485803741D+00
I= 7 X= -1.850045025252D+00 Y= 5.142719733160D+00 Z= -3.439750081861D+00
I= 8 X= -3.968705799272D+00 Y= 2.276155907121D+00 Z= -3.663069922810D+00
I= 9 X= 2.892457758246D+00 Y= -5.397232266540D-01 Z= 4.511845985163D+00
I= 10 X= 2.940843934666D+00 Y= -2.108400509151D+00 Z= 6.145224968019D+00
I= 11 X= 4.740296714447D+00 Y= -4.541663839479D-01 Z= 3.833324575074D+00
I= 12 X= 2.630212703457D+00 Y= 1.412906435511D+00 Z= 5.524905191491D+00
I= 13 X= -2.982482387349D+00 Y= -7.922589686933D-01 Z= 4.514484912094D+00
I= 14 X= -3.845491707627D+00 Y= -2.646141454874D+00 Z= 5.498062233965D+00
I= 15 X= -2.316482332902D+00 Y= 6.502604515514D-01 Z= 6.106073595764D+00
I= 16 X= -5.055991384253D+00 Y= 1.124606637769D-01 Z= 3.870468343534D+00
I= 17 X= -4.759042766909D+00 Y= -2.860217676243D+00 Z= -5.029055692171D-01
I= 18 X= -5.437179756170D+00 Y= -4.539424998572D+00 Z= 4.190969126008D-01

I= 19 X= -6.292421091417D+00 Y= -1.064020448344D+00 Z= -3.380595493844D-01
I= 20 X= -5.119742627278D+00 Y= -3.333513776183D+00 Z= -2.485453909053D+00
I= 21 X= -2.843794412141D-01 Y= -3.713391837086D+00 Z= -4.214450369178D+00
I= 22 X= -1.313219294671D+00 Y= -5.854498192810D+00 Z= -4.374821064820D+00
I= 23 X= -1.791512345189D+00 Y= -2.359403872577D+00 Z= -5.133954639495D+00
I= 24 X= 1.322596666238D+00 Y= -3.700950480026D+00 Z= -5.155640826781D+00
I= 25 X= 4.730955141854D+00 Y= -2.675457933130D+00 Z= -7.688108558637D-01
I= 26 X= 4.693230223436D+00 Y= -2.974937885999D+00 Z= -2.762728447065D+00
I= 27 X= 5.762941681033D+00 Y= -8.608506177381D-01 Z= -5.633359598726D-01
I= 28 X= 5.717814264959D+00 Y= -4.185152482298D+00 Z= 6.847766318272D-02
I= 29 X= 3.179024479826D+00 Y= 3.228775715623D+00 Z= -2.159500762303D+00
I= 30 X= 2.727410569421D+00 Y= 4.180100626313D+00 Z= 4.104591828556D-01
I= 31 X= 4.598787605934D+00 Y= 1.731291468142D+00 Z= -2.157928418800D+00
I= 32 X= 2.418132013509D+00 Y= 4.145375108056D+00 Z= -3.927788843673D+00
I= 33 X= 1.787012254808D+00 Y= 5.952047977247D+00 Z= 5.106319790926D-01
I= 34 X= 3.937547285606D+00 Y= 3.502973991196D+00 Z= 2.290201549073D+00
I= 35 X= 5.004537135753D-03 Y= 1.175199754771D+00 Z= -5.786510410987D-01
I= 36 X= -2.959271853423D+00 Y= 3.659255310484D+00 Z= 2.601885388595D-01
I= 37 X= -2.050894041570D+00 Y= 5.158755000839D+00 Z= 1.062449828529D+00
I= 38 X= -4.074906818983D+00 Y= 2.290728121204D+00 Z= 1.410479367506D+00

Forward Direction:

Total Energy: -692.0011926 Hartrees

Potential Energy: -692.1944970 Hartress

Kinetic Energy: 0.1933044 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.561283335429D+13 Y= -1.254117201981D+13 Z= -2.725262717393D+12

I= 1 X= -1.803569184369D+13 Y= 1.436785756026D+12 Z= 2.464533259948D+12

I= 2 X= 3.584687636176D+12 Y= 5.684060935945D+12 Z= 6.379041882676D+12

I= 3 X= -2.245597041083D+13 Y= -1.847611959680D+11 Z= 4.381168599394D+12

I= 4 X= 1.632907479276D+13 Y= 3.863318603515D+12 Z= -9.602533466199D+12

I= 5 X= -7.142021721081D+12 Y= -1.239217774816D+13 Z= -1.515673642595D+12
I= 6 X= 4.281301161169D+13 Y= -3.793794117618D+13 Z= 8.684637775097D+13
I= 7 X= 2.354377586914D+13 Y= 1.115038403488D+14 Z= -1.069051134431D+14
I= 8 X= 1.904533316429D+13 Y= -1.427302271757D+13 Z= 1.783668986698D+13
I= 9 X= 2.908551139533D+13 Y= -2.677143601986D+12 Z= -4.978352202108D+11
I= 10 X= -1.009691766107D+14 Y= 2.745332204185D+13 Z= -1.114245420284D+14
I= 11 X= -6.348592310756D+13 Y= -8.318593677765D+13 Z= 6.301623305336D+12
I= 12 X= -8.500781659304D+13 Y= 2.701286411727D+13 Z= 7.227872150616D+13
I= 13 X= 1.050629399266D+13 Y= -1.335253147043D+13 Z= -1.220324152808D+13
I= 14 X= -6.571287149353D+12 Y= -2.649415190395D+12 Z= 2.900103731393D+13
I= 15 X= 2.010248904599D+12 Y= 1.280827569442D+14 Z= 6.290701187871D+13
I= 16 X= -6.162601870027D+13 Y= -5.596494068965D+12 Z= -4.514750012866D+12
I= 17 X= -2.796566312334D+13 Y= 1.689709978889D+13 Z= 2.529855411920D+13
I= 18 X= 9.034697908346D+13 Y= 1.129001118531D+13 Z= -9.031509600269D+13
I= 19 X= 1.162632019430D+14 Y= -2.884615370062D+13 Z= -6.292715873456D+13
I= 20 X= 5.724647545497D+13 Y= -4.942309962622D+13 Z= -4.595050586653D+13
I= 21 X= 1.495910436050D+13 Y= -1.208424255578D+13 Z= -8.325952561707D+12
I= 22 X= -1.009045705637D+13 Y= 2.744877839845D+13 Z= 1.229540720061D+13
I= 23 X= 9.659663894897D+13 Y= 6.846563812505D+13 Z= 7.554876110624D+13
I= 24 X= -3.803172615848D+13 Y= 5.704287025087D+13 Z= 8.999053729056D+12
I= 25 X= -1.015091403999D+13 Y= -1.527221351561D+13 Z= 1.167607861527D+13
I= 26 X= 4.103885853334D+13 Y= 1.484513768157D+13 Z= 7.935328460279D+12
I= 27 X= 7.460077519603D+11 Y= 1.647696546722D+13 Z= -2.493071697734D+13
I= 28 X= -6.888443568411D+13 Y= 7.855229793211D+13 Z= -6.319531096039D+13
I= 29 X= -1.668444085639D+13 Y= -1.786939520026D+13 Z= 9.077890091745D+12
I= 30 X= 5.929811771176D+12 Y= -3.318762069296D+12 Z= -2.909945931621D+13
I= 31 X= 7.675343483221D+13 Y= -2.049390967732D+13 Z= -7.702290438166D+13
I= 32 X= 9.431313499726D+12 Y= -5.275705744580D+13 Z= -1.237306026735D+13
I= 33 X= 5.603264920298D+13 Y= -5.251778956655D+13 Z= 2.912389910779D+13
I= 34 X= -1.135897421852D+13 Y= -2.724693911571D+13 Z= 1.637741260210D+13

I= 35 X= -5.024743556575D+12 Y= 6.908613102045D+12 Z= 2.958717559719D+11
I= 36 X= 2.819920439948D+12 Y= 1.353313597186D+13 Z= 1.659142602457D+13
I= 37 X= -7.839942754861D+13 Y= -7.442621209073D+13 Z= 8.562966971800D+13
I= 38 X= 1.102675007044D+14 Y= 5.203187976532D+13 Z= -7.049930865987D+13

Backward Direction:

Total Energy: -692.0011955 Hartrees

Potential Energy: -692.1944970 Hartress

Kinetic Energy: 0.1933015 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.564001013848D+13 Y= -1.128091476388D+13 Z= -6.260931087257D+11
I= 1 X= -1.770829761398D+13 Y= 1.437093091506D+12 Z= 2.464349591519D+12
I= 2 X= 4.385902598840D+12 Y= 5.450907411000D+12 Z= 7.443235546358D+12
I= 3 X= -2.242860314572D+13 Y= -1.445123405804D+12 Z= 2.281724635558D+12
I= 4 X= 1.713041412359D+13 Y= 4.096606666577D+12 Z= -1.066664996560D+13
I= 5 X= -5.744194152375D+12 Y= -2.214764535076D+13 Z= -1.232721983622D+13
I= 6 X= -2.570084881500D+13 Y= -3.792546196147D+13 Z= 8.684694475277D+13
I= 7 X= 1.128236996548D+13 Y= 1.055443923143D+14 Z= -1.215786243709D+14
I= 8 X= 1.403081389003D+13 Y= -2.211731570541D+13 Z= 1.489868360361D+13
I= 9 X= 3.095168521112D+13 Y= -6.035390825655D+12 Z= -1.357588793351D+12
I= 10 X= -1.018241306296D+14 Y= 2.336046316533D+13 Z= -1.133003392396D+14
I= 11 X= -6.113348381608D+13 Y= -8.956675971471D+13 Z= 5.718325701130D+12
I= 12 X= -8.055342564281D+13 Y= 2.399176822625D+13 Z= 7.253575751489D+13
I= 13 X= 1.237232090025D+13 Y= -9.994251500487D+12 Z= -1.134295923092D+13
I= 14 X= -7.424789448238D+12 Y= 1.443961593091D+12 Z= 3.087768308372D+13
I= 15 X= 6.463740428859D+12 Y= 1.311052167336D+14 Z= 6.264976636833D+13
I= 16 X= -5.927439798998D+13 Y= 7.824589787645D+11 Z= -3.930184428749D+12
I= 17 X= -2.829758125592D+13 Y= 1.692408185012D+13 Z= 2.875300031402D+13
I= 18 X= 9.060791399362D+13 Y= 1.282003467552D+13 Z= -8.303273179341D+13
I= 19 X= 1.160282754138D+14 Y= -2.771053000374D+13 Z= -6.162837923659D+13
I= 20 X= 5.590356010007D+13 Y= -5.373261557860D+13 Z= -4.210753898396D+13

I= 21 X= 1.177605598968D+13 Y= -1.208273175767D+13 Z= -8.326966614275D+12
I= 22 X= -1.825272959897D+13 Y= 2.745037435857D+13 Z= 1.229259102650D+13
I= 23 X= 9.463970429626D+13 Y= 7.234016245808D+13 Z= 7.565573718900D+13
I= 24 X= -3.998904610641D+13 Y= 5.317251460528D+13 Z= 8.890700123422D+12
I= 25 X= -1.048244993203D+13 Y= -1.529987707942D+13 Z= 8.221522309544D+12
I= 26 X= 3.969665014622D+13 Y= 1.915368350303D+13 Z= 4.091988506130D+12
I= 27 X= 5.116710926011D+11 Y= 1.533987243750D+13 Z= -2.622902200381D+13
I= 28 X= -6.862334256150D+13 Y= 7.702114444937D+13 Z= -7.047754946489D+13
I= 29 X= -1.528721624727D+13 Y= -8.116884758773D+12 Z= 1.988662945559D+13
I= 30 X= 8.964707731670D+12 Y= -3.238034013130D+12 Z= -1.957175135739D+13
I= 31 X= 7.174150029037D+13 Y= -1.265173401162D+13 Z= -7.408748721176D+13
I= 32 X= -2.827595491202D+12 Y= -4.679713520706D+13 Z= 2.295726787638D+12
I= 33 X= 5.444231082050D+13 Y= -5.862228744447D+13 Z= 4.854540678503D+13
I= 34 X= -1.004060853426D+13 Y= -3.362517507359D+13 Z= 2.308985312054D+13
I= 35 X= -5.390833619039D+12 Y= 6.908978127624D+12 Z= 2.969461203223D+11
I= 36 X= 5.854834247056D+12 Y= 1.345120794163D+13 Z= 7.063122000567D+12
I= 37 X= -7.999320401634D+13 Y= -6.831815751843D+13 Z= 6.620636969580D+13
I= 38 X= 1.115861891679D+14 Y= 5.840739319353D+13 Z= -7.721183312974D+13

Seed: 34617570350

CM Start Point Coordinates: bohr

I= 0 X= -2.078887981588D+00 Y= -2.011845786923D+00 Z= -4.301981636727D-02
I= 1 X= 3.569358573251D-02 Y= -2.564544829712D+00 Z= -1.613453580799D+00
I= 2 X= -1.271244578113D+00 Y= -1.293107696545D+00 Z= 2.405384825228D+00
I= 3 X= 2.088249439304D+00 Y= -2.165602291986D+00 Z= -7.101552376559D-02
I= 4 X= 1.254054328930D+00 Y= -1.334457200327D+00 Z= 2.519823032746D+00
I= 5 X= -2.692526003304D+00 Y= 3.303095645160D+00 Z= -2.430598911528D+00
I= 6 X= -1.736862214497D-01 Y= 2.316703612515D+00 Z= -3.326778567416D+00
I= 7 X= -2.401177471298D+00 Y= 4.830466214549D+00 Z= -3.764981824300D+00
I= 8 X= -4.116788134320D+00 Y= 1.786407589613D+00 Z= -3.067599149543D+00

I= 9 X= 3.022841274496D+00 Y= -6.683862478612D-01 Z= 4.663260225884D+00
I= 10 X= 2.857919706568D+00 Y= -2.408375289878D+00 Z= 6.233366835947D+00
I= 11 X= 4.827253833457D+00 Y= -4.734057801437D-01 Z= 3.950154331926D+00
I= 12 X= 2.063770824834D+00 Y= 9.718004591363D-01 Z= 5.630518768511D+00
I= 13 X= -2.846483914932D+00 Y= -7.903686778862D-01 Z= 4.655860660098D+00
I= 14 X= -1.623557247045D+00 Y= -2.129930823581D+00 Z= 6.182229420736D+00
I= 15 X= -2.857045927935D+00 Y= 1.448889300675D+00 Z= 5.231524804956D+00
I= 16 X= -4.884985101411D+00 Y= -1.651396288999D+00 Z= 3.912876142347D+00
I= 17 X= -4.658474099351D+00 Y= -2.495839436615D+00 Z= -8.644151656555D-01
I= 18 X= -5.505280346873D+00 Y= -4.122941494707D+00 Z= 2.113556594467D-01
I= 19 X= -5.951768273903D+00 Y= -8.789114726653D-01 Z= -3.930865103252D-01
I= 20 X= -4.911980734974D+00 Y= -3.256639086426D+00 Z= -2.842431987421D+00
I= 21 X= -4.225962432399D-02 Y= -3.851138498801D+00 Z= -4.137725790694D+00
I= 22 X= -3.527978824208D-01 Y= -5.973514860505D+00 Z= -4.147718082008D+00
I= 23 X= -1.392233856956D+00 Y= -2.793605892345D+00 Z= -5.657462927888D+00
I= 24 X= 2.387983065744D+00 Y= -3.906552695104D+00 Z= -4.664651678081D+00
I= 25 X= 4.721919189623D+00 Y= -2.589996114069D+00 Z= -6.660486723079D-01
I= 26 X= 5.262045289969D+00 Y= -2.281150482124D+00 Z= -2.447854055608D+00
I= 27 X= 6.132313546115D+00 Y= -1.648727944063D+00 Z= 3.893843738274D-01
I= 28 X= 5.413557373358D+00 Y= -4.510766072017D+00 Z= 7.356990435215D-02
I= 29 X= 2.545208668723D+00 Y= 3.234284745107D+00 Z= -2.430677329489D+00
I= 30 X= 2.639684836880D+00 Y= 3.692251831721D+00 Z= 1.762352924896D-01
I= 31 X= 4.547211297359D+00 Y= 2.311647296097D+00 Z= -3.289957790453D+00
I= 32 X= 1.996081089465D+00 Y= 4.987865711010D+00 Z= -3.635187697253D+00
I= 33 X= 1.914731518436D+00 Y= 5.525721227745D+00 Z= 8.376764904882D-01
I= 34 X= 4.214738549141D+00 Y= 2.775905610810D+00 Z= 7.719962804323D-01
I= 35 X= -5.015330929464D-02 Y= 1.142295073334D+00 Z= -4.682614772839D-01
I= 36 X= -2.600434396144D+00 Y= 3.930878349041D+00 Z= 2.926260846811D-01
I= 37 X= -1.848454620850D+00 Y= 5.811978516912D+00 Z= 4.291807358050D-01
I= 38 X= -4.062260138828D+00 Y= 3.207225388609D+00 Z= 1.519785400175D+00

Forward Direction:

Total Energy: -691.9912881 Hartrees

Potential Energy: -692.1677780 Hartress

Kinetic Energy: 0.1764899 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.506791064284D+13 Y= 2.157299736563D+13 Z= -1.603286473685D+13
I= 1 X= -8.604337783797D+12 Y= -1.226243482819D+13 Z= 6.571651940587D+12
I= 2 X= -1.625748123948D+13 Y= -1.459131404678D+13 Z= -4.846819448197D+12
I= 3 X= 3.190960754450D+12 Y= -1.925305915598D+12 Z= 1.624994322968D+12
I= 4 X= -1.802666580594D+13 Y= 1.614514996241D+13 Z= -1.172075370951D+13
I= 5 X= -2.051437657067D+13 Y= -1.406807353268D+12 Z= 8.108117673996D+12
I= 6 X= 4.763677569572D+13 Y= -1.221773888813D+13 Z= 7.127431186065D+13
I= 7 X= 8.386704935129D+13 Y= 1.177956438700D+14 Z= -3.288928581074D+13
I= 8 X= 6.692592556455D+13 Y= -1.224231166216D+13 Z= 1.285838644862D+13
I= 9 X= -9.827225862501D+12 Y= 5.237535022975D+12 Z= 1.467289422642D+13
I= 10 X= -4.568472611722D+12 Y= -8.004425120698D+13 Z= 6.593836674177D+13
I= 11 X= -4.998837701660D+13 Y= -5.653964748621D+13 Z= 2.741030083794D+12
I= 12 X= -4.553993556413D+13 Y= -1.703562293303D+13 Z= -1.115856041834D+14
I= 13 X= 3.904525685599D+12 Y= -4.735861464017D+12 Z= -2.704103110743D+13
I= 14 X= 6.106521663264D+13 Y= -2.425630960596D+13 Z= 1.354355962130D+14
I= 15 X= 1.123744364646D+13 Y= 6.902068679209D+13 Z= 9.300365085153D+13
I= 16 X= 3.962651511638D+13 Y= 2.305626013810D+13 Z= 9.080899520833D+12
I= 17 X= 1.318201781838D+13 Y= 7.005784519027D+12 Z= 3.057450453094D+11
I= 18 X= -7.020182970174D+13 Y= -3.585922673418D+13 Z= 1.847353209447D+13
I= 19 X= 5.553090659406D+13 Y= 3.995009622624D+13 Z= 8.491181610264D+13
I= 20 X= 7.330980054005D+12 Y= -2.902232798110D+13 Z= -9.866010677214D+13
I= 21 X= 1.574867863013D+13 Y= 2.792732588039D+12 Z= 1.121151870279D+12
I= 22 X= -6.219824046656D+12 Y= -1.142039685090D+13 Z= 8.359850447176D+13
I= 23 X= 2.396881468556D+13 Y= 2.186094511231D+13 Z= 1.748547906668D+13
I= 24 X= -1.571868483443D+14 Y= -6.136500076141D+13 Z= 1.580252407548D+13

I= 25 X= 6.303652763073D+12 Y= -7.990764722136D+12 Z= -1.527155260714D+13
I= 26 X= -1.972984173683D+13 Y= 4.330446141894D+13 Z= 1.085067063729D+14
I= 27 X= 3.270283633912D+13 Y= 5.592515662980D+13 Z= 1.002470453839D+14
I= 28 X= -2.120999018110D+13 Y= -1.552888862085D+13 Z= -1.296240234790D+13
I= 29 X= 8.964277471850D+12 Y= -1.254234451050D+13 Z= 7.349621842148D+12
I= 30 X= -5.696773040206D+12 Y= -6.255527546455D+12 Z= -3.724919160836D+13
I= 31 X= -3.441342274415D+13 Y= -6.649699499936D+13 Z= -3.639449634253D+12
I= 32 X= 7.133606451376D+13 Y= 2.007549932448D+13 Z= 2.629032448296D+13
I= 33 X= -6.877978367449D+13 Y= 7.097446020955D+13 Z= 4.436924898241D+13
I= 34 X= -5.505193764894D+13 Y= 2.978337554569D+13 Z= -3.195258923765D+13
I= 35 X= 5.399486414169D+12 Y= -1.976635201824D+12 Z= 5.549478424134D+12
I= 36 X= -1.437725278606D+13 Y= 1.015744760920D+13 Z= 1.585215331335D+12
I= 37 X= -3.267090828244D+13 Y= -3.144794167753D+13 Z= -4.916932838534D+13
I= 38 X= 6.938914703445D+13 Y= 6.301153611659D+13 Z= -3.039267744457D+13

Backward Direction:

Total Energy: -691.9913497 Hartrees

Potential Energy: -692.1677780 Hartress

Kinetic Energy: 0.1764282 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.515524370932D+13 Y= 2.338948731222D+13 Z= -1.314773022047D+13
I= 1 X= -7.837424645460D+12 Y= -1.226202985087D+13 Z= 6.571421065818D+12
I= 2 X= -1.529953128028D+13 Y= -1.518890521328D+13 Z= -3.343405082794D+12
I= 3 X= 3.278539661140D+12 Y= -3.741956995452D+12 Z= -1.260522627073D+12
I= 4 X= -1.706855318939D+13 Y= 1.674292405359D+13 Z= -1.322409853184D+13
I= 5 X= -1.801561574098D+13 Y= -1.427483733935D+13 Z= -6.519935781736D+12
I= 6 X= -5.926619944144D+13 Y= -1.219987792552D+13 Z= 7.127481651604D+13
I= 7 X= 6.630036451942D+13 Y= 1.117816614295D+14 Z= -5.189965769773D+13
I= 8 X= 5.909265450027D+13 Y= -2.078781730948D+13 Z= 8.841861189806D+12
I= 9 X= -7.471422100015D+12 Y= 9.830962678023D+11 Z= 1.349689511083D+13
I= 10 X= -5.794902941042D+12 Y= -8.532019090823D+13 Z= 6.336140482610D+13

I= 11 X= -4.698705012672D+13 Y= -6.473224494557D+13 Z= 1.971577663319D+12
I= 12 X= -3.980777950276D+13 Y= -2.089500967131D+13 Z= -1.112226042642D+14
I= 13 X= 6.260127012603D+12 Y= -4.813804206605D+11 Z= -2.586437015890D+13
I= 14 X= 5.984060659448D+13 Y= -1.897972856916D+13 Z= 1.380135976257D+14
I= 15 X= 1.696843816618D+13 Y= 7.288182516735D+13 Z= 9.264038478192D+13
I= 16 X= 4.262677945168D+13 Y= 3.124645969271D+13 Z= 9.851973036374D+12
I= 17 X= 1.283501980013D+13 Y= 7.104874321705D+12 Z= 4.732719697549D+12
I= 18 X= -6.969033858918D+13 Y= -3.392429345938D+13 Z= 2.769106938649D+13
I= 19 X= 5.517227282903D+13 Y= 4.133062840545D+13 Z= 8.663605379880D+13
I= 20 X= 5.742613797661D+12 Y= -3.442244098776D+13 Z= -9.374813016359D+13
I= 21 X= 1.173945737726D+13 Y= 2.794690924113D+12 Z= 1.119836949796D+12
I= 22 X= -1.652569736137D+13 Y= -1.141833632206D+13 Z= 8.359484020860D+13
I= 23 X= 2.144331397602D+13 Y= 2.673192483059D+13 Z= 1.771104906738D+13
I= 24 X= -1.597128767075D+14 Y= -6.623052957246D+13 Z= 1.557509129762D+13
I= 25 X= 5.957122115250D+12 Y= -8.090706758013D+12 Z= -1.969865711861D+13
I= 26 X= -2.131729228367D+13 Y= 4.870323997149D+13 Z= 1.035942858647D+14
I= 27 X= 3.234491649340D+13 Y= 5.454279394492D+13 Z= 9.852337544081D+13
I= 28 X= -2.069836411581D+13 Y= -1.746520660656D+13 Z= -2.217964715183D+13
I= 29 X= 1.146228728310D+13 Y= 3.217011233732D+11 Z= 2.197403583566D+13
I= 30 X= -1.061476471579D+12 Y= -5.660664459332D+12 Z= -2.509899997336D+13
I= 31 X= -4.224237261364D+13 Y= -5.795341426542D+13 Z= 3.738923949687D+11
I= 32 X= 5.377238138045D+13 Y= 2.608979436317D+13 Z= 4.529435500509D+13
I= 33 X= -7.088441457424D+13 Y= 6.312732506778D+13 Z= 6.951542721537D+13
I= 34 X= -5.363381634107D+13 Y= 2.143817474595D+13 Z= -2.280594136498D+13
I= 35 X= 4.685900785272D+12 Y= -1.976170743217D+12 Z= 5.550887733527D+12
I= 36 X= -9.741790124360D+12 Y= 9.560976370448D+12 Z= -1.056572477176D+13
I= 37 X= -3.477984294295D+13 Y= -2.359608371162D+13 Z= -7.431812327631D+13
I= 38 X= 7.080800670784D+13 Y= 7.135348293213D+13 Z= -3.953933944066D+13

Seed: 34740595451

CM Start Point Coordinates: bohr

I= 0 X= -2.155813333784D+00 Y= -2.054942232697D+00 Z= 1.210975952899D-01
I= 1 X= 3.352750203347D-02 Y= -2.592986894655D+00 Z= -1.472762096199D+00
I= 2 X= -1.198812337573D+00 Y= -1.034857526060D+00 Z= 2.383887309823D+00
I= 3 X= 2.311179726341D+00 Y= -2.083054038547D+00 Z= -1.406151131583D-01
I= 4 X= 1.404211725146D+00 Y= -1.110023049335D+00 Z= 2.358992394621D+00
I= 5 X= -2.413328773440D+00 Y= 3.344981345033D+00 Z= -2.422777646885D+00
I= 6 X= 1.407440614329D-01 Y= 1.851235648476D+00 Z= -3.230735846918D+00
I= 7 X= -1.269132289157D+00 Y= 5.083561476990D+00 Z= -3.446206465025D+00
I= 8 X= -3.235841418124D+00 Y= 2.078913259413D+00 Z= -3.930310976446D+00
I= 9 X= 3.009105938627D+00 Y= -5.901316741719D-01 Z= 4.504174267746D+00
I= 10 X= 3.442007632528D+00 Y= -2.464046673401D+00 Z= 5.880830160242D+00
I= 11 X= 5.057762148950D+00 Y= -5.950150351591D-03 Z= 3.925971894230D+00
I= 12 X= 1.990519851370D+00 Y= 9.793987684984D-01 Z= 5.501576826750D+00
I= 13 X= -2.799817490287D+00 Y= -6.175238142282D-01 Z= 4.758430408021D+00
I= 14 X= -2.271379958809D+00 Y= -1.912877348513D+00 Z= 6.234903776588D+00
I= 15 X= -2.727686395717D+00 Y= 1.533782511901D+00 Z= 5.366768406806D+00
I= 16 X= -5.114422469881D+00 Y= -9.703452572754D-01 Z= 4.335604595089D+00
I= 17 X= -4.855111718658D+00 Y= -2.603305877571D+00 Z= -9.606299942560D-01
I= 18 X= -5.830850477681D+00 Y= -4.450756249850D+00 Z= -3.916194167027D-01
I= 19 X= -6.205637998752D+00 Y= -1.283565534268D+00 Z= 2.963702504958D-01
I= 20 X= -5.007825381474D+00 Y= -2.055805653235D+00 Z= -2.932088553560D+00
I= 21 X= -1.884338484782D-01 Y= -3.802571598415D+00 Z= -4.137148844657D+00
I= 22 X= -8.897810873094D-01 Y= -5.940410955168D+00 Z= -3.799473678907D+00
I= 23 X= -1.385600341121D+00 Y= -3.262835857744D+00 Z= -5.784992915484D+00
I= 24 X= 1.660634188749D+00 Y= -3.833310175823D+00 Z= -5.299721365622D+00
I= 25 X= 4.852523918868D+00 Y= -2.584336259271D+00 Z= -8.562365462623D-01
I= 26 X= 5.126666598946D+00 Y= -1.588039960532D+00 Z= -3.065193799182D+00
I= 27 X= 6.386129406616D+00 Y= -1.799374749583D+00 Z= 5.033638220066D-01
I= 28 X= 5.066295138281D+00 Y= -4.935900478034D+00 Z= -9.307886480747D-01

I= 29 X= 2.855958848135D+00 Y= 3.007795529396D+00 Z= -2.109356544069D+00
I= 30 X= 2.443579622836D+00 Y= 3.794887832592D+00 Z= 3.762618774396D-01
I= 31 X= 4.154344168099D+00 Y= 1.676665670420D+00 Z= -2.538402191621D+00
I= 32 X= 2.648095202015D+00 Y= 4.251213792404D+00 Z= -3.632995246875D+00
I= 33 X= 1.681555252876D+00 Y= 5.628814236221D+00 Z= 8.820031188320D-01
I= 34 X= 3.611644281303D+00 Y= 2.839783592645D+00 Z= 1.823966316615D+00
I= 35 X= -7.200650890467D-02 Y= 1.118476284375D+00 Z= -5.050106811875D-01
I= 36 X= -2.923985554203D+00 Y= 3.465256801481D+00 Z= 2.582449466063D-01
I= 37 X= -2.447504214706D+00 Y= 5.549474984056D+00 Z= 8.327370242107D-01
I= 38 X= -4.832601912158D+00 Y= 2.647722747326D+00 Z= 1.238484783417D+00

Forward Direction:

Total Energy: -691.9945670 Hartrees

Potential Energy: -692.1761297 Hartress

Kinetic Energy: 0.1815627 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.358034826597D+12 Y= 6.041182917162D+12 Z= -1.808021543212D+12
I= 1 X= -9.518870528701D+12 Y= -8.611054675505D+12 Z= -2.193097542686D+13
I= 2 X= 1.284848167963D+13 Y= 7.410034942283D+12 Z= -3.069304546819D+13
I= 3 X= 5.395744817633D+12 Y= -5.902088814531D+11 Z= 2.263907346083D+13
I= 4 X= -1.177197523543D+13 Y= -6.467053600471D+12 Z= 1.213181427340D+13
I= 5 X= 8.189575000217D+11 Y= -8.840964797176D+12 Z= 2.147972317961D+13
I= 6 X= 2.480846349109D+13 Y= -4.578238696405D+13 Z= -9.578985877372D+13
I= 7 X= -3.308221538831D+13 Y= -7.570064046650D+12 Z= -6.426804938568D+13
I= 8 X= -2.843121783811D+13 Y= 1.208567379193D+13 Z= 8.908969485014D+12
I= 9 X= 2.265510266265D+12 Y= 8.269358368304D+12 Z= -2.612731664318D+13
I= 10 X= 3.915590567242D+13 Y= -8.230845563630D+13 Z= 2.853252177619D+13
I= 11 X= -3.063411736421D+13 Y= -5.324175393897D+13 Z= 2.621754800299D+13
I= 12 X= -2.240963142176D+13 Y= 3.891985060611D+12 Z= 1.299823883966D+13
I= 13 X= 1.833849128259D+13 Y= 8.675803353855D+12 Z= 3.671521543852D+12
I= 14 X= -2.520979065945D+13 Y= 4.234807585424D+13 Z= -1.162761641944D+13

I= 15 X= -8.603544940401D+12 Y= -9.015988249127D+13 Z= -1.217939672989D+13
I= 16 X= 5.334773097995D+13 Y= -9.908340123028D+12 Z= 2.060370229664D+13
I= 17 X= 3.361802505511D+12 Y= -1.728615227360D+13 Z= -9.143311815730D+12
I= 18 X= -6.038474991268D+13 Y= 3.978380493264D+13 Z= -5.023529135921D+13
I= 19 X= -1.326208686304D+14 Y= 3.208990876096D+13 Z= 1.459826621631D+14
I= 20 X= -2.370887648959D+13 Y= -9.110405015872D+13 Z= -1.336217656084D+14
I= 21 X= 5.131421178669D+12 Y= -1.008558241057D+13 Z= 1.881136622420D+13
I= 22 X= -7.110124521086D+12 Y= -8.769083523002D+12 Z= 3.854423271749D+13
I= 23 X= -2.200189583825D+13 Y= 2.687208725064D+13 Z= -5.078114446174D+11
I= 24 X= 1.290347150717D+14 Y= 8.267864204677D+13 Z= -5.389500212393D+13
I= 25 X= -1.066759628316D+13 Y= -2.243893732876D+11 Z= 9.575738297442D+11
I= 26 X= 8.406217625553D+13 Y= -4.852526743698D+13 Z= -1.315657620272D+14
I= 27 X= -5.787108170232D+13 Y= -1.593381069803D+13 Z= 4.629820739114D+13
I= 28 X= -4.823544813248D+13 Y= -2.883252039242D+13 Z= -3.146608086332D+13
I= 29 X= -2.464402207766D+11 Y= 7.552546686775D+12 Z= -3.829523557521D+11
I= 30 X= 6.012977414615D+11 Y= -6.861166635495D+12 Z= 4.673108848681D+12
I= 31 X= -2.772910126840D+13 Y= -1.136618260299D+13 Z= 1.462727359098D+13
I= 32 X= -8.083379685272D+13 Y= 6.810198850978D+13 Z= -5.290080989583D+13
I= 33 X= 2.107471155089D+13 Y= 1.147859767596D+13 Z= -7.756086762197D+13
I= 34 X= -3.953089935716D+12 Y= -2.209842855513D+13 Z= 1.805036294102D+13
I= 35 X= 2.483030738966D+12 Y= 7.101659242614D+12 Z= 3.744945947115D+11
I= 36 X= -1.907557740436D+13 Y= -1.022753834511D+13 Z= 3.154591042299D+13
I= 37 X= 3.629889941916D+13 Y= 1.385669632817D+13 Z= 5.926596198716D+13
I= 38 X= 1.260004215862D+14 Y= 1.391698714468D+14 Z= -3.379769513795D+13

Backward Direction:

Total Energy: -691.9945624 Hartrees

Potential Energy: -692.1761297 Hartress

Kinetic Energy: 0.1815673 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.300652299232D+12 Y= 7.075876409138D+12 Z= -1.868992948710D+11

I= 1 X= -9.035248955416D+12 Y= -8.610830020244D+12 Z= -2.193110151269D+13
I= 2 X= 1.336292101585D+13 Y= 7.028170837757D+12 Z= -2.984151579647D+13
I= 3 X= 5.453262812308D+12 Y= -1.624995707000D+12 Z= 2.101773552702D+13
I= 4 X= -1.125744587172D+13 Y= -6.085087085568D+12 Z= 1.128031774448D+13
I= 5 X= 2.319021945054D+12 Y= -1.598155197537D+13 Z= 1.329889547313D+13
I= 6 X= -3.737691141866D+13 Y= -4.577223339346D+13 Z= -9.578962090706D+13
I= 7 X= -4.307151821374D+13 Y= -1.058727794259D+13 Z= -7.475732868534D+13
I= 8 X= -3.298915215573D+13 Y= 7.655845184669D+12 Z= 6.655711088774D+12
I= 9 X= 3.554437888397D+12 Y= 5.938902333494D+12 Z= -2.678715498237D+13
I= 10 X= 3.845824775771D+13 Y= -8.521484932943D+13 Z= 2.708475200641D+13
I= 11 X= -2.898627093091D+13 Y= -5.774907577050D+13 Z= 2.579056333127D+13
I= 12 X= -1.925365966976D+13 Y= 1.772140773793D+12 Z= 1.320382126041D+13
I= 13 X= 1.962730498042D+13 Y= 1.100628273415D+13 Z= 4.331721059119D+12
I= 14 X= -2.590645502751D+13 Y= 4.525481810964D+13 Z= -1.017928340237D+13
I= 15 X= -5.448213594431D+12 Y= -8.803907450243D+13 Z= -1.238512508333D+13
I= 16 X= 5.499499080916D+13 Y= -5.402337021523D+12 Z= 2.103157763076D+13
I= 17 X= 3.184986389724D+12 Y= -1.722016437216D+13 Z= -6.709205652017D+12
I= 18 X= -6.007193103144D+13 Y= 4.084309161946D+13 Z= -4.518767940737D+13
I= 19 X= -1.328283249173D+14 Y= 3.283563361369D+13 Z= 1.469413754647D+14
I= 20 X= -2.455856456900D+13 Y= -9.405134738446D+13 Z= -1.309232887624D+14
I= 21 X= 2.939485049630D+12 Y= -1.008450163161D+13 Z= 1.881064052256D+13
I= 22 X= -1.274913470106D+13 Y= -8.767947795311D+12 Z= 3.854220809892D+13
I= 23 X= -2.339364927777D+13 Y= 2.953349912135D+13 Z= -3.680061556278D+11
I= 24 X= 1.276426654539D+14 Y= 8.002024681497D+13 Z= -5.403584892767D+13
I= 25 X= -1.084415953414D+13 Y= -2.908420910658D+11 Z= -1.476601983038D+12
I= 26 X= 8.321299286986D+13 Y= -4.557872035056D+13 Z= -1.342644768748D+14
I= 27 X= -5.807815337882D+13 Y= -1.668053322692D+13 Z= 4.533979824408D+13
I= 28 X= -4.792256684443D+13 Y= -2.989255782217D+13 Z= -3.651350854657D+13
I= 29 X= 1.253215210185D+12 Y= 1.469090849359D+13 Z= 7.795866661472D+12
I= 30 X= 3.282985808882D+12 Y= -6.446452610336D+12 Z= 1.134303825197D+13

I= 31 X= -3.228447971659D+13 Y= -6.937271656699D+12 Z= 1.687880576036D+13
I= 32 X= -9.082148468117D+13 Y= 7.111932161494D+13 Z= -4.241506860970D+13
I= 33 X= 1.990564026617D+13 Y= 7.159679449102D+12 Z= -6.368879165684D+13
I= 34 X= -3.221758811359D+12 Y= -2.671746344069D+13 Z= 2.317660968578D+13
I= 35 X= 2.047084709078D+12 Y= 7.101913999434D+12 Z= 3.752752698524D+11
I= 36 X= -1.639377253599D+13 Y= -1.064314904753D+13 Z= 2.487557218566D+13
I= 37 X= 3.512748002222D+13 Y= 1.817824076341D+13 Z= 4.539239025490D+13
I= 38 X= 1.267322165393D+14 Y= 1.437871591569D+14 Z= -3.892393300772D+13

Seed: 34894387040

CM Start Point Coordinates: bohr

I= 0 X= -2.220082018857D+00 Y= -2.051395703802D+00 Z= -2.370064685474D-03
I= 1 X= -7.297794608157D-02 Y= -2.651138265448D+00 Z= -1.432611411817D+00
I= 2 X= -1.320489946920D+00 Y= -1.005299067373D+00 Z= 2.250446706679D+00
I= 3 X= 2.179724511714D+00 Y= -2.072116359535D+00 Z= -4.350042988650D-02
I= 4 X= 1.392976604261D+00 Y= -1.205192078409D+00 Z= 2.408617999374D+00
I= 5 X= -3.081355048642D+00 Y= 3.222208547893D+00 Z= -2.143838154478D+00
I= 6 X= -2.745169151766D-01 Y= 1.521100022202D+00 Z= -3.541095362809D+00
I= 7 X= -2.782902255327D+00 Y= 4.802935122516D+00 Z= -3.669872814478D+00
I= 8 X= -4.677059423946D+00 Y= 1.715112747970D+00 Z= -2.796575788330D+00
I= 9 X= 2.882312738162D+00 Y= -7.726317815089D-01 Z= 4.707955468092D+00
I= 10 X= 3.300678485814D+00 Y= -2.573784095067D+00 Z= 6.098752207023D+00
I= 11 X= 4.900397387592D+00 Y= -6.401237573237D-01 Z= 4.218055019872D+00
I= 12 X= 1.948826618863D+00 Y= 6.128378837869D-01 Z= 5.565275242905D+00
I= 13 X= -3.146017857936D+00 Y= -6.139093631726D-01 Z= 4.459918149356D+00
I= 14 X= -3.384245865712D+00 Y= -2.399451864471D+00 Z= 5.431088943200D+00
I= 15 X= -2.112936983146D+00 Y= 3.006189230552D-01 Z= 6.266913858806D+00
I= 16 X= -5.118985552518D+00 Y= 3.314834357153D-01 Z= 4.098280368167D+00
I= 17 X= -4.975355168212D+00 Y= -2.570162008263D+00 Z= -7.308397854097D-01
I= 18 X= -5.520269901431D+00 Y= -4.408668271109D+00 Z= 2.363377698362D-02

I= 19 X= -6.120446963662D+00 Y= -1.203445872964D+00 Z= 3.325116309070D-01
I= 20 X= -5.007607116125D+00 Y= -2.562548361804D+00 Z= -2.906180446566D+00
I= 21 X= 2.469399374033D-01 Y= -4.010162371679D+00 Z= -4.052879372967D+00
I= 22 X= 1.001757285102D+00 Y= -5.775278818748D+00 Z= -3.811689028650D+00
I= 23 X= -1.635341623070D+00 Y= -3.809158521504D+00 Z= -5.075049111417D+00
I= 24 X= 1.607563797456D+00 Y= -2.588327259669D+00 Z= -5.080710807133D+00
I= 25 X= 4.866442206875D+00 Y= -2.557320156030D+00 Z= -8.197430053232D-01
I= 26 X= 5.152407357641D+00 Y= -2.349796689966D+00 Z= -2.879581270719D+00
I= 27 X= 6.329108578282D+00 Y= -1.079786363373D+00 Z= 4.185700381549D-01
I= 28 X= 5.491455590396D+00 Y= -4.458443601558D+00 Z= 2.805109463155D-02
I= 29 X= 2.853986462365D+00 Y= 3.453194964490D+00 Z= -2.470513146702D+00
I= 30 X= 2.783930785374D+00 Y= 3.427758524086D+00 Z= 2.042004537716D-01
I= 31 X= 4.110654064833D+00 Y= 2.306452851431D+00 Z= -3.384022504246D+00
I= 32 X= 1.464275048945D+00 Y= 5.001760681096D+00 Z= -3.395728832666D+00
I= 33 X= 2.621539887397D+00 Y= 5.004974890638D+00 Z= 1.217702923744D+00
I= 34 X= 4.278237292002D+00 Y= 2.694225333593D+00 Z= 1.427784066642D+00
I= 35 X= 5.607070375056D-02 Y= 1.162765394684D+00 Z= -5.811242467941D-01
I= 36 X= -2.655699666390D+00 Y= 3.791188200470D+00 Z= 4.030921936847D-01
I= 37 X= -2.183169844707D+00 Y= 5.717183703189D+00 Z= 7.437391220466D-01
I= 38 X= -3.504967768031D+00 Y= 2.703263904534D+00 Z= 2.051620583741D+00

Forward Direction:

Total Energy: -692.0054577 Hartrees

Potential Energy: -692.1903294 Hartress

Kinetic Energy: 0.1848717 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.366096405024D+12 Y= -1.385409403445D+13 Z= -5.336518198165D+12

I= 1 X= 1.441220739999D+13 Y= 8.185924384781D+12 Z= -1.826693780633D+13

I= 2 X= 2.017829999391D+13 Y= -9.823371909438D+12 Z= -1.509621973410D+13

I= 3 X= -1.611960196673D+13 Y= -1.610586602576D+13 Z= 7.160957710189D+12

I= 4 X= -1.956994582622D+13 Y= 5.510488780355D+12 Z= -9.996210040307D+11

I= 5 X= -6.930478943710D+12 Y= 1.194679369434D+13 Z= -2.206737000356D+11
I= 6 X= 7.495432007280D+13 Y= 3.514216965840D+12 Z= 6.280900521982D+13
I= 7 X= -5.322845609832D+13 Y= -5.091389634544D+13 Z= -5.715467574830D+13
I= 8 X= -2.118897745753D+13 Y= -2.873181647219D+13 Z= -5.367858691629D+13
I= 9 X= 1.208789052830D+13 Y= 7.731278299812D+12 Z= 1.109255076480D+13
I= 10 X= -5.706536473498D+13 Y= -2.276434354951D+12 Z= -4.065335037542D+13
I= 11 X= 1.760301219282D+14 Y= 2.510978689936D+13 Z= -2.320158954453D+13
I= 12 X= -5.402953599870D+13 Y= -9.278494763314D+13 Z= 6.337241744591D+13
I= 13 X= -1.063566771292D+13 Y= -4.666062078112D+12 Z= 2.312970536714D+12
I= 14 X= 2.254791708314D+13 Y= -1.562781141204D+13 Z= 8.565134337802D+13
I= 15 X= -5.553455327875D+13 Y= 8.431773915432D+13 Z= 8.835078618283D+13
I= 16 X= -3.474021101734D+13 Y= 1.594174361498D+13 Z= 9.140483493792D+12
I= 17 X= 3.607001930846D+12 Y= -2.586375597854D+13 Z= -6.281674615346D+12
I= 18 X= 1.874039960758D+13 Y= 2.164589448523D+12 Z= -5.529747981799D+13
I= 19 X= -8.763826407713D+13 Y= 1.526888141861D+14 Z= 3.982957559571D+13
I= 20 X= -4.913249614567D+13 Y= -1.900962094063D+13 Z= 5.918149123751D+13
I= 21 X= -1.130405197067D+13 Y= -1.332203647307D+11 Z= 1.332467252332D+13
I= 22 X= 3.819343059282D+13 Y= 4.706667100109D+13 Z= -3.174457050780D+13
I= 23 X= 4.677566134970D+13 Y= 6.856200093592D+12 Z= 3.117372827130D+13
I= 24 X= 1.350072459879D+13 Y= 2.666613621796D+13 Z= 2.260976175188D+12
I= 25 X= 2.649506986850D+13 Y= -6.565314983756D+11 Z= 1.579408151427D+13
I= 26 X= -3.527634640414D+13 Y= 8.712719051923D+12 Z= 9.226419422347D+13
I= 27 X= 4.778058075684D+12 Y= -7.632892710705D+13 Z= 1.337452811536D+13
I= 28 X= -1.294447595311D+14 Y= 1.253673570521D+13 Z= 2.536637084412D+12
I= 29 X= -1.343244801940D+13 Y= 2.030305505273D+13 Z= -1.874815723405D+13
I= 30 X= 2.585075675575D+12 Y= -1.027173208999D+13 Z= -1.272630820688D+13
I= 31 X= 8.717892789245D+13 Y= -1.050790945008D+14 Z= 4.000779620256D+13
I= 32 X= 1.215107881636D+13 Y= 8.523034248383D+13 Z= -7.954190103557D+12
I= 33 X= 1.213146116341D+13 Y= 3.728284684758D+13 Z= -2.257113714962D+13
I= 34 X= 7.482571078074D+13 Y= 3.246455603985D+13 Z= 1.012863687290D+14

I= 35 X= 3.417712993348D+12 Y= 2.511410466148D+12 Z= -3.621742315131D+12
I= 36 X= -1.017369631959D+13 Y= -7.209659145044D+12 Z= 8.841370627306D+12
I= 37 X= -5.140861150799D+13 Y= 4.602521369635D+13 Z= 1.086222295864D+14
I= 38 X= 5.142474499287D+13 Y= 7.294666833335D+13 Z= -6.781244337388D+13

Backward Direction:

Total Energy: -692.0054542 Hartrees

Potential Energy: -692.1903294 Hartress

Kinetic Energy: 0.1848752 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.061439052858D+12 Y= -1.178628934146D+13 Z= -2.651110066652D+12
I= 1 X= 1.654245746717D+13 Y= 8.186223397462D+12 Z= -1.826705636723D+13
I= 2 X= 2.042971837665D+13 Y= -1.161816892396D+13 Z= -1.351468195353D+13
I= 3 X= -1.581478713134D+13 Y= -1.817389612044D+13 Z= 4.475169620701D+12
I= 4 X= -1.931841303369D+13 Y= 7.305447202495D+12 Z= -2.581257322710D+12
I= 5 X= -2.023503305297D+12 Y= 2.383115947007D+12 Z= -1.280139587721D+13
I= 6 X= -8.146842119051D+13 Y= 3.534011687779D+12 Z= 6.280824755329D+13
I= 7 X= -7.277180198926D+13 Y= -4.678325588989D+13 Z= -6.967759199163D+13
I= 8 X= -3.268644792331D+13 Y= -2.669359639584D+13 Z= -5.732088590002D+13
I= 9 X= 1.334613142257D+13 Y= 5.385572355430D+12 Z= 1.002326029655D+13
I= 10 X= -5.843645886039D+13 Y= -5.625832654586D+12 Z= -4.304670987317D+13
I= 11 X= 1.777872655543D+14 Y= 2.006441432676D+13 Z= -2.377368401101D+13
I= 12 X= -5.043730443604D+13 Y= -9.506834402161D+13 Z= 6.375375159743D+13
I= 13 X= -9.377617529424D+12 Y= -2.320328997112D+12 Z= 3.382587159131D+12
I= 14 X= 2.117773518444D+13 Y= -1.227813061496D+13 Z= 8.804510331229D+13
I= 15 X= -5.194306892945D+13 Y= 8.660221714749D+13 Z= 8.796930207271D+13
I= 16 X= -3.298377740602D+13 Y= 2.098565357345D+13 Z= 9.713543122219D+12
I= 17 X= 3.772034342288D+12 Y= -2.549441794232D+13 Z= -3.595189160405D+12
I= 18 X= 1.989962217166D+13 Y= 3.214958799582D+12 Z= -5.025519951347D+13
I= 19 X= -8.813182934615D+13 Y= 1.531680507106D+14 Z= 4.116260960641D+13
I= 20 X= -4.946073720252D+13 Y= -2.169874134399D+13 Z= 6.210047184636D+13

I= 21 X= -1.340175694106D+13 Y= -1.319255887030D+11 Z= 1.332380077138D+13
I= 22 X= 3.267902845834D+13 Y= 4.706799452023D+13 Z= -3.174705902829D+13
I= 23 X= 4.515856763971D+13 Y= 9.359963788975D+12 Z= 3.173468828412D+13
I= 24 X= 1.188314827125D+13 Y= 2.416620080228D+13 Z= 1.698418560908D+12
I= 25 X= 2.666027802880D+13 Y= -1.026285833143D+12 Z= 1.310757145388D+13
I= 26 X= -3.560398495573D+13 Y= 1.140059262358D+13 Z= 8.934510707779D+13
I= 27 X= 4.284726647236D+12 Y= -7.680902005999D+13 Z= 1.204164712237D+13
I= 28 X= -1.282857811531D+14 Y= 1.148583304845D+13 Z= -2.504837249612D+12
I= 29 X= -8.525824203929D+12 Y= 2.986338183193D+13 Z= -6.169846972059D+12
I= 30 X= 8.973532628016D+12 Y= -7.555404121540D+12 Z= -5.639880393433D+12
I= 31 X= 7.568891494498D+13 Y= -1.071147035659D+14 Z= 4.364880937115D+13
I= 32 X= -7.391395312711D+12 Y= 8.109847735127D+13 Z= 4.563499456588D+12
I= 33 X= 1.053522671032D+13 Y= 3.240562571087D+13 Z= -6.079775118854D+12
I= 34 X= 7.438544260767D+13 Y= 2.657925216088D+13 Z= 1.094465701474D+14
I= 35 X= 1.813111802033D+12 Y= 2.511676354341D+12 Z= -3.620731398290D+12
I= 36 X= -3.784452059065D+12 Y= -9.927300258447D+12 Z= 1.754562503079D+12
I= 37 X= -5.300696761611D+13 Y= 5.090609076914D+13 Z= 9.212774727908D+13
I= 38 X= 5.098648135013D+13 Y= 7.883112399822D+13 Z= -7.597220539000D+13

Seed: 34979556649

CM Start Point Coordinates: bohr

I= 0 X= -2.169364843330D+00 Y= -2.202269242542D+00 Z= 8.321730432683D-02
I= 1 X= -5.563294525063D-02 Y= -2.566249065010D+00 Z= -1.593010900993D+00
I= 2 X= -1.389197184175D+00 Y= -1.330926892320D+00 Z= 2.404304895505D+00
I= 3 X= 2.202265526836D+00 Y= -2.016848978422D+00 Z= -7.744511423026D-02
I= 4 X= 1.234745465442D+00 Y= -9.642825387272D-01 Z= 2.320993904292D+00
I= 5 X= -3.219428349267D+00 Y= 3.063826917763D+00 Z= -2.274091617721D+00
I= 6 X= 9.573260415407D-02 Y= 1.342920033935D+00 Z= -3.319159671972D+00
I= 7 X= -2.592129838801D+00 Y= 4.488629293583D+00 Z= -3.759147949035D+00
I= 8 X= -4.948689661322D+00 Y= 1.864538722059D+00 Z= -2.686465363515D+00

I= 9 X= 2.854815387230D+00 Y= -6.352891866009D-01 Z= 4.644650408625D+00
I= 10 X= 2.248155390761D+00 Y= -2.564200822527D+00 Z= 5.544772598472D+00
I= 11 X= 4.713325519412D+00 Y= -2.232422562429D-01 Z= 4.961240971819D+00
I= 12 X= 2.384052081627D+00 Y= 9.956294164089D-01 Z= 5.666303664074D+00
I= 13 X= -3.032177925177D+00 Y= -8.763956751431D-01 Z= 4.819975721321D+00
I= 14 X= -3.620480255060D+00 Y= -2.877297018906D+00 Z= 5.666102557738D+00
I= 15 X= -2.198813450974D+00 Y= 6.982967247591D-01 Z= 5.918369348588D+00
I= 16 X= -4.988166331268D+00 Y= -1.991213470856D-01 Z= 4.019392696686D+00
I= 17 X= -5.003639659487D+00 Y= -2.472904692189D+00 Z= -6.825026531558D-01
I= 18 X= -5.884434978289D+00 Y= -4.282629112359D+00 Z= 1.041560860764D-01
I= 19 X= -6.043390449031D+00 Y= -7.558223806331D-01 Z= 7.180100859754D-02
I= 20 X= -5.125710023806D+00 Y= -2.610818195400D+00 Z= -2.815474524811D+00
I= 21 X= -7.063325474662D-02 Y= -3.587420288409D+00 Z= -4.167695332710D+00
I= 22 X= 5.960516313146D-01 Y= -5.381539330333D+00 Z= -4.456052605046D+00
I= 23 X= -2.083244819284D+00 Y= -3.468107094589D+00 Z= -5.042009110573D+00
I= 24 X= 1.310577286697D+00 Y= -2.530796543913D+00 Z= -5.360055804702D+00
I= 25 X= 5.051650016979D+00 Y= -2.116249653627D+00 Z= -5.913164152328D-01
I= 26 X= 5.416364879739D+00 Y= -2.276797339023D+00 Z= -2.485303927417D+00
I= 27 X= 6.717935211842D+00 Y= -7.055653836715D-01 Z= 3.293122074140D-01
I= 28 X= 5.553005279491D+00 Y= -3.965337688818D+00 Z= 1.357228284907D-02
I= 29 X= 3.030663327797D+00 Y= 3.099516083604D+00 Z= -2.428101030742D+00
I= 30 X= 3.190751359884D+00 Y= 3.566840003650D+00 Z= 2.625096463375D-01
I= 31 X= 4.283362948942D+00 Y= 2.061844925653D+00 Z= -3.545370812136D+00
I= 32 X= 2.442190846684D+00 Y= 4.648741743361D+00 Z= -3.425383989805D+00
I= 33 X= 2.149084139219D+00 Y= 5.272238576165D+00 Z= 8.887761189463D-01
I= 34 X= 4.234982557604D+00 Y= 3.186538778196D+00 Z= 1.599749303766D+00
I= 35 X= 5.239065157748D-03 Y= 9.829308633299D-01 Z= -6.027638815425D-01
I= 36 X= -2.572852493858D+00 Y= 4.051388018307D+00 Z= 2.272641328304D-01
I= 37 X= -1.677305102015D+00 Y= 5.876867368532D+00 Z= 5.849795329412D-01
I= 38 X= -3.907544620552D+00 Y= 3.310045390219D+00 Z= 1.662593390271D+00

Forward Direction:

Total Energy: -691.9992363 Hartrees

Potential Energy: -692.1738713 Hartress

Kinetic Energy: 0.1746350 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.447132066981D+13 Y= -2.289127749791D+12 Z= 1.816965338206D+12
I= 1 X= -1.322903580497D+13 Y= -1.274574532352D+13 Z= -6.268480596445D+12
I= 2 X= -1.528028604343D+12 Y= 2.012210920398D+12 Z= -6.134954006389D+12
I= 3 X= 2.774074445488D+13 Y= -1.064392057209D+13 Z= 1.382794051354D+13
I= 4 X= -1.032828453546D+13 Y= 2.064354546919D+13 Z= 1.203316508860D+13
I= 5 X= 2.321089776585D+12 Y= 2.177580873209D+13 Z= -2.629557106531D+13
I= 6 X= 3.910403099487D+13 Y= -3.513369043607D+13 Z= 8.511488460175D+13
I= 7 X= -8.356269699912D+13 Y= -3.924010685595D+13 Z= 6.971453732794D+13
I= 8 X= -5.079269616465D+13 Y= -1.378446199583D+13 Z= -2.246890304878D+13
I= 9 X= 1.521572381327D+13 Y= -9.643359607176D+12 Z= 1.100355643311D+13
I= 10 X= -3.537215790238D+13 Y= -4.963361368207D+12 Z= -1.856093131225D+13
I= 11 X= -1.809441049244D+13 Y= 5.324314718665D+13 Z= -1.539888340745D+13
I= 12 X= -8.242044574589D+13 Y= 1.872537965408D+14 Z= 1.678778633258D+13
I= 13 X= 4.682505362202D+12 Y= -6.387757587187D+12 Z= 2.202276709491D+12
I= 14 X= -1.125587919092D+13 Y= -1.989957696715D+13 Z= 3.096709652139D+13
I= 15 X= 2.025015776230D+13 Y= 7.692628463758D+13 Z= 2.225149613918D+13
I= 16 X= -2.674066930907D+13 Y= 3.418180279447D+13 Z= 6.287904009821D+13
I= 17 X= 6.973364973803D+12 Y= -3.670934923535D+12 Z= -1.373905944491D+13
I= 18 X= 2.544715334654D+13 Y= 6.676422096368D+13 Z= -4.700178079513D+13
I= 19 X= -7.674819257259D+13 Y= 5.158336200372D+13 Z= 1.050974217840D+14
I= 20 X= 6.143261365468D+13 Y= 3.114414324083D+13 Z= 7.336104074682D+13
I= 21 X= 1.374586627912D+13 Y= 1.356606745166D+13 Z= 1.705507571986D+13
I= 22 X= -2.486156437020D+13 Y= -8.146467473783D+12 Z= 5.943492525647D+12
I= 23 X= 7.488786712691D+13 Y= -1.108346929573D+14 Z= -4.938286063166D+13
I= 24 X= 5.678897272444D+13 Y= 3.974415250718D+12 Z= -5.124378529579D+13

I= 25 X= -1.709411320614D+13 Y= -4.121154554604D+12 Z= -8.077536343628D+12
I= 26 X= 7.140731208566D+13 Y= 3.752707433257D+13 Z= -7.976924647222D+13
I= 27 X= 1.539550341238D+13 Y= 6.135955135065D+13 Z= 1.537389142630D+13
I= 28 X= -4.127497453715D+13 Y= -8.788057179243D+13 Z= 1.219024458371D+14
I= 29 X= -7.537208135634D+12 Y= -5.513309225744D+12 Z= 3.328089536095D+12
I= 30 X= 5.665158344695D+12 Y= -1.085994742300D+13 Z= -4.109775101551D+12
I= 31 X= -8.551266876302D+13 Y= 1.024699994810D+13 Z= -4.332587624369D+13
I= 32 X= 5.456573742777D+13 Y= -8.600950404431D+13 Z= -2.642870017674D+13
I= 33 X= -2.079294177345D+13 Y= -2.624723924997D+13 Z= -6.663924595563D+13
I= 34 X= -8.852422043455D+13 Y= -1.981527823560D+13 Z= -2.031580140365D+13
I= 35 X= 8.458796188265D+11 Y= -3.121321998604D+12 Z= -2.122932821333D+12
I= 36 X= -6.618187347894D+10 Y= -1.607633327600D+12 Z= -1.679864317932D+12
I= 37 X= 9.852039295434D+13 Y= 3.779060295466D+13 Z= 3.201734924550D+13
I= 38 X= 5.380183050786D+13 Y= 9.542013952052D+13 Z= -1.674600158174D+13

Backward Direction:

Total Energy: -691.9991414 Hartrees

Potential Energy: -692.1738713 Hartress

Kinetic Energy: 0.1747300 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.457011508672D+13 Y= -1.436931664794D+12 Z= 3.578344645026D+12
I= 1 X= -1.372539846917D+13 Y= -1.274544501531D+13 Z= -6.268687131742D+12
I= 2 X= -5.072213499630D+11 Y= 2.490830169642D+12 Z= -5.341191574267D+12
I= 3 X= 2.764214870094D+13 Y= -1.149616366214D+13 Z= 1.206634409504D+13
I= 4 X= -9.307352788097D+12 Y= 2.016504391565D+13 Z= 1.123955632728D+13
I= 5 X= 2.088835281465D+12 Y= 1.227626673237D+13 Z= -3.593062833658D+13
I= 6 X= 1.260136319228D+13 Y= -3.512494520575D+13 Z= 8.511602852252D+13
I= 7 X= -9.211298641935D+13 Y= -4.953646925342D+13 Z= 5.458700411541D+13
I= 8 X= -5.271038484936D+13 Y= -2.580600481432D+13 Z= -2.498649405740D+13
I= 9 X= 1.729031176839D+13 Y= -1.333995597885D+13 Z= 1.026837895344D+13
I= 10 X= -3.596456571155D+13 Y= -9.247557728385D+12 Z= -2.013771832381D+13

I= 11 X= -1.555631465081D+13 Y= 4.648455716112D+13 Z= -1.596675951777D+13
I= 12 X= -7.773392499643D+13 Y= 1.840063488467D+14 Z= 1.697980058498D+13
I= 13 X= 6.756971264092D+12 Y= -2.691127059028D+12 Z= 2.938055650669D+12
I= 14 X= -1.184664320697D+13 Y= -1.561477499966D+13 Z= 3.254490441256D+13
I= 15 X= 2.493574195597D+13 Y= 8.017517535180D+13 Z= 2.205925279612D+13
I= 16 X= -2.420341210896D+13 Y= 4.093840503415D+13 Z= 6.344827615167D+13
I= 17 X= 6.429195699071D+12 Y= -3.799146441203D+12 Z= -1.005983447758D+13
I= 18 X= 2.529421207615D+13 Y= 6.845665851501D+13 Z= -3.896570738513D+13
I= 19 X= -7.685834617232D+13 Y= 5.297486632765D+13 Z= 1.063351914639D+14
I= 20 X= 5.967966681892D+13 Y= 2.625579394182D+13 Z= 7.748544941031D+13
I= 21 X= 1.018552008641D+13 Y= 1.356762258835D+13 Z= 1.705403316338D+13
I= 22 X= -3.393039462567D+13 Y= -8.144804746568D+12 Z= 5.940627556972D+12
I= 23 X= 7.284649088014D+13 Y= -1.064785423706D+14 Z= -4.948417880813D+13
I= 24 X= 5.474726854544D+13 Y= -3.775594920840D+11 Z= -5.114369709257D+13
I= 25 X= -1.763782061188D+13 Y= -3.993719984591D+12 Z= -1.175690621148D+13
I= 26 X= 6.965509427372D+13 Y= 4.241461217250D+13 Z= -8.389413492344D+13
I= 27 X= 1.528607868860D+13 Y= 5.996635220013D+13 Z= 1.413672374365D+13
I= 28 X= -4.142758142372D+13 Y= -8.957436959936D+13 Z= 1.138661876180D+14
I= 29 X= -7.770157554195D+12 Y= 3.983556841628D+12 Z= 1.296026053537D+13
I= 30 X= 7.082623832591D+12 Y= -1.196950922977D+13 Z= 6.183496882401D+12
I= 31 X= -8.743005884852D+13 Y= 2.226436947930D+13 Z= -4.081137063385D+13
I= 32 X= 4.601858947539D+13 Y= -7.571191869968D+13 Z= -1.130549851205D+13
I= 33 X= -2.232481610329D+13 Y= -3.269046383870D+13 Z= -4.657910810911D+13
I= 34 X= -8.645977429088D+13 Y= -2.619177949011D+13 Z= -1.449119334309D+13
I= 35 X= 1.050641547456D+12 Y= -3.120925124852D+12 Z= -2.121867574987D+12
I= 36 X= 1.350954132149D+12 Y= -4.991783625659D+11 Z= -1.197380868061D+13
I= 37 X= 9.698460807934D+13 Y= 4.423721473737D+13 Z= 1.195608023570D+13
I= 38 X= 5.586583036671D+13 Y= 1.017931693433D+14 Z= -2.257092643614D+13

Seed: 35424570096

CM Start Point Coordinates: bohr

I= 0 X= -2.251967120014D+00 Y= -2.039172531412D+00 Z= -1.513665212197D-01
I= 1 X= 1.011086992933D-01 Y= -2.688037706513D+00 Z= -1.434360083761D+00
I= 2 X= -1.449579235774D+00 Y= -1.380671644455D+00 Z= 2.364865186478D+00
I= 3 X= 2.132628148054D+00 Y= -2.201068066361D+00 Z= 3.637190492846D-02
I= 4 X= 1.294407536355D+00 Y= -1.163609283143D+00 Z= 2.412684197315D+00
I= 5 X= -3.073018412677D+00 Y= 2.941474015926D+00 Z= -2.239141005070D+00
I= 6 X= -5.035374374952D-02 Y= 1.766974310394D+00 Z= -3.037934492074D+00
I= 7 X= -2.555959735138D+00 Y= 4.354266155709D+00 Z= -3.980277158104D+00
I= 8 X= -4.717359204667D+00 Y= 1.386651104173D+00 Z= -2.468982829446D+00
I= 9 X= 3.038229106911D+00 Y= -6.347749242326D-01 Z= 4.593265157915D+00
I= 10 X= 3.083320436978D+00 Y= -2.361745051402D+00 Z= 5.706607843856D+00
I= 11 X= 4.910084327370D+00 Y= 9.137114783059D-02 Z= 4.110722045469D+00
I= 12 X= 2.068876249068D+00 Y= 1.125137386288D+00 Z= 6.005825523903D+00
I= 13 X= -3.140334854314D+00 Y= -9.673158083067D-01 Z= 4.689897014228D+00
I= 14 X= -2.972798975354D+00 Y= -2.476110532384D+00 Z= 6.193384222331D+00
I= 15 X= -2.331460995979D+00 Y= 8.700656646267D-01 Z= 5.560487053516D+00
I= 16 X= -5.298648665943D+00 Y= -8.913737887588D-01 Z= 4.220571498244D+00
I= 17 X= -4.839581257223D+00 Y= -2.501135233749D+00 Z= -7.961842662654D-01
I= 18 X= -5.790510897943D+00 Y= -4.172595490410D+00 Z= -1.407711491685D-01
I= 19 X= -6.001476069708D+00 Y= -7.434536003301D-01 Z= 8.242593153933D-02
I= 20 X= -5.709148919027D+00 Y= -2.011995175010D+00 Z= -3.095258976225D+00
I= 21 X= -1.437138683570D-01 Y= -3.776412331742D+00 Z= -4.211474075933D+00
I= 22 X= -2.716420048359D-01 Y= -6.019629125847D+00 Z= -4.356494472456D+00
I= 23 X= -1.544858750850D+00 Y= -2.783258850245D+00 Z= -5.417712185009D+00
I= 24 X= 1.692260256264D+00 Y= -3.576392680379D+00 Z= -5.027629947384D+00
I= 25 X= 4.924616084076D+00 Y= -2.363063448190D+00 Z= -6.048172836602D-01
I= 26 X= 5.571865353172D+00 Y= -2.044416497720D+00 Z= -2.656167746820D+00
I= 27 X= 6.168121935996D+00 Y= -8.742356487282D-01 Z= 1.115024910720D-01
I= 28 X= 5.812785671048D+00 Y= -4.171362443758D+00 Z= 1.307612625999D-01

I= 29 X= 2.954974909682D+00 Y= 3.243591367703D+00 Z= -2.490993310780D+00
I= 30 X= 2.954304811628D+00 Y= 3.735204431766D+00 Z= 1.472851326543D-01
I= 31 X= 4.482124034479D+00 Y= 2.245548378704D+00 Z= -3.375019285422D+00
I= 32 X= 2.102654099187D+00 Y= 4.775093009051D+00 Z= -3.828325129477D+00
I= 33 X= 2.022216905876D+00 Y= 5.492072202943D+00 Z= 8.188469817219D-01
I= 34 X= 4.299442851306D+00 Y= 2.824214007196D+00 Z= 1.224068595953D+00
I= 35 X= 1.766507266949D-02 Y= 1.131063822284D+00 Z= -5.018874259895D-01
I= 36 X= -2.560299930060D+00 Y= 4.064842951222D+00 Z= 1.712059972689D-01
I= 37 X= -1.586905769560D+00 Y= 5.921828060115D+00 Z= 1.037495764603D+00
I= 38 X= -3.722324883089D+00 Y= 3.361577554936D+00 Z= 1.914937367028D+00

Forward Direction:

Total Energy: -692.0116960 Hartrees

Potential Energy: -692.1889925 Hartress

Kinetic Energy: 0.1772965 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.405758616696D+11 Y= 1.694429326928D+13 Z= 1.609729578694D+13
I= 1 X= 7.719230539144D+12 Y= 1.751639457438D+13 Z= -7.458821239807D+12
I= 2 X= 2.111107072996D+12 Y= -9.728082168717D+12 Z= -1.589152845415D+13
I= 3 X= -7.323001202074D+12 Y= 6.813068859231D+09 Z= 1.659383097969D+13
I= 4 X= -2.623301540234D+13 Y= -3.922343722975D+11 Z= -9.672959633404D+12
I= 5 X= -1.220082657097D+12 Y= 1.134193627182D+13 Z= 1.372659708142D+13
I= 6 X= 2.647352344783D+13 Y= 7.955501732930D+13 Z= 5.795257620355D+13
I= 7 X= -1.562876372970D+13 Y= -1.800143805299D+14 Z= 1.097944554433D+14
I= 8 X= -2.370254407930D+13 Y= -3.769146123778D+13 Z= -9.229107553858D+13
I= 9 X= 1.259954239367D+13 Y= -8.754345089679D+11 Z= 5.593683532878D+12
I= 10 X= 5.044789057568D+13 Y= -1.532910499925D+13 Z= -1.710181987051D+13
I= 11 X= 6.893746333141D+13 Y= -2.995405745660D+13 Z= 8.861085295952D+13
I= 12 X= -2.672196512812D+13 Y= 2.703867200868D+13 Z= -6.432553131579D+12
I= 13 X= -6.787311584690D+12 Y= 1.811076836133D+13 Z= 1.464790301424D+13
I= 14 X= 7.293904616889D+13 Y= -8.649062644545D+13 Z= -9.215869268484D+13

I= 15 X= -4.322567665798D+13 Y= -1.072512167584D+14 Z= -9.692322602398D+13
I= 16 X= -6.028878133753D+12 Y= 4.965809369232D+13 Z= -4.023598671250D+13
I= 17 X= -8.404778136464D+11 Y= -2.829555504794D+12 Z= 7.215539332971D+12
I= 18 X= 9.247269729182D+13 Y= 1.861937078807D+12 Z= -2.559355925273D+13
I= 19 X= 1.163121143691D+14 Y= -3.790660732988D+13 Z= -4.692829135916D+13
I= 20 X= 4.507445157684D+13 Y= 5.119015524472D+13 Z= 5.701925022920D+13
I= 21 X= -3.355541878107D+12 Y= -1.137860509248D+13 Z= -6.554888134806D+12
I= 22 X= 1.588612516274D+13 Y= -5.545664092845D+13 Z= -2.839887990194D+13
I= 23 X= -1.260326099648D+14 Y= 5.085210631364D+13 Z= -8.395164144951D+13
I= 24 X= -6.625856491972D+12 Y= 4.578327912344D+12 Z= -3.231041823829D+13
I= 25 X= 1.268018734523D+13 Y= -8.480830670581D+12 Z= 8.563342648399D+12
I= 26 X= 1.277115836502D+13 Y= 4.763991905371D+12 Z= -1.325629625495D+14
I= 27 X= -1.906118215420D+13 Y= -1.607389144589D+13 Z= -1.966447847961D+13
I= 28 X= 1.750776654877D+13 Y= -2.125271414832D+13 Z= 5.329250570552D+13
I= 29 X= 7.822841239115D+12 Y= 1.665313913221D+13 Z= 5.987174986981D+12
I= 30 X= 4.836314411859D+12 Y= -6.018744884757D+12 Z= -3.560715250719D+12
I= 31 X= 6.286838777937D+11 Y= -6.013333973881D+13 Z= 5.285809463508D+13
I= 32 X= 1.505959322188D+13 Y= 9.262190349987D+13 Z= -1.025418381438D+13
I= 33 X= -4.077610054829D+13 Y= -2.502395160821D+13 Z= -1.162122908862D+14
I= 34 X= -1.085356003563D+14 Y= 3.746155433839D+13 Z= -1.294532118471D+13
I= 35 X= -6.207623504999D+11 Y= -1.077736381267D+12 Z= -3.526603244540D+12
I= 36 X= -6.054276094642D+12 Y= -3.664719362167D+12 Z= 3.305390429605D+12
I= 37 X= -3.565691355296D+13 Y= -8.281125662310D+13 Z= 3.653573905709D+13
I= 38 X= -5.685210952748D+12 Y= -2.416640630043D+13 Z= 2.554745977996D+13

Backward Direction:

Total Energy: -692.0116760 Hartrees

Potential Energy: -692.1889925 Hartress

Kinetic Energy: 0.1773165 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.073054732853D+11 Y= 1.799817148827D+13 Z= 1.772430606475D+13

I= 1 X= 8.262558402102D+12 Y= 1.751661685526D+13 Z= -7.458943895549D+12
I= 2 X= 2.601222006813D+12 Y= -1.016200652058D+13 Z= -1.502945178408D+13
I= 3 X= -7.256138540700D+12 Y= -1.047161926229D+12 Z= 1.496660316608D+13
I= 4 X= -2.574281163857D+13 Y= 4.179244150539D+10 Z= -1.053500984924D+13
I= 5 X= 3.910335005573D+11 Y= 4.274158342017D+12 Z= 5.558387653751D+12
I= 6 X= -3.826646869662D+13 Y= 7.956533770468D+13 Z= 5.795276474136D+13
I= 7 X= -2.578497166858D+13 Y= -1.826445433418D+14 Z= 9.947865523277D+13
I= 8 X= -2.844913062682D+13 Y= -4.172857453828D+13 Z= -9.454858307754D+13
I= 9 X= 1.385491946332D+13 Y= -3.148313294780D+12 Z= 4.932483627851D+12
I= 10 X= 4.973830651067D+13 Y= -1.818217769968D+13 Z= -1.855463506835D+13
I= 11 X= 7.054889257684D+13 Y= -3.437219237017D+13 Z= 8.818821265951D+13
I= 12 X= -2.362584588795D+13 Y= 2.496467554982D+13 Z= -6.224445786786D+12
I= 13 X= -5.532048859754D+12 Y= 2.038367003894D+13 Z= 1.530945346404D+13
I= 14 X= 7.223042740911D+13 Y= -8.363721667032D+13 Z= -9.070533565883D+13
I= 15 X= -4.013018631433D+13 Y= -1.051762754377D+14 Z= -9.713147580428D+13
I= 16 X= -4.418026262740D+12 Y= 5.407493656320D+13 Z= -3.981247477839D+13
I= 17 X= -9.979704725977D+11 Y= -2.751990645568D+12 Z= 9.599816778683D+12
I= 18 X= 9.281460141984D+13 Y= 2.894361556282D+12 Z= -2.067232821745D+13
I= 19 X= 1.160973685051D+14 Y= -3.719113829059D+13 Z= -4.597721731116D+13
I= 20 X= 4.426873345407D+13 Y= 4.832777272747D+13 Z= 5.965990154079D+13
I= 21 X= -5.488589213389D+12 Y= -1.137754204109D+13 Z= -6.555602091853D+12
I= 22 X= 1.039347656115D+13 Y= -5.545552544088D+13 Z= -2.840087412365D+13
I= 23 X= -1.273994058430D+14 Y= 5.344013137791D+13 Z= -8.379696787256D+13
I= 24 X= -7.992949263824D+12 Y= 1.993279346239D+12 Z= -3.246613160688D+13
I= 25 X= 1.252293795897D+13 Y= -8.558846641809D+12 Z= 6.178999485426D+12
I= 26 X= 1.196593706440D+13 Y= 7.625621486574D+12 Z= -1.352038402426D+14
I= 27 X= -1.927555907226D+13 Y= -1.679032642927D+13 Z= -2.061526176954D+13
I= 28 X= 1.784971783602D+13 Y= -2.228586036450D+13 Z= 4.837148134066D+13
I= 29 X= 9.433561053535D+12 Y= 2.371869815800D+13 Z= 1.415340836446D+13
I= 30 X= 7.612597066282D+12 Y= -5.514045230886D+12 Z= 2.960680280371D+12

I= 31 X= -4.115196970605D+12 Y= -5.609696741490D+13 Z= 5.511393830277D+13
I= 32 X= 4.904927605659D+12 Y= 9.525212398626D+13 Z= 5.809319411753D+10
I= 33 X= -4.193457896778D+13 Y= -2.925927449577D+13 Z= -1.025727017445D+14
I= 34 X= -1.078736281178D+14 Y= 3.290274798762D+13 Z= -7.814908208631D+12
I= 35 X= -1.096766562117D+12 Y= -1.077487484566D+12 Z= -3.525832036822D+12
I= 36 X= -3.277850267453D+12 Y= -4.170311517857D+12 Z= -3.216402432018D+12
I= 37 X= -3.681767154038D+13 Y= -7.857332829949D+13 Z= 2.289462071471D+13
I= 38 X= -5.022719247299D+12 Y= -1.960926432027D+13 Z= 2.041707425305D+13

Seed: 36800429431

CM Start Point Coordinates: bohr

I= 0 X= -2.071751979146D+00 Y= -1.981977912764D+00 Z= 2.708274603604D-02
I= 1 X= 6.920647090179D-02 Y= -2.813249448377D+00 Z= -1.474854716689D+00
I= 2 X= -1.327662816506D+00 Y= -1.371958522491D+00 Z= 2.484453365608D+00
I= 3 X= 2.163309989131D+00 Y= -2.190628256031D+00 Z= 9.000596356728D-02
I= 4 X= 1.359630306848D+00 Y= -1.258295270183D+00 Z= 2.502692967862D+00
I= 5 X= -2.882184303792D+00 Y= 3.044064345675D+00 Z= -2.115063653659D+00
I= 6 X= -3.193693302139D-01 Y= 1.548463105614D+00 Z= -3.363274068282D+00
I= 7 X= -2.701147936270D+00 Y= 4.553541689796D+00 Z= -3.657965546191D+00
I= 8 X= -4.279988268300D+00 Y= 1.868605513460D+00 Z= -2.951088645532D+00
I= 9 X= 2.820328953756D+00 Y= -6.044867542481D-01 Z= 4.663834346361D+00
I= 10 X= 2.538429579732D+00 Y= -2.380817327226D+00 Z= 6.097887535650D+00
I= 11 X= 5.073451483137D+00 Y= -2.840683732775D-01 Z= 4.353379493010D+00
I= 12 X= 2.139638266630D+00 Y= 1.084515717637D+00 Z= 5.361163986961D+00
I= 13 X= -2.777240155804D+00 Y= -5.042466839185D-01 Z= 4.677679425686D+00
I= 14 X= -2.969608064765D+00 Y= -2.320766209365D+00 Z= 5.796636542838D+00
I= 15 X= -1.828128369044D+00 Y= 1.062935838755D+00 Z= 5.781120605701D+00
I= 16 X= -4.718055258249D+00 Y= -3.663621635131D-01 Z= 3.754018231308D+00
I= 17 X= -4.834735032627D+00 Y= -2.340591992607D+00 Z= -1.012656413201D+00
I= 18 X= -5.782573087002D+00 Y= -4.128050859842D+00 Z= -9.387555720635D-01

I= 19 X= -5.886679132034D+00 Y= -9.395373311689D-01 Z= -4.588629805861D-01
I= 20 X= -5.095709236269D+00 Y= -1.734382828230D+00 Z= -3.287754961157D+00
I= 21 X= 2.166183680830D-01 Y= -3.589197010640D+00 Z= -4.137899225652D+00
I= 22 X= 5.175525272731D-01 Y= -5.409386153631D+00 Z= -3.954922248267D+00
I= 23 X= -1.587983235922D+00 Y= -3.168377802680D+00 Z= -5.229825434567D+00
I= 24 X= 1.640588613646D+00 Y= -2.421788720056D+00 Z= -5.186611528301D+00
I= 25 X= 4.905084432979D+00 Y= -2.536477961876D+00 Z= -6.857645234941D-01
I= 26 X= 5.114818930106D+00 Y= -2.275001136636D+00 Z= -2.713874230982D+00
I= 27 X= 5.819049166187D+00 Y= -1.040943435571D+00 Z= 5.556244993886D-01
I= 28 X= 5.287975601204D+00 Y= -4.476271305986D+00 Z= -4.296658138666D-01
I= 29 X= 2.370741229464D+00 Y= 3.399570124206D+00 Z= -2.597480881051D+00
I= 30 X= 2.679951596963D+00 Y= 3.255358599857D+00 Z= 1.525899078298D-01
I= 31 X= 3.812242900924D+00 Y= 1.854549879062D+00 Z= -3.844836353389D+00
I= 32 X= 1.354055344277D+00 Y= 4.905238069189D+00 Z= -3.603245819950D+00
I= 33 X= 2.218628111316D+00 Y= 4.852377154700D+00 Z= 1.424852594739D+00
I= 34 X= 4.349849304568D+00 Y= 2.391828102729D+00 Z= 9.368838545450D-01
I= 35 X= -4.784508482724D-03 Y= 1.097242972070D+00 Z= -5.113824852875D-01
I= 36 X= -2.581036405451D+00 Y= 3.898186151255D+00 Z= 2.242850172130D-01
I= 37 X= -1.758871356654D+00 Y= 5.808747782552D+00 Z= 7.209981341170D-01
I= 38 X= -3.971244156628D+00 Y= 3.458956357755D+00 Z= 1.415453439433D+00

Forward Direction:

Total Energy: -692.0061031 Hartrees

Potential Energy: -692.1709785 Hartress

Kinetic Energy: 0.1648754 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.872597129201D+13 Y= -1.181164529755D+12 Z= 6.478413263110D+12

I= 1 X= 1.018737390221D+13 Y= -2.719536502357D+13 Z= -1.001097128973D+13

I= 2 X= 1.531478734573D+13 Y= 3.341392520965D+12 Z= 6.662919714818D+12

I= 3 X= -6.609877487256D+12 Y= 1.771226433533D+13 Z= -2.268683750836D+13

I= 4 X= -7.960021902411D+12 Y= 1.095002749624D+13 Z= -9.448762903796D+12

I= 5 X= 1.246596911806D+13 Y= -2.835342756184D+12 Z= -3.788496299496D+12
I= 6 X= 2.078663470183D+13 Y= 4.385278279799D+12 Z= -8.314358619294D+13
I= 7 X= 5.507366841129D+13 Y= 3.238582227601D+13 Z= -2.167348726799D+11
I= 8 X= -1.094246235279D+14 Y= -6.204933482402D+13 Z= 4.414667076792D+13
I= 9 X= -7.740345443400D+12 Y= 2.383494793695D+12 Z= 1.526345223785D+13
I= 10 X= 6.081983493942D+13 Y= -5.708701861152D+13 Z= 3.204099371429D+13
I= 11 X= 4.251888272183D+13 Y= -3.866215203208D+13 Z= -1.969755951215D+13
I= 12 X= -4.864872205855D+13 Y= 8.241409579503D+12 Z= -2.731715783142D+13
I= 13 X= 8.419366105965D+12 Y= 9.778582131234D+12 Z= -1.115943257641D+13
I= 14 X= -3.659862619404D+13 Y= -9.589518458461D+13 Z= 1.070171774608D+13
I= 15 X= -8.029136029489D+13 Y= -1.360038849730D+14 Z= -1.361626969619D+13
I= 16 X= 2.285371101700D+13 Y= 9.604711742608D+12 Z= -2.300564185254D+13
I= 17 X= 1.630479633280D+12 Y= 2.267760220299D+13 Z= 3.093260128811D+12
I= 18 X= -4.867491222115D+13 Y= 9.810550713746D+12 Z= -1.543228554193D+13
I= 19 X= 5.733786532440D+13 Y= -1.481178119929D+14 Z= -3.851392581752D+13
I= 20 X= 8.865093668041D+12 Y= 2.561764934092D+13 Z= 5.196729006327D+13
I= 21 X= 3.106283012528D+13 Y= -1.001113955748D+12 Z= -5.219504130657D+12
I= 22 X= -5.311641022576D+13 Y= 8.447322742782D+13 Z= 1.672777353153D+13
I= 23 X= -2.150925051923D+13 Y= 6.438774695577D+12 Z= -3.281922637148D+13
I= 24 X= -4.508210095728D+13 Y= 1.263694123812D+13 Z= -3.778979013024D+12
I= 25 X= -1.565413567903D+13 Y= 8.964449672898D+12 Z= 7.592566148371D+12
I= 26 X= -4.458819659391D+13 Y= -6.106986676524D+13 Z= 3.868583941940D+13
I= 27 X= 1.005005650825D+14 Y= 2.998288395828D+13 Z= 8.536657835480D+13
I= 28 X= 1.131240492389D+14 Y= -3.941235024309D+13 Z= -5.433111751584D+12
I= 29 X= 3.019945894026D+11 Y= 5.438829096175D+12 Z= 1.215118282232D+13
I= 30 X= -1.441415274315D+13 Y= 5.579538686280D+12 Z= -3.253515708188D+12
I= 31 X= -2.793449865191D+13 Y= 2.602891704313D+13 Z= -2.619546495500D+12
I= 32 X= 8.025396968334D+12 Y= 4.915346975287D+13 Z= 3.462432530434D+13
I= 33 X= 3.529469707737D+13 Y= -1.139066336296D+13 Z= -1.587550970845D+14
I= 34 X= -2.374823190825D+13 Y= -2.532214913815D+13 Z= 3.412896714794D+13

I= 35 X= -8.007199301565D+11 Y= -3.527009863254D+12 Z= 3.715160276982D+12
I= 36 X= -5.282662371031D+12 Y= 4.673309643068D+12 Z= -1.023830452819D+13
I= 37 X= 4.845821637883D+13 Y= -1.873303903856D+12 Z= 3.990382807810D+13
I= 38 X= -2.288758439948D+13 Y= -1.215460600984D+14 Z= 1.112885259531D+14

Backward Direction:

Total Energy: -692.0061304 Hartrees

Potential Energy: -692.1709785 Hartress

Kinetic Energy: 0.1648482 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.871599462691D+13 Y= -6.237099116683D+11 Z= 7.412913330245D+12
I= 1 X= 1.031966729083D+13 Y= -2.719522746240D+13 Z= -1.001105396119D+13
I= 2 X= 1.567755051296D+13 Y= 3.249363416275D+12 Z= 7.134942554700D+12
I= 3 X= -6.599815350977D+12 Y= 1.715476370259D+13 Z= -2.362145946241D+13
I= 4 X= -7.597203015602D+12 Y= 1.104211657165D+13 Z= -9.920749814687D+12
I= 5 X= 1.306372961879D+13 Y= -7.201169762618D+12 Z= -8.611366388071D+12
I= 6 X= -9.173408345540D+12 Y= 4.390803567183D+12 Z= -8.314332212423D+13
I= 7 X= 4.964551194208D+13 Y= 2.964040922017D+13 Z= -6.798154363322D+12
I= 8 X= -1.116170100913D+14 Y= -6.563634208096D+13 Z= 4.283782712067D+13
I= 9 X= -6.900692880501D+12 Y= 8.731500416611D+11 Z= 1.488047023840D+13
I= 10 X= 6.044141052488D+13 Y= -5.892389231484D+13 Z= 3.120588422976D+13
I= 11 X= 4.357597730944D+13 Y= -4.152724996011D+13 Z= -1.995859833965D+13
I= 12 X= -4.664917600204D+13 Y= 6.884057496598D+12 Z= -2.720314439591D+13
I= 13 X= 9.258953278121D+12 Y= 1.128894157963D+13 Z= -1.077621243216D+13
I= 14 X= -3.697639694113D+13 Y= -9.405807732874D+13 Z= 1.153721039700D+13
I= 15 X= -7.829221783559D+13 Y= -1.346459205071D+14 Z= -1.373037731645D+13
I= 16 X= 2.391043853933D+13 Y= 1.246896992424D+13 Z= -2.274403338735D+13
I= 17 X= 1.478082016395D+12 Y= 2.268698175776D+13 Z= 4.644718737299D+12
I= 18 X= -4.856523947328D+13 Y= 1.049881042508D+13 Z= -1.215675156862D+13
I= 19 X= 5.723479935497D+13 Y= -1.476046060837D+14 Z= -3.793315814874D+13
I= 20 X= 8.256334429508D+12 Y= 2.367695520621D+13 Z= 5.369378852052D+13

I= 21 X= 2.963029202494D+13 Y= -1.000436356635D+12 Z= -5.219958899867D+12
I= 22 X= -5.678879598302D+13 Y= 8.447394356809D+13 Z= 1.672651106957D+13
I= 23 X= -2.238739923656D+13 Y= 8.182903412770D+12 Z= -3.277493738359D+13
I= 24 X= -4.596042127556D+13 Y= 1.089468018299D+13 Z= -3.823882509836D+12
I= 25 X= -1.580636068260D+13 Y= 8.954763145800D+12 Z= 6.041057561747D+12
I= 26 X= -4.519663879748D+13 Y= -5.912960452826D+13 Z= 3.695917193154D+13
I= 27 X= 1.003977658065D+14 Y= 2.946901581870D+13 Z= 8.478602535691D+13
I= 28 X= 1.132337958833D+14 Y= -4.010112023233D+13 Z= -8.708594846357D+12
I= 29 X= 8.994833798114D+11 Y= 9.803336265469D+12 Z= 1.697279410590D+13
I= 30 X= -1.308279113260D+13 Y= 5.594933845073D+12 Z= 1.028102921772D+12
I= 31 X= -3.012576717589D+13 Y= 2.961493991176D+13 Z= -1.311871373989D+12
I= 32 X= 2.598370295721D+12 Y= 5.189910831226D+13 Z= 4.120363542748D+13
I= 33 X= 3.458327118878D+13 Y= -1.413129087333D+13 Z= -1.500434300497D+14
I= 34 X= -2.314460669348D+13 Y= -2.817946608923D+13 Z= 3.712054059968D+13
I= 35 X= -9.547614348137D+11 Y= -3.526845785597D+12 Z= 3.715641413632D+12
I= 36 X= -3.951298839314D+12 Y= 4.657378555349D+12 Z= -1.452019152738D+13
I= 37 X= 4.774524203519D+13 Y= 8.689139955517D+11 Z= 3.119136964295D+13
I= 38 X= -2.228382801385D+13 Y= -1.186899758455D+14 Z= 1.082969108269D+14

Seed: 37466053161

CM Start Point Coordinates: bohr

I= 0 X= -2.182133233745D+00 Y= -2.014413284839D+00 Z= 2.217884946352D-02
I= 1 X= 2.013163361564D-02 Y= -2.550883584280D+00 Z= -1.510869240121D+00
I= 2 X= -1.309538511151D+00 Y= -1.130040086021D+00 Z= 2.465524604124D+00
I= 3 X= 2.196085469610D+00 Y= -2.166504062035D+00 Z= -7.870541950302D-02
I= 4 X= 1.386895743975D+00 Y= -1.315920961035D+00 Z= 2.451565946077D+00
I= 5 X= -2.727247467464D+00 Y= 3.337311238274D+00 Z= -2.418728469990D+00
I= 6 X= 2.181270134073D-01 Y= 1.335400406527D+00 Z= -3.562045288527D+00
I= 7 X= -1.884051650796D+00 Y= 5.104623933290D+00 Z= -3.400260763392D+00
I= 8 X= -4.194564897749D+00 Y= 1.906377668305D+00 Z= -3.403020597536D+00

I= 9 X= 3.046824007611D+00 Y= -5.374945857320D-01 Z= 4.560593659618D+00
I= 10 X= 2.330080939566D+00 Y= -1.679264650366D+00 Z= 6.635030062928D+00
I= 11 X= 5.249988948842D+00 Y= -1.370878210004D+00 Z= 4.112816892681D+00
I= 12 X= 2.928812785800D+00 Y= 1.903876195855D+00 Z= 4.770975907181D+00
I= 13 X= -2.894132314524D+00 Y= -5.417745535303D-01 Z= 4.681856592244D+00
I= 14 X= -2.803239972721D+00 Y= -2.059458318101D+00 Z= 6.367615186784D+00
I= 15 X= -2.495329457930D+00 Y= 1.000410193289D+00 Z= 5.743028121072D+00
I= 16 X= -5.099044855593D+00 Y= -4.078894438582D-01 Z= 4.448281954367D+00
I= 17 X= -4.947198301713D+00 Y= -2.421156402330D+00 Z= -7.493723525847D-01
I= 18 X= -5.480639032860D+00 Y= -4.422466250019D+00 Z= -1.256297042863D-01
I= 19 X= -6.087227964006D+00 Y= -9.638286604323D-01 Z= -1.100146953522D-01
I= 20 X= -5.194804688785D+00 Y= -2.185151237280D+00 Z= -2.847266681560D+00
I= 21 X= -1.946520765537D-02 Y= -3.800476304163D+00 Z= -4.196578701296D+00
I= 22 X= 3.075525908580D-01 Y= -5.912935806701D+00 Z= -4.007489671515D+00
I= 23 X= -2.123422752722D+00 Y= -3.763158822029D+00 Z= -4.564339194669D+00
I= 24 X= 1.006287364582D+00 Y= -2.746398659752D+00 Z= -5.818108115950D+00
I= 25 X= 4.963429919968D+00 Y= -2.790660260342D+00 Z= -9.655864662389D-01
I= 26 X= 4.700272717807D+00 Y= -2.508161642248D+00 Z= -3.358116806190D+00
I= 27 X= 6.272058960056D+00 Y= -1.354828745117D+00 Z= -2.142672992890D-01
I= 28 X= 5.567253866471D+00 Y= -4.855468065148D+00 Z= -4.375809796566D-01
I= 29 X= 3.141318295904D+00 Y= 3.171242643554D+00 Z= -2.071380856724D+00
I= 30 X= 2.381699331746D+00 Y= 4.066330841513D+00 Z= 4.790713285995D-01
I= 31 X= 4.836208432836D+00 Y= 1.696733422917D+00 Z= -2.301880430921D+00
I= 32 X= 2.814078391515D+00 Y= 3.984819797627D+00 Z= -3.986324567152D+00
I= 33 X= 9.355999435715D-01 Y= 5.414249432620D+00 Z= 1.009386177163D+00
I= 34 X= 3.499454279792D+00 Y= 3.487487924034D+00 Z= 2.121768073741D+00
I= 35 X= 2.795594305048D-02 Y= 1.092833394355D+00 Z= -6.016496479729D-01
I= 36 X= -3.046829095604D+00 Y= 3.407948370748D+00 Z= 3.187809253018D-01
I= 37 X= -2.411012605107D+00 Y= 5.060741609400D+00 Z= 1.253219321363D+00
I= 38 X= -4.644345983202D+00 Y= 2.376395646397D+00 Z= 1.274285547492D+00

Forward Direction:

Total Energy: -691.9985512 Hartrees

Potential Energy: -692.1758557 Hartress

Kinetic Energy: 0.1773045 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.951160610920D+12 Y= 1.145492475136D+13 Z= 9.871206494998D+12
I= 1 X= -1.255637902752D+13 Y= 1.005201826624D+13 Z= 7.825561681022D+12
I= 2 X= 8.324900054382D+12 Y= -3.303117743712D+12 Z= 2.359451322907D+12
I= 3 X= 2.087172030280D+13 Y= -2.265584851264D+12 Z= -7.057289634989D+12
I= 4 X= -2.048874171226D+13 Y= -6.783919012713D+12 Z= -2.563818292916D+13
I= 5 X= -7.624444511952D+12 Y= 6.864986717841D+12 Z= -3.861707119308D+11
I= 6 X= 5.226970472751D+13 Y= -6.943996439643D+13 Z= -4.252698430268D+13
I= 7 X= -4.632770652219D+13 Y= -1.347389592255D+12 Z= 1.029550508248D+13
I= 8 X= -1.015170839062D+14 Y= 4.107644078679D+13 Z= -6.470140172648D+13
I= 9 X= 4.938314836405D+12 Y= 1.101013710548D+13 Z= 1.757945963452D+13
I= 10 X= -5.515547467539D+13 Y= 2.497971939394D+13 Z= -2.550977801669D+13
I= 11 X= -2.170882503899D+13 Y= -6.990634131229D+13 Z= 7.007715797228D+12
I= 12 X= 4.174152591879D+13 Y= -5.107813133518D+13 Z= 6.051930205599D+13
I= 13 X= 7.969687366513D+12 Y= -4.623616123425D+12 Z= 7.565696528820D+12
I= 14 X= 5.428910877095D+13 Y= 6.596521604386D+13 Z= -5.400744575365D+13
I= 15 X= 1.228677369043D+13 Y= -2.562172100676D+13 Z= 7.853854003338D+13
I= 16 X= -1.089891046369D+14 Y= 1.001066914042D+14 Z= -8.189797378129D+13
I= 17 X= 9.529413641594D+12 Y= 3.340248988771D+12 Z= 1.369794277474D+13
I= 18 X= -8.588473171935D+13 Y= -1.386500571801D+13 Z= 2.810218856691D+13
I= 19 X= 3.903927185282D+13 Y= 2.294452219604D+13 Z= -8.936686004379D+13
I= 20 X= -8.707313889686D+13 Y= 3.494302403134D+13 Z= -9.395827691249D+13
I= 21 X= -1.092881131603D+13 Y= 1.339051202199D+13 Z= 4.161988508912D+12
I= 22 X= 8.307137488540D+13 Y= -6.216424813624D+13 Z= 5.561023856641D+13
I= 23 X= -4.522946210655D+13 Y= 3.408246823912D+13 Z= -1.056540334478D+14
I= 24 X= -3.221245208479D+13 Y= -5.500180264727D+13 Z= -8.530344278546D+13

I= 25 X= 7.449863566654D+12 Y= -1.135370452910D+13 Z= -5.581999786881D+12
I= 26 X= 5.295306895960D+13 Y= -8.883862637200D+13 Z= 8.502891502372D+13
I= 27 X= -2.615421652901D+13 Y= 8.988078789610D+13 Z= 3.683290731566D+13
I= 28 X= -5.479142760191D+13 Y= 9.634401849110D+13 Z= -7.088914052168D+13
I= 29 X= 2.637280877225D+12 Y= -2.819285890251D+13 Z= -1.939371934310D+12
I= 30 X= -1.457411837186D+13 Y= 1.460626759950D+13 Z= -4.018573649998D+12
I= 31 X= 2.448464760014D+13 Y= -5.085144056956D+13 Z= 2.203472176064D+13
I= 32 X= 6.499783287803D+12 Y= 7.844002426643D+13 Z= -1.372996330659D+13
I= 33 X= 5.437340695051D+13 Y= -1.734762230023D+14 Z= -3.848519497004D+13
I= 34 X= 2.294213722273D+13 Y= 4.179145185499D+13 Z= -1.346246219278D+13
I= 35 X= 4.944680287621D+12 Y= -7.792967207655D+11 Z= 8.934628693457D+11
I= 36 X= -1.064865116805D+13 Y= -9.349142735428D+12 Z= 7.624420744470D+12
I= 37 X= 4.447818682493D+13 Y= 2.019604582900D+13 Z= 4.927063206163D+13
I= 38 X= 3.212510568998D+13 Y= -1.303857274028D+12 Z= -1.633474405734D+13

Backward Direction:

Total Energy: -691.9985289 Hartrees

Potential Energy: -692.1758557 Hartress

Kinetic Energy: 0.1773267 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.035310366601D+12 Y= 1.297482423708D+13 Z= 1.225294587774D+13
I= 1 X= -1.184683661894D+13 Y= 1.005234837731D+13 Z= 7.825376285033D+12
I= 2 X= 9.081157790688D+12 Y= -3.863283234797D+12 Z= 3.610384185282D+12
I= 3 X= 2.095606915631D+13 Y= -3.785621417768D+12 Z= -9.439346028779D+12
I= 4 X= -1.973235169485D+13 Y= -6.223602987214D+12 Z= -2.688906720827D+13
I= 5 X= -5.422367075326D+12 Y= -3.627592881674D+12 Z= -1.240609888994D+13
I= 6 X= -3.905273413762D+13 Y= -6.942504869246D+13 Z= -4.252663393695D+13
I= 7 X= -6.100167549933D+13 Y= -5.787057919127D+12 Z= -5.118873791937D+12
I= 8 X= -1.082106220627D+14 Y= 3.456118595339D+13 Z= -6.801193764251D+13
I= 9 X= 6.832650026247D+12 Y= 7.585121508088D+12 Z= 1.661001286037D+13
I= 10 X= -5.618030754294D+13 Y= 2.070857814204D+13 Z= -2.763683329352D+13

I= 11 X= -1.928709785161D+13 Y= -7.653026551187D+13 Z= 6.380292726620D+12
I= 12 X= 4.637947226374D+13 Y= -5.419350414708D+13 Z= 6.082131170234D+13
I= 13 X= 9.863855330128D+12 Y= -1.198566294999D+12 Z= 8.535674011930D+12
I= 14 X= 5.326573639327D+13 Y= 7.023686985720D+13 Z= -5.187956304130D+13
I= 15 X= 1.692377923730D+13 Y= -2.250493170048D+13 Z= 7.823631599413D+13
I= 16 X= -1.065682396192D+14 Y= 1.067286775965D+14 Z= -8.126924180673D+13
I= 17 X= 9.269295545640D+12 Y= 3.437004146586D+12 Z= 1.727511448940D+13
I= 18 X= -8.542561826408D+13 Y= -1.230818504971D+13 Z= 3.552057188371D+13
I= 19 X= 3.873459025001D+13 Y= 2.404069884190D+13 Z= -8.795813555541D+13
I= 20 X= -8.832229833311D+13 Y= 3.061124515662D+13 Z= -8.999254100970D+13
I= 21 X= -1.415032836622D+13 Y= 1.339210017582D+13 Z= 4.160922015564D+12
I= 22 X= 7.478373596550D+13 Y= -6.216257920305D+13 Z= 5.560726340122D+13
I= 23 X= -4.727472773700D+13 Y= 3.799401203446D+13 Z= -1.054488781747D+14
I= 24 X= -3.425815283295D+13 Y= -5.890891382230D+13 Z= -8.551012846927D+13
I= 25 X= 7.190117304075D+12 Y= -1.145114296644D+13 Z= -9.159273460564D+12
I= 26 X= 5.170465202729D+13 Y= -8.450794933414D+13 Z= 8.106282906487D+13
I= 27 X= -2.645833172231D+13 Y= 8.878314629673D+13 Z= 3.542463150007D+13
I= 28 X= -5.433222284394D+13 Y= 9.478609600187D+13 Z= -7.830725382668D+13
I= 29 X= 4.838757070850D+12 Y= -1.770354918069D+13 Z= 1.007760444382D+13
I= 30 X= -1.063565470535D+13 Y= 1.521404971547D+13 Z= 5.783784438152D+12
I= 31 X= 1.779486210146D+13 Y= -4.433753723101D+13 Z= 2.534272036638D+13
I= 32 X= -8.171811453632D+12 Y= 8.287986887315D+13 Z= 1.679217095572D+12
I= 33 X= 5.265556342970D+13 Y= -1.798232389981D+14 Z= -1.809962053416D+13
I= 34 X= 2.401783364884D+13 Y= 3.500388767413D+13 Z= -5.930775660027D+12
I= 35 X= 4.304849557141D+12 Y= -7.789222796210D+11 Z= 8.946100484095D+11
I= 36 X= -6.710016238979D+12 Y= -9.958242509022D+12 Z= -2.178538144953D+12
I= 37 X= 4.275689213118D+13 Y= 2.654692067980D+13 Z= 2.888286057530D+13
I= 38 X= 3.320148275820D+13 Y= 5.481138356995D+12 Z= -2.386641781696D+13

Seed: 37615231480

CM Start Point Coordinates: bohr

I= 0 X= -2.139770227204D+00 Y= -2.083195554137D+00 Z= 1.830496337602D-02
I= 1 X= -4.442104556224D-02 Y= -2.550833044415D+00 Z= -1.631242873833D+00
I= 2 X= -1.339540647267D+00 Y= -1.311606965107D+00 Z= 2.438457878326D+00
I= 3 X= 2.155864304185D+00 Y= -2.050392319424D+00 Z= -2.352255164723D-01
I= 4 X= 1.345189659860D+00 Y= -1.158014538622D+00 Z= 2.402808099685D+00
I= 5 X= -2.930341275538D+00 Y= 3.274596729253D+00 Z= -2.325620635568D+00
I= 6 X= 9.715967980364D-02 Y= 1.596376662845D+00 Z= -3.189050426562D+00
I= 7 X= -2.312875636545D+00 Y= 4.205809801431D+00 Z= -3.895197570709D+00
I= 8 X= -4.214491551975D+00 Y= 1.447649173864D+00 Z= -2.847184792063D+00
I= 9 X= 2.920357261538D+00 Y= -7.409207772740D-01 Z= 4.663366022327D+00
I= 10 X= 2.976873547468D+00 Y= -2.391987764030D+00 Z= 5.649844844989D+00
I= 11 X= 4.843604057386D+00 Y= -5.919461026949D-01 Z= 3.905166553487D+00
I= 12 X= 2.525575092162D+00 Y= 1.232887843321D+00 Z= 5.356311612326D+00
I= 13 X= -3.076707859469D+00 Y= -7.656846804878D-01 Z= 4.708664135820D+00
I= 14 X= -3.087232617493D+00 Y= -2.433551115859D+00 Z= 6.009049440836D+00
I= 15 X= -2.504411721922D+00 Y= 6.244719083264D-01 Z= 5.846302733834D+00
I= 16 X= -5.152876050734D+00 Y= -5.156603703757D-01 Z= 4.149040933176D+00
I= 17 X= -4.796293445955D+00 Y= -2.269142844453D+00 Z= -8.125358721085D-01
I= 18 X= -5.252509518119D+00 Y= -4.538572445607D+00 Z= -3.064885535870D-01
I= 19 X= -6.343129484842D+00 Y= -1.167282809234D+00 Z= 2.730927088770D-01
I= 20 X= -5.094290762205D+00 Y= -1.947995387313D+00 Z= -2.925946343058D+00
I= 21 X= 3.704716041210D-02 Y= -4.041915614338D+00 Z= -3.905881900738D+00
I= 22 X= 4.380062570716D-01 Y= -6.041383131418D+00 Z= -2.749405509507D+00
I= 23 X= -2.143481848664D+00 Y= -4.069763835548D+00 Z= -5.043112943956D+00
I= 24 X= 1.255753721412D+00 Y= -2.999223039049D+00 Z= -5.620110834193D+00
I= 25 X= 4.871671382907D+00 Y= -2.434296600893D+00 Z= -8.491888698054D-01
I= 26 X= 5.308457000837D+00 Y= -2.234219601570D+00 Z= -3.010351132712D+00
I= 27 X= 5.961826496102D+00 Y= -1.466763510879D+00 Z= 4.974481447723D-01
I= 28 X= 5.407015416634D+00 Y= -4.482243015444D+00 Z= -6.551392387553D-01

I= 29 X= 3.181446598197D+00 Y= 3.320717506244D+00 Z= -2.302884953994D+00
I= 30 X= 2.758052634442D+00 Y= 3.818242424598D+00 Z= 2.482253773325D-01
I= 31 X= 4.500827057706D+00 Y= 2.199238503709D+00 Z= -3.101577208924D+00
I= 32 X= 2.464924315764D+00 Y= 4.661601673220D+00 Z= -3.535273839114D+00
I= 33 X= 1.948012050280D+00 Y= 5.805586213711D+00 Z= 6.985262581698D-01
I= 34 X= 4.217828228042D+00 Y= 3.026829704897D+00 Z= 1.781774025676D+00
I= 35 X= -1.564587655760D-02 Y= 1.101105247406D+00 Z= -5.529750389811D-01
I= 36 X= -2.823587553196D+00 Y= 3.721892649529D+00 Z= 3.158146952563D-01
I= 37 X= -2.073238170083D+00 Y= 5.550481600954D+00 Z= 7.292879878899D-01
I= 38 X= -4.268942219444D+00 Y= 2.897421571688D+00 Z= 1.776469956209D+00

Forward Direction:

Total Energy: -692.0073253 Hartrees

Potential Energy: -692.1786049 Hartress

Kinetic Energy: 0.1712796 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.423002766893D+12 Y= 1.197368369363D+13 Z= 3.949955954748D+12
I= 1 X= 9.344732103953D+12 Y= 6.597813658929D+12 Z= 3.910453730827D+12
I= 2 X= -2.226753080913D+13 Y= -2.026511165375D+12 Z= -1.230752786910D+13
I= 3 X= -1.162974504859D+13 Y= 5.118563264167D+12 Z= -5.041429957669D+12
I= 4 X= 2.392818458880D+13 Y= -2.768215679263D+13 Z= 1.341464950455D+12
I= 5 X= 5.245333672382D+12 Y= -6.404397659019D+12 Z= 3.646988683998D+13
I= 6 X= 3.999388308941D+13 Y= -1.637924979048D+13 Z= 7.430595090564D+13
I= 7 X= -4.911549319996D+13 Y= 6.222491955226D+13 Z= -9.513971174959D+12
I= 8 X= 6.028123980695D+13 Y= 9.232292280039D+13 Z= 3.834010342610D+13
I= 9 X= -1.052163732816D+13 Y= -6.122388750327D+12 Z= -5.514855284935D+12
I= 10 X= -5.059375253669D+13 Y= -4.846782748460D+13 Z= 5.388665381315D+13
I= 11 X= 1.095736852619D+14 Y= 8.110792047372D+13 Z= -8.605538933424D+13
I= 12 X= 7.860202518122D+13 Y= -1.428868091863D+13 Z= 8.649588993760D+13
I= 13 X= -7.527473703992D+11 Y= -9.956104944417D+12 Z= -1.306670460065D+13
I= 14 X= -8.002348220892D+12 Y= 7.169687764329D+13 Z= -4.148372686625D+13

I= 15 X= -4.280369364037D+12 Y= 1.813782475908D+13 Z= 1.045845758559D+14
I= 16 X= -8.330202357670D+13 Y= 1.552188794732D+12 Z= 4.360065200173D+13
I= 17 X= 1.822160056971D+13 Y= -1.201615016346D+12 Z= 4.776873950064D+12
I= 18 X= 1.838793745050D+13 Y= -2.212588312993D+13 Z= 2.570990925137D+13
I= 19 X= 2.361661381629D+13 Y= 4.947053338993D+13 Z= -4.567518909570D+13
I= 20 X= 1.662066260611D+13 Y= -3.561821091085D+13 Z= -9.590938344474D+13
I= 21 X= -4.720177799016D+12 Y= 1.638988185910D+13 Z= -4.909930403988D+12
I= 22 X= -2.900131890946D+13 Y= -8.636704193643D+12 Z= -1.901099796925D+13
I= 23 X= -7.173784083660D+13 Y= -1.656178785114D+13 Z= -9.285479489348D+13
I= 24 X= -5.146430296151D+13 Y= 3.373569398693D+13 Z= 6.931832032657D+13
I= 25 X= 4.540364227729D+12 Y= 2.691799567491D+13 Z= -4.696734571131D+12
I= 26 X= -5.603063958060D+13 Y= 3.850777563667D+13 Z= -3.008390632766D+13
I= 27 X= -7.178934988086D+13 Y= 1.835225972406D+13 Z= -3.411017148390D+13
I= 28 X= -5.609081397228D+13 Y= -1.585836457689D+14 Z= 4.529089168948D+13
I= 29 X= 1.129348823396D+12 Y= -6.052285954075D+12 Z= -7.773603123882D+12
I= 30 X= -1.278041212079D+13 Y= -4.042810832940D+12 Z= 3.182854449374D+11
I= 31 X= 6.806242171834D+13 Y= -5.162782722613D+13 Z= -1.332564426182D+13
I= 32 X= -8.071163450135D+13 Y= 7.266333384615D+13 Z= -2.385516412511D+13
I= 33 X= 6.267697462069D+13 Y= 2.279537135231D+12 Z= -5.021362956299D+13
I= 34 X= 6.585330738376D+13 Y= -4.490067474118D+13 Z= 7.253371012996D+13
I= 35 X= 2.408911061658D+11 Y= -1.734686588982D+12 Z= 6.601930707487D+11
I= 36 X= -4.303441090705D+12 Y= 7.687490419615D+11 Z= 5.040135436755D+12
I= 37 X= -4.138508513772D+13 Y= -2.000692979062D+13 Z= -9.589988003644D+13
I= 38 X= 7.364046940401D+13 Y= -5.435985243411D+13 Z= -4.440267545739D+13

Backward Direction:

Total Energy: -692.0073444 Hartrees

Potential Energy: -692.1786049 Hartress

Kinetic Energy: 0.1712605 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.563503226675D+12 Y= 1.329380163399D+13 Z= 5.821924560266D+12

I= 1 X= 1.037394806281D+13 Y= 6.598047173159D+12 Z= 3.910340091943D+12
I= 2 X= -2.188626992759D+13 Y= -2.879113361479D+12 Z= -1.126368057049D+13
I= 3 X= -1.148911185421D+13 Y= 3.798312466809D+12 Z= -6.913655697249D+12
I= 4 X= 2.430953712575D+13 Y= -2.682943923611D+13 Z= 2.976015049758D+11
I= 5 X= 7.835392311000D+12 Y= -1.384773075968D+13 Z= 2.736707538938D+13
I= 6 X= -5.073170458464D+13 Y= -1.636647119056D+13 Z= 7.430581767248D+13
I= 7 X= -6.171163295690D+13 Y= 6.197410860531D+13 Z= -1.990755322648D+13
I= 8 X= 5.361997638093D+13 Y= 9.052860880237D+13 Z= 3.577014981537D+13
I= 9 X= -9.343847575274D+12 Y= -8.276954062605D+12 Z= -6.268386260735D+12
I= 10 X= -5.147566117464D+13 Y= -5.130503245198D+13 Z= 5.221659288256D+13
I= 11 X= 1.111320533408D+14 Y= 7.676066335827D+13 Z= -8.650055390476D+13
I= 12 X= 8.166700391164D+13 Y= -1.630154534727D+13 Z= 8.674772880672D+13
I= 13 X= 4.249101730802D+11 Y= -7.801516779334D+12 Z= -1.231285298908D+13
I= 14 X= -8.883369318866D+12 Y= 7.453438070014D+13 Z= -3.981320429311D+13
I= 15 X= -1.216018966977D+12 Y= 2.015161973171D+13 Z= 1.043326009867D+14
I= 16 X= -8.174424019648D+13 Y= 5.898178792523D+12 Z= 4.404666433207D+13
I= 17 X= 1.817961815040D+13 Y= -1.033317349181D+12 Z= 7.111014715471D+12
I= 18 X= 1.897620763993D+13 Y= -2.115215948406D+13 Z= 3.036296642650D+13
I= 19 X= 2.332395970686D+13 Y= 5.006385935988D+13 Z= -4.465847631207D+13
I= 20 X= 1.602176417155D+13 Y= -3.824478711562D+13 Z= -9.334272796061D+13
I= 21 X= -6.708222075383D+12 Y= 1.639095432900D+13 Z= -4.910651397456D+12
I= 22 X= -3.415752153318D+13 Y= -8.635590330200D+12 Z= -1.901302938784D+13
I= 23 X= -7.310113910004D+13 Y= -1.416325108652D+13 Z= -9.257669736947D+13
I= 24 X= -5.282794039254D+13 Y= 3.134022658065D+13 Z= 6.903906530570D+13
I= 25 X= 4.498587739394D+12 Y= 2.674928653466D+13 Z= -7.030923484328D+12
I= 26 X= -5.662903766655D+13 Y= 4.113348421058D+13 Z= -3.265073472868D+13
I= 27 X= -7.208170246716D+13 Y= 1.775806401317D+13 Z= -3.512665687296D+13
I= 28 X= -5.550259499468D+13 Y= -1.595579843875D+14 Z= 4.063822463540D+13
I= 29 X= 3.719050498029D+12 Y= 1.388596176086D+12 Z= 1.327213087799D+12
I= 30 X= -8.994445303484D+12 Y= -2.845153811412D+12 Z= 6.616863020592D+12

I= 31 X= 6.140525143380D+13 Y= -4.983310974563D+13 Z= -1.075712658942D+13
I= 32 X= -9.330654809316D+13 Y= 7.291377875985D+13 Z= -1.346544294957D+13
I= 33 X= 6.144755215380D+13 Y= -1.901145867746D+12 Z= -3.649297709344D+13
I= 34 X= 6.611277963439D+13 Y= -4.960888086093D+13 Z= 7.833576435053D+13
I= 35 X= -5.750655425909D+11 Y= -1.734447695375D+12 Z= 6.609945658667D+11
I= 36 X= -5.171290408749D+11 Y= -4.298824531703D+11 Z= -1.258809040656D+12
I= 37 X= -4.261659284724D+13 Y= -1.582346017956D+13 Z= -1.096224872892D+14
I= 38 X= 7.390091512909D+13 Y= -4.965293920679D+13 Z= -5.020456898982D+13

Seed: 40191278813

CM Start Point Coordinates: bohr

I= 0 X= -2.200000282609D+00 Y= -2.214892803029D+00 Z= 1.937639527669D-01
I= 1 X= -9.025134981508D-02 Y= -2.657085588766D+00 Z= -1.370330250423D+00
I= 2 X= -1.304552515561D+00 Y= -1.155206046386D+00 Z= 2.510736347496D+00
I= 3 X= 2.210272641321D+00 Y= -2.120016824077D+00 Z= -4.339832784433D-02
I= 4 X= 1.434437944493D+00 Y= -1.126599944380D+00 Z= 2.275807668810D+00
I= 5 X= -2.729064284813D+00 Y= 3.316764281681D+00 Z= -2.322820135158D+00
I= 6 X= 1.962636611115D-01 Y= 6.879199850286D-01 Z= -3.306080938573D+00
I= 7 X= -1.519518387450D+00 Y= 4.472235979264D+00 Z= -3.265840792612D+00
I= 8 X= -3.714614887486D+00 Y= 1.696450529200D+00 Z= -3.127209471894D+00
I= 9 X= 3.304092604452D+00 Y= -8.253854806403D-01 Z= 4.548940548885D+00
I= 10 X= 3.442752456789D+00 Y= -2.889731557076D+00 Z= 5.382054877612D+00
I= 11 X= 5.151770774518D+00 Y= -4.295071819108D-01 Z= 3.777881679678D+00
I= 12 X= 2.450805791163D+00 Y= 5.732530018860D-01 Z= 6.169493648225D+00
I= 13 X= -3.100106416037D+00 Y= -5.393911212062D-01 Z= 4.540695921770D+00
I= 14 X= -3.318221532888D+00 Y= -2.314293163169D+00 Z= 5.912071844685D+00
I= 15 X= -2.298232723754D+00 Y= 8.271515224685D-01 Z= 6.063860655319D+00
I= 16 X= -4.772141464762D+00 Y= 8.676407965236D-02 Z= 3.621415450329D+00
I= 17 X= -4.897714397141D+00 Y= -2.530123308176D+00 Z= -8.332129845059D-01
I= 18 X= -5.493427185931D+00 Y= -4.491875014814D+00 Z= 9.745876596603D-03

I= 19 X= -5.869192491344D+00 Y= -1.164910830766D+00 Z= 1.403331089415D-01
I= 20 X= -5.331928604350D+00 Y= -2.222547076170D+00 Z= -2.945409593149D+00
I= 21 X= -1.011350616390D-01 Y= -3.703958935129D+00 Z= -4.095745450357D+00
I= 22 X= -1.680978609582D-01 Y= -5.822889147096D+00 Z= -3.779009154496D+00
I= 23 X= -1.680345650070D+00 Y= -2.992579161073D+00 Z= -5.213992892233D+00
I= 24 X= 1.808404040866D+00 Y= -2.822456382967D+00 Z= -4.939134533513D+00
I= 25 X= 4.747847846799D+00 Y= -2.397268790476D+00 Z= -6.692741773942D-01
I= 26 X= 5.476042576002D+00 Y= -2.474730963702D+00 Z= -2.784735888726D+00
I= 27 X= 5.980945590600D+00 Y= -1.121345484063D+00 Z= 1.719591669506D-01
I= 28 X= 5.322108342844D+00 Y= -4.264650809774D+00 Z= -3.605376581965D-01
I= 29 X= 3.264359076361D+00 Y= 3.303744832054D+00 Z= -2.145843022643D+00
I= 30 X= 2.631824737049D+00 Y= 3.995488352970D+00 Z= 2.723628300157D-01
I= 31 X= 4.625281242820D+00 Y= 1.669384310875D+00 Z= -2.644413150203D+00
I= 32 X= 2.290453861308D+00 Y= 4.495745111488D+00 Z= -3.538067486549D+00
I= 33 X= 1.675830136140D+00 Y= 5.946204046751D+00 Z= 5.815914783922D-01
I= 34 X= 3.537674431373D+00 Y= 3.343389961760D+00 Z= 1.817679811408D+00
I= 35 X= -6.523465610346D-02 Y= 1.039384162311D+00 Z= -6.582176479431D-01
I= 36 X= -2.947035723466D+00 Y= 3.643581876809D+00 Z= 3.631276279644D-01
I= 37 X= -2.242254583028D+00 Y= 5.453066339789D+00 Z= 9.258749917588D-01
I= 38 X= -4.390643281607D+00 Y= 2.638687398032D+00 Z= 1.422890021191D+00

Forward Direction:

Total Energy: -692.0054759 Hartrees

Potential Energy: -692.2122426 Hartress

Kinetic Energy: 0.2067667 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.292706256414D+12 Y= -6.157081632323D+12 Z= 1.477697474112D+13

I= 1 X= -7.612517483708D+12 Y= -2.538602251264D+13 Z= 5.778867087238D+12

I= 2 X= 7.320003394014D+12 Y= 9.673923835179D+12 Z= -4.061236002981D+12

I= 3 X= 7.932693432122D+12 Y= -1.669623585836D+12 Z= 1.184234341889D+13

I= 4 X= 7.883844387782D+12 Y= -3.211783887658D+12 Z= 2.817286279093D+12

I= 5 X= -7.580022499291D+12 Y= -9.062677151682D+12 Z= 6.916999095366D+12
I= 6 X= -1.166916330428D+13 Y= -4.197337432177D+13 Z= 6.040786917539D+13
I= 7 X= 1.123519080613D+14 Y= 6.530053149994D+13 Z= -8.174619318977D+13
I= 8 X= -2.598871504005D+12 Y= 5.767831396535D+13 Z= 2.483421270561D+13
I= 9 X= 5.784073944991D+12 Y= 3.993709988038D+12 Z= 1.588093985011D+13
I= 10 X= -2.506566372942D+13 Y= -5.014400699594D+13 Z= -5.737777279403D+13
I= 11 X= -8.897865241211D+13 Y= 4.259100316665D+13 Z= 4.464178025426D+13
I= 12 X= -3.283020744376D+12 Y= 5.953894328917D+13 Z= -7.980980702659D+12
I= 13 X= 3.100581472940D+13 Y= -1.547738816549D+13 Z= -1.070142973048D+13
I= 14 X= -1.107410280707D+14 Y= -3.287368865717D+13 Z= 6.818303239285D+12
I= 15 X= 3.883221792883D+13 Y= 1.265923789150D+14 Z= -2.465612673054D+13
I= 16 X= -1.697670353260D+14 Y= 3.211356553393D+13 Z= -1.028230326002D+14
I= 17 X= 5.759250684261D+12 Y= -1.571605672337D+12 Z= -2.281345004602D+13
I= 18 X= 9.142361189230D+12 Y= -4.819528977048D+13 Z= 7.820194339037D+13
I= 19 X= 4.373352877988D+13 Y= -7.411451950052D+13 Z= -2.968452856051D+13
I= 20 X= -8.377711113378D+13 Y= 5.113107451911D+13 Z= -8.930202851344D+13
I= 21 X= -3.516709293733D+12 Y= 1.931735204550D+13 Z= 1.749823948349D+13
I= 22 X= 2.705776462652D+13 Y= -1.258120323270D+14 Z= 4.473816924604D+13
I= 23 X= 1.051789944311D+13 Y= 3.275562242151D+13 Z= -1.381658509709D+12
I= 24 X= -7.165330432500D+13 Y= -9.045020771179D+13 Z= -6.129867781403D+13
I= 25 X= -1.095239919345D+13 Y= 1.623738213455D+13 Z= 5.360021278185D+11
I= 26 X= 4.832687601777D+13 Y= -2.959040158512D+12 Z= 4.886683734240D+13
I= 27 X= -2.800996494846D+13 Y= 1.058723396253D+14 Z= -2.558843366151D+13
I= 28 X= 1.124928475175D+13 Y= -1.473802912797D+14 Z= 2.286572560391D+13
I= 29 X= -1.628545226432D+13 Y= 3.029307447528D+12 Z= -5.757563884665D+12
I= 30 X= -9.513412686335D+12 Y= -1.220366647924D+13 Z= 5.275670793507D+12
I= 31 X= 7.897011002123D+13 Y= -1.420188638943D+13 Z= 5.659881281807D+13
I= 32 X= 5.730809051738D+12 Y= 3.740073486867D+13 Z= -7.989157041240D+13
I= 33 X= 5.558791728932D+13 Y= 8.454523075913D+13 Z= 6.703687744353D+13
I= 34 X= -4.909429398758D+13 Y= 1.203991519413D+14 Z= -2.003710215949D+13

I= 35 X= 7.819306329165D+11 Y= 2.771558453498D+12 Z= -5.559358696824D+12
I= 36 X= 1.645929482202D+12 Y= -5.080125989698D+12 Z= -5.953552010680D+12
I= 37 X= 8.437937439503D+13 Y= 7.361854280232D+13 Z= -3.875296556095D+11
I= 38 X= -5.292090501849D+13 Y= -9.525068673860D+13 Z= 7.078382448269D+13

Backward Direction:

Total Energy: -692.0054996 Hartrees

Potential Energy: -692.2122426 Hartress

Kinetic Energy: 0.2067429 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.240591019942D+12 Y= -5.543985272267D+12 Z= 1.568469730524D+13
I= 1 X= -7.214994201171D+12 Y= -2.538590369431D+13 Z= 5.778805075379D+12
I= 2 X= 7.550776107046D+12 Y= 9.349290457698D+12 Z= -3.568133835867D+12
I= 3 X= 7.984878147621D+12 Y= -2.282778960683D+12 Z= 1.093449788616D+13
I= 4 X= 8.114664196653D+12 Y= -2.887093935517D+12 Z= 2.324187981716D+12
I= 5 X= -6.509146709180D+12 Y= -1.284500103276D+13 Z= 2.428842781294D+12
I= 6 X= -5.158152633200D+13 Y= -4.196740521200D+13 Z= 6.040789256528D+13
I= 7 X= 1.064728992002D+14 Y= 6.448147296505D+13 Z= -8.715681909802D+13
I= 8 X= -5.527366630093D+12 Y= 5.609189040307D+13 Z= 2.358114016295D+13
I= 9 X= 6.422181922400D+12 Y= 2.833229487150D+12 Z= 1.551373693885D+13
I= 10 X= -2.547684565661D+13 Y= -5.163170835102D+13 Z= -5.818796329677D+13
I= 11 X= -8.814869318448D+13 Y= 4.029803564058D+13 Z= 4.441558854444D+13
I= 12 X= -1.671837616058D+12 Y= 5.846906823486D+13 Z= -7.861979322713D+12
I= 13 X= 3.164385876494D+13 Y= -1.431689570748D+13 Z= -1.033405056638D+13
I= 14 X= -1.111517235587D+14 Y= -3.138582021001D+13 Z= 7.628758238835D+12
I= 15 X= 4.044307244161D+13 Y= 1.276627445319D+14 Z= -2.477520106898D+13
I= 16 X= -1.689373796248D+14 Y= 3.440586348366D+13 Z= -1.025963908326D+14
I= 17 X= 5.703907016303D+12 Y= -1.509864035873D+12 Z= -2.157881091743D+13
I= 18 X= 9.378639334103D+12 Y= -4.766931569114D+13 Z= 8.071180905403D+13
I= 19 X= 4.360307349023D+13 Y= -7.376905023675D+13 Z= -2.917203306534D+13
I= 20 X= -8.414997630112D+13 Y= 4.968988511848D+13 Z= -8.793894668049D+13

I= 21 X= -4.597859855284D+12 Y= 1.931790993997D+13 Z= 1.749786462552D+13
I= 22 X= 2.426514629651D+13 Y= -1.258114496011D+14 Z= 4.473711810090D+13
I= 23 X= 9.804241018608D+12 Y= 3.406421496494D+13 Z= -1.271972494360D+12
I= 24 X= -7.236712782020D+13 Y= -9.175722264797D+13 Z= -6.140893486684D+13
I= 25 X= -1.100762441401D+13 Y= 1.617541394947D+13 Z= -6.986672384912D+11
I= 26 X= 4.795427139800D+13 Y= -1.518271127179D+12 Z= 4.750364966530D+13
I= 27 X= -2.814024314259D+13 Y= 1.055263879024D+14 Z= -2.610079195222D+13
I= 28 X= 1.148556458329D+13 Y= -1.479066177087D+14 Z= 2.035601085380D+13
I= 29 X= -1.521477446125D+13 Y= 6.810417208909D+12 Z= -1.270445008348D+12
I= 30 X= -7.826279279346D+12 Y= -1.177796338755D+13 Z= 8.632597706725D+12
I= 31 X= 7.604335337683D+13 Y= -1.261558281953D+13 Z= 5.785106883978D+13
I= 32 X= -1.474674314251D+11 Y= 3.821972457180D+13 Z= -7.448286509174D+13
I= 33 X= 5.496576434504D+13 Y= 8.234403269682D+13 Z= 7.418573909244D+13
I= 34 X= -4.884228189752D+13 Y= 1.179811924519D+14 Z= -1.719834471810D+13
I= 35 X= 4.536911078049D+11 Y= 2.771686225308D+12 Z= -5.558948482128D+12
I= 36 X= 3.333184935803D+12 Y= -5.506314778664D+12 Z= -9.310679513102D+12
I= 37 X= 8.375607522765D+13 Y= 7.582114514446D+13 Z= -7.537290088309D+12
I= 38 X= -5.266851532056D+13 Y= -9.283351050006D+13 Z= 6.794511251808D+13

Seed: 40595633469

CM Start Point Coordinates: bohr

I= 0 X= -2.201799473271D+00 Y= -1.979945531491D+00 Z= -5.878893093822D-02
I= 1 X= 8.920299028497D-02 Y= -2.467834197966D+00 Z= -1.589150159800D+00
I= 2 X= -1.567402667213D+00 Y= -1.197590826681D+00 Z= 2.553043189696D+00
I= 3 X= 2.125321053029D+00 Y= -2.082998016971D+00 Z= 1.174226425632D-01
I= 4 X= 1.134353274339D+00 Y= -1.207068257874D+00 Z= 2.612592835872D+00
I= 5 X= -3.004490861253D+00 Y= 2.872781346352D+00 Z= -2.202455318896D+00
I= 6 X= -1.272113622338D-01 Y= 1.803155944356D+00 Z= -3.190076925922D+00
I= 7 X= -2.553157185165D+00 Y= 3.970241963942D+00 Z= -3.715402269535D+00
I= 8 X= -4.053008851833D+00 Y= 1.452199720292D+00 Z= -2.884753399534D+00

I= 9 X= 2.748002514691D+00 Y= -4.842136737931D-01 Z= 4.672924615942D+00
I= 10 X= 1.634890671384D+00 Y= -1.709576413786D+00 Z= 6.752518028953D+00
I= 11 X= 4.788914924615D+00 Y= -1.309022286676D+00 Z= 4.187275216588D+00
I= 12 X= 2.669568457373D+00 Y= 1.838576118877D+00 Z= 5.357398813800D+00
I= 13 X= -3.123182141018D+00 Y= -8.970074378306D-01 Z= 4.857283881339D+00
I= 14 X= -3.062388437742D+00 Y= -2.895236602254D+00 Z= 5.436422467301D+00
I= 15 X= -2.030094581936D+00 Y= 4.411495430174D-01 Z= 6.295572165590D+00
I= 16 X= -4.967154930356D+00 Y= 1.282391293364D-01 Z= 4.144372090265D+00
I= 17 X= -4.711939103767D+00 Y= -2.717245950443D+00 Z= -9.988033204506D-01
I= 18 X= -5.602742791150D+00 Y= -4.694004324164D+00 Z= -5.071912295258D-01
I= 19 X= -6.258698793322D+00 Y= -1.532954333974D+00 Z= -3.592541346451D-01
I= 20 X= -4.804457779869D+00 Y= -2.422907989729D+00 Z= -2.890272103780D+00
I= 21 X= 8.676451634961D-02 Y= -3.566023468942D+00 Z= -4.246986740087D+00
I= 22 X= -6.307411955855D-02 Y= -5.591508061425D+00 Z= -4.216344905071D+00
I= 23 X= -1.190213231578D+00 Y= -2.392896472397D+00 Z= -5.673429322694D+00
I= 24 X= 1.707870451023D+00 Y= -3.006385217698D+00 Z= -5.041133922502D+00
I= 25 X= 4.884810033731D+00 Y= -2.511918229869D+00 Z= -1.032748706647D+00
I= 26 X= 4.723722029612D+00 Y= -3.157447061141D+00 Z= -2.928694382903D+00
I= 27 X= 5.954270445910D+00 Y= -6.369939378897D-01 Z= -1.198332358805D+00
I= 28 X= 5.410881492433D+00 Y= -4.063542246847D+00 Z= 1.083679489366D-01
I= 29 X= 2.678123696401D+00 Y= 3.346846884602D+00 Z= -2.632123757362D+00
I= 30 X= 3.310588986265D+00 Y= 3.641678880218D+00 Z= -9.503827854708D-02
I= 31 X= 3.840052488061D+00 Y= 2.198766169849D+00 Z= -3.619454371338D+00
I= 32 X= 1.605505812159D+00 Y= 4.995291624954D+00 Z= -3.714587252593D+00
I= 33 X= 2.659184165645D+00 Y= 4.998584867032D+00 Z= 1.088371798167D+00
I= 34 X= 4.725725378746D+00 Y= 2.483911341139D+00 Z= 6.777000261676D-01
I= 35 X= 4.947193121919D-02 Y= 1.028590249164D+00 Z= -3.700757746606D-01
I= 36 X= -2.632611178354D+00 Y= 4.133471519432D+00 Z= 1.570611314683D-01
I= 37 X= -2.070755344005D+00 Y= 6.317048625688D+00 Z= 5.456654120391D-01
I= 38 X= -3.636598238009D+00 Y= 3.565892735844D+00 Z= 1.811863409746D+00

Forward Direction:

Total Energy: -691.9932622 Hartrees

Potential Energy: -692.1377513 Hartress

Kinetic Energy: 0.1444891 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.364298989091D+13 Y= -1.204927052718D+13 Z= 1.104413055708D+13
I= 1 X= 2.472214959733D+13 Y= -1.082758551846D+12 Z= -5.844605284202D+12
I= 2 X= 1.622741437270D+13 Y= 1.330911098570D+12 Z= -2.951781309235D+13
I= 3 X= -2.523308141688D+12 Y= -8.147141050732D+11 Z= -2.189917606134D+12
I= 4 X= -5.732284014457D+12 Y= 9.546581496918D+12 Z= 1.028177523237D+13
I= 5 X= -7.758102559933D+10 Y= 9.471531223524D+12 Z= 6.243510028035D+12
I= 6 X= 9.770211070700D+12 Y= 4.908202928503D+12 Z= -7.445364966231D+13
I= 7 X= 1.136932383266D+13 Y= -2.098471527725D+13 Z= -8.970620574417D+13
I= 8 X= 2.058216463703D+13 Y= -3.679484474933D+13 Z= -2.055554617125D+13
I= 9 X= 4.550258404920D+12 Y= -3.473169973417D+12 Z= 5.418459955121D+12
I= 10 X= 7.343984646322D+12 Y= -2.230947526871D+13 Z= 3.466114809168D+13
I= 11 X= -5.696927551457D+13 Y= 3.712834464499D+13 Z= -2.462412351283D+13
I= 12 X= 5.293339282428D+13 Y= -1.652683508130D+13 Z= -5.169864737136D+13
I= 13 X= -1.733445632492D+13 Y= 1.524695265670D+13 Z= 3.981606080953D+12
I= 14 X= 4.077847040985D+13 Y= 7.977253358969D+13 Z= -1.368190436546D+13
I= 15 X= -3.029786560350D+12 Y= -1.403006482151D+14 Z= -7.299335984442D+13
I= 16 X= -6.351734145173D+13 Y= 1.095562516135D+13 Z= 3.547539900892D+13
I= 17 X= -1.504691586493D+13 Y= 5.893402430737D+12 Z= 8.029168299212D+12
I= 18 X= 2.921206450425D+13 Y= 3.697077272489D+13 Z= -1.273374846257D+13
I= 19 X= 1.369858020913D+13 Y= -7.497658498235D+13 Z= -1.612596689009D+13
I= 20 X= 6.732246625328D+13 Y= -2.837925114102D+13 Z= -5.996488182229D+13
I= 21 X= -1.103009459164D+13 Y= -1.447843873628D+13 Z= 7.916684693425D+12
I= 22 X= -1.622542666241D+13 Y= 1.294105769618D+14 Z= 5.083860500462D+13
I= 23 X= 6.047510597000D+13 Y= 1.995636252893D+13 Z= -3.655730420293D+12
I= 24 X= 2.360021605709D+13 Y= 4.874732792391D+13 Z= -6.029594547412D+13

I= 25 X= 1.474690974798D+13 Y= -1.016768901983D+12 Z= -1.977488909832D+12
I= 26 X= -5.196071628958D+13 Y= -1.064985058915D+14 Z= -5.508028376502D+13
I= 27 X= 5.449120548149D+13 Y= 9.174510615281D+13 Z= 9.984010126804D+13
I= 28 X= -4.485486182385D+13 Y= 4.824202710259D+13 Z= -2.632801201392D+13
I= 29 X= -1.811398828455D+12 Y= -1.621246880879D+13 Z= -9.004380350278D+12
I= 30 X= -2.402179511190D+12 Y= -1.046919758425D+13 Z= -1.971015610469D+13
I= 31 X= -1.158772478802D+13 Y= 3.327951588102D+13 Z= 1.075786791668D+13
I= 32 X= -4.127030481329D+13 Y= -1.378937591051D+13 Z= -6.834342384953D+13
I= 33 X= -5.047855301964D+13 Y= -4.798249757343D+13 Z= 3.165980467018D+13
I= 34 X= -1.019619929760D+13 Y= 4.578406714346D+12 Z= 4.741068036490D+13
I= 35 X= 3.407302702124D+12 Y= 2.189746876147D+11 Z= 2.983372122459D+12
I= 36 X= -1.156817904764D+12 Y= 2.260715860832D+13 Z= 2.284594723802D+13
I= 37 X= -2.650365226874D+13 Y= -9.302175811977D+13 Z= 2.529284803637D+13
I= 38 X= -8.907131865999D+13 Y= -1.051274756515D+13 Z= 5.034774187934D+13

Backward Direction:

Total Energy: -691.9932920 Hartrees

Potential Energy: -692.1377513 Hartress

Kinetic Energy: 0.1444593 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.375197218365D+13 Y= -1.069051689088D+13 Z= 1.371086926868D+13
I= 1 X= 2.422806103855D+13 Y= -1.082318045566D+12 Z= -5.844900468587D+12
I= 2 X= 1.765657597974D+13 Y= 1.830457173648D+12 Z= -2.828294105177D+13
I= 3 X= -2.632002621061D+12 Y= -2.173552625672D+12 Z= -4.856989376294D+12
I= 4 X= -4.302940644427D+12 Y= 9.047211999404D+12 Z= 9.047106189299D+12
I= 5 X= 3.986495249187D+10 Y= -4.472217037373D+12 Z= -8.155989575751D+12
I= 6 X= -4.069910460195D+13 Y= 4.922019362983D+12 Z= -7.445214081789D+13
I= 7 X= -2.156080638326D+12 Y= -3.480554427426D+13 Z= -1.116695737928D+14
I= 8 X= 1.691433120745D+13 Y= -5.317965664030D+13 Z= -2.434971540195D+13
I= 9 X= 7.521373740798D+12 Y= -8.776487353787D+12 Z= 4.309994446171D+12
I= 10 X= 6.405356931049D+12 Y= -2.851203700888D+13 Z= 3.227482985597D+13

I= 11 X= -5.331493079654D+13 Y= 2.736467819399D+13 Z= -2.545770556104D+13
I= 12 X= 5.971203744560D+13 Y= -2.120563799935D+13 Z= -5.140003803504D+13
I= 13 X= -1.436352619576D+13 Y= 2.055031950948D+13 Z= 5.090929537991D+12
I= 14 X= 3.984218927057D+13 Y= 8.597595523211D+13 Z= -1.129414366913D+13
I= 15 X= 3.747500828177D+12 Y= -1.356197601411D+14 Z= -7.329229817362D+13
I= 16 X= -5.986421584040D+13 Y= 2.071642190255D+13 Z= 3.631094118266D+13
I= 17 X= -1.578210542084D+13 Y= 5.749648226338D+12 Z= 1.333893073674D+13
I= 18 X= 2.910465766375D+13 Y= 3.939672382902D+13 Z= -1.209894886528D+12
I= 19 X= 1.350277397399D+13 Y= -7.301626390494D+13 Z= -1.430137807571D+13
I= 20 X= 6.487751470000D+13 Y= -3.535550791043D+13 Z= -5.402089523488D+13
I= 21 X= -1.612353761057D+13 Y= -1.447618019933D+13 Z= 7.915170257224D+12
I= 22 X= -2.921458740742D+13 Y= 1.294129863279D+14 Z= 5.083443500059D+13
I= 23 X= 5.751776316803D+13 Y= 2.618268503595D+13 Z= -3.745338492123D+12
I= 24 X= 2.064237831558D+13 Y= 4.252710137884D+13 Z= -6.020817481629D+13
I= 25 X= 1.401237232216D+13 Y= -8.741225961909D+11 Z= -7.287453235841D+12
I= 26 X= -5.440460949259D+13 Y= -9.952347860838D+13 Z= -6.102494129702D+13
I= 27 X= 5.429642501033D+13 Y= 8.978237364497D+13 Z= 9.801635587690D+13
I= 28 X= -4.496182991726D+13 Y= 4.581415460423D+13 Z= -3.785204874666D+13
I= 29 X= -1.694941872213D+12 Y= -2.272706938805D+12 Z= 5.390926719967D+12
I= 30 X= 1.207877789136D+11 Y= -1.175606305982D+13 Z= -4.893464724529D+12
I= 31 X= -1.525448178156D+13 Y= 4.965880947453D+13 Z= 1.454767058165D+13
I= 32 X= -5.479130241363D+13 Y= 3.302921407358D+10 Z= -4.638649101678D+13
I= 33 X= -5.273190609606D+13 Y= -5.729657551971D+13 Z= 6.077448192387D+13
I= 34 X= -7.390500292772D+12 Y= -4.733603043924D+12 Z= 5.616497341594D+13
I= 35 X= 3.546411904540D+12 Y= 2.195453113009D+11 Z= 2.984930241865D+12
I= 36 X= 1.365765525693D+12 Y= 2.389238170515D+13 Z= 8.028295360172D+12
I= 37 X= -2.876258352234D+13 Y= -8.370268641220D+13 Z= -3.823666250671D+12
I= 38 X= -8.626605594051D+13 Y= -1.205597300497D+12 Z= 4.159305142460D+13

Seed: 40829322908

CM Start Point Coordinates: bohr

I= 0 X= -2.168492170394D+00 Y= -2.124843749635D+00 Z= -8.589700858429D-02
I= 1 X= -2.537923620738D-02 Y= -2.607765132282D+00 Z= -1.677819076939D+00
I= 2 X= -1.322129738077D+00 Y= -1.502742254949D+00 Z= 2.326715600671D+00
I= 3 X= 2.250910173347D+00 Y= -1.856617514446D+00 Z= 4.868320516547D-02
I= 4 X= 1.375132725921D+00 Y= -1.204308256526D+00 Z= 2.484738957773D+00
I= 5 X= -2.880259382219D+00 Y= 3.115305639000D+00 Z= -2.407940014094D+00
I= 6 X= 7.439257947324D-02 Y= 1.549863868010D+00 Z= -3.044118419788D+00
I= 7 X= -2.278274597449D+00 Y= 4.544453491155D+00 Z= -4.004060545929D+00
I= 8 X= -4.346854678917D+00 Y= 1.802865109121D+00 Z= -2.674239092700D+00
I= 9 X= 2.912450544225D+00 Y= -7.506162891941D-01 Z= 4.725246642141D+00
I= 10 X= 2.760112207579D+00 Y= -2.255227016007D+00 Z= 6.316437051547D+00
I= 11 X= 4.723014548649D+00 Y= -1.124381461448D+00 Z= 4.127795229619D+00
I= 12 X= 2.970710380313D+00 Y= 1.322091715019D+00 Z= 5.518455473801D+00
I= 13 X= -2.984737694280D+00 Y= -8.006537042316D-01 Z= 4.372793519389D+00
I= 14 X= -3.501844919667D+00 Y= -2.935473808747D+00 Z= 5.240604682807D+00
I= 15 X= -1.902940810040D+00 Y= 7.188130626966D-01 Z= 5.664892659303D+00
I= 16 X= -5.064948567500D+00 Y= -5.027192200676D-02 Z= 3.785528920913D+00
I= 17 X= -4.798369381180D+00 Y= -2.301879067676D+00 Z= -7.379773331402D-01
I= 18 X= -5.759182299774D+00 Y= -3.771149788073D+00 Z= 2.780714620588D-01
I= 19 X= -5.782775835900D+00 Y= -8.992421105860D-01 Z= -2.075036991307D-02
I= 20 X= -5.302676053599D+00 Y= -2.262748218001D+00 Z= -2.729800145335D+00
I= 21 X= -2.172376712697D-02 Y= -3.951193903135D+00 Z= -4.085131707478D+00
I= 22 X= -9.611775498124D-02 Y= -6.047137979657D+00 Z= -4.254929235477D+00
I= 23 X= -1.731365775358D+00 Y= -3.373790203404D+00 Z= -5.099253719164D+00
I= 24 X= 2.016249824705D+00 Y= -3.735168565067D+00 Z= -5.562897207727D+00
I= 25 X= 4.921140602937D+00 Y= -1.995408387359D+00 Z= -7.557529427947D-01
I= 26 X= 5.280844181462D+00 Y= -1.416399051303D+00 Z= -2.747001223791D+00
I= 27 X= 6.034209674034D+00 Y= -7.131217805536D-01 Z= 5.971373327695D-01
I= 28 X= 5.463983703962D+00 Y= -4.120142425886D+00 Z= -5.767853883676D-01

I= 29 X= 2.671561552942D+00 Y= 2.979498573728D+00 Z= -2.402913511268D+00
I= 30 X= 3.007413956422D+00 Y= 3.677020419414D+00 Z= 1.447011649307D-01
I= 31 X= 4.026174113374D+00 Y= 1.709487282678D+00 Z= -3.356124707153D+00
I= 32 X= 1.531157846711D+00 Y= 4.401885321937D+00 Z= -3.743480279674D+00
I= 33 X= 2.207574853937D+00 Y= 5.445573004286D+00 Z= 5.056717422439D-01
I= 34 X= 4.208984449640D+00 Y= 2.807356888769D+00 Z= 1.495052460603D+00
I= 35 X= -9.251331690259D-02 Y= 1.045271256536D+00 Z= -4.141439621519D-01
I= 36 X= -2.541485130339D+00 Y= 4.109079026391D+00 Z= 2.458590619144D-01
I= 37 X= -1.440248188296D+00 Y= 5.899397406489D+00 Z= 5.132758369330D-01
I= 38 X= -3.395902686770D+00 Y= 3.475173214560D+00 Z= 1.848705082497D+00

Forward Direction:

Total Energy: -692.0026960 Hartrees

Potential Energy: -692.1821345 Hartress

Kinetic Energy: 0.1794385 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.179200432318D+12 Y= 4.031397734790D+12 Z= -1.535166304321D+13
I= 1 X= 6.227722006301D+12 Y= -1.598158595527D+13 Z= -1.091565874535D+13
I= 2 X= 2.159026099303D+13 Y= -1.962076117875D+13 Z= -8.677203252745D+12
I= 3 X= -1.874086171239D+13 Y= 1.502148510656D+13 Z= -1.523188921358D+13
I= 4 X= 1.426909528151D+13 Y= -8.429165665663D+12 Z= -4.446258149734D+11
I= 5 X= 1.107780483903D+13 Y= 1.434159681770D+13 Z= 2.286256338693D+13
I= 6 X= 4.731718561794D+12 Y= -6.022074561314D+13 Z= -7.969734828147D+13
I= 7 X= -4.133967666921D+13 Y= -4.876410752900D+13 Z= -7.077442988450D+13
I= 8 X= 4.104070142674D+13 Y= 3.052535013087D+13 Z= -6.901640666366D+13
I= 9 X= -2.067664277165D+13 Y= 1.354033884777D+11 Z= -1.136848759276D+13
I= 10 X= 4.222456937540D+13 Y= -2.186371229387D+12 Z= 1.065502386802D+13
I= 11 X= -6.860713303277D+13 Y= -4.623743140815D+13 Z= 3.415750260313D+13
I= 12 X= 7.081640036812D+13 Y= 4.689011131893D+13 Z= 8.231130506435D+12
I= 13 X= -9.859619438150D+12 Y= 2.116327176759D+13 Z= -3.141388417732D+12
I= 14 X= 8.163425885834D+12 Y= -1.153007747697D+14 Z= 1.070295039015D+14

I= 15 X= -2.255409373600D+13 Y= 1.589866383116D+13 Z= 1.074452157381D+14
I= 16 X= 2.601105496856D+13 Y= -1.620609826218D+13 Z= 2.763995956734D+13
I= 17 X= 3.186007312309D+12 Y= -3.367069002593D+12 Z= 6.683947440908D+12
I= 18 X= -3.529787131146D+13 Y= -3.095408435332D+12 Z= -4.486218945748D+12
I= 19 X= 9.024610181779D+12 Y= 6.974975215139D+13 Z= 6.521689722654D+12
I= 20 X= -1.553746280362D+13 Y= 5.088007909501D+13 Z= 8.265763118945D+13
I= 21 X= -1.380135415647D+13 Y= -1.193978206369D+13 Z= -8.239985353037D+12
I= 22 X= 3.350203259382D+13 Y= 4.313274704802D+13 Z= 1.133879411077D+13
I= 23 X= 5.079402607679D+13 Y= -1.068622480824D+13 Z= -5.037275048285D+13
I= 24 X= -6.334585885108D+12 Y= 3.534173691841D+13 Z= -2.130468813452D+11
I= 25 X= 2.750440427115D+13 Y= -8.921025533387D+12 Z= 1.939754539494D+12
I= 26 X= -2.150620684060D+13 Y= -9.877109463579D+12 Z= 1.256257895071D+13
I= 27 X= 3.762057544987D+13 Y= 2.063138037838D+14 Z= 3.107418722416D+13
I= 28 X= -9.368482227093D+13 Y= 3.144070409549D+13 Z= -5.891417493046D+13
I= 29 X= -1.922015087311D+12 Y= -2.142796322666D+13 Z= -1.360638108770D+13
I= 30 X= -3.108193542468D+12 Y= -1.293162081266D+12 Z= 2.265283431162D+12
I= 31 X= -7.001041301925D+13 Y= 1.383046271350D+14 Z= 4.778245860604D+13
I= 32 X= -1.308776303036D+13 Y= -9.720341045630D+12 Z= 1.451279287543D+13
I= 33 X= 1.063877403737D+14 Y= 7.191395119565D+13 Z= 1.049487069762D+13
I= 34 X= -2.399349707756D+13 Y= -2.973100754470D+13 Z= 1.066205667472D+14
I= 35 X= -2.510570212226D+12 Y= 1.169434624790D+12 Z= 5.676629738766D+12
I= 36 X= -1.287090576523D+13 Y= -9.136592256206D+12 Z= 8.633946975370D+12
I= 37 X= -5.641149248895D+12 Y= -8.316172558342D+12 Z= 1.194250950508D+13
I= 38 X= 8.580394802744D+13 Y= 9.242206041420D+13 Z= -9.818974234918D+13

Backward Direction:

Total Energy: -692.0027284 Hartrees

Potential Energy: -692.1821345 Hartress

Kinetic Energy: 0.1794061 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.181604598260D+12 Y= 4.774678863828D+12 Z= -1.407384843953D+13

I= 1 X= 6.337356999105D+12 Y= -1.598139393831D+13 Z= -1.091577664329D+13
I= 2 X= 2.211850436157D+13 Y= -1.968428740960D+13 Z= -8.040936091995D+12
I= 3 X= -1.873833708079D+13 Y= 1.427814486242D+13 Z= -1.650986929901D+13
I= 4 X= 1.479741669583D+13 Y= -8.365556979893D+12 Z= -1.080835660116D+12
I= 5 X= 1.176531019551D+13 Y= 8.250437049968D+12 Z= 1.621582314762D+13
I= 6 X= -3.337133871457D+13 Y= -6.021334990401D+13 Z= -7.969692544310D+13
I= 7 X= -4.860139176709D+13 Y= -5.300755206588D+13 Z= -8.003389030910D+13
I= 8 X= 3.825450680100D+13 Y= 2.511785390840D+13 Z= -7.081092905587D+13
I= 9 X= -1.948150710527D+13 Y= -2.011019099832D+12 Z= -1.189344149111D+13
I= 10 X= 4.171866959405D+13 Y= -4.776620535950D+12 Z= 9.512851627638D+12
I= 11 X= -6.710954378234D+13 Y= -5.028490585508D+13 Z= 3.379331462395D+13
I= 12 X= 7.363823059911D+13 Y= 4.496825185573D+13 Z= 8.384843275538D+12
I= 13 X= -8.664573061403D+12 Y= 2.330971497967D+13 Z= -2.616094325050D+12
I= 14 X= 7.658459297674D+12 Y= -1.127101903952D+14 Z= 1.081722286692D+14
I= 15 X= -1.973283218777D+13 Y= 1.782138816193D+13 Z= 1.072913691876D+14
I= 16 X= 2.750812834780D+13 Y= -1.215981075689D+13 Z= 2.800495382694D+13
I= 17 X= 2.953070578040D+12 Y= -3.368184820246D+12 Z= 8.877522898790D+12
I= 18 X= -3.518227596925D+13 Y= -2.116534366327D+12 Z= 1.706270643308D+11
I= 19 X= 8.891717602193D+12 Y= 7.049203420197D+13 Z= 7.329494652128D+12
I= 20 X= -1.642773127937D+13 Y= 4.810883505227D+13 Z= 8.510156673552D+13
I= 21 X= -1.584237965172D+13 Y= -1.193882897871D+13 Z= -8.240624915705D+12
I= 22 X= 2.827532921599D+13 Y= 4.313375617380D+13 Z= 1.133702147509D+13
I= 23 X= 4.955635899720D+13 Y= -8.199212471619D+12 Z= -5.032984968640D+13
I= 24 X= -7.572488045419D+12 Y= 3.285734100176D+13 Z= -2.567948212442D+11
I= 25 X= 2.727171664283D+13 Y= -8.920348346624D+12 Z= -2.538940740502D+11
I= 26 X= -2.239602920008D+13 Y= -7.106455657358D+12 Z= 1.011839708627D+13
I= 27 X= 3.748806882633D+13 Y= 2.055705732083D+14 Z= 3.026669461959D+13
I= 28 X= -9.356910699177D+13 Y= 3.046109380045D+13 Z= -6.357097796764D+13
I= 29 X= -1.234898738087D+12 Y= -1.533862618123D+13 Z= -6.961411188400D+12
I= 30 X= -1.392063757639D+12 Y= -1.380913082373D+12 Z= 8.332314011275D+12

I= 31 X= -7.279525173235D+13 Y= 1.437105558382D+14 Z= 4.957529881181D+13
I= 32 X= -2.034783652531D+13 Y= -5.476511930165D+12 Z= 2.376933500712D+13
I= 33 X= 1.053967050511D+14 Y= 6.804439213897D+13 Z= 2.275485408288D+13
I= 34 X= -2.307955730206D+13 Y= -3.373273172494D+13 Z= 1.107289502009D+14
I= 35 X= -2.673891182079D+12 Y= 1.169667357196D+12 Z= 5.677302771574D+12
I= 36 X= -1.115480517037D+13 Y= -9.049583327951D+12 Z= 2.566533528207D+12
I= 37 X= -6.634396678738D+12 Y= -4.444401611585D+12 Z= -3.185215815609D+11
I= 38 X= 8.671800089454D+13 Y= 9.642198929996D+13 Z= -1.022982055474D+14

Seed: 40972791204

CM Start Point Coordinates: bohr

I= 0 X= -2.175754614209D+00 Y= -1.850769607603D+00 Z= -2.236896332899D-01
I= 1 X= 1.059746467805D-01 Y= -2.654612061646D+00 Z= -1.600777838255D+00
I= 2 X= -1.485357283445D+00 Y= -1.159748950115D+00 Z= 2.327476962220D+00
I= 3 X= 2.246355852410D+00 Y= -2.046057318713D+00 Z= 1.389440917657D-01
I= 4 X= 1.286142217998D+00 Y= -1.044404712144D+00 Z= 2.400037835194D+00
I= 5 X= -3.000176301194D+00 Y= 3.265082118087D+00 Z= -2.137813251942D+00
I= 6 X= -1.808588206841D-01 Y= 1.339091309027D+00 Z= -3.240940953585D+00
I= 7 X= -2.383562039831D+00 Y= 4.759088138225D+00 Z= -3.396166096711D+00
I= 8 X= -4.447146761292D+00 Y= 2.209590029727D+00 Z= -2.430595826409D+00
I= 9 X= 3.099146007908D+00 Y= -7.159173184709D-01 Z= 4.596179478395D+00
I= 10 X= 3.560221489373D+00 Y= -2.655502061874D+00 Z= 5.876764164958D+00
I= 11 X= 5.068452118795D+00 Y= 1.948835576641D-01 Z= 3.859217012010D+00
I= 12 X= 2.294071132676D+00 Y= 9.884086686881D-01 Z= 5.748401810486D+00
I= 13 X= -3.015979965492D+00 Y= -6.514811840917D-01 Z= 4.538682368841D+00
I= 14 X= -3.147590856534D+00 Y= -2.129249648571D+00 Z= 5.696060774970D+00
I= 15 X= -2.575843299979D+00 Y= 9.118963904571D-01 Z= 5.977306351958D+00
I= 16 X= -5.276047165072D+00 Y= 3.243308809206D-02 Z= 4.324616105282D+00
I= 17 X= -4.818834775684D+00 Y= -2.572850868353D+00 Z= -1.003860273131D+00
I= 18 X= -5.947594279409D+00 Y= -4.104317133046D+00 Z= 4.722658507281D-01

I= 19 X= -6.446958234428D+00 Y= -9.294025045677D-01 Z= -8.366230778350D-01
I= 20 X= -4.823723490809D+00 Y= -3.220219850115D+00 Z= -2.805945739498D+00
I= 21 X= -1.738846291739D-01 Y= -3.954046637129D+00 Z= -3.966779825279D+00
I= 22 X= -5.413141748432D-01 Y= -5.853938955822D+00 Z= -3.954670673055D+00
I= 23 X= -1.987012228732D+00 Y= -3.524831833520D+00 Z= -4.740233103703D+00
I= 24 X= 1.365074754093D+00 Y= -3.647110028999D+00 Z= -5.309597715156D+00
I= 25 X= 4.943183099992D+00 Y= -2.684569960497D+00 Z= -5.905986211582D-01
I= 26 X= 5.553040777188D+00 Y= -2.613685014503D+00 Z= -2.605795893454D+00
I= 27 X= 6.140125270449D+00 Y= -1.221524125152D+00 Z= -2.772826253705D-02
I= 28 X= 5.615495163179D+00 Y= -4.580840708451D+00 Z= 3.565547563473D-01
I= 29 X= 2.725372990323D+00 Y= 3.592361031151D+00 Z= -2.396174266918D+00
I= 30 X= 2.800639078605D+00 Y= 3.716301027327D+00 Z= 3.413678895709D-01
I= 31 X= 4.079267117644D+00 Y= 2.466504049613D+00 Z= -3.381029619671D+00
I= 32 X= 1.756479238760D+00 Y= 5.295497361763D+00 Z= -3.428577267103D+00
I= 33 X= 2.432953151952D+00 Y= 5.601846005066D+00 Z= 1.327449753947D+00
I= 34 X= 4.356067398523D+00 Y= 2.816260025839D+00 Z= 9.934755800210D-01
I= 35 X= 6.384251750956D-02 Y= 1.032485283687D+00 Z= -6.101656195651D-01
I= 36 X= -2.740859269193D+00 Y= 3.673889891349D+00 Z= 4.583074621161D-01
I= 37 X= -1.801838407198D+00 Y= 5.504011976779D+00 Z= 1.047686538360D+00
I= 38 X= -3.965603592619D+00 Y= 2.553838328330D+00 Z= 1.850747169076D+00

Forward Direction:

Total Energy: -691.9997753 Hartrees

Potential Energy: -692.1677174 Hartress

Kinetic Energy: 0.1679421 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.451037876865D+12 Y= -4.713555516146D+12 Z= -1.913142455221D+13

I= 1 X= 1.724884042990D+13 Y= -1.536021415563D+13 Z= -2.527624462622D+13

I= 2 X= 1.555896241310D+13 Y= 2.718287672020D+12 Z= -1.031044798130D+13

I= 3 X= -1.990402588547D+13 Y= 2.132580502564D+13 Z= -6.310882492706D+12

I= 4 X= 2.466896285092D+13 Y= -5.175270680070D+11 Z= 2.888205760425D+12

I= 5 X= -4.246821219954D+11 Y= -8.783839503879D+12 Z= -5.458530867609D+12
I= 6 X= 7.417563877084D+13 Y= -2.772282179841D+13 Z= -6.494532099727D+13
I= 7 X= -5.961240009423D+13 Y= 2.893198251040D+13 Z= 7.396907470090D+13
I= 8 X= 1.139240187957D+13 Y= 3.516643026662D+13 Z= 7.144917444596D+12
I= 9 X= 8.400493510501D+12 Y= -8.502916643003D+11 Z= -1.687658066427D+12
I= 10 X= -5.220659391129D+12 Y= -1.714658151104D+13 Z= 5.155272749786D+13
I= 11 X= 1.105554632858D+13 Y= 2.392276778671D+13 Z= -1.609425750172D+13
I= 12 X= -3.404157468682D+13 Y= 5.912825065864D+13 Z= -1.170001270159D+12
I= 13 X= -3.196606039884D+13 Y= -2.231486396623D+13 Z= 4.687072417475D+12
I= 14 X= 6.389682845865D+13 Y= 2.264571146935D+13 Z= 4.625483323062D+12
I= 15 X= 1.156636475448D+13 Y= 1.705021647851D+11 Z= 2.561453015101D+13
I= 16 X= 7.168320137942D+13 Y= -6.043112395482D+13 Z= -4.694614165689D+13
I= 17 X= -5.255164872353D+11 Y= 9.071274218033D+12 Z= 1.871206289871D+13
I= 18 X= -7.726977262630D+13 Y= 1.218644167127D+13 Z= -1.871740264350D+13
I= 19 X= -3.112105867948D+13 Y= -6.751425663896D+13 Z= 1.582533244179D+13
I= 20 X= 2.323364348800D+13 Y= -1.649440859894D+13 Z= 1.450882767293D+12
I= 21 X= 4.679644466916D+12 Y= 2.624140530129D+12 Z= 1.053757014015D+13
I= 22 X= 1.789123054406D+13 Y= 3.449188491957D+13 Z= 5.199087139832D+13
I= 23 X= -1.579270805194D+14 Y= 4.845096409897D+13 Z= -4.929641556735D+13
I= 24 X= 4.391630398430D+13 Y= -1.537523880117D+13 Z= 4.614308077369D+13
I= 25 X= 3.243113801412D+12 Y= 8.506766861375D+11 Z= 3.189102671670D+12
I= 26 X= -3.341977893156D+13 Y= 1.320148667109D+13 Z= 7.309588408640D+13
I= 27 X= 5.135891715141D+13 Y= 1.934632678747D+13 Z= 5.285907940193D+13
I= 28 X= -1.403965390521D+14 Y= 1.268843863941D+14 Z= -1.127812998064D+12
I= 29 X= -1.551343416193D+13 Y= 1.353651951654D+13 Z= 5.660240070910D+12
I= 30 X= 5.416939146648D+12 Y= 1.511629773451D+13 Z= -2.018728815853D+12
I= 31 X= -2.472238620193D+12 Y= 4.603041330091D+13 Z= -8.253534419184D+13
I= 32 X= 8.735476139843D+13 Y= -1.327519980026D+14 Z= -3.107163795411D+13
I= 33 X= 8.556977866908D+13 Y= 2.596502763548D+13 Z= 8.481461267410D+13
I= 34 X= -8.744130672114D+13 Y= -2.320702303663D+12 Z= -7.649770608188D+13

I= 35 X= -2.179199698096D+11 Y= -5.769871251929D+12 Z= 3.945518782015D+12
I= 36 X= 8.784954581276D+12 Y= 1.188735314718D+13 Z= -1.547271440419D+12
I= 37 X= -5.963243595663D+13 Y= -1.230176447276D+14 Z= -3.310482755912D+12
I= 38 X= -2.107798475218D+13 Y= 1.085935922886D+13 Z= -1.771609890161D+13

Backward Direction:

Total Energy: -691.9997730 Hartrees

Potential Energy: -692.1677174 Hartress

Kinetic Energy: 0.1679444 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.228105529719D+12 Y= -3.505618172849D+12 Z= -1.769390477008D+13
I= 1 X= 1.876867917204D+13 Y= -1.536007497349D+13 Z= -2.527628229877D+13
I= 2 X= 1.552201723142D+13 Y= 1.425671100049D+12 Z= -9.415022548367D+12
I= 3 X= -1.968102835122D+13 Y= 2.011772681761D+13 Z= -7.748612124010D+12
I= 4 X= 2.463206899963D+13 Y= 7.751735466877D+11 Z= 1.992683805016D+12
I= 5 X= 2.893632013797D+12 Y= -1.325669480758D+13 Z= -1.191586760505D+13
I= 6 X= -2.480914479877D+13 Y= -2.771137609001D+13 Z= -6.494605542829D+13
I= 7 X= -7.092952456001D+13 Y= 3.374962198714D+13 Z= 6.865103069439D+13
I= 8 X= 4.110690345886D+12 Y= 3.893467493116D+13 Z= 5.220935305333D+12
I= 9 X= 8.823667028969D+12 Y= -1.673474213963D+12 Z= -2.253279277775D+12
I= 10 X= -6.016123385380D+12 Y= -1.852122325445D+13 Z= 5.027293938995D+13
I= 11 X= 1.171847564539D+13 Y= 2.191321530684D+13 Z= -1.636189796147D+13
I= 12 X= -3.258565187088D+13 Y= 5.825659942170D+13 Z= -9.542251400639D+11
I= 13 X= -3.154298955678D+13 Y= -2.149167018007D+13 Z= 5.252790544030D+12
I= 14 X= 6.310164331550D+13 Y= 2.402042023714D+13 Z= 5.905333782797D+12
I= 15 X= 1.302197708678D+13 Y= 1.042585412445D+12 Z= 2.539869996296D+13
I= 16 X= 7.234582534373D+13 Y= -5.842214832303D+13 Z= -4.667813020699D+13
I= 17 X= -3.064224471824D+11 Y= 9.343228426712D+12 Z= 1.976594455492D+13
I= 18 X= -7.646619990403D+13 Y= 1.254760234868D+13 Z= -1.696593320392D+13
I= 19 X= -3.142807175601D+13 Y= -6.747359351217D+13 Z= 1.646608235565D+13
I= 20 X= 2.336609492906D+13 Y= -1.730772577248D+13 Z= 2.570562931546D+12

I= 21 X= 3.994512732224D+12 Y= 2.624692157466D+12 Z= 1.053719781886D+13
I= 22 X= 1.603194512276D+13 Y= 3.449243414915D+13 Z= 5.198978631892D+13
I= 23 X= -1.585961781907D+14 Y= 4.924735137922D+13 Z= -4.890208547858D+13
I= 24 X= 4.324695024646D+13 Y= -1.616991045045D+13 Z= 4.574793194119D+13
I= 25 X= 3.462232470312D+12 Y= 5.786005914366D+11 Z= 2.135233712065D+12
I= 26 X= -3.328707176341D+13 Y= 1.401413515762D+13 Z= 7.197622901970D+13
I= 27 X= 5.105191407031D+13 Y= 1.930543247171D+13 Z= 5.221831109339D+13
I= 28 X= -1.395931962748D+14 Y= 1.265231429718D+14 Z= -2.878708058006D+12
I= 29 X= -1.219521534435D+13 Y= 1.800767680336D+13 Z= 1.211654708815D+13
I= 30 X= 9.392422290007D+12 Y= 1.714980047529D+13 Z= 6.433270929488D+11
I= 31 X= -9.749037632170D+12 Y= 4.226474589752D+13 Z= -8.061160103461D+13
I= 32 X= 7.603758862504D+13 Y= -1.375706991242D+14 Z= -2.575621079819D+13
I= 33 X= 8.481247949418D+13 Y= 2.400438901024D+13 Z= 9.179010575201D+13
I= 34 X= -8.814859608986D+13 Y= -4.966860770990D+12 Z= -7.222413504971D+13
I= 35 X= -1.328837964393D+12 Y= -5.769773501135D+12 Z= 3.945979331689D+12
I= 36 X= 1.276102871186D+13 Y= 9.853196662268D+12 Z= -4.209446162434D+12
I= 37 X= -6.039036604780D+13 Y= -1.210552473135D+14 Z= -1.028782960827D+13
I= 38 X= -2.178384813101D+13 Y= 1.350564783759D+13 Z= -2.198931346590D+13

Seed: 43070838607

CM Start Point Coordinates: bohr

I= 0 X= -2.262875065920D+00 Y= -2.151419693026D+00 Z= -6.605282888921D-02
I= 1 X= 4.342305018943D-02 Y= -2.744707231618D+00 Z= -1.414235461711D+00
I= 2 X= -1.363019637421D+00 Y= -1.206500744847D+00 Z= 2.346763789937D+00
I= 3 X= 2.203539264181D+00 Y= -2.076625134425D+00 Z= 4.344271275703D-02
I= 4 X= 1.290090904032D+00 Y= -1.294877162076D+00 Z= 2.449460310887D+00
I= 5 X= -2.873806082614D+00 Y= 3.388645749536D+00 Z= -2.493721286993D+00
I= 6 X= -1.425201035584D-01 Y= 2.073209838501D+00 Z= -3.344081464674D+00
I= 7 X= -2.291276585253D+00 Y= 5.136311918916D+00 Z= -3.613432640214D+00
I= 8 X= -4.280593209165D+00 Y= 2.390249821923D+00 Z= -3.780659834548D+00

I= 9 X= 3.219328984098D+00 Y= -8.623280375829D-01 Z= 4.483793382510D+00
I= 10 X= 3.713994916820D+00 Y= -2.725726969248D+00 Z= 5.501776215796D+00
I= 11 X= 5.356859330223D+00 Y= -4.026339135635D-01 Z= 4.063547058870D+00
I= 12 X= 2.359887601631D+00 Y= 2.826247279507D-01 Z= 6.056022959088D+00
I= 13 X= -3.024782988366D+00 Y= -4.489992613960D-01 Z= 4.566447361222D+00
I= 14 X= -2.947986080205D+00 Y= -2.200821317842D+00 Z= 5.871298933937D+00
I= 15 X= -2.326407531903D+00 Y= 9.792209933037D-01 Z= 5.680583709113D+00
I= 16 X= -4.715913099986D+00 Y= -1.278552983770D-01 Z= 3.988948042230D+00
I= 17 X= -4.933580324050D+00 Y= -2.568650486704D+00 Z= -7.902970448946D-01
I= 18 X= -5.903525982378D+00 Y= -3.875811099841D+00 Z= 4.597342203984D-01
I= 19 X= -5.957615780631D+00 Y= -6.361713380032D-01 Z= -8.931314693895D-01
I= 20 X= -4.946447489353D+00 Y= -3.516836190470D+00 Z= -2.844854184375D+00
I= 21 X= 7.914164840388D-03 Y= -3.572577164355D+00 Z= -4.180732818260D+00
I= 22 X= 7.487964656147D-01 Y= -5.571078533201D+00 Z= -4.926557052536D+00
I= 23 X= -1.896666183731D+00 Y= -3.452016805640D+00 Z= -4.620709804669D+00
I= 24 X= 1.563012221356D+00 Y= -2.285012761029D+00 Z= -5.153793301721D+00
I= 25 X= 4.869539143496D+00 Y= -2.363528626426D+00 Z= -6.723434080713D-01
I= 26 X= 5.165477701563D+00 Y= -3.004283901494D+00 Z= -2.745342220703D+00
I= 27 X= 6.524159017443D+00 Y= -6.369371829795D-01 Z= -3.534978125861D-01
I= 28 X= 5.935820803684D+00 Y= -3.863027741569D+00 Z= 5.969429126799D-01
I= 29 X= 2.729039607257D+00 Y= 3.166515952119D+00 Z= -2.486775942659D+00
I= 30 X= 2.615224939873D+00 Y= 3.650075448906D+00 Z= 1.650093424592D-01
I= 31 X= 4.269008150960D+00 Y= 2.010383076724D+00 Z= -3.322190143730D+00
I= 32 X= 1.884437718262D+00 Y= 4.756973325125D+00 Z= -4.056200632676D+00
I= 33 X= 2.396669274683D+00 Y= 5.381971248598D+00 Z= 1.121341716916D+00
I= 34 X= 3.902432578208D+00 Y= 2.774111694230D+00 Z= 1.697219816089D+00
I= 35 X= 8.761357186782D-03 Y= 1.053812761535D+00 Z= -3.683191432936D-01
I= 36 X= -2.768194723552D+00 Y= 3.744272589142D+00 Z= 8.553434752037D-02
I= 37 X= -1.506988331763D+00 Y= 5.511631407339D+00 Z= 7.134714946008D-01
I= 38 X= -4.462157355725D+00 Y= 2.970011236359D+00 Z= 1.195469870285D+00

Forward Direction:

Total Energy: -692.0006440 Hartrees

Potential Energy: -692.1834648 Hartress

Kinetic Energy: 0.1828207 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.583103721456D+13 Y= 1.533372793924D+13 Z= 2.636789000126D+13
I= 1 X= 2.525532674759D+13 Y= 6.795355738720D+12 Z= 5.935545861261D+12
I= 2 X= -6.462605127884D+12 Y= -6.897311273699D+12 Z= 2.539919258046D+12
I= 3 X= -2.751283103246D+13 Y= -4.087925077467D+12 Z= -4.420598793356D+12
I= 4 X= 6.465161144605D+12 Y= 7.186793216206D+12 Z= -1.121170141860D+13
I= 5 X= 2.112787241348D+13 Y= 3.547956423263D+12 Z= 2.479792539769D+13
I= 6 X= 8.335419151717D+13 Y= 1.295204339955D+13 Z= -4.856534794736D+13
I= 7 X= -9.252969052471D+13 Y= -2.002788333843D+13 Z= 5.540033852136D+13
I= 8 X= -2.498209556886D+12 Y= -8.427604682461D+13 Z= -4.204871767180D+13
I= 9 X= -1.639802135662D+11 Y= 1.546479078762D+13 Z= -2.698167307278D+13
I= 10 X= -6.323626730733D+13 Y= 1.611901507670D+13 Z= 5.491707306198D+12
I= 11 X= -1.256063920885D+14 Y= -1.621031174727D+13 Z= -3.718886933874D+12
I= 12 X= -3.498577172070D+13 Y= 2.133359496938D+13 Z= 4.387131408215D+12
I= 13 X= 7.728904056269D+12 Y= -1.568914821641D+13 Z= -1.933440190713D+12
I= 14 X= -6.507499916650D+13 Y= 8.408736225679D+13 Z= -3.656480842368D+13
I= 15 X= -3.935168343971D+13 Y= 6.953571591766D+12 Z= -4.686408579318D+13
I= 16 X= 6.874073457404D+13 Y= 4.424608092510D+11 Z= 7.720061821179D+13
I= 17 X= -1.932308845441D+13 Y= -6.246228916390D+12 Z= 2.163878898128D+13
I= 18 X= -1.043993761110D+14 Y= -4.587157046456D+13 Z= -6.179588907086D+13
I= 19 X= -1.281280767077D+13 Y= -2.939395265929D+13 Z= 3.029364817472D+13
I= 20 X= -4.608058413449D+12 Y= 1.546209033749D+13 Z= -1.272135992821D+14
I= 21 X= -1.580989287876D+13 Y= 1.160847290968D+13 Z= -8.127412265362D+12
I= 22 X= -2.708827318983D+13 Y= -3.072304421373D+13 Z= 3.032905087835D+13
I= 23 X= 7.659865122999D+13 Y= -7.114833645284D+13 Z= 2.935601994653D+13
I= 24 X= -5.264017873409D+13 Y= 1.470042214830D+13 Z= 4.878064117231D+13

I= 25 X= -1.353729628123D+13 Y= -1.531310762134D+13 Z= -4.299901663775D+12
I= 26 X= -4.665873532036D+13 Y= -2.706516287970D+13 Z= -1.189085789900D+14
I= 27 X= 9.349551466530D+13 Y= 2.621071815814D+13 Z= 6.315530670196D+13
I= 28 X= 2.188682033179D+13 Y= 9.960170179284D+13 Z= 2.418673032830D+13
I= 29 X= 9.473136020084D+10 Y= -6.224122406727D+12 Z= -2.551380231798D+12
I= 30 X= -7.674536345052D+12 Y= -6.034532739478D+12 Z= 7.628386099026D+12
I= 31 X= -7.517568703338D+12 Y= -8.151971971800D+12 Z= 3.936471559833D+13
I= 32 X= 1.372570184808D+14 Y= 2.120238802139D+13 Z= 2.099741762608D+12
I= 33 X= -2.893220763962D+13 Y= -2.207745285397D+13 Z= -4.849940597443D+13
I= 34 X= 3.499289411943D+13 Y= -5.555874684192D+13 Z= -6.608060053597D+13
I= 35 X= 3.944440708514D+12 Y= 1.551839454753D+12 Z= -1.093733455413D+12
I= 36 X= -2.019789948603D+12 Y= 1.819827271897D+13 Z= -2.072877813867D+12
I= 37 X= -8.829630301787D+12 Y= -1.626694540081D+14 Z= -5.258969368343D+13
I= 38 X= 4.124312158742D+13 Y= -4.670831441540D+13 Z= -1.840847044859D+13

Backward Direction:

Total Energy: -692.0007040 Hartrees

Potential Energy: -692.1834648 Hartress

Kinetic Energy: 0.1827607 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.622259747333D+13 Y= 1.731588025986D+13 Z= 2.865165948745D+13
I= 1 X= 2.790697467138D+13 Y= 6.795563810229D+12 Z= 5.935502130473D+12
I= 2 X= -6.628466946766D+12 Y= -9.158203027761D+12 Z= 3.992969030294D+12
I= 3 X= -2.712117915238D+13 Y= -6.070313821054D+12 Z= -6.704705686998D+12
I= 4 X= 6.299374681195D+12 Y= 9.447817007978D+12 Z= -1.266493187896D+13
I= 5 X= 2.683170873019D+13 Y= -3.154002012422D+12 Z= 1.471243549566D+13
I= 6 X= -8.342970400442D+13 Y= 1.297075774652D+13 Z= -4.856672017976D+13
I= 7 X= -1.110435026115D+14 Y= -1.074571586132D+13 Z= 4.781729030155D+13
I= 8 X= -1.477070346492D+13 Y= -7.661687215394D+13 Z= -4.508922422619D+13
I= 9 X= 3.518852382449D+11 Y= 1.442721862391D+13 Z= -2.787603351063D+13
I= 10 X= -6.453843828261D+13 Y= 1.419649059175D+13 Z= 3.459396177163D+12

I= 11 X= -1.247266925398D+14 Y= -1.897097557410D+13 Z= -4.119964084022D+12
I= 12 X= -3.296454915964D+13 Y= 2.016790041826D+13 Z= 4.737207602903D+12
I= 13 X= 8.244606009883D+12 Y= -1.465156023355D+13 Z= -1.038974318267D+12
I= 14 X= -6.637685803247D+13 Y= 8.600994052362D+13 Z= -3.453249313110D+13
I= 15 X= -3.733089826045D+13 Y= 8.119860556875D+12 Z= -4.721423154967D+13
I= 16 X= 6.961999576719D+13 Y= 3.202336965266D+12 Z= 7.760219374725D+13
I= 17 X= -1.889332745501D+13 Y= -5.767792892256D+12 Z= 2.307303193546D+13
I= 18 X= -1.030083978623D+14 Y= -4.542344688031D+13 Z= -5.960544637643D+13
I= 19 X= -1.332729767008D+13 Y= -2.946422454542D+13 Z= 3.126609508581D+13
I= 20 X= -4.205104791546D+12 Y= 1.456120747031D+13 Z= -1.257114705602D+14
I= 21 X= -1.662483798143D+13 Y= 1.160926088438D+13 Z= -8.127944823187D+12
I= 22 X= -2.935946352059D+13 Y= -3.072227115880D+13 Z= 3.032748137851D+13
I= 23 X= 7.565845946267D+13 Y= -7.022293585872D+13 Z= 3.004124284489D+13
I= 24 X= -5.358077588600D+13 Y= 1.377753868476D+13 Z= 4.809414034602D+13
I= 25 X= -1.310753953108D+13 Y= -1.579167411987D+13 Z= -5.734108331738D+12
I= 26 X= -4.625541720163D+13 Y= -2.616534312639D+13 Z= -1.204106163583D+14
I= 27 X= 9.298096823918D+13 Y= 2.628076432731D+13 Z= 6.218276763261D+13
I= 28 X= 2.327737147464D+13 Y= 9.915357289674D+13 Z= 2.199728967799D+13
I= 29 X= 5.798474356806D+12 Y= 4.751982556599D+11 Z= 7.532637075024D+12
I= 30 X= -1.011557164942D+12 Y= -2.441922052457D+12 Z= 1.115071981426D+13
I= 31 X= -1.978168309207D+13 Y= -1.580631520480D+13 Z= 4.240512322206D+13
I= 32 X= 1.187428079067D+14 Y= 1.191828021539D+13 Z= 9.678745753623D+12
I= 33 X= -3.007460576952D+13 Y= -2.478608516545D+13 Z= -3.857488811839D+13
I= 34 X= 3.357458500464D+13 Y= -5.944760044849D+13 Z= -5.935036546454D+13
I= 35 X= 2.022121021961D+12 Y= 1.551966895539D+12 Z= -1.093052141115D+12
I= 36 X= 4.644234044092D+12 Y= 1.460465417276D+13 Z= -5.595347328770D+12
I= 37 X= -9.972715369605D+12 Y= -1.599581513983D+14 Z= -6.251727122227D+13
I= 38 X= 3.982729842727D+13 Y= -4.281888906285D+13 Z= -2.513806344122D+13

Seed: 4485029639

CM Start Point Coordinates: bohr

I= 0 X= -2.246199411783D+00 Y= -2.055793799827D+00 Z= -1.602068419222D-02
I= 1 X= -7.851310367045D-02 Y= -2.529552653015D+00 Z= -1.446445075186D+00
I= 2 X= -1.368808420079D+00 Y= -1.286704929415D+00 Z= 2.415622657378D+00
I= 3 X= 2.234005146052D+00 Y= -2.136620590161D+00 Z= -4.147229191144D-02
I= 4 X= 1.269651644429D+00 Y= -1.334150119855D+00 Z= 2.458149910300D+00
I= 5 X= -2.840328469663D+00 Y= 3.136798252086D+00 Z= -2.321253851081D+00
I= 6 X= 1.647704165409D-01 Y= 1.810475587004D+00 Z= -3.230954901793D+00
I= 7 X= -2.746763596149D+00 Y= 4.666471417442D+00 Z= -3.963503990563D+00
I= 8 X= -4.124422953892D+00 Y= 1.869756746562D+00 Z= -3.129829959802D+00
I= 9 X= 3.027655416733D+00 Y= -6.881212525969D-01 Z= 4.578534747255D+00
I= 10 X= 2.807381297390D+00 Y= -1.990208629555D+00 Z= 6.287093555858D+00
I= 11 X= 5.153294009797D+00 Y= -6.273501318593D-01 Z= 4.215567343191D+00
I= 12 X= 2.993140251484D+00 Y= 1.507308739261D+00 Z= 5.459972696363D+00
I= 13 X= -2.975244757802D+00 Y= -8.142493770870D-01 Z= 4.625561981048D+00
I= 14 X= -2.729611807864D+00 Y= -2.185562334403D+00 Z= 6.328696825267D+00
I= 15 X= -2.337903245654D+00 Y= 8.588047254325D-01 Z= 5.474695809580D+00
I= 16 X= -5.013107718052D+00 Y= -4.199201423178D-01 Z= 4.081194281973D+00
I= 17 X= -4.847618452570D+00 Y= -2.520104981025D+00 Z= -8.766963738674D-01
I= 18 X= -5.564625231723D+00 Y= -3.874388124948D+00 Z= 5.488032254159D-01
I= 19 X= -6.316152595932D+00 Y= -6.800835257287D-01 Z= -7.415803321878D-01
I= 20 X= -4.754662664254D+00 Y= -3.741836784095D+00 Z= -2.741938905447D+00
I= 21 X= 2.465364796868D-01 Y= -3.767686758248D+00 Z= -4.211538041690D+00
I= 22 X= 6.296522522562D-01 Y= -5.695389171973D+00 Z= -4.098139406253D+00
I= 23 X= -1.379332825618D+00 Y= -3.277522137097D+00 Z= -5.373699069994D+00
I= 24 X= 1.873402340497D+00 Y= -2.781513326166D+00 Z= -5.083422359901D+00
I= 25 X= 4.842236943448D+00 Y= -2.531424423463D+00 Z= -8.167712725957D-01
I= 26 X= 4.854000312146D+00 Y= -1.856170866131D+00 Z= -3.119255246271D+00
I= 27 X= 6.239934578267D+00 Y= -1.157763967632D+00 Z= 2.964718470570D-01
I= 28 X= 5.239646066374D+00 Y= -4.742611771418D+00 Z= -3.555389353271D-01

I= 29 X= 2.790523117028D+00 Y= 3.138884085930D+00 Z= -2.481881421338D+00
I= 30 X= 3.199857446509D+00 Y= 3.632865775451D+00 Z= 1.108456222570D-01
I= 31 X= 3.779266448506D+00 Y= 1.888306616527D+00 Z= -3.241009440719D+00
I= 32 X= 2.086038612342D+00 Y= 4.714275517674D+00 Z= -3.616167594945D+00
I= 33 X= 2.844477046945D+00 Y= 5.612508743992D+00 Z= 9.532365723532D-01
I= 34 X= 4.277757558657D+00 Y= 2.479319193626D+00 Z= 1.387877904226D+00
I= 35 X= -1.049507892331D-01 Y= 1.185792426879D+00 Z= -3.957473720128D-01
I= 36 X= -2.857442811754D+00 Y= 3.839277277167D+00 Z= 1.307619870722D-01
I= 37 X= -2.236560750625D+00 Y= 5.629840912776D+00 Z= 7.197041390740D-01
I= 38 X= -4.321359304302D+00 Y= 3.101046471638D+00 Z= 9.908748570419D-01

Forward Direction:

Total Energy: -691.9984279 Hartrees

Potential Energy: -692.1842500 Hartress

Kinetic Energy: 0.1858221 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.223479646424D+12 Y= -1.266496861872D+13 Z= -5.658949122766D+12
I= 1 X= -1.021678487134D+13 Y= 9.050859755405D+12 Z= -6.285355779073D+12
I= 2 X= -4.196450441591D+11 Y= -9.739918247322D+12 Z= -1.823001683324D+13
I= 3 X= -1.264531907961D+13 Y= -9.949337975790D+12 Z= 1.560891443178D+13
I= 4 X= -7.492860919368D+12 Y= 1.444920089246D+13 Z= -1.938379629015D+13
I= 5 X= -1.861171501542D+13 Y= -1.514061571074D+13 Z= -1.582342569671D+13
I= 6 X= 3.803562353483D+13 Y= -2.612586256114D+13 Z= -8.345452353874D+13
I= 7 X= 7.568048204681D+13 Y= 3.582937741596D+13 Z= -3.581273308739D+13
I= 8 X= 5.060462439356D+13 Y= 4.127364149458D+13 Z= -4.160653869185D+13
I= 9 X= 1.749208571301D+13 Y= -9.333103821007D+12 Z= 1.014940520137D+12
I= 10 X= 4.087609112999D+11 Y= 3.519788334282D+13 Z= 4.734041346679D+13
I= 11 X= 6.263398458314D+13 Y= 7.868920571250D+13 Z= -4.333328247014D+13
I= 12 X= -7.680209084002D+13 Y= 1.004553771400D+14 Z= 7.320049197055D+13
I= 13 X= 1.692488286408D+12 Y= -1.017967141763D+13 Z= -1.076282354426D+13
I= 14 X= 7.273173082374D+13 Y= -2.652484113370D+12 Z= 3.660885806343D+13

I= 15 X= 4.932751496611D+13 Y= 4.007594742512D+13 Z= 8.074095806872D+13
I= 16 X= 8.504914933663D+13 Y= -7.182953822400D+13 Z= -1.474082566882D+13
I= 17 X= 3.260280964677D+12 Y= 1.209474739976D+12 Z= 1.230564004569D+13
I= 18 X= 2.143336906018D+13 Y= -3.217701487971D+13 Z= -4.684313647506D+13
I= 19 X= -3.699393789046D+13 Y= 5.130730957880D+13 Z= -6.390142848654D+13
I= 20 X= -4.029215274654D+13 Y= -4.405370202753D+12 Z= 8.792464845572D+13
I= 21 X= 1.598856924521D+13 Y= 3.063158654481D+13 Z= 7.977980209032D+12
I= 22 X= 3.716851254647D+13 Y= -1.141145563469D+14 Z= 5.014749738131D+13
I= 23 X= -7.454620052006D+13 Y= 3.379078245176D+13 Z= -1.456177257431D+13
I= 24 X= -1.063566286559D+14 Y= -5.538254749523D+13 Z= -3.763995988212D+12
I= 25 X= -4.911531076782D+12 Y= 6.729049859433D+12 Z= -1.275681772908D+13
I= 26 X= 2.400935479755D+13 Y= 6.677485587962D+13 Z= 3.834451292535D+13
I= 27 X= 2.277725672704D+13 Y= -5.840184566648D+13 Z= 2.084483048487D+13
I= 28 X= -2.550197968812D+12 Y= -1.372946392848D+14 Z= 1.261282329191D+14
I= 29 X= -4.839347912431D+12 Y= -6.580459511268D+12 Z= 1.319135604304D+12
I= 30 X= 3.499972896013D+12 Y= 7.447103494115D+12 Z= -8.482936927315D+12
I= 31 X= 9.043481473469D+13 Y= -3.260701941190D+13 Z= -1.161940417967D+14
I= 32 X= -1.185512420660D+13 Y= 6.852695437695D+11 Z= 1.064602300692D+13
I= 33 X= -8.815906334876D+13 Y= -1.133019210191D+14 Z= -5.624856631442D+13
I= 34 X= -6.145937531838D+12 Y= -4.663564717176D+13 Z= 7.051442461306D+12
I= 35 X= -3.967457772725D+11 Y= -8.312228474755D+11 Z= 6.810635705438D+12
I= 36 X= 3.518134845756D+12 Y= 2.226261603251D+13 Z= 1.866936742503D+13
I= 37 X= -9.275529070207D+12 Y= 1.277761295539D+14 Z= 4.197950885792D+13
I= 38 X= -5.733170564462D+12 Y= -8.492789426356D+13 Z= -1.666735662230D+13

Backward Direction:

Total Energy: -691.9984637 Hartrees

Potential Energy: -692.1842500 Hartress

Kinetic Energy: 0.1857864 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.349080169739D+12 Y= -1.156695625577D+13 Z= -4.127432869490D+12

I= 1 X= -9.307200399172D+12 Y= 9.051047081665D+12 Z= -6.285444158901D+12
I= 2 X= -1.382560372310D+11 Y= -1.049652752831D+13 Z= -1.736732338747D+13
I= 3 X= -1.251961336745D+13 Y= -1.104746264250D+13 Z= 1.407718666682D+13
I= 4 X= -7.211398691139D+12 Y= 1.520590413267D+13 Z= -2.024651072956D+13
I= 5 X= -1.636960742559D+13 Y= -2.111513585077D+13 Z= -2.322137614835D+13
I= 6 X= -3.890440066274D+13 Y= -2.611525679085D+13 Z= -8.345469107144D+13
I= 7 X= 6.522292074064D+13 Y= 3.608813191576D+13 Z= -4.406941815978D+13
I= 8 X= 4.495422588375D+13 Y= 4.028219123265D+13 Z= -4.370451154737D+13
I= 9 X= 1.841110634421D+13 Y= -1.101883801041D+13 Z= 3.996596837914D+11
I= 10 X= -3.237043085430D+11 Y= 3.295113706120D+13 Z= 4.597433264491D+13
I= 11 X= 6.385950696945D+13 Y= 7.525562465308D+13 Z= -4.369061376778D+13
I= 12 X= -7.437766591593D+13 Y= 9.887100831725D+13 Z= 7.340860204508D+13
I= 13 X= 2.611400634552D+12 Y= -8.493919089731D+12 Z= -1.014729421549D+13
I= 14 X= 7.199995441072D+13 Y= -4.055090177429D+11 Z= 3.797528957515D+13
I= 15 X= 5.175144172051D+13 Y= 4.166105131483D+13 Z= 8.053274135953D+13
I= 16 X= 8.627420672361D+13 Y= -6.839695712361D+13 Z= -1.438282672540D+13
I= 17 X= 3.249207385213D+12 Y= 1.360379877761D+12 Z= 1.414688381188D+13
I= 18 X= 2.194723074122D+13 Y= -3.141617889550D+13 Z= -4.320501460427D+13
I= 19 X= -3.724098622111D+13 Y= 5.175430207968D+13 Z= -6.308258841215D+13
I= 20 X= -4.072727777081D+13 Y= -6.442793293907D+12 Z= 8.994567888873D+13
I= 21 X= 1.444001342823D+13 Y= 3.063243878168D+13 Z= 7.977407131961D+12
I= 22 X= 3.314454644282D+13 Y= -1.141136734087D+14 Z= 5.014587938364D+13
I= 23 X= -7.562657273611D+13 Y= 3.565628735393D+13 Z= -1.431751252366D+13
I= 24 X= -1.074372779551D+14 Y= -5.724560064776D+13 Z= -4.009196533568D+12
I= 25 X= -4.922448542186D+12 Y= 6.577826126118D+12 Z= -1.459809632161D+13
I= 26 X= 2.357462719825D+13 Y= 6.881156888817D+13 Z= 3.632335576776D+13
I= 27 X= 2.253043432083D+13 Y= -5.884950964013D+13 Z= 2.002615839769D+13
I= 28 X= -2.036395723932D+12 Y= -1.380559427480D+14 Z= 1.224904558618D+14
I= 29 X= -2.597515813049D+12 Y= -6.079275334582D+11 Z= 8.715500217820D+12
I= 30 X= 6.696304048604D+12 Y= 8.530082657186D+12 Z= -3.531254953229D+12

I= 31 X= 8.478792877547D+13 Y= -3.161502906060D+13 Z= -1.140971637494D+14
I= 32 X= -2.231177401085D+13 Y= 4.261432898995D+11 Z= 1.889958161104D+13
I= 33 X= -8.914759490764D+13 Y= -1.166065381474D+14 Z= -4.535300674783D+13
I= 34 X= -6.017601442673D+12 Y= -5.039781499523D+13 Z= 1.178143777434D+13
I= 35 X= -1.109154663103D+12 Y= -8.310353386456D+11 Z= 6.811277089504D+12
I= 36 X= 6.714778620980D+12 Y= 2.117884838019D+13 Z= 1.371740036574D+13
I= 37 X= -1.026567676955D+13 Y= 1.310829912035D+14 Z= 3.108231736766D+13
I= 38 X= -5.603975231283D+12 Y= -8.116668020933D+13 Z= -2.139719888762D+13

Seed: 4549675668

CM Start Point Coordinates: bohr

I= 0 X= -2.170230184940D+00 Y= -2.087116222471D+00 Z= -7.071878815361D-02
I= 1 X= 6.147326166997D-03 Y= -2.787259173455D+00 Z= -1.455566713067D+00
I= 2 X= -1.276948681820D+00 Y= -1.195385369578D+00 Z= 2.431417499127D+00
I= 3 X= 2.309526432005D+00 Y= -1.980415863248D+00 Z= -6.302171825293D-02
I= 4 X= 1.257926967992D+00 Y= -1.168299862676D+00 Z= 2.285340135034D+00
I= 5 X= -2.887628124565D+00 Y= 3.274704365120D+00 Z= -2.358533144856D+00
I= 6 X= 7.017427009119D-02 Y= 1.705177096547D+00 Z= -3.208692860902D+00
I= 7 X= -2.275904035041D+00 Y= 4.865131830931D+00 Z= -3.886265777625D+00
I= 8 X= -4.356043414885D+00 Y= 2.008004496606D+00 Z= -3.099313535531D+00
I= 9 X= 2.931694098407D+00 Y= -6.705945823910D-01 Z= 4.732808638405D+00
I= 10 X= 2.719897938693D+00 Y= -2.487639561074D+00 Z= 5.813205071608D+00
I= 11 X= 5.024408657334D+00 Y= -4.654807685680D-01 Z= 4.189046235345D+00
I= 12 X= 2.630230108290D+00 Y= 6.551137906306D-01 Z= 6.126892586295D+00
I= 13 X= -2.941062680437D+00 Y= -7.352010504962D-01 Z= 4.568494274434D+00
I= 14 X= -3.409572637428D+00 Y= -2.671907374164D+00 Z= 5.632204071045D+00
I= 15 X= -2.351839530036D+00 Y= 5.809945058487D-01 Z= 6.394437055245D+00
I= 16 X= -4.840901401069D+00 Y= -3.098470451943D-02 Z= 3.631780688131D+00
I= 17 X= -5.040275872470D+00 Y= -2.500448235395D+00 Z= -8.536437485657D-01
I= 18 X= -5.545617376605D+00 Y= -4.365450245451D+00 Z= -3.695278410219D-01

I= 19 X= -6.510863247326D+00 Y= -1.310884678414D+00 Z= -3.805459193352D-01
I= 20 X= -4.938104561894D+00 Y= -2.774522296877D+00 Z= -2.896693153685D+00
I= 21 X= -1.245957440852D-01 Y= -4.047520878386D+00 Z= -4.063132818233D+00
I= 22 X= 1.265488285285D+00 Y= -6.211689088391D+00 Z= -4.327710055604D+00
I= 23 X= -2.370787671519D+00 Y= -4.299902038583D+00 Z= -4.545900892642D+00
I= 24 X= 9.201198293161D-01 Y= -2.641219850789D+00 Z= -5.747114088020D+00
I= 25 X= 4.999238607526D+00 Y= -2.275631786427D+00 Z= -7.696389854745D-01
I= 26 X= 5.093594517991D+00 Y= -2.536644260876D+00 Z= -2.973025047590D+00
I= 27 X= 6.049610420425D+00 Y= -4.989597026474D-01 Z= -1.908890203019D-01
I= 28 X= 5.781819990725D+00 Y= -3.469514369103D+00 Z= 7.045087532265D-01
I= 29 X= 2.831024254047D+00 Y= 3.289575174029D+00 Z= -2.394462591163D+00
I= 30 X= 3.114286176038D+00 Y= 3.558128381173D+00 Z= 3.360337482123D-01
I= 31 X= 4.175158708948D+00 Y= 1.955881512688D+00 Z= -3.452506070940D+00
I= 32 X= 2.227735644529D+00 Y= 4.757185345115D+00 Z= -3.549781144692D+00
I= 33 X= 2.807462868331D+00 Y= 5.324967609756D+00 Z= 1.383089976093D+00
I= 34 X= 4.839776015240D+00 Y= 2.250699477097D+00 Z= 1.071091016446D+00
I= 35 X= -5.580558411117D-02 Y= 1.118347880951D+00 Z= -5.195859389261D-01
I= 36 X= -2.825480194050D+00 Y= 3.913056720114D+00 Z= 3.313278173928D-01
I= 37 X= -1.817553765699D+00 Y= 5.927813376148D+00 Z= 7.262905006640D-01
I= 38 X= -4.111383475073D+00 Y= 2.782358925386D+00 Z= 1.705616860077D+00

Forward Direction:

Total Energy: -691.9949595 Hartrees

Potential Energy: -692.1588750 Hartress

Kinetic Energy: 0.1639155 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.260041961873D+12 Y= -7.124621310938D+12 Z= -3.402452800257D+12

I= 1 X= -1.362369211349D+13 Y= 1.041862026416D+13 Z= 1.036875800836D+13

I= 2 X= 1.016771062631D+13 Y= -8.773899070366D+12 Z= -3.825145771327D+12

I= 3 X= 1.287261358112D+13 Y= 1.374246484459D+13 Z= -9.019608383759D+12

I= 4 X= -3.617226508450D+12 Y= 1.833240756270D+12 Z= 2.917262761092D+11

I= 5 X= -1.910369692946D+13 Y= 1.194679749240D+13 Z= 9.784266485892D+12
I= 6 X= 4.848238634019D+13 Y= 2.735100397685D+13 Z= 9.328256949278D+13
I= 7 X= -2.656018959355D+13 Y= -7.813854891404D+13 Z= 5.500779396289D+13
I= 8 X= -2.126114095467D+13 Y= -1.144877730374D+14 Z= -1.013686851353D+14
I= 9 X= -1.612278000512D+13 Y= -1.770454871163D+13 Z= -9.961078645606D+12
I= 10 X= -1.117214294020D+13 Y= -3.546768357649D+13 Z= 2.937352627622D+13
I= 11 X= -2.272546500025D+13 Y= 3.323442531679D+13 Z= -7.056018846523D+12
I= 12 X= -2.924032085339D+13 Y= -3.908435757969D+13 Z= 9.375870619420D+12
I= 13 X= 1.099689235566D+13 Y= 2.037788648202D+13 Z= 5.872802860122D+12
I= 14 X= -1.944479663297D+13 Y= -1.406449969082D+14 Z= 1.044182403247D+14
I= 15 X= -6.190158785082D+13 Y= -5.637362874389D+13 Z= -1.666085471527D+13
I= 16 X= -6.843887600910D+13 Y= 2.359723312269D+13 Z= -3.304967035687D+13
I= 17 X= 1.754340371380D+12 Y= 4.955476840821D+12 Z= 1.029021551886D+13
I= 18 X= 1.734386243733D+13 Y= -4.697188852923D+13 Z= -1.328782145106D+13
I= 19 X= -1.670880891565D+13 Y= 4.445235080826D+13 Z= -6.772262924638D+13
I= 20 X= -3.620835899979D+13 Y= 6.240938386135D+13 Z= -2.617625627009D+13
I= 21 X= -7.875399349881D+11 Y= 1.217948308379D+13 Z= -6.216605306911D+12
I= 22 X= -4.788789851900D+13 Y= -1.461286803266D+14 Z= 3.959672672992D+13
I= 23 X= 9.285496310911D+13 Y= 3.997743266704D+13 Z= 5.344884488032D+13
I= 24 X= 5.090965293257D+13 Y= 5.120458141129D+13 Z= -1.036067266840D+14
I= 25 X= 1.657225471295D+13 Y= -5.558627383784D+12 Z= -7.711118560897D+11
I= 26 X= -2.196304728261D+13 Y= 5.340876265162D+13 Z= 1.371186837755D+14
I= 27 X= -7.273781097360D+13 Y= -1.214887925387D+13 Z= -3.505694227362D+13
I= 28 X= 1.149126032577D+12 Y= -3.209393630904D+13 Z= 1.478215643893D+13
I= 29 X= -1.657764894197D+13 Y= 2.180213472362D+12 Z= -3.478790724750D+12
I= 30 X= 2.207147453830D+12 Y= 1.453344855436D+13 Z= -1.411369167101D+13
I= 31 X= 5.384481852509D+13 Y= -7.617975206362D+13 Z= -7.572840407127D+13
I= 32 X= 1.302924143192D+13 Y= 8.917764466954D+13 Z= 1.347683586041D+12
I= 33 X= 1.698449244374D+13 Y= -6.367131964029D+13 Z= -5.844158801093D+13
I= 34 X= -1.623884165113D+13 Y= -8.921191224507D+13 Z= -2.561778913457D+13

I= 35 X= 2.715685885735D+12 Y= -2.630424232181D+12 Z= 7.816299356099D+11
I= 36 X= 2.115842176216D+13 Y= 4.793908743995D+11 Z= 2.678793828805D+12
I= 37 X= 2.990853946974D+13 Y= -3.017538497593D+13 Z= 5.023098734826D+13
I= 38 X= -6.494120676982D+12 Y= 5.294100876014D+13 Z= 6.703542091224D+13

Backward Direction:

Total Energy: -691.9950116 Hartrees

Potential Energy: -692.1588750 Hartress

Kinetic Energy: 0.1638634 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.003080823135D+12 Y= -5.412886612059D+12 Z= -1.193368081859D+12
I= 1 X= -1.183107692192D+13 Y= 1.041886402542D+13 Z= 1.036866319618D+13
I= 2 X= 1.035635566356D+13 Y= -1.028551220059D+13 Z= -2.518959469546D+12
I= 3 X= 1.312970224365D+13 Y= 1.203054257785D+13 Z= -1.122900636807D+13
I= 4 X= -3.428488408867D+12 Y= 3.344986424520D+12 Z= -1.014545755166D+12
I= 5 X= -1.499380497293D+13 Y= 4.148003484850D+12 Z= -5.355755345375D+11
I= 6 X= -8.181109508357D+13 Y= 2.736737768998D+13 Z= 9.328191137209D+13
I= 7 X= -4.272769417567D+13 Y= -7.446435752436D+13 Z= 4.485296213729D+13
I= 8 X= -3.083868822305D+13 Y= -1.125273678212D+14 Z= -1.043622016487D+14
I= 9 X= -1.511425249089D+13 Y= -1.958835236839D+13 Z= -1.083998575530D+13
I= 10 X= -1.230655788546D+13 Y= -3.817865218303D+13 Z= 2.740483606792D+13
I= 11 X= -2.130942173348D+13 Y= 2.915723206110D+13 Z= -7.522546962329D+12
I= 12 X= -2.633475345861D+13 Y= -4.092557508047D+13 Z= 9.690799802753D+12
I= 13 X= 1.200526294385D+13 Y= 2.226171211893D+13 Z= 6.751970019328D+12
I= 14 X= -2.057848330877D+13 Y= -1.379338048778D+14 Z= 1.063872438405D+14
I= 15 X= -5.899662564210D+13 Y= -5.453153709621D+13 Z= -1.697590451617D+13
I= 16 X= -6.702340885120D+13 Y= 2.767324502317D+13 Z= -3.258236369536D+13
I= 17 X= 1.903956555514D+12 Y= 5.267171797238D+12 Z= 1.245946921426D+13
I= 18 X= 1.831686506933D+13 Y= -4.612914100480D+13 Z= -9.240346873094D+12
I= 19 X= -1.711936422637D+13 Y= 4.482370522458D+13 Z= -6.663376031355D+13
I= 20 X= -3.644572095568D+13 Y= 6.026360595965D+13 Z= -2.382196236873D+13

I= 21 X= -2.466770674310D+12 Y= 1.218053319463D+13 Z= -6.217312445179D+12
I= 22 X= -5.230839497960D+13 Y= -1.461276084562D+14 Z= 3.959470578996D+13
I= 23 X= 9.154552979098D+13 Y= 4.197945244371D+13 Z= 5.392027110525D+13
I= 24 X= 4.959982284626D+13 Y= 4.920567548280D+13 Z= -1.040794632919D+14
I= 25 X= 1.672200814369D+13 Y= -5.870654049941D+12 Z= -2.940383006100D+12
I= 26 X= -2.219992056777D+13 Y= 5.555351478756D+13 Z= 1.347643110964D+14
I= 27 X= -7.314818625099D+13 Y= -1.252091427127D+13 Z= -3.614569589866D+13
I= 28 X= 2.121917317790D+12 Y= -3.293710123605D+13 Z= 1.073536017388D+13
I= 29 X= -1.246803655736D+13 Y= 9.976261019933D+12 Z= 6.839094898660D+12
I= 30 X= 7.521343583406D+12 Y= 1.682937411105D+13 Z= -8.404113293862D+12
I= 31 X= 4.427350353145D+13 Y= -7.813788440290D+13 Z= -7.273589767075D+13
I= 32 X= -3.137600564581D+12 Y= 8.550240280114D+13 Z= 1.149823500937D+13
I= 33 X= 1.568168797655D+13 Y= -6.761454270932D+13 Z= -4.507169105089D+13
I= 34 X= -1.665099644139D+13 Y= -9.399986994732D+13 Z= -1.891503116492D+13
I= 35 X= 1.368998516624D+12 Y= -2.630210224557D+12 Z= 7.824529999760D+11
I= 36 X= 2.647328353263D+13 Y= -1.817609715456D+12 Z= -3.031088406317D+12
I= 37 X= 2.860404317282D+13 Y= -2.622917546002D+13 Z= 3.685850413013D+13
I= 38 X= -6.904589078119D+12 Y= 5.772833058860D+13 Z= 6.033303726817D+13

Seed: 46230614170

CM Start Point Coordinates: bohr

I= 0 X= -2.287687356561D+00 Y= -2.189923912972D+00 Z= -7.276725748344D-02
I= 1 X= -1.839355284659D-02 Y= -2.762004048837D+00 Z= -1.437969808735D+00
I= 2 X= -1.331007034295D+00 Y= -1.347715323320D+00 Z= 2.317183505436D+00
I= 3 X= 2.101493107203D+00 Y= -2.113431211996D+00 Z= 4.102111696096D-02
I= 4 X= 1.383927627016D+00 Y= -1.171263983736D+00 Z= 2.318568658466D+00
I= 5 X= -2.889487423321D+00 Y= 3.151374508948D+00 Z= -2.170278217176D+00
I= 6 X= -6.987584114928D-02 Y= 1.511656936417D+00 Z= -3.039778257728D+00
I= 7 X= -1.967279569525D+00 Y= 4.370663222874D+00 Z= -3.681867486777D+00
I= 8 X= -4.651559659156D+00 Y= 1.942585282332D+00 Z= -2.826551702260D+00

I= 9 X= 2.889689800523D+00 Y= -4.349870242216D-01 Z= 4.576462612894D+00
I= 10 X= 3.003984090623D+00 Y= -1.778191365123D+00 Z= 6.014878812553D+00
I= 11 X= 4.922019436597D+00 Y= 2.275810908042D-01 Z= 3.882502752811D+00
I= 12 X= 2.216382221962D+00 Y= 1.618362279156D+00 Z= 5.264982173312D+00
I= 13 X= -3.134753173805D+00 Y= -6.113897062562D-01 Z= 4.458204734051D+00
I= 14 X= -3.603091453059D+00 Y= -2.269594316343D+00 Z= 5.937527139159D+00
I= 15 X= -2.317123778774D+00 Y= 9.237843400151D-01 Z= 5.575625482038D+00
I= 16 X= -5.198364060312D+00 Y= 3.018782854725D-01 Z= 3.706388506029D+00
I= 17 X= -4.992509113044D+00 Y= -2.796420742373D+00 Z= -6.718947410702D-01
I= 18 X= -5.769009863497D+00 Y= -4.673405592082D+00 Z= 6.195764860791D-01
I= 19 X= -6.205441077673D+00 Y= -1.223324267973D+00 Z= 2.637924204227D-01
I= 20 X= -5.905755982800D+00 Y= -3.184033722890D+00 Z= -2.542217436809D+00
I= 21 X= 1.304125840755D-01 Y= -3.497257123174D+00 Z= -4.239327107400D+00
I= 22 X= 1.107439096628D+00 Y= -5.517148021648D+00 Z= -4.563949452570D+00
I= 23 X= -1.947476204820D+00 Y= -3.444033234726D+00 Z= -5.034697168254D+00
I= 24 X= 1.429248281289D+00 Y= -2.198315156434D+00 Z= -5.111406574635D+00
I= 25 X= 4.803640928288D+00 Y= -2.528455547317D+00 Z= -7.882020189053D-01
I= 26 X= 5.243490233908D+00 Y= -1.791618962973D+00 Z= -2.810682437949D+00
I= 27 X= 5.784525260387D+00 Y= -1.231304317927D+00 Z= 5.256695264318D-01
I= 28 X= 5.161728195965D+00 Y= -4.797285044285D+00 Z= -9.120175308742D-01
I= 29 X= 2.721697981435D+00 Y= 3.167104452335D+00 Z= -2.283874629889D+00
I= 30 X= 3.113247713763D+00 Y= 3.657337804494D+00 Z= 3.639780096571D-01
I= 31 X= 3.924839166180D+00 Y= 1.959693346509D+00 Z= -3.398726404227D+00
I= 32 X= 1.956510966391D+00 Y= 4.823577891880D+00 Z= -3.369522488604D+00
I= 33 X= 2.061161778850D+00 Y= 5.734722458724D+00 Z= 6.825095013218D-01
I= 34 X= 4.547088562676D+00 Y= 2.578758157123D+00 Z= 1.291484694896D+00
I= 35 X= 7.295178972747D-02 Y= 1.078203840979D+00 Z= -5.425915950508D-01
I= 36 X= -2.654364682535D+00 Y= 3.937815205739D+00 Z= 3.571700193040D-01
I= 37 X= -1.757516746779D+00 Y= 5.789345078633D+00 Z= 8.211330713113D-01
I= 38 X= -4.278002074662D+00 Y= 3.231506764668D+00 Z= 1.472353868735D+00

Forward Direction:

Total Energy: -692.0126924 Hartrees

Potential Energy: -692.1924049 Hartress

Kinetic Energy: 0.1797125 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.086375564246D+13 Y= -9.184956445943D+12 Z= -2.185916913653D+13
I= 1 X= -6.336714966055D+12 Y= 2.396767345990D+13 Z= -1.922345071334D+12
I= 2 X= 2.840690881260D+12 Y= 4.439025159268D+12 Z= 8.296815065240D+12
I= 3 X= -2.270603724620D+13 Y= 1.626243060657D+13 Z= 5.504721863099D+12
I= 4 X= -7.244850251650D+12 Y= 3.248406051202D+12 Z= -1.663779779063D+13
I= 5 X= -6.659847521769D+12 Y= -1.956594794594D+12 Z= 7.392705971125D+12
I= 6 X= 1.322104528788D+13 Y= 3.525787905540D+13 Z= 1.565442169134D+13
I= 7 X= -1.016723429764D+13 Y= -3.982587929718D+13 Z= 9.992759789117D+13
I= 8 X= 5.279728216264D+13 Y= 8.941430351974D+13 Z= 6.015846575060D+13
I= 9 X= 2.213881367295D+13 Y= 1.278321938663D+13 Z= 2.948098944962D+12
I= 10 X= -6.540818261730D+13 Y= -5.116210784058D+13 Z= 2.449789260592D+13
I= 11 X= -5.411856534174D+13 Y= 6.486854519006D+12 Z= 3.462450362979D+12
I= 12 X= 4.498915819717D+13 Y= -3.331974144953D+13 Z= 2.002199545593D+13
I= 13 X= -9.692004452006D+12 Y= 1.736763953152D+12 Z= 2.907777376767D+13
I= 14 X= -7.847290753917D+12 Y= 1.144092688005D+13 Z= -3.316309612045D+13
I= 15 X= 5.879273156582D+13 Y= -6.198294233633D+13 Z= -1.568975902501D+14
I= 16 X= -8.565087371794D+13 Y= 4.151959485543D+13 Z= 1.164480009257D+13
I= 17 X= 8.893136809437D+12 Y= 9.632269083282D+12 Z= -8.452337708629D+10
I= 18 X= -3.708008698174D+13 Y= -8.448044712121D+13 Z= 3.808145297261D+13
I= 19 X= 5.607172791651D+13 Y= -6.917286666433D+13 Z= -9.269012120132D+13
I= 20 X= -4.423005943222D+13 Y= 2.854937742635D+13 Z= -8.123442060180D+13
I= 21 X= 1.340205556358D+13 Y= -1.143032141775D+13 Z= 1.382319447174D+13
I= 22 X= 4.859025136522D+13 Y= 1.495707163664D+13 Z= -5.857741022534D+13
I= 23 X= -1.082725822823D+14 Y= 4.373216609569D+13 Z= 1.318758717255D+11
I= 24 X= 8.378820534900D+13 Y= -3.334047936261D+13 Z= -4.491060758737D+13

I= 25 X= 6.642911745594D+11 Y= -9.459599938827D+12 Z= 1.896174259717D+11
I= 26 X= -7.826320519327D+12 Y= -1.888992859828D+13 Z= -6.428343321089D+13
I= 27 X= 7.035415379847D+13 Y= 2.877640089579D+13 Z= 1.117130889433D+13
I= 28 X= 1.110417023416D+14 Y= -4.412149763675D+13 Z= -1.535537760103D+13
I= 29 X= 1.835935326471D+13 Y= -3.091911133635D+13 Z= -8.404021851966D+12
I= 30 X= -4.684615935836D+12 Y= 1.408371305550D+13 Z= -1.037606224706D+13
I= 31 X= -7.535876911663D+13 Y= 4.235664313643D+13 Z= 2.083860915453D+13
I= 32 X= -1.408592034308D+14 Y= 7.785246302647D+13 Z= 3.524826435570D+13
I= 33 X= 2.671314127458D+13 Y= 5.201936388946D+13 Z= 1.002719411900D+14
I= 34 X= 7.456311819835D+13 Y= -6.656278774726D+13 Z= 8.998446594411D+13
I= 35 X= 2.230242997577D+11 Y= -3.654495949902D+12 Z= 2.971854877146D+12
I= 36 X= -6.246980375817D+12 Y= -7.943365423830D+12 Z= -1.746580863582D+13
I= 37 X= 3.025724113781D+13 Y= 4.220720058079D+13 Z= -7.651978496092D+12
I= 38 X= 4.947741950108D+13 Y= 2.029449977282D+13 Z= -3.679766114555D+13

Backward Direction:

Total Energy: -692.0126917 Hartrees

Potential Energy: -692.1924049 Hartress

Kinetic Energy: 0.1797132 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.085394759824D+13 Y= -8.880694864710D+12 Z= -2.136184458213D+13
I= 1 X= -6.237784089483D+12 Y= 2.396774509783D+13 Z= -1.922387127772D+12
I= 2 X= 3.020853204771D+12 Y= 4.365104154054D+12 Z= 8.551686803141D+12
I= 3 X= -2.269618514864D+13 Y= 1.595814302015D+13 Z= 5.007331955456D+12
I= 4 X= -7.064659020098D+12 Y= 3.322358793192D+12 Z= -1.689265370344D+13
I= 5 X= -6.289744951439D+12 Y= -4.231402844784D+12 Z= 4.846897543313D+12
I= 6 X= -3.869530471856D+12 Y= 3.526088337405D+13 Z= 1.565453750675D+13
I= 7 X= -1.312030525514D+13 Y= -4.109101336761D+13 Z= 9.652923395954D+13
I= 8 X= 5.154581480176D+13 Y= 8.770660178436D+13 Z= 5.946385911536D+13
I= 9 X= 2.256684175240D+13 Y= 1.201195046324D+13 Z= 2.744792147916D+12
I= 10 X= -6.561419686911D+13 Y= -5.210821531343D+13 Z= 2.405356691014D+13

I= 11 X= -5.357687139231D+13 Y= 5.014062165163D+12 Z= 3.326432066175D+12
I= 12 X= 4.601817557618D+13 Y= -3.401574100087D+13 Z= 2.008354674435D+13
I= 13 X= -9.264011219526D+12 Y= 2.508040460470D+12 Z= 2.928120145782D+13
I= 14 X= -8.052972875373D+12 Y= 1.238715225653D+13 Z= -3.271857789692D+13
I= 15 X= 5.982154086561D+13 Y= -6.128662797983D+13 Z= -1.569591897187D+14
I= 16 X= -8.510936943983D+13 Y= 4.299195580246D+13 Z= 1.178111060112D+13
I= 17 X= 8.821861904092D+12 Y= 9.642841629991D+12 Z= 7.122545838755D+11
I= 18 X= -3.700796273637D+13 Y= -8.412928466604D+13 Z= 3.975339672906D+13
I= 19 X= 5.601366051193D+13 Y= -6.891597470472D+13 Z= -9.238652167838D+13
I= 20 X= -4.453086618284D+13 Y= 2.756364420231D+13 Z= -8.034889876040D+13
I= 21 X= 1.267259190763D+13 Y= -1.142997144869D+13 Z= 1.382295954249D+13
I= 22 X= 4.671800314745D+13 Y= 1.495744078014D+13 Z= -5.857806350946D+13
I= 23 X= -1.087251435061D+14 Y= 4.461947654399D+13 Z= 1.625148902196D+11
I= 24 X= 8.333555296815D+13 Y= -3.422682095814D+13 Z= -4.494157090023D+13
I= 25 X= 5.931029193951D+11 Y= -9.470328216365D+12 Z= -6.071851973214D+11
I= 26 X= -8.126963576168D+12 Y= -1.790442529340D+13 Z= -6.516903872384D+13
I= 27 X= 7.029621946894D+13 Y= 2.851917336566D+13 Z= 1.086781597369D+13
I= 28 X= 1.111138585850D+14 Y= -4.447291668124D+13 Z= -1.702728340742D+13
I= 29 X= 1.872931822627D+13 Y= -2.864499848390D+13 Z= -5.858863688727D+12
I= 30 X= -3.934317660512D+12 Y= 1.413546146868D+13 Z= -8.182503549724D+12
I= 31 X= -7.660957229916D+13 Y= 4.406390967348D+13 Z= 2.153262769578D+13
I= 32 X= -1.438117118302D+14 Y= 7.911768657027D+13 Z= 3.864551932631D+13
I= 33 X= 2.634183763732D+13 Y= 5.060972313730D+13 Z= 1.047688897276D+14
I= 34 X= 7.484890639589D+13 Y= -6.804549466212D+13 Z= 9.156941428884D+13
I= 35 X= 1.221062935767D+11 Y= -3.654411981724D+12 Z= 2.972104871865D+12
I= 36 X= -5.496668331194D+12 Y= -7.995395352161D+12 Z= -1.965950378098D+13
I= 37 X= 2.988515139304D+13 Y= 4.361767280986D+13 Z= -1.214936200061D+13
I= 38 X= 4.976330403298D+13 Y= 2.177659457187D+13 Z= -3.838262255173D+13

Seed: 53753451982

CM Start Point Coordinates: bohr

I= 0 X= -2.061682984845D+00 Y= -2.074180072453D+00 Z= -8.791934892340D-02
I= 1 X= 5.375947389092D-03 Y= -2.674532372751D+00 Z= -1.492726333249D+00
I= 2 X= -1.333805807464D+00 Y= -1.298447663709D+00 Z= 2.323602520030D+00
I= 3 X= 2.188449237622D+00 Y= -1.943273305568D+00 Z= -1.714200256588D-02
I= 4 X= 1.240588919407D+00 Y= -1.304049069080D+00 Z= 2.591428264258D+00
I= 5 X= -3.059746368265D+00 Y= 3.285511948263D+00 Z= -2.162609623179D+00
I= 6 X= -1.288518706204D-01 Y= 6.718970980455D-01 Z= -3.418265294990D+00
I= 7 X= -2.421592771902D+00 Y= 4.550349867576D+00 Z= -3.622410433100D+00
I= 8 X= -4.180821303502D+00 Y= 1.779985650568D+00 Z= -2.741363735891D+00
I= 9 X= 2.643251011737D+00 Y= -6.288229444296D-01 Z= 4.918872866412D+00
I= 10 X= 1.920922964853D+00 Y= -1.843570386044D+00 Z= 6.733428318001D+00
I= 11 X= 5.081564839746D+00 Y= -1.212720964152D+00 Z= 4.843395439375D+00
I= 12 X= 2.659235832770D+00 Y= 1.628953613265D+00 Z= 5.468137586043D+00
I= 13 X= -3.026016485141D+00 Y= -9.520766394846D-01 Z= 4.563624184157D+00
I= 14 X= -3.547715352035D+00 Y= -2.891658888629D+00 Z= 5.300610925074D+00
I= 15 X= -2.230558440917D+00 Y= 5.577333436091D-01 Z= 5.975089993214D+00
I= 16 X= -4.970680898905D+00 Y= 2.271395093239D-01 Z= 3.796229783088D+00
I= 17 X= -4.904189884690D+00 Y= -2.643530776679D+00 Z= -6.386539386665D-01
I= 18 X= -5.642921768323D+00 Y= -4.074778829176D+00 Z= 3.849176634261D-01
I= 19 X= -6.221147493369D+00 Y= -8.615736741062D-01 Z= -3.014161363728D-01
I= 20 X= -5.226649342970D+00 Y= -2.643099487328D+00 Z= -2.700537258310D+00
I= 21 X= -5.138207658295D-02 Y= -3.801930939966D+00 Z= -3.887569734405D+00
I= 22 X= 2.700988466477D-01 Y= -5.741283762681D+00 Z= -3.695723264958D+00
I= 23 X= -1.903323739046D+00 Y= -3.780627572293D+00 Z= -4.868287571536D+00
I= 24 X= 1.653924585873D+00 Y= -3.343646242177D+00 Z= -5.058244384965D+00
I= 25 X= 4.795188555620D+00 Y= -2.197357330600D+00 Z= -1.015090412642D+00
I= 26 X= 4.679009977973D+00 Y= -1.881856370861D+00 Z= -3.414461830966D+00
I= 27 X= 6.048904833373D+00 Y= -8.872340650854D-01 Z= -5.412878184404D-02
I= 28 X= 5.740174037741D+00 Y= -4.194334074631D+00 Z= -6.330958222925D-01

I= 29 X= 2.797507252825D+00 Y= 3.222437085963D+00 Z= -2.322902933512D+00
I= 30 X= 2.862408481407D+00 Y= 3.671036263404D+00 Z= 2.194587938932D-01
I= 31 X= 4.108289089438D+00 Y= 2.005903162031D+00 Z= -3.404871578587D+00
I= 32 X= 1.896130472391D+00 Y= 4.593612103692D+00 Z= -3.464452007323D+00
I= 33 X= 1.937024932054D+00 Y= 5.236507275097D+00 Z= 1.127960185883D+00
I= 34 X= 3.863344569685D+00 Y= 2.831086662890D+00 Z= 1.714956085973D+00
I= 35 X= 6.951988714407D-02 Y= 1.108880057625D+00 Z= -6.867650751167D-01
I= 36 X= -2.290418530800D+00 Y= 3.930822421459D+00 Z= 3.054798357672D-01
I= 37 X= -1.653696606766D+00 Y= 5.798921338909D+00 Z= 8.472494344151D-01
I= 38 X= -3.480330677342D+00 Y= 3.028654815755D+00 Z= 2.077338680982D+00

Forward Direction:

Total Energy: -692.0021228 Hartrees

Potential Energy: -692.1892856 Hartress

Kinetic Energy: 0.1871628 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.837543056284D+13 Y= 2.841825180588D+12 Z= -4.641962076435D+11
I= 1 X= -1.440093963600D+13 Y= 1.046157790085D+13 Z= 2.992319501706D+12
I= 2 X= -2.621241755433D+12 Y= -1.467207428884D+13 Z= -1.674942845179D+13
I= 3 X= -1.079562308834D+12 Y= -5.677302349589D+12 Z= 1.735183484395D+12
I= 4 X= -1.685188358345D+13 Y= 2.032224171589D+13 Z= 1.967779583970D+13
I= 5 X= -6.400633015003D+12 Y= -1.426689785729D+12 Z= -6.701413125453D+12
I= 6 X= 5.426578949526D+13 Y= 2.063045722201D+13 Z= -8.327506450186D+13
I= 7 X= 2.789087709990D+13 Y= 1.672870336836D+13 Z= 4.584686155280D+13
I= 8 X= 1.537937671702D+14 Y= 5.416636307496D+13 Z= 1.362550452465D+14
I= 9 X= 7.144119070588D+12 Y= 4.192611053689D+12 Z= 3.368485268399D+12
I= 10 X= -9.546993767419D+13 Y= 4.722269507425D+13 Z= -6.800494211877D+13
I= 11 X= 8.828272060148D+13 Y= 3.101249922050D+13 Z= 4.090661407352D+12
I= 12 X= -3.142385230982D+13 Y= 1.612924798281D+13 Z= 4.748446994870D+13
I= 13 X= -1.559679959826D+13 Y= 1.895821552470D+13 Z= 1.756579367652D+13
I= 14 X= -1.979845433149D+13 Y= -2.765963819522D+12 Z= -1.025137852923D+14

I= 15 X= -4.491096919907D+11 Y= 3.997759652011D+13 Z= -5.363746782273D+13
I= 16 X= 1.705145506105D+14 Y= 1.922368172222D+13 Z= 6.095636512921D+13
I= 17 X= 2.378112323870D+13 Y= -1.110886622933D+13 Z= 6.873229895758D+12
I= 18 X= -2.096905141021D+13 Y= 2.378519109260D+12 Z= -1.821421263674D+13
I= 19 X= 5.566105037165D+13 Y= -5.264615340368D+13 Z= -4.311677492208D+13
I= 20 X= -6.791607167266D+13 Y= 4.542987341543D+13 Z= -2.295086879236D+13
I= 21 X= -1.915746033104D+12 Y= -1.401332928691D+12 Z= -1.034307732605D+13
I= 22 X= -6.455384355306D+13 Y= -4.779950594579D+12 Z= 6.128767697809D+13
I= 23 X= -4.854984635939D+13 Y= -8.104070616316D+12 Z= -3.502413780553D+13
I= 24 X= 1.858473675590D+14 Y= 4.078114511260D+13 Z= -2.361374999226D+13
I= 25 X= 3.735234927890D+12 Y= -1.140765749493D+12 Z= 3.095672839246D+12
I= 26 X= 1.324188507112D+13 Y= 6.080963533254D+13 Z= 7.001197018646D+13
I= 27 X= -1.738498413535D+13 Y= -8.923632999703D+13 Z= 3.352686175366D+12
I= 28 X= -4.407665333672D+13 Y= 2.547304004698D+13 Z= 7.804123265699D+13
I= 29 X= 1.972669839326D+13 Y= -8.786035346360D+12 Z= 5.581324781721D+12
I= 30 X= 5.279702740235D+12 Y= -4.571485177800D+11 Z= -1.345023744611D+13
I= 31 X= -6.503869369294D+13 Y= -1.520962581933D+13 Z= -7.232066161828D+12
I= 32 X= -3.722742747196D+13 Y= -2.096586993821D+12 Z= -4.613330095532D+13
I= 33 X= -1.061614679190D+14 Y= 8.465714578510D+13 Z= 1.246582106166D+14
I= 34 X= -2.308011857113D+13 Y= -2.747391589940D+13 Z= -2.377206187937D+13
I= 35 X= 3.086527905431D+11 Y= -6.653874481578D+12 Z= -2.477658168762D+12
I= 36 X= 5.314623733843D+12 Y= -4.413164881939D+12 Z= -6.201088387125D+12
I= 37 X= 7.183873188994D+13 Y= 2.395267519282D+13 Z= -7.657034663826D+13
I= 38 X= -5.129942904330D+13 Y= -2.877153919453D+13 Z= 3.384220482139D+13

Backward Direction:

Total Energy: -692.0020972 Hartrees

Potential Energy: -692.1892856 Hartress

Kinetic Energy: 0.1871884 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.823881258372D+13 Y= 3.538064066534D+12 Z= 3.406688893481D+11

I= 1 X= -1.347516793677D+13 Y= 1.046165171408D+13 Z= 2.992303495836D+12
I= 2 X= -2.675743840543D+12 Y= -1.546123039417D+13 Z= -1.623845731941D+13
I= 3 X= -9.429115988298D+11 Y= -6.373624103099D+12 Z= 9.301996308548D+11
I= 4 X= -1.690635888083D+13 Y= 2.111144440850D+13 Z= 1.916676203690D+13
I= 5 X= -4.406374201976D+12 Y= -3.803549705344D+12 Z= -1.026221316607D+13
I= 6 X= -4.162190529369D+12 Y= 2.063703311391D+13 Z= -8.327554053937D+13
I= 7 X= 2.138579504258D+13 Y= 1.993994552577D+13 Z= 4.314245502593D+13
I= 8 X= 1.494945607082D+14 Y= 5.680398767658D+13 Z= 1.351828908168D+14
I= 9 X= 7.331693601473D+12 Y= 3.816976019400D+12 Z= 3.053131129479D+12
I= 10 X= -9.592744242897D+13 Y= 4.653550435516D+13 Z= -6.872121831025D+13
I= 11 X= 8.859914985289D+13 Y= 3.002363514881D+13 Z= 3.948420927184D+12
I= 12 X= -3.070075526554D+13 Y= 1.571034429675D+13 Z= 4.760757841036D+13
I= 13 X= -1.540928267429D+13 Y= 1.933385621363D+13 Z= 1.788118676603D+13
I= 14 X= -2.025584427066D+13 Y= -2.078752216745D+12 Z= -1.017975041249D+14
I= 15 X= 2.738311327362D+11 Y= 4.039671307117D+13 Z= -5.376060140649D+13
I= 16 X= 1.708308236554D+14 Y= 2.021226344579D+13 Z= 6.109878460431D+13
I= 17 X= 2.392957051636D+13 Y= -1.094196250957D+13 Z= 7.387550594058D+12
I= 18 X= -2.048304851825D+13 Y= 2.541084444274D+12 Z= -1.742040221131D+13
I= 19 X= 5.548071572358D+13 Y= -5.266594510276D+13 Z= -4.277237886091D+13
I= 20 X= -6.778115986608D+13 Y= 4.509794848712D+13 Z= -2.241127168850D+13
I= 21 X= -2.213042966894D+12 Y= -1.401051963548D+12 Z= -1.034326718778D+13
I= 22 X= -6.537945077261D+13 Y= -4.779674477135D+12 Z= 6.128711814445D+13
I= 23 X= -4.888572524673D+13 Y= -7.765401093775D+12 Z= -3.478481273614D+13
I= 24 X= 1.855113457491D+14 Y= 4.044337039033D+13 Z= -2.385352627781D+13
I= 25 X= 3.883682308250D+12 Y= -1.307717763140D+12 Z= 2.581364324180D+12
I= 26 X= 1.337692689038D+13 Y= 6.114118558172D+13 Z= 6.947240339196D+13
I= 27 X= -1.756533600161D+13 Y= -8.921662313954D+13 Z= 3.008259934497D+12
I= 28 X= -4.359079872959D+13 Y= 2.531046810736D+13 Z= 7.724777212774D+13
I= 29 X= 2.172092217665D+13 Y= -6.410107256804D+12 Z= 9.141599813764D+12
I= 30 X= 7.615121530165D+12 Y= 7.956384250982D+11 Z= -1.218279905511D+13

I= 31 X= -6.933496818302D+13 Y= -1.784557485930D+13 Z= -6.159956947992D+12
I= 32 X= -4.373263810786D+13 Y= -5.308503618642D+12 Z= -4.343032389403D+13
I= 33 X= -1.065663205017D+14 Y= 8.368756606058D+13 Z= 1.281985752057D+14
I= 34 X= -2.356910435587D+13 Y= -2.885607766197D+13 Z= -2.139795547196D+13
I= 35 X= -3.630215899881D+11 Y= -6.653828540592D+12 Z= -2.477416197876D+12
I= 36 X= 7.650406838267D+12 Y= -5.666308155444D+12 Z= -7.468576591201D+12
I= 37 X= 7.143362557829D+13 Y= 2.492320057499D+13 Z= -8.011178531482D+13
I= 38 X= -5.178754684103D+13 Y= -2.738918939203D+13 Z= 3.146832190827D+13

Seed: 5687982974

CM Start Point Coordinates: bohr

I= 0 X= -2.146164320717D+00 Y= -2.328372163154D+00 Z= -6.176536146551D-02
I= 1 X= 4.022029327646D-02 Y= -2.743333130988D+00 Z= -1.560233215679D+00
I= 2 X= -1.360831540744D+00 Y= -1.309537051866D+00 Z= 2.398504840735D+00
I= 3 X= 2.278713216364D+00 Y= -2.207834764770D+00 Z= -1.304361929782D-02
I= 4 X= 1.431108696417D+00 Y= -1.323019320136D+00 Z= 2.626823714542D+00
I= 5 X= -3.299075717034D+00 Y= 3.283453138660D+00 Z= -2.135730733605D+00
I= 6 X= -1.388672872308D-01 Y= 1.202910466398D+00 Z= -3.162791855011D+00
I= 7 X= -2.485637995169D+00 Y= 4.815509162621D+00 Z= -3.734607266677D+00
I= 8 X= -5.051395743260D+00 Y= 2.058627489464D+00 Z= -2.358197118424D+00
I= 9 X= 2.885952546950D+00 Y= -6.341238660043D-01 Z= 4.744948546328D+00
I= 10 X= 1.747264078529D+00 Y= -1.907541512608D+00 Z= 6.393866812276D+00
I= 11 X= 5.144955389163D+00 Y= -1.374690753652D+00 Z= 4.461540030348D+00
I= 12 X= 2.630896188823D+00 Y= 1.491645422815D+00 Z= 5.158369676438D+00
I= 13 X= -3.152240888525D+00 Y= -5.391076881448D-01 Z= 4.436732579227D+00
I= 14 X= -2.807189404033D+00 Y= -1.713005015489D+00 Z= 6.263287086460D+00
I= 15 X= -2.594929612116D+00 Y= 9.922210574097D-01 Z= 5.076771030836D+00
I= 16 X= -4.989109855271D+00 Y= -5.629033031523D-01 Z= 3.881928577653D+00
I= 17 X= -4.722913662564D+00 Y= -2.682520918077D+00 Z= -9.171558635433D-01
I= 18 X= -5.510890691242D+00 Y= -4.016737163761D+00 Z= 8.566739642882D-01

I= 19 X= -5.842987029157D+00 Y= -9.604901634232D-01 Z= -4.248134211976D-01
I= 20 X= -4.806819757197D+00 Y= -3.348065989896D+00 Z= -2.647794838547D+00
I= 21 X= -3.736687089986D-02 Y= -3.653990219265D+00 Z= -4.163397763966D+00
I= 22 X= -8.828510432636D-01 Y= -5.640950902943D+00 Z= -4.195506765628D+00
I= 23 X= -1.401227402362D+00 Y= -2.278703804426D+00 Z= -5.381693005866D+00
I= 24 X= 1.929258425623D+00 Y= -3.486479093974D+00 Z= -5.331876733327D+00
I= 25 X= 5.119369734831D+00 Y= -2.547199102289D+00 Z= -6.635305527349D-01
I= 26 X= 5.484540042125D+00 Y= -2.502508660408D+00 Z= -2.703291865035D+00
I= 27 X= 6.401967214556D+00 Y= -1.163700361216D+00 Z= 8.341473460235D-02
I= 28 X= 5.645849952426D+00 Y= -4.405024387826D+00 Z= 1.921348564983D-02
I= 29 X= 2.754973827314D+00 Y= 3.435107881993D+00 Z= -2.422652365351D+00
I= 30 X= 2.938831196336D+00 Y= 3.568691167143D+00 Z= 6.823819088345D-02
I= 31 X= 4.044113753587D+00 Y= 2.217758412451D+00 Z= -3.731719900450D+00
I= 32 X= 1.610300330700D+00 Y= 4.899015520844D+00 Z= -3.329768660348D+00
I= 33 X= 1.980692834601D+00 Y= 5.277708620763D+00 Z= 1.011643166836D+00
I= 34 X= 4.170553714985D+00 Y= 2.325032357998D+00 Z= 1.254765334526D+00
I= 35 X= -5.530211785770D-02 Y= 1.127107822915D+00 Z= -5.536067491722D-01
I= 36 X= -2.419431782426D+00 Y= 4.045546338226D+00 Z= 3.563150524745D-01
I= 37 X= -1.399263051151D+00 Y= 5.764961823687D+00 Z= 9.153466892031D-01
I= 38 X= -3.350144170955D+00 Y= 3.516817837942D+00 Z= 1.920108163512D+00

Forward Direction:

Total Energy: -691.9953790 Hartrees

Potential Energy: -692.1579395 Hartress

Kinetic Energy: 0.1625605 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.532367809342D+12 Y= -1.592540530433D+13 Z= -1.366160557465D+13

I= 1 X= 9.331210121578D+12 Y= 2.716034008425D+13 Z= 9.259119791972D+12

I= 2 X= 1.852350065173D+13 Y= 1.658872140706D+11 Z= 2.321014850530D+13

I= 3 X= -1.795630096214D+13 Y= 8.253944295957D+12 Z= -1.648309814385D+13

I= 4 X= 3.565676326197D+12 Y= -1.161373754001D+13 Z= -8.333172424729D+12

I= 5 X= -5.069031598314D+12 Y= 1.581921457445D+12 Z= 6.097688856256D+12
I= 6 X= 1.806424910666D+12 Y= -1.440953163400D+13 Z= 3.970166225024D+13
I= 7 X= -7.004482680761D+13 Y= 1.235840352242D+14 Z= -7.245256550869D+13
I= 8 X= 1.460464360660D+13 Y= 4.050943184905D+13 Z= -1.738295286519D+13
I= 9 X= 1.020265323182D+13 Y= -6.666494125423D+12 Z= 6.480518512537D+12
I= 10 X= -2.011435523154D+13 Y= 2.090149942537D+13 Z= 6.541677015149D+13
I= 11 X= -1.255068403347D+13 Y= -4.709540852802D+13 Z= -1.540565666329D+13
I= 12 X= -1.465101351496D+13 Y= -8.022278880926D+12 Z= 2.764952405701D+13
I= 13 X= 1.334705077988D+13 Y= 7.088857327902D+12 Z= 1.601987847746D+13
I= 14 X= 4.731358421513D+13 Y= 3.638591855227D+13 Z= -1.137904195820D+13
I= 15 X= -1.247719672464D+14 Y= -9.826712019370D+13 Z= 4.284347138833D+13
I= 16 X= -9.540609584403D+13 Y= 2.999275034969D+13 Z= -1.109579422078D+12
I= 17 X= 1.568847527623D+12 Y= 2.684834931789D+12 Z= 1.902245620026D+13
I= 18 X= -1.141321415808D+14 Y= -9.074708153451D+13 Z= 2.535458929152D+13
I= 19 X= 7.242363948589D+13 Y= -9.268029821938D+13 Z= -3.002748824087D+13
I= 20 X= 6.202245048237D+11 Y= -2.850061921680D+13 Z= -2.820571660963D+13
I= 21 X= 1.421255926786D+13 Y= -1.357356946977D+13 Z= -9.013860024510D+12
I= 22 X= 1.808962819262D+13 Y= -1.238994365448D+14 Z= 6.160571228378D+13
I= 23 X= 1.299169177760D+13 Y= 8.064171749973D+13 Z= -5.937756947240D+13
I= 24 X= 3.302839656881D+13 Y= 5.947617955951D+13 Z= 2.719168389932D+12
I= 25 X= 1.038256684214D+13 Y= -3.078744188202D+12 Z= -9.700920880197D+12
I= 26 X= 4.289525942462D+13 Y= -7.335831109321D+12 Z= 4.998345764276D+13
I= 27 X= -1.128773191243D+14 Y= 1.357220097116D+13 Z= -1.693737033098D+13
I= 28 X= -9.534462619664D+13 Y= 6.546140844165D+13 Z= 2.238943498963D+12
I= 29 X= 1.291955557958D+13 Y= -2.164683244632D+13 Z= -3.054538055525D+13
I= 30 X= -1.920313640695D+13 Y= 8.243517943430D+12 Z= 4.743042928569D+12
I= 31 X= 3.886156798168D+13 Y= 3.425608369406D+13 Z= 5.703056039222D+13
I= 32 X= -4.589537177778D+13 Y= 1.970279056226D+13 Z= -3.580397391574D+13
I= 33 X= 3.363061486958D+13 Y= -6.400053184899D+13 Z= -8.891772171913D+12
I= 34 X= 3.053193808833D+13 Y= 9.853532483458D+12 Z= -4.376461700655D+13

I= 35 X= -1.778297500550D+12 Y= 7.938660443027D+11 Z= 6.969931043092D+10
I= 36 X= -7.742201439522D+12 Y= 1.597522790672D+13 Z= 1.143476659605D+13
I= 37 X= -1.271952874146D+12 Y= -3.144198481410D+13 Z= -5.047848302302D+13
I= 38 X= 1.714145039814D+13 Y= 4.171797981790D+13 Z= -8.896305709786D+13

Backward Direction:

Total Energy: -691.9953541 Hartrees

Potential Energy: -692.1579395 Hartress

Kinetic Energy: 0.1625854 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.621379417650D+12 Y= -1.514392972303D+13 Z= -1.205101921142D+13
I= 1 X= 8.885743199547D+12 Y= 2.716061422187D+13 Z= 9.258931511519D+12
I= 2 X= 1.945311830056D+13 Y= 5.961847024053D+11 Z= 2.393703711101D+13
I= 3 X= -1.804513133505D+13 Y= 7.472425281850D+12 Z= -1.809388317470D+13
I= 4 X= 4.495407590939D+12 Y= -1.204392746170D+13 Z= -9.059921487122D+12
I= 5 X= -5.266091806603D+12 Y= -7.090041560467D+12 Z= -2.706366817530D+12
I= 6 X= -2.276496291675D+13 Y= -1.440151628331D+13 Z= 3.970270095542D+13
I= 7 X= -7.788205808891D+13 Y= 1.142268568963D+14 Z= -8.625434444634D+13
I= 8 X= 1.282617823626D+13 Y= 2.957633214028D+13 Z= -1.968444060622D+13
I= 9 X= 1.209409120017D+13 Y= -1.003704723588D+13 Z= 5.808430152507D+12
I= 10 X= -2.065740827613D+13 Y= 1.699333738564D+13 Z= 6.397500387435D+13
I= 11 X= -1.023602404875D+13 Y= -5.326008659195D+13 Z= -1.592406182816D+13
I= 12 X= -1.037604871665D+13 Y= -1.098394673554D+13 Z= 2.782535764569D+13
I= 13 X= 1.523837713274D+13 Y= 1.045944159165D+13 Z= 1.669251508407D+13
I= 14 X= 4.677202960716D+13 Y= 4.029463251121D+13 Z= -9.936345584671D+12
I= 15 X= -1.204978568363D+14 Y= -9.530413608743D+13 Z= 4.266742892076D+13
I= 16 X= -9.309220105846D+13 Y= 3.615561536974D+13 Z= -5.899339688456D+11
I= 17 X= 1.074159677436D+12 Y= 2.569243399349D+12 Z= 2.237819388042D+13
I= 18 X= -1.142679372945D+14 Y= -8.920398721078D+13 Z= 3.268170738464D+13
I= 19 X= 7.232196857487D+13 Y= -9.141270091881D+13 Z= -2.889729742598D+13
I= 20 X= -9.758288592230D+11 Y= -3.295661015242D+13 Z= -2.444420635299D+13

I= 21 X= 1.096670905795D+13 Y= -1.357215060151D+13 Z= -9.014811233868D+12
I= 22 X= 9.821376597196D+12 Y= -1.238979196903D+14 Z= 6.160309806777D+13
I= 23 X= 1.112943053744D+13 Y= 8.461289349314D+13 Z= -5.946813166750D+13
I= 24 X= 3.116583552243D+13 Y= 5.550881452948D+13 Z= 2.808606729218D+12
I= 25 X= 9.888299784775D+12 Y= -2.963860874393D+12 Z= -1.305679047756D+13
I= 26 X= 4.129987120844D+13 Y= -2.880582200196D+12 Z= 4.622151044674D+13
I= 27 X= -1.129783260022D+14 Y= 1.230305907502D+13 Z= -1.806701284754D+13
I= 28 X= -9.548011839203D+13 Y= 6.391707495372D+13 Z= -5.088340483953D+12
I= 29 X= 1.272186200225D+13 Y= -1.297731415107D+13 Z= -2.174395826795D+13
I= 30 X= -1.789471859263D+13 Y= 7.241774631468D+12 Z= 1.413005310699D+13
I= 31 X= 3.708339603576D+13 Y= 4.518539350842D+13 Z= 5.932923681461D+13
I= 32 X= -5.372974192745D+13 Y= 2.906107814975D+13 Z= -2.200615170185D+13
I= 33 X= 3.223203682934D+13 Y= -6.987775303517D+13 Z= 9.409991020160D+12
I= 34 X= 3.240920447546D+13 Y= 4.034092621989D+12 Z= -3.844075324622D+13
I= 35 X= -1.596643617970D+12 Y= 7.942279553673D+11 Z= 7.067157506875D+10
I= 36 X= -6.434081146681D+12 Y= 1.697596022463D+13 Z= 2.047143479585D+12
I= 37 X= -2.674095497019D+12 Y= -2.556167080059D+13 Z= -6.878128460840D+13
I= 38 X= 1.901831652505D+13 Y= 4.753425836842D+13 Z= -9.428720785185D+13

Seed: 6289272823

CM Start Point Coordinates: bohr

I= 0 X= -2.160075425058D+00 Y= -2.049933933791D+00 Z= 1.083073471234D-03
I= 1 X= 6.462284707643D-02 Y= -2.649770751980D+00 Z= -1.609583557629D+00
I= 2 X= -1.235747325624D+00 Y= -1.089994153277D+00 Z= 2.338206788268D+00
I= 3 X= 2.180385429370D+00 Y= -2.315967376972D+00 Z= 8.743979442321D-02
I= 4 X= 1.360022618533D+00 Y= -1.058994581604D+00 Z= 2.217714687159D+00
I= 5 X= -2.869866376785D+00 Y= 3.095136795344D+00 Z= -2.312396436393D+00
I= 6 X= 2.141100024323D-01 Y= 1.994886448710D+00 Z= -3.167427073596D+00
I= 7 X= -2.442815829785D+00 Y= 4.752879642873D+00 Z= -3.676727427851D+00
I= 8 X= -3.962554550402D+00 Y= 1.856618869432D+00 Z= -2.745905248181D+00

I= 9 X= 3.031060571993D+00 Y= -4.146702995579D-01 Z= 4.510665545348D+00
I= 10 X= 2.865403781654D+00 Y= -2.257598815189D+00 Z= 5.912253166818D+00
I= 11 X= 4.920318307160D+00 Y= -1.806113413937D-01 Z= 3.509301915460D+00
I= 12 X= 2.076518281364D+00 Y= 1.238007100914D+00 Z= 5.420678527342D+00
I= 13 X= -2.967769203451D+00 Y= -6.173928658255D-01 Z= 4.650023754490D+00
I= 14 X= -3.828163936340D+00 Y= -3.010720553335D+00 Z= 4.980033308772D+00
I= 15 X= -1.830486423091D+00 Y= 1.267197532836D-01 Z= 6.403952952543D+00
I= 16 X= -4.893023272624D+00 Y= 4.001512849420D-01 Z= 4.082481134651D+00
I= 17 X= -4.812987590426D+00 Y= -2.533627454467D+00 Z= -7.174640311979D-01
I= 18 X= -5.338721054531D+00 Y= -4.524786391580D+00 Z= 1.752875159599D-01
I= 19 X= -6.165048448319D+00 Y= -1.074980089092D+00 Z= 2.074247996099D-01
I= 20 X= -5.113594131198D+00 Y= -2.526309922565D+00 Z= -2.626173354763D+00
I= 21 X= 1.241138488512D-01 Y= -3.697556466622D+00 Z= -4.305956168398D+00
I= 22 X= 9.011867858966D-01 Y= -5.690800844762D+00 Z= -4.616963506592D+00
I= 23 X= -1.602888782594D+00 Y= -3.669808346786D+00 Z= -5.165441511598D+00
I= 24 X= 1.543963704074D+00 Y= -2.534622866816D+00 Z= -5.468670506864D+00
I= 25 X= 4.721538027955D+00 Y= -3.003058915092D+00 Z= -8.094246121117D-01
I= 26 X= 5.109726544441D+00 Y= -3.149953684913D+00 Z= -2.977693663459D+00
I= 27 X= 6.098238586056D+00 Y= -1.678792158870D+00 Z= 1.085597730442D-01
I= 28 X= 5.638797511679D+00 Y= -4.466040013184D+00 Z= 2.112456857316D-01
I= 29 X= 2.734157209179D+00 Y= 3.090635963820D+00 Z= -2.114059746692D+00
I= 30 X= 2.710388679590D+00 Y= 3.941573554613D+00 Z= 3.580816752881D-01
I= 31 X= 3.809504993487D+00 Y= 1.336481802989D+00 Z= -2.507235858266D+00
I= 32 X= 2.453319310539D+00 Y= 4.375222642974D+00 Z= -3.681383768749D+00
I= 33 X= 1.512191498747D+00 Y= 5.427997101614D+00 Z= 1.089255663056D+00
I= 34 X= 4.065896555406D+00 Y= 2.839330543759D+00 Z= 1.343251345058D+00
I= 35 X= -4.714954885698D-03 Y= 1.164727452243D+00 Z= -5.049278964250D-01
I= 36 X= -2.844150347581D+00 Y= 3.731358460928D+00 Z= 2.267884483773D-01
I= 37 X= -2.187557603911D+00 Y= 5.569987464330D+00 Z= 1.075185199476D+00
I= 38 X= -3.993601902631D+00 Y= 3.086546934750D+00 Z= 1.622150259813D+00

Forward Direction:

Total Energy: -691.9960859 Hartrees

Potential Energy: -692.1657092 Hartress

Kinetic Energy: 0.1696233 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.910039936453D+13 Y= -5.366680188013D+12 Z= 1.147486115588D+13
I= 1 X= 1.155652568933D+13 Y= 7.724891785268D+12 Z= 1.414093711959D+13
I= 2 X= -1.812886209058D+12 Y= 1.090364998712D+13 Z= -2.809504805766D+13
I= 3 X= -5.206617887397D+12 Y= -1.658673279213D+13 Z= 7.286997520244D+12
I= 4 X= -2.062510451732D+13 Y= 9.644608409777D+12 Z= 7.859159760866D+12
I= 5 X= -4.899615742498D+12 Y= -1.634334587828D+12 Z= 4.744912562377D+12
I= 6 X= 9.062434309044D+12 Y= -2.603892888999D+13 Z= 8.812514774171D+13
I= 7 X= -1.054309684152D+14 Y= 6.559196390898D+12 Z= 3.622873025991D+13
I= 8 X= 4.156031197779D+13 Y= 3.561890832984D+13 Z= -5.440673959823D+12
I= 9 X= 1.725641682373D+13 Y= 1.979787553785D+13 Z= -1.011289579811D+12
I= 10 X= 3.123261335870D+13 Y= -3.161808723615D+13 Z= 3.792738704405D+13
I= 11 X= -1.294511900886D+14 Y= -1.280628858962D+13 Z= -4.909576891336D+13
I= 12 X= 4.817924736199D+12 Y= -4.417148104639D+13 Z= -4.634692509048D+13
I= 13 X= -5.527116786322D+12 Y= -2.750644591584D+13 Z= -9.205460059026D+12
I= 14 X= 2.399550847847D+13 Y= 3.915187366773D+13 Z= -5.065978471250D+13
I= 15 X= -1.736615233939D+13 Y= -4.845964440098D+13 Z= 1.997309391338D+13
I= 16 X= 9.909832007766D+13 Y= -3.819196918161D+13 Z= -4.584627835851D+13
I= 17 X= 1.404939971951D+13 Y= 1.082945142306D+13 Z= 4.680807503300D+11
I= 18 X= -1.377426528059D+14 Y= -9.910839133084D+13 Z= 5.439546627352D+13
I= 19 X= -2.739965262431D+13 Y= -6.512870808732D+13 Z= -3.757133877473D+13
I= 20 X= 3.568402444237D+13 Y= -5.059064647948D+13 Z= -5.360616127761D+13
I= 21 X= -7.286600879182D+12 Y= 1.802786390239D+13 Z= -6.755049999411D+12
I= 22 X= 3.789732148435D+13 Y= -2.034808784076D+13 Z= 2.088036544176D+13
I= 23 X= 1.008784957939D+14 Y= -2.027422404648D+13 Z= 4.652106148151D+13
I= 24 X= -5.133344275355D+13 Y= -3.171928423860D+13 Z= -5.800029848492D+12

I= 25 X= -2.243814104371D+11 Y= -5.110996254764D+12 Z= -1.422746222958D+12
I= 26 X= 6.564716150725D+13 Y= 3.441868415221D+13 Z= -1.204516556734D+14
I= 27 X= 4.510003576627D+13 Y= -7.876165338693D+13 Z= -7.555261602310D+13
I= 28 X= -6.849357113057D+13 Y= 1.143587675511D+13 Z= 1.005023737294D+14
I= 29 X= -1.290125012294D+13 Y= 1.060889538972D+12 Z= 5.081671139979D+12
I= 30 X= -1.447999818872D+13 Y= 4.929881513184D+11 Z= 1.389998271211D+13
I= 31 X= 1.081773655853D+14 Y= 1.374675546488D+13 Z= 8.510639945155D+12
I= 32 X= 3.287540122663D+13 Y= 9.170004212261D+12 Z= -5.287860239973D+13
I= 33 X= -5.760151888389D+13 Y= -8.183976194055D+13 Z= -3.686309734133D+13
I= 34 X= 3.658856751150D+13 Y= -3.718062204420D+13 Z= -1.307778313769D+13
I= 35 X= 1.732947304374D+12 Y= 4.727416076670D+12 Z= 7.454304464746D+11
I= 36 X= 2.684062069317D+12 Y= -5.175401845635D+12 Z= -1.332152479605D+13
I= 37 X= 3.913970085629D+13 Y= 8.598018090504D+13 Z= 6.686361804539D+13
I= 38 X= -1.192448806280D+14 Y= -2.990844926944D+13 Z= 8.406924958603D+12

Backward Direction:

Total Energy: -691.9960695 Hartrees

Potential Energy: -692.1657092 Hartress

Kinetic Energy: 0.1696397 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.917245307908D+13 Y= -4.842430327442D+12 Z= 1.217082435248D+13
I= 1 X= 1.206483998241D+13 Y= 7.724971683124D+12 Z= 1.414090340900D+13
I= 2 X= -1.727942960402D+12 Y= 1.047677718728D+13 Z= -2.769079962399D+13
I= 3 X= -5.134521155341D+12 Y= -1.711103873661D+13 Z= 6.590936579162D+12
I= 4 X= -2.054013047609D+13 Y= 1.007152332057D+13 Z= 7.454890817596D+12
I= 5 X= -3.707666484414D+12 Y= -4.187488342728D+12 Z= 1.452457734135D+12
I= 6 X= -2.971783899012D+13 Y= -2.603389672596D+13 Z= 8.812498931655D+13
I= 7 X= -1.103972511114D+14 Y= 7.329081716364D+12 Z= 3.282341962143D+13
I= 8 X= 3.871056395021D+13 Y= 3.583835812600D+13 Z= -6.387601740942D+12
I= 9 X= 1.761138653774D+13 Y= 1.914006748705D+13 Z= -1.289193810002D+12
I= 10 X= 3.088436820975D+13 Y= -3.253438201075D+13 Z= 3.730695153492D+13

I= 11 X= -1.289637722963D+14 Y= -1.419360315546D+13 Z= -4.924848846340D+13
I= 12 X= 5.802771505034D+12 Y= -4.480370307837D+13 Z= -4.624943982209D+13
I= 13 X= -5.172196417631D+12 Y= -2.684863045485D+13 Z= -8.927462358314D+12
I= 14 X= 2.364752391950D+13 Y= 4.006825143985D+13 Z= -5.003922795832D+13
I= 15 X= -1.638150950132D+13 Y= -4.782712503829D+13 Z= 1.987556677473D+13
I= 16 X= 9.958554520249D+13 Y= -3.680505742720D+13 Z= -4.569329188211D+13
I= 17 X= 1.407708947917D+13 Y= 1.091660744901D+13 Z= 1.208638575266D+12
I= 18 X= -1.374633341010D+14 Y= -9.881297654348D+13 Z= 5.581155587395D+13
I= 19 X= -2.752263031915D+13 Y= -6.497960771537D+13 Z= -3.721746263249D+13
I= 20 X= 3.556341251254D+13 Y= -5.135979654557D+13 Z= -5.279858326660D+13
I= 21 X= -7.880746408006D+12 Y= 1.802821577309D+13 Z= -6.755286814887D+12
I= 22 X= 3.634216011281D+13 Y= -2.034772646998D+13 Z= 2.087969200988D+13
I= 23 X= 1.004367325359D+14 Y= -1.956260355205D+13 Z= 4.665559551796D+13
I= 24 X= -5.177533134887D+13 Y= -3.242987411067D+13 Z= -5.934982149724D+12
I= 25 X= -1.966380867808D+11 Y= -5.198271860385D+12 Z= -2.163313363533D+12
I= 26 X= 6.552671349774D+13 Y= 3.518751124999D+13 Z= -1.212592708388D+14
I= 27 X= 4.497713214387D+13 Y= -7.891100167381D+13 Z= -7.590644074506D+13
I= 28 X= -6.821430436298D+13 Y= 1.114030068024D+13 Z= 9.908647640357D+13
I= 29 X= -1.170940278527D+13 Y= 3.613163782610D+12 Z= 8.373470741387D+12
I= 30 X= -1.288842881652D+13 Y= 1.130133000369D+12 Z= 1.586702685616D+13
I= 31 X= 1.053294441211D+14 Y= 1.352784627976D+13 Z= 9.457182661149D+12
I= 32 X= 2.790940386649D+13 Y= 8.399848347396D+12 Z= -4.947466721216D+13
I= 33 X= -5.802641509950D+13 Y= -8.317875722421D+13 Z= -3.237545408827D+13
I= 34 X= 3.652886109351D+13 Y= -3.876405043623D+13 Z= -1.095202962323D+13
I= 35 X= 1.346152577812D+12 Y= 4.727490130407D+12 Z= 7.457017399251D+11
I= 36 X= 4.275815940244D+12 Y= -5.812892705117D+12 Z= -1.528867726952D+13
I= 37 X= 3.871419655271D+13 Y= 8.732014653591D+13 Z= 6.237518729618D+13
I= 38 X= -1.193041082419D+14 Y= -2.832530809871D+13 Z= 6.281271337081D+12

Seed: 7377033437

CM Start Point Coordinates: bohr

I= 0 X= -2.152551755200D+00 Y= -2.097975380412D+00 Z= -8.731080088538D-02
I= 1 X= 4.392801738056D-02 Y= -2.676207049084D+00 Z= -1.572055480809D+00
I= 2 X= -1.298042710922D+00 Y= -1.198641864564D+00 Z= 2.357340859142D+00
I= 3 X= 2.196046315051D+00 Y= -2.022972275566D+00 Z= 3.583798084527D-02
I= 4 X= 1.455930569708D+00 Y= -1.276710785918D+00 Z= 2.473977251137D+00
I= 5 X= -2.681103886438D+00 Y= 3.254398318691D+00 Z= -2.373331010601D+00
I= 6 X= 5.257186468891D-02 Y= 1.129319340710D+00 Z= -3.117192175678D+00
I= 7 X= -2.033600542124D+00 Y= 4.572312416449D+00 Z= -3.893410301360D+00
I= 8 X= -4.633869062229D+00 Y= 2.234033368102D+00 Z= -3.162170068188D+00
I= 9 X= 2.947731088842D+00 Y= -7.023881828002D-01 Z= 4.638619161485D+00
I= 10 X= 2.371125724057D+00 Y= -1.752184870146D+00 Z= 6.174081682884D+00
I= 11 X= 5.229241023866D+00 Y= -5.960314589924D-01 Z= 4.439785551170D+00
I= 12 X= 2.574908201996D+00 Y= 1.291312750321D+00 Z= 4.956415189877D+00
I= 13 X= -2.806524934262D+00 Y= -5.368349655579D-01 Z= 4.677444005868D+00
I= 14 X= -2.617383630817D+00 Y= -2.266007905075D+00 Z= 5.760182919402D+00
I= 15 X= -2.021520990311D+00 Y= 1.025079684774D+00 Z= 5.876671845010D+00
I= 16 X= -4.749279728486D+00 Y= 7.069308285036D-02 Z= 4.423291868860D+00
I= 17 X= -4.804633396678D+00 Y= -2.334347084491D+00 Z= -7.494713795584D-01
I= 18 X= -5.974594936070D+00 Y= -4.164943957318D+00 Z= 9.373836098245D-02
I= 19 X= -5.871579307842D+00 Y= -2.611760633588D-01 Z= -1.620533334378D-01
I= 20 X= -5.020004214961D+00 Y= -2.891255046563D+00 Z= -2.704090090836D+00
I= 21 X= -1.381032219126D-01 Y= -3.589106335239D+00 Z= -4.257107475673D+00
I= 22 X= 2.716068437862D-02 Y= -5.739269127788D+00 Z= -4.583362909117D+00
I= 23 X= -1.983861139254D+00 Y= -3.061613203729D+00 Z= -5.218541953670D+00
I= 24 X= 1.340411796791D+00 Y= -2.345390517226D+00 Z= -5.656031169797D+00
I= 25 X= 4.803608281812D+00 Y= -2.620124566771D+00 Z= -7.939066629371D-01
I= 26 X= 4.564497978542D+00 Y= -3.463488106607D+00 Z= -2.830976251012D+00
I= 27 X= 5.723206213619D+00 Y= -7.245684212898D-01 Z= -2.183729778345D-01
I= 28 X= 5.517329004300D+00 Y= -3.941266799192D+00 Z= 6.856062427986D-01

I= 29 X= 2.818619327098D+00 Y= 3.155291780053D+00 Z= -2.180597898374D+00
I= 30 X= 2.408753525174D+00 Y= 3.982221754929D+00 Z= 3.288617251845D-01
I= 31 X= 4.298745448765D+00 Y= 1.844455063745D+00 Z= -2.818814723738D+00
I= 32 X= 2.245740142332D+00 Y= 4.253914921521D+00 Z= -4.133812007006D+00
I= 33 X= 1.630676178566D+00 Y= 5.831077361955D+00 Z= 6.401089156519D-01
I= 34 X= 3.602196241557D+00 Y= 3.218172068841D+00 Z= 2.042563359252D+00
I= 35 X= 5.467217025692D-02 Y= 1.027689069299D+00 Z= -5.199784485665D-01
I= 36 X= -2.880221641610D+00 Y= 3.478567945413D+00 Z= 1.207653238933D-01
I= 37 X= -2.135563691967D+00 Y= 5.022626154799D+00 Z= 1.387944624057D+00
I= 38 X= -4.302834786671D+00 Y= 2.354306461641D+00 Z= 1.239736342831D+00

Forward Direction:

Total Energy: -692.0063868 Hartrees

Potential Energy: -692.1945642 Hartress

Kinetic Energy: 0.1881774 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.289933610546D+12 Y= 7.133763873967D+12 Z= -5.294693952785D+11
I= 1 X= -9.553541782273D+12 Y= -3.057178850032D+13 Z= -1.408896376978D+13
I= 2 X= 1.398904073257D+12 Y= 2.716340965267D+13 Z= -8.921553448550D+12
I= 3 X= -2.443657977187D+12 Y= 7.432204767563D+12 Z= 2.698515956873D+12
I= 4 X= 2.858606539751D+12 Y= -1.826650335723D+12 Z= 1.287609986356D+13
I= 5 X= 1.044939943154D+13 Y= 8.640184806226D+12 Z= -2.152635195003D+13
I= 6 X= 3.374640439823D+13 Y= -4.195567727976D+13 Z= 5.746984030473D+13
I= 7 X= -1.140277325961D+14 Y= -3.181495041587D+13 Z= 6.539666340301D+13
I= 8 X= 5.472341860449D+13 Y= -1.960250864853D+13 Z= -4.248305084500D+13
I= 9 X= -1.185952793045D+13 Y= -1.469205118865D+13 Z= -1.592300269100D+13
I= 10 X= 5.696516270384D+13 Y= 8.175406542481D+13 Z= -5.544881852231D+13
I= 11 X= 1.413486494889D+13 Y= 2.503525598255D+13 Z= -8.776196822418D+12
I= 12 X= 6.199249325957D+13 Y= 9.621780622401D+13 Z= 7.409724311113D+13
I= 13 X= 3.254597144296D+12 Y= -8.579232355532D+12 Z= -8.585008907615D+12
I= 14 X= -6.775299571026D+13 Y= 2.580331366202D+13 Z= -5.759377199567D+11

I= 15 X= 8.915443919537D+13 Y= -4.576760562751D+13 Z= -2.033765489264D+13
I= 16 X= 9.029468627687D+13 Y= -6.358670820366D+13 Z= 4.706851818811D+13
I= 17 X= -1.712584666573D+13 Y= 1.910862106649D+13 Z= 8.529126374514D+12
I= 18 X= -7.573470089665D+12 Y= -4.232832961716D+13 Z= 4.117441510135D+13
I= 19 X= 9.993408872607D+12 Y= -1.355859579545D+14 Z= -1.145455723377D+14
I= 20 X= 8.519744578890D+13 Y= 5.032320562324D+13 Z= -3.696547723878D+13
I= 21 X= -1.581254634691D+13 Y= 9.496001040733D+12 Z= 3.753282986005D+12
I= 22 X= 4.497369574980D+13 Y= 1.108421919267D+14 Z= 7.475541759386D+13
I= 23 X= -1.904739364943D+13 Y= 5.287424298584D+13 Z= 6.242407243122D+13
I= 24 X= 8.619840670386D+13 Y= -2.609957035783D+13 Z= -3.631401123807D+13
I= 25 X= -8.680581072543D+12 Y= -1.575990525086D+13 Z= -6.795215260552D+12
I= 26 X= -5.574789732667D+13 Y= 2.540741929641D+13 Z= 3.561595405508D+13
I= 27 X= -2.304201793159D+13 Y= -7.904440293896D+13 Z= -2.467302359172D+13
I= 28 X= -6.315238843348D+12 Y= 4.411764526183D+13 Z= -1.536289114119D+13
I= 29 X= 1.307274383022D+12 Y= 7.449267331665D+11 Z= -4.144930036761D+12
I= 30 X= 8.419730120141D+12 Y= 5.657543727839D+11 Z= -1.809572745418D+12
I= 31 X= 5.403258226400D+13 Y= -5.238561958826D+13 Z= 2.840583387206D+13
I= 32 X= 4.804920671783D+12 Y= -9.477523592736D+12 Z= -2.384485850469D+13
I= 33 X= 7.758765883015D+13 Y= -8.909447378186D+13 Z= -3.490444470484D+13
I= 34 X= -8.922619561277D+13 Y= 9.362002746129D+13 Z= -6.236190383169D+12
I= 35 X= -3.925880071642D+12 Y= -2.878133573079D+12 Z= 5.252699776096D+12
I= 36 X= 2.376429732756D+12 Y= -2.602424565601D+12 Z= 2.511291412341D+13
I= 37 X= 1.441025140770D+14 Y= 1.105177198409D+14 Z= 3.464910629377D+13
I= 38 X= 9.876313380398D+13 Y= 1.407990449455D+13 Z= -5.822925060176D+13

Backward Direction:

Total Energy: -692.0063329 Hartrees

Potential Energy: -692.1945642 Hartress

Kinetic Energy: 0.1882313 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.270790099016D+12 Y= 7.759677995518D+12 Z= 6.083411692884D+11

I= 1 X= -9.590886179630D+12 Y= -3.057161009648D+13 Z= -1.408907792572D+13
I= 2 X= 1.930274708643D+12 Y= 2.722486385036D+13 Z= -8.372360231226D+12
I= 3 X= -2.462687424301D+12 Y= 6.806245191874D+12 Z= 1.560560334386D+12
I= 4 X= 3.390050195582D+12 Y= -1.888030270623D+12 Z= 1.232697324562D+13
I= 5 X= 1.081562365966D+13 Y= 2.986424224870D+12 Z= -2.754343313761D+13
I= 6 X= 5.241879885361D+12 Y= -4.194939397434D+13 Z= 5.747033376738D+13
I= 7 X= -1.201895900750D+14 Y= -3.652044217059D+13 Z= 5.665894610223D+13
I= 8 X= 5.264331582051D+13 Y= -2.536965453762D+13 Z= -4.409012054062D+13
I= 9 X= -1.070629371395D+13 Y= -1.675711424947D+13 Z= -1.639285053864D+13
I= 10 X= 5.653656647613D+13 Y= 7.929884481275D+13 Z= -5.646634480926D+13
I= 11 X= 1.556712731471D+13 Y= 2.118539531461D+13 Z= -9.114212525101D+12
I= 12 X= 6.467124488323D+13 Y= 9.438180207581D+13 Z= 7.422997283165D+13
I= 13 X= 4.407752071106D+12 Y= -6.514149683219D+12 Z= -8.114830511470D+12
I= 14 X= -6.818068647732D+13 Y= 2.825886265319D+13 Z= 4.421345576641D+11
I= 15 X= 9.183265263468D+13 Y= -4.393077902265D+13 Z= -2.047051302709D+13
I= 16 X= 9.172646266557D+13 Y= -5.973797773553D+13 Z= 4.740730362687D+13
I= 17 X= -1.737976258693D+13 Y= 1.908122269496D+13 Z= 1.061900654374D+13
I= 18 X= -7.535634282833D+12 Y= -4.138518186356D+13 Z= 4.565807863158D+13
I= 19 X= 9.890299475570D+12 Y= -1.348482286746D+14 Z= -1.138003716439D+14
I= 20 X= 8.429512352231D+13 Y= 4.763289200376D+13 Z= -3.463180642266D+13
I= 21 X= -1.778564301387D+13 Y= 9.496900014738D+12 Z= 3.752679944542D+12
I= 22 X= 3.993107309020D+13 Y= 1.108431471251D+14 Z= 7.475375131273D+13
I= 23 X= -2.021935582120D+13 Y= 5.528219971558D+13 Z= 6.242882652426D+13
I= 24 X= 8.502623439998D+13 Y= -2.850507866705D+13 Z= -3.631953263071D+13
I= 25 X= -8.934250489031D+12 Y= -1.573293340820D+13 Z= -8.885169748128D+12
I= 26 X= -5.664979856252D+13 Y= 2.809720777913D+13 Z= 3.328203457126D+13
I= 27 X= -2.314474242872D+13 Y= -7.978305733980D+13 Z= -2.541791032690D+13
I= 28 X= -6.277261129052D+12 Y= 4.317377023406D+13 Z= -1.984656741173D+13
I= 29 X= 1.673119142195D+12 Y= 6.397030230918D+12 Z= 1.870481815782D+12
I= 30 X= 9.750202207382D+12 Y= 2.815457129072D+11 Z= 3.995086677562D+12

I= 31 X= 5.195335948780D+13 Y= -4.662028899694D+13 Z= 3.001124588482D+13
I= 32 X= -1.355291921008D+12 Y= -4.771544971430D+12 Z= -1.510980414155D+13
I= 33 X= 7.667064576759D+13 Y= -9.277129575646D+13 Z= -2.332890985763D+13
I= 34 X= -8.824466577409D+13 Y= 8.987740451778D+13 Z= -2.544281724812D+12
I= 35 X= -3.981697418297D+12 Y= -2.877910484200D+12 Z= 5.253327733482D+12
I= 36 X= 3.706815535242D+12 Y= -2.318894173285D+12 Z= 1.930788363651D+13
I= 37 X= 1.431833517389D+14 Y= 1.141965818645D+14 Z= 2.307270378566D+13
I= 38 X= 9.974463882484D+13 Y= 1.782072107913D+13 Z= -6.192127339297D+13

Seed: 8789762236

CM Start Point Coordinates: bohr

I= 0 X= -2.234770043746D+00 Y= -2.192518224700D+00 Z= -7.706728586287D-02
I= 1 X= 7.149393180573D-02 Y= -2.760598971977D+00 Z= -1.623684594134D+00
I= 2 X= -1.385951366381D+00 Y= -1.133151653067D+00 Z= 2.377581433522D+00
I= 3 X= 2.120478479993D+00 Y= -1.986125854784D+00 Z= 2.490733867255D-02
I= 4 X= 1.360274437018D+00 Y= -1.089264058266D+00 Z= 2.397754803473D+00
I= 5 X= -3.170919935891D+00 Y= 3.102718138055D+00 Z= -2.086336843634D+00
I= 6 X= -3.138625170967D-01 Y= 1.959177237253D+00 Z= -3.106435471850D+00
I= 7 X= -2.739373330163D+00 Y= 4.381382393432D+00 Z= -3.604128342540D+00
I= 8 X= -4.423458217009D+00 Y= 1.203319269040D+00 Z= -2.678872677008D+00
I= 9 X= 2.884617550064D+00 Y= -8.683935188042D-01 Z= 4.798189341662D+00
I= 10 X= 2.762841659181D+00 Y= -2.655044730610D+00 Z= 5.898556321110D+00
I= 11 X= 4.929901634305D+00 Y= -4.031552951093D-01 Z= 4.415074200176D+00
I= 12 X= 2.358188527108D+00 Y= 6.858324421306D-01 Z= 5.916877269843D+00
I= 13 X= -2.970278958274D+00 Y= -5.210746834342D-01 Z= 4.421983509659D+00
I= 14 X= -2.409584072471D+00 Y= -1.657843543361D+00 Z= 6.067705065057D+00
I= 15 X= -2.640243182268D+00 Y= 1.380661099012D+00 Z= 5.187054008130D+00
I= 16 X= -4.963518820723D+00 Y= -3.285383637585D-01 Z= 4.337490180593D+00
I= 17 X= -4.981477925220D+00 Y= -2.611079580641D+00 Z= -8.906029320997D-01
I= 18 X= -5.437168410166D+00 Y= -4.765995087581D+00 Z= -5.495101124999D-01

I= 19 X= -6.369194390154D+00 Y= -1.554066274429D+00 Z= 4.876269276513D-01
I= 20 X= -5.468023384118D+00 Y= -1.965784251674D+00 Z= -2.990500342207D+00
I= 21 X= 1.780219518307D-01 Y= -3.860160578287D+00 Z= -4.219713326509D+00
I= 22 X= 1.875391869567D+00 Y= -5.934606361682D+00 Z= -4.017866626142D+00
I= 23 X= -2.150938374087D+00 Y= -4.588218926157D+00 Z= -5.078016577624D+00
I= 24 X= 1.433073268324D+00 Y= -2.286732096638D+00 Z= -5.564150061067D+00
I= 25 X= 4.862189845502D+00 Y= -2.502832969236D+00 Z= -6.183046776065D-01
I= 26 X= 5.000508627533D+00 Y= -2.304781030612D+00 Z= -2.579980718952D+00
I= 27 X= 6.386833404458D+00 Y= -9.498594894185D-01 Z= 3.232339512136D-02
I= 28 X= 5.731982082825D+00 Y= -4.166862540968D+00 Z= 6.088062733412D-03
I= 29 X= 2.629924560415D+00 Y= 3.320727490148D+00 Z= -2.485669763890D+00
I= 30 X= 3.203116011209D+00 Y= 3.401251934396D+00 Z= 1.981710564656D-01
I= 31 X= 3.686970264490D+00 Y= 2.068498080456D+00 Z= -3.819822807299D+00
I= 32 X= 1.748094382342D+00 Y= 5.142091205965D+00 Z= -3.336425675038D+00
I= 33 X= 2.595986896931D+00 Y= 5.133345818464D+00 Z= 1.322988106817D+00
I= 34 X= 4.913346812361D+00 Y= 2.416372202682D+00 Z= 8.964861772036D-01
I= 35 X= -3.972070910850D-03 Y= 1.161428755695D+00 Z= -5.133605770642D-01
I= 36 X= -2.608589733744D+00 Y= 3.987953571978D+00 Z= 3.076043238167D-01
I= 37 X= -2.008924764545D+00 Y= 6.106044232743D+00 Z= 6.311788405463D-01
I= 38 X= -3.768007493832D+00 Y= 3.187834394695D+00 Z= 2.082832514069D+00

Forward Direction:

Total Energy: -691.9885300 Hartrees

Potential Energy: -692.1642589 Hartress

Kinetic Energy: 0.1757289 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.430661311394D+12 Y= -1.614924005289D+11 Z= -3.980366865453D+12

I= 1 X= 8.795089169702D+12 Y= 1.452444969007D+13 Z= 2.826183878571D+12

I= 2 X= 3.713085144232D+12 Y= 1.111441468470D+13 Z= -3.044865732872D+12

I= 3 X= -1.692038276261D+12 Y= 5.242564376877D+12 Z= 9.230071747071D+12

I= 4 X= 2.419398653046D+13 Y= 7.132460670232D+12 Z= 2.535623991439D+13

I= 5 X= -4.292209400212D+12 Y= 1.162595393972D+13 Z= -2.186257194025D+12
I= 6 X= 3.437899943004D+13 Y= -4.262983825984D+13 Z= 5.401069076913D+13
I= 7 X= 5.455572191377D+12 Y= 8.608382677388D+13 Z= -5.220636231793D+13
I= 8 X= -8.917561410824D+13 Y= -9.989105580675D+13 Z= 1.152068228476D+13
I= 9 X= -1.313013467418D+13 Y= 1.665942175024D+13 Z= -7.095053918330D+12
I= 10 X= -2.488663871001D+13 Y= -5.667402174999D+13 Z= 3.749366456127D+13
I= 11 X= -1.740613145156D+13 Y= -3.747449786750D+13 Z= 4.618778100110D+13
I= 12 X= 2.021223688955D+13 Y= -8.790492078549D+13 Z= -6.608862400643D+13
I= 13 X= -9.089101796901D+12 Y= -3.737451642917D+12 Z= 1.315659348897D+13
I= 14 X= 8.877684789791D+13 Y= -4.503586127258D+13 Z= -6.639257564236D+12
I= 15 X= -4.174242802436D+13 Y= -3.267384450182D+13 Z= 1.016671056100D+13
I= 16 X= -1.422835848584D+14 Y= -8.196122038908D+12 Z= -1.680915436689D+13
I= 17 X= 7.850513220906D+12 Y= 2.847678065026D+12 Z= 8.660472279843D+12
I= 18 X= 1.447700383275D+13 Y= 7.612221332172D+13 Z= 1.627501966726D+13
I= 19 X= -2.363137908152D+13 Y= -3.402346190084D+13 Z= 4.430004434104D+13
I= 20 X= -3.020311242684D+13 Y= -7.153503998091D+13 Z= -5.192987570519D+13
I= 21 X= -1.352617588585D+13 Y= 1.201498196171D+13 Z= -9.535616948446D+12
I= 22 X= -3.521534205072D+13 Y= -4.652462387216D+12 Z= -8.825200501643D+13
I= 23 X= 1.511436509878D+14 Y= -8.532588242518D+13 Z= 5.106559747198D+13
I= 24 X= -4.627108252673D+13 Y= 1.769970640077D+13 Z= -6.577609921037D+13
I= 25 X= 8.335917958227D+12 Y= -9.790324332945D+12 Z= 1.296064830212D+13
I= 26 X= 1.876264143701D+12 Y= 5.822504737949D+13 Z= 2.144118861546D+13
I= 27 X= -5.297168500782D+13 Y= -1.081417093433D+13 Z= -5.641053643504D+13
I= 28 X= -1.395217522753D+14 Y= 1.355650770868D+14 Z= -5.526063578960D+13
I= 29 X= 1.427041782539D+12 Y= -7.716145250498D+12 Z= -1.379821322591D+13
I= 30 X= 1.312287088052D+13 Y= -2.098304118693D+13 Z= -3.013547412520D+12
I= 31 X= 4.314284440074D+13 Y= -5.200346905764D+13 Z= 1.002846889204D+14
I= 32 X= -7.188639617540D+13 Y= -2.100544281249D+13 Z= 4.903662765185D+13
I= 33 X= -2.413466835902D+13 Y= 5.368070423993D+13 Z= -7.004110058392D+13
I= 34 X= -1.283144377346D+13 Y= 6.597633344143D+13 Z= -8.010895169413D+13

I= 35 X= 2.730142844461D+12 Y= -1.962490899387D+12 Z= -3.690932076122D+12
I= 36 X= -8.651215668550D+12 Y= -1.208699701808D+13 Z= 6.450838493731D+11
I= 37 X= -1.569955057830D+13 Y= -1.756259187986D+13 Z= 8.578758120717D+13
I= 38 X= 8.649661475388D+13 Y= 1.105639043641D+13 Z= -6.158254453728D+13

Backward Direction:

Total Energy: -691.9885311 Hartrees

Potential Energy: -692.1642589 Hartress

Kinetic Energy: 0.1757279 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.481749019193D+12 Y= 1.146415082014D+12 Z= -1.570455450168D+12
I= 1 X= 8.649148727473D+12 Y= 1.452483123543D+13 Z= 2.825937560957D+12
I= 2 X= 4.868754649640D+12 Y= 1.130302707128D+13 Z= -1.890259001113D+12
I= 3 X= -1.742881025028D+12 Y= 3.934564186376D+12 Z= 6.819854248972D+12
I= 4 X= 2.534981244514D+13 Y= 6.944005979715D+12 Z= 2.420178197339D+13
I= 5 X= -3.638349085189D+12 Y= -4.627535123726D+11 Z= -1.497941563555D+13
I= 6 X= -2.330811905073D+13 Y= -4.261667972404D+13 Z= 5.401179385152D+13
I= 7 X= -7.444725407469D+12 Y= 7.565837865226D+13 Z= -7.095711832875D+13
I= 8 X= -9.338281248400D+13 Y= -1.125775659649D+14 Z= 8.112329379655D+12
I= 9 X= -1.064345558651D+13 Y= 1.220938815284D+13 Z= -8.091397354409D+12
I= 10 X= -2.578358266921D+13 Y= -6.194792214738D+13 Z= 3.533827247975D+13
I= 11 X= -1.432365330151D+13 Y= -4.575035898799D+13 Z= 4.546505531248D+13
I= 12 X= 2.596816108979D+13 Y= -9.185538968306D+13 Z= -6.580955022666D+13
I= 13 X= -6.602590559288D+12 Y= 7.126240731690D+11 Z= 1.415365073066D+13
I= 14 X= 8.788185858918D+13 Y= -3.976125055598D+13 Z= -4.482682260213D+12
I= 15 X= -3.598765949451D+13 Y= -2.872160775385D+13 Z= 9.887360196006D+12
I= 16 X= -1.392021491762D+14 Y= 7.730898395536D+10 Z= -1.608477269117D+13
I= 17 X= 7.289682785913D+12 Y= 2.776570352328D+12 Z= 1.315456573642D+13
I= 18 X= 1.452490226620D+13 Y= 7.815524710408D+13 Z= 2.593845777462D+13
I= 19 X= -2.384222803204D+13 Y= -3.242290882516D+13 Z= 4.589122692852D+13
I= 20 X= -3.216853247889D+13 Y= -7.734348742536D+13 Z= -4.690909567651D+13

I= 21 X= -1.778235480822D+13 Y= 1.201691094238D+13 Z= -9.536910812609D+12
I= 22 X= -4.608819458098D+13 Y= -4.650411189221D+12 Z= -8.825557775423D+13
I= 23 X= 1.486267866682D+14 Y= -8.012996879330D+13 Z= 5.105910211505D+13
I= 24 X= -4.878839231149D+13 Y= 1.250903738508D+13 Z= -6.577123541410D+13
I= 25 X= 7.775621846071D+12 Y= -9.720137811531D+12 Z= 8.466392842825D+12
I= 26 X= -8.825247485838D+10 Y= 6.403238277056D+13 Z= 1.641986743501D+13
I= 27 X= -5.318169852223D+13 Y= -1.241672355174D+13 Z= -5.800103652804D+13
I= 28 X= -1.394735357305D+14 Y= 1.335304671008D+14 Z= -6.492412605921D+13
I= 29 X= 2.080082003309D+12 Y= 4.369035600496D+12 Z= -1.008636523580D+12
I= 30 X= 1.584296589952D+13 Y= -2.168706188753D+13 Z= 9.480142934745D+12
I= 31 X= 3.893734778581D+13 Y= -3.932101150420D+13 Z= 1.036894516681D+14
I= 32 X= -8.478311917802D+13 Y= -1.057889197366D+13 Z= 6.778171159264D+13
I= 33 X= -2.609404171087D+13 Y= 4.577858244732D+13 Z= -4.519753863762D+13
I= 34 X= -1.066947059055D+13 Y= 5.796053942403D+13 Z= -7.227272518343D+13
I= 35 X= 2.656300358179D+12 Y= -1.962010542612D+12 Z= -3.689587851916D+12
I= 36 X= -5.931333275259D+12 Y= -1.138442155116D+13 Z= -1.184940736108D+13
I= 37 X= -1.766356506730D+13 Y= -9.656114279782D+12 Z= 6.094221384627D+13
I= 38 X= 8.865847319676D+13 Y= 1.906825566034D+13 Z= -6.941903414073D+13

Seed: 9047933238

CM Start Point Coordinates: bohr

I= 0 X= -2.169217162699D+00 Y= -1.964461822941D+00 Z= 5.752233370170D-02
I= 1 X= -7.791859897267D-02 Y= -2.852970827319D+00 Z= -1.457284925533D+00
I= 2 X= -1.362799984947D+00 Y= -1.060448988472D+00 Z= 2.449943436340D+00
I= 3 X= 2.088121673961D+00 Y= -2.076416765412D+00 Z= 7.936009480141D-03
I= 4 X= 1.413312876417D+00 Y= -1.365319091333D+00 Z= 2.493732691971D+00
I= 5 X= -2.858854720828D+00 Y= 3.189327999669D+00 Z= -2.445545780114D+00
I= 6 X= 1.419248805725D-01 Y= 1.664535715596D+00 Z= -3.320703886389D+00
I= 7 X= -2.323335352026D+00 Y= 5.047783474506D+00 Z= -3.281508493907D+00
I= 8 X= -4.040306909742D+00 Y= 2.071445103332D+00 Z= -3.133538407447D+00

I= 9 X= 3.033778278560D+00 Y= -8.603501099982D-01 Z= 4.701711962488D+00
I= 10 X= 3.712300572341D+00 Y= -2.672954848343D+00 Z= 5.943755879907D+00
I= 11 X= 4.822834750508D+00 Y= 2.524366648935D-01 Z= 4.074243655235D+00
I= 12 X= 1.918557668195D+00 Y= 1.432604760875D-01 Z= 6.269264903198D+00
I= 13 X= -2.877108296286D+00 Y= -4.765969317312D-01 Z= 4.702523565003D+00
I= 14 X= -2.899237908842D+00 Y= -2.343323131313D+00 Z= 5.695035152461D+00
I= 15 X= -2.206332429852D+00 Y= 8.387108089317D-01 Z= 5.988707872453D+00
I= 16 X= -4.935105608288D+00 Y= 4.084885013011D-01 Z= 4.176390918434D+00
I= 17 X= -4.831410155777D+00 Y= -2.328140223219D+00 Z= -8.539898344215D-01
I= 18 X= -6.017846483340D+00 Y= -3.949271000032D+00 Z= 5.129037269409D-02
I= 19 X= -6.088946970892D+00 Y= -9.115144832027D-01 Z= -4.781313095327D-01
I= 20 X= -5.142389244516D+00 Y= -2.821632395181D+00 Z= -2.730915739024D+00
I= 21 X= 6.184420867857D-02 Y= -3.664360028380D+00 Z= -4.177451372735D+00
I= 22 X= 1.182675587184D+00 Y= -5.879726582433D+00 Z= -4.195472139762D+00
I= 23 X= -1.660754372260D+00 Y= -3.891551753592D+00 Z= -5.172494465680D+00
I= 24 X= 1.489206241423D+00 Y= -2.147412118846D+00 Z= -5.242260481529D+00
I= 25 X= 4.814986238596D+00 Y= -2.349565046959D+00 Z= -8.202346763919D-01
I= 26 X= 4.708816270203D+00 Y= -2.187485242369D+00 Z= -2.983446813681D+00
I= 27 X= 6.281635482040D+00 Y= -1.159949570616D+00 Z= -2.540492267737D-01
I= 28 X= 5.348083641617D+00 Y= -4.227509068493D+00 Z= -3.903482171430D-01
I= 29 X= 2.985218015320D+00 Y= 3.176832283731D+00 Z= -2.301718647018D+00
I= 30 X= 2.662999160557D+00 Y= 3.771221536518D+00 Z= 1.458140910561D-01
I= 31 X= 4.277771358840D+00 Y= 1.747874142727D+00 Z= -2.665051005464D+00
I= 32 X= 2.244886470813D+00 Y= 4.744472068844D+00 Z= -3.600580071151D+00
I= 33 X= 1.454106652376D+00 Y= 5.590836344199D+00 Z= 1.123443598730D+00
I= 34 X= 4.192785836744D+00 Y= 3.361697035679D+00 Z= 1.571046576780D+00
I= 35 X= -2.687797351260D-02 Y= 1.087436624932D+00 Z= -5.461623762330D-01
I= 36 X= -2.800084885772D+00 Y= 3.417267008812D+00 Z= 1.808925531950D-01
I= 37 X= -1.866779292701D+00 Y= 5.059510119903D+00 Z= 9.069709203625D-01
I= 38 X= -4.009523532949D+00 Y= 2.493293557057D+00 Z= 1.629377337404D+00

Forward Direction:

Total Energy: -692.0029568 Hartrees

Potential Energy: -692.1813138 Hartress

Kinetic Energy: 0.1783570 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.112226853663D+13 Y= 5.591219359606D+12 Z= -4.596407200680D+12
I= 1 X= -1.160381954941D+13 Y= 5.538390951887D+12 Z= 1.974816776691D+12
I= 2 X= -2.473622235672D+12 Y= 1.068579647499D+13 Z= -2.426375072492D+12
I= 3 X= 9.056148390165D+11 Y= -5.085960497163D+12 Z= -8.723572625583D+12
I= 4 X= -1.720764313115D+13 Y= 1.183861424728D+13 Z= 5.979249578508D+11
I= 5 X= -2.054979328846D+12 Y= -5.817761619144D+11 Z= 3.605783871417D+12
I= 6 X= 4.296420872071D+13 Y= 9.314680552931D+12 Z= -8.400694175571D+13
I= 7 X= 6.593639666671D+11 Y= -3.161626595566D+13 Z= -1.090763615272D+13
I= 8 X= -5.256597209415D+13 Y= -9.668448686377D+13 Z= -7.918792141441D+13
I= 9 X= 1.039165627977D+13 Y= -7.901190082310D+12 Z= 2.047818583461D+13
I= 10 X= 3.477402244634D+13 Y= 1.145763668648D+14 Z= -1.879876579073D+14
I= 11 X= -2.736322022402D+13 Y= 5.067265669246D+12 Z= -5.802662063244D+12
I= 12 X= -2.683527510092D+13 Y= -3.245198957341D+13 Z= -1.564475182596D+13
I= 13 X= 1.819096319279D+13 Y= -2.531271682098D+13 Z= -2.569135581292D+12
I= 14 X= -1.503847752138D+13 Y= -4.726179703003D+13 Z= 3.050541705558D+12
I= 15 X= 1.937100745057D+13 Y= 3.503099075502D+12 Z= -8.816872067154D+13
I= 16 X= -3.174231743739D+13 Y= 4.037382080063D+13 Z= 3.376597053060D+13
I= 17 X= 1.135427677747D+13 Y= -4.542482131916D+12 Z= -1.510196491680D+13
I= 18 X= -5.515157815071D+13 Y= 4.834198238881D+13 Z= 1.518438172923D+13
I= 19 X= -6.731161928557D+13 Y= -1.645664880651D+13 Z= 3.365076779358D+13
I= 20 X= 9.111012836442D+13 Y= 8.553193205912D+13 Z= 1.445126042029D+14
I= 21 X= 6.235529997532D+11 Y= 1.679962319755D+13 Z= 1.772410067972D+13
I= 22 X= -3.447438326359D+13 Y= -9.062404109017D+13 Z= 3.540757139957D+13
I= 23 X= -4.548534304699D+12 Y= -2.825743122727D+13 Z= -5.404422962867D+13
I= 24 X= -7.686598732353D+11 Y= 1.938045654286D+13 Z= -9.314173556528D+13

I= 25 X= 6.228365473726D+12 Y= 1.172862091651D+13 Z= 3.080870029713D+13
I= 26 X= -1.507923831465D+13 Y= 3.043551759493D+13 Z= 3.191137289050D+13
I= 27 X= 1.266001917145D+13 Y= -2.581408600795D+13 Z= -9.960317661788D+13
I= 28 X= 1.448205114491D+13 Y= -1.489051222632D+14 Z= -5.457300607308D+13
I= 29 X= 1.799144758148D+12 Y= -2.530790407455D+12 Z= -1.188733377303D+13
I= 30 X= -1.445790527815D+13 Y= -1.383254630642D+13 Z= -3.147329040833D+13
I= 31 X= 2.723360320947D+12 Y= 3.919374009062D+13 Z= 3.536611822874D+13
I= 32 X= -6.913965429806D+12 Y= 3.152872007034D+13 Z= -1.125156426179D+13
I= 33 X= 1.492526461335D+13 Y= 5.836655753090D+13 Z= -6.927672566680D+13
I= 34 X= 1.563630148831D+13 Y= -3.788135960922D+13 Z= 6.612834619574D+13
I= 35 X= -4.403487009721D+12 Y= 6.883730063031D+11 Z= 8.556687962561D+12
I= 36 X= 3.722792205423D+11 Y= -4.329061582333D+12 Z= -1.481704084983D+13
I= 37 X= -1.810601928091D+13 Y= 2.422142928311D+12 Z= 7.323811654642D+13
I= 38 X= 8.796901046643D+13 Y= 5.069479380959D+13 Z= 7.636203450708D+13

Backward Direction:

Total Energy: -692.0029437 Hartrees

Potential Energy: -692.1813138 Hartress

Kinetic Energy: 0.1783701 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.127084388257D+13 Y= 7.201311930332D+12 Z= -2.246753035929D+12
I= 1 X= -1.048811368433D+13 Y= 5.538693741689D+12 Z= 1.974662142341D+12
I= 2 X= -1.915456069033D+12 Y= 9.769655038218D+12 Z= -1.138818541388D+12
I= 3 X= 1.054365662659D+12 Y= -6.696210452603D+12 Z= -1.107354658258D+13
I= 4 X= -1.664935732073D+13 Y= 1.275490159577D+13 Z= -6.896315802025D+11
I= 5 X= 8.750145796891D+11 Y= -1.022462895635D+13 Z= -7.948538111005D+12
I= 6 X= -6.383410419584D+13 Y= 9.330325815723D+12 Z= -8.400695634307D+13
I= 7 X= -1.475399527551D+13 Y= -3.314086675054D+13 Z= -2.459654224886D+13
I= 8 X= -6.040393853107D+13 Y= -1.001792715286D+14 Z= -8.242563165473D+13
I= 9 X= 1.198620201343D+13 Y= -1.080629346042D+13 Z= 1.952922406268D+13
I= 10 X= 3.369561805714D+13 Y= 1.108210083439D+14 Z= -1.900845298800D+14

I= 11 X= -2.527830465182D+13 Y= -7.101698456254D+11 Z= -6.379341836811D+12
I= 12 X= -2.277141157747D+13 Y= -3.514125492870D+13 Z= -1.533405413306D+13
I= 13 X= 1.978534329307D+13 Y= -2.240758324967D+13 Z= -1.619735334776D+12
I= 14 X= -1.611567060065D+13 Y= -4.350602519268D+13 Z= 5.148063544696D+12
I= 15 X= 2.343404083418D+13 Y= 6.193600733143D+12 Z= -8.847960120122D+13
I= 16 X= -2.965817049691D+13 Y= 4.614957019114D+13 Z= 3.434378199722D+13
I= 17 X= 1.124089368061D+13 Y= -4.365699078550D+12 Z= -1.199386999975D+13
I= 18 X= -5.449814778736D+13 Y= 4.965752427237D+13 Z= 2.146467087780D+13
I= 19 X= -6.765908537103D+13 Y= -1.561172041838D+13 Z= 3.496072931308D+13
I= 20 X= 9.021537171499D+13 Y= 8.194446664792D+13 Z= 1.479397722816D+14
I= 21 X= -2.074993977206D+12 Y= 1.680103497799D+13 Z= 1.772315189975D+13
I= 22 X= -4.145347141383D+13 Y= -9.062256909997D+13 Z= 3.540490693951D+13
I= 23 X= -6.350942425614D+12 Y= -2.499439200330D+13 Z= -5.373881789753D+13
I= 24 X= -2.571494758480D+12 Y= 1.612142471138D+13 Z= -9.344861713083D+13
I= 25 X= 6.115273122337D+12 Y= 1.155127449609D+13 Z= 2.770053305716D+13
I= 26 X= -1.597333570767D+13 Y= 3.402189460420D+13 Z= 2.848394960369D+13
I= 27 X= 1.231298535015D+13 Y= -2.666021113674D+13 Z= -1.009128057045D+14
I= 28 X= 1.513546303784D+13 Y= -1.502215295936D+14 Z= -6.085287201232D+13
I= 29 X= 4.728647414222D+12 Y= 7.108941491878D+12 Z= -3.356374857215D+11
I= 30 X= -9.963765469319D+12 Y= -1.259821478139D+13 Z= -2.304233378554D+13
I= 31 X= -5.109895718039D+12 Y= 4.268848365067D+13 Z= 3.860181754921D+13
I= 32 X= -2.232554655935D+13 Y= 3.305304993017D+13 Z= 2.432411722526D+12
I= 33 X= 1.333701567266D+13 Y= 5.281727814791D+13 Z= -5.119504729451D+13
I= 34 X= 1.618088203596D+13 Y= -4.402506223910D+13 Z= 7.345488878599D+13
I= 35 X= -5.310710296806D+12 Y= 6.886935625278D+11 Z= 8.557731395319D+12
I= 36 X= 4.866773696974D+12 Y= -5.564639119175D+12 Z= -2.324849732554D+13
I= 37 X= -1.969711989358D+13 Y= 7.975011998653D+12 Z= 5.515406974618D+13
I= 38 X= 8.851464910707D+13 Y= 5.683660245130D+13 Z= 6.903563733909D+13

Seed: 9246416792

CM Start Point Coordinates: bohr

I= 0 X= -2.142278916333D+00 Y= -2.177405270082D+00 Z= -3.543513858014D-02
I= 1 X= 1.658282880849D-01 Y= -2.608206819436D+00 Z= -1.512909263237D+00
I= 2 X= -1.348698833757D+00 Y= -1.463891821735D+00 Z= 2.555481416165D+00
I= 3 X= 2.229026049955D+00 Y= -2.164225445170D+00 Z= 1.381549963045D-01
I= 4 X= 1.191620298536D+00 Y= -1.183112821880D+00 Z= 2.662346831168D+00
I= 5 X= -2.888551046090D+00 Y= 3.135827737678D+00 Z= -2.300631175315D+00
I= 6 X= -1.176834785267D-01 Y= 1.216357661954D+00 Z= -3.316709491471D+00
I= 7 X= -2.188516443301D+00 Y= 4.468299789372D+00 Z= -4.159472417314D+00
I= 8 X= -4.528093484986D+00 Y= 1.741404460065D+00 Z= -2.602905613301D+00
I= 9 X= 3.039443562903D+00 Y= -7.104987672035D-01 Z= 4.558158842399D+00
I= 10 X= 2.434293060496D+00 Y= -2.287508580287D+00 Z= 6.365813670068D+00
I= 11 X= 5.143825689306D+00 Y= -1.221307612584D+00 Z= 3.762368889342D+00
I= 12 X= 2.966987441806D+00 Y= 1.529468692460D+00 Z= 5.099734195026D+00
I= 13 X= -3.283659986254D+00 Y= -9.220398039813D-01 Z= 4.592433493197D+00
I= 14 X= -3.860155495395D+00 Y= -2.395341610116D+00 Z= 6.044197239768D+00
I= 15 X= -2.650668475292D+00 Y= 4.416362599296D-01 Z= 5.818130927849D+00
I= 16 X= -5.153561039913D+00 Y= 5.024519782167D-02 Z= 3.471954696893D+00
I= 17 X= -4.813567602162D+00 Y= -2.239917616590D+00 Z= -8.526754641070D-01
I= 18 X= -5.571179963801D+00 Y= -3.992697632467D+00 Z= -1.962992934030D-01
I= 19 X= -6.160977194233D+00 Y= -8.399278182993D-01 Z= -2.089096360748D-01
I= 20 X= -4.866362238862D+00 Y= -2.294643585727D+00 Z= -3.014695506658D+00
I= 21 X= -2.036086188877D-02 Y= -3.706969971630D+00 Z= -4.058290593593D+00
I= 22 X= -1.245944257115D-01 Y= -6.042771188782D+00 Z= -3.980069872836D+00
I= 23 X= -1.557727365986D+00 Y= -2.881221978135D+00 Z= -4.857208044940D+00
I= 24 X= 1.883498755906D+00 Y= -3.452825006065D+00 Z= -5.259051815648D+00
I= 25 X= 4.858226687575D+00 Y= -2.421919210425D+00 Z= -7.798795154402D-01
I= 26 X= 4.794148154249D+00 Y= -3.043515964082D+00 Z= -2.771866593706D+00
I= 27 X= 5.978687790452D+00 Y= -4.559219417005D-01 Z= -5.885111538850D-01
I= 28 X= 5.983770348200D+00 Y= -3.659579879924D+00 Z= 2.510403028159D-01

I= 29 X= 2.517691363763D+00 Y= 3.410884118469D+00 Z= -2.614543707919D+00
I= 30 X= 2.863436779950D+00 Y= 3.606478293222D+00 Z= 7.977397969232D-02
I= 31 X= 3.365229012013D+00 Y= 2.027956702150D+00 Z= -4.091363912819D+00
I= 32 X= 1.350223830023D+00 Y= 4.858224202834D+00 Z= -3.635302644048D+00
I= 33 X= 2.375124615693D+00 Y= 5.142984514670D+00 Z= 1.581709851285D+00
I= 34 X= 4.525568216851D+00 Y= 2.842780620863D+00 Z= 1.058979409799D+00
I= 35 X= 7.755410864836D-02 Y= 1.129712222661D+00 Z= -4.894412841148D-01
I= 36 X= -2.665391086642D+00 Y= 3.877087295350D+00 Z= 1.876030241893D-01
I= 37 X= -1.451226128166D+00 Y= 5.643194754946D+00 Z= 9.960331447521D-01
I= 38 X= -3.566506261812D+00 Y= 2.840234319905D+00 Z= 1.661805999510D+00

Forward Direction:

Total Energy: -692.0056182 Hartrees

Potential Energy: -692.1629413 Hartress

Kinetic Energy: 0.1573231 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.926935317666D+12 Y= 9.061752984175D+12 Z= 7.952083551302D+12
I= 1 X= 2.484291368968D+13 Y= -2.544397805133D+12 Z= -2.057968552878D+13
I= 2 X= -1.830204653065D+13 Y= -3.940543553997D+11 Z= -2.262906054333D+12
I= 3 X= 1.071123485126D+11 Y= 5.428983589661D+12 Z= -9.638811905299D+12
I= 4 X= 2.212908007446D+13 Y= -3.948733697624D+12 Z= 3.159462709593D+12
I= 5 X= 2.270787918079D+12 Y= 1.820367798278D+13 Z= 1.062003153934D+13
I= 6 X= 4.602980202302D+13 Y= 9.884942251873D+12 Z= -8.930304271564D+13
I= 7 X= -1.571782817735D+12 Y= -4.028145694870D+13 Z= -7.969458594859D+12
I= 8 X= 6.484262798572D+13 Y= -5.024568381834D+12 Z= 2.084774513982D+13
I= 9 X= 5.083735799605D+12 Y= -7.599159752314D+12 Z= 1.567418518955D+13
I= 10 X= 4.873936046267D+13 Y= 6.466965159794D+13 Z= -1.329683057262D+13
I= 11 X= 2.622276351668D+13 Y= -2.535859954263D+13 Z= -6.769017052535D+13
I= 12 X= -7.468455738689D+13 Y= 3.673322214925D+13 Z= 2.988740915904D+13
I= 13 X= -1.286905274370D+13 Y= 2.664773523293D+12 Z= 3.081170494983D+12
I= 14 X= 2.570583154214D+13 Y= -6.900640288593D+13 Z= 9.814779857299D+12

I= 15 X= 1.722006105912D+13 Y= -3.630192652152D+13 Z= -1.574644569089D+13
I= 16 X= -1.234425967675D+14 Y= -7.633361656507D+12 Z= -1.415955976709D+13
I= 17 X= -1.697272169277D+13 Y= -1.051515257763D+12 Z= 1.838082462824D+13
I= 18 X= 7.851001402745D+13 Y= 2.524183840297D+13 Z= -6.400791327436D+13
I= 19 X= 3.488028197922D+13 Y= 1.011280434600D+14 Z= 2.454415266094D+13
I= 20 X= 6.425525075840D+13 Y= -2.146705304522D+13 Z= -1.217593926545D+14
I= 21 X= -1.415501912885D+13 Y= -5.747504995853D+12 Z= 2.018435926630D+13
I= 22 X= -2.212625342915D+13 Y= 3.175775099049D+13 Z= -7.915204246656D+11
I= 23 X= 2.903910047795D+13 Y= 4.773790648778D+13 Z= 1.607577171221D+13
I= 24 X= -5.653945237319D+13 Y= 2.133959357694D+13 Z= 6.158382944009D+13
I= 25 X= 1.409353847932D+13 Y= -5.245782327667D+11 Z= -1.297789619279D+12
I= 26 X= -4.778298791358D+13 Y= 9.613619486617D+12 Z= -8.945129691103D+13
I= 27 X= 7.469854123093D+12 Y= 1.673685206972D+12 Z= 7.205821695192D+12
I= 28 X= 1.009690768112D+14 Y= -1.089602953267D+13 Z= 7.830231357108D+13
I= 29 X= -1.943547567433D+13 Y= 1.070547746945D+13 Z= -4.299797503980D+12
I= 30 X= 9.694175266691D+12 Y= -1.795994473578D+13 Z= -2.793528631588D+13
I= 31 X= 1.488199574153D+13 Y= -7.413586204215D+13 Z= 1.281701988426D+13
I= 32 X= 2.483640201134D+13 Y= -6.007281700120D+13 Z= 1.091972361512D+14
I= 33 X= -4.076716931051D+13 Y= 1.038585695739D+14 Z= 9.008940410399D+13
I= 34 X= -1.743477145289D+13 Y= 6.052121981287D+13 Z= 1.395103735840D+14
I= 35 X= -2.521124145210D+12 Y= -7.362498857680D+11 Z= -2.466138515448D+12
I= 36 X= 6.506391459673D+12 Y= -1.359109588328D+13 Z= -1.114199450930D+13
I= 37 X= -2.115876279772D+13 Y= 1.088012133685D+13 Z= -2.625405674112D+13
I= 38 X= 1.616592052431D+13 Y= -4.493339346167D+13 Z= 3.218930643998D+13

Backward Direction:

Total Energy: -692.0056173 Hartrees

Potential Energy: -692.1629413 Hartress

Kinetic Energy: 0.1573240 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.795790700047D+12 Y= 9.999042158283D+12 Z= 9.189597446426D+12

I= 1 X= 2.576593676165D+13 Y= -2.544256785588D+12 Z= -2.057974417102D+13
I= 2 X= -1.815967262277D+13 Y= -1.169856260651D+12 Z= -1.541632945361D+12
I= 3 X= 2.383324940956D+11 Y= 4.491593657389D+12 Z= -1.087649992527D+13
I= 4 X= 2.227150823518D+13 Y= -3.172857032074D+12 Z= 2.438150915488D+12
I= 5 X= 4.425170608377D+12 Y= 1.369650672964D+13 Z= 4.779620939237D+12
I= 6 X= -2.369711723590D+13 Y= 9.893933016062D+12 Z= -8.930334103287D+13
I= 7 X= -1.044570378697D+13 Y= -3.878081208748D+13 Z= -1.395454420426D+13
I= 8 X= 5.971846094248D+13 Y= -4.499098432827D+12 Z= 1.916528520543D+13
I= 9 X= 5.702268886638D+12 Y= -8.746977858336D+12 Z= 1.518037745404D+13
I= 10 X= 4.811702738174D+13 Y= 6.306149390553D+13 Z= -1.439997570756D+13
I= 11 X= 2.707542675385D+13 Y= -2.779050141165D+13 Z= -6.795977542045D+13
I= 12 X= -7.295696628316D+13 Y= 3.562676524640D+13 Z= 3.006133903259D+13
I= 13 X= -1.225060742455D+13 Y= 3.812604649633D+12 Z= 3.575140508676D+12
I= 14 X= 2.508395126950D+13 Y= -6.739810203755D+13 Z= 1.091813301197D+13
I= 15 X= 1.894729400376D+13 Y= -3.519494850640D+13 Z= -1.592044875881D+13
I= 16 X= -1.225902722256D+14 Y= -5.202165663919D+12 Z= -1.388948757082D+13
I= 17 X= -1.691687970440D+13 Y= -8.927892997825D+11 Z= 1.967822181645D+13
I= 18 X= 7.901592683579D+13 Y= 2.575696398654D+13 Z= -6.153780119244D+13
I= 19 X= 3.465944881730D+13 Y= 1.013822567568D+14 Z= 2.516971113202D+13
I= 20 X= 6.405635620700D+13 Y= -2.280306565497D+13 Z= -1.203457884005D+14
I= 21 X= -1.518936945467D+13 Y= -5.746886476438D+12 Z= 2.018394294325D+13
I= 22 X= -2.483633181521D+13 Y= 3.175838550550D+13 Z= -7.927053925416D+11
I= 23 X= 2.826351753542D+13 Y= 4.897578163796D+13 Z= 1.631974229346D+13
I= 24 X= -5.731525807299D+13 Y= 2.010353413482D+13 Z= 6.133911696826D+13
I= 25 X= 1.414947223076D+13 Y= -6.835115758624D+11 Z= -2.595202083179D+12
I= 26 X= -4.798159433090D+13 Y= 1.094905776152D+13 Z= -9.086496279859D+13
I= 27 X= 7.249146416244D+12 Y= 1.419041959209D+12 Z= 6.580349356556D+12
I= 28 X= 1.014748924516D+14 Y= -1.141143239693D+13 Z= 7.583255100054D+13
I= 29 X= -1.728126950800D+13 Y= 1.521108966917D+13 Z= 1.539461217335D+12
I= 30 X= 1.255226988653D+13 Y= -1.679774280077D+13 Z= -2.449478393469D+13

I= 31 X= 9.761123049877D+12 Y= -7.466031110380D+13 Z= 1.449881783852D+13
I= 32 X= 1.596296240881D+13 Y= -6.157396346291D+13 Z= 1.151798851933D+14
I= 33 X= -4.151778081680D+13 Y= 1.015105092741D+14 Z= 9.797543027062D+13
I= 34 X= -1.756476459954D+13 Y= 5.773115474903D+13 Z= 1.432854603634D+14
I= 35 X= -3.221625902510D+12 Y= -7.361204587311D+11 Z= -2.465660195228D+12
I= 36 X= 9.364822710599D+12 Y= -1.475391058538D+13 Z= -1.458268523496D+13
I= 37 X= -2.191043005179D+13 Y= 1.322989703254D+13 Z= -3.414149245750D+13
I= 38 X= 1.603679658067D+13 Y= -4.214380960510D+13 Z= 2.841440342102D+13

Iridium:

Seed: 10048645518

CM Start Point Coordinates: bohr

I= 0 X= -2.911120778801D+00 Y= 2.322012000037D+00 Z= -7.948228791337D-01
I= 1 X= -3.111404383182D+00 Y= 6.668740944882D-02 Z= -2.003507513781D+00
I= 2 X= -2.330731869335D+00 Y= 1.673306266485D+00 Z= 1.850131492987D+00
I= 3 X= -2.748127634431D+00 Y= -2.020812355122D+00 Z= -2.695886412363D-01
I= 4 X= -2.421263017191D+00 Y= -8.098912189254D-01 Z= 2.335365432186D+00
I= 5 X= 4.481065382102D+00 Y= 2.276916784047D+00 Z= -9.766782950015D-01
I= 6 X= 3.076055886994D+00 Y= 3.293040671683D-01 Z= -2.792117126521D+00
I= 7 X= 6.377454796060D+00 Y= 1.734691212039D+00 Z= -1.462206744061D+00
I= 8 X= 3.846861524266D+00 Y= 3.621250187881D+00 Z= -2.481331353614D+00
I= 9 X= -2.543974978010D+00 Y= -2.257121216520D+00 Z= 4.806778027334D+00
I= 10 X= -4.469491197767D+00 Y= -2.185278454508D+00 Z= 5.779679707292D+00
I= 11 X= -1.835928639417D+00 Y= -4.220681566661D+00 Z= 4.532852232518D+00
I= 12 X= -1.321024057200D+00 Y= -1.563143798556D+00 Z= 6.143493279864D+00
I= 13 X= -2.143130281986D+00 Y= 3.531349942057D+00 Z= 3.969740443223D+00
I= 14 X= -4.105759311488D+00 Y= 4.226573795811D+00 Z= 4.701542607032D+00
I= 15 X= -1.082556687231D+00 Y= 2.878384859675D+00 Z= 5.893392031175D+00
I= 16 X= -8.638553261052D-01 Y= 5.270589280004D+00 Z= 3.611579694849D+00

I= 17 X= -2.913698441643D+00 Y= 4.909675233056D+00 Z= -1.830020538592D+00
I= 18 X= -4.978818889263D+00 Y= 5.388828053691D+00 Z= -1.910002901495D+00
I= 19 X= -1.622480483842D+00 Y= 6.307856113582D+00 Z= -1.144406719033D+00
I= 20 X= -2.412558949294D+00 Y= 4.502359552784D+00 Z= -3.490978096065D+00
I= 21 X= -3.738168470342D+00 Y= -3.647306481671D-01 Z= -4.822939875674D+00
I= 22 X= -5.838768851797D+00 Y= 7.330276223771D-01 Z= -4.950521218331D+00
I= 23 X= -2.670697680180D+00 Y= 6.467945089250D-01 Z= -5.948012839227D+00
I= 24 X= -4.015915125036D+00 Y= -2.489455981019D+00 Z= -5.520188959274D+00
I= 25 X= -3.294842521981D+00 Y= -4.792514837013D+00 Z= -6.363265932108D-01
I= 26 X= -2.647984591590D+00 Y= -5.642469893381D+00 Z= -2.336539386115D+00
I= 27 X= -2.819353775385D+00 Y= -6.279010207637D+00 Z= 8.038588074014D-01
I= 28 X= -5.598115117720D+00 Y= -4.818807583475D+00 Z= -5.394590421086D-01
I= 29 X= 2.547098214536D+00 Y= -3.598719321379D+00 Z= -1.643891983409D+00
I= 30 X= 3.366220293118D+00 Y= -3.137044670173D+00 Z= 9.068907376142D-01
I= 31 X= 8.346386779593D-01 Y= -4.975697165396D+00 Z= -1.582497474557D+00
I= 32 X= 3.893990749198D+00 Y= -3.949146792432D+00 Z= -3.037589064851D+00
I= 33 X= 5.483645347921D+00 Y= -2.609080268053D+00 Z= 1.371837511020D+00
I= 34 X= 2.610809647810D+00 Y= -4.175122378848D+00 Z= 2.547347154936D+00
I= 35 X= 9.302575981117D-01 Y= -1.343350257206D-03 Z= -1.757818876594D-01
I= 36 X= 3.849149083614D+00 Y= 2.390363320742D+00 Z= 1.623052836670D+00
I= 37 X= 5.084459337344D+00 Y= 1.336674502941D+00 Z= 3.340023425663D+00
I= 38 X= 2.622414591008D+00 Y= 3.932698536407D+00 Z= 2.190395477520D+00

Forward Direction:

Total Energy: -651.6116664 Hartrees

Potential Energy: -651.7848924 Hartress

Kinetic Energy: 0.1732260 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.331178067745D+13 Y= 2.774115976601D+13 Z= -9.737494470269D+12

I= 1 X= -8.922475842928D+12 Y= -1.550503795970D+13 Z= 1.108982981732D+13

I= 2 X= -2.424432209277D+12 Y= 1.119030769273D+13 Z= 1.826737239431D+13

I= 3 X= 1.922849214283D+13 Y= 4.011019323462D+12 Z= 3.304066107331D+12
I= 4 X= 3.133240791647D+12 Y= -2.420836272166D+13 Z= 1.542185924959D+12
I= 5 X= -3.123452109631D+13 Y= -7.163909721288D+12 Z= 2.101307495990D+13
I= 6 X= -6.974367583598D+13 Y= 4.140048913498D+13 Z= -5.599109793940D+13
I= 7 X= 1.053551527712D+14 Y= -3.098074509680D+13 Z= -7.055217986981D+13
I= 8 X= 1.835336632249D+13 Y= 2.016714207187D+13 Z= 3.719043205614D+13
I= 9 X= 7.087746506566D+12 Y= 1.465293296432D+13 Z= 5.533102094112D+12
I= 10 X= -6.021318660115D+13 Y= -2.716989327330D+13 Z= -1.723608181516D+13
I= 11 X= 1.668914436913D+13 Y= -1.356728835779D+14 Z= 3.418055518574D+13
I= 12 X= 7.074601970889D+12 Y= 2.559298333919D+13 Z= -9.242269680940D+13
I= 13 X= -5.646056647845D+11 Y= -1.018048698318D+13 Z= -2.745442290188D+13
I= 14 X= -7.395831593951D+13 Y= 7.098706705191D+13 Z= 1.055449282931D+14
I= 15 X= -8.382140594993D+12 Y= 4.738792650685D+13 Z= 4.281825434497D+13
I= 16 X= -3.701119558200D+12 Y= -7.202306537293D+13 Z= 6.688040567710D+13
I= 17 X= 1.059930856170D+13 Y= -1.132158067967D+13 Z= 2.375211358732D+13
I= 18 X= -7.411935102898D+13 Y= -2.005598117341D+12 Z= -3.921926761388D+13
I= 19 X= 2.252332863150D+13 Y= 5.442755714756D+13 Z= 6.805807062750D+11
I= 20 X= -7.903276141436D+13 Y= -2.573474766242D+13 Z= -4.635686186998D+13
I= 21 X= -3.451884621115D+12 Y= 7.759650898277D+11 Z= -9.554200033292D+12
I= 22 X= -3.939692018576D+13 Y= 5.597173466684D+13 Z= 4.322399859054D+13
I= 23 X= -1.121219837575D+13 Y= 5.252700349152D+13 Z= -1.054738997690D+13
I= 24 X= 1.065671036650D+14 Y= -4.359283836748D+13 Z= -2.866763705196D+13
I= 25 X= -2.638995293687D+13 Y= -1.313500539088D+13 Z= -3.268931680729D+12
I= 26 X= 1.580553872438D+13 Y= -4.196148183904D+13 Z= 3.170541222720D+13
I= 27 X= 1.706187545868D+13 Y= 5.687913610308D+13 Z= 1.563364108843D+12
I= 28 X= 9.892926512552D+13 Y= 2.705029847017D+13 Z= -3.854748368397D+13
I= 29 X= 1.636495131231D+13 Y= 7.855453185107D+12 Z= 1.245811917353D+13
I= 30 X= -3.956811220055D+12 Y= -7.446768662299D+12 Z= -1.027498437650D+13
I= 31 X= 5.730631106621D+13 Y= 6.728174793649D+13 Z= 1.737090140849D+13
I= 32 X= -6.690571584692D+13 Y= -1.782456107390D+13 Z= 2.248511638565D+13

I= 33 X= -1.046527407420D+14 Y= -1.301257239140D+14 Z= -2.456770049733D+13
I= 34 X= -1.145064335958D+13 Y= 5.798662594354D+13 Z= -4.177169787326D+13
I= 35 X= 5.959800185911D+11 Y= 4.907252480366D+11 Z= -1.600697743854D+12
I= 36 X= -5.605970218221D+12 Y= 1.454954304493D+13 Z= -2.677311472799D+11
I= 37 X= -1.704694801177D+13 Y= -8.564084829477D+12 Z= 3.993828282236D+12
I= 38 X= 7.367905244517D+13 Y= -3.850617070437D+13 Z= -6.871352254691D+13

Backward Direction:

Total Energy: -651.6116311 Hartrees

Potential Energy: -651.7848924 Hartress

Kinetic Energy: 0.1732613 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.261452065737D+13 Y= 2.753602883151D+13 Z= -9.752818367820D+12
I= 1 X= -8.574908703187D+12 Y= -1.624896820834D+13 Z= 9.852645693666D+12
I= 2 X= -2.876791030836D+12 Y= 1.187198356840D+13 Z= 1.720178475863D+13
I= 3 X= 1.894449253212D+13 Y= 4.073816359930D+12 Z= 1.811046634657D+12
I= 4 X= 5.344143741491D+12 Y= -2.438837614222D+13 Z= 1.260276369939D+11
I= 5 X= -3.108336138753D+13 Y= -8.196922561572D+12 Z= 1.175052426062D+13
I= 6 X= -8.533939848736D+12 Y= 9.772714759963D+13 Z= -2.938992645486D+13
I= 7 X= 1.179208195602D+14 Y= -1.910375416777D+13 Z= -6.939973750258D+13
I= 8 X= 3.537156265818D+13 Y= 3.409300630795D+13 Z= 4.037217239988D+13
I= 9 X= 7.860569672392D+12 Y= 1.498690409431D+13 Z= 4.692212825627D+12
I= 10 X= -5.995415442877D+13 Y= -2.546901094996D+13 Z= -1.920747040699D+13
I= 11 X= 1.650869515236D+13 Y= -1.356605874856D+14 Z= 3.405738785687D+13
I= 12 X= 7.605050184093D+12 Y= 2.573005247374D+13 Z= -9.293007822746D+13
I= 13 X= -4.158203824299D+11 Y= -1.028312042117D+13 Z= -2.782254469593D+13
I= 14 X= -7.374734743729D+13 Y= 7.035565640030D+13 Z= 1.055816521721D+14
I= 15 X= -7.865253702739D+12 Y= 4.686720052874D+13 Z= 4.194181890789D+13
I= 16 X= -3.801537847385D+12 Y= -7.188213572953D+13 Z= 6.698350746354D+13
I= 17 X= 1.084957414683D+13 Y= -1.154686413977D+13 Z= 2.365343212311D+13
I= 18 X= -7.385320315685D+13 Y= -2.142712277919D+12 Z= -3.980713266163D+13

I= 19 X= 2.252277006608D+13 Y= 5.420952448085D+13 Z= 9.291604492071D+11
I= 20 X= -7.873767706010D+13 Y= -2.610752603724D+13 Z= -4.647847303718D+13
I= 21 X= -3.957682353975D+12 Y= 7.845417211843D+11 Z= -1.032519536178D+13
I= 22 X= -3.973368806323D+13 Y= 5.670406572713D+13 Z= 4.139883584727D+13
I= 23 X= -1.089155244390D+13 Y= 5.224597146946D+13 Z= -1.119375925982D+13
I= 24 X= 1.058991333678D+14 Y= -4.361211303594D+13 Z= -2.957742200479D+13
I= 25 X= -2.639351776312D+13 Y= -1.323088800951D+13 Z= -3.483035820081D+12
I= 26 X= 1.541698381318D+13 Y= -4.251248572369D+13 Z= 3.155202018130D+13
I= 27 X= 1.740209453887D+13 Y= 5.719534532638D+13 Z= 1.438546869022D+12
I= 28 X= 9.900972686078D+13 Y= 2.703728703079D+13 Z= -3.815526165724D+13
I= 29 X= 1.503891167529D+13 Y= 8.638393949569D+12 Z= 1.144118911071D+13
I= 30 X= -3.853529335319D+12 Y= -7.223909032175D+12 Z= -1.105687155823D+13
I= 31 X= 5.741144966985D+13 Y= 6.655890782553D+13 Z= 1.688635051603D+13
I= 32 X= -6.859194380843D+13 Y= -1.629812778865D+13 Z= 2.091008430637D+13
I= 33 X= -1.044188736419D+14 Y= -1.302293009550D+14 Z= -2.536439525798D+13
I= 34 X= -1.065937609315D+13 Y= 5.786690983008D+13 Z= -4.228379665410D+13
I= 35 X= 2.768204851638D+11 Y= 3.608381867144D+11 Z= -3.590808110422D+11
I= 36 X= -9.469893645147D+12 Y= 9.932502747498D+12 Z= -2.585136309359D+12
I= 37 X= -1.255659666423D+13 Y= -5.671712724050D+12 Z= -1.710152851384D+12
I= 38 X= 7.639836862451D+13 Y= -3.868969501233D+13 Z= -7.239716629560D+13

Seed: 11811650333

CM Start Point Coordinates: bohr

I= 0 X= -2.472356485179D+00 Y= 2.413228113468D+00 Z= -6.840185832695D-01
I= 1 X= -3.016022654038D+00 Y= -1.680331157971D-02 Z= -2.104861579131D+00
I= 2 X= -2.187175304209D+00 Y= 1.612711968123D+00 Z= 2.033967588068D+00
I= 3 X= -2.910379920739D+00 Y= -2.000766677756D+00 Z= -2.179916251907D-01
I= 4 X= -2.368293242122D+00 Y= -1.052799342394D+00 Z= 2.266535049214D+00
I= 5 X= 4.168050766616D+00 Y= 2.646994259807D+00 Z= -1.643012737666D+00
I= 6 X= 2.325748537357D+00 Y= 3.112043622595D-01 Z= -2.783311517984D+00

I= 7 X= 6.031228148557D+00 Y= 1.847411409810D+00 Z= -2.678921608140D+00
I= 8 X= 3.061873015581D+00 Y= 4.409226560265D+00 Z= -2.512442845105D+00
I= 9 X= -2.581600780281D+00 Y= -2.460988911673D+00 Z= 4.690398777564D+00
I= 10 X= -4.638181795971D+00 Y= -2.671065678080D+00 Z= 4.811714461183D+00
I= 11 X= -1.744890744810D+00 Y= -4.384978886930D+00 Z= 4.740201910746D+00
I= 12 X= -1.579002336615D+00 Y= -1.202650941403D+00 Z= 6.186051715288D+00
I= 13 X= -2.040206858341D+00 Y= 3.498471676517D+00 Z= 4.172953412485D+00
I= 14 X= -4.009506518696D+00 Y= 4.352262427155D+00 Z= 4.550310153265D+00
I= 15 X= -1.002501256291D+00 Y= 2.661735718660D+00 Z= 5.715018130999D+00
I= 16 X= -8.113545578106D-01 Y= 4.922365277045D+00 Z= 3.498422480428D+00
I= 17 X= -2.393495110379D+00 Y= 5.021720470308D+00 Z= -1.642275875603D+00
I= 18 X= -4.352805466473D+00 Y= 5.816809271646D+00 Z= -1.495000833070D+00
I= 19 X= -1.301845799938D+00 Y= 6.122948162017D+00 Z= -5.839353538268D-02
I= 20 X= -1.808934187971D+00 Y= 5.351857268926D+00 Z= -3.915846583713D+00
I= 21 X= -3.491140258194D+00 Y= -2.350676398789D-01 Z= -4.716046691180D+00
I= 22 X= -5.820411702537D+00 Y= -1.408179980540D+00 Z= -4.585444667075D+00
I= 23 X= -3.504188222308D+00 Y= 2.156443591560D+00 Z= -5.463194444591D+00
I= 24 X= -2.060973890536D+00 Y= -1.590075233401D+00 Z= -5.725644976572D+00
I= 25 X= -3.376295203970D+00 Y= -4.812082710320D+00 Z= -7.481950063962D-01
I= 26 X= -3.280882442856D+00 Y= -5.317781075528D+00 Z= -2.888549743126D+00
I= 27 X= -2.016611455664D+00 Y= -6.073358223640D+00 Z= 4.117746667404D-02
I= 28 X= -5.388611777478D+00 Y= -5.395946811971D+00 Z= -1.353916547079D-01
I= 29 X= 3.109862294834D+00 Y= -3.617555688324D+00 Z= -1.047970830240D+00
I= 30 X= 3.088932310399D+00 Y= -2.978049437592D+00 Z= 1.489615544877D+00
I= 31 X= 1.803392045003D+00 Y= -5.092365904814D+00 Z= -1.485086861792D+00
I= 32 X= 4.955891844096D+00 Y= -3.415573810745D+00 Z= -1.995207246117D+00
I= 33 X= 5.173198134976D+00 Y= -2.553720726246D+00 Z= 2.146589364624D+00
I= 34 X= 1.713268293993D+00 Y= -3.990775864004D+00 Z= 2.908996748105D+00
I= 35 X= 8.242031819563D-01 Y= -2.853693094153D-02 Z= -1.990123548397D-01
I= 36 X= 4.035853197975D+00 Y= 2.407573755568D+00 Z= 1.120070389716D+00

I= 37 X= 5.365845157256D+00 Y= 1.313694126855D+00 Z= 2.003854041146D+00

I= 38 X= 3.136819102157D+00 Y= 4.215048050515D+00 Z= 1.870643670952D+00

Forward Direction:

Total Energy: -651.6116593 Hartrees

Potential Energy: -651.7900450 Hartress

Kinetic Energy: 0.1783857 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.569048748538D+12 Y= 1.019628201827D+13 Z= -2.581647375432D+12

I= 1 X= 9.214844956388D+12 Y= -5.458448225495D+12 Z= -3.906096901838D+12

I= 2 X= -2.201916220429D+12 Y= 3.825948876126D+12 Z= -4.721457985738D+12

I= 3 X= -2.160238839872D+12 Y= 1.164075789404D+13 Z= 3.644844684966D+13

I= 4 X= -3.285561946244D+12 Y= -8.797942817035D+12 Z= -2.129219773826D+13

I= 5 X= 7.011790662432D+11 Y= 1.028398983340D+12 Z= 2.395942968555D+13

I= 6 X= -7.291620008683D+13 Y= -1.676557454027D+13 Z= 1.099109152463D+13

I= 7 X= -3.108418038427D+13 Y= 9.313421595708D+13 Z= 3.945000091328D+13

I= 8 X= -3.406347736573D+13 Y= 1.359709733734D+13 Z= -1.590986997786D+13

I= 9 X= -1.438560951748D+13 Y= -4.847300725818D+12 Z= -5.864228137847D+12

I= 10 X= 4.869801599688D+12 Y= -3.818147123369D+13 Z= 7.882489841968D+11

I= 11 X= 1.068742583118D+14 Y= -9.451068607827D+13 Z= -3.817978406139D+13

I= 12 X= 1.037147252680D+14 Y= 2.110610298366D+13 Z= -6.978837959535D+13

I= 13 X= 1.246009005225D+12 Y= 5.873450361291D+12 Z= -2.530701860242D+13

I= 14 X= -3.909013407805D+13 Y= 5.823162154266D+13 Z= -1.225206651019D+12

I= 15 X= 6.182531139842D+13 Y= -7.167753610923D+13 Z= 9.071751730740D+13

I= 16 X= 1.277733364089D+13 Y= -3.243725733746D+13 Z= -1.395175932036D+13

I= 17 X= -9.191917628355D+12 Y= -1.824300500915D+13 Z= -1.129801610736D+13

I= 18 X= 6.520772618350D+13 Y= -5.707996225788D+13 Z= 1.301732440023D+13

I= 19 X= 2.609894654772D+13 Y= 5.368264785853D+13 Z= -1.639901623957D+13

I= 20 X= -2.141127916846D+13 Y= 1.038088796880D+13 Z= 1.135135006944D+13

I= 21 X= 9.484741577795D+12 Y= 3.830584373068D+12 Z= 1.787166337320D+13

I= 22 X= 7.396575885893D+13 Y= 2.894847681325D+13 Z= -2.214995881466D+13

I= 23 X= -4.713331050656D+13 Y= 3.291760070944D+13 Z= 1.368374120370D+13
I= 24 X= 7.452449220590D+13 Y= -1.212714868018D+14 Z= 1.889906922327D+13
I= 25 X= -9.899630565026D+12 Y= -1.139374782921D+13 Z= -1.725954117143D+11
I= 26 X= -4.300300492642D+13 Y= -6.108685716451D+13 Z= -1.826674837686D+14
I= 27 X= 4.761320006353D+13 Y= 8.052249668659D+13 Z= 1.138421816191D+14
I= 28 X= -2.462827306240D+13 Y= 1.726647704619D+13 Z= -4.811865066435D+12
I= 29 X= -8.596497065311D+12 Y= 1.221728872643D+13 Z= 1.142357635302D+13
I= 30 X= 9.429435681353D+12 Y= 2.448068993971D+13 Z= -1.316210571202D+13
I= 31 X= -2.207598607142D+13 Y= -6.829835860504D+13 Z= 3.728113751771D+13
I= 32 X= -1.496498651125D+13 Y= 2.226371857155D+13 Z= -5.871220035165D+13
I= 33 X= -3.931832536461D+13 Y= -8.986604134978D+13 Z= 3.795640840566D+13
I= 34 X= -3.626834247231D+13 Y= -7.552431817500D+13 Z= 1.008164951822D+14
I= 35 X= 7.699576965174D+11 Y= 1.062567867368D+12 Z= 8.023121198294D+11
I= 36 X= -6.296357187246D+12 Y= -6.054004063644D+12 Z= -1.082227091423D+13
I= 37 X= 8.003401344128D+12 Y= -5.219376549178D+12 Z= -1.735295945602D+13
I= 38 X= 8.016028855856D+13 Y= -1.214595490620D+14 Z= -8.904470804275D+13

Backward Direction:

Total Energy: -651.6116691 Hartrees

Potential Energy: -651.7900450 Hartress

Kinetic Energy: 0.1783759 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.299854034241D+12 Y= 9.981282210709D+12 Z= -2.597708506253D+12
I= 1 X= 9.579133594350D+12 Y= -6.238169046736D+12 Z= -5.202802104355D+12
I= 2 X= -2.676038080977D+12 Y= 4.540420260744D+12 Z= -5.838311171504D+12
I= 3 X= -2.457901707663D+12 Y= 1.170657610445D+13 Z= 3.488359802801D+13
I= 4 X= -9.682921850010D+11 Y= -8.986616705135D+12 Z= -2.277648757361D+13
I= 5 X= 8.596110860531D+11 Y= -5.431222913103D+10 Z= 1.425125654544D+13
I= 6 X= -8.761656257392D+12 Y= 4.227096631022D+13 Z= 3.887204860368D+13
I= 7 X= -1.791397783763D+13 Y= 1.055826103689D+14 Z= 4.065788742031D+13
I= 8 X= -1.622653353736D+13 Y= 2.819293659625D+13 Z= -1.257505571990D+13

I= 9 X= -1.357560573001D+13 Y= -4.497262203686D+12 Z= -6.745572689896D+12
I= 10 X= 5.141295847862D+12 Y= -3.639875925349D+13 Z= -1.277983343868D+12
I= 11 X= 1.066851276687D+14 Y= -9.449779841691D+13 Z= -3.830887698493D+13
I= 12 X= 1.042706934170D+14 Y= 2.124976653022D+13 Z= -7.032017119944D+13
I= 13 X= 1.401952357725D+12 Y= 5.765879217736D+12 Z= -2.569285078157D+13
I= 14 X= -3.886901586577D+13 Y= 5.756983365004D+13 Z= -1.186715986851D+12
I= 15 X= 6.236706577030D+13 Y= -7.222331427316D+13 Z= 8.979891645886D+13
I= 16 X= 1.267208420952D+13 Y= -3.228954755125D+13 Z= -1.384369729607D+13
I= 17 X= -8.929611739037D+12 Y= -1.847912688240D+13 Z= -1.140144514817D+13
I= 18 X= 6.548667845912D+13 Y= -5.722367299804D+13 Z= 1.240117710595D+13
I= 19 X= 2.609836111014D+13 Y= 5.345412561721D+13 Z= -1.613847730303D+13
I= 20 X= -2.110199828587D+13 Y= 9.990175182808D+12 Z= 1.122388817207D+13
I= 21 X= 8.954609855477D+12 Y= 3.839573630282D+12 Z= 1.706357536472D+13
I= 22 X= 7.361278903968D+13 Y= 2.971604042204D+13 Z= -2.406293036438D+13
I= 23 X= -4.679723825337D+13 Y= 3.262304820274D+13 Z= 1.300627501462D+13
I= 24 X= 7.382438576850D+13 Y= -1.212916887785D+14 Z= 1.794551440727D+13
I= 25 X= -9.903366899401D+12 Y= -1.149424337185D+13 Z= -3.970001278758D+11
I= 26 X= -4.341025325751D+13 Y= -6.166436991343D+13 Z= -1.828282555187D+14
I= 27 X= 4.796978711604D+13 Y= 8.085391877320D+13 Z= 1.137113594122D+14
I= 28 X= -2.454394030992D+13 Y= 1.725283963018D+13 Z= -4.400773195552D+12
I= 29 X= -9.986332631673D+12 Y= 1.303789686394D+13 Z= 1.035772166286D+13
I= 30 X= 9.537686470813D+12 Y= 2.471427137281D+13 Z= -1.398160958005D+13
I= 31 X= -2.196578923931D+13 Y= -6.905597464268D+13 Z= 3.677327482652D+13
I= 32 X= -1.673233910913D+13 Y= 2.386358874388D+13 Z= -6.036300741398D+13
I= 33 X= -3.907320689097D+13 Y= -8.997460149339D+13 Z= 3.712138456269D+13
I= 34 X= -3.543900724182D+13 Y= -7.564979384180D+13 Z= 1.002797592703D+14
I= 35 X= 4.354433600758D+11 Y= 9.264319230716D+11 Z= 2.103663394021D+12
I= 36 X= -1.034617443920D+13 Y= -1.089317073168D+13 Z= -1.325116672081D+13
I= 37 X= 1.270978403954D+13 Y= -2.187852073776D+12 Z= -2.333135981575D+13
I= 38 X= 8.301043136377D+13 Y= -1.216519027499D+14 Z= -9.290557233748D+13

Seed: 12095833256

CM Start Point Coordinates: bohr

I= 0 X= -2.547402370439D+00 Y= 2.317723926249D+00 Z= -6.756857903578D-01
I= 1 X= -3.023456882533D+00 Y= 2.960210514274D-02 Z= -2.067619996876D+00
I= 2 X= -2.321576974107D+00 Y= 1.770678299767D+00 Z= 1.953939630882D+00
I= 3 X= -2.733038901322D+00 Y= -2.039335143938D+00 Z= -1.443717421658D-01
I= 4 X= -2.391275658480D+00 Y= -8.958128480015D-01 Z= 2.316897235917D+00
I= 5 X= 4.496949829721D+00 Y= 2.283098538667D+00 Z= -9.369315898065D-01
I= 6 X= 2.426440312537D+00 Y= 1.075102662594D+00 Z= -2.964329514893D+00
I= 7 X= 6.109719295896D+00 Y= 6.336114535183D-01 Z= -1.417571756689D+00
I= 8 X= 4.723744592702D+00 Y= 3.811222741288D+00 Z= -2.544496587157D+00
I= 9 X= -2.187755752993D+00 Y= -2.313500580478D+00 Z= 4.654923227380D+00
I= 10 X= -3.696863520626D+00 Y= -1.282168136731D+00 Z= 6.509656450722D+00
I= 11 X= -2.506889250166D+00 Y= -4.627542506239D+00 Z= 4.674289856858D+00
I= 12 X= -3.264654901732D-01 Y= -1.749210434483D+00 Z= 5.612320836036D+00
I= 13 X= -2.218210371653D+00 Y= 3.835794461249D+00 Z= 4.014019636085D+00
I= 14 X= -4.059549639479D+00 Y= 4.418031660977D+00 Z= 4.319966724988D+00
I= 15 X= -1.427617039414D+00 Y= 3.182419058581D+00 Z= 6.031973046029D+00
I= 16 X= -1.540184627923D+00 Y= 5.409472782135D+00 Z= 3.024001256672D+00
I= 17 X= -2.753285569360D+00 Y= 5.029645535243D+00 Z= -1.647135271790D+00
I= 18 X= -4.721950587817D+00 Y= 6.035413865766D+00 Z= -1.410525985558D+00
I= 19 X= -1.520825892016D+00 Y= 6.001738346110D+00 Z= -5.024744552177D-01
I= 20 X= -2.405322920796D+00 Y= 5.502270516675D+00 Z= -3.717769739001D+00
I= 21 X= -3.750759164434D+00 Y= -3.697182225255D-01 Z= -4.739317313703D+00
I= 22 X= -5.754147217249D+00 Y= -1.112468788566D+00 Z= -4.833780906423D+00
I= 23 X= -3.726391861214D+00 Y= 1.505074301956D+00 Z= -5.683034345623D+00
I= 24 X= -2.439381113524D+00 Y= -2.021489548639D+00 Z= -5.476334465520D+00
I= 25 X= -3.573874039712D+00 Y= -4.692569667765D+00 Z= -8.080900372589D-01
I= 26 X= -2.889620382446D+00 Y= -5.394445183527D+00 Z= -2.698142063608D+00

I= 27 X= -2.796488436569D+00 Y= -6.311989926233D+00 Z= 5.583224547308D-01
I= 28 X= -5.638868058534D+00 Y= -4.669285314559D+00 Z= -7.752509725648D-01
I= 29 X= 3.016708231898D+00 Y= -3.352396621024D+00 Z= -1.401975183496D+00
I= 30 X= 3.365017857585D+00 Y= -3.234739329913D+00 Z= 1.137390215706D+00
I= 31 X= 1.795544023790D+00 Y= -4.767670290204D+00 Z= -2.402756080025D+00
I= 32 X= 4.612549486622D+00 Y= -3.002894009893D+00 Z= -2.580230841945D+00
I= 33 X= 5.130558791045D+00 Y= -2.563791598679D+00 Z= 1.771303214524D+00
I= 34 X= 1.944568794585D+00 Y= -4.053944501828D+00 Z= 2.811210179676D+00
I= 35 X= 8.738946120516D-01 Y= -6.369351204341D-02 Z= -2.067292028632D-01
I= 36 X= 3.476068325595D+00 Y= 2.475625891208D+00 Z= 1.423373133300D+00
I= 37 X= 4.810684125275D+00 Y= 1.404932892323D+00 Z= 2.767127381677D+00
I= 38 X= 3.102332472921D+00 Y= 4.722182742198D+00 Z= 1.841868993038D+00

Forward Direction:

Total Energy: -651.5993587 Hartrees

Potential Energy: -651.7893299 Hartress

Kinetic Energy: 0.1899712 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.630876012907D+12 Y= 2.333224924092D+12 Z= 3.353541113020D+12
I= 1 X= -1.058390026452D+13 Y= 5.040210815547D+12 Z= -2.636673915390D+13
I= 2 X= -1.020812271236D+12 Y= 1.205743161967D+13 Z= 2.578005145519D+13
I= 3 X= -1.144921614075D+13 Y= -1.197001145761D+13 Z= -2.516915913030D+12
I= 4 X= 1.102792768608D+13 Y= -3.224738249164D+12 Z= -1.891583101336D+13
I= 5 X= 1.498526213438D+13 Y= 1.325278934118D+13 Z= -4.217235872963D+12
I= 6 X= -3.214341525327D+13 Y= 2.054723226093D+13 Z= 1.018297155560D+13
I= 7 X= 3.066628480410D+13 Y= -7.444407316972D+13 Z= 4.779965964839D+13
I= 8 X= -1.043337544022D+14 Y= -9.696821944579D+13 Z= -2.786598695569D+13
I= 9 X= 4.161592275925D+12 Y= 2.483666837544D+13 Z= -2.956484859367D+12
I= 10 X= 2.056339064184D+12 Y= 4.267241173346D+13 Z= 5.999475237753D+13
I= 11 X= -8.154849374484D+13 Y= 1.170840027228D+13 Z= 3.430786212731D+13
I= 12 X= -1.795997055397D+14 Y= -5.898079805428D+13 Z= -1.380320500798D+14

I= 13 X= 5.270725804601D+12 Y= -2.308488750412D+12 Z= 9.137143009390D+12
I= 14 X= 8.291865498070D+13 Y= -4.259955030269D+12 Z= -2.738604195319D+13
I= 15 X= -6.306275679550D+12 Y= -6.572479136968D+13 Z= -9.121642077130D+13
I= 16 X= -4.991710513064D+13 Y= 1.995732658929D+13 Z= 4.769138540373D+13
I= 17 X= -4.460085849756D+12 Y= 7.654423696531D+12 Z= 2.356722515592D+13
I= 18 X= 1.361793366051D+13 Y= -1.045520867507D+12 Z= -4.474609683197D+13
I= 19 X= 6.768659245943D+12 Y= -1.259534981301D+14 Z= -8.046908444057D+13
I= 20 X= -2.810016817075D+13 Y= -3.925791364701D+13 Z= -8.608775755246D+12
I= 21 X= 1.020992086676D+13 Y= -8.661344914314D+11 Z= 1.336126090645D+13
I= 22 X= -1.534004829398D+14 Y= 5.705065293880D+13 Z= 6.183157551718D+13
I= 23 X= -1.690249875848D+13 Y= -3.519568902343D+13 Z= 8.159346937093D+11
I= 24 X= 6.122822404041D+13 Y= -1.937771425358D+13 Z= 6.438918293177D+13
I= 25 X= 6.337615371014D+12 Y= 7.086947248512D+12 Z= 1.652076305379D+12
I= 26 X= -3.686481143669D+13 Y= -4.416334143955D+13 Z= 5.265412789535D+13
I= 27 X= -1.817277809066D+13 Y= -8.134274070755D+12 Z= -6.383153671577D+13
I= 28 X= 1.006492529955D+14 Y= 4.441861628280D+13 Z= 3.900827403771D+13
I= 29 X= 6.404116638012D+12 Y= -9.504385092255D+12 Z= -2.679490925011D+13
I= 30 X= -2.311660800578D+12 Y= 8.139244304595D+12 Z= -6.398955146190D+12
I= 31 X= -1.331934984862D+13 Y= 4.089466502959D+13 Z= 1.880226515293D+13
I= 32 X= -9.313108105071D+13 Y= -4.242371937827D+13 Z= 8.815815214868D+13
I= 33 X= -2.908652527685D+13 Y= -2.428696148781D+13 Z= -5.975401710273D+13
I= 34 X= 1.122979292295D+14 Y= 4.023708055490D+13 Z= -6.817546309252D+12
I= 35 X= -7.852379733313D+11 Y= -1.301147965320D+12 Z= 1.608583262242D+12
I= 36 X= 2.590200651831D+13 Y= -7.396840171683D+11 Z= -9.142027591223D+12
I= 37 X= -8.303878859448D+13 Y= 1.804336340601D+13 Z= -9.298073166529D+13
I= 38 X= -3.773797432823D+13 Y= -2.281374896484D+13 Z= 5.167215306205D+13

Backward Direction:

Total Energy: -651.5993382 Hartrees

Potential Energy: -651.7893299 Hartress

Kinetic Energy: 0.1899918 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.172028046645D+12 Y= 2.198233803359D+12 Z= 3.343456870886D+12
I= 1 X= -1.035517572813D+13 Y= 4.550650434448D+12 Z= -2.718089657352D+13
I= 2 X= -1.318497380497D+12 Y= 1.250602408236D+13 Z= 2.507881704454D+13
I= 3 X= -1.163610860609D+13 Y= -1.192868642503D+13 Z= -3.499431657398D+12
I= 4 X= 1.248286313681D+13 Y= -3.343200212796D+12 Z= -1.984776649023D+13
I= 5 X= 1.508473624989D+13 Y= 1.257299152546D+13 Z= -1.031267003641D+13
I= 6 X= 8.137056947555D+12 Y= 5.761428317882D+13 Z= 2.768848323948D+13
I= 7 X= 3.893541035442D+13 Y= -6.662814657611D+13 Z= 4.855805081074D+13
I= 8 X= -9.313453955447D+13 Y= -8.780398473071D+13 Z= -2.577216966397D+13
I= 9 X= 4.670166304910D+12 Y= 2.505644574640D+13 Z= -3.509851349552D+12
I= 10 X= 2.226801133091D+12 Y= 4.379171640181D+13 Z= 5.869743485059D+13
I= 11 X= -8.166724249830D+13 Y= 1.171649199926D+13 Z= 3.422680903766D+13
I= 12 X= -1.792506319142D+14 Y= -5.889059656590D+13 Z= -1.383659440706D+14
I= 13 X= 5.368637374748D+12 Y= -2.376029038671D+12 Z= 8.894892008847D+12
I= 14 X= 8.305748764448D+13 Y= -4.675469297015D+12 Z= -2.736187496937D+13
I= 15 X= -5.966126400368D+12 Y= -6.606746705623D+13 Z= -9.179317922915D+13
I= 16 X= -4.998318768489D+13 Y= 2.005006857866D+13 Z= 4.775923390066D+13
I= 17 X= -4.295392833676D+12 Y= 7.506170743571D+12 Z= 2.350228555407D+13
I= 18 X= 1.379307838508D+13 Y= -1.135751981114D+12 Z= -4.513295489714D+13
I= 19 X= 6.768291687995D+12 Y= -1.260969795368D+14 Z= -8.030550084891D+13
I= 20 X= -2.790598116409D+13 Y= -3.950322901608D+13 Z= -8.688804782508D+12
I= 21 X= 9.877069052933D+12 Y= -8.604904431815D+11 Z= 1.285388972697D+13
I= 22 X= -1.536221007775D+14 Y= 5.753258019947D+13 Z= 6.063048527264D+13
I= 23 X= -1.669149035078D+13 Y= -3.538062859593D+13 Z= 3.905765433920D+11
I= 24 X= 6.078865084564D+13 Y= -1.939039839268D+13 Z= 6.379047805217D+13
I= 25 X= 6.335269453412D+12 Y= 7.023849490585D+12 Z= 1.511180158807D+12
I= 26 X= -3.712050891382D+13 Y= -4.452594219590D+13 Z= 5.255318474036D+13
I= 27 X= -1.794888911721D+13 Y= -7.926185334976D+12 Z= -6.391367556237D+13
I= 28 X= 1.007022026842D+14 Y= 4.441005381069D+13 Z= 3.926638474080D+13

I= 29 X= 5.531485810574D+12 Y= -8.989152944580D+12 Z= -2.746412342753D+13
I= 30 X= -2.243693783891D+12 Y= 8.285902201468D+12 Z= -6.913493958700D+12
I= 31 X= -1.325016097081D+13 Y= 4.041898349889D+13 Z= 1.848339531114D+13
I= 32 X= -9.424074207444D+13 Y= -4.141921490361D+13 Z= 8.712166612542D+13
I= 33 X= -2.893262366117D+13 Y= -2.435512273687D+13 Z= -6.027830038129D+13
I= 34 X= 1.128186408239D+14 Y= 4.015829861785D+13 Z= -7.154544671837D+12
I= 35 X= -9.952682320760D+11 Y= -1.386623129121D+12 Z= 2.425657793307D+12
I= 36 X= 2.335926298622D+13 Y= -3.778033397026D+12 Z= -1.066704926610D+13
I= 37 X= -8.008380978705D+13 Y= 1.994675528045D+13 Z= -9.673436741873D+13
I= 38 X= -3.594846588393D+13 Y= -2.293452134788D+13 Z= 4.924804671651D+13

Seed: 12121088233

CM Start Point Coordinates: bohr

I= 0 X= -2.310266333979D+00 Y= 2.423843396353D+00 Z= -5.363933908860D-01
I= 1 X= -2.933386903981D+00 Y= 4.040719839656D-02 Z= -2.014981417307D+00
I= 2 X= -2.407314323526D+00 Y= 1.763735176632D+00 Z= 2.047371933662D+00
I= 3 X= -2.845677370548D+00 Y= -1.898442643185D+00 Z= -2.662230417687D-01
I= 4 X= -2.447602121774D+00 Y= -1.010645481751D+00 Z= 2.418331596271D+00
I= 5 X= 4.148027769449D+00 Y= 2.341330372430D+00 Z= -1.262868109755D+00
I= 6 X= 2.371514958472D+00 Y= 9.124232916591D-01 Z= -2.711133448737D+00
I= 7 X= 5.978221215715D+00 Y= 1.554940761598D+00 Z= -1.724786165582D+00
I= 8 X= 3.603474489291D+00 Y= 3.616289347792D+00 Z= -3.002660669779D+00
I= 9 X= -2.576780182784D+00 Y= -2.266917626725D+00 Z= 4.833017828940D+00
I= 10 X= -4.529269227368D+00 Y= -2.048933478002D+00 Z= 5.073980859531D+00
I= 11 X= -1.732883813801D+00 Y= -4.115979176976D+00 Z= 4.799437705822D+00
I= 12 X= -1.828485758476D+00 Y= -1.049073114442D+00 Z= 6.530626385391D+00
I= 13 X= -2.022982656891D+00 Y= 3.542366420004D+00 Z= 4.179338647236D+00
I= 14 X= -3.933235863352D+00 Y= 3.555549956568D+00 Z= 5.459833467051D+00
I= 15 X= -6.549809394513D-01 Y= 2.832497592598D+00 Z= 5.458894674989D+00
I= 16 X= -1.642344198229D+00 Y= 5.547202573675D+00 Z= 3.416752857187D+00

I= 17 X= -2.378603932221D+00 Y= 5.064814043187D+00 Z= -1.665587755546D+00
I= 18 X= -4.320060222677D+00 Y= 5.710305129915D+00 Z= -1.809434631101D+00
I= 19 X= -1.398447899826D+00 Y= 6.315102393696D+00 Z= -5.616709776105D-01
I= 20 X= -1.159700843461D+00 Y= 5.390871924982D+00 Z= -3.549603724901D+00
I= 21 X= -3.411588590440D+00 Y= -5.065282724888D-01 Z= -4.688816400195D+00
I= 22 X= -5.555901380489D+00 Y= -1.181100391267D+00 Z= -4.896064486244D+00
I= 23 X= -2.814325358591D+00 Y= 1.259998555691D+00 Z= -5.735680963691D+00
I= 24 X= -2.069556395532D+00 Y= -2.167925544199D+00 Z= -5.621116762579D+00
I= 25 X= -3.495263113096D+00 Y= -4.587245565430D+00 Z= -7.993513136903D-01
I= 26 X= -2.353003087045D+00 Y= -5.342023583767D+00 Z= -2.458398078124D+00
I= 27 X= -3.159859974530D+00 Y= -5.689491612524D+00 Z= 1.149310137655D+00
I= 28 X= -5.835182764179D+00 Y= -4.513170454762D+00 Z= -1.211388345521D+00
I= 29 X= 2.849851492986D+00 Y= -3.467064545747D+00 Z= -1.383999655271D+00
I= 30 X= 3.622069420517D+00 Y= -3.016904468655D+00 Z= 1.042229971034D+00
I= 31 X= 1.373701046356D+00 Y= -4.861768350038D+00 Z= -1.884822779829D+00
I= 32 X= 4.063855181545D+00 Y= -3.018483046110D+00 Z= -3.128067268256D+00
I= 33 X= 5.796932754807D+00 Y= -2.020460126452D+00 Z= 9.995084132077D-01
I= 34 X= 3.078385105986D+00 Y= -4.306884456293D+00 Z= 2.528479392411D+00
I= 35 X= 8.499860150591D-01 Y= -9.029464932628D-02 Z= -2.095723916397D-01
I= 36 X= 3.389778035627D+00 Y= 2.804741897577D+00 Z= 1.351884208722D+00
I= 37 X= 4.346036074387D+00 Y= 1.805482929245D+00 Z= 2.784445414350D+00
I= 38 X= 2.274910696000D+00 Y= 4.487389128718D+00 Z= 1.475091513602D+00

Forward Direction:

Total Energy: -651.6121402 Hartrees

Potential Energy: -651.8173059 Hartress

Kinetic Energy: 0.2051658 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.639217252111D+12 Y= 7.978518619140D+11 Z= -9.157172998477D+12

I= 1 X= 1.754394980381D+13 Y= 6.861655333556D+11 Z= 8.009194418797D+12

I= 2 X= -7.844945400605D+12 Y= 3.920428085170D+12 Z= -3.330053281766D+12

I= 3 X= 1.531051064401D+13 Y= 1.781467438858D+13 Z= 1.500726167044D+13
I= 4 X= -1.300387755151D+13 Y= -1.455955589754D+13 Z= 3.317616109828D+11
I= 5 X= 3.395127555347D+12 Y= 2.057190564031D+13 Z= -1.254442007266D+13
I= 6 X= -4.034787279594D+13 Y= -3.346378103503D+13 Z= -1.188451321535D+14
I= 7 X= -2.122521201853D+12 Y= 4.403950044479D+13 Z= -4.312633706375D+13
I= 8 X= 2.114510354398D+13 Y= -1.029248668660D+14 Z= 1.166648620837D+14
I= 9 X= 2.555072592363D+12 Y= 9.067507893149D+12 Z= -2.575434332057D+13
I= 10 X= -7.183741358005D+13 Y= -8.742456633905D+12 Z= -1.044411124423D+13
I= 11 X= -1.075058030169D+13 Y= -9.353854602881D+13 Z= 1.162663920942D+13
I= 12 X= 7.957355849486D+13 Y= 6.495271353502D+13 Z= -3.455222986306D+13
I= 13 X= -1.434799102763D+13 Y= -1.026989701358D+13 Z= 1.072352158865D+13
I= 14 X= -1.482403801863D+10 Y= -3.046240389726D+13 Z= 3.643272310214D+12
I= 15 X= -2.831006792467D+13 Y= -9.595650726984D+12 Z= -1.345086232638D+14
I= 16 X= 3.225950990454D+13 Y= -2.806804702152D+13 Z= -7.716095432158D+13
I= 17 X= -9.988533254871D+12 Y= 2.441465066688D+13 Z= 5.326330306201D+12
I= 18 X= 1.513534500474D+14 Y= -2.231655835864D+13 Z= -6.914178407092D+13
I= 19 X= 4.724937742394D+13 Y= -2.186263430055D+13 Z= 1.624423938963D+13
I= 20 X= -5.388960739211D+13 Y= -5.861102560054D+13 Z= 1.463043850487D+13
I= 21 X= -2.688146921223D+13 Y= -1.863027511747D+13 Z= -9.846116560583D+12
I= 22 X= 1.089795435813D+14 Y= 1.673408007795D+13 Z= -8.382637260883D+12
I= 23 X= 7.816583790508D+13 Y= 1.029509010536D+14 Z= 7.320032254864D+13
I= 24 X= -3.238255720956D+13 Y= 1.672952649976D+13 Z= 2.946046696327D+13
I= 25 X= 2.873997894745D+13 Y= -4.041993785968D+12 Z= -2.290299114325D+13
I= 26 X= -3.628701046009D+13 Y= 6.332111546211D+12 Z= 1.031098462617D+14
I= 27 X= -5.856707954080D+11 Y= -1.787609833029D+11 Z= 4.135126377119D+13
I= 28 X= -9.507332470982D+13 Y= -5.365259482869D+13 Z= 1.119957108473D+13
I= 29 X= -1.416721540613D+13 Y= -1.564190866520D+13 Z= -6.113125637654D+12
I= 30 X= 6.162545561605D+12 Y= -3.102568371294D+12 Z= -3.014049038618D+11
I= 31 X= -1.746461093673D+12 Y= 5.646066507657D+13 Z= -6.559754051221D+13
I= 32 X= 6.875456075697D+13 Y= 7.433832786788D+12 Z= -7.752289220994D+12

I= 33 X= 2.067207728130D+14 Y= 5.648313752071D+13 Z= -2.615926561928D+13
I= 34 X= -5.513209353153D+13 Y= -4.624933642449D+13 Z= -1.159165485014D+13
I= 35 X= -5.686344340742D+11 Y= 9.314522817641D+11 Z= 4.119747282440D+12
I= 36 X= 5.676257649111D+11 Y= -4.040747117837D+12 Z= 1.142666379331D+13
I= 37 X= -4.155250054972D+13 Y= -3.976297051765D+13 Z= -1.759196105953D+13
I= 38 X= 2.996650179360D+13 Y= -8.421135952711D+13 Z= -1.192107250146D+14

Backward Direction:

Total Energy: -651.6121356 Hartrees

Potential Energy: -651.8173059 Hartress

Kinetic Energy: 0.2051703 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.319464409154D+12 Y= 5.977260393362D+11 Z= -9.172122999198D+12
I= 1 X= 1.788303644640D+13 Y= -3.961311917229D+10 Z= 6.802197085076D+12
I= 2 X= -8.286266852207D+12 Y= 4.585471346520D+12 Z= -4.369641010742D+12
I= 3 X= 1.503344050841D+13 Y= 1.787593920318D+13 Z= 1.355067126632D+13
I= 4 X= -1.084691973477D+13 Y= -1.473517706422D+13 Z= -1.049842989662D+12
I= 5 X= 3.542599029702D+12 Y= 1.956409789284D+13 Z= -2.158096829873D+13
I= 6 X= 1.936837050377D+13 Y= 2.148852985064D+13 Z= -9.289301844474D+13
I= 7 X= 1.013654842362D+13 Y= 5.562669761924D+13 Z= -4.200201382144D+13
I= 8 X= 3.774806280506D+13 Y= -8.933878805891D+13 Z= 1.197689692558D+14
I= 9 X= 3.309039190270D+12 Y= 9.393330262451D+12 Z= -2.657471523204D+13
I= 10 X= -7.158470168452D+13 Y= -7.083075146978D+12 Z= -1.236739875237D+13
I= 11 X= -1.092662663257D+13 Y= -9.352654995969D+13 Z= 1.150647711376D+13
I= 12 X= 8.009106399134D+13 Y= 6.508643823524D+13 Z= -3.504723138247D+13
I= 13 X= -1.420283604737D+13 Y= -1.037002623774D+13 Z= 1.036438181686D+13
I= 14 X= 1.909969156531D+11 Y= -3.107840838201D+13 Z= 3.679100136877D+12
I= 15 X= -2.780579286705D+13 Y= -1.010367120458D+13 Z= -1.353636740307D+14
I= 16 X= 3.216154178365D+13 Y= -2.793055600521D+13 Z= -7.706036817415D+13
I= 17 X= -9.744374050505D+12 Y= 2.419486403230D+13 Z= 5.230056628100D+12
I= 18 X= 1.516131040181D+14 Y= -2.245032698848D+13 Z= -6.971530545179D+13

I= 19 X= 4.724883248670D+13 Y= -2.207534705729D+13 Z= 1.648675388278D+13
I= 20 X= -5.360172297826D+13 Y= -5.897470833494D+13 Z= 1.451179459991D+13
I= 21 X= -2.737492568351D+13 Y= -1.862190775121D+13 Z= -1.059829991650D+13
I= 22 X= 1.086509927057D+14 Y= 1.744854255915D+13 Z= -1.016326677904D+13
I= 23 X= 7.847866021098D+13 Y= 1.026767261001D+14 Z= 7.256972441443D+13
I= 24 X= -3.303422930288D+13 Y= 1.671072212483D+13 Z= 2.857288039399D+13
I= 25 X= 2.873650110076D+13 Y= -4.135536907843D+12 Z= -2.311187122856D+13
I= 26 X= -3.666608479115D+13 Y= 5.794551932914D+12 Z= 1.029601969214D+14
I= 27 X= -2.537529196958D+11 Y= 1.297328625142D+11 Z= 4.122949202103D+13
I= 28 X= -9.499482621169D+13 Y= -5.366528879300D+13 Z= 1.158222305635D+13
I= 29 X= -1.546090021581D+13 Y= -1.487807133801D+13 Z= -7.105243019636D+12
I= 30 X= 6.263307410480D+12 Y= -2.885146425399D+12 Z= -1.064214356269D+12
I= 31 X= -1.643887830711D+12 Y= 5.575546196960D+13 Z= -6.607026855748D+13
I= 32 X= 6.710947607194D+13 Y= 8.923021719712D+12 Z= -9.288891157500D+12
I= 33 X= 2.069489336514D+14 Y= 5.638208771729D+13 Z= -2.693652135193D+13
I= 34 X= -5.436013286258D+13 Y= -4.636613151214D+13 Z= -1.209125862657D+13
I= 35 X= -8.800066047103D+11 Y= 8.047344120624D+11 Z= 5.331069266544D+12
I= 36 X= -3.202019500317D+12 Y= -8.545133509357D+12 Z= 9.165802375625D+12
I= 37 X= -3.717171194992D+13 Y= -3.694117111918D+13 Z= -2.315676737305D+13
I= 38 X= 3.261946776092D+13 Y= -8.439040591457D+13 Z= -1.228044893534D+14

Seed: 12310538170

CM Start Point Coordinates: bohr

I= 0 X= -2.589958522675D+00 Y= 2.418892399040D+00 Z= -6.338718361095D-01
I= 1 X= -3.042777838693D+00 Y= 2.947830204093D-02 Z= -1.913411407701D+00
I= 2 X= -2.256646259211D+00 Y= 1.790626437080D+00 Z= 1.994396087219D+00
I= 3 X= -2.983189006927D+00 Y= -2.047213262281D+00 Z= -2.334863555077D-01
I= 4 X= -2.278123663898D+00 Y= -8.745877209996D-01 Z= 2.249151241717D+00
I= 5 X= 4.308015636375D+00 Y= 2.289786389102D+00 Z= -1.059254947658D+00
I= 6 X= 2.546938108610D+00 Y= 1.111254345756D+00 Z= -2.641204058327D+00

I= 7 X= 5.791538021173D+00 Y= 6.711576892128D-01 Z= -1.031473715465D+00
I= 8 X= 4.403933009069D+00 Y= 3.605884338719D+00 Z= -2.446114511500D+00
I= 9 X= -2.063154311795D+00 Y= -2.181761734073D+00 Z= 4.609411243264D+00
I= 10 X= -3.576239415119D+00 Y= -2.107036279289D+00 Z= 6.075873057883D+00
I= 11 X= -1.823373900688D+00 Y= -4.349430643617D+00 Z= 4.478333674533D+00
I= 12 X= -4.623343522732D-01 Y= -1.332586068602D+00 Z= 5.851490903794D+00
I= 13 X= -2.237858174482D+00 Y= 3.638838016672D+00 Z= 4.217995279030D+00
I= 14 X= -4.061296330581D+00 Y= 3.726442927781D+00 Z= 5.243484613105D+00
I= 15 X= -6.421893781228D-01 Y= 3.278615307066D+00 Z= 5.491648827907D+00
I= 16 X= -1.690839054944D+00 Y= 5.615299103207D+00 Z= 3.279014155557D+00
I= 17 X= -2.510070212650D+00 Y= 4.831469566826D+00 Z= -1.762869426116D+00
I= 18 X= -4.210336538080D+00 Y= 5.977756641430D+00 Z= -1.207536304020D+00
I= 19 X= -9.475030436499D-01 Y= 5.589065223562D+00 Z= -1.037415545784D+00
I= 20 X= -1.901438286136D+00 Y= 4.717277974253D+00 Z= -3.707545461418D+00
I= 21 X= -3.498910621798D+00 Y= -1.072173200850D-01 Z= -4.740698755739D+00
I= 22 X= -5.712942159984D+00 Y= 4.563586536149D-01 Z= -5.322021944891D+00
I= 23 X= -2.537774124507D+00 Y= 1.393950679020D+00 Z= -5.711645738365D+00
I= 24 X= -2.420536741047D+00 Y= -1.814575948526D+00 Z= -5.662881429214D+00
I= 25 X= -3.314858135173D+00 Y= -4.805884771701D+00 Z= -5.147147043325D-01
I= 26 X= -3.406373937355D+00 Y= -5.299568640499D+00 Z= -2.738653520118D+00
I= 27 X= -1.728777760591D+00 Y= -5.572536240326D+00 Z= 7.107067394387D-01
I= 28 X= -5.176931787960D+00 Y= -5.479840239793D+00 Z= 9.638200823280D-01
I= 29 X= 3.199690762092D+00 Y= -3.397074944875D+00 Z= -1.285704929838D+00
I= 30 X= 3.218257648977D+00 Y= -3.392441438464D+00 Z= 1.300015455198D+00
I= 31 X= 1.953722978433D+00 Y= -5.124842080074D+00 Z= -1.968476456708D+00
I= 32 X= 4.735388829218D+00 Y= -2.832182459422D+00 Z= -2.647967110668D+00
I= 33 X= 4.715670615745D+00 Y= -2.337958932335D+00 Z= 2.643135773673D+00
I= 34 X= 1.972706156740D+00 Y= -4.273666519212D+00 Z= 2.374813931069D+00
I= 35 X= 8.182692936578D-01 Y= -4.690097944221D-02 Z= -2.681531979617D-01
I= 36 X= 3.500825340923D+00 Y= 2.464586765519D+00 Z= 1.536606956481D+00

I= 37 X= 4.358898415662D+00 Y= 1.690789699572D+00 Z= 3.268707522585D+00

I= 38 X= 2.565999323957D+00 Y= 3.841570851525D+00 Z= 2.271769282198D+00

Forward Direction:

Total Energy: -651.6172046 Hartrees

Potential Energy: -651.7843605 Hartress

Kinetic Energy: 0.1671559 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.350845190939D+12 Y= -2.351474628339D+13 Z= 3.474602954711D+12

I= 1 X= -1.457266744437D+13 Y= -2.019945900436D+13 Z= 8.742766557700D+12

I= 2 X= -1.253503267061D+12 Y= 1.837750063775D+13 Z= -1.647541614714D+13

I= 3 X= 2.009145667309D+13 Y= 1.624750740681D+13 Z= -3.440500565372D+12

I= 4 X= -1.170599145896D+12 Y= 1.269225762774D+12 Z= -5.693935856371D+12

I= 5 X= -1.858326686660D+13 Y= -6.348114714851D+12 Z= -1.722601422074D+13

I= 6 X= -1.330437671778D+14 Y= -1.907899967928D+13 Z= 3.490288505206D+13

I= 7 X= 2.820980629728D+13 Y= -2.558511376007D+13 Z= 1.036721770165D+14

I= 8 X= -2.990402995741D+13 Y= -4.797274178361D+13 Z= 4.351499744680D+13

I= 9 X= -1.514057516529D+13 Y= 1.833685584108D+13 Z= 4.485500453416D+11

I= 10 X= -1.655219936976D+13 Y= -7.038143185062D+13 Z= -1.513793293500D+13

I= 11 X= 3.936645455150D+13 Y= -5.684177628714D+13 Z= 1.021292919268D+13

I= 12 X= 1.651619419597D+13 Y= -4.068448770516D+13 Z= 7.091038051349D+13

I= 13 X= 1.428595261000D+13 Y= -1.327315892201D+13 Z= -1.011940061797D+13

I= 14 X= -1.242688549691D+14 Y= -6.717773886871D+12 Z= 1.268258101772D+14

I= 15 X= 6.689164917899D+13 Y= 3.497875875689D+13 Z= 2.609134699916D+13

I= 16 X= 5.097564562874D+13 Y= -4.812197403040D+13 Z= -1.276927691499D+13

I= 17 X= 9.176714290217D+12 Y= 1.106388816209D+13 Z= 5.043905271979D+12

I= 18 X= -6.731951198057D+13 Y= -4.517298771848D+13 Z= -4.918267958778D+13

I= 19 X= 3.919166417797D+12 Y= -7.432674728843D+13 Z= -1.045812677045D+12

I= 20 X= -4.428926960663D+13 Y= -4.154573476500D+13 Z= 6.465488136790D+12

I= 21 X= 1.840362176445D+13 Y= 9.805400400335D+12 Z= 4.262544501981D+12

I= 22 X= -2.838946513216D+13 Y= 3.798463477827D+13 Z= 3.062691661694D+13

I= 23 X= -4.135788907572D+13 Y= -1.494503481815D+14 Z= 1.312819145505D+13
I= 24 X= 1.478969000950D+13 Y= 6.497128949290D+12 Z= 1.215320860090D+13
I= 25 X= -1.582153685054D+12 Y= -3.636910372141D+12 Z= -2.951937680805D+13
I= 26 X= -1.759068552988D+13 Y= 2.342987989036D+13 Z= 1.443457682360D+14
I= 27 X= -1.855451151916D+13 Y= 2.007936560656D+13 Z= -6.184611535173D+13
I= 28 X= -5.358377242253D+13 Y= -8.823678046824D+13 Z= 4.181812839040D+13
I= 29 X= -1.021570851979D+13 Y= -1.215449418713D+13 Z= -2.318455746699D+12
I= 30 X= 4.332560374956D+12 Y= 5.819010379373D+12 Z= -7.789717871603D+12
I= 31 X= 7.308979051891D+13 Y= -1.080035766351D+13 Z= 6.339396865176D+13
I= 32 X= 1.578730544397D+13 Y= 6.178608032237D+13 Z= 3.721217215203D+13
I= 33 X= 7.895896858198D+13 Y= -3.791365397633D+12 Z= 2.324852196722D+13
I= 34 X= 2.725421588940D+13 Y= -1.943339057307D+13 Z= -1.838974193485D+13
I= 35 X= 1.554309859758D+11 Y= 2.814550750261D+12 Z= -3.075602409688D+11
I= 36 X= 1.724035440196D+13 Y= -3.819194294973D+12 Z= 2.509853724735D+13
I= 37 X= -7.455248041104D+13 Y= 3.358154544864D+13 Z= -8.932006061733D+13
I= 38 X= -1.830944270087D+13 Y= 1.504787729880D+13 Z= 5.995830287690D+13

Backward Direction:

Total Energy: -651.6171997 Hartrees

Potential Energy: -651.7843605 Hartress

Kinetic Energy: 0.1671608 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.424623391327D+12 Y= -2.383064726568D+13 Z= 3.451004202626D+12
I= 1 X= -1.403741516103D+13 Y= -2.134510920652D+13 Z= 6.837506966863D+12
I= 2 X= -1.950134404912D+12 Y= 1.942727930510D+13 Z= -1.811641769467D+13
I= 3 X= 1.965409817912D+13 Y= 1.634421464326D+13 Z= -5.739745774387D+12
I= 4 X= 2.234184322169D+12 Y= 9.920056697863D+11 Z= -7.874815087237D+12
I= 5 X= -1.835048139728D+13 Y= -7.938951183464D+12 Z= -3.149031265384D+13
I= 6 X= -3.878096964376D+13 Y= 6.766387409576D+13 Z= 7.586860400724D+13
I= 7 X= 4.756089294088D+13 Y= -7.294585738094D+12 Z= 1.054469345741D+14
I= 8 X= -3.696062058606D+12 Y= -2.652695542623D+13 Z= 4.841486739463D+13

I= 9 X= -1.395042995886D+13 Y= 1.885117030936D+13 Z= -8.464167362345D+11
I= 10 X= -1.615329065163D+13 Y= -6.776207851712D+13 Z= -1.817386505845D+13
I= 11 X= 3.908856333268D+13 Y= -5.682284034403D+13 Z= 1.002325190130D+13
I= 12 X= 1.733308275669D+13 Y= -4.047340167620D+13 Z= 7.012901476177D+13
I= 13 X= 1.451508146702D+13 Y= -1.343121408708D+13 Z= -1.068630700157D+13
I= 14 X= -1.239439641466D+14 Y= -7.690144259343D+12 Z= 1.268823648312D+14
I= 15 X= 6.768765333580D+13 Y= 3.417684241226D+13 Z= 2.474163923183D+13
I= 16 X= 5.082100179333D+13 Y= -4.790494283526D+13 Z= -1.261050049050D+13
I= 17 X= 9.562122484568D+12 Y= 1.071695235360D+13 Z= 4.891936128478D+12
I= 18 X= -6.690964511812D+13 Y= -4.538414309182D+13 Z= -5.008798987619D+13
I= 19 X= 3.918306226031D+12 Y= -7.466251689223D+13 Z= -6.630006824321D+11
I= 20 X= -4.383484065764D+13 Y= -4.211981227389D+13 Z= 6.278207321594D+12
I= 21 X= 1.762469487597D+13 Y= 9.818608386864D+12 Z= 3.075214163723D+12
I= 22 X= -2.890808658437D+13 Y= 3.911242225565D+13 Z= 2.781617182931D+13
I= 23 X= -4.086409537390D+13 Y= -1.498831365858D+14 Z= 1.213278483392D+13
I= 24 X= 1.376101790168D+13 Y= 6.467446027972D+12 Z= 1.075214268243D+13
I= 25 X= -1.587643510283D+12 Y= -3.784569296743D+12 Z= -2.984909649999D+13
I= 26 X= -1.818905885580D+13 Y= 2.258133567641D+13 Z= 1.441095449806D+14
I= 27 X= -1.803057522473D+13 Y= 2.056632680043D+13 Z= -6.203833350576D+13
I= 28 X= -5.345986161377D+13 Y= -8.825681803941D+13 Z= 4.242214905706D+13
I= 29 X= -1.225780531824D+13 Y= -1.094876791696D+13 Z= -3.884524786877D+12
I= 30 X= 4.491614145933D+12 Y= 6.162213496321D+12 Z= -8.993821627656D+12
I= 31 X= 7.325170362936D+13 Y= -1.191352912061D+13 Z= 6.264776183205D+13
I= 32 X= 1.319051977626D+13 Y= 6.413678269483D+13 Z= 3.478662779282D+13
I= 33 X= 7.931912316531D+13 Y= -3.950873704765D+12 Z= 2.202161458746D+13
I= 34 X= 2.847276494357D+13 Y= -1.961775299955D+13 Z= -1.917837241293D+13
I= 35 X= -3.360736734481D+11 Y= 2.614525091609D+12 Z= 1.604525861686D+12
I= 36 X= 1.128992469054D+13 Y= -1.092942157820D+13 Z= 2.152974071467D+13
I= 37 X= -6.763735370958D+13 Y= 3.803578922752D+13 Z= -9.810417330559D+13
I= 38 X= -1.412170449445D+13 Y= 1.476525044913D+13 Z= 5.428550329637D+13

Seed: 12336245867

CM Start Point Coordinates: bohr

I= 0 X= -2.484004648055D+00 Y= 2.347739158672D+00 Z= -7.069792243844D-01
I= 1 X= -3.018226309191D+00 Y= -2.504334757377D-02 Z= -1.909613687844D+00
I= 2 X= -2.249637553480D+00 Y= 1.832256300026D+00 Z= 1.941546539937D+00
I= 3 X= -2.805681804687D+00 Y= -2.025247446099D+00 Z= -1.862568745814D-01
I= 4 X= -2.508183372502D+00 Y= -8.660624102306D-01 Z= 2.367880252248D+00
I= 5 X= 4.410871852893D+00 Y= 2.129532535049D+00 Z= -1.216448788299D+00
I= 6 X= 2.286458574279D+00 Y= 9.867728771233D-01 Z= -2.633564774394D+00
I= 7 X= 5.531538753450D+00 Y= 5.295828463898D-01 Z= -1.704901335882D+00
I= 8 X= 4.344611773216D+00 Y= 3.757308598575D+00 Z= -2.490544013058D+00
I= 9 X= -2.422775584592D+00 Y= -2.240312798851D+00 Z= 4.700104967146D+00
I= 10 X= -4.229218224128D+00 Y= -2.276798399753D+00 Z= 5.285191882809D+00
I= 11 X= -1.921491095391D+00 Y= -4.233848866559D+00 Z= 4.210954713936D+00
I= 12 X= -1.149955143060D+00 Y= -1.386440366032D+00 Z= 5.975330544872D+00
I= 13 X= -2.284182628094D+00 Y= 3.559064048335D+00 Z= 4.325153301372D+00
I= 14 X= -4.360438507152D+00 Y= 4.537552758974D+00 Z= 3.972569639358D+00
I= 15 X= -1.997977383372D+00 Y= 2.322585072027D+00 Z= 6.665873267798D+00
I= 16 X= -3.106437629924D-01 Y= 5.063150890438D+00 Z= 4.247916994872D+00
I= 17 X= -2.829752614062D+00 Y= 4.945005420266D+00 Z= -1.887524805943D+00
I= 18 X= -4.823174044682D+00 Y= 5.597891882374D+00 Z= -1.955537759278D+00
I= 19 X= -2.229063588659D+00 Y= 6.445185060844D+00 Z= -7.798535278206D-01
I= 20 X= -1.970209272926D+00 Y= 5.100520461938D+00 Z= -3.669728633634D+00
I= 21 X= -3.481809791659D+00 Y= -4.686738712539D-01 Z= -4.741946265246D+00
I= 22 X= -5.403841527479D+00 Y= -4.142289100172D-01 Z= -4.827921895493D+00
I= 23 X= -2.868756864891D+00 Y= 1.144553021318D+00 Z= -5.697142190814D+00
I= 24 X= -2.646911081624D+00 Y= -2.195081020318D+00 Z= -5.781382259631D+00
I= 25 X= -3.295446984377D+00 Y= -4.786884629617D+00 Z= -5.717851710255D-01
I= 26 X= -3.289312443731D+00 Y= -5.240606600496D+00 Z= -2.554081782864D+00

I= 27 X= -1.413236822540D+00 Y= -6.174954607185D+00 Z= 1.105174406036D-01
I= 28 X= -5.176300258809D+00 Y= -5.635092793926D+00 Z= 6.174921984023D-01
I= 29 X= 2.941742810472D+00 Y= -3.513515421648D+00 Z= -1.630038678957D+00
I= 30 X= 3.184709537468D+00 Y= -3.317912664945D+00 Z= 1.152283777317D+00
I= 31 X= 1.303582401881D+00 Y= -4.571370141179D+00 Z= -2.249727937792D+00
I= 32 X= 4.627479743724D+00 Y= -3.025218944755D+00 Z= -2.854706766715D+00
I= 33 X= 4.973001178750D+00 Y= -2.868672791203D+00 Z= 1.980715091316D+00
I= 34 X= 2.081218963178D+00 Y= -4.523598996893D+00 Z= 2.608727454977D+00
I= 35 X= 8.660471515423D-01 Y= 2.469294346671D-02 Z= -2.060847433417D-01
I= 36 X= 3.820082365414D+00 Y= 2.232328098102D+00 Z= 1.400279177023D+00
I= 37 X= 4.847382079973D+00 Y= 8.324726003820D-01 Z= 2.819030420565D+00
I= 38 X= 3.031702140712D+00 Y= 3.854801862434D+00 Z= 2.005879875917D+00

Forward Direction:

Total Energy: -651.5953554 Hartrees

Potential Energy: -651.7726732 Hartress

Kinetic Energy: 0.1773178 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.957461011773D+12 Y= -4.610629304334D+12 Z= 9.902055017221D+12
I= 1 X= 4.839919362135D+12 Y= 1.149944072606D+13 Z= -2.046611937177D+13
I= 2 X= 1.133783032852D+13 Y= 9.495169439600D+12 Z= -1.095196699875D+13
I= 3 X= 1.261039122102D+13 Y= -2.012820585283D+13 Z= -5.810906670057D+12
I= 4 X= 2.833479267073D+09 Y= 4.866188355004D+12 Z= -9.784370706833D+12
I= 5 X= 1.748501220071D+13 Y= -4.689468246753D+12 Z= 1.418164141679D+13
I= 6 X= 1.886248360007D+13 Y= -6.231149899187D+12 Z= -4.599025913073D+13
I= 7 X= -3.197708734204D+13 Y= -7.930268917026D+13 Z= 1.221679175829D+13
I= 8 X= -3.986670195816D+13 Y= -5.416157541910D+13 Z= 4.819469166540D+13
I= 9 X= 7.191768811774D+12 Y= 3.579022578706D+13 Z= 1.198975522434D+13
I= 10 X= -2.639357844012D+13 Y= -9.090741089648D+13 Z= -4.842957500207D+13
I= 11 X= -3.112881759827D+13 Y= -4.176903404803D+13 Z= 2.858912615437D+13
I= 12 X= 1.503622218099D+13 Y= -3.455152872754D+13 Z= -2.123474746086D+13

I= 13 X= -1.297090395322D+13 Y= -4.187556016515D+12 Z= 2.690436225011D+13
I= 14 X= 3.249052677226D+13 Y= -3.108104228406D+11 Z= -1.924012039997D+14
I= 15 X= 1.663251105401D+13 Y= 2.759850847243D+13 Z= -1.820995235964D+13
I= 16 X= 1.334101901352D+13 Y= -4.392149376907D+13 Z= 1.819436846479D+13
I= 17 X= 8.926449818336D+12 Y= 2.571556279795D+13 Z= 1.396606379961D+13
I= 18 X= 2.535256452637D+12 Y= -5.660213659566D+13 Z= 4.978037613256D+13
I= 19 X= -1.035780356658D+14 Y= -1.911404062004D+12 Z= -6.806844428695D+13
I= 20 X= -8.888510663321D+12 Y= -3.008415601342D+13 Z= -3.167521898769D+13
I= 21 X= 1.860337769850D+13 Y= 2.235440954652D+13 Z= -2.724686173859D+13
I= 22 X= -1.331008892795D+13 Y= -8.087714657568D+13 Z= -9.020081182276D+12
I= 23 X= -3.214823151207D+13 Y= -3.805695385161D+13 Z= 8.527282827561D+13
I= 24 X= 5.474387832734D+12 Y= 1.724575064682D+13 Z= 4.254707289833D+13
I= 25 X= -1.317097545716D+13 Y= -9.197362556749D+12 Z= 3.320241375250D+12
I= 26 X= 2.536326839434D+12 Y= -2.413379278211D+13 Z= -3.439791786958D+13
I= 27 X= -1.423236171979D+13 Y= 1.116313577196D+14 Z= 4.011360869887D+13
I= 28 X= 3.116654557344D+13 Y= -1.633136991631D+13 Z= -2.207440286028D+13
I= 29 X= -3.744004363462D+12 Y= -6.426257199329D+12 Z= -2.450067942288D+12
I= 30 X= -9.213273458723D+12 Y= -1.334288593545D+13 Z= -8.072386218834D+12
I= 31 X= -3.333044174938D+13 Y= -8.969791740985D+13 Z= 3.066355980600D+13
I= 32 X= 1.033162275253D+14 Y= 4.061738915948D+13 Z= -1.000185544626D+14
I= 33 X= -5.036346262026D+13 Y= -2.847961404908D+13 Z= -1.549169640695D+13
I= 34 X= -3.033834210484D+13 Y= 3.440238574672D+13 Z= -1.397797136266D+14
I= 35 X= -1.103248450409D+12 Y= -1.373904219784D+12 Z= 2.294837605092D+12
I= 36 X= -7.070762302614D+12 Y= -4.574003707730D+12 Z= -3.081107175956D+12
I= 37 X= -8.931783236320D+13 Y= 9.651173057285D+13 Z= 4.217719359203D+13
I= 38 X= -2.281277810999D+13 Y= 1.455680117157D+14 Z= 1.488289717241D+11

Backward Direction:

Total Energy: -651.5953625 Hartrees

Potential Energy: -651.7726732 Hartress

Kinetic Energy: 0.1773107 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.557684551315D+12 Y= -4.728241839219D+12 Z= 9.893269008026D+12
I= 1 X= 5.039198193753D+12 Y= 1.107290572905D+13 Z= -2.117546319484D+13
I= 2 X= 1.107846882375D+13 Y= 9.886010675068D+12 Z= -1.156292537743D+13
I= 3 X= 1.244755905460D+13 Y= -2.009220095323D+13 Z= -6.666934580540D+12
I= 4 X= 1.270462382470D+12 Y= 4.762977033293D+12 Z= -1.059632999022D+13
I= 5 X= 1.757168014601D+13 Y= -5.281749754662D+12 Z= 8.870925730009D+12
I= 6 X= 5.395729880045D+13 Y= 2.606393580526D+13 Z= -3.073838486096D+13
I= 7 X= -2.477251854769D+13 Y= -7.249297507703D+13 Z= 1.287754859986D+13
I= 8 X= -3.010925984820D+13 Y= -4.617713268315D+13 Z= 5.001895356732D+13
I= 9 X= 7.634869663268D+12 Y= 3.598170929587D+13 Z= 1.150762843546D+13
I= 10 X= -2.624506144207D+13 Y= -8.993220409582D+13 Z= -4.955987750786D+13
I= 11 X= -3.123227878787D+13 Y= -4.176198404245D+13 Z= 2.851850773681D+13
I= 12 X= 1.534035651320D+13 Y= -3.447293966713D+13 Z= -2.152565636252D+13
I= 13 X= -1.288559739281D+13 Y= -4.246401256805D+12 Z= 2.669329833940D+13
I= 14 X= 3.261148629716D+13 Y= -6.728319114990D+11 Z= -1.923801482409D+14
I= 15 X= 1.692886994877D+13 Y= 2.729994841681D+13 Z= -1.871245966405D+13
I= 16 X= 1.328344384600D+13 Y= -4.384069127204D+13 Z= 1.825348223284D+13
I= 17 X= 9.069940461017D+12 Y= 2.558639574182D+13 Z= 1.390948443391D+13
I= 18 X= 2.687853259529D+12 Y= -5.668075148164D+13 Z= 4.944332165720D+13
I= 19 X= -1.035783559226D+14 Y= -2.036413849041D+12 Z= -6.792592023543D+13
I= 20 X= -8.719323024488D+12 Y= -3.029788979775D+13 Z= -3.174494517851D+13
I= 21 X= 1.831337680868D+13 Y= 2.235932698988D+13 Z= -2.768891459407D+13
I= 22 X= -1.350317596164D+13 Y= -8.045726201636D+13 Z= -1.006654460178D+13
I= 23 X= -3.196438805246D+13 Y= -3.821808453461D+13 Z= 8.490223019848D+13
I= 24 X= 5.091404748665D+12 Y= 1.723469945385D+13 Z= 4.202544452767D+13
I= 25 X= -1.317301936305D+13 Y= -9.252337189969D+12 Z= 3.197484022158D+12
I= 26 X= 2.313547527164D+12 Y= -2.444971277564D+13 Z= -3.448586573210D+13
I= 27 X= -1.403729592656D+13 Y= 1.118126573783D+14 Z= 4.004204430109D+13
I= 28 X= 3.121267858571D+13 Y= -1.633883006872D+13 Z= -2.184952099780D+13

I= 29 X= -4.504293805830D+12 Y= -5.977355386107D+12 Z= -3.033128333778D+12
I= 30 X= -9.154056430449D+12 Y= -1.321510859058D+13 Z= -8.520683956520D+12
I= 31 X= -3.327016016568D+13 Y= -9.011236030281D+13 Z= 3.038574086435D+13
I= 32 X= 1.023494228550D+14 Y= 4.149257499874D+13 Z= -1.009216045893D+14
I= 33 X= -5.022937410297D+13 Y= -2.853900030503D+13 Z= -1.594848412226D+13
I= 34 X= -2.988466626166D+13 Y= 3.433374609657D+13 Z= -1.400733272445D+14
I= 35 X= -1.286239679929D+12 Y= -1.448375418479D+12 Z= 3.006722995610D+12
I= 36 X= -9.286156249768D+12 Y= -7.221199834580D+12 Z= -4.409799492575D+12
I= 37 X= -8.674327378791D+13 Y= 9.817008218813D+13 Z= 3.890679615217D+13
I= 38 X= -2.125364871168D+13 Y= 1.454627874108D+14 Z= -1.963200996480D+12

Seed: 12341092432

CM Start Point Coordinates: bohr

I= 0 X= -2.448014816699D+00 Y= 2.366064942488D+00 Z= -5.485625829654D-01
I= 1 X= -3.008905360031D+00 Y= 3.881398373004D-02 Z= -1.926051433937D+00
I= 2 X= -2.344827575105D+00 Y= 1.650388324022D+00 Z= 2.190958570033D+00
I= 3 X= -2.875399304479D+00 Y= -2.011911546936D+00 Z= -2.817645584865D-01
I= 4 X= -2.485405706684D+00 Y= -1.100367143670D+00 Z= 2.501628291174D+00
I= 5 X= 4.432406762876D+00 Y= 2.381936338607D+00 Z= -1.569525435939D+00
I= 6 X= 2.192166891379D+00 Y= 9.512390454923D-01 Z= -3.218730753004D+00
I= 7 X= 5.771514769471D+00 Y= 8.757198594056D-01 Z= -1.539929680018D+00
I= 8 X= 4.306973572413D+00 Y= 3.919661318167D+00 Z= -3.041828681215D+00
I= 9 X= -2.401949284827D+00 Y= -2.555408461897D+00 Z= 4.717874856638D+00
I= 10 X= -3.899681250751D+00 Y= -2.260668706405D+00 Z= 5.994875299466D+00
I= 11 X= -2.614225410165D+00 Y= -4.832288148577D+00 Z= 4.387366562500D+00
I= 12 X= -7.504410826813D-01 Y= -2.145473311053D+00 Z= 5.710754541794D+00
I= 13 X= -2.182719526467D+00 Y= 3.491541389962D+00 Z= 4.317693673718D+00
I= 14 X= -4.181126292921D+00 Y= 3.609731545449D+00 Z= 4.739854497499D+00
I= 15 X= -1.494111474912D+00 Y= 2.248469971281D+00 Z= 5.970573334710D+00
I= 16 X= -9.823647574282D-01 Y= 5.398407435137D+00 Z= 4.253329854904D+00

I= 17 X= -2.497234347481D+00 Y= 4.887417960088D+00 Z= -1.876012884296D+00
I= 18 X= -4.336573332802D+00 Y= 5.416708341865D+00 Z= -3.087829738794D+00
I= 19 X= -1.986651214722D+00 Y= 6.261292612429D+00 Z= -3.672839923576D-01
I= 20 X= -9.138988650634D-01 Y= 4.718143478825D+00 Z= -3.612953707740D+00
I= 21 X= -3.645086492212D+00 Y= -1.150079103645D-01 Z= -4.696476196068D+00
I= 22 X= -5.712867428152D+00 Y= -1.168473894042D-01 Z= -5.069278632779D+00
I= 23 X= -2.776755669023D+00 Y= 1.055269641893D+00 Z= -5.941704067031D+00
I= 24 X= -3.137218329563D+00 Y= -2.002556770193D+00 Z= -5.652903743544D+00
I= 25 X= -3.465563367709D+00 Y= -4.753833532537D+00 Z= -8.522149172479D-01
I= 26 X= -2.236813251983D+00 Y= -5.221292768630D+00 Z= -2.733794077391D+00
I= 27 X= -3.090752702310D+00 Y= -6.127072260843D+00 Z= 1.108475056623D+00
I= 28 X= -5.526151835080D+00 Y= -5.197499321097D+00 Z= -1.541919040509D+00
I= 29 X= 2.754954019226D+00 Y= -3.560293182220D+00 Z= -9.624208224356D-01
I= 30 X= 3.149173412280D+00 Y= -2.927753502131D+00 Z= 1.516567881087D+00
I= 31 X= 1.331412443486D+00 Y= -4.926419002705D+00 Z= -1.632320638931D+00
I= 32 X= 4.314064107610D+00 Y= -3.212116023642D+00 Z= -2.249025609260D+00
I= 33 X= 5.195103372275D+00 Y= -2.298885631524D+00 Z= 2.024485346283D+00
I= 34 X= 2.406019435149D+00 Y= -3.881423688367D+00 Z= 3.137879751746D+00
I= 35 X= 8.774264582297D-01 Y= -2.117198143585D-02 Z= -2.333354102048D-01
I= 36 X= 3.745830848742D+00 Y= 2.655939402519D+00 Z= 1.058831872510D+00
I= 37 X= 5.197204079276D+00 Y= 1.887137143124D+00 Z= 2.578564065381D+00
I= 38 X= 2.964897734108D+00 Y= 4.605829692226D+00 Z= 1.707145230814D+00

Forward Direction:

Total Energy: -651.6159692 Hartrees

Potential Energy: -651.8135306 Hartress

Kinetic Energy: 0.1975613 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.404074768545D+12 Y= 1.292201210530D+12 Z= 2.322015497450D+12

I= 1 X= -1.306625617957D+13 Y= 2.335257991467D+11 Z= -1.430826094927D+13

I= 2 X= 7.706598906164D+12 Y= -5.980361624576D+12 Z= -2.023031569864D+13

I= 3 X= 2.420766282496D+13 Y= -3.227077007504D+13 Z= 1.785254513527D+13
I= 4 X= -3.063661634039D+11 Y= -1.698658371718D+13 Z= 1.933011319124D+13
I= 5 X= -9.157444683096D+11 Y= 3.948501136027D+12 Z= 2.898789280111D+12
I= 6 X= -1.588456845583D+13 Y= -1.983276000181D+13 Z= 6.634026469375D+12
I= 7 X= 8.356469580485D+12 Y= -5.611606489241D+13 Z= -1.242044757240D+13
I= 8 X= -5.187522252674D+13 Y= 2.664858910744D+13 Z= -7.777230462081D+13
I= 9 X= 2.104464364232D+13 Y= -1.765449327760D+13 Z= -1.496530603953D+13
I= 10 X= -5.350106833081D+13 Y= -1.753447997392D+13 Z= 5.035623303634D+13
I= 11 X= -1.544850713833D+13 Y= 1.599268349248D+14 Z= 3.386681357142D+13
I= 12 X= -1.323608438669D+13 Y= -5.771496558789D+12 Z= -2.780903992783D+13
I= 13 X= 5.319985907014D+12 Y= -3.426871278731D+12 Z= 2.476963387075D+12
I= 14 X= -9.425678158896D+13 Y= -8.194295211634D+13 Z= -5.174651226137D+13
I= 15 X= 6.511230832121D+13 Y= 3.214477598966D+13 Z= 2.361406271726D+12
I= 16 X= 1.903047092363D+14 Y= 8.918092193303D+13 Z= -7.821397139071D+13
I= 17 X= -1.573799381632D+13 Y= 3.281709369936D+12 Z= 4.844157557192D+12
I= 18 X= 1.597520599111D+13 Y= -4.496445949419D+13 Z= -3.535899177264D+13
I= 19 X= 4.410828917921D+13 Y= -1.893614556929D+13 Z= 2.755873553990D+13
I= 20 X= 2.400426552743D+13 Y= -2.296368474037D+13 Z= -9.678714601859D+13
I= 21 X= -1.039612515273D+13 Y= 5.303302829448D+12 Z= 6.533482831983D+12
I= 22 X= 1.221869690225D+12 Y= 3.396635604262D+13 Z= -5.685147713291D+13
I= 23 X= 1.384898991430D+13 Y= 5.609204583705D+13 Z= -6.017050295892D+13
I= 24 X= 1.020066781954D+14 Y= -8.146879517115D+13 Z= -7.852646908151D+13
I= 25 X= -1.963816221125D+13 Y= 2.395339578972D+12 Z= -1.104986765497D+13
I= 26 X= -9.060776189629D+12 Y= 9.274682165390D+13 Z= -1.087464440343D+13
I= 27 X= -1.105702393294D+13 Y= 1.355688325130D+13 Z= -1.325253336956D+13
I= 28 X= 7.630406412687D+13 Y= 8.152422173201D+12 Z= -2.406542681272D+13
I= 29 X= -3.988739321654D+12 Y= 9.050902795513D+12 Z= -7.716291955056D+12
I= 30 X= -1.440117683527D+13 Y= 1.285594855299D+12 Z= 9.525002820416D+12
I= 31 X= 1.100856101055D+14 Y= 1.839865266289D+14 Z= 4.107706363270D+13
I= 32 X= -1.844781512730D+13 Y= 2.359618476958D+13 Z= -8.765908023317D+13

I= 33 X= 1.442310470117D+13 Y= 2.341521907986D+13 Z= 7.417243484936D+13
I= 34 X= 7.826027846567D+13 Y= -4.737845345390D+13 Z= 8.029177766510D+13
I= 35 X= -1.144298595271D+12 Y= 1.397741180707D+12 Z= 1.429795085352D+12
I= 36 X= 1.121344113948D+13 Y= 4.004753901605D+12 Z= 7.797552114317D+12
I= 37 X= 1.526849898538D+12 Y= -3.607216250523D+13 Z= 1.114710500433D+14
I= 38 X= -9.648175980833D+13 Y= -3.601323372210D+13 Z= -5.326898224644D+13

Backward Direction:

Total Energy: -651.6159672 Hartrees

Potential Energy: -651.8135306 Hartress

Kinetic Energy: 0.1975633 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -4.043805895412D+12 Y= 1.103995033027D+12 Z= 2.307955931017D+12
I= 1 X= -1.274736579200D+13 Y= -4.490249287082D+11 Z= -1.544336861168D+13
I= 2 X= 7.291562893807D+12 Y= -5.354928839822D+12 Z= -2.120798479867D+13
I= 3 X= 2.394709519482D+13 Y= -3.221315423859D+13 Z= 1.648271035412D+13
I= 4 X= 1.722121621545D+12 Y= -1.715174475418D+13 Z= 1.803079800220D+13
I= 5 X= -7.770565068680D+11 Y= 3.000719177173D+12 Z= -5.599535324526D+12
I= 6 X= 4.027493040022D+13 Y= 3.184654984072D+13 Z= 3.104041273178D+13
I= 7 X= 1.988537978197D+13 Y= -4.521900991160D+13 Z= -1.136308987004D+13
I= 8 X= -3.626114802949D+13 Y= 3.942547082323D+13 Z= -7.485308041087D+13
I= 9 X= 2.175370342131D+13 Y= -1.734807713304D+13 Z= -1.573681598089D+13
I= 10 X= -5.326340814303D+13 Y= -1.597393249633D+13 Z= 4.854749798766D+13
I= 11 X= -1.561406801641D+13 Y= 1.599381165012D+14 Z= 3.375380841639D+13
I= 12 X= -1.274940190045D+13 Y= -5.645736603816D+12 Z= -2.827455878478D+13
I= 13 X= 5.456495345517D+12 Y= -3.521036729697D+12 Z= 2.139214251529D+12
I= 14 X= -9.406321949015D+13 Y= -8.252226689968D+13 Z= -5.171281837223D+13
I= 15 X= 6.558654836926D+13 Y= 3.166701359365D+13 Z= 1.557282980515D+12
I= 16 X= 1.902125761763D+14 Y= 8.931022388253D+13 Z= -7.811937622940D+13
I= 17 X= -1.550837691967D+13 Y= 3.075013393233D+12 Z= 4.753618012475D+12
I= 18 X= 1.621939477563D+13 Y= -4.509026076581D+13 Z= -3.589835377555D+13

I= 19 X= 4.410777670177D+13 Y= -1.913618899641D+13 Z= 2.778680568136D+13
I= 20 X= 2.427500331590D+13 Y= -2.330570625926D+13 Z= -9.689872340399D+13
I= 21 X= -1.086019098440D+13 Y= 5.311171827757D+12 Z= 5.826100083701D+12
I= 22 X= 9.128875535939D+11 Y= 3.463826460396D+13 Z= -5.852605101721D+13
I= 23 X= 1.414318029265D+13 Y= 5.583420094430D+13 Z= -6.076354219475D+13
I= 24 X= 1.013938201810D+14 Y= -8.148647954745D+13 Z= -7.936119032289D+13
I= 25 X= -1.964143291473D+13 Y= 2.307367958156D+12 Z= -1.124630668912D+13
I= 26 X= -9.417272566434D+12 Y= 9.224127950256D+13 Z= -1.101538051882D+13
I= 27 X= -1.074487533144D+13 Y= 1.384700296519D+13 Z= -1.336705230384D+13
I= 28 X= 7.637788719604D+13 Y= 8.140484269976D+12 Z= -2.370556588965D+13
I= 29 X= -5.205371289761D+12 Y= 9.769245395502D+12 Z= -8.649318077444D+12
I= 30 X= -1.430641643784D+13 Y= 1.490066986868D+12 Z= 8.807626874363D+12
I= 31 X= 1.101820740270D+14 Y= 1.833233259495D+14 Z= 4.063249162639D+13
I= 32 X= -1.999491733075D+13 Y= 2.499667648574D+13 Z= -8.910416099968D+13
I= 33 X= 1.463767610769D+13 Y= 2.332018788008D+13 Z= 7.344147305251D+13
I= 34 X= 7.898626057537D+13 Y= -4.748829213689D+13 Z= 7.982193066687D+13
I= 35 X= -1.437125204514D+12 Y= 1.278570722360D+12 Z= 2.568969819152D+12
I= 36 X= 7.668318786227D+12 Y= -2.313478422834D+11 Z= 5.671349306210D+12
I= 37 X= 5.646715429071D+12 Y= -3.341843160538D+13 Z= 1.062376877878D+14
I= 38 X= -9.398680649411D+13 Y= -3.618161597309D+13 Z= -5.664869927433D+13

Seed: 13956542053

CM Start Point Coordinates: bohr

I= 0 X= -2.601298918921D+00 Y= 2.399166560844D+00 Z= -4.070463524216D-01
I= 1 X= -3.073066913369D+00 Y= 2.467064086608D-01 Z= -2.044584087870D+00
I= 2 X= -2.341955363150D+00 Y= 1.752517664335D+00 Z= 2.181491164322D+00
I= 3 X= -2.880492676328D+00 Y= -1.876733176246D+00 Z= -2.917031781346D-01
I= 4 X= -2.393342602356D+00 Y= -1.007209632688D+00 Z= 2.154462066296D+00
I= 5 X= 4.085585862606D+00 Y= 2.155476046922D+00 Z= -1.679025768854D+00
I= 6 X= 2.436441705657D+00 Y= 2.746379001448D-01 Z= -2.774717228248D+00

I= 7 X= 6.003168743754D+00 Y= 1.261540604784D+00 Z= -2.064325355581D+00
I= 8 X= 3.589909247256D+00 Y= 3.432473479760D+00 Z= -3.537465411694D+00
I= 9 X= -2.555435646443D+00 Y= -2.656351878928D+00 Z= 4.327359485575D+00
I= 10 X= -4.713664957693D+00 Y= -3.691407931125D+00 Z= 4.443587342499D+00
I= 11 X= -1.005551989281D+00 Y= -4.169014606222D+00 Z= 4.179143435536D+00
I= 12 X= -2.325338702617D+00 Y= -1.412838206104D+00 Z= 6.658262837628D+00
I= 13 X= -1.903463116267D+00 Y= 3.533280939921D+00 Z= 4.186175868272D+00
I= 14 X= -3.727319970146D+00 Y= 3.519874318783D+00 Z= 5.568118071984D+00
I= 15 X= -1.568806572581D-01 Y= 3.163621556469D+00 Z= 5.402237073280D+00
I= 16 X= -1.553476737660D+00 Y= 5.600542735179D+00 Z= 3.430834511846D+00
I= 17 X= -2.472306475533D+00 Y= 5.105023032834D+00 Z= -1.496628200433D+00
I= 18 X= -4.347313063752D+00 Y= 5.895302282762D+00 Z= -1.150484918400D+00
I= 19 X= -8.426321546018D-01 Y= 6.206760724627D+00 Z= -7.182799483097D-01
I= 20 X= -2.053992519294D+00 Y= 5.392300498583D+00 Z= -3.677612570621D+00
I= 21 X= -3.695722753237D+00 Y= -5.418944959437D-05 Z= -4.810133555071D+00
I= 22 X= -5.634762438138D+00 Y= 2.243594438997D-01 Z= -4.926571811864D+00
I= 23 X= -2.730656425318D+00 Y= 1.517300146873D+00 Z= -5.946422119965D+00
I= 24 X= -3.257921468348D+00 Y= -1.839582821167D+00 Z= -5.320994059460D+00
I= 25 X= -3.143719796547D+00 Y= -4.698697282241D+00 Z= -7.723011513741D-01
I= 26 X= -3.337169260165D+00 Y= -4.929324527511D+00 Z= -2.859344275988D+00
I= 27 X= -8.491303731476D-01 Y= -5.610243279786D+00 Z= -2.207278695187D-01
I= 28 X= -4.582404686379D+00 Y= -5.795338821347D+00 Z= 4.886319497539D-01
I= 29 X= 2.994199027946D+00 Y= -3.634548961265D+00 Z= -5.999388209656D-01
I= 30 X= 3.243921280031D+00 Y= -2.829309476891D+00 Z= 1.827407501896D+00
I= 31 X= 1.730424708123D+00 Y= -5.313269177971D+00 Z= -9.453065053455D-01
I= 32 X= 4.551713036249D+00 Y= -3.424992594810D+00 Z= -2.143957824181D+00
I= 33 X= 4.925875880130D+00 Y= -2.199740227761D+00 Z= 2.414869000920D+00
I= 34 X= 2.033516952244D+00 Y= -3.692086362877D+00 Z= 3.243543314905D+00
I= 35 X= 8.645155907922D-01 Y= -7.954996974957D-02 Z= -2.353930697169D-01
I= 36 X= 3.558600815371D+00 Y= 2.713128172490D+00 Z= 9.297059929719D-01

I= 37 X= 4.854501099263D+00 Y= 2.249461666075D+00 Z= 2.574845306474D+00

I= 38 X= 2.382227032866D+00 Y= 4.254002398878D+00 Z= 1.215386215536D+00

Forward Direction:

Total Energy: -651.6011078 Hartrees

Potential Energy: -651.7904212 Hartress

Kinetic Energy: 0.1893134 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.205053788267D+12 Y= -2.638773469738D+13 Z= 1.732081735417D+13

I= 1 X= 2.921796753950D+13 Y= 1.376663250322D+13 Z= 1.128383160980D+13

I= 2 X= -1.674851305308D+13 Y= -1.688796061808D+13 Z= -1.610706989416D+13

I= 3 X= 1.696619806325D+13 Y= -1.913639343747D+13 Z= 1.440891210589D+13

I= 4 X= -5.262477346988D+12 Y= 1.028329318944D+13 Z= -1.044108132468D+13

I= 5 X= 2.207061792833D+13 Y= -5.040020185133D+12 Z= 2.847652804775D+11

I= 6 X= -1.935163843707D+13 Y= -1.068297213307D+11 Z= -5.555547281657D+13

I= 7 X= -6.216552562922D+13 Y= 7.614852026368D+13 Z= -8.135338034756D+13

I= 8 X= 7.191743625196D+12 Y= -2.988446228842D+13 Z= -4.425387404442D+13

I= 9 X= -1.676958392045D+13 Y= -1.485192166127D+12 Z= -1.205326323010D+13

I= 10 X= 8.837714841240D+13 Y= 6.276143002155D+13 Z= -1.175143705955D+14

I= 11 X= -9.977676861498D+12 Y= 9.366548950194D+13 Z= 2.655383060159D+13

I= 12 X= -8.080282097365D+13 Y= 8.240295030184D+12 Z= 3.477961790549D+13

I= 13 X= -9.001330424487D+12 Y= -2.163799788285D+13 Z= 3.264062531701D+13

I= 14 X= -7.672620438535D+13 Y= 7.073281617203D+13 Z= 4.002420511069D+13

I= 15 X= -1.081421358463D+13 Y= 2.084551994591D+13 Z= -9.230351462056D+13

I= 16 X= -6.822569334694D+12 Y= 3.795110046119D+11 Z= 1.099018377932D+13

I= 17 X= 1.155317440785D+13 Y= 1.365650207292D+13 Z= -1.079075102827D+13

I= 18 X= 2.616561765169D+13 Y= 5.735670179713D+13 Z= 6.272679159498D+13

I= 19 X= -9.171899717293D+13 Y= -9.855714378936D+13 Z= -8.371580919326D+13

I= 20 X= -1.203615323668D+13 Y= 1.932415892850D+13 Z= 3.310305982938D+13

I= 21 X= -6.432036983952D+12 Y= 1.183698505933D+13 Z= 1.487946946206D+13

I= 22 X= 1.110090843461D+14 Y= -7.284944373434D+13 Z= -4.804830705190D+13

I= 23 X= 3.264243629968D+13 Y= 6.111834712303D+12 Z= -3.947298325616D+13
I= 24 X= 1.550309097370D+13 Y= -1.654508699513D+13 Z= -1.295562340178D+13
I= 25 X= -2.011652931577D+13 Y= 6.135873586238D+12 Z= -1.847625783088D+13
I= 26 X= 2.522030528352D+11 Y= 5.734466671327D+13 Z= -4.421811277958D+13
I= 27 X= 2.034208585292D+13 Y= 5.680520261711D+13 Z= 3.541173956120D+13
I= 28 X= 5.144940361493D+13 Y= 7.156109063383D+13 Z= -1.162213893028D+12
I= 29 X= -8.078736662013D+12 Y= 1.278675219050D+13 Z= -8.265644365801D+12
I= 30 X= 2.418966300435D+13 Y= 1.311662244150D+13 Z= 1.348047431106D+13
I= 31 X= 3.224446794995D+13 Y= -3.312672454726D+11 Z= 2.547513796337D+13
I= 32 X= -3.388016301330D+13 Y= -4.681873428192D+13 Z= 2.584836412950D+13
I= 33 X= 1.367060361193D+13 Y= 1.413111798234D+12 Z= -1.353463074037D+14
I= 34 X= -8.246222791690D+13 Y= 1.824628428764D+13 Z= 4.699178906696D+13
I= 35 X= -5.488153209032D+11 Y= -8.790808901434D+11 Z= 3.253509221341D+11
I= 36 X= -1.341476480977D+13 Y= -3.360130228265D+12 Z= -7.837383115426D+12
I= 37 X= 1.123786220493D+14 Y= -6.819820699433D+13 Z= 1.396815500334D+14
I= 38 X= 2.145044683026D+13 Y= 2.775012709143D+13 Z= -3.001503992987D+13

Backward Direction:

Total Energy: -651.6011049 Hartrees

Potential Energy: -651.7904212 Hartress

Kinetic Energy: 0.1893163 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.481636450044D+12 Y= -2.646910413946D+13 Z= 1.731473881216D+13
I= 1 X= 2.935583725899D+13 Y= 1.347153712950D+13 Z= 1.079307684800D+13
I= 2 X= -1.692795057110D+13 Y= -1.661755973211D+13 Z= -1.652975734702D+13
I= 3 X= 1.685354372350D+13 Y= -1.911148368881D+13 Z= 1.381667494178D+13
I= 4 X= -4.385476802690D+12 Y= 1.021188713004D+13 Z= -1.100282990382D+13
I= 5 X= 2.213057856822D+13 Y= -5.449786171249D+12 Z= -3.389417712267D+12
I= 6 X= 4.928473844187D+12 Y= 2.223630850196D+13 Z= -4.500356599945D+13
I= 7 X= -5.718109307506D+13 Y= 8.085977523605D+13 Z= -8.089624015895D+13
I= 8 X= 1.394236444583D+13 Y= -2.436047918900D+13 Z= -4.299177069647D+13

I= 9 X= -1.646302756965D+13 Y= -1.352715586016D+12 Z= -1.238681941269D+13
I= 10 X= 8.847989890419D+13 Y= 6.343612030143D+13 Z= -1.182963627944D+14
I= 11 X= -1.004925579103D+13 Y= 9.367036700052D+13 Z= 2.650497372042D+13
I= 12 X= -8.059240767314D+13 Y= 8.294666345339D+12 Z= 3.457835453189D+13
I= 13 X= -8.942311656044D+12 Y= -2.167870956630D+13 Z= 3.249460216783D+13
I= 14 X= -7.664251935165D+13 Y= 7.048235403921D+13 Z= 4.003877239752D+13
I= 15 X= -1.060917967494D+13 Y= 2.063896317208D+13 Z= -9.265117092703D+13
I= 16 X= -6.862402331673D+12 Y= 4.354136724160D+11 Z= 1.103108124628D+13
I= 17 X= 1.165244744584D+13 Y= 1.356713871324D+13 Z= -1.082989507964D+13
I= 18 X= 2.627119072738D+13 Y= 5.730231261673D+13 Z= 6.249360271204D+13
I= 19 X= -9.171921874186D+13 Y= -9.864363097217D+13 Z= -8.361720487724D+13
I= 20 X= -1.191910190034D+13 Y= 1.917628864896D+13 Z= 3.305482023662D+13
I= 21 X= -6.632672153726D+12 Y= 1.184038715793D+13 Z= 1.457363816144D+13
I= 22 X= 1.108754983774D+14 Y= -7.255894942316D+13 Z= -4.877229573940D+13
I= 23 X= 3.276962716577D+13 Y= 6.000357526318D+12 Z= -3.972937904786D+13
I= 24 X= 1.523812668638D+13 Y= -1.655273269441D+13 Z= -1.331650848657D+13
I= 25 X= -2.011794337726D+13 Y= 6.097839755717D+12 Z= -1.856118668174D+13
I= 26 X= 9.807468548659D+10 Y= 5.712609958834D+13 Z= -4.427895891709D+13
I= 27 X= 2.047704082298D+13 Y= 5.693063357052D+13 Z= 3.536222820906D+13
I= 28 X= 5.148132043188D+13 Y= 7.155592937047D+13 Z= -1.006630882608D+12
I= 29 X= -8.604737809035D+12 Y= 1.309732189401D+13 Z= -8.669030782963D+12
I= 30 X= 2.423063190869D+13 Y= 1.320502433874D+13 Z= 1.317032253046D+13
I= 31 X= 3.228617335749D+13 Y= -6.179967798829D+11 Z= 2.528293079454D+13
I= 32 X= -3.454904033606D+13 Y= -4.621324283786D+13 Z= 2.522359496016D+13
I= 33 X= 1.376337185415D+13 Y= 1.372025814109D+12 Z= -1.356623329202D+14
I= 34 X= -8.214835532871D+13 Y= 1.819879640584D+13 Z= 4.678865445698D+13
I= 35 X= -6.754165744671D+11 Y= -9.306032889498D+11 Z= 8.178640501658D+11
I= 36 X= -1.494747023733D+13 Y= -5.191575095030D+12 Z= -8.756629974655D+12
I= 37 X= 1.141598131159D+14 Y= -6.705088756274D+13 Z= 1.374189475241D+14
I= 38 X= 2.252912003708D+13 Y= 2.767732836826D+13 Z= -3.147623368596D+13

Seed: 16826952480

CM Start Point Coordinates: bohr

I= 0 X= -2.668053294049D+00 Y= 2.333734319354D+00 Z= -5.765275479050D-01
I= 1 X= -2.833571136356D+00 Y= 1.561668468412D-01 Z= -2.096787285390D+00
I= 2 X= -2.263419313900D+00 Y= 1.675219263945D+00 Z= 2.025203535300D+00
I= 3 X= -2.843014402327D+00 Y= -1.948765377096D+00 Z= -3.310796041871D-01
I= 4 X= -2.465307343492D+00 Y= -9.966385183679D-01 Z= 2.160235091601D+00
I= 5 X= 4.208091199663D+00 Y= 2.125918408844D+00 Z= -1.572766505398D+00
I= 6 X= 2.215430760922D+00 Y= 6.263819802704D-01 Z= -2.776233252817D+00
I= 7 X= 5.926320595398D+00 Y= 1.124368327474D+00 Z= -2.282716035994D+00
I= 8 X= 3.766541571818D+00 Y= 3.586416677687D+00 Z= -3.359404221511D+00
I= 9 X= -2.573962130759D+00 Y= -2.461389546161D+00 Z= 4.609301416948D+00
I= 10 X= -4.619356953452D+00 Y= -2.503706128562D+00 Z= 5.402651882163D+00
I= 11 X= -1.660188862551D+00 Y= -4.324021066574D+00 Z= 4.354100025778D+00
I= 12 X= -1.942564335938D+00 Y= -1.855353670710D+00 Z= 6.118963414301D+00
I= 13 X= -2.185898773576D+00 Y= 3.365468908714D+00 Z= 4.469839238186D+00
I= 14 X= -4.023431677844D+00 Y= 3.517783183497D+00 Z= 5.539128422550D+00
I= 15 X= -3.217238249702D-01 Y= 2.640885071426D+00 Z= 5.608905688990D+00
I= 16 X= -1.577631624956D+00 Y= 5.329859164216D+00 Z= 4.071690087620D+00
I= 17 X= -2.617218790179D+00 Y= 4.909224542425D+00 Z= -1.542409239742D+00
I= 18 X= -4.433086662188D+00 Y= 6.022255528734D+00 Z= -1.181979049169D+00
I= 19 X= -7.984484154378D-01 Y= 6.022729228743D+00 Z= -5.363945821060D-01
I= 20 X= -2.453798075626D+00 Y= 4.959941694914D+00 Z= -3.623698160919D+00
I= 21 X= -3.649848140794D+00 Y= 5.892733402699D-02 Z= -4.834203298632D+00
I= 22 X= -5.886443204674D+00 Y= 5.404458224913D-01 Z= -5.197546052371D+00
I= 23 X= -2.460454685465D+00 Y= 1.430971992911D+00 Z= -5.959583808515D+00
I= 24 X= -3.215311900869D+00 Y= -1.632384115772D+00 Z= -5.786673163808D+00
I= 25 X= -3.302510968607D+00 Y= -4.597180509768D+00 Z= -8.237386312376D-01
I= 26 X= -3.439595224736D+00 Y= -4.863498994916D+00 Z= -3.023553175489D+00

I= 27 X= -1.845412346975D+00 Y= -5.742491081890D+00 Z= 3.498575637091D-01
I= 28 X= -5.406227525399D+00 Y= -4.836713019877D+00 Z= -1.649437020510D-01
I= 29 X= 2.505657504335D+00 Y= -3.841844372296D+00 Z= -7.468885390078D-01
I= 30 X= 3.584335503525D+00 Y= -2.694337453746D+00 Z= 1.722272490799D+00
I= 31 X= 1.301940579571D+00 Y= -5.605392660104D+00 Z= -7.992087408782D-01
I= 32 X= 3.574953276142D+00 Y= -3.810783059662D+00 Z= -2.590329689467D+00
I= 33 X= 5.528938902705D+00 Y= -1.811083234068D+00 Z= 1.568335299118D+00
I= 34 X= 2.826251154485D+00 Y= -3.346254753855D+00 Z= 3.896391708090D+00
I= 35 X= 9.111713903748D-01 Y= -7.672859280192D-02 Z= -2.267632526556D-01
I= 36 X= 3.459541004657D+00 Y= 2.944023209043D+00 Z= 8.852212814564D-01
I= 37 X= 4.486615935688D+00 Y= 2.191960470003D+00 Z= 2.882138094480D+00
I= 38 X= 2.469989491017D+00 Y= 4.782033311514D+00 Z= 1.047183864457D+00

Forward Direction:

Total Energy: -651.6127075 Hartrees

Potential Energy: -651.7823133 Hartress

Kinetic Energy: 0.1696058 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.909458011276D+13 Y= 2.692004556929D+13 Z= -1.185247971625D+13
I= 1 X= -1.665510219744D+12 Y= -6.634996356183D+12 Z= 2.380465624681D+13
I= 2 X= 5.347824489694D+12 Y= 4.963456649885D+12 Z= 5.370748046826D+12
I= 3 X= -2.262242651386D+12 Y= 9.354676070460D+12 Z= -5.848769138410D+12
I= 4 X= -1.915372719585D+13 Y= -1.567623771584D+13 Z= -1.125083580670D+13
I= 5 X= 7.708271895534D+12 Y= 1.653094329747D+11 Z= 8.684095289495D+12
I= 6 X= -3.984505462602D+12 Y= -1.728378939850D+13 Z= -9.291236174601D+13
I= 7 X= 1.461908389038D+13 Y= 4.708693703478D+13 Z= -3.908909933286D+12
I= 8 X= 6.588427842903D+13 Y= 7.339173254191D+12 Z= 5.129579923200D+13
I= 9 X= 2.837878569391D+13 Y= -1.820293331348D+13 Z= 6.300501616415D+12
I= 10 X= -1.230951507414D+14 Y= 6.282512069853D+13 Z= 3.804570902257D+13
I= 11 X= 8.933482073088D+13 Y= 4.951187010493D+12 Z= -9.062322269984D+12
I= 12 X= 2.343824722177D+13 Y= 4.235729669383D+13 Z= 1.426969975147D+13

I= 13 X= -3.085477386229D+13 Y= 2.207872194588D+13 Z= -1.882482760493D+12
I= 14 X= 1.925842382964D+13 Y= -2.160343473028D+13 Z= 3.085354847421D+13
I= 15 X= -7.433954491345D+12 Y= 4.229588390704D+13 Z= 2.127128994553D+13
I= 16 X= 5.912088229967D+13 Y= -1.220638163939D+14 Z= 2.791023553473D+13
I= 17 X= 4.005813622578D+12 Y= -1.932833835662D+13 Z= 3.472306130805D+12
I= 18 X= 1.289588299016D+14 Y= -4.143802995866D+13 Z= -1.595686481094D+13
I= 19 X= -6.419401367626D+12 Y= 3.181789595215D+13 Z= -1.600141937978D+13
I= 20 X= 1.295301018000D+13 Y= 5.052097381125D+13 Z= -1.885596767490D+13
I= 21 X= 4.497003981740D+12 Y= 9.207538603781D+12 Z= 9.546068591322D+12
I= 22 X= -3.247109675380D+13 Y= 7.839586017728D+13 Z= -5.063850419794D+13
I= 23 X= -7.823010116937D+13 Y= -1.577754407541D+13 Z= -4.421342208786D+12
I= 24 X= 7.681296555790D+13 Y= -4.347810854083D+13 Z= -1.006985962921D+14
I= 25 X= -1.351617962694D+13 Y= 1.225566936177D+13 Z= 1.627236248489D+13
I= 26 X= 1.829926119287D+13 Y= 7.004707507509D+13 Z= 3.177315096919D+12
I= 27 X= 3.130512098843D+13 Y= -3.850090347251D+13 Z= -6.896974960481D+13
I= 28 X= -8.907471075556D+13 Y= 1.413726834131D+13 Z= 1.151679791453D+13
I= 29 X= -9.027867421911D+12 Y= 1.860539533991D+11 Z= -9.027754336523D+12
I= 30 X= 8.013342309869D+12 Y= -3.917298756339D+12 Z= -4.747317017037D+12
I= 31 X= -3.805281266352D+13 Y= -6.650701984783D+13 Z= 2.299265748992D+13
I= 32 X= 1.240417224487D+14 Y= 4.541997557703D+13 Z= -3.695239785275D+13
I= 33 X= -3.486275098306D+13 Y= 1.089148939181D+13 Z= 4.121887826994D+13
I= 34 X= -5.767607972832D+13 Y= -5.005861354402D+13 Z= 2.923521651775D+13
I= 35 X= 2.156871806906D+10 Y= -2.626371867502D+12 Z= -2.671602885591D+12
I= 36 X= 1.686169146316D+13 Y= 6.457554354227D+11 Z= 2.660494944150D+13
I= 37 X= 6.177364695273D+13 Y= 1.338286243457D+13 Z= -7.881725907845D+13
I= 38 X= -1.141805203012D+13 Y= 1.359430800718D+14 Z= 5.674060021197D+13

Backward Direction:

Total Energy: -651.6127230 Hartrees

Potential Energy: -651.7823133 Hartress

Kinetic Energy: 0.1695903 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.966144142591D+13 Y= 2.675327738011D+13 Z= -1.186493779989D+13
I= 1 X= -1.382943657202D+12 Y= -7.239799824321D+12 Z= 2.279884521909D+13
I= 2 X= 4.980063956824D+12 Y= 5.517648300850D+12 Z= 4.504442236736D+12
I= 3 X= -2.493129820349D+12 Y= 9.405729062727D+12 Z= -7.062570238087D+12
I= 4 X= -1.735629823897D+13 Y= -1.582258576593D+13 Z= -1.240214998510D+13
I= 5 X= 7.831162338018D+12 Y= -6.745135900852D+11 Z= 1.153788797577D+12
I= 6 X= 4.577803697235D+13 Y= 2.850888862797D+13 Z= -7.128603215163D+13
I= 7 X= 2.483477126078D+13 Y= 5.674274187100D+13 Z= -2.971992606844D+12
I= 8 X= 7.971980155481D+13 Y= 1.866067952384D+13 Z= 5.388250355427D+13
I= 9 X= 2.900707864699D+13 Y= -1.793142009430D+13 Z= 5.616872007072D+12
I= 10 X= -1.228845616997D+14 Y= 6.420791098832D+13 Z= 3.644300143346D+13
I= 11 X= 8.918811838846D+13 Y= 4.961183537926D+12 Z= -9.162455351034D+12
I= 12 X= 2.386949319291D+13 Y= 4.246873171856D+13 Z= 1.385720672090D+13
I= 13 X= -3.073381379212D+13 Y= 2.199528259099D+13 Z= -2.181759927760D+12
I= 14 X= 1.942993787051D+13 Y= -2.211676154342D+13 Z= 3.088340440000D+13
I= 15 X= -7.013733666723D+12 Y= 4.187254195798D+13 Z= 2.055876186749D+13
I= 16 X= 5.903924383930D+13 Y= -1.219492428396D+14 Z= 2.799405564888D+13
I= 17 X= 4.209275569916D+12 Y= -1.951149022885D+13 Z= 3.392079668014D+12
I= 18 X= 1.291752038950D+14 Y= -4.154950159487D+13 Z= -1.643478976073D+13
I= 19 X= -6.419855473066D+12 Y= 3.164063886157D+13 Z= -1.579932799830D+13
I= 20 X= 1.319290907873D+13 Y= 5.021791091775D+13 Z= -1.895483561952D+13
I= 21 X= 4.085798465847D+12 Y= 9.214511270923D+12 Z= 8.919261643395D+12
I= 22 X= -3.274488368382D+13 Y= 7.899123368756D+13 Z= -5.212233249982D+13
I= 23 X= -7.796942112645D+13 Y= -1.600601863603D+13 Z= -4.946830160531D+12
I= 24 X= 7.626991633145D+13 Y= -4.349377853399D+13 Z= -1.014382370014D+14
I= 25 X= -1.351907776752D+13 Y= 1.217771831551D+13 Z= 1.609829922328D+13
I= 26 X= 1.798337222406D+13 Y= 6.959911767651D+13 Z= 3.052609801641D+12
I= 27 X= 3.158171370521D+13 Y= -3.824383040023D+13 Z= -6.907122403912D+13
I= 28 X= -8.900929663999D+13 Y= 1.412669024516D+13 Z= 1.183566819626D+13

I= 29 X= -1.010591657082D+13 Y= 8.225723509556D+11 Z= -9.854502313276D+12
I= 30 X= 8.097308839202D+12 Y= -3.736117418397D+12 Z= -5.382978867121D+12
I= 31 X= -3.796733665028D+13 Y= -6.709467736851D+13 Z= 2.259872531601D+13
I= 32 X= 1.226708459157D+14 Y= 4.666094157694D+13 Z= -3.823287389672D+13
I= 33 X= -3.467262075008D+13 Y= 1.080728290597D+13 Z= 4.057117809246D+13
I= 34 X= -5.703279201990D+13 Y= -5.015594083949D+13 Z= 2.881888835048D+13
I= 35 X= -2.379029110195D+11 Y= -2.731967983524D+12 Z= -1.662188054472D+12
I= 36 X= 1.372038313398D+13 Y= -3.107824938363D+12 Z= 2.472093587773D+13
I= 37 X= 6.542423122260D+13 Y= 1.573431498226D+13 Z= -8.345450507468D+13
I= 38 X= -9.207291201004D+12 Y= 1.357938777292D+14 Z= 5.374585639164D+13

Seed: 18114500697

CM Start Point Coordinates: bohr

I= 0 X= -2.288666746520D+00 Y= 2.328098582275D+00 Z= -4.719047495427D-01
I= 1 X= -2.936625590921D+00 Y= 1.179347407909D-01 Z= -1.972921762766D+00
I= 2 X= -2.214861506050D+00 Y= 1.635460102301D+00 Z= 2.229986362782D+00
I= 3 X= -2.967345921557D+00 Y= -1.988548545604D+00 Z= -2.538920806525D-01
I= 4 X= -2.486491844498D+00 Y= -1.170899944059D+00 Z= 2.259514562727D+00
I= 5 X= 4.036878190196D+00 Y= 2.169769479741D+00 Z= -2.214859190456D+00
I= 6 X= 2.378785283435D+00 Y= -1.686071313046D-01 Z= -3.263031526535D+00
I= 7 X= 5.844835575801D+00 Y= 1.225358636407D+00 Z= -2.513279689894D+00
I= 8 X= 3.024744577177D+00 Y= 3.601274916104D+00 Z= -3.795829045155D+00
I= 9 X= -2.959084725754D+00 Y= -2.671169516859D+00 Z= 4.616940334991D+00
I= 10 X= -4.775273681415D+00 Y= -3.132741026954D+00 Z= 5.023087035797D+00
I= 11 X= -1.993775035623D+00 Y= -4.753751925251D+00 Z= 4.292084187440D+00
I= 12 X= -1.822109660796D+00 Y= -2.130629919153D+00 Z= 6.324845538447D+00
I= 13 X= -2.018661373165D+00 Y= 3.165890023023D+00 Z= 4.423805161654D+00
I= 14 X= -3.919650883529D+00 Y= 2.454097114686D+00 Z= 5.850567892813D+00
I= 15 X= 1.328938955012D-01 Y= 2.730901891561D+00 Z= 5.422052960498D+00
I= 16 X= -2.280804594945D+00 Y= 5.297254819158D+00 Z= 3.696159922028D+00

I= 17 X= -2.374843748605D+00 Y= 5.003669548578D+00 Z= -1.444286126275D+00
I= 18 X= -4.228685408009D+00 Y= 5.780861512496D+00 Z= -1.282963016190D+00
I= 19 X= -1.009062887670D+00 Y= 6.463489608704D+00 Z= -2.881850919315D-01
I= 20 X= -1.232621910811D+00 Y= 5.115899833830D+00 Z= -3.245150247848D+00
I= 21 X= -3.419025196653D+00 Y= 1.939018653405D-01 Z= -4.709326646757D+00
I= 22 X= -5.363880521087D+00 Y= 8.382222144310D-01 Z= -5.290202002706D+00
I= 23 X= -1.926077562909D+00 Y= 1.602335793152D+00 Z= -5.743092376912D+00
I= 24 X= -3.316159233991D+00 Y= -2.055284348835D+00 Z= -5.184203888084D+00
I= 25 X= -3.511573005238D+00 Y= -4.524336742618D+00 Z= -1.047722613693D+00
I= 26 X= -2.975449371489D+00 Y= -4.735562645909D+00 Z= -3.142535240717D+00
I= 27 X= -2.514174510877D+00 Y= -5.836263363141D+00 Z= 3.168590228971D-01
I= 28 X= -5.512485175054D+00 Y= -5.169464998881D+00 Z= -1.057060307945D+00
I= 29 X= 2.998205018621D+00 Y= -3.692791801071D+00 Z= -4.341209487230D-01
I= 30 X= 3.445600258319D+00 Y= -2.449974504035D+00 Z= 2.043466012964D+00
I= 31 X= 1.452812517809D+00 Y= -5.216400964933D+00 Z= -2.812505027774D-01
I= 32 X= 4.276202279582D+00 Y= -3.592723524370D+00 Z= -1.933522079611D+00
I= 33 X= 5.108814857637D+00 Y= -1.371133865359D+00 Z= 2.503082735723D+00
I= 34 X= 2.561935436266D+00 Y= -3.248799213583D+00 Z= 3.525560073931D+00
I= 35 X= 8.781425259014D-01 Y= -7.805764560729D-02 Z= -2.215467859324D-01
I= 36 X= 3.469214584596D+00 Y= 3.034771762827D+00 Z= 3.518172458796D-01
I= 37 X= 4.968514589539D+00 Y= 2.521345451422D+00 Z= 1.680351119813D+00
I= 38 X= 2.482018893618D+00 Y= 5.011646250194D+00 Z= 6.007733127948D-01

Forward Direction:

Total Energy: -651.6191107 Hartrees

Potential Energy: -651.7980970 Hartress

Kinetic Energy: 0.1789863 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.364405239469D+12 Y= 1.027285160414D+12 Z= -9.225970160116D+12

I= 1 X= 9.187288420787D+11 Y= 1.449095194587D+12 Z= -9.967498916235D+12

I= 2 X= -1.398719662099D+13 Y= 8.034113638811D+12 Z= -4.546688993720D+12

I= 3 X= -8.364967403033D+12 Y= -1.972168614574D+13 Z= -2.716785227536D+13
I= 4 X= 9.572119944261D+12 Y= 5.112321827299D+12 Z= 2.183587568308D+13
I= 5 X= -1.426755172175D+12 Y= -1.736728506397D+13 Z= -4.410680502866D+12
I= 6 X= -7.524255397510D+13 Y= -2.724479339605D+13 Z= 3.544705321916D+13
I= 7 X= -4.304457951831D+12 Y= -5.551376469167D+13 Z= 5.487435020380D+13
I= 8 X= -1.059807947705D+12 Y= 1.084215650402D+14 Z= -3.160979724583D+13
I= 9 X= -1.709013590636D+13 Y= -7.588910247275D+11 Z= 1.274102204214D+13
I= 10 X= 8.523214668124D+13 Y= 6.305959553420D+13 Z= -1.627014487799D+13
I= 11 X= 1.856585359292D+13 Y= -6.719429601111D+13 Z= 7.201955497764D+13
I= 12 X= -8.058252776595D+13 Y= -8.203380032713D+13 Z= -6.688393761350D+13
I= 13 X= 1.953823687676D+13 Y= 1.008410171889D+12 Z= -2.023065689594D+13
I= 14 X= 4.600118444449D+13 Y= -3.199559225870D+13 Z= 8.425365203760D+13
I= 15 X= 1.338246307260D+13 Y= -3.993150375266D+12 Z= 9.232014980131D+13
I= 16 X= -1.384232261428D+13 Y= -5.983750572309D+11 Z= -6.942697960923D+12
I= 17 X= 1.701821781146D+13 Y= -3.698688541232D+12 Z= 1.348985747391D+13
I= 18 X= -5.219681604660D+13 Y= -1.115177957717D+13 Z= -2.485975667532D+12
I= 19 X= 2.523726933168D+13 Y= 5.166969838685D+13 Z= -6.208205010216D+13
I= 20 X= -4.246681181975D+13 Y= -3.792304892165D+13 Z= -3.661537281365D+13
I= 21 X= -1.771012086972D+13 Y= -7.117346035330D+12 Z= -3.178933698403D+11
I= 22 X= 1.097479539307D+14 Y= 1.294600723346D+12 Z= 2.062358098567D+13
I= 23 X= 9.635447499749D+13 Y= 5.178405130769D+13 Z= 4.888056301103D+13
I= 24 X= 3.328787349016D+12 Y= 7.068138390238D+13 Z= 1.130759135052D+14
I= 25 X= 2.697556445253D+12 Y= 1.375427261290D+13 Z= 6.932028776066D+12
I= 26 X= -2.231328851279D+13 Y= -2.673572456617D+13 Z= -4.925250600108D+12
I= 27 X= 4.045426898710D+12 Y= -3.325297013172D+13 Z= 4.461753806296D+13
I= 28 X= -1.412719119238D+14 Y= -6.044688789132D+13 Z= 1.135549400242D+14
I= 29 X= -1.289387574317D+13 Y= -3.905453702854D+12 Z= 2.572526379157D+13
I= 30 X= 2.792566915742D+12 Y= 1.948801726869D+13 Z= -2.135308696579D+13
I= 31 X= 3.677978955761D+13 Y= -2.693782182755D+12 Z= 8.308098236821D+12
I= 32 X= 1.000110374969D+14 Y= 2.307376354655D+13 Z= -4.061605350129D+13

I= 33 X= 2.126856214078D+12 Y= 4.252904933367D+12 Z= -1.378260742682D+13
I= 34 X= -9.371839772474D+13 Y= 1.616142137927D+12 Z= -1.348456997835D+13
I= 35 X= 2.172691560018D+12 Y= 8.445225928235D+11 Z= -1.012586665026D+12
I= 36 X= -1.269627441502D+13 Y= -1.800260515113D+13 Z= -2.328443739832D+12
I= 37 X= 4.796379750265D+13 Y= 2.568154755971D+13 Z= -8.683086462085D+13
I= 38 X= -1.345039014628D+13 Y= 1.239989030362D+14 Z= 1.125716770480D+14

Backward Direction:

Total Energy: -651.6191241 Hartrees

Potential Energy: -651.7980970 Hartress

Kinetic Energy: 0.1789729 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.567847361441D+12 Y= 9.674333529322D+11 Z= -9.230441269301D+12
I= 1 X= 1.020139785513D+12 Y= 1.232035929346D+12 Z= -1.032847667868D+13
I= 2 X= -1.411918302013D+13 Y= 8.233008716896D+12 Z= -4.857599417856D+12
I= 3 X= -8.447831014119D+12 Y= -1.970336362321D+13 Z= -2.760347605858D+13
I= 4 X= 1.021720323174D+13 Y= 5.059798649400D+12 Z= 2.142267796946D+13
I= 5 X= -1.382650745369D+12 Y= -1.766869102481D+13 Z= -7.113248998336D+12
I= 6 X= -5.738316411627D+13 Y= -1.081015702878D+13 Z= 4.320857488864D+13
I= 7 X= -6.381271225973D+11 Y= -5.204837136023D+13 Z= 5.521060255420D+13
I= 8 X= 3.905653812804D+12 Y= 1.124847656779D+14 Z= -3.068144916181D+13
I= 9 X= -1.686464644678D+13 Y= -6.614470396632D+11 Z= 1.249567268697D+13
I= 10 X= 8.530772545176D+13 Y= 6.355586822828D+13 Z= -1.684534417827D+13
I= 11 X= 1.851320326047D+13 Y= -6.719070833460D+13 Z= 7.198361799386D+13
I= 12 X= -8.042775693642D+13 Y= -8.199380716330D+13 Z= -6.703197815825D+13
I= 13 X= 1.958164850267D+13 Y= 9.784644350381D+11 Z= -2.033806514534D+13
I= 14 X= 4.606273949712D+13 Y= -3.217982126716D+13 Z= 8.426436709550D+13
I= 15 X= 1.353327705471D+13 Y= -4.145084510677D+12 Z= 9.206442901223D+13
I= 16 X= -1.387162202717D+13 Y= -5.572554995077D+11 Z= -6.912615571032D+12
I= 17 X= 1.709123872471D+13 Y= -3.764420325789D+12 Z= 1.346106481914D+13
I= 18 X= -5.211916110301D+13 Y= -1.119178588250D+13 Z= -2.657499212954D+12

I= 19 X= 2.523710635710D+13 Y= 5.160608219728D+13 Z= -6.200952107565D+13
I= 20 X= -4.238071396899D+13 Y= -3.803181584192D+13 Z= -3.665085575357D+13
I= 21 X= -1.785769933242D+13 Y= -7.114843598493D+12 Z= -5.428495116125D+11
I= 22 X= 1.096496939308D+14 Y= 1.508275662293D+12 Z= 2.009104654012D+13
I= 23 X= 9.644803104569D+13 Y= 5.170205355986D+13 Z= 4.869196946793D+13
I= 24 X= 3.133891191287D+12 Y= 7.067576006026D+13 Z= 1.128104622023D+14
I= 25 X= 2.696516328503D+12 Y= 1.372629658852D+13 Z= 6.869558824430D+12
I= 26 X= -2.242665861033D+13 Y= -2.689649299243D+13 Z= -4.970006359301D+12
I= 27 X= 4.144693884508D+12 Y= -3.316070860239D+13 Z= 4.458111967340D+13
I= 28 X= -1.412484352997D+14 Y= -6.045068429065D+13 Z= 1.136693800982D+14
I= 29 X= -1.328077920722D+13 Y= -3.677012194698D+12 Z= 2.542855036544D+13
I= 30 X= 2.822701849699D+12 Y= 1.955304184274D+13 Z= -2.158122106542D+13
I= 31 X= 3.681046623474D+13 Y= -2.904687899989D+12 Z= 8.166719038431D+12
I= 32 X= 9.951904056192D+13 Y= 2.351913660361D+13 Z= -4.107560640635D+13
I= 33 X= 2.195092477537D+12 Y= 4.222683878683D+12 Z= -1.401506198677D+13
I= 34 X= -9.348752676455D+13 Y= 1.581212126324D+12 Z= -1.363398692436D+13
I= 35 X= 2.079569208121D+12 Y= 8.066249673334D+11 Z= -6.503155248823D+11
I= 36 X= -1.382366556784D+13 Y= -1.934973598542D+13 Z= -3.004601570978D+12
I= 37 X= 4.927396383573D+13 Y= 2.652546560835D+13 Z= -8.849513618228D+13
I= 38 X= -1.265696525811D+13 Y= 1.239453554741D+14 Z= 1.114968867549D+14

Seed: 18445319666

CM Start Point Coordinates: bohr

I= 0 X= -2.576563745592D+00 Y= 2.320045432000D+00 Z= -7.110585356502D-01
I= 1 X= -2.959186571192D+00 Y= 3.483788264092D-02 Z= -1.892928536545D+00
I= 2 X= -2.268806886813D+00 Y= 1.966187028078D+00 Z= 1.922514226501D+00
I= 3 X= -2.726900224743D+00 Y= -2.060710841609D+00 Z= -1.269580545089D-01
I= 4 X= -2.531369803963D+00 Y= -7.940229421241D-01 Z= 2.344743913524D+00
I= 5 X= 4.239868225075D+00 Y= 2.771689706475D+00 Z= -7.986466242991D-01
I= 6 X= 2.558570173996D+00 Y= 1.019105493630D+00 Z= -2.551337521957D+00

I= 7 X= 5.996906371714D+00 Y= 2.077946284665D+00 Z= -1.549876098439D+00
I= 8 X= 3.678002578366D+00 Y= 4.625398550977D+00 Z= -1.365050730479D+00
I= 9 X= -2.614477204512D+00 Y= -2.129422193939D+00 Z= 4.917031499889D+00
I= 10 X= -4.617913979313D+00 Y= -3.255795635618D+00 Z= 5.418188517523D+00
I= 11 X= -9.781009418826D-01 Y= -3.739532320492D+00 Z= 4.761651492426D+00
I= 12 X= -2.352387806866D+00 Y= -6.821471382403D-01 Z= 6.718139918441D+00
I= 13 X= -2.170426080330D+00 Y= 3.952118566715D+00 Z= 4.022051267562D+00
I= 14 X= -4.164056021566D+00 Y= 4.110363805320D+00 Z= 4.793605348944D+00
I= 15 X= -8.623433242820D-01 Y= 3.711287672472D+00 Z= 5.743534996771D+00
I= 16 X= -1.475175379292D+00 Y= 5.527594503589D+00 Z= 2.950254417959D+00
I= 17 X= -2.685767581032D+00 Y= 4.933735679215D+00 Z= -2.168865267052D+00
I= 18 X= -4.865166774343D+00 Y= 5.309320341250D+00 Z= -1.850660483759D+00
I= 19 X= -1.531255428412D+00 Y= 6.304098208222D+00 Z= -1.138698008627D+00
I= 20 X= -2.187481681365D+00 Y= 5.000973566118D+00 Z= -4.301436754338D+00
I= 21 X= -3.500047410876D+00 Y= -2.916130423036D-01 Z= -4.636859843575D+00
I= 22 X= -5.453434017130D+00 Y= 9.088082850291D-01 Z= -5.110304787029D+00
I= 23 X= -1.890305394015D+00 Y= 8.188990915214D-01 Z= -5.798475600558D+00
I= 24 X= -3.196809171000D+00 Y= -2.422490226107D+00 Z= -5.113440339757D+00
I= 25 X= -3.055081511982D+00 Y= -4.967213697011D+00 Z= -3.226131079563D-01
I= 26 X= -3.661182277985D+00 Y= -5.143766335404D+00 Z= -2.376635625978D+00
I= 27 X= -1.095104480526D+00 Y= -6.189792337599D+00 Z= 3.616894476026D-01
I= 28 X= -5.052625868267D+00 Y= -5.799061355364D+00 Z= 9.666962702055D-01
I= 29 X= 2.703879807151D+00 Y= -3.431246191366D+00 Z= -2.023727803664D+00
I= 30 X= 3.337262982900D+00 Y= -3.377471269087D+00 Z= 6.366500309604D-01
I= 31 X= 1.348011527521D+00 Y= -4.713938098821D+00 Z= -2.969288918059D+00
I= 32 X= 3.992554929095D+00 Y= -3.032921877793D+00 Z= -3.401411563933D+00
I= 33 X= 5.167185915279D+00 Y= -3.382949750444D+00 Z= 1.409035675752D+00
I= 34 X= 2.242893499994D+00 Y= -4.800245928697D+00 Z= 1.713872538924D+00
I= 35 X= 8.609998164206D-01 Y= -6.989562189885D-02 Z= -2.094107368134D-01
I= 36 X= 3.838844902910D+00 Y= 2.096521379986D+00 Z= 1.900434922453D+00

I= 37 X= 5.135753370289D+00 Y= 1.256260010440D+00 Z= 3.248848474990D+00

I= 38 X= 2.829001595828D+00 Y= 3.689284857283D+00 Z= 3.079994622379D+00

Forward Direction:

Total Energy: -651.6074622 Hartrees

Potential Energy: -651.7886488 Hartress

Kinetic Energy: 0.1811865 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.290928525698D+12 Y= -1.537977513028D+12 Z= -3.675510588102D+12

I= 1 X= -1.568732338355D+13 Y= -1.020313175967D+13 Z= -1.257915214262D+13

I= 2 X= 9.652791152305D+12 Y= 9.073541842542D+12 Z= 9.236547113337D+12

I= 3 X= -4.921968035173D+12 Y= 6.076489362360D+12 Z= -1.263391652694D+13

I= 4 X= 2.434329323346D+12 Y= -7.955467290531D+10 Z= -4.195501890374D+12

I= 5 X= -2.970531876164D+12 Y= -5.115536659606D+12 Z= 4.936854018134D+12

I= 6 X= -9.492247070810D+13 Y= -1.862917685152D+13 Z= 4.678805685414D+13

I= 7 X= -2.439322806998D+13 Y= -1.036049597281D+13 Z= 5.591109363281D+13

I= 8 X= -8.264520062903D+13 Y= 3.963667466264D+13 Z= -3.426862804499D+13

I= 9 X= 1.081199910569D+13 Y= -1.432156595129D+13 Z= 1.729069219956D+13

I= 10 X= -1.024758922713D+14 Y= 1.012721199646D+13 Z= 2.955676477060D+13

I= 11 X= -3.159925087771D+13 Y= 8.294334016317D+13 Z= -9.920493205708D+12

I= 12 X= 1.165846187914D+13 Y= -6.715243839195D+12 Z= -7.892492850765D+13

I= 13 X= -1.020529078744D+12 Y= 2.176920094213D+13 Z= -3.113385839664D+11

I= 14 X= -3.354207513985D+13 Y= 6.567562274464D+11 Z= 6.734175576897D+13

I= 15 X= -2.662676527181D+13 Y= -5.632953566900D+13 Z= 2.253673417523D+13

I= 16 X= 5.678388557344D+13 Y= 9.268435703738D+13 Z= -1.165704152721D+14

I= 17 X= -9.354539283228D+12 Y= -1.233293830480D+13 Z= 7.917741358266D+12

I= 18 X= 1.216549096201D+14 Y= -7.624335696103D+13 Z= 6.739522335733D+13

I= 19 X= 8.289784022880D+13 Y= 1.585702412859D+13 Z= 4.176408840390D+13

I= 20 X= 5.907036989171D+13 Y= 1.463238587873D+13 Z= 1.213942086396D+14

I= 21 X= -2.292885372119D+13 Y= 2.417212038248D+13 Z= -1.803279182533D+12

I= 22 X= 1.149641959744D+14 Y= 3.228218246470D+13 Z= 7.881125239373D+13

I= 23 X= 7.446367910701D+12 Y= -6.089993768367D+13 Z= 4.994870751000D+13
I= 24 X= 1.801319198069D+13 Y= -9.543890427557D+13 Z= 4.298317267526D+13
I= 25 X= 2.994995088802D+12 Y= -7.733259004885D+12 Z= -4.014739310084D+12
I= 26 X= 1.719875643789D+13 Y= -1.602666167649D+13 Z= 5.457087824477D+13
I= 27 X= -4.734596543178D+13 Y= -5.664222588241D+13 Z= -5.619985553651D+13
I= 28 X= 6.644791485107D+13 Y= 8.262219981741D+12 Z= 3.364079596999D+13
I= 29 X= 1.860302403572D+13 Y= -7.178866929198D+12 Z= -2.326655175329D+13
I= 30 X= -4.216861670505D+12 Y= -5.076060309905D+12 Z= 1.240832177670D+13
I= 31 X= 1.268231453494D+13 Y= -1.127217441404D+14 Z= 8.107147827401D+12
I= 32 X= -1.861329598079D+13 Y= -5.975390674886D+13 Z= 4.239929372399D+13
I= 33 X= 1.197844486333D+13 Y= 2.651247509112D+13 Z= -3.062462761940D+13
I= 34 X= 8.903493820205D+13 Y= 1.481534890409D+13 Z= -3.830356157149D+13
I= 35 X= -1.087412969335D+12 Y= 1.543172900869D+12 Z= -2.055460968317D+11
I= 36 X= 1.122935849047D+13 Y= 4.250232253466D+12 Z= -1.761906693984D+13
I= 37 X= 1.771941623101D+14 Y= -9.583138727422D+13 Z= 4.484272948250D+13
I= 38 X= -3.776638727687D+13 Y= 1.073078802555D+13 Z= -6.675526781720D+13

Backward Direction:

Total Energy: -651.6073592 Hartrees

Potential Energy: -651.7886488 Hartress

Kinetic Energy: 0.1812896 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.238827232447D+12 Y= -1.816845282816D+12 Z= -3.696342847931D+12
I= 1 X= -1.521481896240D+13 Y= -1.121447688112D+13 Z= -1.426105730714D+13
I= 2 X= 9.037826390637D+12 Y= 1.000025449041D+13 Z= 7.787920904509D+12
I= 3 X= -5.308054798069D+12 Y= 6.161859565285D+12 Z= -1.466362020165D+13
I= 4 X= 5.439968515788D+12 Y= -3.242761317151D+11 Z= -6.120715681760D+12
I= 5 X= -2.765035949564D+12 Y= -6.519878665042D+12 Z= -7.655234390742D+12
I= 6 X= -1.171014269299D+13 Y= 5.794479139923D+13 Z= 8.295134642628D+13
I= 7 X= -7.310677887396D+12 Y= 5.785825342770D+12 Z= 5.747779557492D+13
I= 8 X= -5.950960441743D+13 Y= 5.856836198238D+13 Z= -2.994317202401D+13

I= 9 X= 1.186262306060D+13 Y= -1.386754479394D+13 Z= 1.614753494887D+13
I= 10 X= -1.021237478017D+14 Y= 1.243949738322D+13 Z= 2.687673631997D+13
I= 11 X= -3.184456478636D+13 Y= 8.296005623479D+13 Z= -1.008793454398D+13
I= 12 X= 1.237958622672D+13 Y= -6.528903522266D+12 Z= -7.961469441406D+13
I= 13 X= -8.182610999434D+11 Y= 2.162967465383D+13 Z= -8.117862819487D+11
I= 14 X= -3.325527141828D+13 Y= -2.016227303095D+11 Z= 6.739168048935D+13
I= 15 X= -2.592407704361D+13 Y= -5.703744300204D+13 Z= 2.134525325193D+13
I= 16 X= 5.664737070569D+13 Y= 9.287594556867D+13 Z= -1.164302522808D+14
I= 17 X= -9.014312659443D+12 Y= -1.263920267438D+13 Z= 7.783587626207D+12
I= 18 X= 1.220167276121D+14 Y= -7.642975849624D+13 Z= 6.659604298923D+13
I= 19 X= 8.289708087748D+13 Y= 1.556061694159D+13 Z= 4.210202318628D+13
I= 20 X= 5.947152594192D+13 Y= 1.412560773371D+13 Z= 1.212288828404D+14
I= 21 X= -2.361646666569D+13 Y= 2.418377999260D+13 Z= -2.851418259404D+12
I= 22 X= 1.145063727455D+14 Y= 3.327775892503D+13 Z= 7.633001245938D+13
I= 23 X= 7.882273966729D+12 Y= -6.128199011472D+13 Z= 4.906999284719D+13
I= 24 X= 1.710511155339D+13 Y= -9.546510745584D+13 Z= 4.174635433575D+13
I= 25 X= 2.990148842960D+12 Y= -7.863607810161D+12 Z= -4.305805815134D+12
I= 26 X= 1.667053068687D+13 Y= -1.677573067974D+13 Z= 5.436234754599D+13
I= 27 X= -4.688345041447D+13 Y= -5.621235136767D+13 Z= -5.636953986810D+13
I= 28 X= 6.655729954582D+13 Y= 8.244531419719D+12 Z= 3.417400702632D+13
I= 29 X= 1.680032314901D+13 Y= -6.114488482675D+12 Z= -2.464902982774D+13
I= 30 X= -4.076453842687D+12 Y= -4.773091045851D+12 Z= 1.134537563572D+13
I= 31 X= 1.282524649761D+13 Y= -1.137044180157D+14 Z= 7.448419161305D+12
I= 32 X= -2.090565931495D+13 Y= -5.767877825505D+13 Z= 4.025809700323D+13
I= 33 X= 1.229637836608D+13 Y= 2.637166600926D+13 Z= -3.170770410659D+13
I= 34 X= 9.011063621536D+13 Y= 1.465259936379D+13 Z= -3.899974055111D+13
I= 35 X= -1.521298320244D+12 Y= 1.366596338825D+12 Z= 1.482385305017D+12
I= 36 X= 5.976500291531D+12 Y= -2.026459935803D+12 Z= -2.076949187456D+13
I= 37 X= 1.832986256484D+14 Y= -9.189931646502D+13 Z= 3.708838221320D+13
I= 38 X= -3.406957947105D+13 Y= 1.048129365001D+13 Z= -7.176304259393D+13

Seed: 18494611204

CM Start Point Coordinates: bohr

I= 0 X= -2.547161465641D+00 Y= 2.370941325005D+00 Z= -5.862846290124D-01
I= 1 X= -2.991789906580D+00 Y= 3.461956254455D-02 Z= -1.974997968353D+00
I= 2 X= -2.377967217663D+00 Y= 1.788694773243D+00 Z= 2.103080312380D+00
I= 3 X= -3.096251729218D+00 Y= -1.955139743311D+00 Z= -2.799428927764D-01
I= 4 X= -2.459368586829D+00 Y= -9.329124356859D-01 Z= 2.289728077780D+00
I= 5 X= 4.325657318583D+00 Y= 1.948530743444D+00 Z= -1.501067380577D+00
I= 6 X= 2.443558404921D+00 Y= 5.717332982365D-01 Z= -2.818256580579D+00
I= 7 X= 5.958733935043D+00 Y= 5.533131672188D-01 Z= -1.782865517791D+00
I= 8 X= 4.522852985840D+00 Y= 3.492514022828D+00 Z= -3.096214105577D+00
I= 9 X= -2.396623612964D+00 Y= -2.511160665219D+00 Z= 4.557822259724D+00
I= 10 X= -4.477559175152D+00 Y= -3.284669986516D+00 Z= 5.017432364456D+00
I= 11 X= -1.113160832716D+00 Y= -4.283140077893D+00 Z= 4.417060408134D+00
I= 12 X= -1.478917590042D+00 Y= -1.184348613208D+00 Z= 6.263691999696D+00
I= 13 X= -2.010223365711D+00 Y= 3.459342409046D+00 Z= 4.233531001680D+00
I= 14 X= -4.017577264033D+00 Y= 3.459966370354D+00 Z= 5.171649302931D+00
I= 15 X= -5.949256902037D-01 Y= 3.075860482278D+00 Z= 5.667235551322D+00
I= 16 X= -1.769552407525D+00 Y= 5.551494230299D+00 Z= 3.311588880596D+00
I= 17 X= -2.590909980683D+00 Y= 5.072217350714D+00 Z= -1.377435995545D+00
I= 18 X= -4.481840496185D+00 Y= 5.981046310126D+00 Z= -1.519153450196D+00
I= 19 X= -1.344684604829D+00 Y= 6.370046456036D+00 Z= -3.949904586223D-01
I= 20 X= -2.459854901043D+00 Y= 5.210889184594D+00 Z= -3.335624830905D+00
I= 21 X= -3.598694592301D+00 Y= -4.533550048441D-02 Z= -4.713778690103D+00
I= 22 X= -5.727977172784D+00 Y= 1.202378588131D+00 Z= -5.440284696665D+00
I= 23 X= -2.010383149423D+00 Y= 1.125456907474D+00 Z= -5.816082269012D+00
I= 24 X= -3.714263034190D+00 Y= -2.088693815731D+00 Z= -5.500859743294D+00
I= 25 X= -3.326215476482D+00 Y= -4.724215130683D+00 Z= -8.108882006980D-01
I= 26 X= -2.603682841122D+00 Y= -5.209214176348D+00 Z= -2.729570817890D+00

I= 27 X= -2.297244311783D+00 Y= -5.919277147707D+00 Z= 8.452191430914D-01
I= 28 X= -5.431886960060D+00 Y= -5.005869663525D+00 Z= -1.074259801471D+00
I= 29 X= 3.046704638455D+00 Y= -3.765637400805D+00 Z= -7.451499518338D-01
I= 30 X= 3.563053760837D+00 Y= -2.699185616700D+00 Z= 1.596680629142D+00
I= 31 X= 1.438412767761D+00 Y= -5.194646516831D+00 Z= -8.399688659680D-01
I= 32 X= 4.286865419115D+00 Y= -3.810923094506D+00 Z= -2.359900485674D+00
I= 33 X= 5.432973047112D+00 Y= -1.962825916095D+00 Z= 1.918224818594D+00
I= 34 X= 2.471409039190D+00 Y= -3.387257253658D+00 Z= 3.338445445479D+00
I= 35 X= 8.646917053541D-01 Y= -5.339783819371D-02 Z= -2.619115140021D-01
I= 36 X= 3.425047454879D+00 Y= 2.664508838084D+00 Z= 1.094018041489D+00
I= 37 X= 4.470903054923D+00 Y= 2.259405443803D+00 Z= 3.135412708672D+00
I= 38 X= 2.141984617686D+00 Y= 4.303071817590D+00 Z= 1.507204378541D+00

Forward Direction:

Total Energy: -651.6151988 Hartrees

Potential Energy: -651.8220983 Hartress

Kinetic Energy: 0.2068995 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.343665430269D+12 Y= 9.817775346331D+12 Z= -1.469796897441D+13
I= 1 X= 3.085491707400D+12 Y= -1.103358929627D+13 Z= 1.988713492039D+13
I= 2 X= 5.204620075445D+12 Y= -1.819137580350D+13 Z= -5.257344026382D+12
I= 3 X= 1.619752902757D+13 Y= 4.828364474761D+12 Z= -1.052068362264D+13
I= 4 X= -8.470125772577D+10 Y= -3.441273852924D+12 Z= 1.722091002195D+13
I= 5 X= 1.787772062821D+13 Y= -8.440397464502D+12 Z= -5.147923887695D+12
I= 6 X= 7.657319203707D+13 Y= -6.373534715217D+13 Z= -5.531061847218D+13
I= 7 X= -1.674556491092D+14 Y= 2.619732607443D+13 Z= 7.401848288139D+13
I= 8 X= -2.275954384686D+13 Y= -1.415914698959D+13 Z= -4.698884455908D+13
I= 9 X= -8.550494818554D+12 Y= -6.633836261697D+12 Z= -7.383051185812D+12
I= 10 X= -4.537423532929D+13 Y= 1.075908350169D+14 Z= 7.123117190180D+13
I= 11 X= 1.069599766132D+13 Y= 3.427744342500D+12 Z= 5.672273875317D+13
I= 12 X= -8.287407880314D+12 Y= 6.988003238541D+13 Z= 4.575209596826D+12

I= 13 X= 2.452131853293D+13 Y= 2.000455998830D+13 Z= -5.785737046130D+11
I= 14 X= -1.293954738032D+14 Y= -3.217596473492D+13 Z= -1.728870572279D+13
I= 15 X= 1.829209083001D+13 Y= -3.349622622555D+13 Z= -1.563894934962D+13
I= 16 X= -3.485401592061D+13 Y= -6.616636207333D+12 Z= -1.834581279425D+13
I= 17 X= -6.131388833805D+12 Y= 1.580418427289D+13 Z= -2.417822999171D+12
I= 18 X= 1.381761568405D+14 Y= -7.411056605976D+13 Z= -3.364820368873D+13
I= 19 X= -7.443020265034D+13 Y= 1.436709341654D+13 Z= -7.761637123665D+13
I= 20 X= -2.604142213808D+12 Y= 5.697603411214D+13 Z= -6.516348561912D+13
I= 21 X= 9.778405659765D+12 Y= -1.629585533352D+13 Z= -1.097049315201D+13
I= 22 X= -9.099010439531D+13 Y= -1.617843570164D+13 Z= 4.524743245044D+13
I= 23 X= 1.901708512314D+13 Y= 1.290287076854D+14 Z= 4.514234385332D+13
I= 24 X= -1.020851898977D+14 Y= 8.837453080715D+12 Z= 6.432885576719D+13
I= 25 X= -2.174722715173D+13 Y= -1.374599006085D+13 Z= 1.458576880839D+13
I= 26 X= -3.186569653332D+13 Y= -3.204564866146D+13 Z= -1.668473335785D+14
I= 27 X= -3.247045528517D+12 Y= -6.131114914342D+13 Z= 9.510086924773D+13
I= 28 X= 2.241245534518D+13 Y= -1.013408462498D+13 Z= -6.307581343001D+13
I= 29 X= 3.536280588610D+12 Y= 1.115483676493D+13 Z= 1.498336489259D+13
I= 30 X= -1.499340233326D+13 Y= 8.065888198521D+12 Z= -3.874014331884D+13
I= 31 X= 2.707142488000D+13 Y= 2.080184420170D+11 Z= 2.873764331791D+13
I= 32 X= 6.451108016660D+13 Y= -5.588651322842D+13 Z= -7.668878905208D+13
I= 33 X= -4.250269396660D+12 Y= 7.555405837511D+12 Z= -6.076964866301D+13
I= 34 X= -3.528561264683D+13 Y= -5.531158517307D+13 Z= 1.107374281122D+14
I= 35 X= 1.361573688518D+12 Y= -9.571819972309D+10 Z= 2.162746375249D+12
I= 36 X= -6.107048810741D+12 Y= 6.442278804561D+12 Z= 9.988031329608D+12
I= 37 X= -1.046105938912D+14 Y= 7.379815699861D+13 Z= -8.166187334835D+13
I= 38 X= 2.664405916626D+13 Y= -4.560725425116D+12 Z= -4.077394879364D+12

Backward Direction:

Total Energy: -651.6152144 Hartrees

Potential Energy: -651.8220983 Hartress

Kinetic Energy: 0.2068839 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.614097697638D+12 Y= 9.738215322524D+12 Z= -1.470391234737D+13
I= 1 X= 3.220295606613D+12 Y= -1.132212261188D+13 Z= 1.940729311198D+13
I= 2 X= 5.029172724609D+12 Y= -1.792698784392D+13 Z= -5.670632144352D+12
I= 3 X= 1.608737979126D+13 Y= 4.852720302268D+12 Z= -1.109975116092D+13
I= 4 X= 7.727973565007D+11 Y= -3.511092050458D+12 Z= 1.667165309146D+13
I= 5 X= 1.793634791314D+13 Y= -8.841051450473D+12 Z= -8.740403781203D+12
I= 6 X= 1.003133855199D+14 Y= -4.188905507620D+13 Z= -4.499335525024D+13
I= 7 X= -1.625820557846D+14 Y= 3.080381649910D+13 Z= 7.446545760045D+13
I= 8 X= -1.615903712788D+13 Y= -8.758001141320D+12 Z= -4.575480670376D+13
I= 9 X= -8.250755384553D+12 Y= -6.504305573482D+12 Z= -7.709190052084D+12
I= 10 X= -4.527376971218D+13 Y= 1.082505221536D+14 Z= 7.046656892179D+13
I= 11 X= 1.062601044050D+13 Y= 3.432513376362D+12 Z= 5.667496831055D+13
I= 12 X= -8.081673560071D+12 Y= 6.993319464015D+13 Z= 4.378421735390D+12
I= 13 X= 2.457902489707D+13 Y= 1.996475361322D+13 Z= -7.213497259534D+11
I= 14 X= -1.293136496763D+14 Y= -3.242085732716D+13 Z= -1.727446237075D+13
I= 15 X= 1.849256538478D+13 Y= -3.369818977721D+13 Z= -1.597887479666D+13
I= 16 X= -3.489296314841D+13 Y= -6.561976654149D+12 Z= -1.830582476815D+13
I= 17 X= -6.034323339122D+12 Y= 1.571680809197D+13 Z= -2.456096602992D+12
I= 18 X= 1.382793822785D+14 Y= -7.416374578338D+13 Z= -3.387620713289D+13
I= 19 X= -7.443041929403D+13 Y= 1.428252945650D+13 Z= -7.751995959356D+13
I= 20 X= -2.489693752917D+12 Y= 5.683145203467D+13 Z= -6.521065250497D+13
I= 21 X= 9.582232035292D+12 Y= -1.629252888526D+13 Z= -1.126952365703D+13
I= 22 X= -9.112071979686D+13 Y= -1.589440112771D+13 Z= 4.453954315559D+13
I= 23 X= 1.914144764190D+13 Y= 1.289197094285D+14 Z= 4.489164955602D+13
I= 24 X= -1.023442621466D+14 Y= 8.829977402054D+12 Z= 6.397599571400D+13
I= 25 X= -2.174860977019D+13 Y= -1.378317813008D+13 Z= 1.450272852698D+13
I= 26 X= -3.201639754064D+13 Y= -3.225935549389D+13 Z= -1.669068266783D+14
I= 27 X= -3.115091574512D+12 Y= -6.118850741232D+13 Z= 9.505245888701D+13
I= 28 X= 2.244366242284D+13 Y= -1.013913111078D+13 Z= -6.292369013513D+13

I= 29 X= 3.021976170677D+12 Y= 1.145850030585D+13 Z= 1.458894861146D+13
I= 30 X= -1.495334445833D+13 Y= 8.152324296681D+12 Z= -3.904339822951D+13
I= 31 X= 2.711220287875D+13 Y= -7.233506744542D+10 Z= 2.854971027674D+13
I= 32 X= 6.385707672240D+13 Y= -5.529448614643D+13 Z= -7.729966517703D+13
I= 33 X= -4.159564051038D+12 Y= 7.515233484220D+12 Z= -6.107864669466D+13
I= 34 X= -3.497871966923D+13 Y= -5.535801706342D+13 Z= 1.105388106234D+14
I= 35 X= 1.237787676989D+12 Y= -1.460948908029D+11 Z= 2.644307449590D+12
I= 36 X= -7.605671345141D+12 Y= 4.651559922624D+12 Z= 9.089225836337D+12
I= 37 X= -1.028690113074D+14 Y= 7.491996339597D+13 Z= -8.387416218973D+13
I= 38 X= 2.769874583260D+13 Y= -4.631905316859D+12 Z= -5.506095951002D+12

Seed: 19329037706

CM Start Point Coordinates: bohr

I= 0 X= -2.320671665392D+00 Y= 2.518487736540D+00 Z= -5.226740943201D-01
I= 1 X= -3.086436630894D+00 Y= 1.578501013748D-01 Z= -1.846691526547D+00
I= 2 X= -2.228563113487D+00 Y= 1.626644655102D+00 Z= 2.053731881932D+00
I= 3 X= -2.932756972307D+00 Y= -1.948466635577D+00 Z= -4.511913723672D-01
I= 4 X= -2.429767355636D+00 Y= -1.124836463910D+00 Z= 2.198915114095D+00
I= 5 X= 3.828510759655D+00 Y= 2.437076734018D+00 Z= -2.142787590583D+00
I= 6 X= 2.029720932637D+00 Y= 2.951192224059D-02 Z= -3.099490503036D+00
I= 7 X= 6.001141979256D+00 Y= 1.618097381851D+00 Z= -2.618597689528D+00
I= 8 X= 3.040265088289D+00 Y= 3.747987215226D+00 Z= -3.596100340849D+00
I= 9 X= -2.590910173706D+00 Y= -2.510645244077D+00 Z= 4.675313827239D+00
I= 10 X= -4.622552995497D+00 Y= -2.431887001146D+00 Z= 4.972408358019D+00
I= 11 X= -2.722798033190D+00 Y= -4.688529922813D+00 Z= 4.277950048002D+00
I= 12 X= -1.026408228887D+00 Y= -1.962342712926D+00 Z= 6.163547166883D+00
I= 13 X= -1.926367546214D+00 Y= 3.100439141503D+00 Z= 4.411632945122D+00
I= 14 X= -3.500961515800D+00 Y= 3.513097694852D+00 Z= 5.174398647141D+00
I= 15 X= -1.165237378712D+00 Y= 2.105161740841D+00 Z= 5.974405113891D+00
I= 16 X= -1.201625124891D+00 Y= 5.142988228248D+00 Z= 4.092125545435D+00

I= 17 X= -2.172557229102D+00 Y= 5.121061168795D+00 Z= -1.447083914874D+00
I= 18 X= -3.951055520323D+00 Y= 6.088869752778D+00 Z= -2.157805759198D+00
I= 19 X= -1.459062917026D+00 Y= 6.404929419249D+00 Z= 2.251792243911D-01
I= 20 X= -1.163336790391D+00 Y= 5.331124847069D+00 Z= -3.311350223259D+00
I= 21 X= -3.504029588455D+00 Y= 8.973278614772D-02 Z= -4.631644191001D+00
I= 22 X= -5.525525764336D+00 Y= 9.545506951087D-01 Z= -4.849535944396D+00
I= 23 X= -2.036738899786D+00 Y= 1.602794176296D+00 Z= -5.812732550100D+00
I= 24 X= -3.192492355756D+00 Y= -1.992177820281D+00 Z= -5.229183202027D+00
I= 25 X= -3.573570768348D+00 Y= -4.698085016134D+00 Z= -1.219961194946D+00
I= 26 X= -3.785286340776D+00 Y= -5.071649173580D+00 Z= -3.218551552011D+00
I= 27 X= -2.107690820862D+00 Y= -6.065109201957D+00 Z= -1.721327977936D-01
I= 28 X= -5.579346887052D+00 Y= -5.334230074031D+00 Z= -4.990194983830D-01
I= 29 X= 3.200926087656D+00 Y= -3.728281808848D+00 Z= -2.792373413239D-01
I= 30 X= 3.533194535928D+00 Y= -2.572928929006D+00 Z= 2.145514545412D+00
I= 31 X= 2.128735399207D+00 Y= -5.613305335409D+00 Z= -9.088380101505D-01
I= 32 X= 4.834070560536D+00 Y= -3.827294569465D+00 Z= -1.502125777388D+00
I= 33 X= 5.466616685747D+00 Y= -1.411859135044D+00 Z= 2.588180339533D+00
I= 34 X= 2.690447063907D+00 Y= -3.575054788308D+00 Z= 3.828419931201D+00
I= 35 X= 8.432881759337D-01 Y= -9.553261068190D-02 Z= -2.300108963722D-01
I= 36 X= 3.421850387069D+00 Y= 2.898728155766D+00 Z= 4.842612895919D-01
I= 37 X= 5.255636122773D+00 Y= 2.800410054445D+00 Z= 2.102770605284D+00
I= 38 X= 2.316202822662D+00 Y= 4.651103280856D+00 Z= 7.973533471167D-01

Forward Direction:

Total Energy: -651.6184445 Hartrees

Potential Energy: -651.7765429 Hartress

Kinetic Energy: 0.1580984 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.289823220422D+13 Y= -5.656451628524D+12 Z= 5.669821154031D+12

I= 1 X= -1.949131926508D+13 Y= -2.869982886091D+13 Z= -1.559519211317D+13

I= 2 X= 6.209110178804D+12 Y= 1.924739494733D+13 Z= 1.647029221663D+13

I= 3 X= -1.170600964172D+13 Y= -5.386363859033D+12 Z= 8.878783922272D+12
I= 4 X= -2.851563898438D+12 Y= -2.271111279032D+13 Z= -8.148542229993D+11
I= 5 X= 1.780336344737D+13 Y= -2.475730340788D+11 Z= -4.589095155142D+11
I= 6 X= -4.919975957674D+13 Y= -5.883110603464D+13 Z= 3.102806473734D+13
I= 7 X= -9.121803927221D+13 Y= 5.833011190381D+12 Z= -1.558657439245D+13
I= 8 X= 6.553596571415D+13 Y= 1.024842162614D+14 Z= 1.123473323013D+13
I= 9 X= -2.727708732734D+13 Y= -1.615339071673D+13 Z= 1.128474440096D+13
I= 10 X= 9.853446241523D+13 Y= -2.298862890042D+13 Z= -6.190568298744D+13
I= 11 X= 2.336723619379D+13 Y= 4.393450668014D+13 Z= 3.007328293061D+13
I= 12 X= 2.198110098983D+13 Y= -1.399620722755D+11 Z= -9.139911854623D+12
I= 13 X= 4.005741861727D+12 Y= -2.775253332380D+12 Z= 3.249982060196D+12
I= 14 X= -7.915699793122D+13 Y= -2.500370740996D+13 Z= -1.741561407986D+13
I= 15 X= -1.295908885780D+12 Y= -1.050180948728D+13 Z= 2.127752832067D+13
I= 16 X= -4.447909439126D+13 Y= -9.939831183466D+13 Z= -2.462547963424D+13
I= 17 X= 2.524095952360D+13 Y= 1.914154039722D+12 Z= -3.603882896747D+12
I= 18 X= -1.020062536307D+14 Y= 5.575368461937D+13 Z= 5.467005206131D+13
I= 19 X= -6.355592960992D+13 Y= -3.413970724586D+13 Z= -2.928625327283D+13
I= 20 X= 3.226293908272D+13 Y= 7.966845949903D+13 Z= -1.098982429673D+14
I= 21 X= 3.249616431784D+12 Y= 1.567655355944D+13 Z= 1.293192817108D+13
I= 22 X= 5.351790570871D+13 Y= -1.734209742485D+13 Z= -1.716777264918D+13
I= 23 X= -6.103177641510D+13 Y= -7.208271330715D+13 Z= -8.891092020561D+13
I= 24 X= -4.694979826519D+12 Y= 4.081136633014D+13 Z= -1.158991006909D+13
I= 25 X= -1.856245072591D+13 Y= 1.105724111286D+13 Z= -5.448820646832D+12
I= 26 X= 6.769915227311D+13 Y= -4.080237362690D+13 Z= -4.987107835971D+13
I= 27 X= -2.080483132003D+13 Y= 2.639538728575D+13 Z= -8.856098809191D+12
I= 28 X= 8.498044710998D+13 Y= 5.722911989509D+12 Z= 9.110705515529D+12
I= 29 X= -1.704143461411D+11 Y= -6.330742257299D+12 Z= -1.213198499449D+13
I= 30 X= 1.943744126655D+11 Y= 2.594139440586D+13 Z= 1.720369260091D+13
I= 31 X= -4.866558338614D+13 Y= -1.012331587842D+13 Z= -2.362250415923D+13
I= 32 X= 1.290264928168D+14 Y= -2.104219781599D+13 Z= -6.595418393061D+13

I= 33 X= -4.479122890878D+13 Y= 3.274472977898D+13 Z= -1.290711041201D+13
I= 34 X= 1.693655175449D+12 Y= 3.142381940525D+13 Z= -4.823174770754D+12
I= 35 X= 2.935568433243D+12 Y= 1.157203619142D+12 Z= 6.725472836409D+11
I= 36 X= -9.540472151045D+12 Y= -8.538592861382D+12 Z= 7.335453410147D+11
I= 37 X= -3.341649563115D+13 Y= 3.937154135588D+13 Z= -1.136858401824D+14
I= 38 X= 4.892455904969D+13 Y= -3.472432950647D+12 Z= -7.777217233776D+13

Backward Direction:

Total Energy: -651.6184449 Hartrees

Potential Energy: -651.7765429 Hartress

Kinetic Energy: 0.1580980 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.319753022032D+13 Y= -5.744503832566D+12 Z= 5.663243389768D+12
I= 1 X= -1.934212649245D+13 Y= -2.901916001451D+13 Z= -1.612625189280D+13
I= 2 X= 6.014935706415D+12 Y= 1.954000348725D+13 Z= 1.601289002198D+13
I= 3 X= -1.182791612965D+13 Y= -5.359408308055D+12 Z= 8.237907131284D+12
I= 4 X= -1.902536498427D+12 Y= -2.278838333248D+13 Z= -1.422738444540D+12
I= 5 X= 1.786824856827D+13 Y= -6.909925383978D+11 Z= -4.434848131304D+12
I= 6 X= -2.292555489401D+13 Y= -3.465295643830D+13 Z= 4.244658522396D+13
I= 7 X= -8.582424209428D+13 Y= 1.093119509443D+13 Z= -1.509188990983D+13
I= 8 X= 7.284100578050D+13 Y= 1.084618765382D+14 Z= 1.260049140065D+13
I= 9 X= -2.694535392341D+13 Y= -1.601003401553D+13 Z= 1.092379370576D+13
I= 10 X= 9.864565165756D+13 Y= -2.225852723220D+13 Z= -6.275189913773D+13
I= 11 X= 2.328977858908D+13 Y= 4.393978476451D+13 Z= 3.002041350375D+13
I= 12 X= 2.220879523835D+13 Y= -8.112531464949D+10 Z= -9.357704712774D+12
I= 13 X= 4.069607763442D+12 Y= -2.819308610401D+12 Z= 3.091966228455D+12
I= 14 X= -7.906643996013D+13 Y= -2.527473966339D+13 Z= -1.739985039910D+13
I= 15 X= -1.074035816539D+12 Y= -1.072533047738D+13 Z= 2.090131947432D+13
I= 16 X= -4.452219882166D+13 Y= -9.933781795656D+13 Z= -2.458122331718D+13
I= 17 X= 2.534838572042D+13 Y= 1.817451388988D+12 Z= -3.646241794980D+12
I= 18 X= -1.018920099799D+14 Y= 5.569482853765D+13 Z= 5.441771170869D+13

I= 19 X= -6.355616936892D+13 Y= -3.423329750379D+13 Z= -2.917955072495D+13
I= 20 X= 3.238960367911D+13 Y= 7.950844483287D+13 Z= -1.099504444138D+14
I= 21 X= 3.032503372433D+12 Y= 1.568023506817D+13 Z= 1.260097936343D+13
I= 22 X= 5.337334850864D+13 Y= -1.702774520601D+13 Z= -1.795122153447D+13
I= 23 X= -6.089413953662D+13 Y= -7.220334596117D+13 Z= -8.918837343557D+13
I= 24 X= -4.981705266949D+12 Y= 4.080309270111D+13 Z= -1.198043415631D+13
I= 25 X= -1.856398092387D+13 Y= 1.101608361572D+13 Z= -5.540724587404D+12
I= 26 X= 6.753236555071D+13 Y= -4.103889137012D+13 Z= -4.993692170767D+13
I= 27 X= -2.065879269250D+13 Y= 2.653111971093D+13 Z= -8.909676457617D+12
I= 28 X= 8.501498521219D+13 Y= 5.717326843130D+12 Z= 9.279066343033D+12
I= 29 X= -7.396152463035D+11 Y= -5.994665886872D+12 Z= -1.256850098643D+13
I= 30 X= 2.387080357290D+11 Y= 2.603705663037D+13 Z= 1.686806847971D+13
I= 31 X= -4.862045276786D+13 Y= -1.043359411632D+13 Z= -2.383049704015D+13
I= 32 X= 1.283026815176D+14 Y= -2.038697818516D+13 Z= -6.663026453214D+13
I= 33 X= -4.469084174193D+13 Y= 3.270026945844D+13 Z= -1.324909066753D+13
I= 34 X= 2.033305687142D+12 Y= 3.137243140930D+13 Z= -5.042992549174D+12
I= 35 X= 2.798569591892D+12 Y= 1.101449756054D+12 Z= 1.205509840934D+12
I= 36 X= -1.119905658008D+13 Y= -1.052045178988D+13 Z= -2.611980041082D+11
I= 37 X= -3.148901777838D+13 Y= 4.061308856281D+13 Z= -1.161342671428D+14
I= 38 X= 5.009182220821D+13 Y= -3.551210535639D+12 Z= -7.935337193508D+13

Seed: 20174731796

CM Start Point Coordinates: bohr

I= 0 X= -2.450465696266D+00 Y= 2.506844251065D+00 Z= -6.820635915849D-01
I= 1 X= -2.971310142946D+00 Y= 1.437364537613D-01 Z= -2.042761843765D+00
I= 2 X= -2.395771922570D+00 Y= 1.808017882343D+00 Z= 2.018692563493D+00
I= 3 X= -2.856548899732D+00 Y= -1.983046790464D+00 Z= -2.752538747815D-01
I= 4 X= -2.463314379166D+00 Y= -8.399026255310D-01 Z= 2.296455806051D+00
I= 5 X= 4.270355301674D+00 Y= 2.219486772829D+00 Z= -1.501892069827D+00
I= 6 X= 2.295556354824D+00 Y= 2.872617234711D-01 Z= -2.748751864472D+00

I= 7 X= 6.248784609603D+00 Y= 1.117127522913D+00 Z= -1.995263105674D+00
I= 8 X= 4.046725094194D+00 Y= 3.659391725963D+00 Z= -3.059225692451D+00
I= 9 X= -2.422588815370D+00 Y= -2.580132949046D+00 Z= 4.533442580835D+00
I= 10 X= -4.320929467010D+00 Y= -2.089731883498D+00 Z= 5.917441794199D+00
I= 11 X= -2.848465029106D+00 Y= -4.680492588360D+00 Z= 4.045252951690D+00
I= 12 X= -5.183669880488D-01 Y= -2.869652878593D+00 Z= 5.940420551757D+00
I= 13 X= -2.213017031392D+00 Y= 3.825609641417D+00 Z= 4.117710282470D+00
I= 14 X= -4.016423716131D+00 Y= 4.616855450070D+00 Z= 4.850915664062D+00
I= 15 X= -1.361251430577D+00 Y= 2.977676109015D+00 Z= 5.825087000541D+00
I= 16 X= -1.519987904435D+00 Y= 5.725287841742D+00 Z= 3.276436484364D+00
I= 17 X= -2.674699243229D+00 Y= 5.088639613605D+00 Z= -1.485218813367D+00
I= 18 X= -4.584110502130D+00 Y= 5.922533377408D+00 Z= -1.067415244434D+00
I= 19 X= -1.022262499143D+00 Y= 6.460224907779D+00 Z= -4.499450134224D-01
I= 20 X= -2.321481420021D+00 Y= 5.095124374921D+00 Z= -3.604767634278D+00
I= 21 X= -3.639801240897D+00 Y= -1.640998221800D-01 Z= -4.706735697947D+00
I= 22 X= -5.734133194829D+00 Y= -4.440407071712D-01 Z= -4.566333347339D+00
I= 23 X= -3.603552195769D+00 Y= 1.768828678543D+00 Z= -6.134443190175D+00
I= 24 X= -2.283490922006D+00 Y= -1.835949812542D+00 Z= -5.567335325276D+00
I= 25 X= -3.379493411741D+00 Y= -4.722087812171D+00 Z= -8.805881350843D-01
I= 26 X= -3.030907938871D+00 Y= -4.873795619838D+00 Z= -3.111882654447D+00
I= 27 X= -1.877404754274D+00 Y= -5.582764513436D+00 Z= -6.418805645034D-05
I= 28 X= -5.045836480911D+00 Y= -5.457805012064D+00 Z= -7.299954353405D-02
I= 29 X= 2.846447809202D+00 Y= -3.567204657052D+00 Z= -1.117063634396D+00
I= 30 X= 3.441378563725D+00 Y= -2.691413901499D+00 Z= 1.417486648159D+00
I= 31 X= 1.373208479593D+00 Y= -4.832450711508D+00 Z= -1.303817324173D+00
I= 32 X= 4.660063146440D+00 Y= -3.367822899463D+00 Z= -2.503570057104D+00
I= 33 X= 5.370408818900D+00 Y= -2.244632965514D+00 Z= 1.641953739805D+00
I= 34 X= 2.950525334129D+00 Y= -3.580068266405D+00 Z= 3.188605759929D+00
I= 35 X= 8.828646093313D-01 Y= -1.170814303607D-01 Z= -1.880114850448D-01
I= 36 X= 3.538716521441D+00 Y= 2.668915569553D+00 Z= 1.099133873097D+00

I= 37 X= 4.415671975279D+00 Y= 1.857889825971D+00 Z= 2.737178918311D+00

I= 38 X= 2.885558024779D+00 Y= 4.387308334305D+00 Z= 1.524099341907D+00

Forward Direction:

Total Energy: -651.6217388 Hartrees

Potential Energy: -651.7913375 Hartress

Kinetic Energy: 0.1695988 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.246247544540D+13 Y= 3.767132272874D+12 Z= 1.908112712640D+13

I= 1 X= 1.124107932288D+13 Y= 1.751381420639D+13 Z= -2.071348146400D+13

I= 2 X= -5.299398236537D+12 Y= -1.434418657899D+13 Z= -1.274724306938D+13

I= 3 X= -1.584085855359D+13 Y= 1.288291248497D+13 Z= -7.798731252372D+12

I= 4 X= 1.239696628348D+13 Y= -2.650452193764D+11 Z= -1.166529465794D+13

I= 5 X= -1.302531412539D+13 Y= 2.689579373353D+11 Z= 2.017826947403D+13

I= 6 X= -5.777026125830D+13 Y= 7.218490333573D+13 Z= -4.166850329176D+13

I= 7 X= 1.289018547279D+13 Y= -5.447411422300D+13 Z= -3.120204579136D+13

I= 8 X= -8.729408639894D+13 Y= -1.059456401862D+14 Z= -1.848586877283D+13

I= 9 X= -4.736586361642D+12 Y= -1.827615965638D+13 Z= 1.151743040569D+13

I= 10 X= 2.923200593837D+13 Y= -3.306312123252D+13 Z= 7.764157795834D+13

I= 11 X= -1.487007003204D+13 Y= 6.531905474249D+13 Z= 4.537670948050D+13

I= 12 X= -7.743985160891D+13 Y= 1.491482034901D+13 Z= -1.451840982691D+14

I= 13 X= -1.586072423900D+12 Y= 1.634234217698D+13 Z= 1.814836368030D+13

I= 14 X= -5.697454290096D+13 Y= 6.744151997030D+13 Z= 4.257361821172D+12

I= 15 X= 4.336649165572D+13 Y= -6.879985173335D+13 Z= 4.768056224427D+13

I= 16 X= -2.244494851535D+13 Y= 4.240391061675D+12 Z= 5.335932705653D+13

I= 17 X= -1.859968324738D+13 Y= -8.255882836534D+12 Z= 3.115927869973D+12

I= 18 X= 1.215240156266D+13 Y= 1.999531542972D+13 Z= -3.553906403107D+13

I= 19 X= 2.116027020066D+13 Y= -9.953367923053D+12 Z= -1.947022883421D+13

I= 20 X= 1.050767030429D+13 Y= 7.038268139239D+13 Z= -1.058691004047D+14

I= 21 X= 6.792116378934D+12 Y= 1.132558442773D+13 Z= 6.888019226773D+12

I= 22 X= -2.970960458710D+12 Y= -2.468639709853D+13 Z= -2.003541081010D+13

I= 23 X= -9.196260278136D+12 Y= 4.728357705403D+13 Z= 7.703058610911D+13
I= 24 X= 8.007642793148D+12 Y= -1.621480531254D+14 Z= 1.112433956985D+13
I= 25 X= 8.291587447134D+11 Y= -1.669256307944D+13 Z= 7.928677067673D+11
I= 26 X= 8.085544445171D+13 Y= 5.253513942832D+13 Z= -6.703065592983D+13
I= 27 X= -7.349373619472D+12 Y= -5.538004553593D+13 Z= 8.904162691882D+12
I= 28 X= -1.206077526383D+14 Y= -1.144355701222D+13 Z= 4.667452470686D+12
I= 29 X= 3.363787535352D+13 Y= -3.312916914860D+12 Z= 2.809077628369D+12
I= 30 X= -2.003928265572D+11 Y= 1.274080038736D+13 Z= -2.610837482682D+13
I= 31 X= 1.378248914283D+13 Y= -3.571367606126D+12 Z= 5.985084047844D+13
I= 32 X= -1.359019965098D+14 Y= -1.885068446685D+13 Z= 9.697595434156D+13
I= 33 X= 3.370592734533D+13 Y= -2.770976193042D+13 Z= 3.228828736098D+13
I= 34 X= 3.022347666443D+13 Y= 2.119155992219D+13 Z= 3.920237086140D+13
I= 35 X= 8.331106155050D+11 Y= 7.734869780651D+10 Z= -2.177238333093D+11
I= 36 X= 4.581271558743D+12 Y= -1.959348797849D+12 Z= -7.612979658725D+12
I= 37 X= -6.795758885707D+13 Y= -2.405710366502D+13 Z= 8.083294739627D+12
I= 38 X= -6.433897239521D+13 Y= 1.005264597048D+13 Z= 8.725519317367D+12

Backward Direction:

Total Energy: -651.6217311 Hartrees

Potential Energy: -651.7913375 Hartress

Kinetic Energy: 0.1696065 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.151454940932D+13 Y= 3.488256464481D+12 Z= 1.906029426622D+13
I= 1 X= 1.171359736880D+13 Y= 1.650243992765D+13 Z= -2.239543511921D+13
I= 2 X= -5.914380724978D+12 Y= -1.341744721255D+13 Z= -1.419591104344D+13
I= 3 X= -1.622695644769D+13 Y= 1.296828515027D+13 Z= -9.828493443387D+12
I= 4 X= 1.540269213062D+13 Y= -5.097737328750D+11 Z= -1.359056395437D+13
I= 5 X= -1.281981227557D+13 Y= -1.135424555848D+12 Z= 7.585818033823D+12
I= 6 X= 2.544446578033D+13 Y= 1.487610792221D+14 Z= -5.504171127381D+12
I= 7 X= 2.997322814739D+13 Y= -3.832732740677D+13 Z= -2.963529867903D+13
I= 8 X= -6.415782318663D+13 Y= -8.701340706420D+13 Z= -1.416028804855D+13

I= 9 X= -3.685932117405D+12 Y= -1.782212540924D+13 Z= 1.037424019704D+13
I= 10 X= 2.958416056173D+13 Y= -3.075076918186D+13 Z= 7.496147224496D+13
I= 11 X= -1.511539101176D+13 Y= 6.533577129904D+13 Z= 4.520926330927D+13
I= 12 X= -7.671870646843D+13 Y= 1.510116603487D+13 Z= -1.458738840641D+14
I= 13 X= -1.383798615107D+12 Y= 1.620281186623D+13 Z= 1.764790155440D+13
I= 14 X= -5.668773091216D+13 Y= 6.658311626319D+13 Z= 4.307287984302D+12
I= 15 X= 4.406920014404D+13 Y= -6.950777947554D+13 Z= 4.648904696182D+13
I= 16 X= -2.258146732328D+13 Y= 4.431985114109D+12 Z= 5.349949408963D+13
I= 17 X= -1.825944681501D+13 Y= -8.562156034848D+12 Z= 2.981770272355D+12
I= 18 X= 1.251422998636D+13 Y= 1.980890852335D+13 Z= -3.633826742877D+13
I= 19 X= 2.115951083055D+13 Y= -1.024978365503D+13 Z= -1.913228430959D+13
I= 20 X= 1.090883791026D+13 Y= 6.987588864129D+13 Z= -1.060344309710D+14
I= 21 X= 6.104483610206D+12 Y= 1.133724437195D+13 Z= 5.839849931647D+12
I= 22 X= -3.428796888113D+12 Y= -2.369079193171D+13 Z= -2.251672227417D+13
I= 23 X= -8.760341654024D+12 Y= 4.690151360141D+13 Z= 7.615184610724D+13
I= 24 X= 7.099536179825D+12 Y= -1.621742570672D+14 Z= 9.887485575677D+12
I= 25 X= 8.243123584676D+11 Y= -1.682291564214D+13 Z= 5.017928097107D+11
I= 26 X= 8.032720346775D+13 Y= 5.178604883052D+13 Z= -6.723919264257D+13
I= 27 X= -6.886845271600D+12 Y= -5.495015863046D+13 Z= 8.734473467029D+12
I= 28 X= -1.204983647902D+14 Y= -1.146124608229D+13 Z= 5.200678902727D+12
I= 29 X= 3.183512249501D+13 Y= -2.248507782471D+12 Z= 1.426559697381D+12
I= 30 X= -5.998095099404D+10 Y= 1.304377838651D+13 Z= -2.717135161204D+13
I= 31 X= 1.392542522730D+13 Y= -4.554069809647D+12 Z= 5.919209282184D+13
I= 32 X= -1.381944259326D+14 Y= -1.677549614662D+13 Z= 9.483469589047D+13
I= 33 X= 3.402387001515D+13 Y= -2.785057507291D+13 Z= 3.120517964886D+13
I= 34 X= 3.129920569121D+13 Y= 2.102880568852D+13 Z= 3.850617180924D+13
I= 35 X= 3.992127557201D+11 Y= -9.923295520124D+10 Z= 1.470256231793D+12
I= 36 X= -6.717380822586D+11 Y= -8.236221944745D+12 Z= -1.076349542009D+13
I= 37 X= -6.185294952616D+13 Y= -2.012491949022D+13 Z= 3.287239135731D+11
I= 38 X= -6.064205800980D+13 Y= 9.803144403710D+12 Z= 3.717600165036D+12

Seed: 20322869887

CM Start Point Coordinates: bohr

I= 0 X= -2.601981391885D+00 Y= 2.264753831924D+00 Z= -4.754655282321D-01
I= 1 X= -3.044328194648D+00 Y= 2.423864374350D-02 Z= -2.095543055876D+00
I= 2 X= -2.113110150634D+00 Y= 1.713023699299D+00 Z= 2.047489966979D+00
I= 3 X= -3.163625568547D+00 Y= -1.981443585706D+00 Z= -1.173821738491D-01
I= 4 X= -2.593876462567D+00 Y= -1.010414226174D+00 Z= 2.227562916224D+00
I= 5 X= 3.900727056258D+00 Y= 2.290497473465D+00 Z= -1.767546952344D+00
I= 6 X= 1.627513865815D+00 Y= 9.591187287498D-01 Z= -2.944030937169D+00
I= 7 X= 5.456618043140D+00 Y= 1.296745821047D+00 Z= -2.654818012156D+00
I= 8 X= 3.360811123946D+00 Y= 4.096373192585D+00 Z= -2.958249556617D+00
I= 9 X= -2.913458141927D+00 Y= -2.601925475042D+00 Z= 4.842792563734D+00
I= 10 X= -4.735222808086D+00 Y= -1.539673883928D+00 Z= 5.759627342479D+00
I= 11 X= -3.079962130531D+00 Y= -4.752204363965D+00 Z= 4.347968409425D+00
I= 12 X= -1.100024277975D+00 Y= -2.593145281076D+00 Z= 6.135126930589D+00
I= 13 X= -1.944204612001D+00 Y= 3.667931458821D+00 Z= 4.070171741566D+00
I= 14 X= -3.733552675800D+00 Y= 4.227237813688D+00 Z= 4.751883537852D+00
I= 15 X= -7.510256038381D-01 Y= 2.965103311869D+00 Z= 5.555519183204D+00
I= 16 X= -4.747089782402D-01 Y= 5.473542366800D+00 Z= 3.482479488716D+00
I= 17 X= -2.390221047366D+00 Y= 4.898043121328D+00 Z= -1.482791520883D+00
I= 18 X= -4.286960800868D+00 Y= 5.776377263452D+00 Z= -8.165455413256D-01
I= 19 X= -6.572720519484D-01 Y= 5.818413379112D+00 Z= -5.754613080466D-01
I= 20 X= -2.484301631405D+00 Y= 4.658619592679D+00 Z= -3.851570843502D+00
I= 21 X= -3.189690813948D+00 Y= -3.731193841937D-01 Z= -4.794152506570D+00
I= 22 X= -4.899471371392D+00 Y= 1.547997048332D-01 Z= -5.603021422262D+00
I= 23 X= -1.830709411619D+00 Y= 1.128008218713D+00 Z= -5.665710315977D+00
I= 24 X= -2.183981852929D+00 Y= -1.887674859144D+00 Z= -5.441541380417D+00
I= 25 X= -3.599787577998D+00 Y= -4.727809984189D+00 Z= -6.693775073506D-01
I= 26 X= -2.920284772647D+00 Y= -5.324713418061D+00 Z= -2.558205527647D+00

I= 27 X= -2.515626478270D+00 Y= -6.047365538374D+00 Z= 5.361205194523D-01
I= 28 X= -5.887809097046D+00 Y= -5.530129679452D+00 Z= -5.287407231526D-01
I= 29 X= 3.405984317527D+00 Y= -3.224298639399D+00 Z= -1.365860469784D+00
I= 30 X= 3.508962158468D+00 Y= -3.081309414948D+00 Z= 1.430342070114D+00
I= 31 X= 2.398334657023D+00 Y= -4.783734399074D+00 Z= -2.358054652609D+00
I= 32 X= 4.953240413172D+00 Y= -2.085705590304D+00 Z= -2.292157504744D+00
I= 33 X= 5.237456220071D+00 Y= -2.150731115311D+00 Z= 2.648021573808D+00
I= 34 X= 2.218294410379D+00 Y= -4.299682350361D+00 Z= 2.497448589572D+00
I= 35 X= 8.456267171047D-01 Y= -2.898468340328D-02 Z= -1.898657016101D-01
I= 36 X= 3.788260314518D+00 Y= 2.470137955387D+00 Z= 1.059985466320D+00
I= 37 X= 5.317799033212D+00 Y= 1.564382127246D+00 Z= 2.608384541461D+00
I= 38 X= 3.260459711524D+00 Y= 4.516516626982D+00 Z= 1.626628649417D+00

Forward Direction:

Total Energy: -651.6088731 Hartrees

Potential Energy: -651.7758248 Hartress

Kinetic Energy: 0.1669518 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.795650252783D+13 Y= -4.939385878345D+12 Z= -5.883343106288D+11
I= 1 X= 1.641317928209D+13 Y= -1.257125649484D+13 Z= 2.975143476922D+13
I= 2 X= 5.738817486301D+11 Y= 5.832029277718D+12 Z= 7.845860196239D+12
I= 3 X= -1.330821603168D+12 Y= 9.398985268044D+11 Z= -1.536372251620D+13
I= 4 X= -1.257880359262D+13 Y= 6.857789785325D+12 Z= -2.845677361691D+13
I= 5 X= -1.996511121055D+13 Y= -1.441252368639D+13 Z= 7.231025395427D+12
I= 6 X= -3.641412271348D+13 Y= -8.447310751734D+12 Z= -8.584841144250D+13
I= 7 X= 1.195287940075D+14 Y= -1.309580410022D+13 Z= 3.866311237266D+13
I= 8 X= -4.986627828759D+13 Y= 1.592197229654D+13 Z= -2.630778559156D+13
I= 9 X= -3.640796037886D+11 Y= -1.932948223476D+13 Z= 9.491239669454D+12
I= 10 X= 4.789138971557D+13 Y= 2.129741100536D+13 Z= -5.282071442524D+13
I= 11 X= -1.158027717425D+13 Y= 7.311094005737D+13 Z= -1.733934953490D+12
I= 12 X= -8.551795996234D+13 Y= -6.612406182981D+12 Z= -3.360892996469D+13

I= 13 X= 1.304679781420D+13 Y= -3.977758793723D+12 Z= 7.388349563934D+12
I= 14 X= -1.487888136111D+14 Y= 2.282724239175D+12 Z= -4.653979506225D+13
I= 15 X= -7.167661490687D+13 Y= -6.225317353731D+13 Z= -5.738767879772D+13
I= 16 X= -5.015826787814D+13 Y= 4.845780171058D+13 Z= -5.475902379863D+13
I= 17 X= -4.222029038502D+12 Y= 6.032876579397D+12 Z= -1.075341125188D+13
I= 18 X= -1.040507563311D+14 Y= 8.363189673299D+13 Z= -9.430902568042D+13
I= 19 X= 8.617401270961D+12 Y= 1.839585842648D+13 Z= 1.781237813658D+13
I= 20 X= -9.287229082859D+13 Y= 8.043121973897D+13 Z= 6.846156011912D+13
I= 21 X= -2.066079698648D+13 Y= 3.502524197764D+11 Z= 1.454417178719D+13
I= 22 X= 5.092144326739D+13 Y= 2.370146320550D+13 Z= -7.873811190894D+12
I= 23 X= -3.761318604411D+12 Y= 9.589170158273D+12 Z= 7.389533641636D+12
I= 24 X= 1.719720104894D+13 Y= -7.564297480560D+13 Z= -9.061376246082D+12
I= 25 X= 6.466929299544D+12 Y= 1.028916311188D+13 Z= -1.572343166793D+13
I= 26 X= -7.932493841356D+13 Y= -8.210271274746D+12 Z= 8.072957934961D+13
I= 27 X= 5.002045120122D+13 Y= -5.898078453851D+13 Z= 1.229720334711D+13
I= 28 X= -5.314048780582D+13 Y= -9.720662955590D+12 Z= 6.298612994569D+13
I= 29 X= 8.431593999921D+12 Y= 4.049192857447D+12 Z= 5.422825415272D+12
I= 30 X= 7.577043145292D+12 Y= 3.513785490106D+12 Z= 8.870392536938D+12
I= 31 X= -1.419359737757D+13 Y= -2.676296686489D+12 Z= 4.521901692195D+13
I= 32 X= -1.001264771448D+14 Y= 9.384859482953D+12 Z= 1.154852994315D+14
I= 33 X= 6.295980711318D+13 Y= 5.722270808749D+13 Z= 3.198705619715D+13
I= 34 X= -6.588145986691D+13 Y= -9.081016189324D+13 Z= -1.506845094738D+13
I= 35 X= 2.225492867587D+12 Y= 2.064482965917D+11 Z= -1.302687571369D+12
I= 36 X= 1.347283088990D+12 Y= 1.355519306363D+13 Z= -8.487987525327D+12
I= 37 X= 1.613499216319D+13 Y= -1.734725682138D+13 Z= 5.444409135227D+13
I= 38 X= 1.686167859520D+13 Y= -8.379085322288D+13 Z= 6.624437119903D+13

Backward Direction:

Total Energy: -651.6089078 Hartrees

Potential Energy: -651.7758248 Hartress

Kinetic Energy: 0.1669170 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.706301211994D+13 Y= -5.202246958221D+12 Z= -6.079708225226D+11
I= 1 X= 1.685856249045D+13 Y= -1.352455156362D+13 Z= 2.816606903245D+13
I= 2 X= -5.784739025048D+09 Y= 6.705549682373D+12 Z= 6.480383471011D+12
I= 3 X= -1.694747429864D+12 Y= 1.020368578420D+12 Z= -1.727692352723D+13
I= 4 X= -9.745684644087D+12 Y= 6.627115058371D+12 Z= -3.027148234516D+13
I= 5 X= -1.977141051494D+13 Y= -1.573625807155D+13 Z= -4.638291568438D+12
I= 6 X= 4.202191303047D+13 Y= 6.373139946956D+13 Z= -5.176085325063D+13
I= 7 X= 1.356308253846D+14 Y= 2.123736871723D+12 Z= 4.013988742044D+13
I= 8 X= -2.805863878829D+13 Y= 3.376700245793D+13 Z= -2.223060578814D+13
I= 9 X= 6.262397443475D+11 Y= -1.890152137178D+13 Z= 8.413698333338D+12
I= 10 X= 4.822332150064D+13 Y= 2.347697386437D+13 Z= -5.534691231270D+13
I= 11 X= -1.181151034951D+13 Y= 7.312669664213D+13 Z= -1.891765352571D+12
I= 12 X= -8.483822731655D+13 Y= -6.436761590422D+12 Z= -3.425910410595D+13
I= 13 X= 1.323745584633D+13 Y= -4.109276433689D+12 Z= 6.916626989999D+12
I= 14 X= -1.485184720919D+14 Y= 1.473615250650D+12 Z= -4.649273596623D+13
I= 15 X= -7.101426017544D+13 Y= -6.292044780485D+13 Z= -5.851077008425D+13
I= 16 X= -5.028694694598D+13 Y= 4.863839327957D+13 Z= -5.462690599769D+13
I= 17 X= -3.901331036790D+12 Y= 5.744191434423D+12 Z= -1.087986471223D+13
I= 18 X= -1.037097062842D+14 Y= 8.345619442414D+13 Z= -9.506233402277D+13
I= 19 X= 8.616685485441D+12 Y= 1.811646468091D+13 Z= 1.813091585972D+13
I= 20 X= -9.249416066516D+13 Y= 7.995353008241D+13 Z= 6.830572383793D+13
I= 21 X= -2.130894173188D+13 Y= 3.612427794702D+11 Z= 1.355619469061D+13
I= 22 X= 5.048989857135D+13 Y= 2.463989472010D+13 Z= -1.021263079699D+13
I= 23 X= -3.350433049807D+12 Y= 9.229047093548D+12 Z= 6.561256189563D+12
I= 24 X= 1.634124339723D+13 Y= -7.566767395954D+13 Z= -1.022720262649D+13
I= 25 X= 6.462361221638D+12 Y= 1.016629617842D+13 Z= -1.599779128875D+13
I= 26 X= -7.982284461669D+13 Y= -8.916344579947D+12 Z= 8.053301807240D+13
I= 27 X= 5.045641838942D+13 Y= -5.857558432886D+13 Z= 1.213725870266D+13
I= 28 X= -5.303738167013D+13 Y= -9.737336216608D+12 Z= 6.348873530206D+13

I= 29 X= 6.732366076491D+12 Y= 5.052477199847D+12 Z= 4.119699998479D+12
I= 30 X= 7.709391723462D+12 Y= 3.799364665497D+12 Z= 7.868458286695D+12
I= 31 X= -1.405886954800D+13 Y= -3.602566207267D+12 Z= 4.459809852996D+13
I= 32 X= -1.022872614520D+14 Y= 1.134087797719D+13 Z= 1.134670049508D+14
I= 33 X= 6.325949159647D+13 Y= 5.708998128193D+13 Z= 3.096614706033D+13
I= 34 X= -6.486750568701D+13 Y= -9.096356979638D+13 Z= -1.572467005108D+13
I= 35 X= 1.816512038388D+12 Y= 4.000702717506D+10 Z= 2.883585026306D+11
I= 36 X= -3.604067069469D+12 Y= 7.638775812550D+12 Z= -1.145758167870D+13
I= 37 X= 2.188906630245D+13 Y= -1.364088236771D+13 Z= 4.713483473091D+13
I= 38 X= 2.034629387205D+13 Y= -8.402602690478D+13 Z= 6.152403695640D+13

Seed: 2072860618

CM Start Point Coordinates: bohr

I= 0 X= -2.694112566818D+00 Y= 2.274449723602D+00 Z= -6.947020834831D-01
I= 1 X= -3.060397276271D+00 Y= -9.968766764410D-02 Z= -1.841439220554D+00
I= 2 X= -2.493801999581D+00 Y= 1.794351969053D+00 Z= 1.935360322786D+00
I= 3 X= -3.047367038398D+00 Y= -2.009718113282D+00 Z= -1.205136390385D-01
I= 4 X= -2.238352352599D+00 Y= -9.050083582994D-01 Z= 2.381984390704D+00
I= 5 X= 4.357431910331D+00 Y= 2.753591701964D+00 Z= -6.955780716469D-01
I= 6 X= 2.716076777475D+00 Y= 1.362918934906D+00 Z= -2.678387643190D+00
I= 7 X= 5.982166059724D+00 Y= 1.546955781398D+00 Z= -1.699300682508D+00
I= 8 X= 4.043463300179D+00 Y= 4.599529273485D+00 Z= -1.495166280445D+00
I= 9 X= -2.210160169230D+00 Y= -2.036794959715D+00 Z= 4.818790575914D+00
I= 10 X= -4.017923357152D+00 Y= -1.414635893565D+00 Z= 6.367786634877D+00
I= 11 X= -2.422237708521D+00 Y= -4.268373907949D+00 Z= 4.775865073825D+00
I= 12 X= -1.493793578856D-01 Y= -1.877297860998D+00 Z= 5.930041439938D+00
I= 13 X= -2.231090898178D+00 Y= 3.721963927103D+00 Z= 3.955419018224D+00
I= 14 X= -4.391376938125D+00 Y= 3.925478029735D+00 Z= 4.812662522768D+00
I= 15 X= -8.231959386196D-01 Y= 3.246669524387D+00 Z= 5.500815857860D+00
I= 16 X= -1.830665666367D+00 Y= 5.474811887978D+00 Z= 3.226106501180D+00

I= 17 X= -2.996723407207D+00 Y= 4.853184832050D+00 Z= -2.059869491393D+00
I= 18 X= -4.973534043738D+00 Y= 5.403642763274D+00 Z= -2.828771703226D+00
I= 19 X= -2.018381529056D+00 Y= 6.436796782318D+00 Z= -7.054184809692D-01
I= 20 X= -1.673878201855D+00 Y= 4.809663082870D+00 Z= -3.768269754693D+00
I= 21 X= -3.376484095791D+00 Y= -2.500535003652D-01 Z= -4.677964539966D+00
I= 22 X= -5.598728238554D+00 Y= -3.556895498980D-01 Z= -4.901964762481D+00
I= 23 X= -2.049568145274D+00 Y= 1.179284694677D+00 Z= -5.503827629438D+00
I= 24 X= -2.852542795541D+00 Y= -2.305292409885D+00 Z= -5.045018048606D+00
I= 25 X= -3.667412561965D+00 Y= -4.712933438286D+00 Z= -4.572062918771D-01
I= 26 X= -3.634809439770D+00 Y= -5.410620790101D+00 Z= -2.339071966833D+00
I= 27 X= -2.417481107562D+00 Y= -6.252571990125D+00 Z= 6.889344551953D-01
I= 28 X= -5.797221885697D+00 Y= -4.997331170132D+00 Z= 2.339175042182D-01
I= 29 X= 2.820546908458D+00 Y= -3.520874587494D+00 Z= -1.684037603217D+00
I= 30 X= 3.311753766161D+00 Y= -3.511730807462D+00 Z= 9.279909999850D-01
I= 31 X= 1.565944999961D+00 Y= -4.911205887848D+00 Z= -2.654848522435D+00
I= 32 X= 4.222113697524D+00 Y= -2.769922393295D+00 Z= -3.220324850121D+00
I= 33 X= 5.053647422067D+00 Y= -3.012207521597D+00 Z= 1.546801553174D+00
I= 34 X= 2.259369182217D+00 Y= -4.391508777602D+00 Z= 2.573359321832D+00
I= 35 X= 9.116339291818D-01 Y= -3.464222276419D-02 Z= -2.563294264736D-01
I= 36 X= 3.800992352555D+00 Y= 2.169481134271D+00 Z= 1.924870997584D+00
I= 37 X= 5.085005634381D+00 Y= 9.992514855796D-01 Z= 2.951417911689D+00
I= 38 X= 2.600410801954D+00 Y= 3.420239338815D+00 Z= 3.099486117276D+00

Forward Direction:

Total Energy: -651.6183433 Hartrees

Potential Energy: -651.8125569 Hartress

Kinetic Energy: 0.1942136 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -7.532976859971D+12 Y= 2.291767723550D+12 Z= 1.706636264021D+13

I= 1 X= -6.728370581740D+12 Y= 9.096984389119D+12 Z= 2.027978264759D+13

I= 2 X= 1.346151831009D+13 Y= 5.336999853267D+11 Z= 6.878210332789D+12

I= 3 X= 4.061792275528D+12 Y= -1.461133166949D+12 Z= -4.367259538410D+10
I= 4 X= 1.152416606521D+13 Y= 8.289654127004D+12 Z= -1.473690114018D+13
I= 5 X= -8.084932721480D+12 Y= 3.331890858319D+12 Z= 1.179529341974D+13
I= 6 X= -3.004354329541D+13 Y= -3.800469375731D+13 Z= -1.208507376207D+14
I= 7 X= 1.929722908520D+13 Y= -1.220896038042D+13 Z= 6.014205018343D+13
I= 8 X= 2.218797354461D+13 Y= 1.083251310599D+14 Z= -1.036404791320D+14
I= 9 X= 4.327749482492D+12 Y= -1.139677563907D+13 Z= 2.698438947778D+13
I= 10 X= -6.286604101170D+13 Y= -8.508168326693D+13 Z= -3.944395256492D+13
I= 11 X= -1.041353230338D+13 Y= -2.765351007649D+13 Z= -9.968471772726D+13
I= 12 X= 2.992518857524D+13 Y= 4.615300770230D+13 Z= -6.905151033174D+13
I= 13 X= 7.002335721527D+12 Y= -1.941848747503D+12 Z= -1.828730071372D+13
I= 14 X= -9.978944671678D+13 Y= 6.500563110240D+13 Z= 7.522265182943D+13
I= 15 X= 1.551501010237D+13 Y= 5.932111285667D+13 Z= -8.677833767305D+13
I= 16 X= 5.171335099575D+13 Y= 4.745668950679D+13 Z= 2.914016400859D+13
I= 17 X= 4.255803406590D+12 Y= -1.308234774629D+13 Z= -7.584940330189D+12
I= 18 X= 2.672575604782D+13 Y= -6.969700689019D+12 Z= -1.400801622593D+13
I= 19 X= -5.827719210894D+13 Y= -1.457590584572D+14 Z= -6.228553724802D+13
I= 20 X= 1.910038173646D+13 Y= -1.772290457980D+13 Z= 5.909409992712D+13
I= 21 X= 2.483633080740D+13 Y= -9.904713787563D+11 Z= 5.061531974243D+12
I= 22 X= -1.059590750892D+14 Y= 7.359446540075D+13 Z= 4.835729530696D+12
I= 23 X= -8.368408547126D+13 Y= -3.571372305782D+13 Z= 7.260126423570D+13
I= 24 X= -7.170088018624D+12 Y= -6.672804125196D+13 Z= -5.299664641854D+13
I= 25 X= -9.837620879138D+12 Y= 6.473865089735D+12 Z= -2.297762975979D+13
I= 26 X= -2.958004238426D+13 Y= 6.151774812771D+13 Z= 1.526541750860D+13
I= 27 X= 2.853041245344D+13 Y= 4.097260290081D+13 Z= 7.137305427138D+13
I= 28 X= -3.728647819582D+13 Y= -2.642933319873D+13 Z= 5.891980623176D+13
I= 29 X= -9.300258706452D+12 Y= -1.066416763607D+13 Z= -8.358295583164D+12
I= 30 X= -4.660792928592D+11 Y= -1.062098742284D+13 Z= 7.343936000431D+12
I= 31 X= 1.403873503519D+14 Y= 5.576995936630D+13 Z= -5.135488818437D+12
I= 32 X= -8.724070036871D+13 Y= -7.602979032622D+13 Z= -1.518215458062D+13

I= 33 X= 2.239246931129D+13 Y= 7.578577229756D+13 Z= 7.370418797727D+13
I= 34 X= -4.669706545029D+13 Y= -5.594811654455D+13 Z= 2.065982842464D+13
I= 35 X= 1.092891642608D+10 Y= 2.027646165031D+12 Z= -5.997352690241D+11
I= 36 X= 1.181988245157D+12 Y= -1.908967724176D+13 Z= 1.666923771420D+13
I= 37 X= -5.607065947021D+13 Y= 6.121995276846D+12 Z= -1.707085483744D+14
I= 38 X= -4.532868323690D+12 Y= 3.310145835098D+13 Z= -6.370857517377D+13

Backward Direction:

Total Energy: -651.6183063 Hartrees

Potential Energy: -651.8125569 Hartress

Kinetic Energy: 0.1942506 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.285761887401D+12 Y= 2.070301570062D+12 Z= 1.704981845206D+13
I= 1 X= -6.353125576688D+12 Y= 8.293812635373D+12 Z= 1.894407765961D+13
I= 2 X= 1.297313673232D+13 Y= 1.269659856332D+12 Z= 5.727766601286D+12
I= 3 X= 3.755176880624D+12 Y= -1.393335403106D+12 Z= -1.655585905251D+12
I= 4 X= 1.391113017608D+13 Y= 8.095305671607D+12 Z= -1.626583256753D+13
I= 5 X= -7.921735692485D+12 Y= 2.216615958262D+12 Z= 1.795136669754D+12
I= 6 X= 3.604051653945D+13 Y= 2.280743372934D+13 Z= -9.213123116144D+13
I= 7 X= 3.286353945294D+13 Y= 6.138327088814D+11 Z= 6.138626516518D+13
I= 8 X= 4.056138239146D+13 Y= 1.233599556798D+14 Z= -1.002053667922D+14
I= 9 X= 5.162114996553D+12 Y= -1.103620933749D+13 Z= 2.607653755135D+13
I= 10 X= -6.258638128078D+13 Y= -8.324535433085D+13 Z= -4.157232901687D+13
I= 11 X= -1.060835125526D+13 Y= -2.764023480813D+13 Z= -9.981769326200D+13
I= 12 X= 3.049787806606D+13 Y= 4.630099207661D+13 Z= -6.959929614039D+13
I= 13 X= 7.162969243555D+12 Y= -2.052655206944D+12 Z= -1.868473720547D+13
I= 14 X= -9.956167813291D+13 Y= 6.432393924495D+13 Z= 7.526230013751D+13
I= 15 X= 1.607305831243D+13 Y= 5.875891983024D+13 Z= -8.772456641537D+13
I= 16 X= 5.160493609081D+13 Y= 4.760884182031D+13 Z= 2.925147611561D+13
I= 17 X= 4.525998429996D+12 Y= -1.332557123416D+13 Z= -7.691480108768D+12
I= 18 X= 2.701309812029D+13 Y= -7.117733665534D+12 Z= -1.464269478799D+13

I= 19 X= -5.827779512944D+13 Y= -1.459944537554D+14 Z= -6.201716233373D+13
I= 20 X= 1.941896455907D+13 Y= -1.812536846811D+13 Z= 5.896280447156D+13
I= 21 X= 2.429025481129D+13 Y= -9.812117656966D+11 Z= 4.229139862078D+12
I= 22 X= -1.063226608501D+14 Y= 7.438511428424D+13 Z= 2.865223330059D+12
I= 23 X= -8.333790548879D+13 Y= -3.601713455119D+13 Z= 7.190342253011D+13
I= 24 X= -7.891250894626D+12 Y= -6.674885082890D+13 Z= -5.397888040544D+13
I= 25 X= -9.841469585618D+12 Y= 6.370347038415D+12 Z= -2.320878368833D+13
I= 26 X= -2.999953914109D+13 Y= 6.092286607645D+13 Z= 1.509981037122D+13
I= 27 X= 2.889772424511D+13 Y= 4.131399285798D+13 Z= 7.123829744219D+13
I= 28 X= -3.719960904391D+13 Y= -2.644338077206D+13 Z= 5.934326212862D+13
I= 29 X= -1.073189504852D+13 Y= -9.818878834154D+12 Z= -9.456206984411D+12
I= 30 X= -3.545727469802D+11 Y= -1.038038077800D+13 Z= 6.499784684705D+12
I= 31 X= 1.405008614778D+14 Y= 5.498955722093D+13 Z= -5.658626022950D+12
I= 32 X= -8.906120796470D+13 Y= -7.438180235480D+13 Z= -1.688261141489D+13
I= 33 X= 2.264495997973D+13 Y= 7.567394709519D+13 Z= 7.284404991060D+13
I= 34 X= -4.584278708589D+13 Y= -5.607736602737D+13 Z= 2.010694960775D+13
I= 35 X= -3.336462953833D+11 Y= 1.887415787262D+12 Z= 7.407555259184D+11
I= 36 X= -2.989631564639D+12 Y= -2.407438698357D+13 Z= 1.416729029101D+13
I= 37 X= -5.122272732482D+13 Y= 9.244696070914D+12 Z= -1.768667554681D+14
I= 38 X= -1.597004452252D+12 Y= 3.290331942284D+13 Z= -6.768555906033D+13

Seed: 20872618492

CM Start Point Coordinates: bohr

I= 0 X= -2.543563515248D+00 Y= 2.286017375515D+00 Z= -5.565410771608D-01
I= 1 X= -2.865103430390D+00 Y= 9.188647813610D-02 Z= -2.069752437493D+00
I= 2 X= -2.303505500795D+00 Y= 1.750425920645D+00 Z= 2.033989586845D+00
I= 3 X= -2.931453528693D+00 Y= -2.021039591232D+00 Z= -1.511337851451D-01
I= 4 X= -2.275325164735D+00 Y= -1.029217955891D+00 Z= 2.268453659474D+00
I= 5 X= 4.270698684918D+00 Y= 2.528112848158D+00 Z= -1.217021817590D+00
I= 6 X= 2.005174018596D+00 Y= 1.135726353050D+00 Z= -2.838698133717D+00

I= 7 X= 5.678248104039D+00 Y= 1.372938764961D+00 Z= -2.059698086367D+00
I= 8 X= 3.848533514356D+00 Y= 4.212637245103D+00 Z= -2.108997846465D+00
I= 9 X= -2.177015786436D+00 Y= -2.189861087392D+00 Z= 4.925662313482D+00
I= 10 X= -4.278740474241D+00 Y= -2.542496914560D+00 Z= 5.369100103184D+00
I= 11 X= -1.017479086716D+00 Y= -4.065951404158D+00 Z= 5.083839497902D+00
I= 12 X= -1.217288210673D+00 Y= -3.751208700939D-01 Z= 6.139188370887D+00
I= 13 X= -2.392471017417D+00 Y= 3.639695844121D+00 Z= 4.117102504953D+00
I= 14 X= -4.284963353680D+00 Y= 3.440032728647D+00 Z= 5.132695157139D+00
I= 15 X= -5.882649649781D-01 Y= 3.331470130103D+00 Z= 5.674416677318D+00
I= 16 X= -2.521220096133D+00 Y= 5.766347973386D+00 Z= 3.379057379687D+00
I= 17 X= -2.536345358222D+00 Y= 4.814466592159D+00 Z= -1.640782241383D+00
I= 18 X= -4.633952042035D+00 Y= 5.449107938514D+00 Z= -1.852126885834D+00
I= 19 X= -1.417511204049D+00 Y= 6.241905710199D+00 Z= -5.938404407701D-01
I= 20 X= -2.089518814449D+00 Y= 4.544639785667D+00 Z= -3.713704868286D+00
I= 21 X= -3.067085963954D+00 Y= -3.120191699792D-01 Z= -4.679170347271D+00
I= 22 X= -5.048639889941D+00 Y= -1.660556064173D+00 Z= -5.618272030171D+00
I= 23 X= -2.909166143594D+00 Y= 1.521828419207D+00 Z= -5.761460276449D+00
I= 24 X= -1.215944345418D+00 Y= -1.415159390484D+00 Z= -5.380872155699D+00
I= 25 X= -3.697295680218D+00 Y= -4.651828218279D+00 Z= -5.649000606481D-01
I= 26 X= -3.465914016262D+00 Y= -5.311373283428D+00 Z= -2.472601848643D+00
I= 27 X= -2.876497189746D+00 Y= -5.893492394119D+00 Z= 7.179677529273D-01
I= 28 X= -5.629691263250D+00 Y= -4.567542758273D+00 Z= 2.947729425468D-01
I= 29 X= 2.658139404542D+00 Y= -3.380557438393D+00 Z= -1.495264018882D+00
I= 30 X= 3.189100888883D+00 Y= -3.385697466119D+00 Z= 1.079645453098D+00
I= 31 X= 1.449798255937D+00 Y= -4.836904283315D+00 Z= -2.186940816113D+00
I= 32 X= 4.074533935968D+00 Y= -3.115747071475D+00 Z= -2.828135684098D+00
I= 33 X= 4.930736779806D+00 Y= -2.710213132683D+00 Z= 1.643286071050D+00
I= 34 X= 2.107024028520D+00 Y= -4.697260746786D+00 Z= 2.535913596467D+00
I= 35 X= 8.759117233674D-01 Y= -4.573075617922D-02 Z= -2.371305894839D-01
I= 36 X= 3.545137692508D+00 Y= 2.419483273356D+00 Z= 1.435017303069D+00

I= 37 X= 4.930895946112D+00 Y= 1.865716115566D+00 Z= 2.915125750783D+00

I= 38 X= 2.753423100855D+00 Y= 4.399064736892D+00 Z= 2.433282981215D+00

Forward Direction:

Total Energy: -651.6109624 Hartrees

Potential Energy: -651.7996927 Hartress

Kinetic Energy: 0.1887304 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.548976903449D+12 Y= 1.116958158816D+13 Z= 4.390079729190D+11

I= 1 X= -1.388036800197D+13 Y= 7.400623346845D+12 Z= -4.212752958806D+12

I= 2 X= 8.548989782182D+12 Y= 6.072422965463D+12 Z= 1.649230918765D+13

I= 3 X= 1.090964994716D+13 Y= -1.090121563575D+13 Z= -4.249516731650D+11

I= 4 X= 4.592436843427D+12 Y= 3.222434619524D+13 Z= -3.151886226663D+13

I= 5 X= -9.374339836229D+12 Y= 1.844532348931D+13 Z= 1.131932947937D+11

I= 6 X= -4.779995295000D+13 Y= -7.464789042422D+12 Z= 7.868806263653D+13

I= 7 X= 9.837429116641D+13 Y= -3.697964193702D+13 Z= -6.904076190831D+12

I= 8 X= -7.605844837259D+13 Y= -8.346137753325D+13 Z= -1.090828056255D+13

I= 9 X= -1.325973987938D+13 Y= -1.311042616092D+13 Z= -7.578349383928D+12

I= 10 X= 7.202374387153D+13 Y= 4.114645075810D+13 Z= 2.343783682353D+13

I= 11 X= 2.107411281749D+12 Y= 1.170832045157D+14 Z= 4.276626053997D+13

I= 12 X= 3.962762723606D+13 Y= 8.904477523161D+12 Z= 1.091274385993D+14

I= 13 X= -1.460313761184D+13 Y= -2.562423923119D+12 Z= -2.260771157825D+12

I= 14 X= 1.866135831279D+14 Y= -3.679005868805D+13 Z= -6.518194233771D+13

I= 15 X= 2.034368738007D+13 Y= -4.287465491547D+13 Z= -3.676746539571D+13

I= 16 X= 4.544209483478D+13 Y= -1.207573395795D+13 Z= -5.306912582090D+13

I= 17 X= -2.008825964427D+13 Y= 3.659163539203D+10 Z= 6.370801096719D+12

I= 18 X= 9.903167738407D+13 Y= -1.942084493974D+13 Z= 2.001198546667D+13

I= 19 X= 9.142616139170D+11 Y= -3.502760167431D+13 Z= -5.035172313928D+13

I= 20 X= 9.245727841969D+13 Y= -6.478504869543D+13 Z= -8.107627217430D+13

I= 21 X= -9.350433708613D+12 Y= -1.062051172090D+12 Z= 1.592758835341D+13

I= 22 X= 8.164311013169D+12 Y= -3.749945018226D+13 Z= -6.060910038586D+13

I= 23 X= 2.900090934333D+13 Y= 9.153022431833D+13 Z= -6.432847420916D+13
I= 24 X= -9.807535233297D+13 Y= -2.226004622729D+13 Z= -2.319007257052D+13
I= 25 X= 9.397021434887D+12 Y= -7.768491007024D+12 Z= -1.698881088405D+13
I= 26 X= -1.051746629430D+14 Y= 5.691966481333D+13 Z= -4.756431632766D+12
I= 27 X= -5.579401164401D+13 Y= -1.482254162158D+13 Z= 4.580061069166D+13
I= 28 X= 8.404378186782D+13 Y= 2.664480704031D+13 Z= -3.087077960751D+13
I= 29 X= 8.204119836524D+12 Y= 1.598831618130D+13 Z= -1.954102929564D+13
I= 30 X= 3.009918424401D+12 Y= 2.202697948074D+13 Z= 1.068126626170D+13
I= 31 X= 6.767465385094D+13 Y= -1.641727870838D+13 Z= 4.355805591056D+13
I= 32 X= -9.402202920632D+13 Y= -7.763703565139D+11 Z= 2.134556505163D+13
I= 33 X= 4.097665642841D+12 Y= -4.713530967634D+13 Z= 2.847719283651D+13
I= 34 X= -8.501968562521D+13 Y= -5.690220133475D+13 Z= 1.183089465107D+14
I= 35 X= 5.039004568245D+11 Y= -3.228683203288D+12 Z= 1.131682142889D+12
I= 36 X= 2.755319548373D+11 Y= -1.252326753249D+12 Z= 1.362307392739D+13
I= 37 X= 2.342222435631D+13 Y= -3.731776264095D+13 Z= -4.482029916999D+13
I= 38 X= -7.365408360308D+13 Y= -6.537811612441D+13 Z= 9.415011914304D+12

Backward Direction:

Total Energy: -651.6109655 Hartrees

Potential Energy: -651.7996927 Hartress

Kinetic Energy: 0.1887272 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.202040073462D+12 Y= 1.106751424746D+13 Z= 4.313832358568D+11
I= 1 X= -1.370742844177D+13 Y= 7.030464734724D+12 Z= -4.828340722078D+12
I= 2 X= 8.323908851119D+12 Y= 6.411605566097D+12 Z= 1.596210297321D+13
I= 3 X= 1.076833978693D+13 Y= -1.086996961050D+13 Z= -1.167835857696D+12
I= 4 X= 5.692519505931D+12 Y= 3.213477661710D+13 Z= -3.222350250459D+13
I= 5 X= -9.299127048311D+12 Y= 1.793132556987D+13 Z= -4.495589479584D+12
I= 6 X= -1.734372268516D+13 Y= 2.056176020709D+13 Z= 9.192405182961D+13
I= 7 X= 1.046266109156D+14 Y= -3.106998778199D+13 Z= -6.330653521311D+12
I= 8 X= -6.759067608044D+13 Y= -7.653226207610D+13 Z= -9.325136721955D+12

I= 9 X= -1.287520496692D+13 Y= -1.294425158991D+13 Z= -7.996752057030D+12
I= 10 X= 7.215263094588D+13 Y= 4.199276160872D+13 Z= 2.245692971895D+13
I= 11 X= 2.017624865389D+12 Y= 1.170893227029D+14 Z= 4.270497596653D+13
I= 12 X= 3.989156324001D+13 Y= 8.972679239938D+12 Z= 1.088749799828D+14
I= 13 X= -1.452910627062D+13 Y= -2.613491414736D+12 Z= -2.443938131455D+12
I= 14 X= 1.867185550773D+14 Y= -3.710423073985D+13 Z= -6.516366957225D+13
I= 15 X= 2.060087565875D+13 Y= -4.313375340701D+13 Z= -3.720355484111D+13
I= 16 X= 4.539212953439D+13 Y= -1.200561136090D+13 Z= -5.301782529336D+13
I= 17 X= -1.996373457970D+13 Y= -7.550303284120D+10 Z= 6.321699994184D+12
I= 18 X= 9.916410502403D+13 Y= -1.948906906320D+13 Z= 1.971948047323D+13
I= 19 X= 9.139836879107D+11 Y= -3.513608855067D+13 Z= -5.022803690717D+13
I= 20 X= 9.260410403366D+13 Y= -6.497053265524D+13 Z= -8.113678244759D+13
I= 21 X= -9.602104327196D+12 Y= -1.057783682413D+12 Z= 1.554396292421D+13
I= 22 X= 7.996744860838D+12 Y= -3.713506300731D+13 Z= -6.151724965220D+13
I= 23 X= 2.916045366557D+13 Y= 9.139039075670D+13 Z= -6.465008924588D+13
I= 24 X= -9.840771541782D+13 Y= -2.226963675097D+13 Z= -2.364275578680D+13
I= 25 X= 9.395247677192D+12 Y= -7.816199480626D+12 Z= -1.709534303771D+13
I= 26 X= -1.053679968544D+14 Y= 5.664550089233D+13 Z= -4.832755173227D+12
I= 27 X= -5.562472827229D+13 Y= -1.466520487168D+13 Z= 4.573850516834D+13
I= 28 X= 8.408381734876D+13 Y= 2.663833291897D+13 Z= -3.067562104069D+13
I= 29 X= 7.544320085257D+12 Y= 1.637788532067D+13 Z= -2.004702487954D+13
I= 30 X= 3.061308562767D+12 Y= 2.213786811863D+13 Z= 1.029222135576D+13
I= 31 X= 6.772696783931D+13 Y= -1.677694346586D+13 Z= 4.331695711721D+13
I= 32 X= -9.486104846258D+13 Y= -1.686040490025D+10 Z= 2.056187371940D+13
I= 33 X= 4.214031284438D+12 Y= -4.718684667975D+13 Z= 2.808078009849D+13
I= 34 X= -8.462597345379D+13 Y= -5.696176868145D+13 Z= 1.180541406682D+14
I= 35 X= 3.450957161520D+11 Y= -3.293311324496D+12 Z= 1.749475547487D+12
I= 36 X= -1.647046859648D+12 Y= -3.549635182955D+12 Z= 1.246999878279D+13
I= 37 X= 2.565649595445D+13 Y= -3.587860023400D+13 Z= -4.765843856055D+13
I= 38 X= -7.230102892248D+13 Y= -6.546943261556D+13 Z= 7.582135161456D+12

Seed: 21012156505

CM Start Point Coordinates: bohr

I= 0 X= -2.531556752771D+00 Y= 2.423350706040D+00 Z= -6.272395745899D-01
I= 1 X= -2.959295158787D+00 Y= 1.874022255406D-02 Z= -2.110184697310D+00
I= 2 X= -2.245563932022D+00 Y= 1.621985724971D+00 Z= 1.957873825705D+00
I= 3 X= -3.121090007353D+00 Y= -1.953178127555D+00 Z= -3.635728654777D-01
I= 4 X= -2.535963732956D+00 Y= -9.812682688050D-01 Z= 2.182094567466D+00
I= 5 X= 4.526903555765D+00 Y= 2.001753628900D+00 Z= -1.863610084490D+00
I= 6 X= 2.539819458158D+00 Y= -3.015042115326D-01 Z= -3.209989176339D+00
I= 7 X= 5.769544265626D+00 Y= 8.761928911835D-02 Z= -1.459953237473D+00
I= 8 X= 4.410852784942D+00 Y= 3.324915138673D+00 Z= -3.587078485245D+00
I= 9 X= -2.584054235125D+00 Y= -2.831028743356D+00 Z= 4.514395377515D+00
I= 10 X= -4.440490856191D+00 Y= -2.777214407796D+00 Z= 4.826833197077D+00
I= 11 X= -1.964403469054D+00 Y= -4.691366945513D+00 Z= 4.452821853807D+00
I= 12 X= -1.811065714747D+00 Y= -2.101027944607D+00 Z= 6.338341814238D+00
I= 13 X= -2.049312458690D+00 Y= 3.314895514651D+00 Z= 4.360678090724D+00
I= 14 X= -3.936167310915D+00 Y= 3.385403683915D+00 Z= 5.599082586726D+00
I= 15 X= -4.633809104296D-01 Y= 2.256787209757D+00 Z= 5.482808339434D+00
I= 16 X= -1.910664949682D+00 Y= 5.456550986302D+00 Z= 4.192348295117D+00
I= 17 X= -2.421793005698D+00 Y= 5.015237115348D+00 Z= -1.696756340351D+00
I= 18 X= -4.339006879362D+00 Y= 5.799222248692D+00 Z= -1.128033346388D+00
I= 19 X= -1.451235999546D+00 Y= 6.206589496878D+00 Z= -7.483161377055D-01
I= 20 X= -2.016389956518D+00 Y= 5.231985068991D+00 Z= -3.644107679174D+00
I= 21 X= -3.635584314737D+00 Y= -1.681387797190D-02 Z= -4.797617348649D+00
I= 22 X= -5.626282369839D+00 Y= 2.710415197040D-02 Z= -5.283733404902D+00
I= 23 X= -2.716628116461D+00 Y= 1.869699994621D+00 Z= -5.641543552824D+00
I= 24 X= -2.814466744943D+00 Y= -1.841661500359D+00 Z= -5.878752215199D+00
I= 25 X= -3.617665463694D+00 Y= -4.758243095325D+00 Z= -7.317350232951D-01
I= 26 X= -3.073277251255D+00 Y= -5.370960737544D+00 Z= -2.892530271910D+00

I= 27 X= -2.408850528662D+00 Y= -6.309403439740D+00 Z= 5.532186750247D-02
I= 28 X= -5.324955534068D+00 Y= -5.434726830387D+00 Z= -7.446665747278D-01
I= 29 X= 2.821245973320D+00 Y= -3.630531629642D+00 Z= -8.669424269303D-01
I= 30 X= 3.708974878948D+00 Y= -2.799236888665D+00 Z= 1.606437628375D+00
I= 31 X= 1.633058423310D+00 Y= -5.230103071046D+00 Z= -7.746285375795D-01
I= 32 X= 4.156409584765D+00 Y= -3.599937223387D+00 Z= -2.717576295921D+00
I= 33 X= 5.486252897786D+00 Y= -2.053336576667D+00 Z= 2.049907338277D+00
I= 34 X= 3.429134002214D+00 Y= -3.796141073222D+00 Z= 3.328632979045D+00
I= 35 X= 8.589089058851D-01 Y= -1.992464132988D-02 Z= -1.466097391212D-01
I= 36 X= 3.631203322349D+00 Y= 3.101241137725D+00 Z= 6.673689254150D-01
I= 37 X= 4.828351664993D+00 Y= 2.622052105999D+00 Z= 2.278953457241D+00
I= 38 X= 2.542907781903D+00 Y= 4.780578896027D+00 Z= 6.101048172257D-01

Forward Direction:

Total Energy: -651.6113753 Hartrees

Potential Energy: -651.7602713 Hartress

Kinetic Energy: 0.1488960 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.310855863461D+13 Y= -2.046184522244D+12 Z= 9.430424007541D+11
I= 1 X= -1.542191024003D+13 Y= -5.228949322935D+12 Z= 9.763821299243D+12
I= 2 X= 5.778391007372D+12 Y= 1.238148233445D+13 Z= -9.413969425674D+12
I= 3 X= 8.296648710990D+11 Y= -2.190887830523D+13 Z= -2.266872661133D+13
I= 4 X= 2.257824895439D+12 Y= 1.119830146763D+13 Z= 4.293484927566D+12
I= 5 X= 5.468773574377D+12 Y= 1.013017279324D+13 Z= -1.870995555262D+12
I= 6 X= -5.712435647646D+13 Y= -7.463892201420D+12 Z= 7.995284975627D+12
I= 7 X= 1.486270125521D+13 Y= -1.681898680999D+13 Z= 5.794947178482D+13
I= 8 X= 7.117466225461D+13 Y= -7.606323098112D+13 Z= 9.274616778913D+13
I= 9 X= 9.987216347495D+12 Y= -1.593378488003D+13 Z= 9.258192573293D+12
I= 10 X= -7.252079579188D+12 Y= 6.522989020664D+13 Z= 3.135943858498D+13
I= 11 X= 6.804230228417D+13 Y= 4.898487318096D+13 Z= -4.987716368766D+13
I= 12 X= -3.348793184699D+13 Y= -1.309297299625D+14 Z= -2.377049351479D+13

I= 13 X= -7.412641298150D+12 Y= 1.884377353573D+12 Z= -1.936803354271D+12
I= 14 X= -3.056230106374D+12 Y= -1.419259241035D+13 Z= 6.356726992922D+11
I= 15 X= 1.235008914581D+14 Y= 1.262039551423D+13 Z= 5.533795240606D+13
I= 16 X= 1.401366871465D+13 Y= -2.739245940415D+13 Z= 3.012511129862D+13
I= 17 X= 5.699039475542D+12 Y= 3.006916755461D+12 Z= 1.347833788344D+13
I= 18 X= 4.225784186083D+13 Y= -1.252887892032D+12 Z= -3.371838147887D+13
I= 19 X= 8.726613554719D+12 Y= -1.555410716049D+13 Z= -5.656665671307D+13
I= 20 X= 6.659342259389D+13 Y= 7.564923140084D+12 Z= -9.140628703726D+13
I= 21 X= 5.321027508538D+12 Y= -1.925113229676D+13 Z= -4.187006863131D+12
I= 22 X= -9.097874521893D+13 Y= 1.716420795616D+13 Z= -6.040735089910D+12
I= 23 X= 4.264329367345D+13 Y= 5.734228835911D+13 Z= -9.101408796076D+13
I= 24 X= -9.426808764300D+11 Y= 2.410980487421D+13 Z= 2.683160936264D+13
I= 25 X= -3.211824289794D+13 Y= -1.886707306941D+13 Z= 8.007039131671D+12
I= 26 X= 3.823940222726D+13 Y= 5.084372726746D+13 Z= 5.737987217059D+12
I= 27 X= 1.089550573080D+13 Y= -1.378543364214D+12 Z= -4.086821127177D+13
I= 28 X= 3.425806988654D+13 Y= 1.937327014285D+13 Z= 4.747115766513D+13
I= 29 X= -7.049471353824D+12 Y= -5.851717713041D+12 Z= 1.706986239630D+13
I= 30 X= 1.910448235716D+13 Y= 1.582240204786D+13 Z= 7.499216382745D+12
I= 31 X= -8.231194727797D+13 Y= 5.684818946442D+13 Z= -1.901462025364D+13
I= 32 X= 1.744931019436D+14 Y= 1.276714756505D+13 Z= -2.426731816378D+13
I= 33 X= -3.922390663206D+13 Y= -1.842329210308D+13 Z= -7.905587080878D+13
I= 34 X= -1.219371936951D+13 Y= 2.008665203023D+12 Z= -2.072971769996D+13
I= 35 X= -5.859147025938D+11 Y= 2.356058524522D+12 Z= -5.568632859176D+11
I= 36 X= -6.635095792587D+12 Y= -9.750907721714D+12 Z= -1.444132037377D+13
I= 37 X= -3.944443733118D+13 Y= 1.988361679403D+13 Z= 9.632354891662D+13
I= 38 X= 9.354723211142D+13 Y= -7.532711468609D+12 Z= 2.377481067991D+12

Backward Direction:

Total Energy: -651.6113692 Hartrees

Potential Energy: -651.7602713 Hartress

Kinetic Energy: 0.1489021 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.340619928972D+13 Y= -2.133749137215D+12 Z= 9.365010608900D+11
I= 1 X= -1.527354362158D+13 Y= -5.546512182735D+12 Z= 9.235702259418D+12
I= 2 X= 5.585291772640D+12 Y= 1.267247055734D+13 Z= -9.868838759938D+12
I= 3 X= 7.084334410479D+11 Y= -2.188207201968D+13 Z= -2.330605455298D+13
I= 4 X= 3.201597062964D+12 Y= 1.112145881095D+13 Z= 3.688966860697D+12
I= 5 X= 5.533299395646D+12 Y= 9.689208719324D+12 Z= -5.824917442637D+12
I= 6 X= -3.099564499348D+13 Y= 1.658037108444D+13 Z= 1.935057549617D+13
I= 7 X= 2.022663032397D+13 Y= -1.174903406297D+13 Z= 5.844141695724D+13
I= 8 X= 7.843925072134D+13 Y= -7.011867195301D+13 Z= 9.410436308359D+13
I= 9 X= 1.031711278536D+13 Y= -1.579122201616D+13 Z= 8.899240640137D+12
I= 10 X= -7.141506041687D+12 Y= 6.595594894264D+13 Z= 3.051790834259D+13
I= 11 X= 6.796527359976D+13 Y= 4.899012203448D+13 Z= -4.992974034749D+13
I= 12 X= -3.326149845005D+13 Y= -1.308712190125D+14 Z= -2.398708034207D+13
I= 13 X= -7.349129058821D+12 Y= 1.840566031543D+12 Z= -2.093944174473D+12
I= 14 X= -2.966173604510D+12 Y= -1.446212382229D+13 Z= 6.513490848235D+11
I= 15 X= 1.237215358986D+14 Y= 1.239811226482D+13 Z= 5.496382681730D+13
I= 16 X= 1.397080297450D+13 Y= -2.733230051003D+13 Z= 3.016912254900D+13
I= 17 X= 5.805870801881D+12 Y= 2.910749595064D+12 Z= 1.343621354664D+13
I= 18 X= 4.237145288750D+13 Y= -1.311418064694D+12 Z= -3.396932451075D+13
I= 19 X= 8.726375117116D+12 Y= -1.564717916160D+13 Z= -5.646054502395D+13
I= 20 X= 6.671938579364D+13 Y= 7.405794556626D+12 Z= -9.145819941667D+13
I= 21 X= 5.105116708716D+12 Y= -1.924747117363D+13 Z= -4.516123042555D+12
I= 22 X= -9.112250193622D+13 Y= 1.747681944585D+13 Z= -6.819845635567D+12
I= 23 X= 4.278016838459D+13 Y= 5.722232371101D+13 Z= -9.129000479104D+13
I= 24 X= -1.227818572014D+12 Y= 2.410157706353D+13 Z= 2.644324780160D+13
I= 25 X= -3.211976462195D+13 Y= -1.890800265726D+13 Z= 7.915644107017D+12
I= 26 X= 3.807353908635D+13 Y= 5.060851923665D+13 Z= 5.672508475798D+12
I= 27 X= 1.104073567315D+13 Y= -1.243562555617D+12 Z= -4.092149223651D+13
I= 28 X= 3.429241673391D+13 Y= 1.936771592323D+13 Z= 4.763858619870D+13

I= 29 X= -7.615520310243D+12 Y= -5.517502364236D+12 Z= 1.663576360887D+13
I= 30 X= 1.914857048282D+13 Y= 1.591753454291D+13 Z= 7.165450777877D+12
I= 31 X= -8.226706657314D+13 Y= 5.653962938949D+13 Z= -1.922146137527D+13
I= 32 X= 1.737732987392D+14 Y= 1.341873891898D+13 Z= -2.493965497639D+13
I= 33 X= -3.912407535810D+13 Y= -1.846750622336D+13 Z= -7.939595735275D+13
I= 34 X= -1.185594967277D+13 Y= 1.957561768523D+12 Z= -2.094831823832D+13
I= 35 X= -7.221549138530D+11 Y= 2.300613398209D+12 Z= -2.685200457344D+10
I= 36 X= -8.284495821530D+12 Y= -1.172179212271D+13 Z= -1.543055533644D+13
I= 37 X= -3.752763287271D+13 Y= 2.111828894032D+13 Z= 9.388868010074D+13
I= 38 X= 9.470803156251D+13 Y= -7.611052825344D+12 Z= 8.050373512345D+11

Seed: 21165468539

CM Start Point Coordinates: bohr

I= 0 X= -2.433282876308D+00 Y= 2.400484115955D+00 Z= -4.690112422040D-01
I= 1 X= -3.072697415097D+00 Y= 4.121021105329D-02 Z= -1.924106807939D+00
I= 2 X= -2.324500064276D+00 Y= 1.729631428847D+00 Z= 2.148635644913D+00
I= 3 X= -3.232396252001D+00 Y= -1.922834690106D+00 Z= -3.448753343982D-01
I= 4 X= -2.495278183036D+00 Y= -1.050042892923D+00 Z= 2.127801141688D+00
I= 5 X= 4.273481126474D+00 Y= 2.294335689091D+00 Z= -1.691633695273D+00
I= 6 X= 2.803047445136D+00 Y= 4.459598310728D-01 Z= -2.976980346014D+00
I= 7 X= 5.728906754546D+00 Y= 9.964121088725D-01 Z= -1.880152892522D+00
I= 8 X= 3.953668023763D+00 Y= 3.696500514276D+00 Z= -3.123014424993D+00
I= 9 X= -2.491602842006D+00 Y= -2.675201503912D+00 Z= 4.660218439027D+00
I= 10 X= -4.293880627248D+00 Y= -2.164702117327D+00 Z= 5.521009541686D+00
I= 11 X= -2.478002894196D+00 Y= -4.908940869002D+00 Z= 4.048881978101D+00
I= 12 X= -9.864287856799D-01 Y= -2.596149195529D+00 Z= 5.937625120196D+00
I= 13 X= -1.914168219279D+00 Y= 3.492697758936D+00 Z= 4.445580079605D+00
I= 14 X= -3.991737345011D+00 Y= 3.890960329734D+00 Z= 4.910788945151D+00
I= 15 X= -8.428135042349D-01 Y= 2.389520635399D+00 Z= 6.036756520194D+00
I= 16 X= -8.964028605972D-01 Y= 5.451296473980D+00 Z= 4.308052724650D+00

I= 17 X= -2.150682855473D+00 Y= 5.004124889223D+00 Z= -1.526322040352D+00
I= 18 X= -4.141069559540D+00 Y= 5.581170780382D+00 Z= -1.808984652871D+00
I= 19 X= -1.071596884075D+00 Y= 6.181700421734D+00 Z= -1.525158823388D-02
I= 20 X= -1.430230297523D+00 Y= 4.900409364020D+00 Z= -3.760067283280D+00
I= 21 X= -3.639363635555D+00 Y= -7.986239497950D-02 Z= -4.735701610993D+00
I= 22 X= -5.742545911387D+00 Y= -1.042039770076D+00 Z= -4.971302822888D+00
I= 23 X= -3.300854592910D+00 Y= 1.879093662474D+00 Z= -5.663810422845D+00
I= 24 X= -2.164187568804D+00 Y= -1.824663190632D+00 Z= -5.758786636173D+00
I= 25 X= -3.741402124409D+00 Y= -4.713951444118D+00 Z= -8.224290699678D-01
I= 26 X= -3.770588729790D+00 Y= -5.159351647567D+00 Z= -2.894521579095D+00
I= 27 X= -2.371679888457D+00 Y= -6.113329832198D+00 Z= -9.290476370724D-03
I= 28 X= -5.634258116506D+00 Y= -5.074530858244D+00 Z= -2.363861134709D-01
I= 29 X= 3.374340189029D+00 Y= -3.456322721425D+00 Z= -7.307502429216D-01
I= 30 X= 3.371492827717D+00 Y= -2.695703590042D+00 Z= 1.847307249365D+00
I= 31 X= 1.645945205394D+00 Y= -4.953098690623D+00 Z= -1.097511572897D+00
I= 32 X= 4.864370292691D+00 Y= -3.358227071300D+00 Z= -2.169212289907D+00
I= 33 X= 5.198834522767D+00 Y= -2.136846084304D+00 Z= 2.592994900572D+00
I= 34 X= 2.135215724107D+00 Y= -3.748615319834D+00 Z= 3.231450814439D+00
I= 35 X= 8.691942118114D-01 Y= -9.544771113630D-02 Z= -2.614578673605D-01
I= 36 X= 3.362493701414D+00 Y= 3.185022736554D+00 Z= 9.165830455113D-01
I= 37 X= 4.508635475123D+00 Y= 2.422690285791D+00 Z= 2.562001719674D+00
I= 38 X= 1.998306420179D+00 Y= 5.021382546560D+00 Z= 8.237043780555D-01

Forward Direction:

Total Energy: -651.6190756 Hartrees

Potential Energy: -651.7992116 Hartress

Kinetic Energy: 0.1801360 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.821335398950D+12 Y= -1.042802069837D+13 Z= 4.750925129385D+12

I= 1 X= -1.630586851926D+13 Y= -1.917193671821D+13 Z= -1.566364398639D+13

I= 2 X= 2.080719338227D+13 Y= -4.258238629123D+12 Z= 2.534744136025D+13

I= 3 X= 3.197530807478D+12 Y= -1.803065940741D+13 Z= 1.297975096830D+13
I= 4 X= 1.002772237946D+13 Y= 1.774640465241D+13 Z= -8.801393598078D+12
I= 5 X= -2.448582110534D+13 Y= 6.391915666211D+12 Z= 7.183317985400D+12
I= 6 X= -4.142621452721D+13 Y= -1.640713189886D+13 Z= 5.645364549488D+13
I= 7 X= 9.909692849066D+13 Y= -4.499853768479D+13 Z= 2.904598732458D+12
I= 8 X= 6.692615636421D+13 Y= -1.769887424724D+13 Z= 2.940760418782D+13
I= 9 X= -4.915331123394D+12 Y= 1.115176684480D+11 Z= 1.720877489551D+13
I= 10 X= -6.868840331460D+13 Y= 2.966829098431D+13 Z= -2.240707792339D+13
I= 11 X= -3.654576171373D+13 Y= -4.236130402441D+13 Z= -7.882569407924D+13
I= 12 X= 5.968481030743D+13 Y= 1.530366502426D+13 Z= -6.253782617496D+13
I= 13 X= -2.464966921121D+13 Y= -6.996376125133D+11 Z= -2.466215196622D+13
I= 14 X= -5.982958939391D+13 Y= 5.973955565925D+13 Z= -7.730307121601D+12
I= 15 X= 1.026315565949D+14 Y= -1.079859985396D+14 Z= 9.243225325488D+13
I= 16 X= 1.495049504882D+13 Y= 4.680403963017D+13 Z= 5.975608057443D+13
I= 17 X= -5.485596379530D+12 Y= -3.324274704019D+12 Z= -1.576778655417D+12
I= 18 X= -5.732051683514D+13 Y= -1.001075858363D+13 Z= 2.726621345289D+13
I= 19 X= 5.266849706876D+13 Y= 2.850342074031D+13 Z= 8.192632788065D+12
I= 20 X= -5.026971419700D+12 Y= -7.961301828758D+13 Z= 2.704653318144D+13
I= 21 X= 1.423684223115D+13 Y= 4.298946785761D+12 Z= 1.212121242624D+13
I= 22 X= -4.577493489097D+13 Y= -7.025833546642D+12 Z= 3.335668891294D+13
I= 23 X= -7.455712524800D+10 Y= 1.897789173279D+13 Z= 3.817615692156D+13
I= 24 X= -3.894184490375D+13 Y= 1.858971569639D+13 Z= -8.763810890072D+12
I= 25 X= -9.284772364992D+11 Y= -1.134752997730D+13 Z= -1.917305468536D+13
I= 26 X= 5.343659332237D+13 Y= 6.699192691732D+13 Z= 9.486932862661D+13
I= 27 X= -7.610916073541D+13 Y= 1.232840225890D+14 Z= -7.539065653903D+13
I= 28 X= -7.699125502510D+13 Y= 1.943298685712D+13 Z= 1.177480658067D+14
I= 29 X= 7.194293775237D+12 Y= 1.415498276227D+13 Z= 1.872455771451D+13
I= 30 X= -4.941294709475D+12 Y= -1.816967613908D+13 Z= -1.830505415004D+13
I= 31 X= -1.803134446775D+13 Y= -1.240554088776D+13 Z= 2.101001355486D+13
I= 32 X= 7.301458879113D+13 Y= 2.810117998191D+13 Z= -2.709539849806D+13

I= 33 X= 5.460718293296D+13 Y= -6.836264153416D+12 Z= -1.416314695223D+12
I= 34 X= 1.341521798777D+14 Y= 8.258860172718D+13 Z= -9.607085856786D+13
I= 35 X= 6.806642110857D+11 Y= 1.110816315032D+12 Z= -1.701037900542D+12
I= 36 X= 2.053791771112D+12 Y= -3.560700781576D+11 Z= -1.873906264849D+12
I= 37 X= 9.105431490241D+13 Y= 4.697699929949D+13 Z= 6.842158076423D+13
I= 38 X= -1.467009193595D+13 Y= 6.067171409861D+13 Z= -6.946446709607D+13

Backward Direction:

Total Energy: -651.6190577 Hartrees

Potential Energy: -651.7992116 Hartress

Kinetic Energy: 0.1801539 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.014664238240D+12 Y= -1.048489721974D+13 Z= 4.746676283925D+12
I= 1 X= -1.620949880068D+13 Y= -1.937820578063D+13 Z= -1.600667723465D+13
I= 2 X= 2.068176814172D+13 Y= -4.069230794523D+12 Z= 2.505198656143D+13
I= 3 X= 3.118786418001D+12 Y= -1.801324771189D+13 Z= 1.256578241640D+13
I= 4 X= 1.064073802395D+13 Y= 1.769649244702D+13 Z= -9.194050898170D+12
I= 5 X= -2.444390914801D+13 Y= 6.105492855178D+12 Z= 4.615096485734D+12
I= 6 X= -2.445463024540D+13 Y= -7.894753943232D+11 Z= 6.382933526898D+13
I= 7 X= 1.025810028715D+14 Y= -4.170541202364D+13 Z= 3.224135689011D+12
I= 8 X= 7.164478076217D+13 Y= -1.383765879404D+13 Z= 3.028980329298D+13
I= 9 X= -4.701050941581D+12 Y= 2.041176289120D+11 Z= 1.697562206679D+13
I= 10 X= -6.861658163378D+13 Y= 3.013989353446D+13 Z= -2.295368357121D+13
I= 11 X= -3.659579475323D+13 Y= -4.235789469460D+13 Z= -7.885984460837D+13
I= 12 X= 5.983188734193D+13 Y= 1.534167009332D+13 Z= -6.267850749699D+13
I= 13 X= -2.460841561147D+13 Y= -7.280947199429D+11 Z= -2.476422085570D+13
I= 14 X= -5.977109429330D+13 Y= 5.956448483315D+13 Z= -7.720124715014D+12
I= 15 X= 1.027748734898D+14 Y= -1.081303798984D+14 Z= 9.218924456668D+13
I= 16 X= 1.492265213405D+13 Y= 4.684311510222D+13 Z= 5.978466754942D+13
I= 17 X= -5.416205401258D+12 Y= -3.386738905513D+12 Z= -1.604140004445D+12
I= 18 X= -5.724672218715D+13 Y= -1.004877614106D+13 Z= 2.710321647843D+13

I= 19 X= 5.266834219418D+13 Y= 2.844296696610D+13 Z= 8.261556329652D+12
I= 20 X= -4.945153568106D+12 Y= -7.971637831397D+13 Z= 2.701281412791D+13
I= 21 X= 1.409660001735D+13 Y= 4.301324819522D+12 Z= 1.190743904694D+13
I= 22 X= -4.586831030473D+13 Y= -6.822780578013D+12 Z= 3.285062720881D+13
I= 23 X= 1.434817613645D+10 Y= 1.889997015136D+13 Z= 3.799693852089D+13
I= 24 X= -3.912705261023D+13 Y= 1.858437141094D+13 Z= -9.016066371874D+12
I= 25 X= -9.294656504825D+11 Y= -1.137411528852D+13 Z= -1.923241920730D+13
I= 26 X= 5.332885895084D+13 Y= 6.683915043063D+13 Z= 9.482679770759D+13
I= 27 X= -7.601482840070D+13 Y= 1.233716977167D+14 Z= -7.542526454823D+13
I= 28 X= -7.696894544598D+13 Y= 1.942937918214D+13 Z= 1.178568169553D+14
I= 29 X= 6.826623614532D+12 Y= 1.437206824711D+13 Z= 1.844259416768D+13
I= 30 X= -4.912657807955D+12 Y= -1.810788399135D+13 Z= -1.852184750783D+13
I= 31 X= -1.800219275272D+13 Y= -1.260596230174D+13 Z= 2.087566244000D+13
I= 32 X= 7.254704944523D+13 Y= 2.852441316185D+13 Z= -2.753210663293D+13
I= 33 X= 5.467202711407D+13 Y= -6.864982893809D+12 Z= -1.637213740537D+12
I= 34 X= 1.343715740462D+14 Y= 8.255540811797D+13 Z= -9.621284786889D+13
I= 35 X= 5.921710515211D+11 Y= 1.074802612919D+12 Z= -1.356775569168D+12
I= 36 X= 9.824441985840D+11 Y= -1.636233884620D+12 Z= -2.516451710295D+12
I= 37 X= 9.229935174401D+13 Y= 4.777896545878D+13 Z= 6.684004156708D+13
I= 38 X= -1.391610888128D+13 Y= 6.062082843303D+13 Z= -7.048582864079D+13

Seed: 2121407000

CM Start Point Coordinates: bohr

I= 0 X= -2.575018813635D+00 Y= 2.314431329748D+00 Z= -5.586824937271D-01
I= 1 X= -3.064610472457D+00 Y= 7.125618416945D-02 Z= -1.875344626274D+00
I= 2 X= -2.378476336670D+00 Y= 1.631458282776D+00 Z= 2.174579514907D+00
I= 3 X= -3.054322968994D+00 Y= -2.003914331578D+00 Z= -2.540223446793D-01
I= 4 X= -2.594850533538D+00 Y= -1.030637417339D+00 Z= 2.241077507813D+00
I= 5 X= 3.899283426669D+00 Y= 2.694915995695D+00 Z= -1.494311553473D+00
I= 6 X= 2.179019877187D+00 Y= 1.042911047744D+00 Z= -2.748106730790D+00

I= 7 X= 5.409521373216D+00 Y= 1.594624089392D+00 Z= -2.370307317656D+00
I= 8 X= 3.314560643668D+00 Y= 4.192861216971D+00 Z= -2.373951415572D+00
I= 9 X= -2.502438794512D+00 Y= -2.271982785526D+00 Z= 4.718653467583D+00
I= 10 X= -4.187995597286D+00 Y= -1.533630839011D+00 Z= 5.929607787765D+00
I= 11 X= -3.006504725318D+00 Y= -4.782985248481D+00 Z= 4.475891072724D+00
I= 12 X= -6.178346268845D-01 Y= -2.185207690444D+00 Z= 5.767503199893D+00
I= 13 X= -2.039186868885D+00 Y= 3.749445583528D+00 Z= 4.161531856324D+00
I= 14 X= -4.151556871863D+00 Y= 4.175782875469D+00 Z= 4.894593158864D+00
I= 15 X= -1.052706161627D+00 Y= 3.468837774069D+00 Z= 6.143618505103D+00
I= 16 X= -1.463610124736D+00 Y= 5.418736202444D+00 Z= 3.241393367401D+00
I= 17 X= -2.405198360671D+00 Y= 4.796649694409D+00 Z= -1.719003956976D+00
I= 18 X= -4.485626657097D+00 Y= 5.751965912799D+00 Z= -2.106783863781D+00
I= 19 X= -1.460240345147D+00 Y= 6.328903849769D+00 Z= -5.516088337285D-01
I= 20 X= -1.447717680979D+00 Y= 5.067023794590D+00 Z= -3.445953517148D+00
I= 21 X= -3.756414336237D+00 Y= -1.629916542705D-01 Z= -4.782158713912D+00
I= 22 X= -5.678104727199D+00 Y= 8.684268826951D-01 Z= -5.233728685696D+00
I= 23 X= -2.231861424965D+00 Y= 1.090877758405D+00 Z= -5.347962456863D+00
I= 24 X= -3.945697996108D+00 Y= -2.339148013639D+00 Z= -5.174794696895D+00
I= 25 X= -3.566358503363D+00 Y= -4.783691368441D+00 Z= -1.020381768330D+00
I= 26 X= -2.902642043783D+00 Y= -4.965509414019D+00 Z= -2.908926946894D+00
I= 27 X= -3.070671232134D+00 Y= -6.076796788482D+00 Z= 5.046827193009D-01
I= 28 X= -5.655725058229D+00 Y= -5.066212093785D+00 Z= -9.366468501716D-01
I= 29 X= 3.190551694298D+00 Y= -3.384401210233D+00 Z= -1.078471533577D+00
I= 30 X= 3.327673874850D+00 Y= -2.994001666506D+00 Z= 1.551791606948D+00
I= 31 X= 2.079867683321D+00 Y= -4.755740278997D+00 Z= -1.894168748966D+00
I= 32 X= 4.467970721847D+00 Y= -3.125417553704D+00 Z= -2.626915484414D+00
I= 33 X= 4.973936439359D+00 Y= -2.341692490049D+00 Z= 2.383376816535D+00
I= 34 X= 2.232439480650D+00 Y= -4.561690536521D+00 Z= 2.796531823198D+00
I= 35 X= 9.214313338983D-01 Y= -9.186088176572D-02 Z= -2.129425707929D-01
I= 36 X= 3.775019598440D+00 Y= 2.600608108962D+00 Z= 1.134861178929D+00

I= 37 X= 4.995261343939D+00 Y= 1.589262090439D+00 Z= 2.295296974292D+00

I= 38 X= 2.935583869029D+00 Y= 4.120566224731D+00 Z= 1.955167900929D+00

Forward Direction:

Total Energy: -651.6170802 Hartrees

Potential Energy: -651.8038407 Hartress

Kinetic Energy: 0.1867605 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.826511792579D+13 Y= -3.439883956101D+12 Z= -2.596339526145D+13

I= 1 X= -1.345913153092D+13 Y= 6.701616503149D+12 Z= 1.031466772189D+12

I= 2 X= 1.341319937161D+13 Y= -1.486331527186D+13 Z= -1.314307972153D+13

I= 3 X= -2.555063474272D+12 Y= 1.527263770500D+11 Z= -1.234043463553D+13

I= 4 X= -5.127649720367D+12 Y= -2.654705163435D+13 Z= 7.033483342196D+12

I= 5 X= 2.571096371030D+12 Y= -1.070756931258D+13 Z= 9.848646082202D+12

I= 6 X= -6.234318333314D+13 Y= -2.843289133087D+13 Z= 6.428103957898D+13

I= 7 X= 1.005611350060D+14 Y= 7.175751702320D+12 Z= -3.880586239198D+12

I= 8 X= -2.517073296240D+13 Y= -5.681418525495D+12 Z= 3.346376026880D+13

I= 9 X= 1.863264001033D+13 Y= 4.793608621023D+12 Z= -1.491870200664D+12

I= 10 X= -1.089807773663D+14 Y= -8.447091242908D+11 Z= 2.005215937260D+13

I= 11 X= -2.020359672294D+13 Y= -3.446198653384D+11 Z= 3.568147838916D+13

I= 12 X= 2.658093650266D+12 Y= -3.010420398858D+13 Z= -7.768417781793D+13

I= 13 X= 1.514782416826D+12 Y= 7.039398011569D+12 Z= -1.027401480067D+13

I= 14 X= -1.025054747787D+14 Y= 1.320621763397D+14 Z= -1.570883919660D+13

I= 15 X= 8.571714146732D+13 Y= -8.805539533226D+13 Z= 3.904647006220D+13

I= 16 X= -8.239164972207D+13 Y= 5.661746095393D+13 Z= 6.844308769789D+13

I= 17 X= -1.835924733493D+13 Y= 3.400656228883D+12 Z= -1.715242316658D+13

I= 18 X= 5.737786265329D+13 Y= -2.160127214172D+13 Z= -5.042396207956D+13

I= 19 X= -2.440833205052D+13 Y= 1.179482751379D+13 Z= -1.295370253239D+13

I= 20 X= -3.408651437681D+13 Y= 1.452261564297D+13 Z= 8.180473287300D+13

I= 21 X= -1.652016518213D+13 Y= 2.472115541669D+13 Z= 2.796808135418D+13

I= 22 X= 3.302558270409D+13 Y= -1.811122845233D+13 Z= -8.916436525297D+13

I= 23 X= 1.730988468843D+12 Y= -2.108756958369D+12 Z= -2.642487903997D+13
I= 24 X= 4.696143638312D+13 Y= -8.958541744054D+13 Z= -4.571681470335D+13
I= 25 X= -1.280234130299D+13 Y= -1.111293181118D+12 Z= 3.068672736448D+13
I= 26 X= -9.643392356311D+12 Y= 3.461391502874D+13 Z= 2.363890884493D+13
I= 27 X= -5.974450328430D+13 Y= 2.870772799218D+13 Z= -3.995914921921D+13
I= 28 X= 2.826622745598D+13 Y= 4.827171216233D+13 Z= 1.417507333922D+13
I= 29 X= 1.341138728081D+12 Y= 5.197353519974D+12 Z= 9.221647014671D+12
I= 30 X= 3.077777223602D+13 Y= 4.314542275409D+12 Z= 8.844363946602D+12
I= 31 X= -1.655636424307D+13 Y= 1.411711071668D+13 Z= -1.836847134235D+12
I= 32 X= -1.262034990243D+14 Y= 7.807491876381D+12 Z= 9.238109098867D+13
I= 33 X= -1.816957449391D+14 Y= 1.091334525710D+13 Z= -4.061195636143D+13
I= 34 X= -2.460997710323D+13 Y= 1.790427177534D+13 Z= -7.707620486935D+13
I= 35 X= 1.087581503284D+12 Y= 6.444081659209D+11 Z= -1.816911194915D+11
I= 36 X= 1.862712012369D+13 Y= -1.293814485675D+13 Z= 2.975866698876D+12
I= 37 X= -1.489024150075D+13 Y= -5.880572883899D+13 Z= -9.630540239344D+13
I= 38 X= -1.035456695888D+14 Y= -6.017903675287D+12 Z= -6.576744116493D+13

Backward Direction:

Total Energy: -651.6170368 Hartrees

Potential Energy: -651.8038407 Hartress

Kinetic Energy: 0.1868039 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.773012584357D+13 Y= -3.597276353007D+12 Z= -2.597515294580D+13
I= 1 X= -1.319245100475D+13 Y= 6.130815393137D+12 Z= 8.220294941067D+10
I= 2 X= 1.306611452222D+13 Y= -1.434028055563D+13 Z= -1.396068137946D+13
I= 3 X= -2.772970050283D+12 Y= 2.009091447767D+11 Z= -1.348599522329D+13
I= 4 X= -3.431273130777D+12 Y= -2.668517192303D+13 Z= 5.946896630363D+12
I= 5 X= 2.687077848903D+12 Y= -1.150017705664D+13 Z= 2.741697235590D+12
I= 6 X= -1.537831623914D+13 Y= 1.478529914029D+13 Z= 8.469152596901D+13
I= 7 X= 1.102024912573D+14 Y= 1.628870230453D+13 Z= -2.996342880313D+12
I= 8 X= -1.211304996037D+13 Y= 5.003586930374D+12 Z= 3.590503876632D+13

I= 9 X= 1.922561001647D+13 Y= 5.049857230601D+12 Z= -2.137065805718D+12
I= 10 X= -1.087820277470D+14 Y= 4.603399970043D+11 Z= 1.853955682140D+13
I= 11 X= -2.034205138325D+13 Y= -3.351853479011D+11 Z= 3.558697484222D+13
I= 12 X= 3.065094757907D+12 Y= -2.999903389088D+13 Z= -7.807348028414D+13
I= 13 X= 1.628942044952D+12 Y= 6.960649661442D+12 Z= -1.055646645400D+13
I= 14 X= -1.023436033492D+14 Y= 1.315777090154D+14 Z= -1.568066178655D+13
I= 15 X= 8.611373726043D+13 Y= -8.845493677411D+13 Z= 3.837400067415D+13
I= 16 X= -8.246869844025D+13 Y= 5.672559312935D+13 Z= 6.852219540488D+13
I= 17 X= -1.816722412312D+13 Y= 3.227801248331D+12 Z= -1.722813925578D+13
I= 18 X= 5.758207198818D+13 Y= -2.170647678604D+13 Z= -5.087501783921D+13
I= 19 X= -2.440876062706D+13 Y= 1.162753590898D+13 Z= -1.276297283070D+13
I= 20 X= -3.386010271922D+13 Y= 1.423659109761D+13 Z= 8.171142333393D+13
I= 21 X= -1.690825251709D+13 Y= 2.472773607547D+13 Z= 2.737651381012D+13
I= 22 X= 3.276718821276D+13 Y= -1.754932713897D+13 Z= -9.056477197719D+13
I= 23 X= 1.977012952472D+12 Y= -2.324386569108D+12 Z= -2.692082379444D+13
I= 24 X= 4.644891765162D+13 Y= -8.960020646382D+13 Z= -4.641487243453D+13
I= 25 X= -1.280507651708D+13 Y= -1.184861778470D+12 Z= 3.052245002694D+13
I= 26 X= -9.941521883371D+12 Y= 3.419114202098D+13 Z= 2.352121454949D+13
I= 27 X= -5.948346076311D+13 Y= 2.895034829066D+13 Z= -4.005491870419D+13
I= 28 X= 2.832796395083D+13 Y= 4.826172877152D+13 Z= 1.447601655922D+13
I= 29 X= 3.236980502057D+11 Y= 5.798086530315D+12 Z= 8.441379226829D+12
I= 30 X= 3.085701812633D+13 Y= 4.485537506034D+12 Z= 8.244439326515D+12
I= 31 X= -1.647569373454D+13 Y= 1.356249159958D+13 Z= -2.208632242078D+12
I= 32 X= -1.274973041827D+14 Y= 8.978690141283D+12 Z= 9.117260395612D+13
I= 33 X= -1.815163039228D+14 Y= 1.083387290039D+13 Z= -4.122324250558D+13
I= 34 X= -2.400285535217D+13 Y= 1.781241626842D+13 Z= -7.746912685679D+13
I= 35 X= 8.426975018700D+11 Y= 5.447487165257D+11 Z= 7.709738984808D+11
I= 36 X= 1.566241773911D+13 Y= -1.648069704145D+13 Z= 1.197773333006D+12
I= 37 X= -1.144489492524D+13 Y= -5.658647614678D+13 Z= -1.006819400722D+14
I= 38 X= -1.014591988533D+14 Y= -6.158717791585D+12 Z= -6.859381896965D+13

Seed: 21461384799

CM Start Point Coordinates: bohr

I= 0 X= -2.579625063413D+00 Y= 2.405489850422D+00 Z= -5.565980574755D-01
I= 1 X= -3.001159794731D+00 Y= -1.253341462140D-02 Z= -1.978989136105D+00
I= 2 X= -2.302561284505D+00 Y= 1.756234366773D+00 Z= 1.971142484641D+00
I= 3 X= -3.042888555117D+00 Y= -1.912717587479D+00 Z= -1.431666963055D-01
I= 4 X= -2.370899526888D+00 Y= -8.467115698079D-01 Z= 2.276273915758D+00
I= 5 X= 3.941930173731D+00 Y= 2.390308632447D+00 Z= -1.381512121381D+00
I= 6 X= 2.223970600994D+00 Y= 7.250505085226D-01 Z= -2.712106988419D+00
I= 7 X= 5.307344798403D+00 Y= 1.005459567031D+00 Z= -2.127513026235D+00
I= 8 X= 3.484875977456D+00 Y= 4.240008515147D+00 Z= -2.676370172851D+00
I= 9 X= -2.521996557563D+00 Y= -2.480701466243D+00 Z= 4.600316415153D+00
I= 10 X= -4.400449072310D+00 Y= -2.658950087725D+00 Z= 5.264126815638D+00
I= 11 X= -1.672427836646D+00 Y= -4.248241291605D+00 Z= 4.006809914501D+00
I= 12 X= -1.566999383031D+00 Y= -1.569499308300D+00 Z= 5.967651078231D+00
I= 13 X= -1.835212504438D+00 Y= 3.373968654314D+00 Z= 4.147209414281D+00
I= 14 X= -3.623452365564D+00 Y= 4.256848691180D+00 Z= 4.941827501398D+00
I= 15 X= -7.009357624123D-01 Y= 1.789242867255D+00 Z= 5.436494676790D+00
I= 16 X= -8.896890426296D-01 Y= 5.164307088779D+00 Z= 3.560397359385D+00
I= 17 X= -2.508466791175D+00 Y= 4.828721645624D+00 Z= -1.979335243385D+00
I= 18 X= -4.215159411211D+00 Y= 5.880735169152D+00 Z= -2.306469442366D+00
I= 19 X= -1.246001931565D+00 Y= 6.019521002382D+00 Z= -1.066066290082D+00
I= 20 X= -2.064277899586D+00 Y= 4.582631175362D+00 Z= -4.054209308698D+00
I= 21 X= -3.663853456342D+00 Y= -2.396826794336D-01 Z= -4.760390835972D+00
I= 22 X= -5.464112659403D+00 Y= -9.050260802123D-01 Z= -5.235256683930D+00
I= 23 X= -3.458910725579D+00 Y= 1.840626424043D+00 Z= -5.518326422995D+00
I= 24 X= -1.999688509675D+00 Y= -1.624757588723D+00 Z= -5.656692389440D+00
I= 25 X= -3.693471294259D+00 Y= -4.536302780747D+00 Z= -8.132564921101D-01
I= 26 X= -3.719947344114D+00 Y= -4.921487684132D+00 Z= -3.210697848289D+00

I= 27 X= -2.330174496881D+00 Y= -6.061984661512D+00 Z= 1.734610118757D-01
I= 28 X= -5.547869087609D+00 Y= -4.800616714371D+00 Z= 4.090186722399D-02
I= 29 X= 3.309843519678D+00 Y= -3.393168245457D+00 Z= -1.055882871166D+00
I= 30 X= 3.666384590797D+00 Y= -2.922504004840D+00 Z= 1.349685204129D+00
I= 31 X= 1.686303367346D+00 Y= -4.938025159591D+00 Z= -1.295265509277D+00
I= 32 X= 4.461084248484D+00 Y= -3.076117049900D+00 Z= -2.528853323335D+00
I= 33 X= 5.407243943995D+00 Y= -2.010605388063D+00 Z= 2.078538412186D+00
I= 34 X= 2.767245124550D+00 Y= -3.969193488997D+00 Z= 3.070034038572D+00
I= 35 X= 8.529445252094D-01 Y= -4.634521275534D-02 Z= -1.941458829279D-01
I= 36 X= 3.673906500427D+00 Y= 2.290628919023D+00 Z= 1.348399506442D+00
I= 37 X= 5.032955422373D+00 Y= 1.762639653636D+00 Z= 2.670808024614D+00
I= 38 X= 3.152295889211D+00 Y= 4.043875765872D+00 Z= 2.343928115684D+00

Forward Direction:

Total Energy: -651.6131081 Hartrees

Potential Energy: -651.7985760 Hartress

Kinetic Energy: 0.1854679 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.398996535101D+12 Y= 9.803999971482D+12 Z= -2.334956929313D+13
I= 1 X= -4.387113370802D+12 Y= 1.653345267105D+12 Z= -1.109048613944D+13
I= 2 X= -5.792481208857D+12 Y= -6.655297776441D+12 Z= 2.851182408302D+13
I= 3 X= 9.886013090015D+12 Y= -1.891370494115D+13 Z= 2.720181825913D+13
I= 4 X= 4.413624755000D+12 Y= 6.241211244545D+12 Z= -1.614394511057D+13
I= 5 X= -9.752722204279D+12 Y= -3.582385790074D+12 Z= 2.785774449633D+12
I= 6 X= 5.983038736516D+12 Y= -7.640130165925D+13 Z= 7.948356319538D+13
I= 7 X= 3.353779597605D+13 Y= -6.084750409913D+13 Z= -7.436367523844D+13
I= 8 X= -6.793495804116D+13 Y= 1.868499818403D+13 Z= 1.276782265451D+13
I= 9 X= -1.261348201598D+13 Y= 4.024466400743D+13 Z= -1.495936229493D+13
I= 10 X= 6.249216404159D+11 Y= -6.865383052037D+13 Z= 6.005250461652D+13
I= 11 X= -4.686370449733D+13 Y= -3.411024386498D+13 Z= -4.903849890900D+13
I= 12 X= -2.248123032082D+13 Y= 1.423696937474D+13 Z= -6.027838584301D+13

I= 13 X= 1.348826553778D+13 Y= -1.371354063611D+13 Z= 7.314047438571D+12
I= 14 X= -1.390113976628D+14 Y= 6.509996252776D+13 Z= 3.025618431185D+13
I= 15 X= -7.501740304503D+13 Y= 4.062516922050D+13 Z= -6.127415379237D+13
I= 16 X= 6.789630081883D+13 Y= 3.586100134517D+13 Z= -3.320890568036D+13
I= 17 X= -6.788920638540D+12 Y= 5.525868258012D+12 Z= 1.750876953763D+13
I= 18 X= -5.386342919366D+12 Y= -5.832145934672D+13 Z= -6.790108177089D+13
I= 19 X= 5.740958566806D+13 Y= 6.212562756822D+13 Z= -1.333433060661D+13
I= 20 X= 3.462901672214D+13 Y= 8.693351741875D+12 Z= -1.521678025597D+14
I= 21 X= -1.556277251378D+13 Y= 1.407501534071D+12 Z= -1.971787326615D+12
I= 22 X= 5.247401551350D+13 Y= 2.393675711690D+13 Z= 1.192418437276D+14
I= 23 X= 1.255643145621D+13 Y= -8.826386075811D+13 Z= 2.124524510087D+13
I= 24 X= 5.745470629045D+13 Y= -9.668574941608D+13 Z= -1.716098205077D+13
I= 25 X= -2.026968715635D+11 Y= 9.427561397492D+12 Z= -1.626466734093D+13
I= 26 X= -7.860497877810D+11 Y= -4.875158107048D+13 Z= 5.735824206000D+13
I= 27 X= -4.091061125655D+13 Y= -9.362444688671D+11 Z= 2.378432239292D+13
I= 28 X= 5.216408521091D+13 Y= -3.008083376763D+13 Z= 4.660275468922D+13
I= 29 X= 6.768349515643D+12 Y= 7.419827278497D+12 Z= -2.536614972545D+12
I= 30 X= -7.956513967695D+12 Y= 1.007444643595D+12 Z= 5.124097378757D+12
I= 31 X= 1.437595601290D+14 Y= -1.759406112504D+12 Z= -2.706613820452D+12
I= 32 X= -9.118888676130D+13 Y= -2.379528951790D+13 Z= 2.444990287393D+13
I= 33 X= 3.103229472327D+13 Y= 3.983627191208D+13 Z= -9.301579446190D+11
I= 34 X= 4.552989561369D+13 Y= 5.323355489989D+13 Z= -1.259144038871D+14
I= 35 X= 1.572080617373D+12 Y= -2.643389830943D+12 Z= 2.014225837512D+12
I= 36 X= -1.528510173499D+13 Y= 1.704272830447D+13 Z= -1.016919763348D+13
I= 37 X= 8.685916331933D+12 Y= 5.111479113920D+13 Z= -9.641295541175D+13
I= 38 X= 7.762709926172D+13 Y= 3.667328876238D+12 Z= -1.048179151266D+13

Backward Direction:

Total Energy: -651.6131184 Hartrees

Potential Energy: -651.7985760 Hartress

Kinetic Energy: 0.1854576 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.097616117920D+12 Y= 9.715335135081D+12 Z= -2.335619282380D+13
I= 1 X= -4.236882572059D+12 Y= 1.331792328715D+12 Z= -1.162524083159D+13
I= 2 X= -5.988006673716D+12 Y= -6.360653377262D+12 Z= 2.805123945594D+13
I= 3 X= 9.763258423179D+12 Y= -1.888656184329D+13 Z= 2.655648248910D+13
I= 4 X= 5.369255128958D+12 Y= 6.163403083033D+12 Z= -1.675605876085D+13
I= 5 X= -9.687385639144D+12 Y= -4.028890438226D+12 Z= -1.217827238601D+12
I= 6 X= 3.244004938380D+13 Y= -5.205492965365D+13 Z= 9.098152942352D+13
I= 7 X= 3.896912114993D+13 Y= -5.571384896061D+13 Z= -7.386554892652D+13
I= 8 X= -6.057909227401D+13 Y= 2.470424875678D+13 Z= 1.414308325379D+13
I= 9 X= -1.227944053500D+13 Y= 4.038901813007D+13 Z= -1.532282434778D+13
I= 10 X= 7.368845008713D+11 Y= -6.791864908137D+13 Z= 5.920040081340D+13
I= 11 X= -4.694170102540D+13 Y= -3.410492906201D+13 Z= -4.909173617885D+13
I= 12 X= -2.225195185766D+13 Y= 1.429621549503D+13 Z= -6.049769402015D+13
I= 13 X= 1.355257579435D+13 Y= -1.375790243502D+13 Z= 7.154932192319D+12
I= 14 X= -1.389202096204D+14 Y= 6.482704453190D+13 Z= 3.027205767159D+13
I= 15 X= -7.479398626514D+13 Y= 4.040009305415D+13 Z= -6.165298015746D+13
I= 16 X= 6.785289648483D+13 Y= 3.592191611631D+13 Z= -3.316434144503D+13
I= 17 X= -6.680747008360D+12 Y= 5.428492787984D+12 Z= 1.746611592043D+13
I= 18 X= -5.271304403348D+12 Y= -5.838072492878D+13 Z= -6.815517781577D+13
I= 19 X= 5.740934424015D+13 Y= 6.203138614809D+13 Z= -1.322688566442D+13
I= 20 X= 3.475656260334D+13 Y= 8.532223755802D+12 Z= -1.522203672068D+14
I= 21 X= -1.578139616704D+13 Y= 1.411208658650D+12 Z= -2.305038748891D+12
I= 22 X= 5.232845253710D+13 Y= 2.425329648342D+13 Z= 1.184529438961D+14
I= 23 X= 1.269502596254D+13 Y= -8.838533272963D+13 Z= 2.096586145805D+13
I= 24 X= 5.716598592002D+13 Y= -9.669408060882D+13 Z= -1.755422325332D+13
I= 25 X= -2.042377178848D+11 Y= 9.386117541050D+12 Z= -1.635721071397D+13
I= 26 X= -9.539969453932D+11 Y= -4.898974441986D+13 Z= 5.729194059749D+13
I= 27 X= -4.076355655033D+13 Y= -7.995676664197D+11 Z= 2.373037197466D+13
I= 28 X= 5.219886361485D+13 Y= -3.008645777288D+13 Z= 4.677228690522D+13

I= 29 X= 6.195188331852D+12 Y= 7.758241940982D+12 Z= -2.976168076327D+12
I= 30 X= -7.911871887235D+12 Y= 1.103772451394D+12 Z= 4.786138113142D+12
I= 31 X= 1.438050047490D+14 Y= -2.071843148727D+12 Z= -2.916053835639D+12
I= 32 X= -9.191773406612D+13 Y= -2.313551111600D+13 Z= 2.376911835925D+13
I= 33 X= 3.113338034764D+13 Y= 3.979150225544D+13 Z= -1.274517568670D+12
I= 34 X= 4.587190928634D+13 Y= 5.318180936635D+13 Z= -1.261357510729D+14
I= 35 X= 1.434128590080D+12 Y= -2.699531608660D+12 Z= 2.550896546203D+12
I= 36 X= -1.695522596867D+13 Y= 1.504708035264D+13 Z= -1.117086202501D+13
I= 37 X= 1.062680484287D+13 Y= 5.236497656393D+13 Z= -9.887841759790D+13
I= 38 X= 7.880248379478D+13 Y= 3.588003187008D+12 Z= -1.207399249643D+13

Seed: 21530788848

CM Start Point Coordinates: bohr

I= 0 X= -2.724354249961D+00 Y= 2.360106087306D+00 Z= -5.394835343676D-01
I= 1 X= -2.899703273436D+00 Y= 6.194391974297D-02 Z= -1.943155810712D+00
I= 2 X= -2.417708964306D+00 Y= 1.697931697600D+00 Z= 2.067896170493D+00
I= 3 X= -2.915578013619D+00 Y= -1.832759859574D+00 Z= -2.203258942016D-01
I= 4 X= -2.383545269012D+00 Y= -9.823152551244D-01 Z= 2.386591886069D+00
I= 5 X= 4.143886723249D+00 Y= 2.362175194456D+00 Z= -1.196397364379D+00
I= 6 X= 2.727712437514D+00 Y= 8.151917340888D-01 Z= -2.990490112949D+00
I= 7 X= 5.972956719033D+00 Y= 1.242778302112D+00 Z= -1.774151743081D+00
I= 8 X= 3.487115355370D+00 Y= 4.148865449975D+00 Z= -2.093812516853D+00
I= 9 X= -2.445571491544D+00 Y= -2.058622158073D+00 Z= 5.109150079317D+00
I= 10 X= -4.197379103884D+00 Y= -7.725771093836D-01 Z= 5.797858801844D+00
I= 11 X= -2.656223865099D+00 Y= -4.068526991814D+00 Z= 5.368715060349D+00
I= 12 X= -7.063821324924D-01 Y= -1.419452847599D+00 Z= 6.088569363185D+00
I= 13 X= -2.349183132370D+00 Y= 3.599445284258D+00 Z= 4.121351297235D+00
I= 14 X= -4.318654533184D+00 Y= 4.329681309110D+00 Z= 4.541969107943D+00
I= 15 X= -1.667226503237D+00 Y= 2.757897898608D+00 Z= 6.130587073661D+00
I= 16 X= -1.113407536371D+00 Y= 5.534221575383D+00 Z= 3.646645475556D+00

I= 17 X= -2.508291809846D+00 Y= 4.968592617127D+00 Z= -1.740184614912D+00
I= 18 X= -4.526610212173D+00 Y= 5.602059545668D+00 Z= -2.346159913461D+00
I= 19 X= -2.013270582574D+00 Y= 6.683727928586D+00 Z= -2.385955784373D-01
I= 20 X= -8.913942831090D-01 Y= 4.938811764718D+00 Z= -3.658551717658D+00
I= 21 X= -3.479692445918D+00 Y= -2.177522230774D-01 Z= -4.675739926584D+00
I= 22 X= -5.320735184141D+00 Y= -2.767917817209D-01 Z= -4.706207711108D+00
I= 23 X= -3.001568747669D+00 Y= 1.417432058558D+00 Z= -5.957006996607D+00
I= 24 X= -2.676187292014D+00 Y= -2.226845643425D+00 Z= -4.730260113429D+00
I= 25 X= -3.504279843475D+00 Y= -4.678271250803D+00 Z= -7.832698070981D-01
I= 26 X= -2.814056669592D+00 Y= -5.584058657994D+00 Z= -2.284556247975D+00
I= 27 X= -2.398972341914D+00 Y= -5.384030789068D+00 Z= 7.755916843942D-01
I= 28 X= -5.670970124661D+00 Y= -5.228148048700D+00 Z= -4.890882323072D-01
I= 29 X= 3.130776519609D+00 Y= -3.508498753462D+00 Z= -1.561619948362D+00
I= 30 X= 3.447738907470D+00 Y= -2.936247399572D+00 Z= 1.134191972341D+00
I= 31 X= 1.935991550169D+00 Y= -4.614547772983D+00 Z= -2.421471569526D+00
I= 32 X= 4.528542546594D+00 Y= -2.814570134988D+00 Z= -2.903826468920D+00
I= 33 X= 5.236620455904D+00 Y= -2.359774386859D+00 Z= 1.480117843625D+00
I= 34 X= 2.593941078711D+00 Y= -4.394565558982D+00 Z= 2.287160774761D+00
I= 35 X= 8.834690019716D-01 Y= -9.492692265694D-02 Z= -2.581552269683D-01
I= 36 X= 3.569580284538D+00 Y= 2.354471095572D+00 Z= 1.620090681467D+00
I= 37 X= 4.805519513251D+00 Y= 1.666319659507D+00 Z= 2.747420553504D+00
I= 38 X= 2.319763627724D+00 Y= 4.010597732056D+00 Z= 2.160215282750D+00

Forward Direction:

Total Energy: -651.6167339 Hartrees

Potential Energy: -651.7591866 Hartress

Kinetic Energy: 0.1424527 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.675912203863D+11 Y= -7.598736253212D+11 Z= -1.675330235742D+13

I= 1 X= -7.361450216850D+12 Y= 3.480470900353D+12 Z= 1.581344521713D+13

I= 2 X= -6.613585164758D+12 Y= -4.572743616000D+12 Z= -7.527396782560D+12

I= 3 X= 3.988349421807D+12 Y= -1.421699963729D+13 Z= -1.156312749404D+13
I= 4 X= -2.058095950727D+12 Y= -1.977807485290D+12 Z= -6.758596616844D+12
I= 5 X= 1.259108659244D+13 Y= -6.295540143684D+12 Z= -5.559686819186D+12
I= 6 X= -3.562031728207D+13 Y= 1.392070979703D+13 Z= 1.024059263023D+13
I= 7 X= -1.171415358122D+14 Y= 4.611300284130D+13 Z= -8.242213149680D+12
I= 8 X= -9.209120447961D+13 Y= 1.124864366146D+13 Z= 6.594435189273D+13
I= 9 X= 2.054786121457D+13 Y= -3.795961304198D+12 Z= -1.543853785371D+13
I= 10 X= 6.089790057072D+13 Y= 7.700494518083D+12 Z= 3.142525727318D+13
I= 11 X= -1.103239356830D+14 Y= 4.488236136165D+13 Z= 5.386212824872D+13
I= 12 X= -2.629253712148D+13 Y= 7.292144454845D+13 Z= 9.685179405004D+13
I= 13 X= 3.003033006987D+12 Y= -7.715655689164D+12 Z= 1.126614993692D+13
I= 14 X= -1.500898559500D+12 Y= 2.919726062932D+13 Z= 7.069692524608D+13
I= 15 X= -2.465036922179D+13 Y= -3.540481737392D+13 Z= -2.847949300043D+13
I= 16 X= 4.118638155239D+13 Y= 6.575832815695D+13 Z= -2.870215067467D+12
I= 17 X= -2.839820888835D+11 Y= -1.472206398043D+12 Z= 1.316040252383D+13
I= 18 X= 1.014804878552D+14 Y= -3.224945866783D+13 Z= -4.530475089664D+12
I= 19 X= -1.738722679574D+13 Y= -5.959690229828D+13 Z= 6.677790791387D+13
I= 20 X= -7.000663282563D+12 Y= -6.744773545762D+13 Z= -6.763169642693D+13
I= 21 X= 1.681026391924D+12 Y= -1.821395378895D+13 Z= -8.747815192764D+12
I= 22 X= -5.531230093920D+12 Y= 1.767554458966D+13 Z= -4.477619191257D+13
I= 23 X= -6.216772275763D+13 Y= 1.444143961459D+13 Z= -5.802613027836D+13
I= 24 X= -9.520205967935D+13 Y= 7.258273617575D+13 Z= 6.342270066116D+13
I= 25 X= 6.321628973209D+12 Y= 1.650760135819D+13 Z= 2.509327806307D+13
I= 26 X= -4.346298798730D+13 Y= -1.611879058788D+13 Z= -1.569844252452D+13
I= 27 X= -1.316050173703D+13 Y= -5.365556800287D+12 Z= -5.474537005069D+13
I= 28 X= -6.005186240421D+13 Y= 3.340283718991D+13 Z= -7.146382817664D+13
I= 29 X= 4.949109884767D+12 Y= -1.460631179911D+13 Z= -1.587149976906D+13
I= 30 X= 1.695026308844D+13 Y= -1.880314762261D+12 Z= 1.966295236555D+12
I= 31 X= -3.785208880516D+13 Y= -4.494051786134D+13 Z= -9.005617373882D+13
I= 32 X= -5.623844983678D+13 Y= -3.787298864706D+13 Z= 7.607507985616D+13

I= 33 X= 7.908983912992D+13 Y= -2.883567570138D+13 Z= 2.370491289283D+13
I= 34 X= -1.280658950007D+12 Y= 3.014814908811D+11 Z= 2.764855778063D+13
I= 35 X= 7.293492987015D+11 Y= 1.744756267056D+12 Z= -8.604528858214D+11
I= 36 X= -2.043133860300D+13 Y= 1.911989854753D+13 Z= 2.619309409655D+13
I= 37 X= -3.529303814095D+13 Y= -2.917359529268D+12 Z= -7.082301920064D+13
I= 38 X= 1.926714172367D+13 Y= -5.499016454199D+10 Z= 3.265855829982D+13

Backward Direction:

Total Energy: -651.6167327 Hartrees

Potential Energy: -651.7591866 Hartress

Kinetic Energy: 0.1424539 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.757227014154D+10 Y= -8.790710018785D+11 Z= -1.676220675917D+13
I= 1 X= -7.159486084255D+12 Y= 3.048188296968D+12 Z= 1.509454290773D+13
I= 2 X= -6.876441594665D+12 Y= -4.176635752366D+12 Z= -8.146587893032D+12
I= 3 X= 3.823323074900D+12 Y= -1.418050956830D+13 Z= -1.243069047588D+13
I= 4 X= -7.733856091791D+11 Y= -2.082409591685D+12 Z= -7.581497140814D+12
I= 5 X= 1.267892239827D+13 Y= -6.895802710341D+12 Z= -1.094196497729D+13
I= 6 X= -5.259563114596D+10 Y= 4.665097529368D+13 Z= 2.569798756373D+13
I= 7 X= -1.098398846689D+14 Y= 5.301447857135D+13 Z= -7.572552537578D+12
I= 8 X= -8.220227977352D+13 Y= 1.934067763068D+13 Z= 6.779319592106D+13
I= 9 X= 2.099693290047D+13 Y= -3.601897533276D+12 Z= -1.592716135306D+13
I= 10 X= 6.104841884981D+13 Y= 8.688842338294D+12 Z= 3.027972381272D+13
I= 11 X= -1.104287910218D+14 Y= 4.488950636741D+13 Z= 5.379055824351D+13
I= 12 X= -2.598430454664D+13 Y= 7.300109261116D+13 Z= 9.655696511751D+13
I= 13 X= 3.089489079976D+12 Y= -7.775293873902D+12 Z= 1.105224191511D+13
I= 14 X= -1.378309093074D+12 Y= 2.883036086097D+13 Z= 7.071826473582D+13
I= 15 X= -2.435001685832D+13 Y= -3.570740055150D+13 Z= -2.898877164832D+13
I= 16 X= 4.112803054713D+13 Y= 6.584021947968D+13 Z= -2.810304735397D+12
I= 17 X= -1.385578937152D+11 Y= -1.603113993687D+12 Z= 1.310306074932D+13
I= 18 X= 1.016351409212D+14 Y= -3.232913289210D+13 Z= -4.872071403534D+12

I= 19 X= -1.738755136835D+13 Y= -5.972359660471D+13 Z= 6.692235250057D+13
I= 20 X= -6.829195820775D+12 Y= -6.766434932295D+13 Z= -6.770236218162D+13
I= 21 X= 1.387117707863D+12 Y= -1.820897008168D+13 Z= -9.195824759818D+12
I= 22 X= -5.726918996659D+12 Y= 1.810108714615D+13 Z= -4.583675653813D+13
I= 23 X= -6.198140198175D+13 Y= 1.427813767524D+13 Z= -5.840172220436D+13
I= 24 X= -9.559020351495D+13 Y= 7.257153606300D+13 Z= 6.289404329119D+13
I= 25 X= 6.319557525218D+12 Y= 1.645188593381D+13 Z= 2.496886654208D+13
I= 26 X= -4.368876927365D+13 Y= -1.643896764301D+13 Z= -1.578757549107D+13
I= 27 X= -1.296280740894D+13 Y= -5.181814108882D+12 Z= -5.481789878375D+13
I= 28 X= -6.000510774438D+13 Y= 3.339527650830D+13 Z= -7.123591600464D+13
I= 29 X= 4.178575459871D+12 Y= -1.415136098587D+13 Z= -1.646241696273D+13
I= 30 X= 1.701027807206D+13 Y= -1.750815603886D+12 Z= 1.511956638249D+12
I= 31 X= -3.779099492065D+13 Y= -4.536054541802D+13 Z= -9.033773631979D+13
I= 32 X= -5.721828230752D+13 Y= -3.698600958545D+13 Z= 7.515986103268D+13
I= 33 X= 7.922573450182D+13 Y= -2.889586219426D+13 Z= 2.324196991407D+13
I= 34 X= -8.208697774976D+11 Y= 2.319169143070D+11 Z= 2.735098768728D+13
I= 35 X= 5.438922426390D+11 Y= 1.669281560920D+12 Z= -1.389747621968D+11
I= 36 X= -2.267658522479D+13 Y= 1.643703116459D+13 Z= 2.484649750623D+13
I= 37 X= -3.268378710846D+13 Y= -1.236661448247D+12 Z= -7.413748559998D+13
I= 38 X= 2.084728055759D+13 Y= -1.616323746275D+11 Z= 3.051806849900D+13

Seed: 21876514586

CM Start Point Coordinates: bohr

I= 0 X= -2.492942748228D+00 Y= 2.281027424785D+00 Z= -7.401355224764D-01
I= 1 X= -3.000101725974D+00 Y= -7.977338600694D-02 Z= -2.003397896946D+00
I= 2 X= -2.379043093877D+00 Y= 1.828545899252D+00 Z= 2.022133903278D+00
I= 3 X= -2.781935181152D+00 Y= -2.041309378634D+00 Z= -2.050109069782D-01
I= 4 X= -2.433960733753D+00 Y= -8.014366078094D-01 Z= 2.395749718216D+00
I= 5 X= 4.208489177280D+00 Y= 2.556800281420D+00 Z= -8.795843519801D-01
I= 6 X= 2.476768873767D+00 Y= 1.283221996339D+00 Z= -2.829827096106D+00

I= 7 X= 5.846195229865D+00 Y= 1.538529241093D+00 Z= -1.779684039690D+00
I= 8 X= 3.843631632712D+00 Y= 4.531204728895D+00 Z= -1.601681382131D+00
I= 9 X= -2.385143073166D+00 Y= -2.171867590128D+00 Z= 4.864613910419D+00
I= 10 X= -3.850705351114D+00 Y= -6.742667259671D-01 Z= 6.732949256999D+00
I= 11 X= -3.133035431110D+00 Y= -4.360673523551D+00 Z= 4.237321899681D+00
I= 12 X= -1.748115484798D-02 Y= -2.107587580354D+00 Z= 5.772013429723D+00
I= 13 X= -2.309541868559D+00 Y= 3.873481714301D+00 Z= 3.969234168856D+00
I= 14 X= -4.128987248681D+00 Y= 3.843724064926D+00 Z= 4.486543051555D+00
I= 15 X= -1.162528038588D+00 Y= 3.450032328811D+00 Z= 5.570909488285D+00
I= 16 X= -1.714610234415D+00 Y= 5.788057470429D+00 Z= 3.205268230484D+00
I= 17 X= -2.600635497640D+00 Y= 4.781938881082D+00 Z= -1.823804425747D+00
I= 18 X= -4.306112748461D+00 Y= 5.639646927018D+00 Z= -1.461068578551D+00
I= 19 X= -1.167259707168D+00 Y= 6.037398543792D+00 Z= -8.354744800530D-01
I= 20 X= -2.363146029408D+00 Y= 5.140702824992D+00 Z= -3.821188848072D+00
I= 21 X= -3.668911696743D+00 Y= -3.945862839917D-01 Z= -4.736400590057D+00
I= 22 X= -5.748555405898D+00 Y= -7.439284908865D-01 Z= -5.061181779099D+00
I= 23 X= -3.188532756132D+00 Y= 1.529564020837D+00 Z= -5.635085968729D+00
I= 24 X= -2.619826525308D+00 Y= -1.924349282108D+00 Z= -5.265001288247D+00
I= 25 X= -3.480061790906D+00 Y= -4.755910122754D+00 Z= -5.796153850376D-01
I= 26 X= -2.694620350673D+00 Y= -5.424085087248D+00 Z= -2.585546069767D+00
I= 27 X= -2.765737114453D+00 Y= -5.791833420541D+00 Z= 1.064875335584D+00
I= 28 X= -5.680953093946D+00 Y= -4.805848819976D+00 Z= -3.909278921586D-01
I= 29 X= 3.008394122176D+00 Y= -3.476705454690D+00 Z= -1.729477078514D+00
I= 30 X= 3.434756093445D+00 Y= -3.383916256780D+00 Z= 8.777806348697D-01
I= 31 X= 1.735082636440D+00 Y= -4.983101772491D+00 Z= -2.389150459723D+00
I= 32 X= 4.368920533797D+00 Y= -3.080743544574D+00 Z= -2.975483034740D+00
I= 33 X= 5.296585152260D+00 Y= -2.694591483476D+00 Z= 1.838981966927D+00
I= 34 X= 2.157569132056D+00 Y= -4.571022205697D+00 Z= 2.080096903861D+00
I= 35 X= 8.778469735303D-01 Y= -4.314749532115D-02 Z= -2.198176241959D-01
I= 36 X= 3.713631188854D+00 Y= 2.265955343229D+00 Z= 1.760036269641D+00

I= 37 X= 4.904932167251D+00 Y= 1.235823230822D+00 Z= 2.804429330349D+00

I= 38 X= 2.612659794393D+00 Y= 3.663362965429D+00 Z= 2.917255800122D+00

Forward Direction:

Total Energy: -651.6052764 Hartrees

Potential Energy: -651.7918032 Hartress

Kinetic Energy: 0.1865268 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 7.184592566080D+12 Y= -1.168507678097D+13 Z= -9.831792903219D+12

I= 1 X= 1.708610146962D+13 Y= 1.851353674530D+13 Z= -1.072991184034D+12

I= 2 X= 2.039780761474D+12 Y= -3.361220434446D+13 Z= -1.085284316644D+13

I= 3 X= 5.532143984595D+11 Y= -9.694247116219D+12 Z= 5.377479465675D+12

I= 4 X= -3.097213437485D+12 Y= -2.922306907770D+12 Z= -1.548364065087D+13

I= 5 X= 1.625514202969D+13 Y= 8.874652424618D+12 Z= -1.945504753025D+13

I= 6 X= 1.199798568719D+13 Y= 1.443216597687D+13 Z= -5.064512805610D+13

I= 7 X= 1.568289957482D+12 Y= -1.261485801211D+12 Z= 4.632616485341D+13

I= 8 X= -8.084914150976D+13 Y= -1.412747748882D+14 Z= 7.298528900606D+13

I= 9 X= -2.395867162865D+12 Y= 9.028876799747D+12 Z= 6.199859715938D+12

I= 10 X= 4.847823652095D+13 Y= -1.003178298300D+14 Z= 9.146398339961D+13

I= 11 X= -2.866057734990D+13 Y= -5.468896562171D+12 Z= -4.539296293073D+13

I= 12 X= -1.071159698438D+14 Y= 2.138853921314D+13 Z= -5.305468243976D+13

I= 13 X= 1.316554160635D+13 Y= 3.424272185928D+13 Z= 2.524534401731D+13

I= 14 X= 1.188213410653D+14 Y= -5.052621188985D+12 Z= -4.027503373664D+13

I= 15 X= 2.396053262832D+13 Y= 3.294063592829D+13 Z= -4.759220487404D+13

I= 16 X= 2.925577928554D+12 Y= 3.962002843327D+13 Z= 4.101215223228D+13

I= 17 X= 5.231153709734D+12 Y= 8.299030863823D+12 Z= -7.773751062252D+12

I= 18 X= 6.677460030254D+13 Y= -5.759334023798D+13 Z= 1.752565999118D+13

I= 19 X= 1.936159484686D+13 Y= 7.837196831243D+13 Z= 2.107226389619D+13

I= 20 X= -1.172099735195D+13 Y= 7.406081316372D+13 Z= 4.327296976136D+13

I= 21 X= -7.396862910615D+12 Y= 1.720970332773D+12 Z= -6.816099424371D+12

I= 22 X= 1.083654427251D+14 Y= 6.197776815087D+13 Z= 7.760376905396D+13

I= 23 X= -5.367481864220D+13 Y= 3.078501703915D+13 Z= -3.534958291599D+13
I= 24 X= -1.706309539220D+13 Y= -8.386026354159D+12 Z= 2.860557282819D+13
I= 25 X= -2.488320669505D+13 Y= -6.840357917348D+12 Z= 2.123758101254D+13
I= 26 X= -3.280405569862D+13 Y= -4.964081545576D+13 Z= -1.061577496142D+14
I= 27 X= -9.965263553552D+12 Y= -9.331893656422D+13 Z= 6.320299556646D+13
I= 28 X= 4.119654516003D+13 Y= -3.312498734553D+13 Z= -2.373201482223D+13
I= 29 X= 1.735916022987D+13 Y= -4.065764278878D+12 Z= 4.554446324799D+13
I= 30 X= -1.438457809019D+13 Y= -8.564256721228D+12 Z= -1.000560359998D+13
I= 31 X= 2.659787746601D+13 Y= 2.266608340911D+13 Z= -1.480017796175D+13
I= 32 X= 7.942217242537D+13 Y= -1.462215830219D+13 Z= -1.229460205030D+14
I= 33 X= 4.278173856047D+13 Y= -1.652099155473D+13 Z= 1.469156651249D+13
I= 34 X= -8.243475523823D+13 Y= 5.879306357025D+13 Z= 4.546732102649D+12
I= 35 X= -2.268916933993D+12 Y= 1.273300867039D+12 Z= -2.220885019380D+12
I= 36 X= -3.128443183412D+12 Y= -1.857329858860D+13 Z= 2.026582283385D+13
I= 37 X= 2.152299190053D+13 Y= 1.788669145661D+13 Z= -6.802470650065D+13
I= 38 X= -3.593230242708D+13 Y= 1.177667579522D+13 Z= 3.904824383900D+12

Backward Direction:

Total Energy: -651.6052609 Hartrees

Potential Energy: -651.7918032 Hartress

Kinetic Energy: 0.1865423 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.946195556103D+12 Y= -1.175521216881D+13 Z= -9.837032228276D+12
I= 1 X= 1.720493657269D+13 Y= 1.825918292766D+13 Z= -1.495991197304D+12
I= 2 X= 1.885116806344D+12 Y= -3.337913563692D+13 Z= -1.121717340227D+13
I= 3 X= 4.561133793145D+11 Y= -9.672776467102D+12 Z= 4.867007947080D+12
I= 4 X= -2.341293632673D+12 Y= -2.983854480532D+12 Z= -1.596783290961D+13
I= 5 X= 1.630682436205D+13 Y= 8.521459687219D+12 Z= -2.262196424115D+13
I= 6 X= 3.292592898875D+13 Y= 3.369055838541D+13 Z= -4.155004212553D+13
I= 7 X= 5.864560116792D+12 Y= 2.799322315319D+12 Z= 4.672019119986D+13
I= 8 X= -7.503052715865D+13 Y= -1.365134457888D+14 Z= 7.407314342118D+13

I= 9 X= -2.131634698299D+12 Y= 9.143063354802D+12 Z= 5.912355079859D+12
I= 10 X= 4.856680103989D+13 Y= -9.973628886502D+13 Z= 9.078995486893D+13
I= 11 X= -2.872227392107D+13 Y= -5.464692461692D+12 Z= -4.543507451108D+13
I= 12 X= -1.069346066979D+14 Y= 2.143540389965D+13 Z= -5.322815891664D+13
I= 13 X= 1.321641210573D+13 Y= 3.420763092694D+13 Z= 2.511948116323D+13
I= 14 X= 1.188934723450D+14 Y= -5.268503946964D+12 Z= -4.026247764765D+13
I= 15 X= 2.413725907651D+13 Y= 3.276259687372D+13 Z= -4.789186293608D+13
I= 16 X= 2.891244360205D+12 Y= 3.966821305104D+13 Z= 4.104740329483D+13
I= 17 X= 5.316720879804D+12 Y= 8.222005216959D+12 Z= -7.807490794881D+12
I= 18 X= 6.686559771611D+13 Y= -5.764022031347D+13 Z= 1.732466572845D+13
I= 19 X= 1.936140388259D+13 Y= 7.829742174679D+13 Z= 2.115725465832D+13
I= 20 X= -1.162010641174D+13 Y= 7.393335819654D+13 Z= 4.323139023374D+13
I= 21 X= -7.569797922471D+12 Y= 1.723902730277D+12 Z= -7.079706940782D+12
I= 22 X= 1.082502999437D+14 Y= 6.222815612553D+13 Z= 7.697973593830D+13
I= 23 X= -5.356518806448D+13 Y= 3.068893066450D+13 Z= -3.557058010632D+13
I= 24 X= -1.729147807623D+13 Y= -8.392616460575D+12 Z= 2.829451237547D+13
I= 25 X= -2.488442553125D+13 Y= -6.873140709059D+12 Z= 2.116437763593D+13
I= 26 X= -3.293690474348D+13 Y= -4.982920669365D+13 Z= -1.062101951943D+14
I= 27 X= -9.848940796101D+12 Y= -9.321082290262D+13 Z= 6.316031987230D+13
I= 28 X= 4.122405546085D+13 Y= -3.312943602362D+13 Z= -2.359791197480D+13
I= 29 X= 1.690578003083D+13 Y= -3.798072551041D+12 Z= 4.519676930088D+13
I= 30 X= -1.434926544953D+13 Y= -8.488059795430D+12 Z= -1.027293510120D+13
I= 31 X= 2.663382493147D+13 Y= 2.241894042300D+13 Z= -1.496584856103D+13
I= 32 X= 7.884564186990D+13 Y= -1.410026241995D+13 Z= -1.234845325788D+14
I= 33 X= 4.286169899856D+13 Y= -1.655640510944D+13 Z= 1.441917222040D+13
I= 34 X= -8.216421663702D+13 Y= 5.875213197707D+13 Z= 4.371642730696D+12
I= 35 X= -2.378039322484D+12 Y= 1.228891770879D+12 Z= -1.796369403693D+12
I= 36 X= -4.449539722881D+12 Y= -2.015188990399D+13 Z= 1.947348934313D+13
I= 37 X= 2.305826756723D+13 Y= 1.887560928582D+13 Z= -6.997492882656D+13
I= 38 X= -3.500255336533D+13 Y= 1.171392783252D+13 Z= 2.645366453110D+12

Seed: 22402754432

CM Start Point Coordinates: bohr

I= 0 X= -2.665578585543D+00 Y= 2.418139275123D+00 Z= -6.481125483434D-01
I= 1 X= -2.986816207235D+00 Y= -8.516347093451D-02 Z= -1.907351622427D+00
I= 2 X= -2.443898267656D+00 Y= 1.722063565597D+00 Z= 1.882161812107D+00
I= 3 X= -2.935648518726D+00 Y= -2.025472003170D+00 Z= -1.532683999572D-01
I= 4 X= -2.521213950975D+00 Y= -9.119571533685D-01 Z= 2.356239546126D+00
I= 5 X= 4.150587568705D+00 Y= 2.341504497699D+00 Z= -1.064807153089D+00
I= 6 X= 1.994099937220D+00 Y= 1.208455935361D+00 Z= -2.722564070026D+00
I= 7 X= 5.698366477376D+00 Y= 1.105426338045D+00 Z= -1.666701574488D+00
I= 8 X= 4.023378604697D+00 Y= 4.406762387014D+00 Z= -2.053229673988D+00
I= 9 X= -2.138691615744D+00 Y= -2.110018662963D+00 Z= 4.881906087139D+00
I= 10 X= -3.920807846367D+00 Y= -2.299574240644D+00 Z= 5.988935350052D+00
I= 11 X= -1.514772082037D+00 Y= -4.122829743472D+00 Z= 4.375943438139D+00
I= 12 X= -5.343276833824D-01 Y= -1.031762093715D+00 Z= 6.036318850989D+00
I= 13 X= -2.209564853350D+00 Y= 3.756287132403D+00 Z= 4.006856274511D+00
I= 14 X= -4.402486853923D+00 Y= 4.626364810207D+00 Z= 4.470628683187D+00
I= 15 X= -1.371259411460D+00 Y= 2.896693317109D+00 Z= 5.844709325954D+00
I= 16 X= -7.329752219220D-01 Y= 5.323885842376D+00 Z= 3.415117228039D+00
I= 17 X= -2.724679965306D+00 Y= 4.825385878930D+00 Z= -2.012401172758D+00
I= 18 X= -4.745664591838D+00 Y= 5.442780302361D+00 Z= -2.220371019587D+00
I= 19 X= -1.425692151046D+00 Y= 6.300257653781D+00 Z= -1.051361042062D+00
I= 20 X= -2.056642227997D+00 Y= 4.965113883208D+00 Z= -4.157719207574D+00
I= 21 X= -3.410314948835D+00 Y= -2.747163917900D-01 Z= -4.639931906018D+00
I= 22 X= -5.428171183639D+00 Y= -4.074523244069D-01 Z= -4.898065886851D+00
I= 23 X= -2.383062525955D+00 Y= 1.190574348585D+00 Z= -5.796840630969D+00
I= 24 X= -2.508211460701D+00 Y= -1.992188022253D+00 Z= -5.539174241098D+00
I= 25 X= -3.232668581943D+00 Y= -4.763218731736D+00 Z= -6.397520226927D-01
I= 26 X= -3.113954552809D+00 Y= -5.480701411090D+00 Z= -2.709910105669D+00

I= 27 X= -2.124263318140D+00 Y= -5.700552819998D+00 Z= 3.862192401061D-01
I= 28 X= -5.228392925927D+00 Y= -5.113086102491D+00 Z= 1.939467063192D-01
I= 29 X= 2.807382778433D+00 Y= -3.056219062157D+00 Z= -1.721223834651D+00
I= 30 X= 3.069214039158D+00 Y= -3.268991940413D+00 Z= 1.004105541020D+00
I= 31 X= 1.762181888908D+00 Y= -4.279005821722D+00 Z= -3.070344521607D+00
I= 32 X= 4.397832409870D+00 Y= -2.477314392705D+00 Z= -2.910735227740D+00
I= 33 X= 4.697855853844D+00 Y= -2.973586723589D+00 Z= 2.341633778855D+00
I= 34 X= 1.460905954101D+00 Y= -4.775343271076D+00 Z= 1.884147642440D+00
I= 35 X= 8.725065533527D-01 Y= -5.085666221535D-02 Z= -1.989071657660D-01
I= 36 X= 3.925363850360D+00 Y= 2.097615713295D+00 Z= 1.702012887479D+00
I= 37 X= 5.680744808110D+00 Y= 1.118848465161D+00 Z= 3.013069004030D+00
I= 38 X= 3.278390175748D+00 Y= 3.884625957089D+00 Z= 2.656762630222D+00

Forward Direction:

Total Energy: -651.6171870 Hartrees

Potential Energy: -651.8096835 Hartress

Kinetic Energy: 0.1924965 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.269256534016D+12 Y= -1.597666024056D+13 Z= 6.597399823968D+12
I= 1 X= 8.158694334244D+12 Y= -6.464277830098D+12 Z= 1.631350988550D+13
I= 2 X= -5.846148607906D+12 Y= 3.950082353633D+12 Z= -2.385890238475D+13
I= 3 X= 1.198166662075D+13 Y= 7.480599442881D+12 Z= -4.153403017279D+12
I= 4 X= 7.956459238061D+12 Y= 3.460469263603D+13 Z= -2.600352872719D+13
I= 5 X= -8.840442746620D+12 Y= 1.055645938149D+13 Z= -5.769545546771D+12
I= 6 X= 4.288710671519D+13 Y= -6.802420217332D+13 Z= -5.727024797135D+13
I= 7 X= -8.032420979221D+13 Y= -2.330037319238D+13 Z= 1.383657117325D+13
I= 8 X= -2.620354298097D+13 Y= -1.124257538955D+14 Z= -9.732778121862D+11
I= 9 X= 2.914508101404D+12 Y= 3.186195496437D+11 Z= 1.729439186036D+13
I= 10 X= -8.970566112216D+13 Y= -2.752357564421D+12 Z= -6.812439650956D+13
I= 11 X= 5.780158796011D+13 Y= -3.575186233358D+13 Z= -2.549321314497D+13
I= 12 X= 9.489361643901D+13 Y= -4.325318808232D+13 Z= -8.554614362418D+13

I= 13 X= -1.168821503115D+13 Y= 1.457605476848D+12 Z= 1.480063980086D+13
I= 14 X= 1.053030515362D+14 Y= 4.643047171714D+13 Z= -3.587281415147D+13
I= 15 X= 8.128963409770D+13 Y= -2.068667794698D+12 Z= -3.769554035326D+12
I= 16 X= -5.000914545892D+13 Y= -9.426336519148D+13 Z= 7.372294807453D+12
I= 17 X= -2.699490302477D+12 Y= -1.884962237528D+13 Z= 1.169720993964D+13
I= 18 X= -1.860278698843D+13 Y= 9.269118775083D+13 Z= -5.628006607252D+13
I= 19 X= -1.156827349402D+14 Y= -8.556706745573D+13 Z= -5.354710423081D+13
I= 20 X= -5.109837033324D+12 Y= -5.005022070761D+13 Z= -4.882467220601D+13
I= 21 X= 1.412692800611D+13 Y= -1.645097214217D+13 Z= 3.300524538563D+12
I= 22 X= 1.602043658425D+13 Y= -1.164530742672D+13 Z= 7.268942786304D+13
I= 23 X= -4.242532675395D+13 Y= -2.103387126330D+13 Z= -2.157988200635D+13
I= 24 X= -8.710032916059D+13 Y= 1.370281087011D+14 Z= 9.848874630412D+13
I= 25 X= 1.354026322663D+13 Y= 3.922287132641D+12 Z= 1.907244924306D+12
I= 26 X= -1.522682897837D+13 Y= -1.186187138134D+13 Z= -4.597918467173D+13
I= 27 X= 1.510930021290D+13 Y= 4.862528532593D+13 Z= 9.544205189652D+12
I= 28 X= -6.864321447641D+13 Y= -8.717376268276D+13 Z= -5.455014934808D+13
I= 29 X= -4.179841404575D+13 Y= -2.769552814490D+12 Z= -1.464699901151D+13
I= 30 X= -1.347275523279D+13 Y= -5.210099395803D+11 Z= 1.295346621997D+13
I= 31 X= 8.400781047833D+13 Y= -4.798555720099D+12 Z= 4.038652914799D+13
I= 32 X= -2.567167126211D+12 Y= 2.066965085876D+13 Z= 2.306815851416D+13
I= 33 X= -4.401753819270D+13 Y= -7.205541485015D+13 Z= 8.755840703067D+13
I= 34 X= 1.473673493207D+14 Y= 6.786463600751D+13 Z= -5.553296583383D+13
I= 35 X= 1.259397443353D+12 Y= 1.146958954483D+12 Z= 2.890820774557D+11
I= 36 X= 8.344766021117D+12 Y= 6.649841481900D+12 Z= 2.854916818447D+12
I= 37 X= -5.661592170326D+13 Y= 3.514901080613D+12 Z= 1.978114889808D+13
I= 38 X= 7.563134416921D+12 Y= -4.561283726018D+12 Z= 2.706391957416D+13

Backward Direction:

Total Energy: -651.6172479 Hartrees

Potential Energy: -651.8096835 Hartress

Kinetic Energy: 0.1924356 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.585081874393D+11 Y= -1.618575938224D+13 Z= 6.581779489584D+12
I= 1 X= 8.512985074691D+12 Y= -7.222599228992D+12 Z= 1.505239273623D+13
I= 2 X= -6.307258201740D+12 Y= 4.644945083595D+12 Z= -2.494510355490D+13
I= 3 X= 1.169217310523D+13 Y= 7.544611272880D+12 Z= -5.675304588566D+12
I= 4 X= 1.021013156962D+13 Y= 3.442119689898D+13 Z= -2.744708225231D+13
I= 5 X= -8.686358888940D+12 Y= 9.503463156229D+12 Z= -1.521127804522D+13
I= 6 X= 1.052809302070D+14 Y= -1.060791815355D+13 Z= -3.015448327345D+13
I= 7 X= -6.751546322330D+13 Y= -1.119362475452D+13 Z= 1.501130725783D+13
I= 8 X= -8.856133758645D+12 Y= -9.823049719382D+13 Z= 2.270012524794D+12
I= 9 X= 3.702281345404D+12 Y= 6.590512693580D+11 Z= 1.643723579385D+13
I= 10 X= -8.944161803936D+13 Y= -1.018572079383D+12 Z= -7.013392113723D+13
I= 11 X= 5.761764798577D+13 Y= -3.573932837985D+13 Z= -2.561876311494D+13
I= 12 X= 9.543432604695D+13 Y= -4.311346738531D+13 Z= -8.606334021174D+13
I= 13 X= -1.153655153664D+13 Y= 1.352986619493D+12 Z= 1.442539678008D+13
I= 14 X= 1.055181011702D+14 Y= 4.578684658750D+13 Z= -3.583537986266D+13
I= 15 X= 8.181652003030D+13 Y= -2.599467095343D+12 Z= -4.662943900734D+12
I= 16 X= -5.011150630639D+13 Y= -9.411970930507D+13 Z= 7.477391073996D+12
I= 17 X= -2.444383392547D+12 Y= -1.907926388975D+13 Z= 1.159661950519D+13
I= 18 X= -1.833149055572D+13 Y= 9.255142114245D+13 Z= -5.687930322127D+13
I= 19 X= -1.156833043147D+14 Y= -8.578931790620D+13 Z= -5.329371577912D+13
I= 20 X= -4.809044354926D+12 Y= -5.043021039074D+13 Z= -4.894863591593D+13
I= 21 X= 1.361134574229D+13 Y= -1.644222959560D+13 Z= 2.514614492167D+12
I= 22 X= 1.567715401715D+13 Y= -1.089880959853D+13 Z= 7.082895778810D+13
I= 23 X= -4.209847800140D+13 Y= -2.132033977736D+13 Z= -2.223875514384D+13
I= 24 X= -8.778122118384D+13 Y= 1.370084611702D+14 Z= 9.756136177702D+13
I= 25 X= 1.353662943922D+13 Y= 3.824549687695D+12 Z= 1.688998992074D+12
I= 26 X= -1.562290038980D+13 Y= -1.242353430089D+13 Z= -4.613554404589D+13
I= 27 X= 1.545610075019D+13 Y= 4.894761154051D+13 Z= 9.416973389920D+12
I= 28 X= -6.856119622921D+13 Y= -8.718702582620D+13 Z= -5.415033988058D+13

I= 29 X= -4.315010559991D+13 Y= -1.971466251699D+12 Z= -1.568360134006D+13
I= 30 X= -1.336747538493D+13 Y= -2.938391434695D+11 Z= 1.215645361985D+13
I= 31 X= 8.411498295884D+13 Y= -5.535378996780D+12 Z= 3.989260473773D+13
I= 32 X= -4.286014762781D+12 Y= 2.222561262597D+13 Z= 2.146265782112D+13
I= 33 X= -4.377914699028D+13 Y= -7.216099556419D+13 Z= 8.674630040198D+13
I= 34 X= 1.481739234630D+14 Y= 6.774260401664D+13 Z= -5.605497103982D+13
I= 35 X= 9.340638466310D+11 Y= 1.014559259639D+12 Z= 1.554717788836D+12
I= 36 X= 4.406095931701D+12 Y= 1.943485658174D+12 Z= 4.926820141150D+11
I= 37 X= -5.203870559576D+13 Y= 6.463225420589D+12 Z= 1.396682563280D+13
I= 38 X= 1.033505510690D+13 Y= -4.748358266248D+12 Z= 2.330901662650D+13

Seed: 23239193623

CM Start Point Coordinates: bohr

I= 0 X= -2.698184218655D+00 Y= 2.287310709157D+00 Z= -6.322002029363D-01
I= 1 X= -2.866270337086D+00 Y= -1.220491106195D-01 Z= -1.985824106290D+00
I= 2 X= -2.564585910431D+00 Y= 1.737236266939D+00 Z= 2.042400626798D+00
I= 3 X= -2.954575277674D+00 Y= -2.102996546625D+00 Z= -9.796541034724D-02
I= 4 X= -2.403035344418D+00 Y= -7.850031308202D-01 Z= 2.445507677547D+00
I= 5 X= 4.538907283814D+00 Y= 2.253830162118D+00 Z= -9.112324233960D-01
I= 6 X= 2.608064509713D+00 Y= 8.494709144325D-01 Z= -2.888455907199D+00
I= 7 X= 5.861028144770D+00 Y= 1.010409964381D+00 Z= -1.517110779053D+00
I= 8 X= 4.773033511031D+00 Y= 4.278648456318D+00 Z= -1.701707397899D+00
I= 9 X= -1.985194877599D+00 Y= -2.334468309576D+00 Z= 4.664614415707D+00
I= 10 X= -3.570667928427D+00 Y= -2.613908322999D+00 Z= 6.116739886396D+00
I= 11 X= -1.554438566145D+00 Y= -4.327239506942D+00 Z= 3.990478102365D+00
I= 12 X= -4.047627883893D-01 Y= -1.864559461078D+00 Z= 5.932859014237D+00
I= 13 X= -1.888987643863D+00 Y= 3.644941786025D+00 Z= 4.251578544881D+00
I= 14 X= -3.402843167234D+00 Y= 4.413778195449D+00 Z= 5.684170434602D+00
I= 15 X= -4.838868963129D-01 Y= 3.004999165166D+00 Z= 5.281777947191D+00
I= 16 X= -1.148052843588D+00 Y= 5.278015389610D+00 Z= 3.364984145094D+00

I= 17 X= -2.353641375658D+00 Y= 4.759623882214D+00 Z= -2.069394054271D+00
I= 18 X= -4.686565074724D+00 Y= 5.272652458524D+00 Z= -3.226936367828D+00
I= 19 X= -1.698511658324D+00 Y= 6.585825919043D+00 Z= -7.064295603787D-01
I= 20 X= -9.135305183707D-01 Y= 4.743529776710D+00 Z= -3.756541702969D+00
I= 21 X= -3.508154093017D+00 Y= -4.622498373929D-01 Z= -4.830078110203D+00
I= 22 X= -5.587324018174D+00 Y= -4.958358158352D-01 Z= -4.771729622583D+00
I= 23 X= -2.422661157352D+00 Y= 1.060699073610D+00 Z= -5.896532697298D+00
I= 24 X= -2.467516727458D+00 Y= -2.356662254784D+00 Z= -5.805552499782D+00
I= 25 X= -3.418625260565D+00 Y= -4.756802641857D+00 Z= -5.552958043653D-01
I= 26 X= -2.776910112189D+00 Y= -5.114399386757D+00 Z= -2.507707987628D+00
I= 27 X= -2.022694469336D+00 Y= -6.205954306294D+00 Z= 7.271032175830D-01
I= 28 X= -5.480094009135D+00 Y= -5.191725697564D+00 Z= -5.342524112485D-01
I= 29 X= 2.980727830517D+00 Y= -3.175474045536D+00 Z= -1.587060647752D+00
I= 30 X= 3.006641854751D+00 Y= -2.995229425564D+00 Z= 1.067342868459D+00
I= 31 X= 2.066085687751D+00 Y= -4.423280664063D+00 Z= -2.851728319348D+00
I= 32 X= 4.852350506498D+00 Y= -2.466206533676D+00 Z= -2.379118432557D+00
I= 33 X= 4.619740468195D+00 Y= -2.343378723120D+00 Z= 1.928081454315D+00
I= 34 X= 1.597979189322D+00 Y= -4.123904853754D+00 Z= 2.273272172910D+00
I= 35 X= 7.815797629003D-01 Y= -1.554594675305D-02 Z= -2.297103073116D-01
I= 36 X= 3.881363532828D+00 Y= 2.269989799375D+00 Z= 1.704210125578D+00
I= 37 X= 4.841158299617D+00 Y= 1.189054540528D+00 Z= 2.902818282721D+00
I= 38 X= 3.419332251443D+00 Y= 4.212935708759D+00 Z= 2.570494165382D+00

Forward Direction:

Total Energy: -651.6121763 Hartrees

Potential Energy: -651.7718873 Hartress

Kinetic Energy: 0.1597111 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.462663858485D+13 Y= -1.296846226196D+13 Z= 9.674152200398D+12

I= 1 X= -1.550888132289D+11 Y= 1.298222657902D+13 Z= -9.117888409707D+12

I= 2 X= -1.060418462534D+13 Y= -1.370052148008D+13 Z= 1.567378456381D+13

I= 3 X= -1.167174213451D+13 Y= -1.763662693700D+13 Z= 3.235506671014D+12
I= 4 X= -9.759380633346D+12 Y= -1.698663380521D+13 Z= 2.823815483218D+13
I= 5 X= 7.112966789710D+12 Y= 7.837263350179D+12 Z= -1.957618879887D+13
I= 6 X= 7.584132590522D+12 Y= 7.060146071130D+12 Z= -7.768821789694D+13
I= 7 X= 7.402061957403D+13 Y= -2.030703692878D+13 Z= 3.127995048121D+13
I= 8 X= -1.489274554675D+13 Y= -7.705334619976D+13 Z= 7.154766632976D+13
I= 9 X= 3.797688034759D+12 Y= 2.061633360395D+12 Z= -2.767743170797D+12
I= 10 X= -7.172773972819D+13 Y= -8.633860902653D+12 Z= -1.421430823052D+13
I= 11 X= -3.118226674090D+13 Y= 4.626685587584D+13 Z= -6.332443522207D+13
I= 12 X= 1.400967631735D+13 Y= 5.744314326428D+13 Z= 8.087935815482D+13
I= 13 X= -2.677110994060D+13 Y= 6.813875663568D+12 Z= -1.278808173077D+13
I= 14 X= -3.449645701959D+13 Y= 6.045387500409D+13 Z= -7.718829196471D+12
I= 15 X= 1.213589414324D+14 Y= 4.389645216973D+13 Z= 5.977463312236D+13
I= 16 X= 6.331401963974D+12 Y= 1.311068108669D+13 Z= 1.522035237847D+14
I= 17 X= -6.076999432910D+11 Y= 1.788560233834D+13 Z= 1.833169559672D+11
I= 18 X= 8.478565273486D+13 Y= -4.050986537002D+13 Z= -2.594509057176D+13
I= 19 X= 1.573956750210D+13 Y= -4.368712651157D+13 Z= -1.661148668682D+13
I= 20 X= 1.905670160649D+13 Y= 2.598940064280D+12 Z= -9.660431022418D+13
I= 21 X= 5.893253606220D+12 Y= -6.121522455572D+12 Z= 5.055185449381D+12
I= 22 X= -4.741119491833D+12 Y= -3.895491780947D+13 Z= 4.822110252420D+13
I= 23 X= 4.783046091396D+13 Y= 6.484669507529D+13 Z= 8.794269463320D+12
I= 24 X= -9.760083884569D+13 Y= 5.490156639168D+13 Z= -8.098528479541D+13
I= 25 X= -1.986267247700D+13 Y= -5.288485770183D+12 Z= -1.960401844725D+13
I= 26 X= 2.122571169961D+13 Y= -4.740116584144D+13 Z= -8.916571848056D+12
I= 27 X= 9.140472390833D+13 Y= -6.352919299098D+13 Z= 9.023931659201D+13
I= 28 X= 1.250078811171D+13 Y= 2.931176951523D+13 Z= 7.663072074454D+12
I= 29 X= 1.783944807675D+13 Y= -5.399240468806D+11 Z= 5.236601245428D+12
I= 30 X= 3.012629086075D+12 Y= -4.485131760377D+12 Z= -1.530015011013D+13
I= 31 X= -1.266754882523D+13 Y= -4.594641137320D+13 Z= -5.366022749156D+13
I= 32 X= -6.528073838305D+13 Y= -7.160802686605D+13 Z= 9.856661430851D+12

I= 33 X= -1.036813204288D+13 Y= 7.631140962107D+13 Z= 7.141767773020D+13
I= 34 X= -3.264908252349D+13 Y= -7.152238220427D+13 Z= 7.175233195184D+13
I= 35 X= 8.616092113360D+11 Y= 2.833736260894D+12 Z= -1.873377870465D+12
I= 36 X= 5.385843381556D+12 Y= -3.353600285931D+12 Z= 1.834839393792D+13
I= 37 X= -5.335986170008D+13 Y= -1.599585949020D+13 Z= -2.143870753593D+13
I= 38 X= 7.283282227058D+12 Y= -5.473145734598D+13 Z= 4.487682289301D+13

Backward Direction:

Total Energy: -651.6121828 Hartrees

Potential Energy: -651.7718873 Hartress

Kinetic Energy: 0.1597046 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.433327596074D+13 Y= -1.305476829867D+13 Z= 9.667704880260D+12
I= 1 X= -8.854687800103D+09 Y= 1.266922809310D+13 Z= -9.638416724616D+12
I= 2 X= -1.079450841908D+13 Y= -1.341371566983D+13 Z= 1.522545312788D+13
I= 3 X= -1.179123109016D+13 Y= -1.761020594066D+13 Z= 2.607339130039D+12
I= 4 X= -8.829173427162D+12 Y= -1.706237199213D+13 Z= 2.764232558449D+13
I= 5 X= 7.176565168948D+12 Y= 7.402637317429D+12 Z= -2.347328043610D+13
I= 6 X= 3.333729259677D+13 Y= 3.075881793574D+13 Z= -6.649613849088D+13
I= 7 X= 7.930745216843D+13 Y= -1.530995528309D+13 Z= 3.176482485720D+13
I= 8 X= -7.732571993483D+12 Y= -7.119422911062D+13 Z= 7.288634010332D+13
I= 9 X= 4.122842826046D+12 Y= 2.202147150744D+12 Z= -3.121535839072D+12
I= 10 X= -7.161875547369D+13 Y= -7.918237905300D+12 Z= -1.504374303505D+13
I= 11 X= -3.125818827759D+13 Y= 4.627202928914D+13 Z= -6.337625619373D+13
I= 12 X= 1.423285516221D+13 Y= 5.750081323010D+13 Z= 8.066588435356D+13
I= 13 X= -2.670851056957D+13 Y= 6.770694047523D+12 Z= -1.294296394585D+13
I= 14 X= -3.440769490776D+13 Y= 6.018821760435D+13 Z= -7.703378129237D+12
I= 15 X= 1.215764145248D+14 Y= 4.367736382806D+13 Z= 5.940588488874D+13
I= 16 X= 6.289152343029D+12 Y= 1.316997530733D+13 Z= 1.522469024519D+14
I= 17 X= -5.024041199434D+11 Y= 1.779081740246D+13 Z= 1.417980789936D+11
I= 18 X= 8.489763081300D+13 Y= -4.056755427863D+13 Z= -2.619242674998D+13

I= 19 X= 1.573933249710D+13 Y= -4.377886077475D+13 Z= -1.650690016348D+13
I= 20 X= 1.918085430562D+13 Y= 2.442098659631D+12 Z= -9.665547646315D+13
I= 21 X= 5.680446126090D+12 Y= -6.117913955967D+12 Z= 4.730799700936D+12
I= 22 X= -4.882809968777D+12 Y= -3.864679951895D+13 Z= 4.745319023446D+13
I= 23 X= 4.796536831763D+13 Y= 6.472845468771D+13 Z= 8.522318419180D+12
I= 24 X= -9.788187821688D+13 Y= 5.489345683518D+13 Z= -8.136806437764D+13
I= 25 X= -1.986417233382D+13 Y= -5.328827070149D+12 Z= -1.969409984024D+13
I= 26 X= 2.106223252599D+13 Y= -4.763299319365D+13 Z= -8.981109454377D+12
I= 27 X= 9.154786642795D+13 Y= -6.339615228335D+13 Z= 9.018680144423D+13
I= 28 X= 1.253464127794D+13 Y= 2.930629513923D+13 Z= 7.828094126863D+12
I= 29 X= 1.728153501871D+13 Y= -2.105124200720D+11 Z= 4.808741818313D+12
I= 30 X= 3.056083528442D+12 Y= -4.391366615945D+12 Z= -1.562911845761D+13
I= 31 X= -1.262331319551D+13 Y= -4.625053647342D+13 Z= -5.386409565586D+13
I= 32 X= -6.599019575816D+13 Y= -7.096580092119D+13 Z= 9.193988206048D+12
I= 33 X= -1.026973565574D+13 Y= 7.626783099771D+13 Z= 7.108247929524D+13
I= 34 X= -3.231616763233D+13 Y= -7.157275112211D+13 Z= 7.153687338871D+13
I= 35 X= 7.273271990466D+11 Y= 2.779088053932D+12 Z= -1.350984512398D+12
I= 36 X= 3.760150398034D+12 Y= -5.296156900717D+12 Z= 1.737337738296D+13
I= 37 X= -5.147060772909D+13 Y= -1.477893345182D+13 Z= -2.383857965724D+13
I= 38 X= 8.427397346208D+12 Y= -5.480867269189D+13 Z= 4.332698012363D+13

Seed: 23251358091

CM Start Point Coordinates: bohr

I= 0 X= -2.573937152731D+00 Y= 2.387334898189D+00 Z= -5.342020670589D-01
I= 1 X= -3.033985107389D+00 Y= 1.256298407636D-01 Z= -1.979213459472D+00
I= 2 X= -2.283687465290D+00 Y= 1.747562749920D+00 Z= 2.123907086208D+00
I= 3 X= -2.926887168531D+00 Y= -2.038746536550D+00 Z= -1.925555801477D-01
I= 4 X= -2.473945981157D+00 Y= -9.234170889509D-01 Z= 2.349812723045D+00
I= 5 X= 4.164253740545D+00 Y= 2.287922993143D+00 Z= -1.788113954566D+00
I= 6 X= 2.043743672491D+00 Y= 6.502433117715D-01 Z= -2.750143080608D+00

I= 7 X= 5.790475666637D+00 Y= 9.664532199646D-01 Z= -2.403112355094D+00
I= 8 X= 3.355129925901D+00 Y= 3.646041089454D+00 Z= -3.006358869375D+00
I= 9 X= -2.677643750110D+00 Y= -2.395547942630D+00 Z= 4.784110692225D+00
I= 10 X= -4.834856221544D+00 Y= -2.877054502581D+00 Z= 5.047839316350D+00
I= 11 X= -1.691470375444D+00 Y= -4.358019010585D+00 Z= 4.831463655485D+00
I= 12 X= -1.932930735335D+00 Y= -1.723155721996D+00 Z= 6.816625744492D+00
I= 13 X= -2.078610190244D+00 Y= 3.567979369971D+00 Z= 4.143168353846D+00
I= 14 X= -3.805819690242D+00 Y= 4.412440959487D+00 Z= 4.320203870029D+00
I= 15 X= -1.244852313304D+00 Y= 2.773395911712D+00 Z= 5.838031134877D+00
I= 16 X= -4.102107195251D-01 Y= 5.134576716365D+00 Z= 3.586056142775D+00
I= 17 X= -2.540796943948D+00 Y= 5.018490845114D+00 Z= -1.617401426889D+00
I= 18 X= -4.493705681277D+00 Y= 5.594607506304D+00 Z= -1.428258538847D+00
I= 19 X= -1.623578942729D+00 Y= 6.307062108036D+00 Z= -1.728344392635D-01
I= 20 X= -1.883247827076D+00 Y= 5.167643842463D+00 Z= -3.748005452351D+00
I= 21 X= -3.521961651189D+00 Y= -9.469753154994D-02 Z= -4.761282171147D+00
I= 22 X= -5.516876009898D+00 Y= 3.552985506727D-01 Z= -5.477992883553D+00
I= 23 X= -2.591230773031D+00 Y= 1.227900214154D+00 Z= -5.929702356917D+00
I= 24 X= -2.942400591739D+00 Y= -1.716891414954D+00 Z= -5.873137603015D+00
I= 25 X= -3.543696475894D+00 Y= -4.653435305858D+00 Z= -1.034448435531D+00
I= 26 X= -2.524656135632D+00 Y= -5.372886144033D+00 Z= -2.815025657595D+00
I= 27 X= -2.478939447757D+00 Y= -5.782253662379D+00 Z= 5.318163652287D-01
I= 28 X= -5.822242069859D+00 Y= -5.200742821748D+00 Z= -1.341595362034D+00
I= 29 X= 3.435495877823D+00 Y= -3.553371559220D+00 Z= -1.239243582747D+00
I= 30 X= 3.504903398513D+00 Y= -3.020025440409D+00 Z= 1.557574840893D+00
I= 31 X= 2.367454978537D+00 Y= -5.292093039410D+00 Z= -1.732927544798D+00
I= 32 X= 4.972130257916D+00 Y= -3.061280242999D+00 Z= -2.696833870168D+00
I= 33 X= 5.030598770362D+00 Y= -2.176348538451D+00 Z= 2.119197542220D+00
I= 34 X= 2.418821832320D+00 Y= -4.352366954591D+00 Z= 2.763123039628D+00
I= 35 X= 8.465638626460D-01 Y= -8.432933923537D-02 Z= -1.694959580142D-01
I= 36 X= 3.772318253218D+00 Y= 2.825022199226D+00 Z= 8.946304814319D-01

I= 37 X= 5.228530942242D+00 Y= 2.307849588482D+00 Z= 2.368638805161D+00

I= 38 X= 2.650321667293D+00 Y= 4.266609430590D+00 Z= 1.376758345048D+00

Forward Direction:

Total Energy: -651.6086643 Hartrees

Potential Energy: -651.8217919 Hartress

Kinetic Energy: 0.2131276 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.544950618068D+13 Y= 1.438417643258D+13 Z= 1.341306009538D+13

I= 1 X= -1.569147949359D+13 Y= 3.208438178754D+12 Z= -1.537800991514D+13

I= 2 X= 1.630048197285D+12 Y= -3.974435708775D+12 Z= 2.789362818479D+13

I= 3 X= 8.237960423514D+12 Y= 7.622532501364D+12 Z= -9.353785463950D+11

I= 4 X= -1.443172348341D+13 Y= -4.810965223127D+12 Z= -2.553029067203D+13

I= 5 X= -8.860505829573D+12 Y= -1.500245099698D+13 Z= 2.109402427279D+13

I= 6 X= 6.158095539005D+13 Y= -4.583299625274D+13 Z= -4.298010389067D+13

I= 7 X= 1.383995154012D+13 Y= -5.244777464950D+12 Z= -7.501916731066D+13

I= 8 X= -2.844750470748D+13 Y= 1.416087399819D+14 Z= 1.351995003061D+13

I= 9 X= 1.867340032263D+13 Y= -1.218422555310D+13 Z= 7.365554540269D+12

I= 10 X= -5.655532352013D+12 Y= -2.091432205919D+13 Z= -9.407143121918D+13

I= 11 X= -3.887428558068D+13 Y= 6.379479140706D+13 Z= 3.536123923530D+13

I= 12 X= -4.616933919166D+13 Y= -1.563348922487D+13 Z= -1.005273976252D+14

I= 13 X= 2.418657633394D+13 Y= -6.175730772429D+12 Z= -5.500038657511D+12

I= 14 X= -5.437745656331D+13 Y= 2.286626890017D+13 Z= 3.320521932601D+13

I= 15 X= -9.364968779020D+13 Y= 2.140284764228D+13 Z= -9.393837821905D+13

I= 16 X= -6.509481177724D+13 Y= 3.470386214525D+12 Z= -9.215578323368D+13

I= 17 X= 6.742458875507D+11 Y= -2.479528736111D+13 Z= 8.771965006244D+12

I= 18 X= -1.300594922060D+14 Y= 4.631617600724D+13 Z= -2.161953123604D+13

I= 19 X= 2.289138393090D+13 Y= 9.840474262977D+11 Z= 8.037162810045D+13

I= 20 X= -1.201105747101D+14 Y= 5.093648489754D+13 Z= 3.527013609127D+13

I= 21 X= -2.476230577186D+13 Y= 2.474255666929D+13 Z= 5.319206011656D+12

I= 22 X= 1.401674683771D+14 Y= 2.393307583682D+13 Z= -2.623975396563D+13

I= 23 X= -3.290134818872D+13 Y= -7.657772992650D+13 Z= 3.137953919873D+13
I= 24 X= 1.553495454223D+13 Y= -3.176550170828D+13 Z= -1.878716145930D+13
I= 25 X= 1.165101513027D+13 Y= -2.037143780787D+13 Z= 3.752657052802D+13
I= 26 X= -1.782829935005D+13 Y= 3.192172365742D+13 Z= -1.240616829602D+14
I= 27 X= -1.361194390988D+13 Y= 7.985872600632D+13 Z= -4.587273859756D+13
I= 28 X= -1.957886093337D+13 Y= 7.823593776067D+13 Z= -7.361058127186D+13
I= 29 X= -1.844676069724D+12 Y= 2.015367267974D+13 Z= 1.401522630127D+13
I= 30 X= -1.242379849422D+12 Y= -1.545369402442D+13 Z= 4.325696977686D+12
I= 31 X= -8.031537071336D+13 Y= -8.311736123407D+13 Z= -3.807122867254D+13
I= 32 X= 3.340920832514D+13 Y= -5.133223300170D+13 Z= -3.564107822773D+13
I= 33 X= -2.180470800255D+13 Y= 6.984177161419D+13 Z= -1.109697949561D+14
I= 34 X= 1.215350323814D+13 Y= -1.303921799107D+13 Z= 1.802438297178D+13
I= 35 X= 1.970814947452D+12 Y= 3.611768948592D+11 Z= -2.659634041086D+12
I= 36 X= 1.928869857636D+13 Y= 1.227402503497D+13 Z= 6.245088909617D+12
I= 37 X= 6.888933482959D+13 Y= -7.759055057348D+13 Z= 1.031601646724D+14
I= 38 X= -1.850327319019D+12 Y= -4.058074500329D+13 Z= -2.182589407706D+13

Backward Direction:

Total Energy: -651.6086641 Hartrees

Potential Energy: -651.8217919 Hartress

Kinetic Energy: 0.2131278 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.587225303104D+13 Y= 1.425980610496D+13 Z= 1.340376925767D+13
I= 1 X= -1.548075048452D+13 Y= 2.757395293697D+12 Z= -1.612811128116D+13
I= 2 X= 1.355784275368D+12 Y= -3.561137480694D+12 Z= 2.724756530093D+13
I= 3 X= 8.065772232475D+12 Y= 7.660606173232D+12 Z= -1.840592189032D+12
I= 4 X= -1.309125904284D+13 Y= -4.920106869649D+12 Z= -2.638890358824D+13
I= 5 X= -8.768858111459D+12 Y= -1.562876386759D+13 Z= 1.547816499470D+13
I= 6 X= 9.869225171024D+13 Y= -1.168229654398D+13 Z= -2.685188602668D+13
I= 7 X= 2.145848111048D+13 Y= 1.956209812685D+12 Z= -7.432044464411D+13
I= 8 X= -1.812941859684D+13 Y= 1.500519535660D+14 Z= 1.544903054147D+13

I= 9 X= 1.914196090371D+13 Y= -1.198173976583D+13 Z= 6.855725665044D+12
I= 10 X= -5.498481853601D+12 Y= -1.988308174070D+13 Z= -9.526667876042D+13
I= 11 X= -3.898369144664D+13 Y= 6.380224649453D+13 Z= 3.528656321990D+13
I= 12 X= -4.584772988825D+13 Y= -1.555038457764D+13 Z= -1.008350215965D+14
I= 13 X= 2.427678444595D+13 Y= -6.237957145840D+12 Z= -5.723229899701D+12
I= 14 X= -5.424954693353D+13 Y= 2.248344634061D+13 Z= 3.322748491492D+13
I= 15 X= -9.333630067292D+13 Y= 2.108713290198D+13 Z= -9.446975864291D+13
I= 16 X= -6.515569511516D+13 Y= 3.555831473686D+12 Z= -9.209327290046D+13
I= 17 X= 8.259812331553D+11 Y= -2.493187610854D+13 Z= 8.712134705243D+12
I= 18 X= -1.298981274721D+14 Y= 4.623304406969D+13 Z= -2.197595220434D+13
I= 19 X= 2.289104528281D+13 Y= 8.518548122083D+11 Z= 8.052234132083D+13
I= 20 X= -1.199316658742D+14 Y= 5.071047038582D+13 Z= 3.519640357088D+13
I= 21 X= -2.506896956138D+13 Y= 2.474775665461D+13 Z= 4.851753642187D+12
I= 22 X= 1.399632869298D+14 Y= 2.437708616832D+13 Z= -2.734634517572D+13
I= 23 X= -3.270694142755D+13 Y= -7.674811888349D+13 Z= 3.098764725989D+13
I= 24 X= 1.512996596740D+13 Y= -3.177718789279D+13 Z= -1.933876159602D+13
I= 25 X= 1.164885378532D+13 Y= -2.042957117855D+13 Z= 3.739675977108D+13
I= 26 X= -1.806387913750D+13 Y= 3.158765150326D+13 Z= -1.241546841389D+14
I= 27 X= -1.340567000711D+13 Y= 8.005044279651D+13 Z= -4.594841494915D+13
I= 28 X= -1.953007720337D+13 Y= 7.822804896033D+13 Z= -7.337277812315D+13
I= 29 X= -2.648650290782D+12 Y= 2.062836753514D+13 Z= 1.339866437168D+13
I= 30 X= -1.179760324744D+12 Y= -1.531857483799D+13 Z= 3.851640907703D+12
I= 31 X= -8.025162546069D+13 Y= -8.355561722378D+13 Z= -3.836501056278D+13
I= 32 X= 3.238685290457D+13 Y= -5.040676065375D+13 Z= -3.659601589004D+13
I= 33 X= -2.166291501760D+13 Y= 6.977897313596D+13 Z= -1.114528288182D+14
I= 34 X= 1.263324642511D+13 Y= -1.311180154595D+13 Z= 1.771389887339D+13
I= 35 X= 1.777309391133D+12 Y= 2.824267230917D+11 Z= -1.906845074126D+12
I= 36 X= 1.694601231912D+13 Y= 9.474726068490D+12 Z= 4.840052467467D+12
I= 37 X= 7.161182263145D+13 Y= -7.583691324213D+13 Z= 9.970185643499D+13
I= 38 X= -2.016133241711D+11 Y= -4.069201529374D+13 Z= -2.405927725458D+13

Seed: 23568097734

CM Start Point Coordinates: bohr

I= 0 X= -2.617492734408D+00 Y= 2.283466188241D+00 Z= -7.194146138941D-01
I= 1 X= -3.014432265570D+00 Y= -2.444402061186D-02 Z= -2.062480694587D+00
I= 2 X= -2.526571871806D+00 Y= 1.700332715308D+00 Z= 2.071678029223D+00
I= 3 X= -2.794355026420D+00 Y= -2.039941403847D+00 Z= -3.583030190905D-01
I= 4 X= -2.237255206868D+00 Y= -9.226476390001D-01 Z= 2.158777349050D+00
I= 5 X= 4.345259659665D+00 Y= 2.502325152884D+00 Z= -1.108340450503D+00
I= 6 X= 2.429475020813D+00 Y= 6.145108316871D-01 Z= -3.131826607227D+00
I= 7 X= 5.699106210201D+00 Y= 1.679871841031D+00 Z= -2.121606148662D+00
I= 8 X= 4.067081756764D+00 Y= 4.516653415505D+00 Z= -1.996280459330D+00
I= 9 X= -1.852439873356D+00 Y= -2.359193403440D+00 Z= 4.828148443591D+00
I= 10 X= -3.602799520863D+00 Y= -2.386534092795D+00 Z= 5.878304119552D+00
I= 11 X= -1.356020103455D+00 Y= -4.463753238937D+00 Z= 4.793353646385D+00
I= 12 X= -3.975127343136D-01 Y= -1.253187999822D+00 Z= 5.663048525067D+00
I= 13 X= -2.298719286388D+00 Y= 3.735978169681D+00 Z= 3.929688071222D+00
I= 14 X= -3.759749512853D+00 Y= 4.767753083329D+00 Z= 4.696360733275D+00
I= 15 X= -1.014810904558D+00 Y= 3.669490760498D+00 Z= 5.460084221941D+00
I= 16 X= -1.352811302034D+00 Y= 5.620757901188D+00 Z= 3.169180299711D+00
I= 17 X= -2.794390397789D+00 Y= 4.995252998838D+00 Z= -1.712866398926D+00
I= 18 X= -4.579620121752D+00 Y= 5.709907495363D+00 Z= -2.010111886503D+00
I= 19 X= -1.488573056883D+00 Y= 5.981326529287D+00 Z= -2.930584325077D-01
I= 20 X= -2.012910092646D+00 Y= 5.511388025148D+00 Z= -3.410408998167D+00
I= 21 X= -3.671150805248D+00 Y= -2.111746937612D-01 Z= -4.818218236041D+00
I= 22 X= -5.449524120739D+00 Y= -7.896755838146D-01 Z= -5.134930732500D+00
I= 23 X= -2.852548368926D+00 Y= 1.252222119906D+00 Z= -6.209975830270D+00
I= 24 X= -2.820389698130D+00 Y= -1.980081557141D+00 Z= -5.451232726374D+00
I= 25 X= -3.392255409133D+00 Y= -4.580596851560D+00 Z= -8.487256340413D-01
I= 26 X= -3.561552261136D+00 Y= -5.432920264829D+00 Z= -2.642591688418D+00

I= 27 X= -2.663325848320D+00 Y= -6.072769979810D+00 Z= 1.140410598892D-01
I= 28 X= -5.570500459270D+00 Y= -4.612661932473D+00 Z= -2.428742787436D-01
I= 29 X= 2.675627992030D+00 Y= -3.458283332670D+00 Z= -1.221673413713D+00
I= 30 X= 3.075201452745D+00 Y= -3.135721665040D+00 Z= 1.399719710619D+00
I= 31 X= 1.540874591114D+00 Y= -4.906812275564D+00 Z= -1.982075709781D+00
I= 32 X= 4.289335662095D+00 Y= -3.242115681300D+00 Z= -2.475265369828D+00
I= 33 X= 4.855002058562D+00 Y= -2.625726860958D+00 Z= 1.784092659180D+00
I= 34 X= 2.225054726590D+00 Y= -4.140191533619D+00 Z= 2.954839093852D+00
I= 35 X= 8.642434866624D-01 Y= -6.142804166107D-02 Z= -2.023023635064D-01
I= 36 X= 3.946922040132D+00 Y= 2.256661660493D+00 Z= 1.526366187082D+00
I= 37 X= 5.567141321576D+00 Y= 1.675754201310D+00 Z= 2.578059656837D+00
I= 38 X= 2.983982955304D+00 Y= 3.833087572850D+00 Z= 2.257959035840D+00

Forward Direction:

Total Energy: -651.6117132 Hartrees

Potential Energy: -651.8028152 Hartress

Kinetic Energy: 0.1911021 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.690558598116D+13 Y= 2.021072570742D+13 Z= -1.475040973984D+13
I= 1 X= -1.042913240676D+13 Y= -1.040727861708D+13 Z= 2.981908820380D+12
I= 2 X= 2.057516562146D+13 Y= -2.291193552494D+13 Z= 2.206211617990D+13
I= 3 X= 6.346098801196D+12 Y= -7.846208274170D+12 Z= 1.301909224612D+13
I= 4 X= 4.840989697984D+12 Y= -1.571718212873D+13 Z= 1.787315098975D+13
I= 5 X= -7.152023994939D+12 Y= 3.101208068202D+13 Z= 8.670325044658D+12
I= 6 X= -1.880133544024D+13 Y= -3.543839845155D+13 Z= 1.148014500985D+13
I= 7 X= -7.731150754882D+13 Y= 7.920317010591D+13 Z= -3.071592013498D+13
I= 8 X= 8.877323679513D+13 Y= -6.721129760893D+13 Z= -3.773849617631D+13
I= 9 X= 3.161674447743D+12 Y= 1.771745811125D+13 Z= -2.874632945675D+12
I= 10 X= -5.751336600374D+13 Y= 4.839220745278D+13 Z= -8.117292105375D+12
I= 11 X= 1.224156331741D+14 Y= -1.440361182701D+14 Z= -5.439424955063D+12
I= 12 X= 1.003825953841D+14 Y= 2.285038892927D+12 Z= -4.393247319242D+13

I= 13 X= -1.924143337583D+13 Y= -1.075008694908D+13 Z= 2.501913221813D+11
I= 14 X= -3.229919028074D+12 Y= 3.879925855710D+13 Z= 2.999252520291D+13
I= 15 X= -9.824547322647D+13 Y= 2.307395179275D+13 Z= -2.286622033011D+13
I= 16 X= -5.418159097514D+13 Y= -2.955968590132D+13 Z= 3.273841802955D+13
I= 17 X= -9.110785770805D+12 Y= 7.434873706100D+11 Z= -2.436210567450D+12
I= 18 X= 7.030350287910D+13 Y= -1.366162841634D+13 Z= -4.363927680635D+13
I= 19 X= 6.068668871834D+13 Y= 7.882590334579D+13 Z= 5.011295361272D+13
I= 20 X= -3.174197180949D+13 Y= 5.209304615906D+13 Z= -4.353832553268D+12
I= 21 X= -7.505598689246D+10 Y= 1.524315671842D+13 Z= 3.524639164497D+12
I= 22 X= 1.910057032512D+13 Y= -2.085813875613D+13 Z= -9.632078382399D+13
I= 23 X= -6.081424697109D+13 Y= -4.620947503899D+13 Z= 1.342508465276D+13
I= 24 X= -1.413561903056D+13 Y= -8.688069969799D+13 Z= 3.923850622913D+13
I= 25 X= 4.808702748380D+12 Y= -1.389685479132D+13 Z= -1.076458474240D+13
I= 26 X= 2.857682835330D+13 Y= -2.207819275997D+13 Z= -6.914985801896D+13
I= 27 X= -1.953386391899D+13 Y= 4.033302361037D+13 Z= -5.425912436145D+13
I= 28 X= -1.218645260371D+14 Y= 4.680260062992D+13 Z= 6.804431096384D+13
I= 29 X= -3.985069374883D+12 Y= -1.170136690928D+13 Z= 1.416934503149D+13
I= 30 X= -9.848798754189D+12 Y= -1.961798670223D+13 Z= 4.626133876135D+12
I= 31 X= -4.775715962941D+13 Y= -5.060834746513D+13 Z= 7.271515757596D+13
I= 32 X= 9.819704629192D+13 Y= 2.686119427024D+13 Z= -7.922350844388D+13
I= 33 X= 8.142905645142D+13 Y= 4.425530835870D+13 Z= -2.938687484390D+13
I= 34 X= -4.240835910054D+13 Y= 1.535828735281D+14 Z= -1.107069325086D+14
I= 35 X= 2.749546265901D+12 Y= 8.555589025817D+11 Z= -1.319916250975D+12
I= 36 X= -7.969464545726D+11 Y= 3.066718710538D+12 Z= -1.488404473065D+13
I= 37 X= 2.421491887522D+12 Y= -1.445842821431D+13 Z= 8.453174460529D+13
I= 38 X= 1.810187727018D+13 Y= 2.863065252948D+13 Z= -7.451658931919D+12

Backward Direction:

Total Energy: -651.6117359 Hartrees

Potential Energy: -651.8028152 Hartress

Kinetic Energy: 0.1910793 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.758735285237D+13 Y= 2.001015279219D+13 Z= -1.476539313813D+13
I= 1 X= -1.008928822316D+13 Y= -1.113467870188D+13 Z= 1.772214983502D+12
I= 2 X= 2.013285823229D+13 Y= -2.224540651768D+13 Z= 2.102020595036D+13
I= 3 X= 6.068409674363D+12 Y= -7.784806590401D+12 Z= 1.155924773319D+13
I= 4 X= 7.002766285589D+12 Y= -1.589319564362D+13 Z= 1.648845980278D+13
I= 5 X= -7.004223060091D+12 Y= 3.000202143120D+13 Z= -3.864113665905D+11
I= 6 X= 4.104831749492D+13 Y= 1.963667916126D+13 Z= 3.749023728297D+13
I= 7 X= -6.502505043311D+13 Y= 9.081625376525D+13 Z= -2.958908508656D+13
I= 8 X= 1.054132880555D+14 Y= -5.359486669675D+13 Z= -3.462745424561D+13
I= 9 X= 3.917325453492D+12 Y= 1.804400838777D+13 Z= -3.696837615974D+12
I= 10 X= -5.726008953418D+13 Y= 5.005529609175D+13 Z= -1.004487634850D+13
I= 11 X= 1.222391935503D+14 Y= -1.440240953970D+14 Z= -5.559855500210D+12
I= 12 X= 1.009012570209D+14 Y= 2.419062342830D+12 Z= -4.442858057683D+13
I= 13 X= -1.909595411228D+13 Y= -1.085043986743D+13 Z= -1.097507885838D+11
I= 14 X= -3.023638259440D+12 Y= 3.818187788639D+13 Z= 3.002843306879D+13
I= 15 X= -9.774007159506D+13 Y= 2.256479636844D+13 Z= -2.372318132943D+13
I= 16 X= -5.427977796281D+13 Y= -2.942188772499D+13 Z= 3.283922889213D+13
I= 17 X= -8.866081095308D+12 Y= 5.232097192121D+11 Z= -2.532699326334D+12
I= 18 X= 7.056373693610D+13 Y= -1.379569589346D+13 Z= -4.421407946952D+13
I= 19 X= 6.068614256801D+13 Y= 7.861271537666D+13 Z= 5.035600989896D+13
I= 20 X= -3.145344424022D+13 Y= 5.172855093356D+13 Z= -4.472741516211D+12
I= 21 X= -5.696148700719D+11 Y= 1.525154277885D+13 Z= 2.770775385917D+12
I= 22 X= 1.877128544671D+13 Y= -2.014208012532D+13 Z= -9.810539137453D+13
I= 23 X= -6.050072580282D+13 Y= -4.648426251454D+13 Z= 1.279307772536D+13
I= 24 X= -1.478874699695D+13 Y= -8.689954608073D+13 Z= 3.834893673763D+13
I= 25 X= 4.805217135256D+12 Y= -1.399060689501D+13 Z= -1.097393147858D+13
I= 26 X= 2.819690714964D+13 Y= -2.261695331159D+13 Z= -6.929984168278D+13
I= 27 X= -1.920120451230D+13 Y= 4.064220664993D+13 Z= -5.438116815987D+13
I= 28 X= -1.217858521641D+14 Y= 4.678987830218D+13 Z= 6.842781780375D+13

I= 29 X= -5.281644352377D+12 Y= -1.093582312339D+13 Z= 1.317501119989D+13
I= 30 X= -9.747811798637D+12 Y= -1.940007902314D+13 Z= 3.861620262651D+12
I= 31 X= -4.765435720965D+13 Y= -5.131512603626D+13 Z= 7.224137342486D+13
I= 32 X= 9.654828638975D+13 Y= 2.835371014116D+13 Z= -8.076354323845D+13
I= 33 X= 8.165772701181D+13 Y= 4.415403280499D+13 Z= -3.016586701076D+13
I= 34 X= -4.163467382899D+13 Y= 1.534658175129D+14 Z= -1.112076524307D+14
I= 35 X= 2.437478470707D+12 Y= 7.285579374515D+11 Z= -1.058881018694D+11
I= 36 X= -4.575013330099D+12 Y= -1.447730745562D+12 Z= -1.714995704769D+13
I= 37 X= 6.812067428547D+12 Y= -1.163032474594D+13 Z= 7.895450618726D+13
I= 38 X= 2.076077012186D+13 Y= 2.845120614225D+13 Z= -1.105345195503D+13

Seed: 24369831866

CM Start Point Coordinates: bohr

I= 0 X= -2.509248899659D+00 Y= 2.426836644333D+00 Z= -8.571993669450D-01
I= 1 X= -3.124480374013D+00 Y= -7.159313403221D-02 Z= -2.015443233787D+00
I= 2 X= -2.310500290173D+00 Y= 1.745538323664D+00 Z= 1.877102352875D+00
I= 3 X= -2.887838816900D+00 Y= -2.007300877040D+00 Z= -1.316601261442D-01
I= 4 X= -2.391991465116D+00 Y= -7.601237190207D-01 Z= 2.341363632235D+00
I= 5 X= 4.260138534529D+00 Y= 2.472518533380D+00 Z= -1.021584434576D+00
I= 6 X= 2.465309504907D+00 Y= 9.688086682509D-01 Z= -2.840815507685D+00
I= 7 X= 5.801235392585D+00 Y= 1.240650111468D+00 Z= -1.965186725956D+00
I= 8 X= 3.482893706078D+00 Y= 4.106066706565D+00 Z= -1.814574159497D+00
I= 9 X= -2.193655490508D+00 Y= -2.138512098492D+00 Z= 4.667155993771D+00
I= 10 X= -4.205672865277D+00 Y= -3.291909297240D+00 Z= 5.206491464973D+00
I= 11 X= -8.437096614197D-01 Y= -3.960711752128D+00 Z= 4.340133548640D+00
I= 12 X= -1.256189551980D+00 Y= -8.871290575053D-01 Z= 6.226580476689D+00
I= 13 X= -1.969968257177D+00 Y= 3.731696972361D+00 Z= 3.853108442000D+00
I= 14 X= -4.044647887313D+00 Y= 3.999690725481D+00 Z= 4.688924902746D+00
I= 15 X= -1.067980208009D+00 Y= 2.998024644803D+00 Z= 5.453536066601D+00
I= 16 X= -1.111436031752D+00 Y= 5.462188731222D+00 Z= 2.831138614404D+00

I= 17 X= -2.564250282677D+00 Y= 4.928418015517D+00 Z= -1.944872233944D+00
I= 18 X= -4.488555211545D+00 Y= 5.608356683830D+00 Z= -2.003922544527D+00
I= 19 X= -1.273722020187D+00 Y= 6.514956527405D+00 Z= -8.012254339881D-01
I= 20 X= -1.606274251622D+00 Y= 4.910481992433D+00 Z= -3.806334990779D+00
I= 21 X= -3.975205380414D+00 Y= -3.765579100422D-01 Z= -4.666878823817D+00
I= 22 X= -6.156664597019D+00 Y= -5.818012677684D-01 Z= -5.122532605732D+00
I= 23 X= -3.349810482755D+00 Y= 1.151162442523D+00 Z= -6.116347181217D+00
I= 24 X= -3.297044785550D+00 Y= -2.126932735291D+00 Z= -5.485868336986D+00
I= 25 X= -3.318765144219D+00 Y= -4.740060031919D+00 Z= -7.923184116503D-01
I= 26 X= -3.071755112251D+00 Y= -5.366560903997D+00 Z= -2.712728928968D+00
I= 27 X= -2.518235743333D+00 Y= -5.761801109104D+00 Z= 7.135091191132D-01
I= 28 X= -5.393972239326D+00 Y= -5.227539605590D+00 Z= -2.912018246787D-01
I= 29 X= 3.393934639976D+00 Y= -3.235301473164D+00 Z= -1.638113849610D+00
I= 30 X= 3.117974998757D+00 Y= -3.348721248895D+00 Z= 1.074597236718D+00
I= 31 X= 2.275309729910D+00 Y= -4.357656552767D+00 Z= -3.240216789312D+00
I= 32 X= 5.052196474812D+00 Y= -2.261738871337D+00 Z= -2.938242972826D+00
I= 33 X= 4.708367066298D+00 Y= -2.323768582058D+00 Z= 2.744499894178D+00
I= 34 X= 1.699738282376D+00 Y= -5.088209365957D+00 Z= 1.854456309161D+00
I= 35 X= 8.358840639315D-01 Y= -5.537989000202D-02 Z= -1.515402071745D-01
I= 36 X= 3.867975345193D+00 Y= 2.225796569932D+00 Z= 1.662155949771D+00
I= 37 X= 5.122459917002D+00 Y= 8.913334536072D-01 Z= 2.768712569762D+00
I= 38 X= 3.131615851037D+00 Y= 3.835179744960D+00 Z= 2.661217192376D+00

Forward Direction:

Total Energy: -651.6046557 Hartrees

Potential Energy: -651.7858510 Hartress

Kinetic Energy: 0.1811953 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 4.507325113540D+12 Y= 9.546199952488D+12 Z= 2.851652854242D+13

I= 1 X= -6.806033980573D+12 Y= 2.156497765206D+12 Z= -2.268128311453D+13

I= 2 X= 1.597727478788D+13 Y= -1.083943462168D+13 Z= -2.756918164074D+13

I= 3 X= -1.892591755775D+13 Y= 1.733136751289D+13 Z= 1.548281670000D+13
I= 4 X= -3.442115552284D+12 Y= -3.582862286069D+12 Z= -1.597820490452D+13
I= 5 X= 1.038448780540D+13 Y= -1.819793020605D+13 Z= -7.862202873539D+12
I= 6 X= -1.106889374351D+14 Y= -2.047221168657D+13 Z= -3.248225628730D+13
I= 7 X= 7.557745469476D+13 Y= 2.072751872005D+13 Z= -4.679467306525D+13
I= 8 X= 1.511173599247D+13 Y= 9.939380682802D+13 Z= -5.788427810694D+13
I= 9 X= 5.582862190166D+12 Y= 1.386329148643D+13 Z= 6.654016112580D+12
I= 10 X= 9.184475747317D+13 Y= 5.608746881907D+13 Z= 5.716147921724D+12
I= 11 X= -2.871955764248D+13 Y= -2.372722454179D+13 Z= 4.132782010107D+12
I= 12 X= -1.500343876798D+14 Y= -2.702759311341D+13 Z= -1.220658092452D+14
I= 13 X= -1.777818938794D+13 Y= 9.898436656021D+12 Z= -1.816754588170D+12
I= 14 X= -2.716878959784D+13 Y= 2.667081646907D+13 Z= 1.394659200009D+14
I= 15 X= -1.352473910531D+13 Y= -9.001271383030D+12 Z= -1.830604626799D+12
I= 16 X= 1.012286920368D+13 Y= 1.013517441768D+14 Z= -3.859770518040D+13
I= 17 X= -1.400739175964D+13 Y= -2.607514217497D+13 Z= 2.126505988502D+13
I= 18 X= -8.109593728091D+13 Y= 5.028565433704D+13 Z= 3.323895132621D+13
I= 19 X= -1.042859217129D+13 Y= 3.357664307618D+13 Z= -7.002830902179D+12
I= 20 X= 4.361129493546D+13 Y= -6.816619687996D+13 Z= 7.307899029253D+12
I= 21 X= -1.432553735349D+12 Y= 1.847081077871D+13 Z= 1.020306523088D+13
I= 22 X= -1.135842668243D+14 Y= 3.533887650034D+13 Z= -1.123217227123D+13
I= 23 X= 5.265055083221D+12 Y= -7.316073285333D+13 Z= 9.704163213659D+13
I= 24 X= 4.040147261124D+13 Y= -2.534815845585D+13 Z= 3.906398272309D+13
I= 25 X= -8.822114556382D+12 Y= -1.696479715658D+13 Z= -8.277805111882D+12
I= 26 X= -3.849778619297D+13 Y= -3.101906826976D+13 Z= -5.011910560427D+12
I= 27 X= 1.517523187436D+13 Y= 1.068469986449D+13 Z= -2.153984841323D+13
I= 28 X= 4.446528231700D+13 Y= 2.249662245543D+13 Z= -4.368127259970D+13
I= 29 X= 1.724873299798D+13 Y= -7.519332235832D+12 Z= -6.783559742934D+12
I= 30 X= -9.008837802313D+12 Y= 1.496730860767D+11 Z= 1.487097794253D+13
I= 31 X= -7.130214173693D+13 Y= -8.569629022237D+13 Z= -1.827105647339D+12
I= 32 X= 1.065863220569D+13 Y= -1.991032809403D+13 Z= 2.254105895055D+13

I= 33 X= 9.859794256433D+12 Y= -8.002314057468D+13 Z= 5.412264377534D+13
I= 34 X= 4.642313378881D+13 Y= 4.965412047940D+13 Z= -7.959149260100D+13
I= 35 X= 3.755243709756D+12 Y= 5.692894574457D+11 Z= 4.411470111207D+11
I= 36 X= -1.159444177629D+13 Y= 6.353621839093D+12 Z= 2.698881005168D+12
I= 37 X= -2.957503671593D+13 Y= 3.923430586610D+13 Z= -6.882954469585D+13
I= 38 X= 9.569789788852D+11 Y= -1.265379368555D+14 Z= -5.257932851040D+13

Backward Direction:

Total Energy: -651.6046413 Hartrees

Potential Energy: -651.7858510 Hartress

Kinetic Energy: 0.1812097 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.915192617088D+12 Y= 9.371997088651D+12 Z= 2.850351506531D+13
I= 1 X= -6.510870350763D+12 Y= 1.524731619703D+12 Z= -2.373193409637D+13
I= 2 X= 1.559311916371D+13 Y= -1.026053661137D+13 Z= -2.847410813620D+13
I= 3 X= -1.916709788374D+13 Y= 1.738469649388D+13 Z= 1.421490326437D+13
I= 4 X= -1.564555607232D+12 Y= -3.735734662944D+12 Z= -1.718084569570D+13
I= 5 X= 1.051285681071D+13 Y= -1.907519328604D+13 Z= -1.572821714878D+13
I= 6 X= -5.870793644730D+13 Y= 2.736194479534D+13 Z= -9.891805619391D+12
I= 7 X= 8.624856652332D+13 Y= 3.081378795756D+13 Z= -4.581598712730D+13
I= 8 X= 2.956405907909D+13 Y= 1.112200359565D+14 Z= -5.518225619218D+13
I= 9 X= 6.239164999853D+12 Y= 1.414690900807D+13 Z= 5.939909686467D+12
I= 10 X= 9.206473475578D+13 Y= 5.753190514002D+13 Z= 4.041990201229D+12
I= 11 X= -2.887280010859D+13 Y= -2.371678236036D+13 Z= 4.028184907928D+12
I= 12 X= -1.495839163843D+14 Y= -2.691119021353D+13 Z= -1.224966915813D+14
I= 13 X= -1.765183681091D+13 Y= 9.811277501185D+12 Z= -2.129373797904D+12
I= 14 X= -2.698962931087D+13 Y= 2.613460508070D+13 Z= 1.394971069357D+14
I= 15 X= -1.308578445645D+13 Y= -9.443486287760D+12 Z= -2.574897843259D+12
I= 16 X= 1.003759121329D+13 Y= 1.014714255275D+14 Z= -3.851014828978D+13
I= 17 X= -1.379485930238D+13 Y= -2.626645912214D+13 Z= 2.118125685391D+13
I= 18 X= -8.086991714902D+13 Y= 5.016921319191D+13 Z= 3.273972005879D+13

I= 19 X= -1.042906652871D+13 Y= 3.339148370798D+13 Z= -6.791730107129D+12
I= 20 X= 4.386188873847D+13 Y= -6.848277058850D+13 Z= 7.204623462484D+12
I= 21 X= -1.862091160656D+12 Y= 1.847809429234D+13 Z= 9.548314668957D+12
I= 22 X= -1.138702594201D+14 Y= 3.596079229500D+13 Z= -1.278215096608D+13
I= 23 X= 5.537356482045D+12 Y= -7.339939302123D+13 Z= 9.649271746041D+13
I= 24 X= 3.983421375590D+13 Y= -2.536452703845D+13 Z= 3.829136817385D+13
I= 25 X= -8.825141904492D+12 Y= -1.704622332795D+13 Z= -8.459628269231D+12
I= 26 X= -3.882775777673D+13 Y= -3.148699600555D+13 Z= -5.142175320416D+12
I= 27 X= 1.546415533521D+13 Y= 1.095323348241D+13 Z= -2.164584666713D+13
I= 28 X= 4.453361264709D+13 Y= 2.248557278051D+13 Z= -4.334818679910D+13
I= 29 X= 1.612262345643D+13 Y= -6.854437280284D+12 Z= -7.647164883682D+12
I= 30 X= -8.921127968916D+12 Y= 3.389316489800D+11 Z= 1.420697771809D+13
I= 31 X= -7.121285512672D+13 Y= -8.631014603705D+13 Z= -2.238599668702D+12
I= 32 X= 9.226640772833D+12 Y= -1.861403872389D+13 Z= 2.120349814120D+13
I= 33 X= 1.005840066600D+13 Y= -8.011110106223D+13 Z= 5.344606854472D+13
I= 34 X= 4.709509984056D+13 Y= 4.955245424446D+13 Z= -8.002638105159D+13
I= 35 X= 3.484204605389D+12 Y= 4.589857720650D+11 Z= 1.495562456126D+12
I= 36 X= -1.487579243475D+13 Y= 2.432703500132D+12 Z= 7.308764381243D+11
I= 37 X= -2.576170613998D+13 Y= 4.169058826449D+13 Z= -7.367352325831D+13
I= 38 X= 3.266297498576D+12 Y= -1.266937907755D+14 Z= -5.570758067767D+13

Seed: 25704926461

CM Start Point Coordinates: bohr

I= 0 X= -2.582470915500D+00 Y= 2.335115372572D+00 Z= -6.358193850650D-01
I= 1 X= -3.092150118609D+00 Y= -6.506936559968D-02 Z= -1.951261069040D+00
I= 2 X= -2.381029576385D+00 Y= 1.860595042937D+00 Z= 1.979895840110D+00
I= 3 X= -2.938367136324D+00 Y= -2.009812957294D+00 Z= -1.118587890073D-01
I= 4 X= -2.478239448628D+00 Y= -7.747060119941D-01 Z= 2.356381154574D+00
I= 5 X= 4.282920371180D+00 Y= 2.556610096829D+00 Z= -6.497988825931D-01
I= 6 X= 2.323742871790D+00 Y= 1.488476931746D+00 Z= -2.731572691897D+00

I= 7 X= 6.065521697514D+00 Y= 1.549868237492D+00 Z= -1.370312072143D+00
I= 8 X= 4.091117493115D+00 Y= 4.431351376484D+00 Z= -1.741376104168D+00
I= 9 X= -2.554235337133D+00 Y= -2.025571850143D+00 Z= 4.845012233848D+00
I= 10 X= -4.256385816365D+00 Y= -4.334774650574D-01 Z= 6.225458843752D+00
I= 11 X= -3.620029578340D+00 Y= -4.332432312796D+00 Z= 4.606867187787D+00
I= 12 X= -1.711574004805D-01 Y= -2.030437735431D+00 Z= 5.760906265087D+00
I= 13 X= -2.006320732618D+00 Y= 3.822917604268D+00 Z= 3.956608917994D+00
I= 14 X= -4.128046458216D+00 Y= 4.431094528963D+00 Z= 4.638218889846D+00
I= 15 X= -8.123954457459D-01 Y= 3.087584260410D+00 Z= 5.348638519537D+00
I= 16 X= -1.143447776783D+00 Y= 5.535435997024D+00 Z= 3.106794898598D+00
I= 17 X= -2.641429883685D+00 Y= 4.835146044138D+00 Z= -2.056147851483D+00
I= 18 X= -4.550238511485D+00 Y= 5.730478593458D+00 Z= -2.070427532869D+00
I= 19 X= -1.612786771891D+00 Y= 6.400912047045D+00 Z= -1.178559569735D+00
I= 20 X= -2.112667009975D+00 Y= 4.722909975550D+00 Z= -3.855982866886D+00
I= 21 X= -3.689031404722D+00 Y= -4.614981832024D-01 Z= -4.691085030459D+00
I= 22 X= -5.592653096617D+00 Y= -1.169967677102D+00 Z= -5.168514923327D+00
I= 23 X= -3.238900600354D+00 Y= 1.315491761404D+00 Z= -5.906011799480D+00
I= 24 X= -2.572816253047D+00 Y= -2.065961725606D+00 Z= -5.356173257906D+00
I= 25 X= -3.139416567047D+00 Y= -4.693048261837D+00 Z= -5.874807526766D-01
I= 26 X= -2.758240657739D+00 Y= -5.257116067025D+00 Z= -2.428584992203D+00
I= 27 X= -1.613737442601D+00 Y= -5.755641881101D+00 Z= 4.784902856913D-01
I= 28 X= -4.925857575932D+00 Y= -5.713900727490D+00 Z= 3.307618456855D-01
I= 29 X= 2.820858012624D+00 Y= -3.279467120397D+00 Z= -2.034896453745D+00
I= 30 X= 3.355050904151D+00 Y= -3.370783277371D+00 Z= 6.819875367689D-01
I= 31 X= 1.647525568414D+00 Y= -4.898827109213D+00 Z= -2.675481216643D+00
I= 32 X= 4.252282608279D+00 Y= -2.424574912779D+00 Z= -3.147434596777D+00
I= 33 X= 5.161927835529D+00 Y= -2.551314067074D+00 Z= 1.107296047679D+00
I= 34 X= 2.471220445629D+00 Y= -4.606453719283D+00 Z= 1.957614308907D+00
I= 35 X= 8.848216219449D-01 Y= -7.705919325544D-02 Z= -1.944724999229D-01
I= 36 X= 3.642670665812D+00 Y= 2.312500851926D+00 Z= 1.870549601121D+00

I= 37 X= 4.757608998955D+00 Y= 1.070993287450D+00 Z= 3.015283054865D+00

I= 38 X= 2.491658018207D+00 Y= 3.811688118137D+00 Z= 2.900662567939D+00

Forward Direction:

Total Energy: -651.6079289 Hartrees

Potential Energy: -651.7979181 Hartress

Kinetic Energy: 0.1899892 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.866284023118D+12 Y= 1.268999844351D+13 Z= -5.251213855373D+12

I= 1 X= -2.871730194133D+12 Y= -1.603138443049D+13 Z= 1.938450648103D+12

I= 2 X= 5.027222753426D+12 Y= 2.130033233215D+13 Z= -3.828693038786D+12

I= 3 X= 7.151525053681D+12 Y= 2.982309299587D+12 Z= -1.267626635792D+13

I= 4 X= 6.679984415449D+12 Y= 6.448320370130D+11 Z= 1.281258422424D+13

I= 5 X= -7.633036608650D+12 Y= 4.322423084982D+12 Z= -2.588110175808D+13

I= 6 X= -7.899485147162D+13 Y= 2.468672845686D+13 Z= 4.778849662611D+13

I= 7 X= 4.740485053689D+13 Y= -5.334491381411D+13 Z= 1.635919637362D+13

I= 8 X= -2.588200179315D+13 Y= -8.215305875612D+13 Z= 4.877620590559D+13

I= 9 X= 1.589029571645D+13 Y= 1.304068320488D+13 Z= -3.667267686427D+12

I= 10 X= -4.752670342210D+13 Y= -2.966316876669D+13 Z= -2.454082110243D+13

I= 11 X= 6.578344856813D+13 Y= -8.877167527418D+13 Z= -2.027144479900D+11

I= 12 X= 2.336788271871D+12 Y= -9.368707485946D+13 Z= -5.580284868821D+12

I= 13 X= -1.635773907745D+13 Y= -1.013922444244D+13 Z= 1.456594882864D+13

I= 14 X= -1.208086793224D+14 Y= -5.271453257252D+12 Z= 8.849369307108D+13

I= 15 X= -3.917352730290D+13 Y= 1.012205217617D+14 Z= -1.903622595187D+13

I= 16 X= 5.897776459168D+13 Y= 7.425877498239D+13 Z= -7.733788239543D+13

I= 17 X= -1.256879148525D+13 Y= 4.780603030313D+12 Z= -1.267732364380D+13

I= 18 X= -1.365990632027D+13 Y= 5.998995842903D+13 Z= 3.154304256908D+13

I= 19 X= -5.418838649395D+13 Y= -2.251669595447D+13 Z= 1.316572204354D+14

I= 20 X= 2.036072634974D+13 Y= -8.117607155491D+13 Z= -1.126121735089D+14

I= 21 X= 4.581175560227D+12 Y= 1.882815116811D+11 Z= 5.500177296813D+12

I= 22 X= 7.472677343899D+12 Y= -8.781795312952D+13 Z= -2.983431667475D+13

I= 23 X= 4.583526864454D+13 Y= -3.715966088748D+13 Z= 4.715174848877D+13
I= 24 X= -8.693919379155D+13 Y= 4.759238205440D+13 Z= 1.163735402869D+14
I= 25 X= -1.105041076331D+13 Y= -4.936666026482D+12 Z= -1.659533067116D+13
I= 26 X= -5.407629892859D+13 Y= -5.049982792951D+13 Z= 6.467661889114D+13
I= 27 X= -3.248190801202D+13 Y= 6.117274256597D+12 Z= 2.982604786345D+13
I= 28 X= 1.110860802145D+14 Y= 4.152365159257D+12 Z= -1.193193883736D+13
I= 29 X= -2.825168052016D+13 Y= -8.674142393998D+12 Z= 2.558443013624D+13
I= 30 X= 1.699546557119D+13 Y= -1.135666970198D+13 Z= -1.094198385365D+13
I= 31 X= 5.306059369319D+13 Y= 1.041981702474D+13 Z= 7.919088877676D+12
I= 32 X= 9.126095983092D+13 Y= -2.402806162110D+13 Z= -1.089117719235D+14
I= 33 X= 3.813639767670D+13 Y= 6.178696723343D+13 Z= 5.139915345556D+13
I= 34 X= -1.075225799752D+14 Y= 2.268402828283D+13 Z= 1.532073759958D+13
I= 35 X= 1.505789946719D+12 Y= 1.030710658187D+12 Z= -8.962859581499D+11
I= 36 X= 5.621110035637D+12 Y= -4.685385443789D+12 Z= 2.168460245097D+13
I= 37 X= -8.827152860669D+12 Y= -1.027247660086D+14 Z= 2.638006933566D+13
I= 38 X= -2.991411214639D+13 Y= 9.943300505830D+13 Z= -4.975230560478D+13

Backward Direction:

Total Energy: -651.6079394 Hartrees

Potential Energy: -651.7979181 Hartress

Kinetic Energy: 0.1899786 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.633253919674D+12 Y= 1.262144197749D+13 Z= -5.256335228156D+12
I= 1 X= -2.755570363012D+12 Y= -1.628001211306D+13 Z= 1.524973416205D+12
I= 2 X= 4.876040667477D+12 Y= 2.152815408500D+13 Z= -4.184821295912D+12
I= 3 X= 7.056610019393D+12 Y= 3.003296591995D+12 Z= -1.317524589466D+13
I= 4 X= 7.418886588186D+12 Y= 5.846700534151D+11 Z= 1.233929233628D+13
I= 5 X= -7.582517772859D+12 Y= 3.977181589146D+12 Z= -2.897672331564D+13
I= 6 X= -5.853804811465D+13 Y= 4.351156665513D+13 Z= 5.667882959943D+13
I= 7 X= 5.160440099162D+13 Y= -4.937552457504D+13 Z= 1.674435221060D+13
I= 8 X= -2.019437888761D+13 Y= -7.749891899572D+13 Z= 4.983957001465D+13

I= 9 X= 1.614857965645D+13 Y= 1.315229913618D+13 Z= -3.948299879089D+12
I= 10 X= -4.744013270770D+13 Y= -2.909471973539D+13 Z= -2.519967557920D+13
I= 11 X= 6.572314094387D+13 Y= -8.876756581761D+13 Z= -2.438779949295D+11
I= 12 X= 2.514068485160D+12 Y= -9.364126521476D+13 Z= -5.749855961273D+12
I= 13 X= -1.630801380014D+13 Y= -1.017352539196D+13 Z= 1.444291946197D+13
I= 14 X= -1.207381718954D+14 Y= -5.482475954361D+12 Z= 8.850596649591D+13
I= 15 X= -3.900077940445D+13 Y= 1.010464908048D+14 Z= -1.932913796900D+13
I= 16 X= 5.894420396077D+13 Y= 7.430587484420D+13 Z= -7.730342491612D+13
I= 17 X= -1.248515063739D+13 Y= 4.705311420496D+12 Z= -1.271030381308D+13
I= 18 X= -1.357095748000D+13 Y= 5.994413373613D+13 Z= 3.134657316670D+13
I= 19 X= -5.418857316175D+13 Y= -2.258956429121D+13 Z= 1.317402978532D+14
I= 20 X= 2.045934600612D+13 Y= -8.130065719921D+13 Z= -1.126528169762D+14
I= 21 X= 4.412133748748D+12 Y= 1.911478955549D+11 Z= 5.242504240006D+12
I= 22 X= 7.360126717314D+12 Y= -8.757320199777D+13 Z= -3.044430126033D+13
I= 23 X= 4.594243118241D+13 Y= -3.725358412375D+13 Z= 4.693572649404D+13
I= 24 X= -8.716243501890D+13 Y= 4.758594030530D+13 Z= 1.160694825791D+14
I= 25 X= -1.105160215431D+13 Y= -4.968710797413D+12 Z= -1.666688605813D+13
I= 26 X= -5.420615721478D+13 Y= -5.068397800949D+13 Z= 6.462535398731D+13
I= 27 X= -3.236820395057D+13 Y= 6.222954011592D+12 Z= 2.978433289458D+13
I= 28 X= 1.111129712018D+14 Y= 4.148016623283D+12 Z= -1.180085496635D+13
I= 29 X= -2.869485400609D+13 Y= -8.412477070958D+12 Z= 2.524456364286D+13
I= 30 X= 1.702998323561D+13 Y= -1.128218815746D+13 Z= -1.120329705895D+13
I= 31 X= 5.309573189160D+13 Y= 1.017823784223D+13 Z= 7.757147933150D+12
I= 32 X= 9.069740840974D+13 Y= -2.351791490762D+13 Z= -1.094381607557D+14
I= 33 X= 3.821455800644D+13 Y= 6.175235092533D+13 Z= 5.113289143621D+13
I= 34 X= -1.072581318697D+14 Y= 2.264401816180D+13 Z= 1.514958992366D+13
I= 35 X= 1.399124172484D+12 Y= 9.873013212750D+11 Z= -4.813272427357D+11
I= 36 X= 4.329754657519D+12 Y= -6.228438749837D+12 Z= 2.091010635174D+13
I= 37 X= -7.326440059932D+12 Y= -1.017581111711D+14 Z= 2.447375135350D+13
I= 38 X= -2.900529403974D+13 Y= 9.937166970901D+13 Z= -5.098341001793D+13

Seed: 27693154100

CM Start Point Coordinates: bohr

I= 0 X= -2.674504623341D+00 Y= 2.514949446183D+00 Z= -6.627560072084D-01
I= 1 X= -3.045619132993D+00 Y= 2.786484017966D-01 Z= -2.072243525058D+00
I= 2 X= -2.170346514419D+00 Y= 1.629175694479D+00 Z= 2.070689359585D+00
I= 3 X= -2.920992232915D+00 Y= -1.969258436142D+00 Z= -4.688481089829D-01
I= 4 X= -2.413323921642D+00 Y= -1.029740285988D+00 Z= 2.053707631719D+00
I= 5 X= 4.058344740590D+00 Y= 2.311840995507D+00 Z= -1.746087136653D+00
I= 6 X= 2.783687943234D+00 Y= 3.048899136569D-01 Z= -2.891038640544D+00
I= 7 X= 5.764007599182D+00 Y= 1.099934471760D+00 Z= -2.181275272313D+00
I= 8 X= 3.776771261081D+00 Y= 3.668171178573D+00 Z= -3.537211724416D+00
I= 9 X= -2.473145433576D+00 Y= -2.709076019341D+00 Z= 4.414420612968D+00
I= 10 X= -4.067868654886D+00 Y= -2.386515522159D+00 Z= 5.549642682317D+00
I= 11 X= -2.225082691495D+00 Y= -4.844187207474D+00 Z= 3.887086064045D+00
I= 12 X= -9.542591039425D-01 Y= -2.200590070300D+00 Z= 5.794796776815D+00
I= 13 X= -1.625350010064D+00 Y= 3.237163054661D+00 Z= 4.366251225561D+00
I= 14 X= -3.447146068687D+00 Y= 3.290031064914D+00 Z= 5.124790364818D+00
I= 15 X= -3.134061558229D-02 Y= 2.805829706657D+00 Z= 5.240705401019D+00
I= 16 X= -1.145980488076D+00 Y= 5.032686343244D+00 Z= 3.464282079906D+00
I= 17 X= -2.767812181634D+00 Y= 5.078865786318D+00 Z= -1.501276858101D+00
I= 18 X= -4.744183216841D+00 Y= 5.779017007919D+00 Z= -1.556316909182D+00
I= 19 X= -1.546246509398D+00 Y= 6.193505730426D+00 Z= -6.215418343826D-01
I= 20 X= -1.655769149053D+00 Y= 5.328468026525D+00 Z= -3.317313814517D+00
I= 21 X= -3.950682728432D+00 Y= 9.576742844942D-02 Z= -4.825797325811D+00
I= 22 X= -6.349064284260D+00 Y= -4.705002574338D-01 Z= -4.823432074173D+00
I= 23 X= -3.856369587821D+00 Y= 1.915872443642D+00 Z= -6.299889305319D+00
I= 24 X= -3.090066963430D+00 Y= -1.456524466160D+00 Z= -5.759477897177D+00
I= 25 X= -3.273416335691D+00 Y= -4.654452810979D+00 Z= -8.460137531228D-01
I= 26 X= -3.117517555433D+00 Y= -5.597675363890D+00 Z= -2.920144595991D+00

I= 27 X= -2.380817798689D+00 Y= -5.783528710824D+00 Z= 5.399074317845D-01
I= 28 X= -5.629307110013D+00 Y= -4.814787364658D+00 Z= -7.992860310227D-01
I= 29 X= 3.217072945776D+00 Y= -3.927657207919D+00 Z= -3.525740216906D-01
I= 30 X= 3.019236498990D+00 Y= -2.910887031487D+00 Z= 2.226848095749D+00
I= 31 X= 1.731357572648D+00 Y= -5.435353915795D+00 Z= -9.593808669793D-01
I= 32 X= 4.657061645979D+00 Y= -3.808434971488D+00 Z= -1.943432102289D+00
I= 33 X= 4.476603640484D+00 Y= -2.000205970641D+00 Z= 3.400243117465D+00
I= 34 X= 1.713502561048D+00 Y= -3.387360610341D+00 Z= 3.803546762209D+00
I= 35 X= 8.997680390623D-01 Y= -5.926035139065D-02 Z= -2.386456060529D-01
I= 36 X= 3.537163252029D+00 Y= 3.000706301448D+00 Z= 9.434135673590D-01
I= 37 X= 5.064048123030D+00 Y= 2.105799335536D+00 Z= 2.434944358930D+00
I= 38 X= 2.544064544944D+00 Y= 4.743347588373D+00 Z= 1.200682833712D+00

Forward Direction:

Total Energy: -651.6182129 Hartrees

Potential Energy: -651.7760614 Hartress

Kinetic Energy: 0.1578485 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.682673345835D+13 Y= 1.464174300411D+13 Z= 2.066780312632D+13
I= 1 X= -4.299448420522D+10 Y= 1.621939664262D+13 Z= -1.569816144860D+13
I= 2 X= 5.881966148509D+12 Y= -5.606728142569D+12 Z= -3.168757930638D+13
I= 3 X= -1.002311905305D+13 Y= 1.371647070675D+12 Z= 1.701490630719D+13
I= 4 X= 1.908775522594D+13 Y= 6.056142594403D+12 Z= -7.279390733052D+12
I= 5 X= 6.178028952974D+12 Y= -6.239485927992D+12 Z= 1.275824266172D+13
I= 6 X= 5.925980310678D+13 Y= -2.716360823504D+13 Z= -7.081276734271D+13
I= 7 X= -1.261733056818D+14 Y= 5.535649482965D+13 Z= 4.879273070641D+13
I= 8 X= -2.483849773086D+13 Y= -1.937913738784D+13 Z= -2.634369019398D+13
I= 9 X= 1.160759619190D+13 Y= 1.065539975118D+13 Z= 1.636804687910D+13
I= 10 X= -3.658284616077D+13 Y= 1.110050222960D+13 Z= 3.112305608373D+13
I= 11 X= -6.560526760376D+12 Y= 2.981743891127D+13 Z= -5.405349423803D+13
I= 12 X= -8.782830773184D+13 Y= -1.003481641705D+14 Z= -6.109516456227D+13

I= 13 X= 1.487177521375D+12 Y= -2.042425651330D+13 Z= 1.159396991112D+13
I= 14 X= -1.152217156358D+13 Y= 3.630623485591D+13 Z= 2.660039133059D+13
I= 15 X= -6.001245184545D+13 Y= -5.402829007362D+13 Z= -1.834030471263D+13
I= 16 X= -5.090556064620D+13 Y= 8.468036717100D+13 Z= -4.696311696254D+13
I= 17 X= 1.560936206791D+13 Y= -1.232194030260D+12 Z= 2.099835877943D+13
I= 18 X= 5.791699329191D+13 Y= 3.471781009117D+13 Z= 1.852197027032D+13
I= 19 X= -1.807549397903D+13 Y= 7.478472861409D+13 Z= 8.297159307342D+12
I= 20 X= -2.746904930349D+12 Y= -2.911235855860D+13 Z= -1.254284331313D+14
I= 21 X= 8.119194484267D+11 Y= -2.713130087837D+13 Z= 1.049402290970D+13
I= 22 X= 1.851781941143D+13 Y= -6.324763925968D+11 Z= -5.391577542503D+13
I= 23 X= -4.013748353666D+12 Y= 2.058818872630D+13 Z= 4.120388752771D+13
I= 24 X= -3.867757389015D+13 Y= 7.912836142666D+13 Z= 8.730705555996D+12
I= 25 X= 5.794997874960D+12 Y= 1.052656737571D+11 Z= -7.068020760212D+12
I= 26 X= -2.565952748223D+13 Y= -1.065226214527D+13 Z= 3.281139666286D+13
I= 27 X= -4.607410860597D+13 Y= -6.235777163866D+13 Z= 2.543721021322D+13
I= 28 X= -5.903161158946D+13 Y= -2.479254896674D+13 Z= -8.373859219498D+12
I= 29 X= 5.731873419152D+12 Y= -1.461134035634D+13 Z= -1.497967602818D+13
I= 30 X= -6.500572454419D+12 Y= -1.072085943716D+13 Z= 2.974521190009D+13
I= 31 X= -1.360573661489D+13 Y= 1.025089588508D+14 Z= -3.105049116938D+13
I= 32 X= -8.789969558824D+13 Y= -5.862585014584D+13 Z= -2.576664979434D+12
I= 33 X= 3.532574038025D+13 Y= 1.683189405999D+13 Z= -2.522303716429D+13
I= 34 X= 3.950308761660D+12 Y= 6.574784450084D+13 Z= -1.493671294049D+14
I= 35 X= -4.038743337450D+11 Y= 1.810945413931D+12 Z= -5.265601200439D+11
I= 36 X= 8.955061404720D+12 Y= -6.950451935799D+12 Z= -1.113205855928D+13
I= 37 X= -3.027925274166D+13 Y= -5.032869383879D+13 Z= -3.946294775999D+13
I= 38 X= 6.426581154066D+13 Y= 1.436650169853D+12 Z= -4.441598995380D+13

Backward Direction:

Total Energy: -651.6182454 Hartrees

Potential Energy: -651.7760614 Hartress

Kinetic Energy: 0.1578161 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.705944845217D+13 Y= 1.457327924277D+13 Z= 2.066268867762D+13
I= 1 X= 7.300827257078D+10 Y= 1.597110516163D+13 Z= -1.611107956688D+13
I= 2 X= 5.730988497860D+12 Y= -5.379214457483D+12 Z= -3.204322599815D+13
I= 3 X= -1.011790574104D+13 Y= 1.392605982838D+12 Z= 1.651660150409D+13
I= 4 X= 1.982565823333D+13 Y= 5.996061962243D+12 Z= -7.752042624239D+12
I= 5 X= 6.228479473671D+12 Y= -6.584260575341D+12 Z= 9.666807093270D+12
I= 6 X= 7.968894418427D+13 Y= -8.364225527666D+12 Z= -6.193445613405D+13
I= 7 X= -1.219794339803D+14 Y= 5.932051655282D+13 Z= 4.917736572305D+13
I= 8 X= -1.915856579878D+13 Y= -1.473129108638D+13 Z= -2.528176399427D+13
I= 9 X= 1.186553086954D+13 Y= 1.076686475282D+13 Z= 1.608739470553D+13
I= 10 X= -3.649639251661D+13 Y= 1.166818258598D+13 Z= 3.046509252773D+13
I= 11 X= -6.620752838937D+12 Y= 2.982154280999D+13 Z= -5.409460211910D+13
I= 12 X= -8.765126724815D+13 Y= -1.003024164718D+14 Z= -6.126450635533D+13
I= 13 X= 1.536835563330D+12 Y= -2.045851107981D+13 Z= 1.147110690724D+13
I= 14 X= -1.145175947348D+13 Y= 3.609549750823D+13 Z= 2.661264816323D+13
I= 15 X= -5.983993753376D+13 Y= -5.420208570058D+13 Z= -1.863282065004D+13
I= 16 X= -5.093907589396D+13 Y= 8.472740334202D+13 Z= -4.692870608222D+13
I= 17 X= 1.569288981048D+13 Y= -1.307383826076D+12 Z= 2.096542320857D+13
I= 18 X= 5.800582184947D+13 Y= 3.467204736354D+13 Z= 1.832576654705D+13
I= 19 X= -1.807568040211D+13 Y= 7.471195881783D+13 Z= 8.380124385881D+12
I= 20 X= -2.648418635970D+12 Y= -2.923677572579D+13 Z= -1.254690216372D+14
I= 21 X= 6.431062199086D+11 Y= -2.712843837295D+13 Z= 1.023669828456D+13
I= 22 X= 1.840542097816D+13 Y= -3.880562166224D+11 Z= -5.452493516871D+13
I= 23 X= -3.906730723130D+12 Y= 2.049439249151D+13 Z= 4.098815764160D+13
I= 24 X= -3.890051325230D+13 Y= 7.912192838204D+13 Z= 8.427059005542D+12
I= 25 X= 5.793808093211D+12 Y= 7.326423460710D+10 Z= -7.139479386568D+12
I= 26 X= -2.578921017090D+13 Y= -1.083616321979D+13 Z= 3.276020108160D+13
I= 27 X= -4.596055830514D+13 Y= -6.225223478819D+13 Z= 2.539555165932D+13
I= 28 X= -5.900475696572D+13 Y= -2.479689161817D+13 Z= -8.242952604819D+12

I= 29 X= 5.289299204853D+12 Y= -1.435002886490D+13 Z= -1.531908294432D+13
I= 30 X= -6.466101465170D+12 Y= -1.064647860979D+13 Z= 2.948425205004D+13
I= 31 X= -1.357064593264D+13 Y= 1.022677063389D+14 Z= -3.121221313062D+13
I= 32 X= -8.846248496042D+13 Y= -5.811639326690D+13 Z= -3.102342014505D+12
I= 33 X= 3.540379501846D+13 Y= 1.679732456148D+13 Z= -2.548893913641D+13
I= 34 X= 4.214399273419D+12 Y= 6.570788848363D+13 Z= -1.495380456501D+14
I= 35 X= -5.103958708857D+11 Y= 1.767594776269D+12 Z= -1.121625234636D+11
I= 36 X= 7.665452234514D+12 Y= -8.491418679850D+12 Z= -1.190550736182D+13
I= 37 X= -2.878056924828D+13 Y= -4.936334614206D+13 Z= -4.136668796329D+13
I= 38 X= 6.517340071422D+13 Y= 1.375397756467D+12 Z= -4.564542962696D+13

Seed: 2820608934

CM Start Point Coordinates: bohr

I= 0 X= -2.602182603388D+00 Y= 2.366136730435D+00 Z= -4.279749199123D-01
I= 1 X= -2.775622731018D+00 Y= 1.170602999883D-01 Z= -1.946953612807D+00
I= 2 X= -2.499987671022D+00 Y= 1.843777734218D+00 Z= 2.112331668816D+00
I= 3 X= -2.916047828464D+00 Y= -2.019743601050D+00 Z= -2.651549969727D-01
I= 4 X= -2.559859194471D+00 Y= -9.342213728901D-01 Z= 2.267518790345D+00
I= 5 X= 3.638745851818D+00 Y= 2.483857916974D+00 Z= -1.996993462514D+00
I= 6 X= 2.483934286044D+00 Y= -2.562132992136D-01 Z= -2.868144045341D+00
I= 7 X= 5.604663619704D+00 Y= 2.034974968164D+00 Z= -2.605196559540D+00
I= 8 X= 2.646855181878D+00 Y= 3.961240282715D+00 Z= -3.044892209488D+00
I= 9 X= -2.643400881027D+00 Y= -2.245164385314D+00 Z= 4.720029232044D+00
I= 10 X= -4.464030442184D+00 Y= -1.389386001376D+00 Z= 5.892782051873D+00
I= 11 X= -2.962813360538D+00 Y= -4.403593158338D+00 Z= 4.358273353461D+00
I= 12 X= -7.698387809633D-01 Y= -2.185484182845D+00 Z= 5.798919883677D+00
I= 13 X= -2.098151181277D+00 Y= 3.343204188505D+00 Z= 4.532975022400D+00
I= 14 X= -4.294428450345D+00 Y= 3.835440464051D+00 Z= 4.731978601815D+00
I= 15 X= -1.541361761636D+00 Y= 1.625009157609D+00 Z= 6.407118195831D+00
I= 16 X= -8.668179953689D-01 Y= 5.119971246737D+00 Z= 4.311754241152D+00

I= 17 X= -2.248715655416D+00 Y= 5.111009735795D+00 Z= -1.484647634762D+00
I= 18 X= -4.157051715038D+00 Y= 5.791869038034D+00 Z= -1.586943103742D+00
I= 19 X= -9.310651693092D-01 Y= 6.124239719939D+00 Z= -6.264966144692D-01
I= 20 X= -1.773298282138D+00 Y= 4.973014778228D+00 Z= -3.473852788325D+00
I= 21 X= -3.312525496879D+00 Y= 1.492198314803D-01 Z= -4.871673104490D+00
I= 22 X= -5.282286427519D+00 Y= 4.095851035673D-01 Z= -5.383710480297D+00
I= 23 X= -2.393479257576D+00 Y= 1.564808268529D+00 Z= -5.888520225709D+00
I= 24 X= -2.937590546357D+00 Y= -1.700642166588D+00 Z= -5.773813856004D+00
I= 25 X= -3.353443567381D+00 Y= -4.734963482395D+00 Z= -8.757086466586D-01
I= 26 X= -3.272495595500D+00 Y= -4.964134884931D+00 Z= -2.760863882371D+00
I= 27 X= -2.039956039500D+00 Y= -6.245808265846D+00 Z= 1.519055638953D-01
I= 28 X= -5.083290767667D+00 Y= -5.333243701770D+00 Z= -3.457033045149D-01
I= 29 X= 2.932472517024D+00 Y= -3.726384504788D+00 Z= -6.745344875986D-01
I= 30 X= 3.588407266473D+00 Y= -2.586344386519D+00 Z= 1.670293239489D+00
I= 31 X= 1.448227976246D+00 Y= -5.132114597446D+00 Z= -9.373819925647D-01
I= 32 X= 4.275150864984D+00 Y= -3.546718534800D+00 Z= -2.411984519829D+00
I= 33 X= 5.517490054513D+00 Y= -1.766827142319D+00 Z= 2.215249265606D+00
I= 34 X= 2.249006074799D+00 Y= -3.103366535512D+00 Z= 3.274864437749D+00
I= 35 X= 8.855040403066D-01 Y= -1.226626772520D-01 Z= -2.434297193662D-01
I= 36 X= 3.512801918366D+00 Y= 2.668953967149D+00 Z= 8.519699787586D-01
I= 37 X= 5.202638990451D+00 Y= 1.927699069316D+00 Z= 2.145043338893D+00
I= 38 X= 2.606173808031D+00 Y= 4.279615254015D+00 Z= 2.026666507327D+00

Forward Direction:

Total Energy: -651.5981671 Hartrees

Potential Energy: -651.8028014 Hartress

Kinetic Energy: 0.2046343 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.383108330819D+12 Y= 1.853479461088D+13 Z= -2.425153902049D+12

I= 1 X= 5.558005327978D+12 Y= -9.455579021926D+11 Z= -8.138917841814D+12

I= 2 X= 2.597976088898D+12 Y= 1.796217627312D+13 Z= -2.050929706626D+13

I= 3 X= 3.008761173468D+13 Y= -1.201781459678D+13 Z= -6.812657373116D+12
I= 4 X= -1.633822576408D+12 Y= -2.043398741138D+13 Z= 2.986857174070D+12
I= 5 X= -1.054671296984D+13 Y= 1.053516384168D+12 Z= 6.716517056856D+12
I= 6 X= -5.472380366035D+13 Y= -1.288281926749D+12 Z= -4.403369031677D+13
I= 7 X= 1.232983992108D+14 Y= -8.117102351104D+13 Z= -7.787600513439D+13
I= 8 X= -1.827747850156D+13 Y= -1.156714979379D+14 Z= -7.993666442552D+13
I= 9 X= 1.461605055167D+13 Y= 2.160811602408D+12 Z= 5.235988142207D+12
I= 10 X= 4.869362823037D+13 Y= 1.442887548713D+13 Z= 4.047722252092D+13
I= 11 X= 2.557978789147D+12 Y= 6.548184821476D+13 Z= -8.848095368671D+13
I= 12 X= -1.086827921135D+14 Y= -2.151247798141D+13 Z= -9.930031458235D+13
I= 13 X= 1.088915344618D+13 Y= 2.914233226342D+13 Z= 2.187850764462D+13
I= 14 X= 5.292790515746D+13 Y= -1.114426071284D+13 Z= -2.405562747811D+13
I= 15 X= -8.192229158365D+13 Y= 2.531945182959D+13 Z= 4.939979334183D+13
I= 16 X= 3.478512195524D+12 Y= -6.908768366071D+12 Z= -8.663537681206D+13
I= 17 X= -1.284165525058D+13 Y= -5.217261773082D+12 Z= -3.558939708521D+12
I= 18 X= 1.116586063233D+14 Y= -3.780780002384D+13 Z= 1.626792021872D+13
I= 19 X= -4.188083107850D+13 Y= -4.396101214116D+13 Z= -2.014101983721D+12
I= 20 X= 4.957832615946D+13 Y= 4.739485668970D+13 Z= -7.112368908829D+13
I= 21 X= -2.558263179513D+13 Y= -2.427452132239D+13 Z= -5.959433352388D+12
I= 22 X= 1.230945953612D+14 Y= 2.256632041706D+13 Z= -1.397479477648D+13
I= 23 X= 2.947367202535D+13 Y= 6.817754440972D+13 Z= -5.269302061858D+13
I= 24 X= 1.008118611452D+13 Y= 2.307835906294D+13 Z= 4.042656079007D+13
I= 25 X= 7.615268259398D+12 Y= -2.095994001488D+12 Z= 2.525807474119D+13
I= 26 X= -1.160763454667D+14 Y= 6.000495294929D+13 Z= 1.853461454611D+13
I= 27 X= -6.445297063975D+13 Y= 2.132622873713D+13 Z= -2.910495111913D+13
I= 28 X= 2.181324629642D+13 Y= -9.295652244899D+13 Z= -7.990809453028D+13
I= 29 X= -7.277073882417D+12 Y= -8.410183842932D+12 Z= -1.235329955510D+13
I= 30 X= 5.573904890152D+12 Y= 8.418689590693D+12 Z= 4.827648818688D+12
I= 31 X= 1.343906680851D+14 Y= 9.484604322699D+12 Z= -8.099947726679D+13
I= 32 X= -7.213463024428D+13 Y= -1.286754976716D+13 Z= 1.822812826747D+13

I= 33 X= -1.856269223305D+14 Y= -5.582373366841D+13 Z= 3.047954556749D+13
I= 34 X= -1.433414529057D+13 Y= 3.180931039247D+13 Z= 9.635828657900D+12
I= 35 X= -8.104921226346D+11 Y= 1.067580860933D+12 Z= 2.634470366997D+12
I= 36 X= -2.874586273743D+12 Y= -2.722098436597D+12 Z= 7.059230006820D+12
I= 37 X= 7.711312855782D+13 Y= -5.654494682141D+13 Z= -2.667927010495D+13
I= 38 X= 3.227933149964D+13 Y= -6.957014423586D+13 Z= -4.018064449156D+13

Backward Direction:

Total Energy: -651.5981058 Hartrees

Potential Energy: -651.8028014 Hartress

Kinetic Energy: 0.2046956 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -9.051439736257D+12 Y= 1.833817435265D+13 Z= -2.439842026477D+12
I= 1 X= 5.891152258458D+12 Y= -1.658623233346D+12 Z= -9.324772439984D+12
I= 2 X= 2.164385181372D+12 Y= 1.861557010217D+13 Z= -2.153067454316D+13
I= 3 X= 2.981539498028D+13 Y= -1.195762294630D+13 Z= -8.243732968433D+12
I= 4 X= 4.853522350368D+11 Y= -2.060653225633D+13 Z= 1.629453869065D+12
I= 5 X= -1.040182472650D+13 Y= 6.336220744679D+10 Z= -2.161739729881D+12
I= 6 X= 3.946401947301D+12 Y= 5.270144013165D+13 Z= -1.853617468112D+13
I= 7 X= 1.353427291227D+14 Y= -6.978679698963D+13 Z= -7.677137644033D+13
I= 8 X= -1.965350017271D+12 Y= -1.023234038012D+14 Z= -7.688693128621D+13
I= 9 X= 1.535681006753D+13 Y= 2.480926605939D+12 Z= 4.429986524016D+12
I= 10 X= 4.894191342564D+13 Y= 1.605918991603D+13 Z= 3.858762486648D+13
I= 11 X= 2.385016233242D+12 Y= 6.549363415303D+13 Z= -8.859901092982D+13
I= 12 X= -1.081743516544D+14 Y= -2.138109571117D+13 Z= -9.978664525879D+13
I= 13 X= 1.103176577449D+13 Y= 2.904395698388D+13 Z= 2.152565885272D+13
I= 14 X= 5.313012078617D+13 Y= -1.174947476532D+13 Z= -2.402042724456D+13
I= 15 X= -8.142684981381D+13 Y= 2.482033024736D+13 Z= 4.855972033162D+13
I= 16 X= 3.382260165496D+12 Y= -6.773685753529D+12 Z= -8.653655261511D+13
I= 17 X= -1.260177293144D+13 Y= -5.433198447924D+12 Z= -3.653526978446D+12
I= 18 X= 1.119137119890D+14 Y= -3.793922545612D+13 Z= 1.570444510124D+13

I= 19 X= -4.188136646982D+13 Y= -4.416999884996D+13 Z= -1.775835565656D+12
I= 20 X= 4.986116775783D+13 Y= 4.703754451527D+13 Z= -7.124025473138D+13
I= 21 X= -2.606744448591D+13 Y= -2.426630052523D+13 Z= -6.698440861379D+12
I= 22 X= 1.227717996467D+14 Y= 2.326826780366D+13 Z= -1.572423335418D+13
I= 23 X= 2.978101468731D+13 Y= 6.790817212555D+13 Z= -5.331257268772D+13
I= 24 X= 9.440929232134D+12 Y= 2.305988408152D+13 Z= 3.955452189634D+13
I= 25 X= 7.611851331739D+12 Y= -2.187898547521D+12 Z= 2.505285356730D+13
I= 26 X= -1.164487796263D+14 Y= 5.947680966383D+13 Z= 1.838758658871D+13
I= 27 X= -6.412686690624D+13 Y= 2.162931875817D+13 Z= -2.922458981560D+13
I= 28 X= 2.189036974945D+13 Y= -9.296899406165D+13 Z= -7.953214540374D+13
I= 29 X= -8.548097468919D+12 Y= -7.659726503274D+12 Z= -1.332803821213D+13
I= 30 X= 5.672901713240D+12 Y= 8.632302998898D+12 Z= 4.078201350103D+12
I= 31 X= 1.344914445925D+14 Y= 8.791754121785D+12 Z= -8.146392462907D+13
I= 32 X= -7.375089830576D+13 Y= -1.140444666205D+13 Z= 1.671844268655D+13
I= 33 X= -1.854027581426D+14 Y= -5.592301340125D+13 Z= 2.971590487312D+13
I= 34 X= -1.357570690701D+13 Y= 3.169456118192D+13 Z= 9.144976343334D+12
I= 35 X= -1.116410048246D+12 Y= 9.430826830259D+11 Z= 3.824573861968D+12
I= 36 X= -6.578199405233D+12 Y= -7.147582376300D+12 Z= 4.837971654908D+12
I= 37 X= 8.141717974290D+13 Y= -5.377257632733D+13 Z= -3.214659879742D+13
I= 38 X= 3.488582598001D+13 Y= -6.974605430574D+13 Z= -4.371145756478D+13

Seed: 28766904189

CM Start Point Coordinates: bohr

I= 0 X= -2.306533998526D+00 Y= 2.358763965760D+00 Z= -5.448211498808D-01
I= 1 X= -2.758786632367D+00 Y= 1.691460113513D-01 Z= -2.012173302347D+00
I= 2 X= -2.224352192125D+00 Y= 1.601137715156D+00 Z= 2.176648843039D+00
I= 3 X= -2.911164270535D+00 Y= -1.947184684231D+00 Z= -2.884258308174D-01
I= 4 X= -2.545199282751D+00 Y= -9.865698248979D-01 Z= 2.105975284673D+00
I= 5 X= 3.781763653694D+00 Y= 2.284234489348D+00 Z= -2.312736264532D+00
I= 6 X= 1.854346786163D+00 Y= -9.514565146308D-02 Z= -3.059917510355D+00

I= 7 X= 5.710673098970D+00 Y= 1.125173875380D+00 Z= -2.599308593055D+00
I= 8 X= 3.545814384622D+00 Y= 3.372605746814D+00 Z= -4.436724557456D+00
I= 9 X= -2.363770789116D+00 Y= -2.611475526195D+00 Z= 4.509286787456D+00
I= 10 X= -4.487953827255D+00 Y= -2.724525874024D+00 Z= 5.003364908044D+00
I= 11 X= -1.552815327400D+00 Y= -4.304415434391D+00 Z= 4.168156873922D+00
I= 12 X= -1.378632279266D+00 Y= -1.394589038688D+00 Z= 6.005533318355D+00
I= 13 X= -1.998853667414D+00 Y= 3.447130863750D+00 Z= 4.442643693546D+00
I= 14 X= -3.940525757651D+00 Y= 3.352885639554D+00 Z= 5.433468361707D+00
I= 15 X= -7.388080799603D-01 Y= 2.408925312056D+00 Z= 6.030143854977D+00
I= 16 X= -8.245916761445D-01 Y= 5.388795768011D+00 Z= 4.016401720710D+00
I= 17 X= -2.337533469292D+00 Y= 5.016318636887D+00 Z= -1.263497698805D+00
I= 18 X= -4.542285982225D+00 Y= 5.459034465231D+00 Z= -9.360282232123D-01
I= 19 X= -1.323977751507D+00 Y= 6.397670503113D+00 Z= -2.070768980692D-02
I= 20 X= -1.617366427200D+00 Y= 5.536756590384D+00 Z= -3.294713490015D+00
I= 21 X= -3.271236343746D+00 Y= 3.666326003642D-01 Z= -4.765661867853D+00
I= 22 X= -5.421030772815D+00 Y= 7.519068613205D-01 Z= -5.385100935837D+00
I= 23 X= -2.281473611313D+00 Y= 1.980868536153D+00 Z= -5.251247491865D+00
I= 24 X= -2.790340156692D+00 Y= -1.211370160396D+00 Z= -6.287067579989D+00
I= 25 X= -3.526166348495D+00 Y= -4.562979117716D+00 Z= -1.238823130513D+00
I= 26 X= -2.863493009598D+00 Y= -4.555431850146D+00 Z= -3.313536640299D+00
I= 27 X= -2.414588953116D+00 Y= -5.936357237332D+00 Z= -2.862463745816D-02
I= 28 X= -5.377701676092D+00 Y= -4.990188701236D+00 Z= -1.245466748375D+00
I= 29 X= 3.124653986329D+00 Y= -3.708405008491D+00 Z= -3.267955193886D-01
I= 30 X= 3.464743523686D+00 Y= -2.541557654897D+00 Z= 2.172435976994D+00
I= 31 X= 1.553208739680D+00 Y= -5.555236250515D+00 Z= -3.202984496858D-01
I= 32 X= 4.728981490673D+00 Y= -3.838082769633D+00 Z= -1.491855870759D+00
I= 33 X= 5.384428335490D+00 Y= -1.517568552038D+00 Z= 2.243096452418D+00
I= 34 X= 2.696929719103D+00 Y= -3.159765469004D+00 Z= 4.123675124427D+00
I= 35 X= 8.269258091786D-01 Y= -1.504136187304D-01 Z= -1.921692387368D-01
I= 36 X= 3.337055617309D+00 Y= 3.166159402185D+00 Z= 2.705088845428D-01

I= 37 X= 4.818415850374D+00 Y= 2.836570421161D+00 Z= 1.808237769085D+00

I= 38 X= 2.191995725500D+00 Y= 5.045343466496D+00 Z= 8.099276884657D-01

Forward Direction:

Total Energy: -651.6169976 Hartrees

Potential Energy: -651.7853007 Hartress

Kinetic Energy: 0.1683031 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.144970214440D+13 Y= 5.926309202253D+12 Z= 1.292567128268D+12

I= 1 X= 1.896867961130D+13 Y= 1.889045716738D+13 Z= 1.185191543937D+13

I= 2 X= -5.011010664828D+12 Y= 9.759595920561D+12 Z= -1.298635027630D+13

I= 3 X= -1.686840858069D+12 Y= -1.855811957714D+13 Z= 1.138829088863D+13

I= 4 X= -1.327597313632D+13 Y= 5.525746451495D+12 Z= 3.785534326096D+12

I= 5 X= 1.472550398483D+13 Y= -9.827394136781D+12 Z= -5.629437646073D+12

I= 6 X= 1.055047653414D+13 Y= -3.338822724540D+13 Z= -5.755514291454D+13

I= 7 X= -1.298131198217D+14 Y= -8.956562319885D+12 Z= -1.280532826744D+13

I= 8 X= 3.647181317221D+13 Y= 4.862266472792D+13 Z= -3.122985103430D+13

I= 9 X= -1.205746420752D+13 Y= -1.279164062594D+13 Z= -1.378090621090D+11

I= 10 X= -4.737906469441D+13 Y= 2.341071650772D+13 Z= 1.605306709188D+13

I= 11 X= 1.282119548744D+14 Y= -5.484782538501D+13 Z= -1.112611569733D+12

I= 12 X= 1.224788391150D+14 Y= 1.094450589694D+14 Z= -1.101901646920D+13

I= 13 X= 6.193996067191D+12 Y= -2.132043237301D+13 Z= -1.765715862992D+12

I= 14 X= 5.674180257627D+13 Y= -3.784478758293D+12 Z= -2.748805178731D+13

I= 15 X= -6.206636449567D+13 Y= 1.455917322885D+13 Z= 4.143326911455D+13

I= 16 X= 1.714651332229D+13 Y= 1.027418471492D+14 Z= -2.814368030348D+13

I= 17 X= -2.309455974713D+13 Y= -5.674291865458D+12 Z= -1.811734679828D+13

I= 18 X= 1.655096404788D+13 Y= -4.339881544155D+13 Z= 3.856907095962D+13

I= 19 X= 9.502740450599D+13 Y= 7.792279266308D+13 Z= 7.366910962956D+13

I= 20 X= 2.017628779373D+13 Y= 1.998992834728D+13 Z= 2.224041825764D+13

I= 21 X= -6.681615653070D+11 Y= -1.745752195140D+13 Z= -6.787817554287D+12

I= 22 X= -6.374972248804D+13 Y= -6.865483491119D+13 Z= -1.755862565146D+13

I= 23 X= 5.374351825133D+13 Y= 7.512762416468D+13 Z= 1.326976290780D+13
I= 24 X= -7.417436572793D+13 Y= -8.279343992795D+13 Z= 7.579337067966D+12
I= 25 X= -4.312158592291D+12 Y= -9.831982713406D+12 Z= -2.250399899193D+13
I= 26 X= -2.365857994314D+13 Y= 7.140337947530D+13 Z= 4.850890239156D+13
I= 27 X= 1.046318069941D+14 Y= 6.380152666416D+12 Z= 1.144815332717D+13
I= 28 X= -9.365346475186D+13 Y= -8.712468388632D+12 Z= 4.070700816853D+13
I= 29 X= -6.022369571962D+11 Y= 1.564930126208D+12 Z= -8.949492635432D+12
I= 30 X= 4.117284937133D+12 Y= 2.771708564512D+11 Z= 1.872054953655D+13
I= 31 X= -6.774779405871D+13 Y= -5.773827907079D+13 Z= -5.996908453276D+13
I= 32 X= 6.197836612965D+13 Y= -2.645823864643D+13 Z= -9.341692679125D+13
I= 33 X= -8.183203565051D+13 Y= 4.945881058044D+13 Z= -9.591309221750D+13
I= 34 X= -2.571896996094D+13 Y= 2.374182790476D+13 Z= 2.480148941078D+13
I= 35 X= 9.168197926560D+11 Y= 1.097307403163D+12 Z= 2.207922880008D+11
I= 36 X= 7.464627018108D+12 Y= 1.471756865390D+13 Z= 3.074495013478D+13
I= 37 X= -3.385817515986D+13 Y= -1.802788484648D+12 Z= 1.048579586440D+13
I= 38 X= 5.073159984660D+13 Y= 1.961617977867D+13 Z= 3.438634926905D+13

Backward Direction:

Total Energy: -651.6169533 Hartrees

Potential Energy: -651.7853007 Hartress

Kinetic Energy: 0.1683474 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.214795074132D+13 Y= 5.720887433716D+12 Z= 1.277221506950D+12
I= 1 X= 1.931673953244D+13 Y= 1.814547217513D+13 Z= 1.061297723725D+13
I= 2 X= -5.464010842083D+12 Y= 1.044223827662D+13 Z= -1.405344870136D+13
I= 3 X= -1.971243124486D+12 Y= -1.849523350652D+13 Z= 9.893154613249D+12
I= 4 X= -1.106193556716D+13 Y= 5.345477806610D+12 Z= 2.367368209443D+12
I= 5 X= 1.487687800784D+13 Y= -1.086187158207D+13 Z= -1.490512079174D+13
I= 6 X= 7.184699570589D+13 Y= 2.301829117335D+13 Z= -3.091625628068D+13
I= 7 X= -1.172296374250D+14 Y= 2.937267814362D+12 Z= -1.165125196836D+13
I= 8 X= 5.351413791316D+13 Y= 6.256827305944D+13 Z= -2.804359961766D+13

I= 9 X= -1.128354533027D+13 Y= -1.245719599239D+13 Z= -9.798905414119D+11
I= 10 X= -4.711966526499D+13 Y= 2.511401034887D+13 Z= 1.407888346881D+13
I= 11 X= 1.280312498137D+14 Y= -5.483551185798D+13 Z= -1.235953524250D+12
I= 12 X= 1.230100394069D+14 Y= 1.095823224393D+14 Z= -1.152711725271D+13
I= 13 X= 6.342992295806D+12 Y= -2.142321132446D+13 Z= -2.134359580425D+12
I= 14 X= 5.695307018769D+13 Y= -4.416784615629D+12 Z= -2.745127584699D+13
I= 15 X= -6.154874476972D+13 Y= 1.403770896532D+13 Z= 4.055559106971D+13
I= 16 X= 1.704595266489D+13 Y= 1.028829765985D+14 Z= -2.804043233690D+13
I= 17 X= -2.284393934033D+13 Y= -5.899894735074D+12 Z= -1.821616817706D+13
I= 18 X= 1.681748925802D+13 Y= -4.353612400691D+13 Z= 3.798037243722D+13
I= 19 X= 9.502684514570D+13 Y= 7.770445087455D+13 Z= 7.391804179490D+13
I= 20 X= 2.047179050826D+13 Y= 1.961662143969D+13 Z= 2.211863466307D+13
I= 21 X= -1.174676415960D+12 Y= -1.744893315661D+13 Z= -7.559905999004D+12
I= 22 X= -6.408696783214D+13 Y= -6.792146554387D+13 Z= -1.938637611448D+13
I= 23 X= 5.406461880284D+13 Y= 7.484619369970D+13 Z= 1.262247720930D+13
I= 24 X= -7.484328307287D+13 Y= -8.281274192066D+13 Z= 6.668262221516D+12
I= 25 X= -4.315728475756D+12 Y= -9.928001272029D+12 Z= -2.271840669087D+13
I= 26 X= -2.404768575015D+13 Y= 7.085159438093D+13 Z= 4.835529286760D+13
I= 27 X= 1.049725084346D+14 Y= 6.696810208821D+12 Z= 1.132315911487D+13
I= 28 X= -9.357288894105D+13 Y= -8.725498276395D+12 Z= 4.109978628494D+13
I= 29 X= -1.930156654975D+12 Y= 2.348980942383D+12 Z= -9.967864500501D+12
I= 30 X= 4.220713255893D+12 Y= 5.003464575612D+11 Z= 1.793755379548D+13
I= 31 X= -6.764250639314D+13 Y= -5.846214402713D+13 Z= -6.045432241721D+13
I= 32 X= 6.028974743029D+13 Y= -2.492964118596D+13 Z= -9.499419195004D+13
I= 33 X= -8.159783697279D+13 Y= 4.935508668767D+13 Z= -9.671091653330D+13
I= 34 X= -2.492658083382D+13 Y= 2.362194206047D+13 Z= 2.428866458022D+13
I= 35 X= 5.972077553324D+11 Y= 9.672361876688D+11 Z= 1.464169585311D+12
I= 36 X= 3.595225318827D+12 Y= 1.009398231441D+13 Z= 2.842425935539D+13
I= 37 X= -2.936145738850D+13 Y= 1.093684424405D+12 Z= 4.773727625958D+12
I= 38 X= 5.345477147045D+13 Y= 1.943239527071D+13 Z= 3.069748285041D+13

Seed: 28801055485

CM Start Point Coordinates: bohr

I= 0 X= -2.469703134690D+00 Y= 2.304077068386D+00 Z= -5.312516366338D-01
I= 1 X= -3.022574883446D+00 Y= 1.372701183686D-01 Z= -2.016830214587D+00
I= 2 X= -2.283601099356D+00 Y= 1.664756311838D+00 Z= 2.137535830475D+00
I= 3 X= -3.020072991063D+00 Y= -2.017705483488D+00 Z= -3.697594829768D-01
I= 4 X= -2.582792570310D+00 Y= -1.007700116271D+00 Z= 2.151832734518D+00
I= 5 X= 4.362255772868D+00 Y= 2.258433649435D+00 Z= -1.375563294974D+00
I= 6 X= 2.812553324333D+00 Y= 4.733856982157D-01 Z= -2.930866732561D+00
I= 7 X= 6.055419613975D+00 Y= 9.114422190674D-01 Z= -1.327060901033D+00
I= 8 X= 4.110574147308D+00 Y= 3.664439629965D+00 Z= -2.954579120656D+00
I= 9 X= -2.364652856450D+00 Y= -2.516826745007D+00 Z= 4.398610365239D+00
I= 10 X= -4.248805879026D+00 Y= -3.977369528312D+00 Z= 4.875747109077D+00
I= 11 X= -8.512753615007D-01 Y= -4.143871291902D+00 Z= 4.097372027506D+00
I= 12 X= -1.695927800660D+00 Y= -1.230481327408D+00 Z= 6.020470516192D+00
I= 13 X= -2.005579775003D+00 Y= 3.469406383158D+00 Z= 4.455402749667D+00
I= 14 X= -3.793164363693D+00 Y= 3.936940624395D+00 Z= 5.512000575106D+00
I= 15 X= -8.265469477707D-01 Y= 2.796024698884D+00 Z= 5.873444609914D+00
I= 16 X= -1.284650390798D+00 Y= 5.430448751384D+00 Z= 3.796556625010D+00
I= 17 X= -2.317385116004D+00 Y= 4.935626013295D+00 Z= -1.734079607061D+00
I= 18 X= -4.304033569773D+00 Y= 6.065015529916D+00 Z= -2.406141270785D+00
I= 19 X= -1.180228189939D+00 Y= 6.144153388100D+00 Z= -4.962812611255D-01
I= 20 X= -1.601255131054D+00 Y= 4.994253098862D+00 Z= -3.569642028019D+00
I= 21 X= -3.762573234187D+00 Y= 2.513507286492D-02 Z= -4.660329312864D+00
I= 22 X= -5.625562089136D+00 Y= 1.015651958619D+00 Z= -4.595631257351D+00
I= 23 X= -2.468395348335D+00 Y= 1.267092660119D+00 Z= -6.068323563955D+00
I= 24 X= -3.802106629716D+00 Y= -1.939143883650D+00 Z= -5.507198837780D+00
I= 25 X= -3.489556393152D+00 Y= -4.653885757718D+00 Z= -6.920405931504D-01
I= 26 X= -3.130160117273D+00 Y= -5.622138241318D+00 Z= -2.801781367755D+00

I= 27 X= -2.568103143677D+00 Y= -5.936785255739D+00 Z= 5.402264802730D-01
I= 28 X= -5.577789118347D+00 Y= -5.158881806494D+00 Z= -2.868010589113D-02
I= 29 X= 2.720272659869D+00 Y= -3.772256287973D+00 Z= -8.100461381929D-01
I= 30 X= 3.717315427838D+00 Y= -2.617884542284D+00 Z= 1.638847884528D+00
I= 31 X= 1.286486176789D+00 Y= -5.322746944297D+00 Z= -7.438109178551D-01
I= 32 X= 3.856336326294D+00 Y= -3.284225059138D+00 Z= -2.422990150254D+00
I= 33 X= 5.445884174211D+00 Y= -1.972063750890D+00 Z= 2.017866660856D+00
I= 34 X= 2.757068219422D+00 Y= -3.511689143867D+00 Z= 3.334001452154D+00
I= 35 X= 8.791703851987D-01 Y= -8.668776042975D-02 Z= -2.536708686405D-01
I= 36 X= 3.224992838499D+00 Y= 2.996156539525D+00 Z= 1.115767853208D+00
I= 37 X= 4.465621328249D+00 Y= 2.636917894530D+00 Z= 3.068158577007D+00
I= 38 X= 2.122909912111D+00 Y= 5.018316707267D+00 Z= 1.134578564677D+00

Forward Direction:

Total Energy: -651.6158288 Hartrees

Potential Energy: -651.8073639 Hartress

Kinetic Energy: 0.1915351 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.260120881406D+12 Y= -4.871850735700D+12 Z= 1.452886287412D+13
I= 1 X= 5.803345577899D+12 Y= 1.562611433660D+13 Z= 7.872135295636D+12
I= 2 X= 8.595965779563D+12 Y= 2.271705475020D+13 Z= 7.476408395478D+11
I= 3 X= -1.341612693234D+13 Y= -7.572509497821D+11 Z= 1.895962275310D+12
I= 4 X= -1.143515877166D+13 Y= -2.026695862503D+13 Z= -5.431166182191D+12
I= 5 X= 1.712002509762D+13 Y= -2.801888508352D+13 Z= -3.728430301210D+11
I= 6 X= -1.761051392739D+13 Y= -5.998250619111D+13 Z= -1.044035906565D+14
I= 7 X= 9.734255859562D+13 Y= 3.920341130753D+13 Z= 9.313719275380D+12
I= 8 X= -7.407959422968D+13 Y= 1.338742798578D+14 Z= 1.921831806373D+13
I= 9 X= -1.234565402065D+13 Y= 1.207598658130D+13 Z= -2.710503692663D+12
I= 10 X= 3.706497332415D+13 Y= 5.214992491454D+13 Z= 2.404600956407D+12
I= 11 X= 5.011062042308D+13 Y= -2.735709089091D+13 Z= -6.425079253169D+13
I= 12 X= -9.019169962608D+13 Y= -6.930156954653D+13 Z= 7.826168495157D+12

I= 13 X= 2.167083225137D+13 Y= 1.426926529480D+13 Z= -9.515774020554D+12
I= 14 X= -1.084926297245D+14 Y= 1.694152733422D+13 Z= 6.088463200685D+13
I= 15 X= -1.237774220376D+13 Y= -3.699838358740D+13 Z= 4.521185657629D+13
I= 16 X= -9.794984484744D+13 Y= 3.417848048136D+13 Z= -2.379154066168D+13
I= 17 X= 8.834986272978D+12 Y= -6.603290735990D+12 Z= 5.213479289762D+11
I= 18 X= -3.967508513113D+13 Y= -3.512289514830D+13 Z= -1.201497253145D+13
I= 19 X= 8.082886490252D+13 Y= 4.808200533074D+13 Z= 7.845655792388D+13
I= 20 X= -3.582132069570D+13 Y= 7.072132734830D+13 Z= 9.400216464492D+12
I= 21 X= -4.525650949678D+12 Y= -2.093144222705D+13 Z= -1.983940414345D+13
I= 22 X= 7.413902007886D+13 Y= 6.154828383091D+13 Z= 9.489451727939D+12
I= 23 X= 1.656549054271D+12 Y= -1.784555970951D+13 Z= -4.132430720615D+13
I= 24 X= 9.812015204603D+12 Y= 1.112235980929D+14 Z= 2.964353915185D+12
I= 25 X= -1.588001034571D+13 Y= -1.873094691780D+13 Z= 2.146609030300D+12
I= 26 X= -3.508525587996D+13 Y= -4.243439578839D+13 Z= -4.707751982528D+12
I= 27 X= 1.051463839853D+14 Y= -2.729825498738D+13 Z= 2.422545686263D+13
I= 28 X= 1.333847840919D+14 Y= 1.366245532119D+14 Z= 5.171468691617D+13
I= 29 X= 9.490755296093D+12 Y= 1.856440464304D+13 Z= 8.462006710167D+12
I= 30 X= 9.329256044235D+11 Y= 1.416615860403D+13 Z= -8.032768572085D+12
I= 31 X= -4.475735150741D+12 Y= 2.156398763904D+12 Z= -1.902416242457D+13
I= 32 X= -3.622526674621D+13 Y= -3.301743991430D+12 Z= -1.205264028430D+14
I= 33 X= -1.043690935265D+13 Y= 4.644185927793D+13 Z= 2.932510121568D+13
I= 34 X= -5.568505722437D+13 Y= -3.150348956406D+13 Z= 1.019619065837D+14
I= 35 X= -1.357768774435D+12 Y= -1.928900480850D+12 Z= -9.042547225272D+11
I= 36 X= -4.843491033664D+12 Y= 9.052049589286D+12 Z= 9.427320944150D+12
I= 37 X= 4.894703971863D+13 Y= -3.391980419593D+13 Z= 1.213627469033D+14
I= 38 X= 1.055341506749D+14 Y= -7.366169011275D+13 Z= -7.004171412667D+12

Backward Direction:

Total Energy: -651.6158704 Hartrees

Potential Energy: -651.8073639 Hartress

Kinetic Energy: 0.1914935 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.029426247618D+11 Y= -5.065189785454D+12 Z= 1.451441986556D+13
I= 1 X= 6.130932935125D+12 Y= 1.492494867277D+13 Z= 6.706070293075D+12
I= 2 X= 8.169610653047D+12 Y= 2.335954471254D+13 Z= -2.566918421835D+11
I= 3 X= -1.368380091829D+13 Y= -6.980637811970D+11 Z= 4.887685338265D+11
I= 4 X= -9.351348847839D+12 Y= -2.043662403429D+13 Z= -6.765917077412D+12
I= 5 X= 1.726249544413D+13 Y= -2.899251552249D+13 Z= -9.102939059526D+12
I= 6 X= 4.008060058826D+13 Y= -6.893767099145D+12 Z= -7.933157873608D+13
I= 7 X= 1.091858921805D+14 Y= 5.039765733268D+13 Z= 1.039991387219D+13
I= 8 X= -5.803968328651D+13 Y= 1.469996203821D+14 Z= 2.221715711060D+13
I= 9 X= -1.161725633682D+13 Y= 1.239075948945D+13 Z= -3.503054718163D+12
I= 10 X= 3.730911511043D+13 Y= 5.375303258473D+13 Z= 5.465369947209D+11
I= 11 X= 4.994054426551D+13 Y= -2.734550163482D+13 Z= -6.436687962577D+13
I= 12 X= -8.969174405088D+13 Y= -6.917237979281D+13 Z= 7.347953726141D+12
I= 13 X= 2.181106465967D+13 Y= 1.417253170590D+13 Z= -9.862734453802D+12
I= 14 X= -1.082937886811D+14 Y= 1.634641312042D+13 Z= 6.091924482615D+13
I= 15 X= -1.189056839428D+13 Y= -3.748917580579D+13 Z= 4.438580274068D+13
I= 16 X= -9.804449062158D+13 Y= 3.431130882471D+13 Z= -2.369436564133D+13
I= 17 X= 9.070865417734D+12 Y= -6.815623850249D+12 Z= 4.283391340881D+11
I= 18 X= -3.942423669547D+13 Y= -3.525212736330D+13 Z= -1.256904436672D+13
I= 19 X= 8.082833842466D+13 Y= 4.787650621096D+13 Z= 7.869084814680D+13
I= 20 X= -3.554319916285D+13 Y= 7.036997801988D+13 Z= 9.285596075696D+12
I= 21 X= -5.002373065026D+12 Y= -2.092335861740D+13 Z= -2.056607906076D+13
I= 22 X= 7.382161119307D+13 Y= 6.223851708563D+13 Z= 7.769207862920D+12
I= 23 X= 1.958762762285D+12 Y= -1.811043669399D+13 Z= -4.193352016350D+13
I= 24 X= 9.182442956760D+12 Y= 1.112054314251D+14 Z= 2.106867645109D+12
I= 25 X= -1.588337025060D+13 Y= -1.882131775739D+13 Z= 1.944812597765D+12
I= 26 X= -3.545147484680D+13 Y= -4.295372539629D+13 Z= -4.852326330794D+12
I= 27 X= 1.054670456853D+14 Y= -2.700022294669D+13 Z= 2.410781469619D+13
I= 28 X= 1.334606205108D+14 Y= 1.366122897316D+14 Z= 5.208436219839D+13

I= 29 X= 8.240942606829D+12 Y= 1.930233831387D+13 Z= 7.503534537492D+12
I= 30 X= 1.030270362709D+12 Y= 1.437620722103D+13 Z= -8.769709226567D+12
I= 31 X= -4.376640408356D+12 Y= 1.475110879196D+12 Z= -1.948085906558D+13
I= 32 X= -3.781456245230D+13 Y= -1.863057223690D+12 Z= -1.220108947240D+14
I= 33 X= -1.021648602608D+13 Y= 4.634423632783D+13 Z= 2.857420418944D+13
I= 34 X= -5.493927569620D+13 Y= -3.161632383389D+13 Z= 1.014792456316D+14
I= 35 X= -1.658581526908D+12 Y= -2.051321026852D+12 Z= 2.659882705997D+11
I= 36 X= -8.485298096497D+12 Y= 4.700418327606D+12 Z= 7.243131051787D+12
I= 37 X= 5.317926470115D+13 Y= -3.119369915045D+13 Z= 1.159866572436D+14
I= 38 X= 1.080971478615D+14 Y= -7.383466458674D+13 Z= -1.047606211875D+13

Seed: 29461475743

CM Start Point Coordinates: bohr

I= 0 X= -2.411113980514D+00 Y= 2.269884915542D+00 Z= -6.945200804222D-01
I= 1 X= -3.219354509842D+00 Y= 8.571109946292D-02 Z= -2.117899810390D+00
I= 2 X= -2.160040963664D+00 Y= 1.580368861296D+00 Z= 2.045125026278D+00
I= 3 X= -3.115313511796D+00 Y= -1.991815215703D+00 Z= -4.322692611673D-01
I= 4 X= -2.603595252293D+00 Y= -1.133294410753D+00 Z= 2.118287137175D+00
I= 5 X= 4.102377220589D+00 Y= 2.019595733607D+00 Z= -1.776021902953D+00
I= 6 X= 2.482350546134D+00 Y= -2.785271274921D-01 Z= -2.884524395722D+00
I= 7 X= 5.947393076177D+00 Y= 1.057594426236D+00 Z= -1.998068716829D+00
I= 8 X= 3.946416084776D+00 Y= 3.192760753622D+00 Z= -3.320666461969D+00
I= 9 X= -2.671020366821D+00 Y= -2.688794762231D+00 Z= 4.441490076753D+00
I= 10 X= -4.518804375199D+00 Y= -3.159441565080D+00 Z= 5.222430291277D+00
I= 11 X= -1.699447084268D+00 Y= -4.721309185981D+00 Z= 4.219864273031D+00
I= 12 X= -1.875072180461D+00 Y= -1.437180985415D+00 Z= 6.300987930612D+00
I= 13 X= -1.964231142260D+00 Y= 3.330563122472D+00 Z= 4.237253439018D+00
I= 14 X= -3.911229156855D+00 Y= 3.433610464005D+00 Z= 5.511531561690D+00
I= 15 X= -2.416835135716D-01 Y= 3.004464720595D+00 Z= 5.490367837823D+00
I= 16 X= -1.467863692531D+00 Y= 5.354222518402D+00 Z= 3.315162450627D+00

I= 17 X= -2.239878309246D+00 Y= 4.952151232627D+00 Z= -1.514843520720D+00
I= 18 X= -3.850665356306D+00 Y= 6.557659953214D+00 Z= -6.514012696301D-01
I= 19 X= -5.116634425955D-01 Y= 5.725343610217D+00 Z= -3.162295266841D-01
I= 20 X= -2.416308735748D+00 Y= 5.361825264906D+00 Z= -3.754695592740D+00
I= 21 X= -4.139795774001D+00 Y= -1.392512367132D-02 Z= -4.870047285681D+00
I= 22 X= -5.978827022736D+00 Y= 8.639097794856D-01 Z= -5.293732783477D+00
I= 23 X= -2.755504532917D+00 Y= 1.148935589883D+00 Z= -6.259231916417D+00
I= 24 X= -3.804880923078D+00 Y= -1.893660832816D+00 Z= -5.872362131636D+00
I= 25 X= -3.613472660446D+00 Y= -4.734157067360D+00 Z= -1.023401408804D+00
I= 26 X= -3.704618698587D+00 Y= -5.238037946449D+00 Z= -2.950494639799D+00
I= 27 X= -2.180299016492D+00 Y= -6.074174486167D+00 Z= -3.414227673543D-02
I= 28 X= -5.614888342697D+00 Y= -4.984897155440D+00 Z= -9.400761785552D-02
I= 29 X= 3.097504891457D+00 Y= -3.765500990814D+00 Z= -6.743557906631D-01
I= 30 X= 3.662314285352D+00 Y= -2.486394570040D+00 Z= 1.777863881417D+00
I= 31 X= 1.692594430914D+00 Y= -5.580954348552D+00 Z= -7.225083486703D-01
I= 32 X= 4.618074643266D+00 Y= -3.861331452973D+00 Z= -2.342463157306D+00
I= 33 X= 5.570443178477D+00 Y= -1.273864503934D+00 Z= 1.686379649704D+00
I= 34 X= 3.161670585933D+00 Y= -3.149844166669D+00 Z= 3.710688170912D+00
I= 35 X= 9.119597583117D-01 Y= -3.211827908645D-02 Z= -1.577770395545D-01
I= 36 X= 3.403760928948D+00 Y= 2.953783881062D+00 Z= 8.086473211666D-01
I= 37 X= 4.897955488614D+00 Y= 2.537275365900D+00 Z= 2.302271914811D+00
I= 38 X= 2.776260716448D+00 Y= 5.062264920209D+00 Z= 1.256596320254D+00

Forward Direction:

Total Energy: -651.6075027 Hartrees

Potential Energy: -651.7983202 Hartress

Kinetic Energy: 0.1908175 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.909361247992D+12 Y= 1.260729502815D+13 Z= -1.559678082118D+13

I= 1 X= -5.980836894011D+12 Y= -8.550652693942D+12 Z= 1.543478191782D+13

I= 2 X= -5.883253005249D+12 Y= -2.357360623619D+13 Z= -1.127831333695D+13

I= 3 X= -1.919779790181D+12 Y= 1.575682337705D+13 Z= 1.740067102095D+13
I= 4 X= 1.848415000903D+13 Y= 1.707874360283D+13 Z= -1.155496336133D+13
I= 5 X= 5.370134456127D+12 Y= -1.672099830855D+13 Z= 1.941017754478D+13
I= 6 X= -4.037672414741D+13 Y= 3.454517924464D+13 Z= -8.515495805912D+13
I= 7 X= -1.164609562034D+14 Y= 2.702776435999D+13 Z= 8.306264120745D+12
I= 8 X= 1.859185617821D+13 Y= 3.735431517853D+13 Z= 2.536900127378D+13
I= 9 X= -1.771796327637D+13 Y= 5.458455768484D+12 Z= 2.121855269025D+12
I= 10 X= 6.417771260989D+13 Y= 1.984761605875D+13 Z= 3.743766798599D+13
I= 11 X= 1.007845193294D+14 Y= -1.259477978906D+14 Z= 3.220765421327D+12
I= 12 X= -4.212656668866D+13 Y= 5.158533663201D+13 Z= -1.107784779967D+12
I= 13 X= -1.564506408232D+13 Y= -9.446060536224D+12 Z= 1.811609003500D+13
I= 14 X= 8.376666168011D+13 Y= 1.349803833987D+13 Z= -4.540060372216D+11
I= 15 X= -4.033925943009D+13 Y= 9.950666754156D+12 Z= -3.753912421361D+13
I= 16 X= -1.465372403890D+13 Y= 8.633079504803D+13 Z= 2.372786177004D+13
I= 17 X= 1.425844092330D+12 Y= 2.901052214697D+13 Z= 9.270891397602D+12
I= 18 X= 1.398114052294D+14 Y= -7.085716180722D+13 Z= -8.226845610173D+13
I= 19 X= 7.136870781271D+13 Y= -1.264104230518D+14 Z= -3.305468189189D+13
I= 20 X= -2.515606989341D+13 Y= -2.970131845694D+13 Z= -9.140926319790D+13
I= 21 X= -7.892998498735D+12 Y= -1.529622536529D+13 Z= -1.942998640855D+13
I= 22 X= 6.095211177487D+13 Y= -2.978186305955D+13 Z= 1.873467863106D+13
I= 23 X= 1.102226225302D+13 Y= -2.657741530541D+13 Z= -6.076586966281D+13
I= 24 X= -2.631132684811D+13 Y= 1.237564979866D+14 Z= -1.571305906658D+13
I= 25 X= -7.486302029598D+12 Y= 1.646915204563D+12 Z= -8.634748441598D+10
I= 26 X= -7.742158806173D+13 Y= -4.124405974302D+13 Z= -5.979713852039D+13
I= 27 X= 3.836682418244D+13 Y= -4.455748311182D+13 Z= 1.843050014718D+13
I= 28 X= -4.158859792417D+13 Y= 1.353373177039D+13 Z= -9.840498240300D+12
I= 29 X= -2.542214183704D+12 Y= 6.283436535457D+12 Z= -3.135782852220D+12
I= 30 X= -1.106602944515D+13 Y= 4.774783151389D+12 Z= 3.271379292327D+12
I= 31 X= -3.211609631357D+13 Y= -4.812297274331D+13 Z= 1.587320941845D+13
I= 32 X= 7.382899236918D+13 Y= 4.841010035430D+12 Z= 2.727272155579D+13

I= 33 X= 1.029066472992D+14 Y= 8.669676213277D+13 Z= 5.658001485866D+13
I= 34 X= 2.112619605039D+13 Y= -9.051061383161D+13 Z= -5.304765114542D+13
I= 35 X= -3.006789174546D+11 Y= -1.071086439505D+12 Z= 6.246451640624D+11
I= 36 X= 3.035607166456D+13 Y= 1.357179986844D+12 Z= 6.748507270224D+12
I= 37 X= 2.854485055280D+13 Y= 2.861584260664D+13 Z= -1.467800970746D+14
I= 38 X= -9.170054846421D+13 Y= 5.846331095347D+13 Z= -4.306435391959D+13

Backward Direction:

Total Energy: -651.6075478 Hartrees

Potential Energy: -651.7983202 Hartress

Kinetic Energy: 0.1907725 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.217939376992D+12 Y= 1.240388165392D+13 Z= -1.561197641087D+13
I= 1 X= -5.636179928897D+12 Y= -9.288354021780D+12 Z= 1.420795672477D+13
I= 2 X= -6.331824230987D+12 Y= -2.289763802547D+13 Z= -1.233497881815D+13
I= 3 X= -2.201401475408D+12 Y= 1.581909461506D+13 Z= 1.592015258488D+13
I= 4 X= 2.067654109311D+13 Y= 1.690023743269D+13 Z= -1.295926416985D+13
I= 5 X= 5.520028506480D+12 Y= -1.774536174358D+13 Z= 1.022518208584D+13
I= 6 X= 2.032050336262D+13 Y= 9.040021518642D+13 Z= -5.877651790503D+13
I= 7 X= -1.040005016104D+14 Y= 3.880530936830D+13 Z= 9.449057099910D+12
I= 8 X= 3.546755933607D+13 Y= 5.116357829813D+13 Z= 2.852410093769D+13
I= 9 X= -1.695161093993D+13 Y= 5.789630559956D+12 Z= 1.288006758425D+12
I= 10 X= 6.443457592037D+13 Y= 2.153425691449D+13 Z= 3.548278582108D+13
I= 11 X= 1.006055810176D+14 Y= -1.259356047558D+14 Z= 3.098629370088D+12
I= 12 X= -4.160055989566D+13 Y= 5.172125808394D+13 Z= -1.610917902813D+12
I= 13 X= -1.549752458179D+13 Y= -9.547834624795D+12 Z= 1.775105052138D+13
I= 14 X= 8.397586374385D+13 Y= 1.287191449575D+13 Z= -4.175896512810D+11
I= 15 X= -3.982670044091D+13 Y= 9.434300804347D+12 Z= -3.840822126106D+13
I= 16 X= -1.475330151729D+13 Y= 8.647054468488D+13 Z= 2.383010029082D+13
I= 17 X= 1.674014205598D+12 Y= 2.878712498391D+13 Z= 9.173036191073D+12
I= 18 X= 1.400753246454D+14 Y= -7.099312791491D+13 Z= -8.285139896105D+13

I= 19 X= 7.136815391786D+13 Y= -1.266266301246D+14 Z= -3.280818350803D+13
I= 20 X= -2.486345628331D+13 Y= -3.007097556053D+13 Z= -9.152985611920D+13
I= 21 X= -8.394561183899D+12 Y= -1.528772054628D+13 Z= -2.019452620283D+13
I= 22 X= 6.061816365924D+13 Y= -2.905566381325D+13 Z= 1.692479795319D+13
I= 23 X= 1.134022341934D+13 Y= -2.685609423856D+13 Z= -6.140682689568D+13
I= 24 X= -2.697370422038D+13 Y= 1.237373847090D+14 Z= -1.661522640433D+13
I= 25 X= -7.489837011217D+12 Y= 1.551835411377D+12 Z= -2.986589333786D+11
I= 26 X= -7.780688960602D+13 Y= -4.179045007559D+13 Z= -5.994924621495D+13
I= 27 X= 3.870419460557D+13 Y= -4.424392150186D+13 Z= 1.830672799733D+13
I= 28 X= -4.150880990130D+13 Y= 1.352082927816D+13 Z= -9.451560285052D+12
I= 29 X= -3.857150907766D+12 Y= 7.059821742657D+12 Z= -4.144198168450D+12
I= 30 X= -1.096361234058D+13 Y= 4.995776781068D+12 Z= 2.496038845064D+12
I= 31 X= -3.201183803716D+13 Y= -4.883976052126D+13 Z= 1.539271566702D+13
I= 32 X= 7.215688317193D+13 Y= 6.354662509540D+12 Z= 2.571087720397D+13
I= 33 X= 1.031385562347D+14 Y= 8.659405233634D+13 Z= 5.578999081281D+13
I= 34 X= 2.191083804403D+13 Y= -9.062932756509D+13 Z= -5.355546212831D+13
I= 35 X= -6.171661319342D+11 Y= -1.199885957829D+12 Z= 1.855866051084D+12
I= 36 X= 2.652450082630D+13 Y= -3.221201882477D+12 Z= 4.450505717320D+12
I= 37 X= 3.299760424050D+13 Y= 3.148399691145D+13 Z= -1.524363188360D+14
I= 38 X= -8.900400108850D+13 Y= 5.828132329681D+13 Z= -4.671715456226D+13

Seed: 30047930840

CM Start Point Coordinates: bohr

I= 0 X= -2.605199170032D+00 Y= 2.324759284584D+00 Z= -5.699309942317D-01
I= 1 X= -3.042219424407D+00 Y= 1.121981373871D-01 Z= -1.846041562466D+00
I= 2 X= -2.523305281127D+00 Y= 1.745397517627D+00 Z= 2.019587383086D+00
I= 3 X= -2.853575980092D+00 Y= -2.080537612683D+00 Z= -8.524222464289D-02
I= 4 X= -2.721840410490D+00 Y= -1.007442249038D+00 Z= 2.269550060792D+00
I= 5 X= 4.380071871302D+00 Y= 2.176774718840D+00 Z= -1.254276717311D+00
I= 6 X= 2.179792089619D+00 Y= 7.377932574254D-01 Z= -2.712236246180D+00

I= 7 X= 6.247664373547D+00 Y= 1.567737516523D+00 Z= -1.869285000811D+00
I= 8 X= 3.966678625419D+00 Y= 4.124508202978D+00 Z= -2.449903487058D+00
I= 9 X= -2.457743890668D+00 Y= -2.323031444495D+00 Z= 4.748927897831D+00
I= 10 X= -4.454249304801D+00 Y= -3.106034231764D+00 Z= 5.886893215889D+00
I= 11 X= -1.648031819340D+00 Y= -3.947924001755D+00 Z= 4.384439592615D+00
I= 12 X= -1.155102576757D+00 Y= -1.678983717560D+00 Z= 6.118078924200D+00
I= 13 X= -1.767217556029D+00 Y= 3.614440797815D+00 Z= 3.871694477179D+00
I= 14 X= -3.475218208980D+00 Y= 4.040652048267D+00 Z= 4.655785749940D+00
I= 15 X= -3.465002716842D-01 Y= 3.206577947551D+00 Z= 5.320076410648D+00
I= 16 X= -1.291777622088D+00 Y= 5.355217373507D+00 Z= 3.323466149616D+00
I= 17 X= -2.522208159886D+00 Y= 5.059903245185D+00 Z= -1.693814296753D+00
I= 18 X= -4.271660685199D+00 Y= 6.047859216955D+00 Z= -6.927206882855D-01
I= 19 X= -5.360581281236D-01 Y= 5.968017567691D+00 Z= -9.907932579731D-01
I= 20 X= -2.587690978891D+00 Y= 4.789686646815D+00 Z= -3.619396722509D+00
I= 21 X= -3.334812968396D+00 Y= -2.121076019514D-01 Z= -4.689921180440D+00
I= 22 X= -5.127434899122D+00 Y= -9.435129474082D-01 Z= -5.731295335167D+00
I= 23 X= -2.518682323041D+00 Y= 1.129041739049D+00 Z= -5.738136565722D+00
I= 24 X= -2.397713764640D+00 Y= -2.117928099032D+00 Z= -5.309524067304D+00
I= 25 X= -3.418333210493D+00 Y= -4.872279169400D+00 Z= -7.739020539381D-01
I= 26 X= -2.652946433016D+00 Y= -5.225846180546D+00 Z= -2.473742703702D+00
I= 27 X= -2.691354196647D+00 Y= -6.032516078030D+00 Z= 6.729072328569D-01
I= 28 X= -5.371831571779D+00 Y= -5.429995213219D+00 Z= -7.671890520488D-01
I= 29 X= 3.036530358359D+00 Y= -3.413018457098D+00 Z= -1.435746851312D+00
I= 30 X= 3.420418343746D+00 Y= -2.859984944209D+00 Z= 1.198118579719D+00
I= 31 X= 1.211298027756D+00 Y= -5.104544596184D+00 Z= -1.471671583899D+00
I= 32 X= 4.244911532741D+00 Y= -2.903020940659D+00 Z= -2.931550115447D+00
I= 33 X= 5.109570816214D+00 Y= -1.779007830782D+00 Z= 1.597739482411D+00
I= 34 X= 2.511207791339D+00 Y= -3.717020206007D+00 Z= 2.748867567901D+00
I= 35 X= 8.357691777169D-01 Y= -4.566736150042D-02 Z= -2.093865265849D-01
I= 36 X= 3.607286606015D+00 Y= 2.379708559370D+00 Z= 1.372417407572D+00

I= 37 X= 4.865068111075D+00 Y= 1.946298478093D+00 Z= 2.935099359658D+00

I= 38 X= 2.602442709357D+00 Y= 4.139354739210D+00 Z= 1.919018524151D+00

Forward Direction:

Total Energy: -651.6017593 Hartrees

Potential Energy: -651.7597744 Hartress

Kinetic Energy: 0.1580151 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.012437551854D+12 Y= 1.732757086049D+13 Z= -2.136633550205D+13

I= 1 X= 9.099020834416D+12 Y= -1.204405549660D+13 Z= 2.795499781147D+13

I= 2 X= 3.872518215955D+11 Y= 1.099743882191D+13 Z= 7.735414020009D+12

I= 3 X= -9.253962089301D+12 Y= 1.232960734109D+13 Z= -7.635244937158D+12

I= 4 X= 6.578714929454D+12 Y= 1.332890707519D+13 Z= 2.543843353926D+13

I= 5 X= -9.165849463707D+12 Y= -2.289274108373D+12 Z= -1.802006180707D+13

I= 6 X= -4.383883069802D+13 Y= -1.076309184582D+13 Z= -7.826110564496D+13

I= 7 X= -6.218818339417D+13 Y= 1.839528622646D+13 Z= 5.863375218952D+13

I= 8 X= 3.286052372271D+13 Y= -1.874181360465D+13 Z= 4.371587558269D+13

I= 9 X= -3.991519337290D+12 Y= -5.256186354306D+12 Z= -9.358617599188D+12

I= 10 X= 3.141671184797D+13 Y= -8.764044059646D+12 Z= -3.877997374625D+13

I= 11 X= 2.706435266261D+13 Y= 1.518152629944D+14 Z= 4.589983819844D+13

I= 12 X= 3.840845284858D+13 Y= 9.116807639732D+12 Z= -2.458957113338D+13

I= 13 X= -1.938129316337D+13 Y= -6.943507969572D+12 Z= 8.478487194464D+12

I= 14 X= 1.974000224825D+12 Y= 9.005965749147D+12 Z= -3.606819850632D+13

I= 15 X= -2.001606735579D+13 Y= 6.259734538300D+13 Z= -4.614497490306D+13

I= 16 X= 5.849486331472D+13 Y= 2.559649946340D+13 Z= 3.857246554312D+13

I= 17 X= -1.417446612209D+13 Y= 1.431058802183D+13 Z= -2.068403272715D+13

I= 18 X= -1.076714308587D+14 Y= 8.385832398376D+13 Z= 4.123653333434D+13

I= 19 X= -7.603198691069D+13 Y= 1.356679971390D+13 Z= 3.258414108842D+13

I= 20 X= 1.664309247232D+13 Y= 2.179547827701D+13 Z= 5.614899083890D+13

I= 21 X= -9.338049929262D+12 Y= 2.304501706429D+13 Z= 9.610490165122D+12

I= 22 X= 8.579198157386D+13 Y= -3.947979515319D+13 Z= 2.268792532725D+13

I= 23 X= 2.404377434078D+13 Y= -4.427120021042D+13 Z= -9.395031207931D+13
I= 24 X= 5.295600396374D+13 Y= -2.375723142749D+13 Z= 1.438940238350D+13
I= 25 X= -5.175019551929D+12 Y= -3.903999809600D+12 Z= 5.084168979279D+12
I= 26 X= 1.063303863111D+13 Y= -3.299773859638D+13 Z= -8.060828535705D+13
I= 27 X= 6.020268552445D+13 Y= 4.241681985459D+13 Z= -5.232205179762D+13
I= 28 X= -8.632683916262D+13 Y= -4.025896093805D+13 Z= -4.307540728759D+13
I= 29 X= -1.399528342867D+13 Y= -2.801394022037D+13 Z= -4.297876071220D+12
I= 30 X= 2.982270048240D+13 Y= 1.732257063655D+12 Z= -2.268736263249D+12
I= 31 X= 6.020769623580D+13 Y= 7.001670891448D+13 Z= -3.824700871375D+13
I= 32 X= -4.478038022987D+13 Y= -3.744782472753D+13 Z= -4.106513689537D+13
I= 33 X= -5.638384750397D+13 Y= -5.749101321727D+13 Z= 5.539947323010D+13
I= 34 X= 3.289652448656D+13 Y= 3.718122371672D+13 Z= -8.488757842744D+13
I= 35 X= 1.858387311105D+12 Y= -2.603433852025D+12 Z= 1.178838881970D+12
I= 36 X= 3.100631417335D+12 Y= -5.877933645805D+12 Z= 7.112546519508D+12
I= 37 X= -1.081756030670D+14 Y= -2.638233763943D+13 Z= -2.071588130868D+13
I= 38 X= 3.123274429425D+13 Y= -4.877268974442D+13 Z= -4.893777924586D+13

Backward Direction:

Total Energy: -651.6017384 Hartrees

Potential Energy: -651.7597744 Hartress

Kinetic Energy: 0.1580360 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.501560961031D+12 Y= 1.717727313975D+13 Z= -2.137756319377D+13
I= 1 X= 9.353680374283D+12 Y= -1.258912697220D+13 Z= 2.704852334326D+13
I= 2 X= 5.581229150134D+10 Y= 1.149689703923D+13 Z= 6.954666864404D+12
I= 3 X= -9.462046230738D+12 Y= 1.237561820476D+13 Z= -8.729167828930D+12
I= 4 X= 8.198625046731D+12 Y= 1.319701274542D+13 Z= 2.440082619610D+13
I= 5 X= -9.055096007190D+12 Y= -3.046153987435D+12 Z= -2.480665530751D+13
I= 6 X= 1.009031383599D+12 Y= 3.050698013842D+13 Z= -5.877064958113D+13
I= 7 X= -5.298142433720D+13 Y= 2.709745823122D+13 Z= 5.947813707968D+13
I= 8 X= 4.532961397564D+13 Y= -8.538449248192D+12 Z= 4.604711014206D+13

I= 9 X= -3.425278257078D+12 Y= -5.011488498607D+12 Z= -9.974730138674D+12
I= 10 X= 3.160650256081D+13 Y= -7.517821798293D+12 Z= -4.022439368968D+13
I= 11 X= 2.693213903713D+13 Y= 1.518242722375D+14 Z= 4.580959452913D+13
I= 12 X= 3.879710782535D+13 Y= 9.217237049217D+12 Z= -2.496132526054D+13
I= 13 X= -1.927227943345D+13 Y= -7.018706632309D+12 Z= 8.208767432220D+12
I= 14 X= 2.128575078552D+12 Y= 8.543336438079D+12 Z= -3.604129122904D+13
I= 15 X= -1.963734865290D+13 Y= 6.221581381141D+13 Z= -4.678713182343D+13
I= 16 X= 5.842128766618D+13 Y= 2.569975743542D+13 Z= 3.864800735830D+13
I= 17 X= -1.399109861748D+13 Y= 1.414552471445D+13 Z= -2.075633581197D+13
I= 18 X= -1.074764265358D+14 Y= 8.375786158290D+13 Z= 4.080580952551D+13
I= 19 X= -7.603239616774D+13 Y= 1.340704900453D+13 Z= 3.276627338710D+13
I= 20 X= 1.685929831633D+13 Y= 2.152234667787D+13 Z= 5.605988735334D+13
I= 21 X= -9.708643699028D+12 Y= 2.305130109142D+13 Z= 9.045588330851D+12
I= 22 X= 8.554523456789D+13 Y= -3.894322230542D+13 Z= 2.135064383040D+13
I= 23 X= 2.427870894042D+13 Y= -4.447711002313D+13 Z= -9.442390144918D+13
I= 24 X= 5.246658771009D+13 Y= -2.377135381542D+13 Z= 1.372281055114D+13
I= 25 X= -5.177631468092D+12 Y= -3.974252203219D+12 Z= 4.927296664361D+12
I= 26 X= 1.034834769828D+13 Y= -3.340145453529D+13 Z= -8.072067442853D+13
I= 27 X= 6.045196120609D+13 Y= 4.264850371206D+13 Z= -5.241350434747D+13
I= 28 X= -8.626788551975D+13 Y= -4.026849431139D+13 Z= -4.278802948714D+13
I= 29 X= -1.496686159168D+13 Y= -2.744028606463D+13 Z= -5.042972230213D+12
I= 30 X= 2.989837425496D+13 Y= 1.895544451826D+12 Z= -2.841618467281D+12
I= 31 X= 6.028473041036D+13 Y= 6.948709000677D+13 Z= -3.860203510181D+13
I= 32 X= -4.601586536910D+13 Y= -3.632941981430D+13 Z= -4.221914973634D+13
I= 33 X= -5.621249503661D+13 Y= -5.756690325001D+13 Z= 5.481574163755D+13
I= 34 X= 3.347627939959D+13 Y= 3.709350872192D+13 Z= -8.526278892354D+13
I= 35 X= 1.624541787384D+12 Y= -2.698601016320D+12 Z= 2.088561233616D+12
I= 36 X= 2.695670109385D+11 Y= -9.260800492180D+12 Z= 5.414603119546D+12
I= 37 X= -1.048855601564D+14 Y= -2.426312076826D+13 Z= -2.489514062164D+13
I= 38 X= 3.322516453630D+13 Y= -4.890715647067D+13 Z= -5.163675424094D+13

Seed: 3117303747

CM Start Point Coordinates: bohr

I= 0 X= -2.532944671148D+00 Y= 2.302541096992D+00 Z= -7.090693959208D-01
I= 1 X= -2.864215282771D+00 Y= -1.375557339876D-01 Z= -2.000423169211D+00
I= 2 X= -2.306972148084D+00 Y= 1.858580131790D+00 Z= 2.019232037269D+00
I= 3 X= -2.683424629435D+00 Y= -2.168891764173D+00 Z= -1.826866769104D-01
I= 4 X= -2.387751458051D+00 Y= -8.544580770881D-01 Z= 2.348230913972D+00
I= 5 X= 4.401646365541D+00 Y= 2.529980290644D+00 Z= -9.971832914488D-01
I= 6 X= 2.193212223461D+00 Y= 8.984258485674D-01 Z= -2.690414043045D+00
I= 7 X= 5.999864860197D+00 Y= 1.192018748284D+00 Z= -2.127329902046D+00
I= 8 X= 4.224888181504D+00 Y= 4.378643743178D+00 Z= -1.980877456883D+00
I= 9 X= -2.347481335864D+00 Y= -2.034269718104D+00 Z= 4.853305139313D+00
I= 10 X= -4.280242417562D+00 Y= -1.636705771655D+00 Z= 5.877535808588D+00
I= 11 X= -2.014587179598D+00 Y= -4.316639000964D+00 Z= 5.004818726584D+00
I= 12 X= -1.138105530407D+00 Y= -1.346056824527D+00 Z= 6.462970505182D+00
I= 13 X= -2.214189636964D+00 Y= 3.724760484511D+00 Z= 3.902641967319D+00
I= 14 X= -4.220407012983D+00 Y= 4.652998480802D+00 Z= 4.152488442313D+00
I= 15 X= -1.440933543350D+00 Y= 3.000209061513D+00 Z= 5.736044870913D+00
I= 16 X= -8.056714657434D-01 Y= 5.209951552636D+00 Z= 3.692136684014D+00
I= 17 X= -2.800323632617D+00 Y= 5.046074706996D+00 Z= -1.780584861124D+00
I= 18 X= -4.763957542437D+00 Y= 5.508129699665D+00 Z= -2.103575258321D+00
I= 19 X= -1.975507378623D+00 Y= 6.647834622684D+00 Z= -5.982403622529D-01
I= 20 X= -1.750337173362D+00 Y= 5.185754862022D+00 Z= -3.702868313939D+00
I= 21 X= -3.626465208205D+00 Y= -2.513228923047D-01 Z= -4.817536603221D+00
I= 22 X= -5.534232464070D+00 Y= 9.555923699132D-01 Z= -5.081943434960D+00
I= 23 X= -2.010569513323D+00 Y= 9.943026868148D-01 Z= -5.972114982136D+00
I= 24 X= -3.778243220275D+00 Y= -2.366127216452D+00 Z= -5.282535698291D+00
I= 25 X= -2.911983692134D+00 Y= -4.868757318096D+00 Z= -6.179732855301D-01
I= 26 X= -3.109469930519D+00 Y= -5.061491249631D+00 Z= -2.576061454609D+00

I= 27 X= -9.442969111722D-01 Y= -5.958735887041D+00 Z= 2.176884515477D-01
I= 28 X= -4.533554925766D+00 Y= -5.593394530403D+00 Z= 7.897405914202D-01
I= 29 X= 2.734826390417D+00 Y= -3.537510435488D+00 Z= -1.768230887002D+00
I= 30 X= 3.094727790238D+00 Y= -3.396970886430D+00 Z= 1.005887089529D+00
I= 31 X= 1.497867675477D+00 Y= -5.008395333405D+00 Z= -2.750625808120D+00
I= 32 X= 4.623565092944D+00 Y= -2.669095744198D+00 Z= -2.830724540611D+00
I= 33 X= 5.030891547768D+00 Y= -2.453395959413D+00 Z= 1.949283548488D+00
I= 34 X= 1.853843793274D+00 Y= -4.041660184149D+00 Z= 2.419056515869D+00
I= 35 X= 8.282621497325D-01 Y= -3.495301835795D-02 Z= -1.975603156829D-01
I= 36 X= 3.874476336086D+00 Y= 2.128383094792D+00 Z= 1.571265055352D+00
I= 37 X= 4.748319249370D+00 Y= 6.653162820695D-01 Z= 2.894918396789D+00
I= 38 X= 3.214112530430D+00 Y= 3.799538977288D+00 Z= 2.667425449453D+00

Forward Direction:

Total Energy: -651.6145322 Hartrees

Potential Energy: -651.7973536 Hartress

Kinetic Energy: 0.1828214 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.365003673172D+12 Y= -1.498930310520D+13 Z= 4.295201412267D+12
I= 1 X= 7.250456451394D+12 Y= -9.940896623623D+12 Z= -8.650942554966D+12
I= 2 X= -6.364705312797D+12 Y= 2.751503083397D+13 Z= -7.863725476467D+11
I= 3 X= 1.639129442373D+13 Y= -9.956554193407D+11 Z= 9.979380635731D+12
I= 4 X= -9.545653480570D+12 Y= 1.679095958246D+12 Z= -8.225219743853D+12
I= 5 X= 6.150029357280D+12 Y= -1.705580891911D+13 Z= 4.112901846184D+12
I= 6 X= -7.947645200774D+13 Y= -6.626353548683D+13 Z= 3.899068868317D+13
I= 7 X= -1.880784589317D+12 Y= 3.415762427119D+13 Z= -1.184563716177D+13
I= 8 X= -1.240862110877D+13 Y= 3.674218750689D+13 Z= 6.501521208144D+13
I= 9 X= -9.777536858760D+12 Y= 3.474993974322D+12 Z= -8.625686958408D+12
I= 10 X= -1.782275636743D+13 Y= -1.942151123913D+13 Z= -6.158524242922D+13
I= 11 X= 1.769132171498D+13 Y= -1.087762523238D+14 Z= 3.817962506610D+13
I= 12 X= -1.205572774109D+13 Y= -3.115769975212D+13 Z= -2.687993939151D+13

I= 13 X= 1.091200474680D+13 Y= 9.627369512053D+12 Z= 9.801674743886D+12
I= 14 X= -7.727826208713D+13 Y= -4.365071304745D+13 Z= 7.853155407362D+13
I= 15 X= 3.233925503989D+12 Y= 6.856528744879D+13 Z= 7.440509055167D+13
I= 16 X= 6.872879057882D+13 Y= -8.197018135448D+13 Z= -4.043017292854D+13
I= 17 X= -1.679090181229D+12 Y= -6.554328180917D+12 Z= -2.046649235469D+13
I= 18 X= 4.737816165201D+13 Y= 9.184642952184D+13 Z= 1.415752661484D+13
I= 19 X= -2.443922354488D+13 Y= -4.632751504887D+13 Z= -2.192655925404D+13
I= 20 X= -1.119979036667D+13 Y= 8.186109893647D+13 Z= 1.717576378581D+14
I= 21 X= -1.844835525772D+13 Y= -6.102939421345D+12 Z= -8.403228434235D+12
I= 22 X= -4.352665329789D+13 Y= -2.601545242465D+13 Z= 3.873489816564D+13
I= 23 X= 3.951349899933D+13 Y= -1.191200629649D+14 Z= 4.832849429072D+13
I= 24 X= -2.732349707576D+12 Y= 1.145530614523D+14 Z= 3.066266750648D+13
I= 25 X= 9.427142522421D+12 Y= -1.481526018065D+13 Z= -2.798116759655D+13
I= 26 X= -7.865525761201D+12 Y= 1.862400511135D+13 Z= -2.594880157968D+13
I= 27 X= -1.216046281049D+14 Y= 1.674463105302D+14 Z= -7.330206623293D+13
I= 28 X= 3.808540405880D+13 Y= -3.869861806840D+12 Z= 2.922338115777D+12
I= 29 X= -1.124379245394D+13 Y= -1.458267154973D+12 Z= -1.392402933019D+13
I= 30 X= 1.035629037989D+13 Y= -2.504400282445D+12 Z= 4.081007391627D+11
I= 31 X= -5.431985220427D+13 Y= 3.871692761402D+13 Z= -3.339099505972D+13
I= 32 X= 4.565281929066D+13 Y= -7.296794199639D+12 Z= -3.511050750953D+13
I= 33 X= 1.278902562596D+14 Y= 3.549735875901D+13 Z= 1.920635075853D+13
I= 34 X= -7.800507098329D+13 Y= -3.622837833331D+13 Z= 2.575915794614D+13
I= 35 X= 4.788132049731D+11 Y= 3.103906502806D+11 Z= 3.415082122267D+12
I= 36 X= -1.133434869878D+12 Y= 2.002058576210D+13 Z= -2.496080074015D+13
I= 37 X= 7.328197417766D+13 Y= -2.033095579858D+13 Z= 8.086497410937D+13
I= 38 X= -7.678766844062D+12 Y= 7.059697878727D+12 Z= 6.145021682771D+13

Backward Direction:

Total Energy: -651.6145335 Hartrees

Potential Energy: -651.7973536 Hartress

Kinetic Energy: 0.1828201 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.200698300213D+12 Y= -1.523516091041D+13 Z= 4.276835096708D+12
I= 1 X= 7.667029870723D+12 Y= -1.083252742534D+13 Z= -1.013375827948D+13
I= 2 X= -6.906875845394D+12 Y= 2.833204722627D+13 Z= -2.063522869771D+12
I= 3 X= 1.605090928528D+13 Y= -9.203906047278D+11 Z= 8.189935792408D+12
I= 4 X= -6.895795954156D+12 Y= 1.463342517638D+12 Z= -9.922543316778D+12
I= 5 X= 6.331200445638D+12 Y= -1.829391702056D+13 Z= -6.988643653282D+12
I= 6 X= -6.114082281017D+12 Y= 1.246266295322D+12 Z= 7.087327968075D+13
I= 7 X= 1.317968051502D+13 Y= 4.839268321427D+13 Z= -1.046438789418D+13
I= 8 X= 7.988382597262D+12 Y= 5.343290482989D+13 Z= 6.882865789386D+13
I= 9 X= -8.851276713771D+12 Y= 3.875272019501D+12 Z= -9.633527104630D+12
I= 10 X= -1.751229572624D+13 Y= -1.738293427281D+13 Z= -6.394803220654D+13
I= 11 X= 1.747504595434D+13 Y= -1.087615149579D+14 Z= 3.803200398565D+13
I= 12 X= -1.141996387891D+13 Y= -3.099341679482D+13 Z= -2.748805675503D+13
I= 13 X= 1.109032998429D+13 Y= 9.504359142559D+12 Z= 9.360465732696D+12
I= 14 X= -7.702540771706D+13 Y= -4.440748450556D+13 Z= 7.857556913969D+13
I= 15 X= 3.853435556339D+12 Y= 6.794117608643D+13 Z= 7.335464687053D+13
I= 16 X= 6.860843515892D+13 Y= -8.180127142236D+13 Z= -4.030660122134D+13
I= 17 X= -1.379136652370D+12 Y= -6.824339614176D+12 Z= -2.058476612476D+13
I= 18 X= 4.769715074864D+13 Y= 9.168209259639D+13 Z= 1.345294633850D+13
I= 19 X= -2.443989300519D+13 Y= -4.658883610572D+13 Z= -2.162862628648D+13
I= 20 X= -1.084611972217D+13 Y= 8.141430882214D+13 Z= 1.716118818976D+14
I= 21 X= -1.905457450525D+13 Y= -6.092659975468D+12 Z= -9.327297839048D+12
I= 22 X= -4.393028335561D+13 Y= -2.513772372001D+13 Z= 3.654736603154D+13
I= 23 X= 3.989780626195D+13 Y= -1.194568913243D+14 Z= 4.755379429983D+13
I= 24 X= -3.532939401059D+12 Y= 1.145299599767D+14 Z= 2.957225306630D+13
I= 25 X= 9.422869933327D+12 Y= -1.493017941628D+13 Z= -2.823778015816D+13
I= 26 X= -8.331224703469D+12 Y= 1.796360444735D+13 Z= -2.613264821180D+13
I= 27 X= -1.211968616283D+14 Y= 1.678253002031D+14 Z= -7.345166480366D+13
I= 28 X= 3.818184073825D+13 Y= -3.885456555584D+12 Z= 3.392432242273D+12

I= 29 X= -1.283310514426D+13 Y= -5.198806574709D+11 Z= -1.514286156357D+13
I= 30 X= 1.048007793893D+13 Y= -2.237293909527D+12 Z= -5.290229973810D+11
I= 31 X= -5.419383929336D+13 Y= 3.785057420523D+13 Z= -3.397174910247D+13
I= 32 X= 4.363180617394D+13 Y= -5.467301534041D+12 Z= -3.699824781330D+13
I= 33 X= 1.281705555343D+14 Y= 3.537321744302D+13 Z= 1.825147953303D+13
I= 34 X= -7.705670482989D+13 Y= -3.637186298496D+13 Z= 2.514538663529D+13
I= 35 X= 9.628746279575D+10 Y= 1.547156997778D+11 Z= 4.903210750664D+12
I= 36 X= -5.764504984010D+12 Y= 1.448687430430D+13 Z= -2.773830552062D+13
I= 37 X= 7.866384375284D+13 Y= -1.686432964577D+13 Z= 7.402851964469D+13
I= 38 X= -4.419555290583D+12 Y= 6.839736498372D+12 Z= 5.703521927179D+13

Seed: 3126505819

CM Start Point Coordinates: bohr

I= 0 X= -2.572149651513D+00 Y= 2.276428862814D+00 Z= -7.680471716944D-01
I= 1 X= -2.980809116148D+00 Y= -8.620963070296D-02 Z= -1.952530342938D+00
I= 2 X= -2.443147914303D+00 Y= 1.979537085768D+00 Z= 1.890014500496D+00
I= 3 X= -2.678885084876D+00 Y= -1.922187748752D+00 Z= 2.703294783309D-02
I= 4 X= -2.415224404227D+00 Y= -6.794870873938D-01 Z= 2.499377109103D+00
I= 5 X= 4.289510518460D+00 Y= 2.447871473180D+00 Z= -3.511012587936D-01
I= 6 X= 2.635936801639D+00 Y= 1.375506589303D+00 Z= -2.719099596134D+00
I= 7 X= 6.095886517624D+00 Y= 1.389658140944D+00 Z= -1.188178167565D+00
I= 8 X= 4.210262089351D+00 Y= 4.581553416462D+00 Z= -1.109272933295D+00
I= 9 X= -2.316496746119D+00 Y= -1.825764781354D+00 Z= 5.153738277901D+00
I= 10 X= -3.982572534629D+00 Y= -1.306419558518D+00 Z= 6.822397172884D+00
I= 11 X= -2.691051891986D+00 Y= -4.119164374639D+00 Z= 4.888760046536D+00
I= 12 X= -2.932678761085D-01 Y= -1.136129997569D+00 Z= 5.853704709975D+00
I= 13 X= -2.220683690213D+00 Y= 3.877651910487D+00 Z= 3.970824285809D+00
I= 14 X= -4.467347805135D+00 Y= 3.776110420781D+00 Z= 4.971300606375D+00
I= 15 X= -6.394243915128D-01 Y= 2.987269666097D+00 Z= 4.979308246069D+00
I= 16 X= -2.021828726530D+00 Y= 5.885614195800D+00 Z= 3.208881831879D+00

I= 17 X= -2.654394758258D+00 Y= 4.840052825438D+00 Z= -2.272870716218D+00
I= 18 X= -4.858725808381D+00 Y= 5.358504694396D+00 Z= -2.709741519541D+00
I= 19 X= -1.868292232455D+00 Y= 6.218417540694D+00 Z= -1.051731502017D+00
I= 20 X= -1.712355526461D+00 Y= 4.795660995029D+00 Z= -4.217908009571D+00
I= 21 X= -3.408490615664D+00 Y= -5.455633236727D-01 Z= -4.674688028008D+00
I= 22 X= -5.583833102387D+00 Y= -4.661895291822D-01 Z= -5.100547454526D+00
I= 23 X= -2.686445902140D+00 Y= 1.077385638796D+00 Z= -5.845546255412D+00
I= 24 X= -2.468982548479D+00 Y= -2.221062966557D+00 Z= -5.497076183328D+00
I= 25 X= -3.189643780380D+00 Y= -4.732264387627D+00 Z= -3.100853021370D-01
I= 26 X= -3.310032062156D+00 Y= -5.252760437110D+00 Z= -2.469675110608D+00
I= 27 X= -1.859317332200D+00 Y= -5.967971527080D+00 Z= 7.611349063669D-01
I= 28 X= -5.165717517366D+00 Y= -5.400466680232D+00 Z= 4.249677901557D-01
I= 29 X= 2.951760095347D+00 Y= -3.061535565565D+00 Z= -2.439398241431D+00
I= 30 X= 3.265327029294D+00 Y= -3.404800813405D+00 Z= 3.188452965681D-01
I= 31 X= 1.871186491771D+00 Y= -4.391902514980D+00 Z= -3.476812857276D+00
I= 32 X= 4.525291356813D+00 Y= -1.877640416244D+00 Z= -3.687123021675D+00
I= 33 X= 5.025473467129D+00 Y= -2.911387197743D+00 Z= 8.827625282567D-01
I= 34 X= 2.277739557465D+00 Y= -4.777135816850D+00 Z= 1.487839523205D+00
I= 35 X= 8.407455531166D-01 Y= -7.093534057801D-02 Z= -2.159232695594D-01
I= 36 X= 3.654877434997D+00 Y= 1.847557781791D+00 Z= 2.213723138384D+00
I= 37 X= 4.918296873027D+00 Y= 5.005420473303D-01 Z= 3.188959134919D+00
I= 38 X= 2.512121300780D+00 Y= 3.422431986294D+00 Z= 3.594363942387D+00

Forward Direction:

Total Energy: -651.6222355 Hartrees

Potential Energy: -651.7982732 Hartress

Kinetic Energy: 0.1760377 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.154797713520D+13 Y= 1.262140065695D+13 Z= 1.570642318912D+13

I= 1 X= -5.008086582657D+12 Y= 1.428740368799D+13 Z= -9.420884271711D+12

I= 2 X= 1.839906538403D+13 Y= -1.712747318286D+13 Z= -6.482012117563D+12

I= 3 X= 2.707455936459D+13 Y= 2.652223224231D+13 Z= 1.428627951771D+13
I= 4 X= -1.262908873478D+13 Y= 1.494789229990D+13 Z= -2.911892164129D+13
I= 5 X= 1.501955844864D+12 Y= 4.601709642760D+12 Z= 3.110517417534D+13
I= 6 X= 1.115708908979D+13 Y= -4.374461978019D+13 Z= 6.227612127532D+13
I= 7 X= 2.643237720653D+13 Y= -4.737111739443D+12 Z= -7.391979377645D+13
I= 8 X= 2.269800155543D+12 Y= -9.950729987726D+13 Z= -1.676055229834D+13
I= 9 X= -4.968239368751D+11 Y= -1.785566493280D+13 Z= 7.592028133485D+12
I= 10 X= 1.855001660597D+12 Y= -2.697329107248D+13 Z= -1.109575927142D+14
I= 11 X= -5.131512066504D+13 Y= 2.628056723588D+13 Z= 7.033684383843D+13
I= 12 X= 2.897368303855D+13 Y= -9.134769407609D+12 Z= 5.570769710066D+12
I= 13 X= -1.244640938832D+13 Y= -1.330934995456D+13 Z= 9.547044761302D+12
I= 14 X= 7.287344467202D+13 Y= -4.355200695868D+13 Z= 1.152260696683D+13
I= 15 X= -8.864292903497D+13 Y= -1.715686828419D+12 Z= -3.903801607136D+13
I= 16 X= 3.934047070671D+13 Y= 6.449491958425D+13 Z= 3.545960080524D+13
I= 17 X= -1.720229080460D+11 Y= -1.720532534256D+12 Z= -1.867314688378D+11
I= 18 X= 9.803263087850D+13 Y= -5.854660823485D+13 Z= 1.387470598718D+13
I= 19 X= -5.049385927574D+13 Y= 4.647246744654D+12 Z= -1.037581998919D+14
I= 20 X= 4.666332576459D+13 Y= -1.018023932522D+13 Z= -2.411728581750D+13
I= 21 X= -9.949090568891D+12 Y= -9.320982896123D+12 Z= 8.050718699468D+12
I= 22 X= 9.008593559933D+13 Y= -3.198521909230D+13 Z= 5.165176746760D+13
I= 23 X= 3.759628443002D+13 Y= 7.363657945055D+13 Z= -8.379992709111D+13
I= 24 X= -5.246589404766D+13 Y= 3.544215927618D+13 Z= -2.742458660582D+13
I= 25 X= -6.877574834169D+12 Y= -1.891628053674D+13 Z= 2.379092566541D+13
I= 26 X= -3.318989661004D+13 Y= -2.668908086277D+13 Z= -1.289655854136D+14
I= 27 X= -5.616726307673D+13 Y= -1.089207771360D+13 Z= -2.024978110280D+13
I= 28 X= -8.807961012687D+13 Y= -9.314241734504D+13 Z= -6.269478814627D+13
I= 29 X= 1.223291165986D+13 Y= 1.092995749809D+13 Z= -1.076610547653D+13
I= 30 X= 6.163530320437D+12 Y= 1.534756880893D+12 Z= -1.591438252342D+13
I= 31 X= 4.025362607822D+13 Y= -2.626835502860D+13 Z= -6.320620503225D+12
I= 32 X= -3.618760124502D+13 Y= -7.233211429554D+13 Z= 9.867729366796D+13

I= 33 X= -2.842600927248D+13 Y= -1.187668441581D+14 Z= -4.179931658674D+13
I= 34 X= 7.853037584796D+13 Y= 3.342850589205D+13 Z= -3.981421788749D+13
I= 35 X= -8.035513754700D+11 Y= 1.291652926587D+12 Z= 7.928030167484D+11
I= 36 X= 2.275217935281D+12 Y= 3.233874285130D+12 Z= -1.520724253644D+13
I= 37 X= -3.992868002507D+13 Y= 1.859182025009D+13 Z= -6.236739661285D+13
I= 38 X= 3.236684150274D+12 Y= 5.016387516500D+13 Z= 6.717738334814D+13

Backward Direction:

Total Energy: -651.6221954 Hartrees

Potential Energy: -651.7982732 Hartress

Kinetic Energy: 0.1760778 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.217125292107D+13 Y= 1.243803557037D+13 Z= 1.569272526510D+13
I= 1 X= -4.697398781772D+12 Y= 1.362240971793D+13 Z= -1.052679438218D+13
I= 2 X= 1.799470504342D+13 Y= -1.651812795396D+13 Z= -7.434533344973D+12
I= 3 X= 2.682069412650D+13 Y= 2.657836606803D+13 Z= 1.295168000367D+13
I= 4 X= -1.065277827237D+13 Y= 1.478697957998D+13 Z= -3.038481548780D+13
I= 5 X= 1.637076438230D+12 Y= 3.678306792400D+12 Z= 2.282544582168D+13
I= 6 X= 6.587203781447D+13 Y= 6.605380589118D+12 Z= 8.605471973359D+13
I= 7 X= 3.766473759911D+13 Y= 5.879646183191D+12 Z= -7.288963371990D+13
I= 8 X= 1.748224512217D+13 Y= -8.705906864142D+13 Z= -1.391641718129D+13
I= 9 X= 1.939972116182D+11 Y= -1.755713051023D+13 Z= 6.840363182847D+12
I= 10 X= 2.086548687325D+12 Y= -2.545288443480D+13 Z= -1.127198029805D+14
I= 11 X= -5.147642293571D+13 Y= 2.629155862702D+13 Z= 7.022674543415D+13
I= 12 X= 2.944784694323D+13 Y= -9.012244282157D+12 Z= 5.117225055474D+12
I= 13 X= -1.231341127988D+13 Y= -1.340109325774D+13 Z= 9.217983301621D+12
I= 14 X= 7.306202791944D+13 Y= -4.411642045387D+13 Z= 1.155543417570D+13
I= 15 X= -8.818088751369D+13 Y= -2.181160090301D+12 Z= -3.982145549023D+13
I= 16 X= 3.925070751826D+13 Y= 6.462089558848D+13 Z= 3.555176276208D+13
I= 17 X= 5.168772261692D+10 Y= -1.921911821197D+12 Z= -2.749421311959D+11
I= 18 X= 9.827053856971D+13 Y= -5.866917361633D+13 Z= 1.334921758662D+13

I= 19 X= -5.049435858276D+13 Y= 4.452348894429D+12 Z= -1.035359962187D+14
I= 20 X= 4.692709958192D+13 Y= -1.051346326543D+13 Z= -2.422599317666D+13
I= 21 X= -1.040121957200D+13 Y= -9.313316305799D+12 Z= 7.361531445071D+12
I= 22 X= 8.978490118456D+13 Y= -3.133059356003D+13 Z= 5.002026743728D+13
I= 23 X= 3.788290755246D+13 Y= 7.338536692159D+13 Z= -8.437771200704D+13
I= 24 X= -5.306298795289D+13 Y= 3.542492978696D+13 Z= -2.823783691933D+13
I= 25 X= -6.880761407353D+12 Y= -1.900198932925D+13 Z= 2.359953949274D+13
I= 26 X= -3.353722308634D+13 Y= -2.718161932205D+13 Z= -1.291027014726D+14
I= 27 X= -5.586314364844D+13 Y= -1.060942053029D+13 Z= -2.036135435100D+13
I= 28 X= -8.800768595275D+13 Y= -9.315404818529D+13 Z= -6.234418365875D+13
I= 29 X= 1.104757423474D+13 Y= 1.162982269239D+13 Z= -1.167513204344D+13
I= 30 X= 6.255853263895D+12 Y= 1.733969524233D+12 Z= -1.661330592705D+13
I= 31 X= 4.034760872606D+13 Y= -2.691449667456D+13 Z= -6.753757105481D+12
I= 32 X= -3.769490845948D+13 Y= -7.096764641319D+13 Z= 9.726938366769D+13
I= 33 X= -2.821695713189D+13 Y= -1.188594309407D+14 Z= -4.251147638131D+13
I= 34 X= 7.923768404396D+13 Y= 3.332149250811D+13 Z= -4.027197935321D+13
I= 35 X= -1.088845818472D+12 Y= 1.175547804280D+12 Z= 1.902675584121D+12
I= 36 X= -1.178715802552D+12 Y= -8.932652810521D+11 Z= -1.727875457026D+13
I= 37 X= -3.591478681459D+13 Y= 2.117729115239D+13 Z= -6.746614487809D+13
I= 38 X= 5.667461588649D+12 Y= 4.999982408885D+13 Z= 6.388460033301D+13

Seed: 31882016875

CM Start Point Coordinates: bohr

I= 0 X= -2.299580832672D+00 Y= 2.257531158813D+00 Z= -8.320849751520D-01
I= 1 X= -2.972851725712D+00 Y= -7.803606015750D-02 Z= -1.972640926162D+00
I= 2 X= -2.272978238065D+00 Y= 1.744924426087D+00 Z= 2.176897228558D+00
I= 3 X= -2.882533129323D+00 Y= -2.125037756139D+00 Z= -1.765154767970D-01
I= 4 X= -2.417669494178D+00 Y= -1.045302412033D+00 Z= 2.309156329463D+00
I= 5 X= 3.773516620936D+00 Y= 2.474637181704D+00 Z= -1.300588135178D+00
I= 6 X= 2.088825992083D+00 Y= 1.063002115339D+00 Z= -3.098932841995D+00

I= 7 X= 5.744521513199D+00 Y= 1.772944452122D+00 Z= -1.852472354548D+00
I= 8 X= 3.750000087672D+00 Y= 4.360984945448D+00 Z= -2.737990696223D+00
I= 9 X= -2.676291869567D+00 Y= -2.391148146078D+00 Z= 4.672012536301D+00
I= 10 X= -4.652749411950D+00 Y= -2.584108035249D+00 Z= 5.548266635738D+00
I= 11 X= -2.320432677616D+00 Y= -4.513676561441D+00 Z= 4.370171101078D+00
I= 12 X= -1.261536835192D+00 Y= -1.265651600173D+00 Z= 5.683004123946D+00
I= 13 X= -1.991931010175D+00 Y= 3.749891878956D+00 Z= 4.147640068702D+00
I= 14 X= -3.796819208059D+00 Y= 3.916199475490D+00 Z= 5.079636798944D+00
I= 15 X= -5.916481860677D-01 Y= 3.496247798639D+00 Z= 5.703501872245D+00
I= 16 X= -1.417749992795D+00 Y= 5.850174241827D+00 Z= 3.325413749484D+00
I= 17 X= -2.323317901539D+00 Y= 4.838555258675D+00 Z= -1.874862877673D+00
I= 18 X= -4.273737410028D+00 Y= 5.489173534789D+00 Z= -2.703457753142D+00
I= 19 X= -1.464722444351D+00 Y= 5.886939969545D+00 Z= -6.469060588305D-01
I= 20 X= -9.261521565942D-01 Y= 5.183786708044D+00 Z= -3.553874560754D+00
I= 21 X= -3.804203060643D+00 Y= 8.409776560630D-02 Z= -4.744954720721D+00
I= 22 X= -5.949897796247D+00 Y= 1.003928515166D+00 Z= -4.669475542042D+00
I= 23 X= -2.649918542276D+00 Y= 8.842190057439D-01 Z= -6.066808999026D+00
I= 24 X= -3.794874724708D+00 Y= -1.919029952702D+00 Z= -5.568557849339D+00
I= 25 X= -3.426629134036D+00 Y= -4.891549274642D+00 Z= -7.360352301552D-01
I= 26 X= -2.995596707192D+00 Y= -5.451559221620D+00 Z= -2.511432219525D+00
I= 27 X= -2.553214932044D+00 Y= -5.902660964224D+00 Z= 7.875716947473D-01
I= 28 X= -5.729627529778D+00 Y= -5.058370640139D+00 Z= -3.189840705584D-01
I= 29 X= 3.010549018304D+00 Y= -3.494736822002D+00 Z= -1.387586608097D+00
I= 30 X= 3.454839320816D+00 Y= -3.084078362545D+00 Z= 1.292042734125D+00
I= 31 X= 1.809622151896D+00 Y= -4.895287329357D+00 Z= -2.058995441217D+00
I= 32 X= 4.409874969602D+00 Y= -2.686931215017D+00 Z= -2.827613809618D+00
I= 33 X= 5.119769253220D+00 Y= -2.480053530212D+00 Z= 1.870796815666D+00
I= 34 X= 2.586836789389D+00 Y= -4.150047700395D+00 Z= 2.743946306743D+00
I= 35 X= 8.858540039698D-01 Y= -6.432895480978D-02 Z= -1.883632134733D-01
I= 36 X= 3.554071725990D+00 Y= 2.647763052948D+00 Z= 1.357338207353D+00

I= 37 X= 4.993075891191D+00 Y= 2.075510713271D+00 Z= 2.969352659236D+00

I= 38 X= 2.329310958438D+00 Y= 4.054927426273D+00 Z= 1.713975255998D+00

Forward Direction:

Total Energy: -651.6183070 Hartrees

Potential Energy: -651.7752751 Hartress

Kinetic Energy: 0.1569681 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.323971524458D+13 Y= -8.420412934322D+12 Z= -8.025225721667D+12

I= 1 X= -7.406233490427D+12 Y= 1.540710170400D+13 Z= 1.699078724905D+12

I= 2 X= 4.463558362922D+12 Y= -3.554029784738D+13 Z= -7.096692661777D+12

I= 3 X= -6.040860693271D+12 Y= 1.115222789466D+13 Z= -1.464716846870D+12

I= 4 X= 1.013477134235D+13 Y= 4.901403104664D+12 Z= -9.181843212630D+12

I= 5 X= -4.700793514454D+12 Y= -7.112603261424D+12 Z= 1.827564769319D+13

I= 6 X= 1.256164210843D+13 Y= 3.402141003497D+12 Z= -5.453894927169D+13

I= 7 X= -2.681035777756D+13 Y= 3.259058794014D+13 Z= 7.406335144803D+12

I= 8 X= -2.926840073834D+13 Y= 1.422116446651D+13 Z= -2.235732612109D+11

I= 9 X= -1.086040821659D+13 Y= 2.614623803218D+12 Z= 3.240115402473D+12

I= 10 X= 1.146559008879D+10 Y= -1.835105795040D+13 Z= 3.669271792430D+13

I= 11 X= 5.010296767290D+13 Y= -1.181500302442D+14 Z= 9.551108817826D+12

I= 12 X= -8.039398947582D+12 Y= 1.000308819295D+13 Z= 2.900094787672D+13

I= 13 X= -1.824490506236D+12 Y= -1.004130777236D+13 Z= 6.320919086018D+12

I= 14 X= -6.747076568371D+13 Y= 5.252557329663D+13 Z= 9.647279058354D+13

I= 15 X= 2.717138071885D+13 Y= 2.862140292574D+13 Z= 7.586984712908D+12

I= 16 X= 2.066887032744D+13 Y= 8.441755789419D+13 Z= -2.430866655084D+13

I= 17 X= 4.290593538947D+12 Y= 7.827219395994D+12 Z= 9.858030691129D+12

I= 18 X= -3.939386160291D+13 Y= 6.984069306388D+13 Z= -1.492425179456D+13

I= 19 X= 3.105857315189D+12 Y= -4.330952879132D+13 Z= -8.248695292941D+13

I= 20 X= -7.399270889630D+13 Y= 3.645804022141D+13 Z= -4.907044965377D+13

I= 21 X= -8.241188220981D+12 Y= -9.525556091612D+12 Z= 4.245158412113D+12

I= 22 X= 5.058129680361D+13 Y= 1.076545087494D+13 Z= 4.512564133142D+13

I= 23 X= -3.677698420218D+13 Y= -1.261260592502D+14 Z= 1.069764834008D+13
I= 24 X= -2.078493868601D+13 Y= 7.220011765240D+13 Z= -1.041770503682D+14
I= 25 X= -8.584268346450D+12 Y= -6.117272423622D+12 Z= 7.255988677549D+12
I= 26 X= 1.461241322026D+13 Y= -2.074842692184D+13 Z= -9.379039284581D+13
I= 27 X= -2.432849469454D+13 Y= 5.597709416158D+13 Z= 6.207292866637D+13
I= 28 X= -1.079138439019D+14 Y= -4.577896733461D+13 Z= 2.462418699609D+13
I= 29 X= -2.350685356597D+13 Y= -3.352845176182D+12 Z= -1.596811409329D+13
I= 30 X= 8.509349523397D+12 Y= 1.102413088537D+13 Z= 1.692785594214D+13
I= 31 X= 1.288184692904D+14 Y= 9.721106854484D+13 Z= 1.219232497224D+14
I= 32 X= 2.716258533874D+13 Y= 5.288603829230D+13 Z= 6.876254095049D+13
I= 33 X= 1.258671340692D+12 Y= -5.043836076350D+13 Z= 5.176416631075D+13
I= 34 X= -1.304766734796D+13 Y= -7.292546866430D+13 Z= -5.072093397617D+13
I= 35 X= 1.270406927661D+12 Y= 1.043141326266D+12 Z= -3.055021652016D+12
I= 36 X= 1.724675267339D+13 Y= -3.077630436579D+12 Z= 1.049080459827D+13
I= 37 X= -2.563950137669D+13 Y= 9.170983767466D+13 Z= -9.233450928280D+12
I= 38 X= 5.229966318992D+13 Y= -5.641194190551D+13 Z= 6.120723485150D+13

Backward Direction:

Total Energy: -651.6182998 Hartrees

Potential Energy: -651.7752751 Hartress

Kinetic Energy: 0.1569753 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.265585028947D+13 Y= -8.592183521987D+12 Z= -8.038057500376D+12
I= 1 X= -7.115191028342D+12 Y= 1.478415647709D+13 Z= 6.630972645830D+11
I= 2 X= 4.084766439240D+12 Y= -3.496948259387D+13 Z= -7.988984287884D+12
I= 3 X= -6.278673584055D+12 Y= 1.120481227988D+13 Z= -2.714927274819D+12
I= 4 X= 1.198611620241D+13 Y= 4.750665180382D+12 Z= -1.036769235346D+13
I= 5 X= -4.574216837873D+12 Y= -7.977617714749D+12 Z= 1.051946119500D+13
I= 6 X= 6.381686793038D+13 Y= 5.056842187176D+13 Z= -3.226391361647D+13
I= 7 X= -1.628823938451D+13 Y= 4.253602950292D+13 Z= 8.371356357303D+12
I= 8 X= -1.501786555636D+13 Y= 2.588227204659D+13 Z= 2.440722168194D+12

I= 9 X= -1.021326890862D+13 Y= 2.894281367586D+12 Z= 2.535979555244D+12
I= 10 X= 2.283714879191D+11 Y= -1.692678930813D+13 Z= 3.504193532742D+13
I= 11 X= 4.995186483363D+13 Y= -1.181397338588D+14 Z= 9.447972130648D+12
I= 12 X= -7.595217266045D+12 Y= 1.011786583778D+13 Z= 2.857608165235D+13
I= 13 X= -1.699902106299D+12 Y= -1.012724998271D+13 Z= 6.012664764119D+12
I= 14 X= -6.729410689292D+13 Y= 5.199684866527D+13 Z= 9.650354206903D+13
I= 15 X= 2.760420653299D+13 Y= 2.818536236605D+13 Z= 6.853083554962D+12
I= 16 X= 2.058478301930D+13 Y= 8.453556821404D+13 Z= -2.422233215608D+13
I= 17 X= 4.500158552783D+12 Y= 7.638573677898D+12 Z= 9.775397745633D+12
I= 18 X= -3.917099723432D+13 Y= 6.972587771048D+13 Z= -1.541651263136D+13
I= 19 X= 3.105389588338D+12 Y= -4.349210290543D+13 Z= -8.227879959108D+13
I= 20 X= -7.374561396775D+13 Y= 3.614588661881D+13 Z= -4.917228325684D+13
I= 21 X= -8.664728307216D+12 Y= -9.518374273391D+12 Z= 3.599549685309D+12
I= 22 X= 5.029929732883D+13 Y= 1.137868328542D+13 Z= 4.359730393058D+13
I= 23 X= -3.650848476229D+13 Y= -1.263613871693D+14 Z= 1.015639778348D+13
I= 24 X= -2.134427728761D+13 Y= 7.218397761414D+13 Z= -1.049388774267D+14
I= 25 X= -8.587253428784D+12 Y= -6.197561697221D+12 Z= 7.076704191418D+12
I= 26 X= 1.428704880751D+13 Y= -2.120982130482D+13 Z= -9.391883881209D+13
I= 27 X= -2.404360528642D+13 Y= 5.624187842778D+13 Z= 6.196841039664D+13
I= 28 X= -1.078464676263D+14 Y= -4.578986272555D+13 Z= 2.495262213994D+13
I= 29 X= -2.461724000945D+13 Y= -2.697233695051D+12 Z= -1.681966130519D+13
I= 30 X= 8.595834724578D+12 Y= 1.121074696018D+13 Z= 1.627312669969D+13
I= 31 X= 1.289065092540D+14 Y= 9.660578357688D+13 Z= 1.215175011106D+14
I= 32 X= 2.575058782454D+13 Y= 5.416422846068D+13 Z= 6.744365558774D+13
I= 33 X= 1.454504745099D+12 Y= -5.052509311897D+13 Z= 5.109703763839D+13
I= 34 X= -1.238508349924D+13 Y= -7.302571540225D+13 Z= -5.114975037702D+13
I= 35 X= 1.003152156703D+12 Y= 9.343777354105D+11 Z= -2.015328288591D+12
I= 36 X= 1.401121726979D+13 Y= -6.943803673288D+12 Z= 8.550277931847D+12
I= 37 X= -2.187941372515D+13 Y= 9.413182468061D+13 Z= -1.400979633179D+13
I= 38 X= 5.457673827224D+13 Y= -5.656561974341D+13 Z= 5.812266032844D+13

Seed: 31995162837

CM Start Point Coordinates: bohr

I= 0 X= -2.371993974197D+00 Y= 2.317661192036D+00 Z= -6.232867554458D-01
I= 1 X= -2.866511443017D+00 Y= -4.925659152097D-02 Z= -2.030232192891D+00
I= 2 X= -2.421731909624D+00 Y= 1.797146286768D+00 Z= 2.165507250908D+00
I= 3 X= -2.900875609400D+00 Y= -1.883454655955D+00 Z= -1.653740593951D-01
I= 4 X= -2.425523126210D+00 Y= -9.595490430550D-01 Z= 2.366354751210D+00
I= 5 X= 3.804629657918D+00 Y= 2.553712602700D+00 Z= -1.405759829652D+00
I= 6 X= 2.172787305105D+00 Y= 8.094072813349D-01 Z= -3.120791357495D+00
I= 7 X= 5.634255238810D+00 Y= 1.629875315657D+00 Z= -2.132789624430D+00
I= 8 X= 3.489444629619D+00 Y= 4.368365094505D+00 Z= -2.436858276179D+00
I= 9 X= -2.514085208871D+00 Y= -2.406306959944D+00 Z= 4.793179481945D+00
I= 10 X= -4.735291205665D+00 Y= -2.174547883741D+00 Z= 5.141960833859D+00
I= 11 X= -2.228869880662D+00 Y= -4.421764816802D+00 Z= 4.396629609374D+00
I= 12 X= -1.263090077102D+00 Y= -1.567426556035D+00 Z= 6.229077050736D+00
I= 13 X= -2.190708179033D+00 Y= 3.715090420321D+00 Z= 4.294916654980D+00
I= 14 X= -3.615220881456D+00 Y= 2.986881401545D+00 Z= 5.992489617778D+00
I= 15 X= -3.060036901129D-01 Y= 2.810828216313D+00 Z= 5.422848310773D+00
I= 16 X= -2.169523663614D+00 Y= 5.674608977429D+00 Z= 3.621664820825D+00
I= 17 X= -2.410244755979D+00 Y= 5.002725874917D+00 Z= -1.829650632409D+00
I= 18 X= -4.582579702230D+00 Y= 5.631684553457D+00 Z= -2.103930032578D+00
I= 19 X= -1.820226356299D+00 Y= 6.661696346618D+00 Z= -3.527487893603D-01
I= 20 X= -1.139048698867D+00 Y= 4.874105197651D+00 Z= -3.539292158625D+00
I= 21 X= -3.197129866904D+00 Y= -3.163782541018D-01 Z= -4.768312303468D+00
I= 22 X= -5.211445512926D+00 Y= -1.458543808083D-01 Z= -5.227520522330D+00
I= 23 X= -2.060932879464D+00 Y= 1.299895782402D+00 Z= -5.940429900044D+00
I= 24 X= -2.593508567236D+00 Y= -2.208893526132D+00 Z= -5.746030433914D+00
I= 25 X= -3.641729690020D+00 Y= -4.620544134617D+00 Z= -4.506588022388D-01
I= 26 X= -3.730049083595D+00 Y= -5.266204512250D+00 Z= -2.580802675556D+00

I= 27 X= -2.389361751937D+00 Y= -5.744148391664D+00 Z= 7.228070051699D-01
I= 28 X= -5.354429851647D+00 Y= -4.996753413819D+00 Z= 1.594717414641D-01
I= 29 X= 3.099707664318D+00 Y= -3.363881087744D+00 Z= -1.505265904011D+00
I= 30 X= 3.213270702172D+00 Y= -2.970898225152D+00 Z= 1.161408001181D+00
I= 31 X= 1.940261050795D+00 Y= -4.778147882927D+00 Z= -2.422904283053D+00
I= 32 X= 4.804503089535D+00 Y= -3.217791599786D+00 Z= -2.584268043404D+00
I= 33 X= 5.075066425147D+00 Y= -2.656160573591D+00 Z= 2.412257809153D+00
I= 34 X= 1.916559157032D+00 Y= -4.178474915958D+00 Z= 2.338283465363D+00
I= 35 X= 8.753441048606D-01 Y= -8.348847448392D-02 Z= -2.172647851388D-01
I= 36 X= 3.616670933776D+00 Y= 2.419854730762D+00 Z= 1.217121845778D+00
I= 37 X= 5.303452476640D+00 Y= 1.928289400813D+00 Z= 2.783014823005D+00
I= 38 X= 2.510037273212D+00 Y= 3.949744922418D+00 Z= 2.227117046671D+00

Forward Direction:

Total Energy: -651.6209813 Hartrees

Potential Energy: -651.8103169 Hartress

Kinetic Energy: 0.1893355 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.847882465665D+11 Y= -4.100183437705D+12 Z= -6.514001818180D+12
I= 1 X= 8.035835283447D+12 Y= 7.818184601274D+12 Z= 2.251299512548D+12
I= 2 X= 1.942386218624D+13 Y= -3.020714607239D+13 Z= -1.138780124551D+13
I= 3 X= -3.507696293978D+12 Y= 9.791629668670D+12 Z= 7.829462562733D+12
I= 4 X= -4.296608672801D+12 Y= 2.039008574874D+13 Z= 2.011951927663D+12
I= 5 X= -1.091436995928D+13 Y= 2.892458207172D+12 Z= -1.474513744703D+13
I= 6 X= -1.719104479516D+12 Y= 1.864867129142D+13 Z= -5.903837729434D+13
I= 7 X= -1.335374259817D+14 Y= 6.904388432813D+13 Z= 6.859915175598D+13
I= 8 X= 2.146616759896D+13 Y= -5.815409445405D+12 Z= -7.337821479055D+13
I= 9 X= 1.071055575582D+12 Y= -9.553074335846D+12 Z= 1.213575133749D+13
I= 10 X= 2.662584725690D+12 Y= 3.405791927886D+13 Z= 4.222244854572D+12
I= 11 X= 3.156875361265D+13 Y= 7.997719250650D+13 Z= -4.101218330377D+12
I= 12 X= -7.982714893311D+13 Y= -9.456044607579D+13 Z= -2.250634975214D+13

I= 13 X= 1.045875091818D+13 Y= 1.726427687180D+13 Z= 1.953400522395D+13
I= 14 X= -9.938811420841D+12 Y= -2.203350738569D+13 Z= 3.740543006325D+13
I= 15 X= -1.106351776389D+13 Y= -1.564171717009D+13 Z= -1.431943788606D+13
I= 16 X= -2.098081877702D+13 Y= -7.784870928886D+13 Z= 6.632551464777D+12
I= 17 X= -3.080904286240D+12 Y= 5.260323905177D+12 Z= -2.876403077435D+12
I= 18 X= 9.006050141311D+13 Y= -1.734157858661D+14 Z= 4.180150430085D+13
I= 19 X= 8.119807824755D+13 Y= 1.163352133161D+13 Z= 1.321847664180D+13
I= 20 X= 3.572778623371D+13 Y= 6.415248753151D+13 Z= 9.751889638189D+13
I= 21 X= 9.766407317119D+12 Y= -4.297659840730D+12 Z= -5.300739666555D+12
I= 22 X= -3.768882692287D+13 Y= 6.059841951787D+13 Z= -7.380013579382D+13
I= 23 X= -7.382653802532D+13 Y= -5.502381936298D+13 Z= -5.800408573313D+13
I= 24 X= 3.470354480247D+13 Y= -6.687124001284D+13 Z= -7.996016880807D+13
I= 25 X= 8.103695419666D+12 Y= -5.985602944532D+09 Z= -4.701152765430D+12
I= 26 X= -4.444192094728D+12 Y= -8.142922156121D+13 Z= -1.833830668299D+14
I= 27 X= -1.790277591755D+13 Y= 1.063979616584D+13 Z= 1.076455841885D+14
I= 28 X= 3.307389143818D+13 Y= -5.538638971514D+12 Z= 5.320771120724D+13
I= 29 X= -8.514963514587D+11 Y= -8.517219346193D+12 Z= -1.016329088317D+12
I= 30 X= 7.334470238843D+12 Y= 6.525717704105D+12 Z= -1.293505353584D+13
I= 31 X= 3.573812546773D+13 Y= -4.562059794004D+12 Z= 8.296424951494D+13
I= 32 X= -1.017890489930D+14 Y= 3.211450198736D+13 Z= 7.325070411705D+13
I= 33 X= -7.267078527967D+13 Y= -9.161984447320D+13 Z= -1.038904975881D+13
I= 34 X= -7.007990592075D+13 Y= -5.550310098033D+13 Z= 9.244218041574D+13
I= 35 X= -1.429511547548D+12 Y= 8.549431894229D+11 Z= 1.016205465841D+12
I= 36 X= 1.318786948167D+13 Y= 1.317887843344D+13 Z= -1.001223992009D+13
I= 37 X= -9.878157154160D+13 Y= -4.421921529179D+13 Z= 3.403565980938D+13
I= 38 X= -1.688149382006D+13 Y= -6.529540350269D+13 Z= -2.231240613848D+13

Backward Direction:

Total Energy: -651.6209830 Hartrees

Potential Energy: -651.8103169 Hartress

Kinetic Energy: 0.1893339 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.704269243187D+11 Y= -4.163247626249D+12 Z= -6.518712902145D+12
I= 1 X= 8.142689183554D+12 Y= 7.589475273163D+12 Z= 1.870947253505D+12
I= 2 X= 1.928479178012D+13 Y= -2.999757584354D+13 Z= -1.171539893797D+13
I= 3 X= -3.595007383467D+12 Y= 9.810935603147D+12 Z= 7.370457861829D+12
I= 4 X= -3.616902301281D+12 Y= 2.033474353249D+13 Z= 1.576576954715D+12
I= 5 X= -1.086789834911D+13 Y= 2.574875107086D+12 Z= -1.759275892800D+13
I= 6 X= 1.709883936974D+13 Y= 3.596539189043D+13 Z= -5.086027714051D+13
I= 7 X= -1.296743148565D+14 Y= 7.269527318934D+13 Z= 6.895345153110D+13
I= 8 X= 2.669813695761D+13 Y= -1.534127605816D+12 Z= -7.240004015861D+13
I= 9 X= 1.308647560644D+12 Y= -9.450400311129D+12 Z= 1.187723352505D+13
I= 10 X= 2.742219975788D+12 Y= 3.458082805557D+13 Z= 3.616173300051D+12
I= 11 X= 3.151327740614D+13 Y= 7.998097273774D+13 Z= -4.139084136481D+12
I= 12 X= -7.966407120762D+13 Y= -9.451830639429D+13 Z= -2.266233596563D+13
I= 13 X= 1.050449254929D+13 Y= 1.723272387895D+13 Z= 1.942083213119D+13
I= 14 X= -9.873952564701D+12 Y= -2.222762438350D+13 Z= 3.741672022833D+13
I= 15 X= -1.090460924231D+13 Y= -1.580180595982D+13 Z= -1.458888379410D+13
I= 16 X= -2.101169075192D+13 Y= -7.780538275128D+13 Z= 6.664248444662D+12
I= 17 X= -3.003964183449D+12 Y= 5.191064147573D+12 Z= -2.906741099363D+12
I= 18 X= 9.014232426766D+13 Y= -1.734579393998D+14 Z= 4.162077468955D+13
I= 19 X= 8.119790651569D+13 Y= 1.156649071689D+13 Z= 1.329489846481D+13
I= 20 X= 3.581850514789D+13 Y= 6.403788284767D+13 Z= 9.748150899537D+13
I= 21 X= 9.610907978238D+12 Y= -4.295023095844D+12 Z= -5.537769715901D+12
I= 22 X= -3.779236076438D+13 Y= 6.082356285644D+13 Z= -7.436125257961D+13
I= 23 X= -7.372796061788D+13 Y= -5.511021811698D+13 Z= -5.820280151950D+13
I= 24 X= 3.449818813919D+13 Y= -6.687716569892D+13 Z= -8.023986747920D+13
I= 25 X= 8.102599472337D+12 Y= -3.546316266919D+10 Z= -4.766975625549D+12
I= 26 X= -4.563647025027D+12 Y= -8.159861879423D+13 Z= -1.834302247382D+14
I= 27 X= -1.779818105795D+13 Y= 1.073700958005D+13 Z= 1.076072111385D+14
I= 28 X= 3.309862810058D+13 Y= -5.542639129273D+12 Z= 5.332829353000D+13

I= 29 X= -1.259165803668D+12 Y= -8.276516865986D+12 Z= -1.328967795216D+12
I= 30 X= 7.366222585257D+12 Y= 6.594232295905D+12 Z= -1.317543210913D+13
I= 31 X= 3.577044862858D+13 Y= -4.784285302329D+12 Z= 8.281528218007D+13
I= 32 X= -1.023074525235D+14 Y= 3.258377922276D+13 Z= 7.276648596645D+13
I= 33 X= -7.259888661960D+13 Y= -9.165168755831D+13 Z= -1.063398068481D+13
I= 34 X= -6.983664358876D+13 Y= -5.553990576076D+13 Z= 9.228474392784D+13
I= 35 X= -1.527631986215D+12 Y= 8.150115122565D+11 Z= 1.397920520654D+12
I= 36 X= 1.199996868759D+13 Y= 1.175944403027D+13 Z= -1.072468867743D+13
I= 37 X= -9.740108560774D+13 Y= -4.333000224376D+13 Z= 3.228206301692D+13
I= 38 X= -1.604548401767D+13 Y= -6.535182508442D+13 Z= -2.344488286385D+13

Seed: 32631781433

CM Start Point Coordinates: bohr

I= 0 X= -2.672354987035D+00 Y= 2.271188380580D+00 Z= -6.342538044977D-01
I= 1 X= -3.048939628320D+00 Y= -8.323843096559D-02 Z= -1.930598215399D+00
I= 2 X= -2.366488852273D+00 Y= 1.744147098799D+00 Z= 1.967338645907D+00
I= 3 X= -3.085320603471D+00 Y= -2.056048689602D+00 Z= -1.794096835874D-01
I= 4 X= -2.477305841597D+00 Y= -1.033844596971D+00 Z= 2.267241845533D+00
I= 5 X= 4.212341455627D+00 Y= 2.321658879435D+00 Z= -1.233751571024D+00
I= 6 X= 2.154883476874D+00 Y= 7.813338816345D-01 Z= -2.899456491968D+00
I= 7 X= 5.875017633090D+00 Y= 1.630587539022D+00 Z= -1.894290103837D+00
I= 8 X= 3.711498094625D+00 Y= 3.931064107146D+00 Z= -2.400214251988D+00
I= 9 X= -2.798913804808D+00 Y= -2.418098190732D+00 Z= 4.730992883329D+00
I= 10 X= -4.963611714324D+00 Y= -3.440327207278D+00 Z= 4.858051157229D+00
I= 11 X= -1.319999078967D+00 Y= -4.112554270591D+00 Z= 4.544766931770D+00
I= 12 X= -2.583261390563D+00 Y= -1.013048343684D+00 Z= 6.599498841749D+00
I= 13 X= -2.007810976258D+00 Y= 3.612498792078D+00 Z= 4.079497566443D+00
I= 14 X= -3.939636105684D+00 Y= 4.234255266940D+00 Z= 4.615920704799D+00
I= 15 X= -1.570720008242D+00 Y= 2.738889492631D+00 Z= 5.741914188679D+00
I= 16 X= -7.657394776089D-01 Y= 5.216856876953D+00 Z= 3.727106280090D+00

I= 17 X= -2.375647360727D+00 Y= 5.015257721250D+00 Z= -1.835574590121D+00
I= 18 X= -4.291269716717D+00 Y= 5.500637048528D+00 Z= -2.444279642935D+00
I= 19 X= -1.477047361265D+00 Y= 6.413588524163D+00 Z= -4.720057935536D-01
I= 20 X= -1.295724384680D+00 Y= 4.819646568075D+00 Z= -3.615113291302D+00
I= 21 X= -3.531140819000D+00 Y= -3.100681762887D-01 Z= -4.741511179636D+00
I= 22 X= -5.662098444573D+00 Y= -7.196854994740D-01 Z= -5.141543224931D+00
I= 23 X= -2.479038082483D+00 Y= 1.607479728520D+00 Z= -5.328664318054D+00
I= 24 X= -2.229760477597D+00 Y= -1.899959641521D+00 Z= -5.475026104211D+00
I= 25 X= -3.666967001735D+00 Y= -4.728031572356D+00 Z= -5.867232074751D-01
I= 26 X= -3.329554655720D+00 Y= -5.193210446422D+00 Z= -2.702195381356D+00
I= 27 X= -2.553682525483D+00 Y= -6.037405042507D+00 Z= 3.507626055793D-01
I= 28 X= -5.324972659822D+00 Y= -5.408776762313D+00 Z= 3.964878089215D-02
I= 29 X= 2.737907666825D+00 Y= -3.621266661253D+00 Z= -1.510205224220D+00
I= 30 X= 3.921096153581D+00 Y= -2.795054867049D+00 Z= 9.584161398446D-01
I= 31 X= 1.522451322601D+00 Y= -5.491186552807D+00 Z= -1.384506214987D+00
I= 32 X= 3.859667442404D+00 Y= -3.291419277165D+00 Z= -3.586243971977D+00
I= 33 X= 6.047295067141D+00 Y= -2.177764796025D+00 Z= 7.697267244900D-01
I= 34 X= 3.199782611844D+00 Y= -3.862017618422D+00 Z= 2.837560444333D+00
I= 35 X= 8.892642668299D-01 Y= -2.490814164434D-02 Z= -1.760680216334D-01
I= 36 X= 3.663657378611D+00 Y= 2.444491976764D+00 Z= 1.364649816115D+00
I= 37 X= 4.937792229057D+00 Y= 1.732580903558D+00 Z= 2.788713050122D+00
I= 38 X= 2.907891678413D+00 Y= 4.480251191439D+00 Z= 1.840497289229D+00

Forward Direction:

Total Energy: -651.6164600 Hartrees

Potential Energy: -651.8071101 Hartress

Kinetic Energy: 0.1906501 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.389760365105D+13 Y= 1.679969204531D+13 Z= -1.874594899187D+11

I= 1 X= 3.520395398814D+12 Y= -8.664124381406D+12 Z= -2.428861763680D+13

I= 2 X= -1.848217627172D+12 Y= -1.582595302981D+13 Z= -9.766724285793D+12

I= 3 X= 8.006953128467D+12 Y= -1.172963124959D+13 Z= 4.707063121946D+12
I= 4 X= -2.200590113326D+13 Y= -8.644799430118D+12 Z= 1.777471208308D+13
I= 5 X= 1.005725183534D+13 Y= -1.697029903819D+12 Z= 1.692356777171D+13
I= 6 X= 3.835700461839D+13 Y= 5.560328405814D+13 Z= -5.902999622564D+13
I= 7 X= -3.755587800574D+13 Y= -2.174627650457D+13 Z= -7.219185099000D+12
I= 8 X= -1.392135879983D+14 Y= 7.076969131697D+13 Z= -5.753516862836D+13
I= 9 X= -6.609877290180D+12 Y= 1.168126195058D+13 Z= -2.809955277525D+12
I= 10 X= 1.180672658426D+13 Y= -2.021081248983D+13 Z= -4.689370892480D+13
I= 11 X= -2.072928546374D+13 Y= -8.454480835618D+13 Z= -2.166470359844D+13
I= 12 X= 5.815594518885D+13 Y= 5.447623282370D+13 Z= 1.151458360364D+12
I= 13 X= 2.210964177775D+12 Y= -3.947539400776D+12 Z= 1.166481798798D+13
I= 14 X= 5.775820316894D+13 Y= -3.740745872274D+13 Z= 3.735959211225D+13
I= 15 X= -7.605254258343D+13 Y= 1.341568999736D+13 Z= 1.072644364094D+14
I= 16 X= 5.869551368068D+13 Y= 1.382059621074D+14 Z= 3.185257111498D+13
I= 17 X= 1.611464464942D+13 Y= -1.711425738892D+13 Z= -2.060418620814D+13
I= 18 X= -6.611680899167D+13 Y= 7.049936305280D+12 Z= -5.101143567221D+13
I= 19 X= -1.004038378787D+13 Y= -2.221081248239D+13 Z= 4.282585751505D+13
I= 20 X= -4.222086869237D+13 Y= 4.352458999527D+13 Z= 1.103657850713D+14
I= 21 X= 1.470652001778D+12 Y= -1.394918912125D+12 Z= 2.011925739016D+13
I= 22 X= 1.955118948300D+12 Y= -2.959142793750D+13 Z= 4.779281584390D+13
I= 23 X= 1.289357193707D+14 Y= 1.288634065778D+14 Z= -4.691564686704D+13
I= 24 X= 4.166964664823D+13 Y= 1.972593535937D+12 Z= -7.179364595895D+13
I= 25 X= 8.662760453103D+12 Y= -2.220881392048D+12 Z= -1.576830294487D+13
I= 26 X= 1.296904272692D+13 Y= 1.088167042594D+14 Z= 7.081760890547D+13
I= 27 X= -3.128869169328D+13 Y= -4.045816183369D+13 Z= 1.570540627376D+13
I= 28 X= 7.856711711257D+13 Y= 1.688083499341D+13 Z= 1.095916272126D+14
I= 29 X= 1.708575172905D+13 Y= -2.062247800506D+13 Z= 5.531492829647D+12
I= 30 X= 1.061070722834D+13 Y= 6.682249555789D+12 Z= 1.992504001015D+13
I= 31 X= -1.324027920415D+14 Y= -1.248288480297D+14 Z= -2.134891860492D+13
I= 32 X= -2.425219909507D+13 Y= -2.896546053667D+13 Z= -1.533305918816D+13

I= 33 X= -4.359535075494D+13 Y= -1.037036674065D+13 Z= -5.139099550971D+13
I= 34 X= -3.684397222148D+13 Y= -7.258385846256D+13 Z= -7.313528123563D+13
I= 35 X= -7.973962481069D+11 Y= 2.777095588749D+12 Z= -6.517671261406D+11
I= 36 X= 9.017745488337D+12 Y= -1.104751481576D+11 Z= -1.908863230966D+13
I= 37 X= -4.122432467473D+13 Y= -3.360648683430D+13 Z= 6.345239331692D+12
I= 38 X= -2.039613238698D+13 Y= 3.164268198058D+13 Z= 1.779010586783D+13

Backward Direction:

Total Energy: -651.6164650 Hartrees

Potential Energy: -651.8071101 Hartress

Kinetic Energy: 0.1906450 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.412803664402D+13 Y= 1.673189963764D+13 Z= -1.925237862947D+11
I= 1 X= 3.635260634772D+12 Y= -8.909981117776D+12 Z= -2.469748668204D+13
I= 2 X= -1.997714793690D+12 Y= -1.560067034335D+13 Z= -1.011888350906D+13
I= 3 X= 7.913095919574D+12 Y= -1.170887786059D+13 Z= 4.213644693367D+12
I= 4 X= -2.127523399889D+13 Y= -8.704290911913D+12 Z= 1.730669501428D+13
I= 5 X= 1.010720764362D+13 Y= -2.038423694910D+12 Z= 1.386244680740D+13
I= 6 X= 5.858581761473D+13 Y= 7.421832008689D+13 Z= -5.023874570431D+13
I= 7 X= -3.340313139179D+13 Y= -1.782112596971D+13 Z= -6.838321813990D+12
I= 8 X= -1.335893534501D+14 Y= 7.537196085155D+13 Z= -5.648365567656D+13
I= 9 X= -6.354471928481D+12 Y= 1.179163392736D+13 Z= -3.087855376744D+12
I= 10 X= 1.189233245448D+13 Y= -1.964869879661D+13 Z= -4.754522049557D+13
I= 11 X= -2.078892098056D+13 Y= -8.454074469829D+13 Z= -2.170540837532D+13
I= 12 X= 5.833124960674D+13 Y= 5.452153192111D+13 Z= 9.837771324900D+11
I= 13 X= 2.260135267751D+12 Y= -3.981458067566D+12 Z= 1.154315977629D+13
I= 14 X= 5.782792479231D+13 Y= -3.761612957654D+13 Z= 3.737172874640D+13
I= 15 X= -7.588171995481D+13 Y= 1.324359860905D+13 Z= 1.069747888850D+14
I= 16 X= 5.866232708130D+13 Y= 1.382525370416D+14 Z= 3.188664456128D+13
I= 17 X= 1.619735331349D+13 Y= -1.718870987544D+13 Z= -2.063679881086D+13
I= 18 X= -6.602885149212D+13 Y= 7.004622324935D+12 Z= -5.120571541351D+13

I= 19 X= -1.004056838672D+13 Y= -2.228286870191D+13 Z= 4.290800904030D+13
I= 20 X= -4.212334816494D+13 Y= 4.340139286240D+13 Z= 1.103255945770D+14
I= 21 X= 1.303494147170D+12 Y= -1.392084471719D+12 Z= 1.986445609019D+13
I= 22 X= 1.843822685955D+12 Y= -2.934940453602D+13 Z= 4.718962952109D+13
I= 23 X= 1.290416875825D+14 Y= 1.287705301122D+14 Z= -4.712926130385D+13
I= 24 X= 4.144889341760D+13 Y= 1.966223578532D+12 Z= -7.209431495515D+13
I= 25 X= 8.661582342626D+12 Y= -2.252569025709D+12 Z= -1.583906084579D+13
I= 26 X= 1.284063171053D+13 Y= 1.086346065152D+14 Z= 7.076691535741D+13
I= 27 X= -3.117625486404D+13 Y= -4.035365987401D+13 Z= 1.566415622769D+13
I= 28 X= 7.859370840041D+13 Y= 1.687653492169D+13 Z= 1.097212501617D+14
I= 29 X= 1.664751739448D+13 Y= -2.036372893415D+13 Z= 5.195414135204D+12
I= 30 X= 1.064484019655D+13 Y= 6.755901004183D+12 Z= 1.966663912973D+13
I= 31 X= -1.323680454613D+14 Y= -1.250677348198D+14 Z= -2.150905472119D+13
I= 32 X= -2.480946975923D+13 Y= -2.846099939225D+13 Z= -1.585358143821D+13
I= 33 X= -4.351806151731D+13 Y= -1.040459725126D+13 Z= -5.165429005216D+13
I= 34 X= -3.658247137796D+13 Y= -7.262342267201D+13 Z= -7.330452147645D+13
I= 35 X= -9.028732342072D+11 Y= 2.734170047664D+12 Z= -2.414331105185D+11
I= 36 X= 7.740782225197D+12 Y= -1.636331179954D+12 Z= -1.985449667859D+13
I= 37 X= -3.974033726483D+13 Y= -3.265060533560D+13 Z= 4.460167198080D+12
I= 38 X= -1.949744302349D+13 Y= 3.158203020806D+13 Z= 1.657272207472D+13

Seed: 3292668439

CM Start Point Coordinates: bohr

I= 0 X= -2.586381768777D+00 Y= 2.339726242303D+00 Z= -5.651511084334D-01
I= 1 X= -2.894055667052D+00 Y= -2.787156696947D-02 Z= -2.109999990031D+00
I= 2 X= -2.336931655780D+00 Y= 1.672912873161D+00 Z= 1.978282603630D+00
I= 3 X= -2.766733449966D+00 Y= -1.893615892795D+00 Z= -2.092490878087D-01
I= 4 X= -2.421337694517D+00 Y= -9.581750666365D-01 Z= 2.184679944265D+00
I= 5 X= 4.115319103772D+00 Y= 2.588502953004D+00 Z= -1.504478355680D+00
I= 6 X= 2.124092230733D+00 Y= 6.372441078448D-01 Z= -3.115760385842D+00

I= 7 X= 5.548046770796D+00 Y= 1.628498051824D+00 Z= -2.098524651904D+00
I= 8 X= 3.583821245611D+00 Y= 4.487962280967D+00 Z= -2.411631780425D+00
I= 9 X= -2.445619177621D+00 Y= -2.264968706354D+00 Z= 4.704804319985D+00
I= 10 X= -4.051136607085D+00 Y= -1.595552249249D+00 Z= 5.992598213303D+00
I= 11 X= -2.608948684873D+00 Y= -4.411346091112D+00 Z= 4.917286588033D+00
I= 12 X= -6.346459619994D-01 Y= -1.671091711373D+00 Z= 5.795910074236D+00
I= 13 X= -1.983540877553D+00 Y= 3.470622958512D+00 Z= 4.245741021098D+00
I= 14 X= -3.769795067105D+00 Y= 3.624512171188D+00 Z= 4.929830088649D+00
I= 15 X= -7.560371351419D-01 Y= 2.857590890475D+00 Z= 5.773435522413D+00
I= 16 X= -1.246926689291D+00 Y= 5.476679286478D+00 Z= 3.640279167446D+00
I= 17 X= -2.362161372553D+00 Y= 4.940957185118D+00 Z= -1.680169201242D+00
I= 18 X= -4.364440271519D+00 Y= 5.678903217544D+00 Z= -1.907421631200D+00
I= 19 X= -1.072210311089D+00 Y= 5.769048719975D+00 Z= -2.504853740635D-01
I= 20 X= -1.056467632577D+00 Y= 4.962387357266D+00 Z= -3.517262568020D+00
I= 21 X= -3.419869087229D+00 Y= -1.556307453018D-01 Z= -4.902572142933D+00
I= 22 X= -5.253499387039D+00 Y= -7.067464147980D-01 Z= -5.395579388641D+00
I= 23 X= -2.924371643022D+00 Y= 1.737895384645D+00 Z= -5.586532971317D+00
I= 24 X= -2.049953766755D+00 Y= -1.732869352257D+00 Z= -5.940459126885D+00
I= 25 X= -3.409377879640D+00 Y= -4.723701776049D+00 Z= -5.579340645336D-01
I= 26 X= -4.037131909881D+00 Y= -4.867280127346D+00 Z= -3.033347201484D+00
I= 27 X= -1.421209219051D+00 Y= -5.605606429350D+00 Z= 1.899266703646D-02
I= 28 X= -5.259182130854D+00 Y= -5.167926089161D+00 Z= 7.476056031372D-01
I= 29 X= 2.952288355312D+00 Y= -3.542137222328D+00 Z= -1.250902305907D+00
I= 30 X= 3.329154483849D+00 Y= -2.947356993468D+00 Z= 1.325278703642D+00
I= 31 X= 1.526874217646D+00 Y= -5.151534012349D+00 Z= -1.764294665925D+00
I= 32 X= 4.569014558689D+00 Y= -3.597046497509D+00 Z= -2.611140177171D+00
I= 33 X= 5.118906954204D+00 Y= -2.338731386634D+00 Z= 2.199212953765D+00
I= 34 X= 2.373608478062D+00 Y= -3.974392588181D+00 Z= 2.672013084413D+00
I= 35 X= 8.270951897525D-01 Y= -7.697225648762D-02 Z= -2.051945696094D-01
I= 36 X= 3.637526131053D+00 Y= 2.585518902633D+00 Z= 1.320526081981D+00

I= 37 X= 4.740648159703D+00 Y= 1.796778399352D+00 Z= 2.587558556477D+00

I= 38 X= 2.488556992254D+00 Y= 3.983795224714D+00 Z= 2.176578948605D+00

Forward Direction:

Total Energy: -651.6170711 Hartrees

Potential Energy: -651.7956052 Hartress

Kinetic Energy: 0.1785340 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.374707921942D+12 Y= 1.866943486758D+13 Z= 1.034703979109D+13

I= 1 X= 1.200786565074D+13 Y= 1.235226374506D+13 Z= 5.112760943978D+12

I= 2 X= -1.099398192502D+13 Y= 2.029658390494D+12 Z= -1.432993835324D+13

I= 3 X= 3.330166366865D+12 Y= -1.886226686242D+13 Z= -2.916215980371D+12

I= 4 X= 2.864220123986D+13 Y= -3.155135130290D+11 Z= -3.817673386006D+12

I= 5 X= 3.639028570502D+12 Y= 3.361026980243D+12 Z= -4.104981766990D+12

I= 6 X= 3.253615161975D+13 Y= -6.259716719707D+13 Z= -9.021277432501D+13

I= 7 X= -8.872125472416D+13 Y= -1.946925238536D+13 Z= 4.847719431225D+13

I= 8 X= 2.466036020151D+13 Y= 1.908197396752D+13 Z= 9.347741344794D+13

I= 9 X= -8.495884615293D+12 Y= -5.477453605373D+12 Z= -2.174381649350D+13

I= 10 X= -5.239881272073D+13 Y= -3.967701803278D+13 Z= 1.085167401937D+14

I= 11 X= -2.025038543518D+12 Y= -7.825344882666D+13 Z= 1.898100667453D+13

I= 12 X= -6.211707800172D+13 Y= 2.364157984780D+13 Z= -1.862214188739D+13

I= 13 X= 6.042597578676D+12 Y= 2.282611177693D+12 Z= 1.298040041984D+13

I= 14 X= 5.457534819288D+13 Y= -5.401625233077D+13 Z= -5.036919798669D+13

I= 15 X= 3.089903883470D+13 Y= 5.450112169158D+13 Z= -4.140624022830D+12

I= 16 X= 2.796015751467D+12 Y= 4.762448595932D+13 Z= 1.556394975544D+13

I= 17 X= 1.733709087159D+13 Y= 1.181329149451D+13 Z= 1.027166431912D+13

I= 18 X= -1.295864671224D+14 Y= 8.944368622885D+13 Z= -9.079615977690D+13

I= 19 X= -1.842154076874D+13 Y= -3.764707944682D+13 Z= -2.322352107788D+13

I= 20 X= -1.917389330994D+13 Y= 3.065789567351D+13 Z= -1.002813174089D+14

I= 21 X= -8.088964056185D+12 Y= -5.641759783405D+12 Z= -1.909760502536D+13

I= 22 X= 2.019192966758D+13 Y= -4.209688257180D+13 Z= 1.322965307557D+13

I= 23 X= 6.267152969344D+13 Y= -5.814724354739D+13 Z= 2.333250059596D+13
I= 24 X= -3.270257468035D+13 Y= 1.069535532562D+14 Z= -2.635578800706D+13
I= 25 X= -5.997201397402D+12 Y= -1.385274285497D+12 Z= -1.161920721138D+13
I= 26 X= -1.873391563917D+13 Y= -1.439419698845D+13 Z= 2.895550489976D+13
I= 27 X= -7.527184224198D+13 Y= 1.891096250437D+14 Z= -9.310651497210D+13
I= 28 X= -8.540823395227D+12 Y= 5.279700466564D+13 Z= 8.500632640181D+13
I= 29 X= -2.334400006709D+12 Y= -2.219899964541D+13 Z= -2.732234949277D+12
I= 30 X= -3.747381732960D+12 Y= -2.525988239400D+12 Z= 3.891076108283D+12
I= 31 X= 5.231640024915D+13 Y= -7.780333691234D+12 Z= 7.060167644661D+13
I= 32 X= 6.057534917539D+13 Y= -1.206455400585D+13 Z= -8.521173993923D+13
I= 33 X= 2.990439788883D+13 Y= 9.147918620464D+13 Z= -4.527744133361D+13
I= 34 X= -5.007171583906D+13 Y= -7.945850917650D+13 Z= 5.897723071432D+13
I= 35 X= -1.845897068474D+12 Y= -1.024342682278D+12 Z= 2.872944121716D+12
I= 36 X= 1.966443749131D+13 Y= 1.663239697628D+12 Z= 3.268814523642D+12
I= 37 X= -5.511488758937D+13 Y= -3.067355916845D+13 Z= -8.274149916989D+13
I= 38 X= 1.613876201627D+13 Y= 7.754534331164D+13 Z= 5.816582837476D+12

Backward Direction:

Total Energy: -651.6170576 Hartrees

Potential Energy: -651.7956052 Hartress

Kinetic Energy: 0.1785476 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.780965721960D+12 Y= 1.854991555027D+13 Z= 1.033811133858D+13
I= 1 X= 1.221037527100D+13 Y= 1.191881358708D+13 Z= 4.391916946411D+12
I= 2 X= -1.125754830518D+13 Y= 2.426836105268D+12 Z= -1.495080184119D+13
I= 3 X= 3.164694298746D+12 Y= -1.882567823690D+13 Z= -3.786122168602D+12
I= 4 X= 2.993038146363D+13 Y= -4.203981389286D+11 Z= -4.642796487117D+12
I= 5 X= 3.727101611990D+12 Y= 2.759143161281D+12 Z= -9.501796959780D+12
I= 6 X= 6.819993839003D+13 Y= -2.977850028985D+13 Z= -7.471363040056D+13
I= 7 X= -8.139988249860D+13 Y= -1.254913640737D+13 Z= 4.914866361590D+13
I= 8 X= 3.457599397222D+13 Y= 2.719586377130D+13 Z= 9.533125103279D+13

I= 9 X= -8.045600027905D+12 Y= -5.282865685647D+12 Z= -2.223375972016D+13
I= 10 X= -5.224788790477D+13 Y= -3.868600077640D+13 Z= 1.073681127564D+14
I= 11 X= -2.130177085386D+12 Y= -7.824628452000D+13 Z= 1.890924336230D+13
I= 12 X= -6.180801292118D+13 Y= 2.372144303077D+13 Z= -1.891776712780D+13
I= 13 X= 6.129287161944D+12 Y= 2.222811915469D+12 Z= 1.276591465229D+13
I= 14 X= 5.469826876100D+13 Y= -5.438414306278D+13 Z= -5.034780085992D+13
I= 15 X= 3.120020242148D+13 Y= 5.419772126273D+13 Z= -4.651278185687D+12
I= 16 X= 2.737507143201D+12 Y= 4.770659846315D+13 Z= 1.562402190148D+13
I= 17 X= 1.748290784421D+13 Y= 1.168203033063D+13 Z= 1.021416766988D+13
I= 18 X= -1.294313963526D+14 Y= 8.936379680853D+13 Z= -9.113867871430D+13
I= 19 X= -1.842186621839D+13 Y= -3.777411594423D+13 Z= -2.307868635837D+13
I= 20 X= -1.900196272929D+13 Y= 3.044069675486D+13 Z= -1.003521740237D+14
I= 21 X= -8.383666560170D+12 Y= -5.636762616412D+12 Z= -1.954682462362D+13
I= 22 X= 1.999571222786D+13 Y= -4.167019066164D+13 Z= 1.216622396366D+13
I= 23 X= 6.285835370585D+13 Y= -5.831098655297D+13 Z= 2.295589422964D+13
I= 24 X= -3.309176686007D+13 Y= 1.069423228920D+14 Z= -2.688587323272D+13
I= 25 X= -5.999278439653D+12 Y= -1.441140190281D+12 Z= -1.174395475786D+13
I= 26 X= -1.896030673957D+13 Y= -1.471523880664D+13 Z= 2.886613119294D+13
I= 27 X= -7.507361395976D+13 Y= 1.892938640089D+14 Z= -9.317923960330D+13
I= 28 X= -8.493942452284D+12 Y= 5.278942356574D+13 Z= 8.523485414192D+13
I= 29 X= -3.107015573251D+12 Y= -2.174282005197D+13 Z= -3.324748154989D+12
I= 30 X= -3.687204653340D+12 Y= -2.396139315338D+12 Z= 3.435510383847D+12
I= 31 X= 5.237765914298D+13 Y= -8.201495704600D+12 Z= 7.031935339179D+13
I= 32 X= 5.959287026827D+13 Y= -1.117517929499D+13 Z= -8.612943068257D+13
I= 33 X= 3.004066030214D+13 Y= 9.141883715295D+13 Z= -4.574163467820D+13
I= 34 X= -4.961068481605D+13 Y= -7.952826164035D+13 Z= 5.867885691301D+13
I= 35 X= -2.031855026969D+12 Y= -1.100021239093D+12 Z= 3.596370890848D+12
I= 36 X= 1.741312666620D+13 Y= -1.026873861030D+12 Z= 1.918580900513D+12
I= 37 X= -5.249858921118D+13 Y= -2.898832167494D+13 Z= -8.606491763725D+13
I= 38 X= 1.772316865771D+13 Y= 7.743841307228D+13 Z= 3.670311772466D+12

Seed: 33848100429

CM Start Point Coordinates: bohr

I= 0 X= -2.696344797790D+00 Y= 2.273523509096D+00 Z= -8.136523579467D-01
I= 1 X= -3.073306850712D+00 Y= -9.316993561533D-02 Z= -1.918302152729D+00
I= 2 X= -2.392628136061D+00 Y= 2.090157705897D+00 Z= 1.866814965124D+00
I= 3 X= -2.720225817342D+00 Y= -1.937574597872D+00 Z= -9.348668679030D-02
I= 4 X= -2.378212900150D+00 Y= -7.061628899977D-01 Z= 2.386434076138D+00
I= 5 X= 4.291120730982D+00 Y= 2.443539952967D+00 Z= -9.268331480604D-01
I= 6 X= 1.874940351778D+00 Y= 1.083658201031D+00 Z= -2.826186461797D+00
I= 7 X= 5.916422695135D+00 Y= 1.446986935206D+00 Z= -1.686965189513D+00
I= 8 X= 3.962697746683D+00 Y= 4.389546872018D+00 Z= -1.894679587501D+00
I= 9 X= -2.572726415145D+00 Y= -2.179511917603D+00 Z= 4.763671867599D+00
I= 10 X= -4.579475667615D+00 Y= -2.033474131913D+00 Z= 5.583069577563D+00
I= 11 X= -1.774435663264D+00 Y= -4.366577592052D+00 Z= 4.346618490682D+00
I= 12 X= -1.347237152140D+00 Y= -1.112129464812D+00 Z= 6.206089118382D+00
I= 13 X= -2.124831924020D+00 Y= 3.938533697418D+00 Z= 3.940606650832D+00
I= 14 X= -3.811893604898D+00 Y= 4.421963442828D+00 Z= 4.547649479682D+00
I= 15 X= -9.127653793202D-01 Y= 2.786896624126D+00 Z= 5.653021619885D+00
I= 16 X= -1.135345101900D+00 Y= 5.562754819884D+00 Z= 3.044869869331D+00
I= 17 X= -2.923716946686D+00 Y= 4.940280438545D+00 Z= -1.908067177533D+00
I= 18 X= -4.555792903554D+00 Y= 5.796920579824D+00 Z= -1.501316004806D+00
I= 19 X= -1.360672809906D+00 Y= 6.409887531065D+00 Z= -1.356031920174D+00
I= 20 X= -2.794938350341D+00 Y= 4.620718322100D+00 Z= -4.027356502635D+00
I= 21 X= -3.310131457057D+00 Y= -5.636727590889D-01 Z= -4.628140140848D+00
I= 22 X= -5.546066350156D+00 Y= -2.664694236767D-01 Z= -5.121771096855D+00
I= 23 X= -2.296804985825D+00 Y= 1.101323612554D+00 Z= -5.716178021944D+00
I= 24 X= -2.703528268908D+00 Y= -2.338981185083D+00 Z= -5.187128045381D+00
I= 25 X= -3.061398145415D+00 Y= -4.745088843325D+00 Z= -5.150973557304D-01
I= 26 X= -3.534428329101D+00 Y= -5.553529787058D+00 Z= -2.482855232511D+00

I= 27 X= -1.875469019007D+00 Y= -6.411942788664D+00 Z= 5.214054895492D-01
I= 28 X= -5.223038026310D+00 Y= -4.966460556296D+00 Z= -7.951826173934D-02
I= 29 X= 2.929461658727D+00 Y= -3.147871506797D+00 Z= -2.039596601838D+00
I= 30 X= 3.155265378107D+00 Y= -3.372563098972D+00 Z= 6.235379599162D-01
I= 31 X= 1.245374329953D+00 Y= -4.470929525809D+00 Z= -2.771352489920D+00
I= 32 X= 4.161432062670D+00 Y= -2.110363589402D+00 Z= -3.527730163166D+00
I= 33 X= 5.032973022113D+00 Y= -2.473455697625D+00 Z= 1.620229606507D+00
I= 34 X= 2.234093017031D+00 Y= -4.967350045174D+00 Z= 1.774262529992D+00
I= 35 X= 8.666590797446D-01 Y= -5.932557114161D-02 Z= -1.605263722197D-01
I= 36 X= 3.836945571693D+00 Y= 1.933737178523D+00 Z= 1.813554288444D+00
I= 37 X= 5.305194818462D+00 Y= 7.506493285822D-01 Z= 2.429861835842D+00
I= 38 X= 3.057552547070D+00 Y= 3.650695869346D+00 Z= 2.807577170032D+00

Forward Direction:

Total Energy: -651.6192124 Hartrees

Potential Energy: -651.7929534 Hartress

Kinetic Energy: 0.1737410 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.108131681480D+13 Y= -5.297779183554D+12 Z= 1.230810973029D+13
I= 1 X= -1.446812460875D+13 Y= -4.528672709244D+12 Z= -2.489717486098D+13
I= 2 X= 6.646654758411D+12 Y= 1.741914397583D+13 Z= -2.256772335655D+12
I= 3 X= 1.841569313642D+13 Y= 1.328147761175D+12 Z= 1.110869313133D+13
I= 4 X= 3.756498432468D+10 Y= 4.220671214989D+12 Z= 5.708770468354D+11
I= 5 X= 4.370796176352D+12 Y= 5.482500743840D+12 Z= 9.200563829705D+12
I= 6 X= -4.626688059790D+13 Y= -7.428028147621D+13 Z= 7.303165024425D+13
I= 7 X= 1.302605127523D+14 Y= -1.351993014584D+14 Z= -6.979964428848D+12
I= 8 X= -8.806759402063D+13 Y= -3.878996613449D+13 Z= 2.310690182537D+13
I= 9 X= -8.284373738986D+12 Y= 1.474036412257D+13 Z= 1.511266836672D+13
I= 10 X= 2.901487916150D+13 Y= 2.404073139808D+13 Z= -9.142934510559D+13
I= 11 X= 7.467076438525D+13 Y= -3.019045047391D+13 Z= -5.238855976116D+13
I= 12 X= 6.751613626882D+13 Y= -1.089601271475D+14 Z= -4.098764457567D+13

I= 13 X= -6.475180574890D+11 Y= 6.450778484899D+11 Z= -1.158683325521D+13
I= 14 X= -9.083085957118D+13 Y= 5.941769513330D+13 Z= 2.678734949240D+13
I= 15 X= -5.106882647873D+12 Y= 5.566397381123D+13 Z= 1.403703919644D+13
I= 16 X= 9.672952855331D+12 Y= 4.347867843809D+13 Z= 4.232894960392D+13
I= 17 X= -2.140639408369D+13 Y= 9.439010959205D+12 Z= 9.863486100825D+12
I= 18 X= 7.991183289761D+13 Y= -8.819339106007D+12 Z= -6.069195386479D+13
I= 19 X= -7.694726946007D+13 Y= -5.178084460037D+13 Z= -7.345033516070D+13
I= 20 X= 6.911121780881D+12 Y= -4.452090340407D+13 Z= -4.097390241719D+13
I= 21 X= -3.216782142588D+12 Y= -8.264197627751D+12 Z= 4.356588098417D+12
I= 22 X= 1.356526039068D+13 Y= 5.820040362977D+13 Z= 5.847610598030D+13
I= 23 X= 9.991202255645D+13 Y= 2.856649211274D+13 Z= -7.338344777774D+13
I= 24 X= 4.916175661936D+13 Y= -5.085235610945D+13 Z= 8.324596193794D+12
I= 25 X= -1.175781337972D+13 Y= -1.053234657251D+13 Z= 3.897037012699D+12
I= 26 X= -2.244421404725D+13 Y= -4.272898268278D+13 Z= -4.844077484994D+13
I= 27 X= 3.832369135158D+13 Y= 6.561632356498D+13 Z= -5.522380336906D+13
I= 28 X= -5.746076530401D+13 Y= 2.097526025595D+13 Z= -5.760875671562D+13
I= 29 X= 2.550704130765D+13 Y= 2.448947343922D+12 Z= -3.170018453535D+13
I= 30 X= -2.575554225499D+12 Y= -1.661248765612D+12 Z= 1.427107576821D+13
I= 31 X= -4.910207640942D+13 Y= -4.277931260835D+13 Z= 5.900063802425D+13
I= 32 X= 2.369696886204D+13 Y= -8.567906722354D+12 Z= -3.202398724349D+12
I= 33 X= -1.278150704620D+14 Y= -2.144648485942D+13 Z= 3.739870758488D+12
I= 34 X= -6.836555457395D+12 Y= 2.799800428808D+13 Z= 2.247311582787D+13
I= 35 X= -1.116505708984D+12 Y= -1.507854247451D+12 Z= -4.757811650262D+11
I= 36 X= -1.310333326993D+12 Y= 2.235004898924D+13 Z= 5.176094928696D+12
I= 37 X= 6.297201994370D+13 Y= -1.995846655182D+13 Z= 4.643237937955D+13
I= 38 X= -4.849138595746D+13 Y= 1.459520468056D+13 Z= 1.344641167193D+14

Backward Direction:

Total Energy: -651.6193444 Hartrees

Potential Energy: -651.7929534 Hartress

Kinetic Energy: 0.1736090 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.974374006649D+13 Y= -5.691288576165D+12 Z= 1.227871339600D+13
I= 1 X= -1.380137517272D+13 Y= -5.955778484602D+12 Z= -2.727050570989D+13
I= 2 X= 5.778880005901D+12 Y= 1.872682514913D+13 Z= -4.300924018011D+12
I= 3 X= 1.787088737434D+13 Y= 1.448613374262D+12 Z= 8.244584948069D+12
I= 4 X= 4.278812569885D+12 Y= 3.875345570740D+12 Z= -2.145785806811D+12
I= 5 X= 4.660770801256D+12 Y= 3.500838357238D+12 Z= -8.568090731581D+12
I= 6 X= 7.115376193458D+13 Y= 3.377299341158D+13 Z= 1.240615492859D+14
I= 7 X= 1.543656431619D+14 Y= -1.124152805224D+14 Z= -4.769196467653D+12
I= 8 X= -5.542103026021D+13 Y= -1.207552438816D+13 Z= 2.921053859912D+13
I= 9 X= -6.801841727905D+12 Y= 1.538103188543D+13 Z= 1.349956292664D+13
I= 10 X= 2.951178906973D+13 Y= 2.730358970435D+13 Z= -9.521112444156D+13
I= 11 X= 7.432460273856D+13 Y= -3.016686247820D+13 Z= -5.262483568485D+13
I= 12 X= 6.853371246873D+13 Y= -1.086971829410D+14 Z= -4.196097097968D+13
I= 13 X= -3.620983776682D+11 Y= 4.481927611121D+11 Z= -1.229301335617D+13
I= 14 X= -9.042615178372D+13 Y= 5.820643940178D+13 Z= 2.685779810173D+13
I= 15 X= -4.115321596841D+12 Y= 5.466504809856D+13 Z= 1.235574438004D+13
I= 16 X= 9.480317166513D+12 Y= 4.374902838706D+13 Z= 4.252673314505D+13
I= 17 X= -2.092630141167D+13 Y= 9.006842315275D+12 Z= 9.674182211153D+12
I= 18 X= 8.042239307990D+13 Y= -9.082369696424D+12 Z= -6.181967464957D+13
I= 19 X= -7.694834097463D+13 Y= -5.219910380606D+13 Z= -7.297347650236D+13
I= 20 X= 7.477191759173D+12 Y= -4.523601637655D+13 Z= -4.120719310935D+13
I= 21 X= -4.187070507817D+12 Y= -8.247744792144D+12 Z= 2.877562492686D+12
I= 22 X= 1.291922753745D+13 Y= 5.960525830394D+13 Z= 5.497483646569D+13
I= 23 X= 1.005271281638D+14 Y= 2.802737917750D+13 Z= -7.462339915173D+13
I= 24 X= 4.788036730687D+13 Y= -5.088933133679D+13 Z= 6.579325903755D+12
I= 25 X= -1.176465190269D+13 Y= -1.071628134323D+13 Z= 3.486314024706D+12
I= 26 X= -2.318959166882D+13 Y= -4.378599148877D+13 Z= -4.873503183102D+13
I= 27 X= 3.897634476737D+13 Y= 6.622291808189D+13 Z= -5.546324437460D+13
I= 28 X= -5.730641291953D+13 Y= 2.095029998399D+13 Z= -5.685634434405D+13

I= 29 X= 2.296325601374D+13 Y= 3.950888271080D+12 Z= -3.365099480185D+13
I= 30 X= -2.377425201426D+12 Y= -1.233729833645D+12 Z= 1.277115596313D+13
I= 31 X= -4.890038558289D+13 Y= -4.416596048184D+13 Z= 5.807110816901D+13
I= 32 X= 2.046222249932D+13 Y= -5.639699725153D+12 Z= -6.223834377756D+12
I= 33 X= -1.273664355418D+14 Y= -2.164518009115D+13 Z= 2.211545091039D+12
I= 34 X= -5.318641527901D+12 Y= 2.776834894611D+13 Z= 2.149073995676D+13
I= 35 X= -1.728759901567D+12 Y= -1.757020854042D+12 Z= 1.906053287617D+12
I= 36 X= -8.722624267410D+12 Y= 1.349302927335D+13 Z= 7.305406596397D+11
I= 37 X= 7.158600809164D+13 Y= -1.440993435798D+13 Z= 3.549024543830D+13
I= 38 X= -4.327483261929D+13 Y= 1.424314398599D+13 Z= 1.273976621931D+14

Seed: 33982230834

CM Start Point Coordinates: bohr

I= 0 X= -2.701495658468D+00 Y= 2.358817093957D+00 Z= -7.787712137447D-01
I= 1 X= -3.097379158613D+00 Y= -1.396545717977D-01 Z= -1.930673057260D+00
I= 2 X= -2.434226940551D+00 Y= 1.917561599471D+00 Z= 2.018790150985D+00
I= 3 X= -2.909488459423D+00 Y= -1.914476262120D+00 Z= -2.621093456479D-02
I= 4 X= -2.341671932441D+00 Y= -8.339285739800D-01 Z= 2.421274847532D+00
I= 5 X= 4.387265730647D+00 Y= 2.194324144967D+00 Z= -6.461031275970D-01
I= 6 X= 2.507587988593D+00 Y= 1.212317365713D+00 Z= -2.835774460351D+00
I= 7 X= 6.065438217136D+00 Y= 8.647708461335D-01 Z= -1.282182796874D+00
I= 8 X= 4.617690331462D+00 Y= 4.000829623713D+00 Z= -1.829914814579D+00
I= 9 X= -2.551106373333D+00 Y= -2.062133706443D+00 Z= 4.891120710432D+00
I= 10 X= -4.424311858878D+00 Y= -2.594816689045D+00 Z= 5.416414660069D+00
I= 11 X= -1.597676753269D+00 Y= -3.925683999550D+00 Z= 5.037883963828D+00
I= 12 X= -2.163870396707D+00 Y= -8.386486572447D-01 Z= 6.747421259666D+00
I= 13 X= -2.437142668928D+00 Y= 3.955868622211D+00 Z= 3.940667864671D+00
I= 14 X= -4.515502528500D+00 Y= 4.163297948176D+00 Z= 4.744246886419D+00
I= 15 X= -1.690461401321D+00 Y= 2.867070347037D+00 Z= 5.421256152876D+00
I= 16 X= -1.489650676840D+00 Y= 5.741715603767D+00 Z= 3.281644710608D+00

I= 17 X= -2.553595745576D+00 Y= 4.818625850194D+00 Z= -2.109842717145D+00
I= 18 X= -4.408928331171D+00 Y= 6.216423459918D+00 Z= -1.169939945031D+00
I= 19 X= -8.103025493558D-01 Y= 6.187993001778D+00 Z= -1.545881752864D+00
I= 20 X= -2.955865741548D+00 Y= 4.681626268628D+00 Z= -4.299844153075D+00
I= 21 X= -3.975019253062D+00 Y= -4.055545932165D-01 Z= -4.586184240536D+00
I= 22 X= -6.096039414494D+00 Y= 7.604243526432D-01 Z= -4.664441510433D+00
I= 23 X= -2.634668889890D+00 Y= 8.045330965248D-01 Z= -5.843407079956D+00
I= 24 X= -3.937680149896D+00 Y= -2.687441262388D+00 Z= -5.217130192450D+00
I= 25 X= -3.232056132640D+00 Y= -4.654770166046D+00 Z= -6.923426563855D-01
I= 26 X= -2.620461025481D+00 Y= -5.339374884188D+00 Z= -2.764077086734D+00
I= 27 X= -2.620717491783D+00 Y= -6.166697914700D+00 Z= 9.294761277058D-01
I= 28 X= -5.343833107623D+00 Y= -4.994058115745D+00 Z= -1.253988073256D+00
I= 29 X= 2.843142567780D+00 Y= -3.388002619732D+00 Z= -2.030165178488D+00
I= 30 X= 3.754378192258D+00 Y= -3.182149055432D+00 Z= 5.312860925933D-01
I= 31 X= 1.893065048300D+00 Y= -5.161885382114D+00 Z= -2.882098419325D+00
I= 32 X= 4.159639811090D+00 Y= -2.722885596116D+00 Z= -3.825429871172D+00
I= 33 X= 5.592373540004D+00 Y= -2.583473125485D+00 Z= 9.384779808603D-01
I= 34 X= 3.150381204770D+00 Y= -4.652445541423D+00 Z= 1.908317851814D+00
I= 35 X= 9.168876604124D-01 Y= -6.534984208521D-02 Z= -1.834945895221D-01
I= 36 X= 3.544031264403D+00 Y= 2.245139936551D+00 Z= 1.875889686024D+00
I= 37 X= 4.059604885885D+00 Y= 1.659093829873D+00 Z= 3.599416377432D+00
I= 38 X= 2.887741583669D+00 Y= 4.188270687189D+00 Z= 2.245741297113D+00

Forward Direction:

Total Energy: -651.6074317 Hartrees

Potential Energy: -651.7660941 Hartress

Kinetic Energy: 0.1586624 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.134034098629D+13 Y= 1.532147071333D+13 Z= -1.272906819531D+13

I= 1 X= -1.947063612682D+13 Y= 1.657701111181D+13 Z= 7.004824473279D+12

I= 2 X= 7.580432018177D+12 Y= 1.075653307247D+13 Z= -8.062992714037D+12

I= 3 X= 4.619028882356D+11 Y= -7.757907928085D+12 Z= -9.251470404356D+12
I= 4 X= 1.409907974457D+13 Y= 4.769929811936D+12 Z= 6.118548711127D+12
I= 5 X= 6.706475798537D+12 Y= 1.161377939658D+13 Z= -1.161327055553D+13
I= 6 X= -1.292194816446D+12 Y= -6.768154810315D+12 Z= 4.846828399582D+13
I= 7 X= -5.464250050888D+13 Y= 3.844656691428D+12 Z= -6.374502251260D+12
I= 8 X= -8.929835551864D+13 Y= -8.307534729596D+13 Z= 3.627549188251D+13
I= 9 X= -1.732373945982D+13 Y= 2.554747998994D+11 Z= 2.116856312758D+12
I= 10 X= 5.175875332239D+13 Y= 5.798050351172D+13 Z= 2.000710360617D+13
I= 11 X= 2.378773434363D+13 Y= -1.101417303066D+14 Z= -5.313323535641D+13
I= 12 X= -1.009956148870D+14 Y= 2.128282174753D+13 Z= -5.576277156937D+13
I= 13 X= -2.166171876765D+13 Y= 1.396024949051D+13 Z= 8.202646430683D+12
I= 14 X= -5.105520058442D+13 Y= -3.185456903420D+12 Z= 6.849938393150D+13
I= 15 X= 6.320848888582D+13 Y= -1.465547257091D+13 Z= 3.545889565664D+13
I= 16 X= 8.150987188135D+13 Y= 5.196974587455D+13 Z= 2.263673873075D+13
I= 17 X= -1.170012605301D+13 Y= -2.583351899761D+13 Z= -7.769161326901D+12
I= 18 X= -6.734260654626D+12 Y= 1.110059487012D+13 Z= 3.567396133925D+13
I= 19 X= 1.058750911533D+13 Y= -4.435777474551D+13 Z= -1.043244454427D+14
I= 20 X= -1.568637847464D+13 Y= 2.033231418005D+13 Z= 1.392457966226D+14
I= 21 X= 6.432036814701D+12 Y= -8.116226771516D+12 Z= 1.749414266077D+13
I= 22 X= 5.934549449601D+13 Y= 1.073004322140D+13 Z= 8.347988233274D+13
I= 23 X= 5.933199128944D+13 Y= 1.306087435069D+14 Z= -3.969210926719D+13
I= 24 X= 8.218447688091D+13 Y= 1.243714286966D+13 Z= 3.835561040078D+13
I= 25 X= -1.553379508788D+13 Y= -1.815083362428D+13 Z= 1.244786159566D+13
I= 26 X= 1.490779096745D+13 Y= 4.071943639908D+13 Z= 5.848165669734D+13
I= 27 X= 1.278158815087D+12 Y= -2.153625950998D+13 Z= -1.811575058293D+13
I= 28 X= 9.440351519776D+13 Y= 4.635623206755D+12 Z= -4.350152276363D+13
I= 29 X= -3.517303230318D+12 Y= -7.529292762332D+12 Z= -9.158919648368D+12
I= 30 X= 1.878117354350D+12 Y= 1.808823249693D+13 Z= 6.303974227064D+12
I= 31 X= -7.443523852693D+13 Y= -5.289243945371D+13 Z= -1.012917836157D+14
I= 32 X= -3.416090868295D+13 Y= -6.232845539993D+12 Z= 4.813922916752D+13

I= 33 X= -5.019555259313D+13 Y= 2.807968388661D+13 Z= 2.358145642236D+13
I= 34 X= 4.796297579439D+13 Y= 8.527929597597D+13 Z= -6.088337938636D+13
I= 35 X= 8.992155512515D+11 Y= -3.465954720708D+12 Z= -3.882114650691D+11
I= 36 X= 6.038199861911D+12 Y= 1.371544043461D+13 Z= -8.108429569264D+12
I= 37 X= 2.164621028085D+13 Y= 1.435860513385D+13 Z= -1.182339399017D+13
I= 38 X= -1.183494931299D+13 Y= 6.456126588788D+13 Z= -5.670776809144D+12

Backward Direction:

Total Energy: -651.6074555 Hartrees

Potential Energy: -651.7660941 Hartress

Kinetic Energy: 0.1586386 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.102106508056D+13 Y= 1.522754109947D+13 Z= -1.273608502072D+13
I= 1 X= -1.931148486148D+13 Y= 1.623636487096D+13 Z= 6.438316898093D+12
I= 2 X= 7.373296558159D+12 Y= 1.106867298709D+13 Z= -8.550926123109D+12
I= 3 X= 3.318592437380D+11 Y= -7.729153116967D+12 Z= -9.935125185761D+12
I= 4 X= 1.511145393197D+13 Y= 4.687501525186D+12 Z= 5.470088726251D+12
I= 5 X= 6.775691945484D+12 Y= 1.114076201298D+13 Z= -1.585459974583D+13
I= 6 X= 2.673579102488D+13 Y= 1.902386602722D+13 Z= 6.064898116287D+13
I= 7 X= -4.888867188794D+13 Y= 9.283140103292D+12 Z= -5.846797995997D+12
I= 8 X= -8.150571014723D+13 Y= -7.669868320051D+13 Z= 3.773241326590D+13
I= 9 X= -1.696986312588D+13 Y= 4.084004406804D+11 Z= 1.731812461931D+12
I= 10 X= 5.187736436054D+13 Y= 5.875933885205D+13 Z= 1.910440324181D+13
I= 11 X= 2.370510651119D+13 Y= -1.101360999145D+14 Z= -5.318963377011D+13
I= 12 X= -1.007527222295D+14 Y= 2.134558581176D+13 Z= -5.599510192237D+13
I= 13 X= -2.159358987441D+13 Y= 1.391325355876D+13 Z= 8.034083173273D+12
I= 14 X= -5.095859794648D+13 Y= -3.474580333958D+12 Z= 6.851619982067D+13
I= 15 X= 6.344517178906D+13 Y= -1.489391339970D+13 Z= 3.505757518803D+13
I= 16 X= 8.146389026300D+13 Y= 5.203427766779D+13 Z= 2.268394911980D+13
I= 17 X= -1.158552924152D+13 Y= -2.593667646761D+13 Z= -7.814347647111D+12
I= 18 X= -6.612391332516D+12 Y= 1.103781019340D+13 Z= 3.540477747528D+13

I= 19 X= 1.058725335216D+13 Y= -4.445761206975D+13 Z= -1.042106205842D+14
I= 20 X= -1.555125911495D+13 Y= 2.016161867632D+13 Z= 1.391901107721D+14
I= 21 X= 6.200431638957D+12 Y= -8.112299521747D+12 Z= 1.714110329840D+13
I= 22 X= 5.919128822140D+13 Y= 1.106537818670D+13 Z= 8.264413889367D+13
I= 23 X= 5.947881530994D+13 Y= 1.304800587321D+14 Z= -3.998808226383D+13
I= 24 X= 8.187861275841D+13 Y= 1.242831698800D+13 Z= 3.793901915658D+13
I= 25 X= -1.553542742584D+13 Y= -1.819473835152D+13 Z= 1.234982314499D+13
I= 26 X= 1.472987137790D+13 Y= 4.046713128648D+13 Z= 5.841141836419D+13
I= 27 X= 1.433945387224D+12 Y= -2.139146706054D+13 Z= -1.817290448653D+13
I= 28 X= 9.444035868801D+13 Y= 4.629665261598D+12 Z= -4.332192399905D+13
I= 29 X= -4.124497813043D+12 Y= -7.170783575294D+12 Z= -9.624572717031D+12
I= 30 X= 1.925410210377D+12 Y= 1.819028009510D+13 Z= 5.945947477211D+12
I= 31 X= -7.438709547554D+13 Y= -5.322342850494D+13 Z= -1.015136598467D+14
I= 32 X= -3.493303378057D+13 Y= -5.533890547546D+12 Z= 4.741802075145D+13
I= 33 X= -5.008846466817D+13 Y= 2.803225588260D+13 Z= 2.321664927101D+13
I= 34 X= 4.832529769317D+13 Y= 8.522447787599D+13 Z= -6.111786981671D+13
I= 35 X= 7.530721517690D+11 Y= -3.525430107873D+12 Z= 1.803258969279D+11
I= 36 X= 4.268906310888D+12 Y= 1.160129408282D+13 Z= -9.169571201813D+12
I= 37 X= 2.370234566331D+13 Y= 1.568302457374D+13 Z= -1.443525140166D+13
I= 38 X= -1.058977231925D+13 Y= 6.447722996230D+13 Z= -7.357520153585D+12

Seed: 34617570350

CM Start Point Coordinates: bohr

I= 0 X= -2.482672485033D+00 Y= 2.273990689360D+00 Z= -5.613673156048D-01
I= 1 X= -2.928727342421D+00 Y= 2.135885962268D-01 Z= -2.077356253726D+00
I= 2 X= -2.415150793276D+00 Y= 1.770279888338D+00 Z= 2.138239460738D+00
I= 3 X= -2.840567637552D+00 Y= -1.816438175539D+00 Z= -3.971592399460D-01
I= 4 X= -2.467940151884D+00 Y= -9.477149243821D-01 Z= 2.256443095147D+00
I= 5 X= 4.024820342218D+00 Y= 2.287199172447D+00 Z= -1.591898932678D+00
I= 6 X= 2.566652928855D+00 Y= 2.778975074260D-01 Z= -2.943312816482D+00

I= 7 X= 5.784330463058D+00 Y= 1.646343515452D+00 Z= -1.907225634266D+00
I= 8 X= 3.228284695545D+00 Y= 3.492842252315D+00 Z= -3.205607617618D+00
I= 9 X= -2.327462010455D+00 Y= -2.265787135354D+00 Z= 4.699641170819D+00
I= 10 X= -4.233323964203D+00 Y= -2.308003026528D+00 Z= 5.331767110905D+00
I= 11 X= -1.412963782735D+00 Y= -3.965536794557D+00 Z= 4.298846137794D+00
I= 12 X= -1.184731383136D+00 Y= -1.150110502087D+00 Z= 6.016446820928D+00
I= 13 X= -1.978641391262D+00 Y= 3.621270107794D+00 Z= 4.302817467911D+00
I= 14 X= -3.597519624724D+00 Y= 3.353037199931D+00 Z= 6.056088971794D+00
I= 15 X= 3.083616999224D-01 Y= 2.923309075000D+00 Z= 5.276046316721D+00
I= 16 X= -1.733693738649D+00 Y= 5.577499557505D+00 Z= 3.527831275440D+00
I= 17 X= -2.452132259795D+00 Y= 5.009674433898D+00 Z= -1.667017030105D+00
I= 18 X= -4.856218161527D+00 Y= 5.160418656325D+00 Z= -2.622204471720D+00
I= 19 X= -1.701528411688D+00 Y= 6.151864151629D+00 Z= 8.816561495384D-03
I= 20 X= -1.258641662878D+00 Y= 5.272855337434D+00 Z= -3.483123894666D+00
I= 21 X= -3.561341362538D+00 Y= 2.035210133038D-01 Z= -4.785775581252D+00
I= 22 X= -5.436250116817D+00 Y= 3.982058824897D-01 Z= -4.608227030642D+00
I= 23 X= -2.616525956358D+00 Y= 1.660066972736D+00 Z= -5.926851245564D+00
I= 24 X= -3.276026616298D+00 Y= -1.646679647191D+00 Z= -5.703053470834D+00
I= 25 X= -3.296089624996D+00 Y= -4.547962061074D+00 Z= -9.557951475266D-01
I= 26 X= -2.986497858543D+00 Y= -4.729902734611D+00 Z= -2.935413916452D+00
I= 27 X= -2.060178890580D+00 Y= -5.843135682359D+00 Z= 2.671192901719D-01
I= 28 X= -5.144185187234D+00 Y= -5.257748049953D+00 Z= -7.678982444339D-01
I= 29 X= 3.177151534779D+00 Y= -3.606844600543D+00 Z= -9.679681507531D-01
I= 30 X= 3.533488987024D+00 Y= -2.712866739254D+00 Z= 1.639822937366D+00
I= 31 X= 1.704798235217D+00 Y= -5.082741642400D+00 Z= -1.321866173492D+00
I= 32 X= 4.518606815733D+00 Y= -3.113469864717D+00 Z= -2.421081097657D+00
I= 33 X= 5.416378464682D+00 Y= -1.919951389869D+00 Z= 2.215775513332D+00
I= 34 X= 2.359870906895D+00 Y= -3.365733043350D+00 Z= 2.994850429649D+00
I= 35 X= 8.239619733639D-01 Y= -1.695066690851D-01 Z= -2.087109288152D-01
I= 36 X= 3.447281707630D+00 Y= 2.853871280085D+00 Z= 1.123811249327D+00

I= 37 X= 5.145790872410D+00 Y= 2.448624078419D+00 Z= 2.580564180981D+00

I= 38 X= 2.350079864666D+00 Y= 4.662905356829D+00 Z= 1.649404295936D+00

Forward Direction:

Total Energy: -651.6048077 Hartrees

Potential Energy: -651.7842497 Hartress

Kinetic Energy: 0.1794421 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.327721645094D+13 Y= 3.722878185194D+12 Z= 3.193348465905D+13

I= 1 X= 1.359972482977D+11 Y= -8.152056846711D+12 Z= 3.627160023554D+12

I= 2 X= -1.262104402043D+12 Y= -1.114976819482D+13 Z= -5.840467515374D+12

I= 3 X= 1.157990730126D+13 Y= 6.697649559625D+12 Z= -3.783861736358D+12

I= 4 X= -9.254720401674D+12 Y= 1.206622825257D+13 Z= -7.654291587645D+12

I= 5 X= -4.709003356652D+12 Y= 9.599866962900D+12 Z= -4.453842588325D+12

I= 6 X= 5.202887214589D+12 Y= -2.742930635003D+13 Z= -8.994702042575D+13

I= 7 X= -9.889444612066D+12 Y= -4.282033363426D+13 Z= 4.486683803201D+13

I= 8 X= -9.397086666828D+13 Y= 3.332024048844D+13 Z= 8.302933752817D+13

I= 9 X= -1.966302731413D+11 Y= 1.015173061406D+13 Z= -5.998256264044D+12

I= 10 X= -4.764745770565D+13 Y= 1.204514393582D+13 Z= 2.462047515546D+13

I= 11 X= 1.535700166345D+12 Y= -7.742907578914D+13 Z= -2.482157605400D+13

I= 12 X= 1.457413130928D+13 Y= 1.040953235045D+14 Z= -6.684920163150D+12

I= 13 X= 1.607787717790D+13 Y= -8.951937940207D+12 Z= 5.790026952449D+12

I= 14 X= -9.092309894712D+13 Y= 1.003863759427D+13 Z= 2.907438005368D+13

I= 15 X= 4.449186766835D+13 Y= 6.334047948721D+13 Z= -7.151462342401D+12

I= 16 X= -3.102664642568D+13 Y= -9.881177209523D+12 Z= 2.101442490475D+13

I= 17 X= -2.346448287873D+13 Y= 1.716140781849D+13 Z= -1.541423289978D+13

I= 18 X= 1.182873389165D+14 Y= 5.963015819561D+13 Z= -2.532471152917D+13

I= 19 X= -4.760283796952D+13 Y= -4.355313900292D+13 Z= -7.772154033650D+13

I= 20 X= 1.571128885609D+13 Y= 2.981886966775D+13 Z= -8.491863927648D+13

I= 21 X= 8.922043681342D+12 Y= -1.192610811081D+13 Z= 1.072029356168D+13

I= 22 X= 3.216056665258D+13 Y= 2.921265007605D+13 Z= 1.408243900375D+13

I= 23 X= 6.580921291156D+13 Y= 5.059243403322D+13 Z= -6.981016132926D+13
I= 24 X= 1.650884149644D+13 Y= 4.260025850854D+13 Z= -3.688278404572D+13
I= 25 X= -1.603519160993D+13 Y= 1.158948996651D+13 Z= -1.715921692315D+13
I= 26 X= 3.813069877413D+13 Y= -5.590557737002D+13 Z= 9.388511581800D+13
I= 27 X= 9.893222325913D+13 Y= -9.335366642558D+13 Z= 9.009909433389D+13
I= 28 X= 1.356665625204D+13 Y= -8.716992942744D+13 Z= 2.426441156800D+13
I= 29 X= -1.645293520602D+11 Y= 9.487251830810D+12 Z= 1.258073821806D+13
I= 30 X= -2.035165832476D+13 Y= -1.551807611593D+12 Z= -1.287737412046D+13
I= 31 X= -4.241985536567D+13 Y= -1.055348295591D+14 Z= 7.456050431061D+13
I= 32 X= 6.454899002795D+13 Y= 1.273389542902D+13 Z= -1.234017775702D+14
I= 33 X= -4.639559030523D+13 Y= 1.312426622127D+13 Z= -9.856597681180D+12
I= 34 X= 6.246251611877D+13 Y= 6.557134695318D+13 Z= -3.822600247046D+13
I= 35 X= 1.620517355654D+12 Y= -2.229263965638D+12 Z= -8.308318089931D+11
I= 36 X= 1.894968571868D+13 Y= -6.015924319975D+12 Z= 2.648201655268D+13
I= 37 X= -6.254218309241D+13 Y= -3.061921648360D+13 Z= -7.900188033149D+13
I= 38 X= -3.625642680140D+13 Y= 8.470134234878D+13 Z= 1.195738434791D+14

Backward Direction:

Total Energy: -651.6048020 Hartrees

Potential Energy: -651.7842497 Hartress

Kinetic Energy: 0.1794478 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.413331309474D+13 Y= 3.471018192248D+12 Z= 3.191466996141D+13
I= 1 X= 5.627405766492D+11 Y= -9.065455249053D+12 Z= 2.108143954013D+12
I= 2 X= -1.817511076428D+12 Y= -1.031280578197D+13 Z= -7.148797221422D+12
I= 3 X= 1.123121225574D+13 Y= 6.774751832138D+12 Z= -5.616992736252D+12
I= 4 X= -6.540171254646D+12 Y= 1.184520757002D+13 Z= -9.393052337720D+12
I= 5 X= -4.523409293855D+12 Y= 8.331532625764D+12 Z= -1.582641283279D+13
I= 6 X= 8.035627042642D+13 Y= 4.172862874477D+13 Z= -5.728607193064D+13
I= 7 X= 5.538695312006D+12 Y= -2.823775071417D+13 Z= 4.628180807663D+13
I= 8 X= -7.307590591817D+13 Y= 5.041843237769D+13 Z= 8.693588192780D+13

I= 9 X= 7.522428904415D+11 Y= 1.056178074552D+13 Z= -7.030701059896D+12
I= 10 X= -4.732941770929D+13 Y= 1.413348918386D+13 Z= 2.220000201071D+13
I= 11 X= 1.314144412280D+12 Y= -7.741397863530D+13 Z= -2.497280103859D+13
I= 12 X= 1.522541623054D+13 Y= 1.042636171381D+14 Z= -7.307883644335D+12
I= 13 X= 1.626055591618D+13 Y= -9.077951390793D+12 Z= 5.338046595916D+12
I= 14 X= -9.066407158177D+13 Y= 9.263390895071D+12 Z= 2.911946966786D+13
I= 15 X= 4.512650197248D+13 Y= 6.270113153626D+13 Z= -8.227550763521D+12
I= 16 X= -3.114994010320D+13 Y= -9.708143638476D+12 Z= 2.114101339430D+13
I= 17 X= -2.315720650961D+13 Y= 1.688480453156D+13 Z= -1.553539411388D+13
I= 18 X= 1.186141155752D+14 Y= 5.946180927560D+13 Z= -2.604649289730D+13
I= 19 X= -4.760352377126D+13 Y= -4.382083975716D+13 Z= -7.741633385351D+13
I= 20 X= 1.607359375303D+13 Y= 2.936117195657D+13 Z= -8.506795360880D+13
I= 21 X= 8.301024653911D+12 Y= -1.191557771103D+13 Z= 9.773664622494D+12
I= 22 X= 3.174708267372D+13 Y= 3.011180698504D+13 Z= 1.184150211393D+13
I= 23 X= 6.620290235659D+13 Y= 5.024738259942D+13 Z= -7.060377426647D+13
I= 24 X= 1.568870680662D+13 Y= 4.257659304958D+13 Z= -3.799981904421D+13
I= 25 X= -1.603956850543D+13 Y= 1.147176517760D+13 Z= -1.742209422899D+13
I= 26 X= 3.765363061787D+13 Y= -5.658210056303D+13 Z= 9.369678089331D+13
I= 27 X= 9.934994463565D+13 Y= -9.296542438284D+13 Z= 8.994584358569D+13
I= 28 X= 1.366544726159D+13 Y= -8.718590488996D+13 Z= 2.474598221618D+13
I= 29 X= -1.792642321633D+12 Y= 1.044854738783D+13 Z= 1.133215033449D+13
I= 30 X= -2.022484870900D+13 Y= -1.278180305129D+12 Z= -1.383737608824D+13
I= 31 X= -4.229076606898D+13 Y= -1.064223334666D+14 Z= 7.396557217805D+13
I= 32 X= 6.247863742438D+13 Y= 1.460805194768D+13 Z= -1.253356037410D+14
I= 33 X= -4.610844801580D+13 Y= 1.299709421525D+13 Z= -1.083478041070D+13
I= 34 X= 6.343403496800D+13 Y= 6.542435937712D+13 Z= -3.885475793099D+13
I= 35 X= 1.228652918317D+12 Y= -2.388739446799D+12 Z= 6.936268681520D+11
I= 36 X= 1.420555615579D+13 Y= -1.168473162937D+13 Z= 2.363670386809D+13
I= 37 X= -5.702892462070D+13 Y= -2.706795873759D+13 Z= -8.600523483026D+13
I= 38 X= -3.291764732033D+13 Y= 8.447601099559D+13 Z= 1.150510615089D+14

Seed: 34740595451

CM Start Point Coordinates: bohr

I= 0 X= -2.370879722361D+00 Y= 2.377501360816D+00 Z= -6.873447287033D-01
I= 1 X= -2.994997689827D+00 Y= -1.498493126910D-01 Z= -2.049921165631D+00
I= 2 X= -2.366263766548D+00 Y= 1.839463638228D+00 Z= 2.033175053232D+00
I= 3 X= -2.699507132333D+00 Y= -1.872796057789D+00 Z= -4.122322977815D-02
I= 4 X= -2.278442086770D+00 Y= -7.999556018897D-01 Z= 2.338796014510D+00
I= 5 X= 4.249932363999D+00 Y= 2.322440231486D+00 Z= -9.840814097335D-01
I= 6 X= 2.239154586288D+00 Y= 1.234950377233D+00 Z= -3.064631969616D+00
I= 7 X= 6.111344277751D+00 Y= 1.568784429587D+00 Z= -1.827597884602D+00
I= 8 X= 3.754019000063D+00 Y= 4.162690817014D+00 Z= -1.636516927095D+00
I= 9 X= -2.541582263427D+00 Y= -2.012731065303D+00 Z= 4.954113230376D+00
I= 10 X= -4.239807392820D+00 Y= -1.298844974084D+00 Z= 5.741782806330D+00
I= 11 X= -3.004471103088D+00 Y= -4.261115255589D+00 Z= 4.751936510222D+00
I= 12 X= -8.803403909064D-01 Y= -1.201079206560D+00 Z= 6.012934808639D+00
I= 13 X= -1.994082125950D+00 Y= 3.479843380968D+00 Z= 4.188591377243D+00
I= 14 X= -3.742831852488D+00 Y= 3.127228075681D+00 Z= 5.648883555820D+00
I= 15 X= -1.595745888929D-01 Y= 3.235625946549D+00 Z= 5.355157941353D+00
I= 16 X= -2.401920378233D+00 Y= 5.763166517797D+00 Z= 3.162243725936D+00
I= 17 X= -2.510272782196D+00 Y= 5.063732502702D+00 Z= -1.811717967110D+00
I= 18 X= -4.320571506284D+00 Y= 5.751851712837D+00 Z= -1.969718575782D+00
I= 19 X= -9.398874718640D-01 Y= 6.236209346581D+00 Z= -6.667897988834D-01
I= 20 X= -1.609580502484D+00 Y= 4.708995738660D+00 Z= -3.676989299492D+00
I= 21 X= -3.472639170217D+00 Y= -5.235150222119D-01 Z= -4.697832825661D+00
I= 22 X= -5.560661878901D+00 Y= -7.662258418806D-02 Z= -4.945943779801D+00
I= 23 X= -2.501021967553D+00 Y= 1.067182730761D+00 Z= -5.656483596345D+00
I= 24 X= -2.987433530707D+00 Y= -2.281037348176D+00 Z= -5.146591992586D+00
I= 25 X= -3.201182631242D+00 Y= -4.674354448239D+00 Z= -6.366088339660D-01
I= 26 X= -2.813419577521D+00 Y= -4.787819073857D+00 Z= -2.977868174749D+00

I= 27 X= -1.718278907954D+00 Y= -5.995596293816D+00 Z= 1.979229792982D-01
I= 28 X= -4.925085790319D+00 Y= -5.512301314134D+00 Z= -9.749956847548D-02
I= 29 X= 3.081687665787D+00 Y= -3.354279380638D+00 Z= -1.643311588280D+00
I= 30 X= 3.345194409957D+00 Y= -3.248695212144D+00 Z= 9.939966830338D-01
I= 31 X= 1.900782263140D+00 Y= -4.793649537564D+00 Z= -2.291903312807D+00
I= 32 X= 4.412950629651D+00 Y= -2.252139684648D+00 Z= -2.824891221077D+00
I= 33 X= 4.994066798610D+00 Y= -2.394927856068D+00 Z= 2.139936760773D+00
I= 34 X= 1.965835375391D+00 Y= -4.497050623245D+00 Z= 2.225157940632D+00
I= 35 X= 8.117610238871D-01 Y= -6.409913369310D-02 Z= -2.401691000246D-01
I= 36 X= 3.480287175149D+00 Y= 2.328547956478D+00 Z= 1.603969246173D+00
I= 37 X= 4.642333623033D+00 Y= 1.375813768216D+00 Z= 2.881417036340D+00
I= 38 X= 2.490016275979D+00 Y= 4.160435031274D+00 Z= 2.254595381816D+00

Forward Direction:

Total Energy: -651.6099106 Hartrees

Potential Energy: -651.7930129 Hartress

Kinetic Energy: 0.1831023 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.258692803818D+13 Y= -1.428642737320D+12 Z= -1.223478991537D+12
I= 1 X= 1.265504158198D+13 Y= -5.474388134476D+12 Z= 3.593233770467D+12
I= 2 X= 2.746954405466D+12 Y= -3.283099802813D+12 Z= 1.027412231686D+13
I= 3 X= 9.913702504585D+12 Y= 1.365327024144D+13 Z= 6.497718715770D+12
I= 4 X= -5.736783971095D+12 Y= -2.334500548950D+13 Z= -2.866732850999D+13
I= 5 X= -1.815256279134D+12 Y= 1.345105516900D+13 Z= -2.191510285702D+13
I= 6 X= -8.930792288694D+13 Y= -4.902928249844D+12 Z= -1.743114967127D+13
I= 7 X= 1.031232963621D+14 Y= -7.076808861964D+13 Z= 2.643197948797D+13
I= 8 X= -8.752278932138D+13 Y= 4.624589891492D+13 Z= -2.728333242637D+13
I= 9 X= 5.088468677227D+12 Y= 1.440939355879D+13 Z= 1.570741262945D+13
I= 10 X= -2.145537618528D+13 Y= -4.932090340086D+13 Z= 3.963857140174D+13
I= 11 X= -2.418077138800D+13 Y= 9.796393445769D+13 Z= -3.743066523205D+13
I= 12 X= -1.024636379837D+14 Y= -4.831643369433D+13 Z= -4.786204587602D+13

I= 13 X= 7.210333421801D+12 Y= -1.898266043117D+13 Z= -2.573433006809D+13
I= 14 X= 2.233821087332D+13 Y= 1.411722899342D+13 Z= 5.006647530463D+12
I= 15 X= 7.133206869617D+13 Y= 2.723695110948D+13 Z= 1.000815673801D+14
I= 16 X= 4.014888932155D+13 Y= -3.587250699996D+13 Z= 7.932713628003D+12
I= 17 X= -1.014470671435D+13 Y= -4.548025841360D+12 Z= -6.389280938526D+12
I= 18 X= -8.378206707357D+13 Y= 1.126271410459D+12 Z= 2.972106429170D+13
I= 19 X= 8.675206508267D+12 Y= 8.978826108546D+13 Z= 1.163091361185D+13
I= 20 X= 9.172244735042D+13 Y= 6.189939493962D+13 Z= 6.480354379702D+13
I= 21 X= -1.240443025334D+13 Y= 4.515140402825D+12 Z= -2.013326391199D+13
I= 22 X= 1.364366411045D+14 Y= 1.956925384549D+13 Z= 1.930603669392D+13
I= 23 X= -4.036083146835D+13 Y= -2.602426667898D+13 Z= 6.693733736113D+13
I= 24 X= 1.811037496338D+13 Y= -3.495329431179D+13 Z= 1.313770750175D+13
I= 25 X= -1.966389875728D+12 Y= 1.158139375842D+13 Z= -3.364557718756D+12
I= 26 X= -2.290303011558D+13 Y= -2.198956982406D+13 Z= -3.124685161239D+13
I= 27 X= 7.174465266109D+13 Y= -9.273246332032D+13 Z= 1.191472167017D+14
I= 28 X= -6.169298614322D+13 Y= 1.369244777000D+13 Z= -4.394904397409D+12
I= 29 X= -3.336741467715D+13 Y= -1.808289008682D+13 Z= 7.872096309159D+11
I= 30 X= -2.030231208357D+12 Y= 8.390877417543D+11 Z= 2.683128891250D+13
I= 31 X= 9.863657154708D+13 Y= 1.442706886129D+14 Z= 4.720413497639D+13
I= 32 X= 6.866643819217D+13 Y= 3.319829015070D+13 Z= 3.522908087987D+13
I= 33 X= -1.480474758170D+13 Y= -1.437816858256D+13 Z= 3.443096388800D+13
I= 34 X= 1.629981539759D+13 Y= -2.861841659288D+13 Z= 1.159128274292D+13
I= 35 X= 2.239497813427D+12 Y= 1.869454727592D+12 Z= -1.084699467811D+12
I= 36 X= -6.533170122756D+12 Y= -1.967149086210D+13 Z= 1.983147990809D+13
I= 37 X= 1.413778079048D+12 Y= 3.063769528136D+13 Z= 6.012205798626D+12
I= 38 X= 7.319547916172D+13 Y= -7.679057320273D+13 Z= 1.971932556887D+13

Backward Direction:

Total Energy: -651.6099174 Hartrees

Potential Energy: -651.7930129 Hartress

Kinetic Energy: 0.1830955 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.308310472867D+13 Y= -1.574615809593D+12 Z= -1.234383618857D+12
I= 1 X= 1.290237357884D+13 Y= -6.003775790641D+12 Z= 2.712842088194D+12
I= 2 X= 2.425051675278D+12 Y= -2.798012934107D+12 Z= 9.515840283801D+12
I= 3 X= 9.711605751117D+12 Y= 1.369795719480D+13 Z= 5.435272227786D+12
I= 4 X= -4.163484950602D+12 Y= -2.347310470666D+13 Z= -2.967507986711D+13
I= 5 X= -1.707689627018D+12 Y= 1.271595365828D+13 Z= -2.850641974867D+13
I= 6 X= -4.575050769351D+13 Y= 3.517964373769D+13 Z= 1.498490397173D+12
I= 7 X= 1.120651412631D+14 Y= -6.231631184744D+13 Z= 2.725206814864D+13
I= 8 X= -7.541248314349D+13 Y= 5.615567291435D+13 Z= -2.501917652581D+13
I= 9 X= 5.638416793802D+12 Y= 1.464705051010D+13 Z= 1.510902803650D+13
I= 10 X= -2.127104650342D+13 Y= -4.811053978133D+13 Z= 3.823571301173D+13
I= 11 X= -2.430918073127D+13 Y= 9.797268447488D+13 Z= -3.751831224258D+13
I= 12 X= -1.020861661326D+14 Y= -4.821889402732D+13 Z= -4.822310319302D+13
I= 13 X= 7.316210397292D+12 Y= -1.905569533669D+13 Z= -2.599628894603D+13
I= 14 X= 2.248833800043D+13 Y= 1.366791131860D+13 Z= 5.032780584256D+12
I= 15 X= 7.169989018847D+13 Y= 2.686639768425D+13 Z= 9.945788780415D+13
I= 16 X= 4.007743072066D+13 Y= -3.577222015860D+13 Z= 8.006081818128D+12
I= 17 X= -9.966615410717D+12 Y= -4.708339637918D+12 Z= -6.459503582621D+12
I= 18 X= -8.359267379073D+13 Y= 1.028699699025D+12 Z= 2.930273407459D+13
I= 19 X= 8.674809015259D+12 Y= 8.963310702631D+13 Z= 1.180780526357D+13
I= 20 X= 9.193243211040D+13 Y= 6.163412239784D+13 Z= 6.471700416464D+13
I= 21 X= -1.276436061317D+13 Y= 4.521243615959D+12 Z= -2.068191132720D+13
I= 22 X= 1.361969939558D+14 Y= 2.009038741389D+13 Z= 1.800723398266D+13
I= 23 X= -4.013265685883D+13 Y= -2.622425166727D+13 Z= 6.647737499560D+13
I= 24 X= 1.763504109905D+13 Y= -3.496701034218D+13 Z= 1.249029610097D+13
I= 25 X= -1.968926636132D+12 Y= 1.151316279912D+13 Z= -3.516916208905D+12
I= 26 X= -2.317952938693D+13 Y= -2.238166929035D+13 Z= -3.135600680968D+13
I= 27 X= 7.198675571226D+13 Y= -9.250744590629D+13 Z= 1.190583955952D+14
I= 28 X= -6.163572882473D+13 Y= 1.368318870911D+13 Z= -4.115795570385D+12

I= 29 X= -3.431103676868D+13 Y= -1.752574218666D+13 Z= 6.355277668655D+10
I= 30 X= -1.956734860436D+12 Y= 9.976767181162D+11 Z= 2.627489074963D+13
I= 31 X= 9.871138914889D+13 Y= 1.437563088940D+14 Z= 4.685932407490D+13
I= 32 X= 6.746650274993D+13 Y= 3.428451421612D+13 Z= 3.410827346076D+13
I= 33 X= -1.463832558557D+13 Y= -1.445187496504D+13 Z= 3.386402851438D+13
I= 34 X= 1.686288851784D+13 Y= -2.870360768673D+13 Z= 1.122686850799D+13
I= 35 X= 2.012380934497D+12 Y= 1.777025891358D+12 Z= -2.011533557257D+11
I= 36 X= -9.282773824937D+12 Y= -2.295701951281D+13 Z= 1.818239292233D+13
I= 37 X= 4.609153701999D+12 Y= 3.269593406278D+13 Z= 1.953199978843D+12
I= 38 X= 7.513056975030D+13 Y= -7.692117080107D+13 Z= 1.709801054801D+13

Seed: 34894387040

CM Start Point Coordinates: bohr

I= 0 X= -2.713563385097D+00 Y= 2.392738222413D+00 Z= -5.589399065502D-01
I= 1 X= -3.083291563819D+00 Y= 1.624104560965D-02 Z= -2.077259246611D+00
I= 2 X= -2.439746138762D+00 Y= 1.647821483506D+00 Z= 1.891481817631D+00
I= 3 X= -2.866011122430D+00 Y= -1.944147773167D+00 Z= -3.184592487523D-01
I= 4 X= -2.556970625687D+00 Y= -1.114475248223D+00 Z= 2.170258675526D+00
I= 5 X= 4.312728682170D+00 Y= 2.185723900005D+00 Z= -2.029357646877D+00
I= 6 X= 2.436168777720D+00 Y= -2.658105458744D-01 Z= -3.034292964292D+00
I= 7 X= 6.275114398183D+00 Y= 1.148564998031D+00 Z= -2.213346813721D+00
I= 8 X= 3.466458202734D+00 Y= 3.507601142594D+00 Z= -3.428647510345D+00
I= 9 X= -2.564754121272D+00 Y= -2.723203823814D+00 Z= 4.587186886351D+00
I= 10 X= -4.486417840849D+00 Y= -2.731110374829D+00 Z= 5.528943865319D+00
I= 11 X= -1.897621004605D+00 Y= -4.589143417095D+00 Z= 4.283731393180D+00
I= 12 X= -1.894289874494D+00 Y= -1.525154517655D+00 Z= 6.179832338982D+00
I= 13 X= -1.819857138434D+00 Y= 3.198849416804D+00 Z= 4.338090898480D+00
I= 14 X= -3.286015558419D+00 Y= 3.948007175772D+00 Z= 5.275888786232D+00
I= 15 X= -5.343801025283D-01 Y= 2.267764699334D+00 Z= 5.867430669056D+00
I= 16 X= -6.804469208313D-01 Y= 4.799625790148D+00 Z= 4.044263349575D+00

I= 17 X= -2.832487003967D+00 Y= 5.140856821414D+00 Z= -1.355191943300D+00
I= 18 X= -4.538535382559D+00 Y= 5.796516028280D+00 Z= -7.568049419704D-01
I= 19 X= -1.634290776377D+00 Y= 6.384147134465D+00 Z= -3.428237543383D-01
I= 20 X= -2.593364667023D+00 Y= 5.419704009205D+00 Z= -3.507831630970D+00
I= 21 X= -3.532662175011D+00 Y= -2.048987447939D-01 Z= -4.867415319332D+00
I= 22 X= -5.528127529997D+00 Y= -5.443954601829D-01 Z= -5.229966323341D+00
I= 23 X= -2.846245330116D+00 Y= 1.437853247216D+00 Z= -5.910602493850D+00
I= 24 X= -1.995106158135D+00 Y= -1.913662251755D+00 Z= -5.740026877430D+00
I= 25 X= -3.663128716008D+00 Y= -4.564882012901D+00 Z= -1.004632483196D+00
I= 26 X= -2.609491377728D+00 Y= -4.751520000508D+00 Z= -3.207730625669D+00
I= 27 X= -2.984066148320D+00 Y= -6.001229782625D+00 Z= 6.928756532601D-01
I= 28 X= -5.715772093354D+00 Y= -4.730658057696D+00 Z= -1.048223536263D+00
I= 29 X= 2.969105199815D+00 Y= -3.758208350460D+00 Z= -5.214250117196D-01
I= 30 X= 3.126679476031D+00 Y= -2.710292288548D+00 Z= 1.927878171352D+00
I= 31 X= 1.369042293128D+00 Y= -5.228353573480D+00 Z= -1.185721415039D+00
I= 32 X= 4.439388334702D+00 Y= -3.586277504563D+00 Z= -1.855585642248D+00
I= 33 X= 4.586862948609D+00 Y= -1.869633735376D+00 Z= 2.576965832078D+00
I= 34 X= 2.239962415729D+00 Y= -3.790539793976D+00 Z= 3.389256570098D+00
I= 35 X= 9.186682421768D-01 Y= -2.024311684367D-02 Z= -1.939277281187D-01
I= 36 X= 3.782122140820D+00 Y= 2.764247639171D+00 Z= 6.220161498238D-01
I= 37 X= 5.181244911124D+00 Y= 2.331159371015D+00 Z= 2.050447642197D+00
I= 38 X= 2.625689331312D+00 Y= 4.476360302745D+00 Z= 1.312848767832D+00

Forward Direction:

Total Energy: -651.6182828 Hartrees

Potential Energy: -651.7964640 Hartress

Kinetic Energy: 0.1781812 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.025000222573D+12 Y= 1.508692752559D+13 Z= 9.041450433399D+12

I= 1 X= -2.408515772713D+13 Y= 8.069020251329D+12 Z= 1.578171029913D+13

I= 2 X= -1.045663357073D+13 Y= -3.230228712939D+13 Z= -1.767501676903D+12

I= 3 X= 2.227676061749D+12 Y= 8.961651212311D+11 Z= 1.793339856103D+13
I= 4 X= 3.569565198405D+12 Y= 6.061456707872D+11 Z= -1.091633183267D+13
I= 5 X= 8.299237686699D+12 Y= -4.451603483589D+12 Z= 2.462511005719D+13
I= 6 X= 4.298624469746D+12 Y= -3.019632825030D+13 Z= -8.402755856398D+13
I= 7 X= -6.506262553699D+12 Y= -5.534247736856D+13 Z= 1.366803993321D+13
I= 8 X= 8.725044939310D+11 Y= 4.285869049440D+13 Z= -1.520324736590D+14
I= 9 X= -4.646835489085D+12 Y= 1.433890517550D+13 Z= 1.344244625289D+13
I= 10 X= -1.776470044527D+13 Y= 1.076128220083D+13 Z= 6.194231527335D+13
I= 11 X= 1.073232270894D+14 Y= -5.214179979976D+13 Z= -1.046117028380D+14
I= 12 X= -6.317732377782D+13 Y= -2.603874831064D+13 Z= -3.265649464299D+13
I= 13 X= -6.618859123833D+12 Y= -9.477810284909D+12 Z= -1.166376029749D+13
I= 14 X= -5.866151819380D+13 Y= -1.185221369385D+12 Z= 2.079915932637D+13
I= 15 X= 5.347956149884D+13 Y= -3.255328003123D+13 Z= -2.028989270213D+13
I= 16 X= 1.136673589373D+13 Y= 1.259768027721D+14 Z= 4.864807913954D+13
I= 17 X= 1.413826087147D+13 Y= -3.297327052331D+12 Z= -1.876086435771D+13
I= 18 X= 3.231591300037D+12 Y= -1.272990869321D+13 Z= -2.786342199274D+13
I= 19 X= -4.974426406716D+13 Y= 2.527421557806D+13 Z= 1.180782371030D+13
I= 20 X= -5.616892236068D+13 Y= -3.925003980229D+13 Z= 1.182310142700D+14
I= 21 X= -6.262921764517D+12 Y= 9.273646844200D+12 Z= -1.899529102013D+13
I= 22 X= 1.025083937578D+14 Y= 7.736579094782D+12 Z= 1.189310180771D+14
I= 23 X= 3.664762236393D+13 Y= -2.967386603459D+13 Z= 2.228663397131D+13
I= 24 X= 4.723834833999D+13 Y= 9.649400296899D+12 Z= 6.205645413345D+12
I= 25 X= 1.769811164042D+12 Y= -2.047118380517D+12 Z= -1.760711151481D+13
I= 26 X= 2.378751622288D+13 Y= -5.899909184270D+13 Z= 2.913618396855D+13
I= 27 X= -7.401150124403D+13 Y= 2.033147656125D+12 Z= -5.123407712190D+13
I= 28 X= 2.217218790349D+12 Y= -1.103743499030D+13 Z= -2.325442212687D+13
I= 29 X= -1.614316226192D+13 Y= -1.899386880967D+13 Z= 1.591648025212D+13
I= 30 X= -9.604932607573D+10 Y= 1.322306093237D+13 Z= -8.569111013249D+12
I= 31 X= -5.340385760033D+12 Y= -1.645855707068D+13 Z= -3.424725413171D+13
I= 32 X= 1.225729090998D+14 Y= 1.175414474623D+14 Z= -2.942779587436D+13

I= 33 X= 5.189165879621D+13 Y= -5.164764881938D+13 Z= -6.128702361675D+13
I= 34 X= -8.740414014209D+13 Y= -1.251116609110D+14 Z= 9.224195010972D+12
I= 35 X= 1.673187981493D+11 Y= 9.363439374654D+11 Z= -3.183443352567D+11
I= 36 X= 1.025799964562D+13 Y= 6.378183280964D+12 Z= -1.723440166079D+12
I= 37 X= 6.747933252677D+12 Y= -8.450300944917D+12 Z= 1.193398978040D+14
I= 38 X= 5.095880364126D+13 Y= 6.183178441763D+13 Z= 2.144543953907D+13

Backward Direction:

Total Energy: -651.6183334 Hartrees

Potential Energy: -651.7964640 Hartress

Kinetic Energy: 0.1781306 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.821095237062D+12 Y= 1.473274379774D+13 Z= 9.014991844898D+12
I= 1 X= -2.348504041080D+13 Y= 6.784533391446D+12 Z= 1.364556009834D+13
I= 2 X= -1.123768658473D+13 Y= -3.112529008348D+13 Z= -3.607369484621D+12
I= 3 X= 1.737315884325D+12 Y= 1.004591910136D+12 Z= 1.535551723661D+13
I= 4 X= 7.386960435841D+12 Y= 2.953304105671D+11 Z= -1.336150288883D+13
I= 5 X= 8.560233475355D+12 Y= -6.235226914152D+12 Z= 8.632179690130D+12
I= 6 X= 1.099847445442D+14 Y= 6.705855928823D+13 Z= -3.809737183402D+13
I= 7 X= 1.518990306026D+13 Y= -3.483539513993D+13 Z= 1.565787309312D+13
I= 8 X= 3.025650873242D+13 Y= 6.690340390106D+13 Z= -1.465388085350D+14
I= 9 X= -3.312461460352D+12 Y= 1.491554731179D+13 Z= 1.199054774950D+13
I= 10 X= -1.731744961533D+13 Y= 1.369806425128D+13 Z= 5.853847096760D+13
I= 11 X= 1.070116593659D+14 Y= -5.212056908849D+13 Z= -1.048243663441D+14
I= 12 X= -6.226143984312D+13 Y= -2.580208163414D+13 Z= -3.353255092392D+13
I= 13 X= -6.361963082644D+12 Y= -9.655019508863D+12 Z= -1.229936774711D+13
I= 14 X= -5.829725519380D+13 Y= -2.275429326419D+12 Z= 2.086256760145D+13
I= 15 X= 5.437203012977D+13 Y= -3.345237732783D+13 Z= -2.180316602423D+13
I= 16 X= 1.119335139949D+13 Y= 1.262201350917D+14 Z= 4.882609703034D+13
I= 17 X= 1.457037510896D+13 Y= -3.686306588228D+12 Z= -1.893125001388D+13
I= 18 X= 3.691128250617D+12 Y= -1.296665312026D+13 Z= -2.887844312182D+13

I= 19 X= -4.974522850234D+13 Y= 2.489775543082D+13 Z= 1.223702713605D+13
I= 20 X= -5.565942302876D+13 Y= -3.989368740668D+13 Z= 1.180210376637D+14
I= 21 X= -7.136243614631D+12 Y= 9.288455453683D+12 Z= -2.032650906193D+13
I= 22 X= 1.019269226952D+14 Y= 9.001038532754D+12 Z= 1.157796506315D+14
I= 23 X= 3.720125691548D+13 Y= -3.015910230143D+13 Z= 2.117059809390D+13
I= 24 X= 4.608501565772D+13 Y= 9.616120220013D+12 Z= 4.634790051986D+12
I= 25 X= 1.763656053759D+12 Y= -2.212671488730D+12 Z= -1.797678858424D+13
I= 26 X= 2.311662849166D+13 Y= -5.995046765760D+13 Z= 2.887133378746D+13
I= 27 X= -7.342407124623D+13 Y= 2.579121683916D+12 Z= -5.144958940401D+13
I= 28 X= 2.356145848297D+12 Y= -1.105990084240D+13 Z= -2.257720266803D+13
I= 29 X= -1.843273241196D+13 Y= -1.764202550879D+13 Z= 1.416062571470D+13
I= 30 X= 8.227952141306D+10 Y= 1.360785543037D+13 Z= -9.919135175869D+12
I= 31 X= -5.158851064060D+12 Y= -1.770662922042D+13 Z= -3.508389070364D+13
I= 32 X= 1.196614296073D+14 Y= 1.201770218335D+14 Z= -3.214728202682D+13
I= 33 X= 5.229545904243D+13 Y= -5.182648729204D+13 Z= -6.266261488229D+13
I= 34 X= -8.603792011027D+13 Y= -1.253183654699D+14 Z= 8.339993631003D+12
I= 35 X= -3.837492988850D+11 Y= 7.120779880785D+11 Z= 1.825459654716D+12
I= 36 X= 3.586461717672D+12 Y= -1.593703339770D+12 Z= -5.724724542716D+12
I= 37 X= 1.450107585568D+13 Y= -3.456265591508D+12 Z= 1.094912744537D+14
I= 38 X= 5.565403670627D+13 Y= 6.151490718046D+13 Z= 1.508517659005D+13

Seed: 36800429431

CM Start Point Coordinates: bohr

I= 0 X= -2.727655135094D+00 Y= 2.408567553418D+00 Z= -6.007032543871D-01
I= 1 X= -2.956375933159D+00 Y= 1.717358416975D-01 Z= -1.990233859664D+00
I= 2 X= -2.258244450155D+00 Y= 1.705312298551D+00 Z= 2.080033117874D+00
I= 3 X= -2.825010157399D+00 Y= -1.890452915824D+00 Z= -2.074191618443D-01
I= 4 X= -2.471939523540D+00 Y= -9.421675069044D-01 Z= 2.243538986198D+00
I= 5 X= 4.266255939758D+00 Y= 2.227286070800D+00 Z= -1.433141281095D+00
I= 6 X= 2.521250473846D+00 Y= 7.247120135254D-01 Z= -2.991260187959D+00

I= 7 X= 5.844213202637D+00 Y= 1.212264272990D+00 Z= -2.070557567428D+00
I= 8 X= 3.553373321227D+00 Y= 3.720891506174D+00 Z= -2.990279234025D+00
I= 9 X= -2.214688566247D+00 Y= -2.402811825176D+00 Z= 4.618538848322D+00
I= 10 X= -4.047216888621D+00 Y= -3.431431295508D+00 Z= 5.516750049181D+00
I= 11 X= -8.203088231631D-01 Y= -4.046949504194D+00 Z= 3.673656823964D+00
I= 12 X= -1.262305029281D+00 Y= -1.302123876341D+00 Z= 5.901872389310D+00
I= 13 X= -1.817213327363D+00 Y= 3.568216969768D+00 Z= 4.237075127615D+00
I= 14 X= -3.522108033522D+00 Y= 3.814255571703D+00 Z= 5.156183126117D+00
I= 15 X= -2.760189788985D-01 Y= 2.561815549094D+00 Z= 5.581831461973D+00
I= 16 X= -1.237090208512D+00 Y= 5.339895166962D+00 Z= 3.416274824863D+00
I= 17 X= -2.697612408114D+00 Y= 4.964190676223D+00 Z= -1.541511102391D+00
I= 18 X= -4.461118578830D+00 Y= 6.177601521106D+00 Z= -1.354959397286D+00
I= 19 X= -1.879472894281D+00 Y= 6.357775331941D+00 Z= -5.752278791962D-01
I= 20 X= -1.635170414598D+00 Y= 5.071982310881D+00 Z= -3.340656660263D+00
I= 21 X= -3.262391935901D+00 Y= -6.517992588649D-02 Z= -4.872886251648D+00
I= 22 X= -5.171781602420D+00 Y= 7.520887820887D-01 Z= -5.549585621967D+00
I= 23 X= -1.482682581201D+00 Y= 1.402733138217D+00 Z= -5.818258718055D+00
I= 24 X= -2.763234680274D+00 Y= -2.056654754803D+00 Z= -5.388336046785D+00
I= 25 X= -3.717672474563D+00 Y= -4.648226479560D+00 Z= -8.803281806230D-01
I= 26 X= -3.478243378075D+00 Y= -5.106676419106D+00 Z= -2.889038870842D+00
I= 27 X= -2.394628813826D+00 Y= -5.816300107831D+00 Z= 1.018226796962D-01
I= 28 X= -5.569597554844D+00 Y= -4.727108493101D+00 Z= -5.865440840947D-01
I= 29 X= 2.994327966380D+00 Y= -3.481998393720D+00 Z= -7.859239750673D-01
I= 30 X= 3.641292833961D+00 Y= -2.717738599004D+00 Z= 1.692825956158D+00
I= 31 X= 1.715999540322D+00 Y= -5.035613983005D+00 Z= -1.193820545481D+00
I= 32 X= 4.289162433927D+00 Y= -3.245632460954D+00 Z= -2.793387839099D+00
I= 33 X= 5.279148201489D+00 Y= -1.827428023558D+00 Z= 2.061283028308D+00
I= 34 X= 2.800432909863D+00 Y= -3.441262500792D+00 Z= 3.431871026948D+00
I= 35 X= 8.199745934418D-01 Y= -1.217351540793D-01 Z= -2.342770795771D-01
I= 36 X= 3.468274897127D+00 Y= 2.778698857878D+00 Z= 1.097239832761D+00

I= 37 X= 4.522926892535D+00 Y= 2.042229904612D+00 Z= 2.644718122775D+00

I= 38 X= 2.249828408902D+00 Y= 4.217878096482D+00 Z= 1.367008447158D+00

Forward Direction:

Total Energy: -651.6195215 Hartrees

Potential Energy: -651.7873943 Hartress

Kinetic Energy: 0.1678728 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.560676218139D+12 Y= -2.322171625451D+13 Z= -1.826903862938D+12

I= 1 X= -5.705253790189D+12 Y= -1.960854248505D+13 Z= -8.780742103587D+12

I= 2 X= 1.595315834470D+13 Y= 2.259016422446D+10 Z= 1.268420137669D+12

I= 3 X= 1.005661169904D+12 Y= 2.258006675046D+13 Z= -1.312094657935D+12

I= 4 X= -6.486639171760D+12 Y= -1.102480461630D+13 Z= 1.974229381724D+13

I= 5 X= 4.209194215108D+12 Y= -1.285827966495D+12 Z= -2.117636909101D+13

I= 6 X= -1.605179505538D+13 Y= -1.636809201979D+13 Z= -3.966840581098D+13

I= 7 X= -6.384128887030D+13 Y= -3.779401874790D+13 Z= -2.139369525325D+12

I= 8 X= 3.058217639147D+13 Y= -4.558411589276D+13 Z= 9.719858975293D+13

I= 9 X= 1.897747702399D+13 Y= 2.366096543650D+12 Z= -1.431670196232D+13

I= 10 X= -5.306949120268D+13 Y= -1.091814088487D+13 Z= -4.065195581866D+13

I= 11 X= -9.952870340379D+13 Y= 9.648039156991D+13 Z= 3.740558331951D+13

I= 12 X= -6.056753601617D+12 Y= 1.252320990820D+13 Z= -9.632082421159D+13

I= 13 X= -7.147369058313D+12 Y= -4.591708107278D+12 Z= 1.355594323927D+13

I= 14 X= 6.722972370108D+13 Y= 2.813128298480D+13 Z= -6.070900044983D+13

I= 15 X= -8.771858845012D+13 Y= 5.986485866933D+13 Z= -7.670729515740D+13

I= 16 X= -1.104772114077D+13 Y= -2.508319934637D+13 Z= 4.553704068106D+13

I= 17 X= -1.567652494917D+13 Y= 2.318764431486D+13 Z= -5.632765175564D+12

I= 18 X= 5.570659530897D+13 Y= 6.900245902606D+12 Z= 2.259329266250D+13

I= 19 X= -2.290639674475D+13 Y= -3.075001478072D+13 Z= 8.352168738584D+12

I= 20 X= 4.830889228749D+13 Y= -1.187084943712D+13 Z= -8.708054804161D+13

I= 21 X= 7.775860533124D+12 Y= 9.689111622526D+12 Z= -1.702347494989D+13

I= 22 X= -2.603816331140D+13 Y= -4.471267989464D+13 Z= -9.772027024972D+13

I= 23 X= 3.695392800446D+13 Y= 2.728505941205D+13 Z= -6.196939530647D+13
I= 24 X= 7.658051514902D+12 Y= -1.266100023724D+14 Z= -5.074352321357D+13
I= 25 X= -1.311219407755D+12 Y= 4.407288071489D+12 Z= 8.183435958330D+12
I= 26 X= -3.498317593276D+12 Y= 5.815578441878D+12 Z= -1.030618852416D+14
I= 27 X= -6.457317710285D+13 Y= 7.967530885585D+13 Z= 6.477521056676D+11
I= 28 X= 2.372650913033D+13 Y= -5.635959819459D+13 Z= 4.460167831285D+13
I= 29 X= 2.205330393450D+11 Y= -1.440070545481D+13 Z= -1.597391638650D+13
I= 30 X= -8.179815378709D+11 Y= 7.796679736301D+11 Z= 1.973062352104D+13
I= 31 X= -3.280594918465D+13 Y= -6.484548476728D+13 Z= -1.178543229695D+13
I= 32 X= 3.629707300657D+13 Y= -2.315179294280D+13 Z= 4.319705891291D+13
I= 33 X= -7.306832124844D+13 Y= 4.178523331001D+13 Z= -7.095669270814D+13
I= 34 X= 8.302639086092D+13 Y= -1.806840068536D+13 Z= -1.228735144313D+13
I= 35 X= 4.375993025199D+11 Y= 1.378758013967D+12 Z= 2.935309296694D+12
I= 36 X= -2.583922140505D+12 Y= 6.859135097602D+12 Z= 4.973098572165D+11
I= 37 X= 5.011587041525D+13 Y= 4.040951337670D+13 Z= 1.754705137306D+14
I= 38 X= -3.286783857246D+13 Y= -1.002330573551D+14 Z= 4.941935342031D+13

Backward Direction:

Total Energy: -651.6195257 Hartrees

Potential Energy: -651.7873943 Hartress

Kinetic Energy: 0.1678686 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.804597781146D+12 Y= -2.329347694112D+13 Z= -1.832264602128D+12
I= 1 X= -5.583664830639D+12 Y= -1.986879063250D+13 Z= -9.213544609993D+12
I= 2 X= 1.579491024796D+13 Y= 2.610599461248D+11 Z= 8.956470067471D+11
I= 3 X= 9.063099553404D+11 Y= 2.260203495626D+13 Z= -1.834395709821D+12
I= 4 X= -5.713201880299D+12 Y= -1.108777847672D+13 Z= 1.924688101273D+13
I= 5 X= 4.262074217199D+12 Y= -1.647205498160D+12 Z= -2.441667510769D+13
I= 6 X= 5.361126958987D+12 Y= 3.336589361068D+12 Z= -3.036255272553D+13
I= 7 X= -5.944545806625D+13 Y= -3.363910651669D+13 Z= -1.736212118450D+12
I= 8 X= 3.653562979197D+13 Y= -4.071244899010D+13 Z= 9.831165382195D+13

I= 9 X= 1.924783274814D+13 Y= 2.482929226638D+12 Z= -1.461086915662D+13
I= 10 X= -5.297887431458D+13 Y= -1.032312344465D+13 Z= -4.134160411931D+13
I= 11 X= -9.959182971512D+13 Y= 9.648469309427D+13 Z= 3.736249585714D+13
I= 12 X= -5.871187593429D+12 Y= 1.257116062660D+13 Z= -9.649832078872D+13
I= 13 X= -7.095319698851D+12 Y= -4.627612227934D+12 Z= 1.342716367297D+13
I= 14 X= 6.730352653445D+13 Y= 2.791039742432D+13 Z= -6.069615338527D+13
I= 15 X= -8.753776658786D+13 Y= 5.968269378059D+13 Z= -7.701389742026D+13
I= 16 X= -1.108285033663D+13 Y= -2.503389811391D+13 Z= 4.557310864633D+13
I= 17 X= -1.558897486239D+13 Y= 2.310883369697D+13 Z= -5.667286783452D+12
I= 18 X= 5.579970147832D+13 Y= 6.852279442133D+12 Z= 2.238764061058D+13
I= 19 X= -2.290659213562D+13 Y= -3.082628886656D+13 Z= 8.439129060909D+12
I= 20 X= 4.841212125909D+13 Y= -1.200125800796D+13 Z= -8.712309111951D+13
I= 21 X= 7.598917975695D+12 Y= 9.692111973851D+12 Z= -1.729319123912D+13
I= 22 X= -2.615597437490D+13 Y= -4.445648947372D+13 Z= -9.835876455364D+13
I= 23 X= 3.706609915689D+13 Y= 2.718674634738D+13 Z= -6.219551382618D+13
I= 24 X= 7.424376340664D+12 Y= -1.266167452068D+14 Z= -5.106179209349D+13
I= 25 X= -1.312466484525D+12 Y= 4.373745581162D+12 Z= 8.108536186653D+12
I= 26 X= -3.634245256377D+12 Y= 5.622821469496D+12 Z= -1.031155461792D+14
I= 27 X= -6.445415870825D+13 Y= 7.978592791304D+13 Z= 6.040874535122D+11
I= 28 X= 2.375465695228D+13 Y= -5.636414996063D+13 Z= 4.473888883437D+13
I= 29 X= -2.433536745205D+11 Y= -1.412681030940D+13 Z= -1.632966770236D+13
I= 30 X= -7.818505711047D+11 Y= 8.576306668273D+11 Z= 1.945709694949D+13
I= 31 X= -3.276916868312D+13 Y= -6.509835497950D+13 Z= -1.195494210263D+13
I= 32 X= 3.570718208059D+13 Y= -2.261780277978D+13 Z= 4.264606749718D+13
I= 33 X= -7.298650782748D+13 Y= 4.174899909063D+13 Z= -7.123539939469D+13
I= 34 X= 8.330319885376D+13 Y= -1.811028081849D+13 Z= -1.246649829200D+13
I= 35 X= 3.259481391565D+11 Y= 1.333319792609D+12 Z= 3.369662526941D+12
I= 36 X= -3.935633428834D+12 Y= 5.243961919654D+12 Z= -3.133849651041D+11
I= 37 X= 5.168672416383D+13 Y= 4.142134813325D+13 Z= 1.734750974567D+14
I= 38 X= -3.191654374607D+13 Y= -1.002972594236D+14 Z= 4.813070913819D+13

Seed: 37466053161

CM Start Point Coordinates: bohr

I= 0 X= -2.506921927149D+00 Y= 2.376769641741D+00 Z= -5.991172324874D-01
I= 1 X= -2.827908342523D+00 Y= -7.912879599713D-02 Z= -1.909649006927D+00
I= 2 X= -2.557010756726D+00 Y= 2.008688716883D+00 Z= 1.894362391589D+00
I= 3 X= -2.752171207965D+00 Y= -1.952247535496D+00 Z= -6.808497374235D-02
I= 4 X= -2.435910647538D+00 Y= -7.308003681291D-01 Z= 2.430569096786D+00
I= 5 X= 4.020740751278D+00 Y= 2.927060832957D+00 Z= -9.716695817785D-01
I= 6 X= 2.558123190192D+00 Y= 8.775657815900D-01 Z= -2.850535196473D+00
I= 7 X= 5.623414150512D+00 Y= 2.594443907652D+00 Z= -2.447437447443D+00
I= 8 X= 2.756248152182D+00 Y= 4.672964330514D+00 Z= -1.682042246421D+00
I= 9 X= -2.498650815739D+00 Y= -2.197892842881D+00 Z= 4.806260775757D+00
I= 10 X= -4.459744765637D+00 Y= -2.279793199698D+00 Z= 5.573440462722D+00
I= 11 X= -2.049970308169D+00 Y= -4.181099059506D+00 Z= 4.487262092275D+00
I= 12 X= -1.291953898232D+00 Y= -1.523485649580D+00 Z= 6.281881789767D+00
I= 13 X= -2.292423462805D+00 Y= 3.885435928326D+00 Z= 3.902666228155D+00
I= 14 X= -4.132085130239D+00 Y= 4.772294029361D+00 Z= 4.652485601056D+00
I= 15 X= -1.585052539394D+00 Y= 3.151755893514D+00 Z= 5.663752364561D+00
I= 16 X= -1.191743699729D+00 Y= 5.266546683148D+00 Z= 3.266441254040D+00
I= 17 X= -2.770532241430D+00 Y= 4.963623058365D+00 Z= -1.991361963552D+00
I= 18 X= -4.770967146521D+00 Y= 5.193406945424D+00 Z= -2.588811421891D+00
I= 19 X= -2.527582911007D+00 Y= 6.925225890063D+00 Z= -4.553231504952D-01
I= 20 X= -1.611522819606D+00 Y= 4.948147097054D+00 Z= -3.802382494144D+00
I= 21 X= -3.483312279659D+00 Y= -4.655360164032D-01 Z= -4.643019361152D+00
I= 22 X= -5.403908307093D+00 Y= 8.282888938527D-01 Z= -5.158730448053D+00
I= 23 X= -1.633234091162D+00 Y= 3.752474718340D-01 Z= -6.223180876863D+00
I= 24 X= -3.729585057718D+00 Y= -2.870235285155D+00 Z= -4.981017048190D+00
I= 25 X= -3.295179670084D+00 Y= -4.730781385249D+00 Z= -5.611010759773D-01
I= 26 X= -3.333869148632D+00 Y= -5.512646245599D+00 Z= -2.744847234595D+00

I= 27 X= -2.026267726096D+00 Y= -5.995678634405D+00 Z= 5.965615124628D-01
I= 28 X= -5.159185853630D+00 Y= -5.308829392590D+00 Z= 4.040278787630D-01
I= 29 X= 2.724858608104D+00 Y= -3.410571420701D+00 Z= -1.949836326777D+00
I= 30 X= 3.230700894778D+00 Y= -3.506631198583D+00 Z= 7.062339557330D-01
I= 31 X= 1.127157048591D+00 Y= -4.423972561419D+00 Z= -2.694096120106D+00
I= 32 X= 4.184704181918D+00 Y= -3.371688943117D+00 Z= -3.178029201529D+00
I= 33 X= 4.971984452983D+00 Y= -2.838774006128D+00 Z= 1.520410631035D+00
I= 34 X= 1.781857184570D+00 Y= -4.566908311443D+00 Z= 1.880010565712D+00
I= 35 X= 9.138841093623D-01 Y= -8.056330300659D-02 Z= -1.749272723586D-01
I= 36 X= 3.886907542654D+00 Y= 2.136565821907D+00 Z= 1.680110477161D+00
I= 37 X= 5.353333848705D+00 Y= 7.238906871276D-01 Z= 2.691466553483D+00
I= 38 X= 2.991613998438D+00 Y= 3.387833005203D+00 Z= 2.818814337203D+00

Forward Direction:

Total Energy: -651.6084430 Hartrees

Potential Energy: -651.7826649 Hartress

Kinetic Energy: 0.1742220 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 6.561410561720D+12 Y= -1.744926842268D+13 Z= -2.333837957233D+13
I= 1 X= -5.431701641234D+12 Y= -1.553661241044D+13 Z= 2.648693445169D+12
I= 2 X= 8.149790137750D+12 Y= -9.582096182000D+12 Z= 6.884964542215D+12
I= 3 X= 9.317048900809D+11 Y= 9.610936221497D+12 Z= -4.578414407899D+11
I= 4 X= 1.896675051557D+12 Y= -5.594896172597D+12 Z= 1.225232965270D+13
I= 5 X= -2.511664072778D+12 Y= 1.248778417374D+13 Z= 5.733706546072D+12
I= 6 X= -6.122609253249D+13 Y= -1.221708535712D+13 Z= 2.876561499674D+12
I= 7 X= 7.522073205053D+13 Y= -2.427504859138D+13 Z= 8.930269480034D+13
I= 8 X= -5.272951947731D+13 Y= 6.755049773006D+13 Z= 1.108282896362D+12
I= 9 X= -2.324633119475D+13 Y= 1.105757990027D+13 Z= -2.002275084054D+13
I= 10 X= 6.609306575876D+13 Y= -2.507926009172D+13 Z= 8.241485983057D+13
I= 11 X= 6.765995815293D+13 Y= -3.139749984867D+13 Z= -4.763389859208D+13
I= 12 X= 7.618214688346D+13 Y= -1.856827736631D+13 Z= 6.227327394657D+13

I= 13 X= -1.654762620550D+13 Y= -7.777537303001D+12 Z= 3.821690391942D+12
I= 14 X= -1.072210642458D+14 Y= 8.681382222598D+13 Z= -8.593598110717D+13
I= 15 X= 8.828212769939D+13 Y= -1.279433504893D+14 Z= 8.346159312337D+13
I= 16 X= -4.678188804479D+13 Y= 3.093926775002D+13 Z= 2.296123079678D+13
I= 17 X= -4.814057819006D+12 Y= 4.997544392707D+12 Z= 3.273119661743D+12
I= 18 X= -8.471195666847D+13 Y= 4.126512737361D+13 Z= 1.877268857670D+13
I= 19 X= -3.657406076161D+13 Y= -3.875694981577D+13 Z= -1.479725092209D+13
I= 20 X= 3.394171776015D+13 Y= 2.149601131524D+13 Z= -1.110842910970D+14
I= 21 X= -5.622318309894D+12 Y= 1.644277109534D+13 Z= 1.216067360143D+13
I= 22 X= -3.015246834656D+13 Y= -4.205168359957D+12 Z= 7.080379218555D+13
I= 23 X= 4.828855158996D+13 Y= -4.485540928733D+13 Z= -3.219493102498D+13
I= 24 X= 1.619827987717D+14 Y= -9.758490351195D+13 Z= -5.600596219833D+11
I= 25 X= -1.108861984657D+13 Y= 6.827728847307D+12 Z= 1.169727858415D+13
I= 26 X= 2.868036765272D+13 Y= -7.424941098257D+13 Z= -7.367514087849D+13
I= 27 X= -1.951210533985D+13 Y= -1.914136227364D+13 Z= -7.545853187661D+13
I= 28 X= 2.424537740144D+13 Y= 2.220531625294D+13 Z= -5.774466581940D+13
I= 29 X= 2.038970450391D+12 Y= 9.546369292159D+12 Z= -1.036785273639D+13
I= 30 X= 8.098268596248D+12 Y= 2.536437464930D+13 Z= 5.959257618068D+12
I= 31 X= 1.203051440233D+13 Y= 1.053247081770D+13 Z= 7.539002662345D+13
I= 32 X= 1.136297396184D+13 Y= -6.609891341577D+13 Z= -6.238610565986D+12
I= 33 X= -1.118878684887D+14 Y= -5.273977908223D+13 Z= -1.448098554259D+14
I= 34 X= -1.537056866313D+13 Y= 1.543071763343D+12 Z= -4.068221104012D+12
I= 35 X= 1.937849760975D+12 Y= -4.532529835588D+11 Z= 2.184791202635D+09
I= 36 X= 2.380013851121D+12 Y= 1.208253728792D+12 Z= 3.005523233167D+12
I= 37 X= -2.246473857072D+13 Y= -5.736139618418D+13 Z= -1.402226485578D+13
I= 38 X= -9.555560259598D+12 Y= 3.551368202852D+12 Z= 6.699943165736D+11

Backward Direction:

Total Energy: -651.6085132 Hartrees

Potential Energy: -651.7826649 Hartress

Kinetic Energy: 0.1741518 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 5.832716501738D+12 Y= -1.766364711719D+13 Z= -2.335439430425D+13
I= 1 X= -5.068465397843D+12 Y= -1.631408069609D+13 Z= 1.355734298689D+12
I= 2 X= 7.677037971364D+12 Y= -8.869688836606D+12 Z= 5.771337836658D+12
I= 3 X= 6.349019421691D+11 Y= 9.676564288907D+12 Z= -2.018169563452D+12
I= 4 X= 4.207250442717D+12 Y= -5.783025001456D+12 Z= 1.077232778810D+13
I= 5 X= -2.353689744776D+12 Y= 1.140820080855D+13 Z= -3.946420614472D+12
I= 6 X= 2.743114998288D+12 Y= 4.664890461110D+13 Z= 3.067697317873D+13
I= 7 X= 8.835288715158D+13 Y= -1.186261639849D+13 Z= 9.050709184507D+13
I= 8 X= -3.494410485678D+13 Y= 8.210417101353D+13 Z= 4.433463198778D+12
I= 9 X= -2.243866743333D+13 Y= 1.140660719408D+13 Z= -2.090154927346D+13
I= 10 X= 6.636377567941D+13 Y= -2.330169819020D+13 Z= 8.035459664663D+13
I= 11 X= 6.747137387753D+13 Y= -3.138464942491D+13 Z= -4.776261858071D+13
I= 12 X= 7.673650889140D+13 Y= -1.842502885574D+13 Z= 6.174301863505D+13
I= 13 X= -1.639213334800D+13 Y= -7.884797684937D+12 Z= 3.436972844421D+12
I= 14 X= -1.070005848074D+14 Y= 8.615394619091D+13 Z= -8.589760163957D+13
I= 15 X= 8.882231700239D+13 Y= -1.284875519614D+14 Z= 8.254564602063D+13
I= 16 X= -4.688683339613D+13 Y= 3.108655080948D+13 Z= 2.306898063956D+13
I= 17 X= -4.552509709619D+12 Y= 4.762104650836D+12 Z= 3.169989415623D+12
I= 18 X= -8.443381026445D+13 Y= 4.112183179638D+13 Z= 1.815832126787D+13
I= 19 X= -3.657464451232D+13 Y= -3.898481187904D+13 Z= -1.453746465791D+13
I= 20 X= 3.425010515694D+13 Y= 2.110642725961D+13 Z= -1.112113847721D+14
I= 21 X= -6.150918530321D+12 Y= 1.645173438458D+13 Z= 1.135492008096D+13
I= 22 X= -3.050441846723D+13 Y= -3.439822163979D+12 Z= 6.889634702450D+13
I= 23 X= 4.862365297141D+13 Y= -4.514911085982D+13 Z= -3.287044007646D+13
I= 24 X= 1.612847148768D+14 Y= -9.760504712537D+13 Z= -1.510859712455D+12
I= 25 X= -1.109234538257D+13 Y= 6.727523625643D+12 Z= 1.147352215255D+13
I= 26 X= 2.827429581661D+13 Y= -7.482525535005D+13 Z= -7.383544817812D+13
I= 27 X= -1.915654841618D+13 Y= -1.881089763397D+13 Z= -7.558897615732D+13
I= 28 X= 2.432946653512D+13 Y= 2.219171822563D+13 Z= -5.733476154410D+13

I= 29 X= 6.531499838195D+11 Y= 1.036460677224D+13 Z= -1.143062827532D+13
I= 30 X= 8.206206658915D+12 Y= 2.559728129002D+13 Z= 5.142121217365D+12
I= 31 X= 1.214039288374D+13 Y= 9.777043460368D+12 Z= 7.488363110014D+13
I= 32 X= 9.600727075377D+12 Y= -6.450366511180D+13 Z= -7.884648605764D+12
I= 33 X= -1.116434581384D+14 Y= -5.284802560796D+13 Z= -1.456424669657D+14
I= 34 X= -1.454362929794D+13 Y= 1.417958583709D+12 Z= -4.603406436873D+12
I= 35 X= 1.604301803279D+12 Y= -5.889956435755D+11 Z= 1.299776586898D+12
I= 36 X= -1.658103871133D+12 Y= -3.616933053642D+12 Z= 5.836442741322D+11
I= 37 X= -1.777195216186D+13 Y= -5.433862949022D+13 Z= -1.998339419006D+13
I= 38 X= -6.713651240400D+12 Y= 3.359570208670D+12 Z= -3.179716317246D+12

Seed: 37615231480

CM Start Point Coordinates: bohr

I= 0 X= -2.475578514713D+00 Y= 2.310293157245D+00 Z= -5.939935574612D-01
I= 1 X= -2.882711760932D+00 Y= -1.603445782798D-01 Z= -1.962687224962D+00
I= 2 X= -2.377188411003D+00 Y= 1.856823306529D+00 Z= 1.957731848184D+00
I= 3 X= -2.776609724465D+00 Y= -2.025967544954D+00 Z= -1.544268423254D-01
I= 4 X= -2.341498100921D+00 Y= -8.078732497081D-01 Z= 2.315560684592D+00
I= 5 X= 4.209914629231D+00 Y= 2.523509008050D+00 Z= -1.463958707195D+00
I= 6 X= 2.487802941999D+00 Y= 4.904621281357D-01 Z= -2.721007443628D+00
I= 7 X= 5.631988551800D+00 Y= 1.287999531175D+00 Z= -1.779973720889D+00
I= 8 X= 3.692160878613D+00 Y= 4.066703825665D+00 Z= -2.690779874810D+00
I= 9 X= -2.149938691314D+00 Y= -2.355259781157D+00 Z= 4.696784777365D+00
I= 10 X= -4.538152925949D+00 Y= -3.192783275164D+00 Z= 4.851373582892D+00
I= 11 X= -1.136983817598D+00 Y= -4.240594479245D+00 Z= 4.327796145864D+00
I= 12 X= -1.654703021212D+00 Y= -1.007827973831D+00 Z= 6.269579665619D+00
I= 13 X= -2.279306874170D+00 Y= 3.545383955070D+00 Z= 4.182389843492D+00
I= 14 X= -4.188151352407D+00 Y= 4.097015721094D+00 Z= 5.043465117974D+00
I= 15 X= -9.996341595395D-01 Y= 2.717105373929D+00 Z= 5.682005355551D+00
I= 16 X= -1.630619409837D+00 Y= 5.693858382658D+00 Z= 3.295529095534D+00

I= 17 X= -2.770809764422D+00 Y= 4.958813404208D+00 Z= -1.686874492373D+00
I= 18 X= -4.457964557920D+00 Y= 6.242475090328D+00 Z= -1.310587807703D+00
I= 19 X= -1.380330904705D+00 Y= 6.235794750182D+00 Z= -6.054523024594D-01
I= 20 X= -2.096030862387D+00 Y= 4.933385406780D+00 Z= -3.826583886872D+00
I= 21 X= -3.140787079777D+00 Y= -2.110322861316D-01 Z= -4.657137976449D+00
I= 22 X= -5.276935919379D+00 Y= -4.510489361831D-01 Z= -5.195168345231D+00
I= 23 X= -2.527051499408D+00 Y= 1.349893329144D+00 Z= -5.495214952503D+00
I= 24 X= -2.318959983451D+00 Y= -1.978705937732D+00 Z= -5.464104318706D+00
I= 25 X= -3.366696049861D+00 Y= -4.741582360785D+00 Z= -7.278737017185D-01
I= 26 X= -3.234365641692D+00 Y= -5.285256647934D+00 Z= -2.785374677559D+00
I= 27 X= -2.100976046129D+00 Y= -5.809872109133D+00 Z= 3.782604282938D-01
I= 28 X= -5.510043007361D+00 Y= -4.951830160605D+00 Z= -3.611386543876D-01
I= 29 X= 2.647525771501D+00 Y= -3.888136929222D+00 Z= -1.310143949928D+00
I= 30 X= 3.045103552044D+00 Y= -3.205066635879D+00 Z= 1.242289941912D+00
I= 31 X= 8.915790364712D-01 Y= -4.815671544190D+00 Z= -2.258061043060D+00
I= 32 X= 3.938983514681D+00 Y= -3.499597336531D+00 Z= -2.387800296391D+00
I= 33 X= 4.948308138304D+00 Y= -2.447600967440D+00 Z= 1.803892945088D+00
I= 34 X= 2.037228180563D+00 Y= -4.136826010168D+00 Z= 2.917552534915D+00
I= 35 X= 8.533543412366D-01 Y= -2.958605116148D-02 Z= -2.110043416490D-01
I= 36 X= 3.848105970442D+00 Y= 2.563912688433D+00 Z= 1.362635938403D+00
I= 37 X= 5.339862770901D+00 Y= 1.737531826106D+00 Z= 2.412649249379D+00
I= 38 X= 3.227564024455D+00 Y= 4.302284985403D+00 Z= 2.193723130744D+00

Forward Direction:

Total Energy: -651.6233961 Hartrees

Potential Energy: -651.7892062 Hartress

Kinetic Energy: 0.1658101 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.949284214397D+12 Y= -2.295768627627D+13 Z= 4.036327150297D+12

I= 1 X= 2.053293354555D+13 Y= 3.079384017511D+12 Z= -7.099879300608D+12

I= 2 X= -5.479043605225D+12 Y= -9.417454778183D+12 Z= -1.938092391083D+12

I= 3 X= -7.474158263885D+12 Y= -2.106505728808D+13 Z= 1.168059127826D+13
I= 4 X= 1.508884461907D+13 Y= -7.033220076134D+12 Z= -1.719621196467D+13
I= 5 X= -1.001319446731D+13 Y= 2.638476574780D+12 Z= 2.314713850619D+13
I= 6 X= 3.409195142997D+13 Y= -5.585424514258D+13 Z= -6.891225185709D+13
I= 7 X= 8.161648520374D+12 Y= 1.180605954769D+13 Z= -5.954457046804D+13
I= 8 X= 8.932721316227D+13 Y= -1.130386984674D+14 Z= 7.119976300068D+13
I= 9 X= -2.244222769659D+13 Y= 1.613936588326D+11 Z= 6.998242657076D+12
I= 10 X= 1.177919300443D+14 Y= 1.750703953937D+13 Z= 2.078131204299D+13
I= 11 X= 3.537414600732D+13 Y= -1.168627381631D+14 Z= 1.032467798175D+12
I= 12 X= -3.875250636234D+13 Y= -2.433001400097D+13 Z= -4.578778837838D+13
I= 13 X= -2.954236255039D+12 Y= 1.219658805054D+13 Z= 1.020176889996D+13
I= 14 X= 8.601464981424D+13 Y= 2.721508777842D+13 Z= 3.853038696425D+13
I= 15 X= 2.555769937527D+13 Y= 2.733849059881D+13 Z= 4.279759564285D+13
I= 16 X= 2.148022345466D+13 Y= 3.198552515461D+13 Z= 7.240079154027D+12
I= 17 X= 1.558808410304D+13 Y= 3.932645700527D+12 Z= 1.672249016232D+13
I= 18 X= -3.538989835054D+13 Y= 6.360212104952D+13 Z= 5.319641256748D+13
I= 19 X= -6.822024124409D+13 Y= -3.468439002368D+13 Z= -7.358290661478D+13
I= 20 X= 8.959352177336D+12 Y= -3.035775238537D+13 Z= -3.760304311995D+13
I= 21 X= -1.995347163076D+13 Y= -3.143064149254D+12 Z= -1.034091418637D+13
I= 22 X= 1.067114917715D+14 Y= -8.802340503636D+13 Z= 7.964199315284D+13
I= 23 X= 3.508741779568D+13 Y= 1.476765386924D+13 Z= 5.331337253720D+13
I= 24 X= -2.418217081674D+13 Y= 1.180161323048D+13 Z= 9.008711285093D+13
I= 25 X= -3.513777579511D+12 Y= 3.510908202619D+13 Z= 3.909904422825D+12
I= 26 X= 2.880095619515D+13 Y= -3.514055816895D+13 Z= -2.130590382354D+13
I= 27 X= 9.796723574539D+13 Y= -5.961407906611D+13 Z= -7.447800139354D+13
I= 28 X= -1.074590870456D+14 Y= 3.462736443117D+13 Z= -1.972277582783D+13
I= 29 X= -5.575032797841D+12 Y= -8.024707474729D+11 Z= 2.708151190174D+13
I= 30 X= -2.227804794155D+12 Y= 1.075703436620D+13 Z= -1.425673310353D+13
I= 31 X= 5.074018567536D+12 Y= -9.289627128474D+12 Z= -2.616309773339D+13
I= 32 X= 1.391428418766D+13 Y= 3.158061440929D+13 Z= -4.893911029979D+13

I= 33 X= -4.847643068060D+13 Y= -2.816778520188D+12 Z= -1.028777993593D+13
I= 34 X= 2.922690483701D+12 Y= -6.992564459152D+13 Z= 3.804627307495D+13
I= 35 X= 2.687964617995D+11 Y= 8.884926445541D+11 Z= -2.157961392581D+12
I= 36 X= -6.317495824244D+12 Y= 2.138193608794D+13 Z= -1.307295971292D+13
I= 37 X= 4.662140782822D+13 Y= 1.640959007309D+13 Z= -4.800967361469D+13
I= 38 X= -8.355870070508D+12 Y= -1.145554369477D+14 Z= -2.311879035411D+13

Backward Direction:

Total Energy: -651.6233857 Hartrees

Potential Energy: -651.7892062 Hartress

Kinetic Energy: 0.1658206 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.657531128503D+12 Y= -2.316604950827D+13 Z= 4.020761790640D+12
I= 1 X= 2.088597738498D+13 Y= 2.323731481255D+12 Z= -8.356558032864D+12
I= 2 X= -5.938530353549D+12 Y= -8.725037571524D+12 Z= -3.020470748828D+12
I= 3 X= -7.762632925085D+12 Y= -2.100127074356D+13 Z= 1.016404593713D+13
I= 4 X= 1.733458530198D+13 Y= -7.216070012888D+12 Z= -1.863468500066D+13
I= 5 X= -9.859652896856D+12 Y= 1.589186299837D+12 Z= 1.373863555993D+13
I= 6 X= 9.626618400016D+13 Y= 1.359966072364D+12 Z= -4.189191929404D+13
I= 7 X= 2.092531555448D+13 Y= 2.387019908685D+13 Z= -5.837396879006D+13
I= 8 X= 1.066135693306D+14 Y= -9.889340102972D+13 Z= 7.443163879272D+13
I= 9 X= -2.165722696797D+13 Y= 5.006272524709D+11 Z= 6.144103293862D+12
I= 10 X= 1.180550438475D+14 Y= 1.923472308077D+13 Z= 1.877885980446D+13
I= 11 X= 3.519085340591D+13 Y= -1.168502483186D+14 Z= 9.073596933950D+11
I= 12 X= -3.821369974915D+13 Y= -2.419078503822D+13 Z= -4.630316472568D+13
I= 13 X= -2.803106529010D+12 Y= 1.209233739257D+13 Z= 9.827846521867D+12
I= 14 X= 8.622894259717D+13 Y= 2.657372784489D+13 Z= 3.856768950717D+13
I= 15 X= 2.608273097642D+13 Y= 2.680955941156D+13 Z= 4.190734999857D+13
I= 16 X= 2.137822285436D+13 Y= 3.212867545706D+13 Z= 7.344805538690D+12
I= 17 X= 1.584229318255D+13 Y= 3.703812395563D+12 Z= 1.662225375074D+13
I= 18 X= -3.511955672584D+13 Y= 6.346284634484D+13 Z= 5.259928438756D+13

I= 19 X= -6.822080861495D+13 Y= -3.490585827876D+13 Z= -7.333040994024D+13
I= 20 X= 9.259086244317D+12 Y= -3.073640471393D+13 Z= -3.772657054464D+13
I= 21 X= -2.046723934039D+13 Y= -3.134352373429D+12 Z= -1.112405827455D+13
I= 22 X= 1.063694173624D+14 Y= -8.727953445545D+13 Z= 7.778807087500D+13
I= 23 X= 3.541311622585D+13 Y= 1.448219355771D+13 Z= 5.265681825931D+13
I= 24 X= -2.486066648408D+13 Y= 1.178203484540D+13 Z= 8.916299219825D+13
I= 25 X= -3.517398576928D+12 Y= 3.501168856133D+13 Z= 3.692426592123D+12
I= 26 X= 2.840627873029D+13 Y= -3.570024435183D+13 Z= -2.146171289984D+13
I= 27 X= 9.831281574826D+13 Y= -5.929288725616D+13 Z= -7.460478540957D+13
I= 28 X= -1.073773574545D+14 Y= 3.461414796227D+13 Z= -1.932437345852D+13
I= 29 X= -6.921967162598D+12 Y= -7.192996459046D+09 Z= 2.604855782654D+13
I= 30 X= -2.122895472066D+12 Y= 1.098340565075D+13 Z= -1.505094067022D+13
I= 31 X= 5.180813862178D+12 Y= -1.002385720390D+13 Z= -2.665528380921D+13
I= 32 X= 1.220148592213D+13 Y= 3.313110007416D+13 Z= -5.053896053908D+13
I= 33 X= -4.823887847968D+13 Y= -2.921987651590D+12 Z= -1.109702840827D+13
I= 34 X= 3.726425941594D+12 Y= -7.004724710054D+13 Z= 3.752610503109D+13
I= 35 X= -5.539214547307D+10 Y= 7.565589216562D+11 Z= -8.967800019594D+11
I= 36 X= -1.024230402711D+13 Y= 1.669214396916D+13 Z= -1.542688078874D+13
I= 37 X= 5.118251472527D+13 Y= 1.934753798354D+13 Z= -5.380353375550D+13
I= 38 X= -5.593704970290D+12 Y= -1.147418530918D+14 Z= -2.686047816942D+13

Seed: 38791410059

CM Start Point Coordinates: bohr

I= 0 X= -2.668628714193D+00 Y= 2.195672908320D+00 Z= -7.282801793175D-01
I= 1 X= -3.167539448210D+00 Y= -4.134608796824D-02 Z= -1.881519155871D+00
I= 2 X= -2.559206711949D+00 Y= 1.849859451700D+00 Z= 1.907869389259D+00
I= 3 X= -2.806658361720D+00 Y= -2.127530448092D+00 Z= -9.808052512859D-03
I= 4 X= -2.325983314644D+00 Y= -8.213071213436D-01 Z= 2.335232022023D+00
I= 5 X= 4.448762578712D+00 Y= 2.235395444768D+00 Z= -8.504273205875D-01
I= 6 X= 2.590259722923D+00 Y= 1.180539202096D+00 Z= -2.552669432496D+00

I= 7 X= 5.781122954968D+00 Y= 1.013744960400D+00 Z= -1.579164934025D+00
I= 8 X= 4.304904999763D+00 Y= 4.147873053757D+00 Z= -1.912442891412D+00
I= 9 X= -2.671990986988D+00 Y= -2.220854364242D+00 Z= 4.739412777729D+00
I= 10 X= -4.858425353706D+00 Y= -2.498289337811D+00 Z= 5.371840174169D+00
I= 11 X= -1.603786697583D+00 Y= -4.222164759195D+00 Z= 4.308519285246D+00
I= 12 X= -1.677680136260D+00 Y= -1.458471911718D+00 Z= 6.217674269069D+00
I= 13 X= -2.204379584537D+00 Y= 3.465510547774D+00 Z= 4.145890671781D+00
I= 14 X= -4.173940483667D+00 Y= 4.820443992472D+00 Z= 4.132326190389D+00
I= 15 X= -1.469056151018D+00 Y= 2.408716783332D+00 Z= 6.035541960026D+00
I= 16 X= -1.406265553770D-01 Y= 4.928709077516D+00 Z= 3.525231673786D+00
I= 17 X= -2.709848022695D+00 Y= 4.745998158032D+00 Z= -1.967435688863D+00
I= 18 X= -4.733612209080D+00 Y= 5.464458691761D+00 Z= -2.373183611379D+00
I= 19 X= -1.778188526178D+00 Y= 6.287665952693D+00 Z= -6.309722194567D-01
I= 20 X= -1.467684460510D+00 Y= 4.493489887989D+00 Z= -3.851503370174D+00
I= 21 X= -3.694030422965D+00 Y= -5.129730551836D-01 Z= -4.695731349971D+00
I= 22 X= -5.764909993037D+00 Y= -6.257312220541D-01 Z= -5.271081313752D+00
I= 23 X= -2.650084249014D+00 Y= 9.363812372681D-01 Z= -5.791706362617D+00
I= 24 X= -2.934915536390D+00 Y= -2.151163107046D+00 Z= -5.144959247940D+00
I= 25 X= -3.316678747575D+00 Y= -4.928317235817D+00 Z= -4.035444942326D-01
I= 26 X= -3.366325268031D+00 Y= -4.878520069993D+00 Z= -2.548458630212D+00
I= 27 X= -1.796947473604D+00 Y= -6.064981718287D+00 Z= 5.979314031613D-01
I= 28 X= -4.938767284554D+00 Y= -5.312398944605D+00 Z= 9.033888507608D-01
I= 29 X= 2.600142698160D+00 Y= -3.316258892616D+00 Z= -1.734419039514D+00
I= 30 X= 3.155980322579D+00 Y= -3.141259790099D+00 Z= 8.417102537579D-01
I= 31 X= 8.671585610700D-01 Y= -4.401945070173D+00 Z= -2.265325971787D+00
I= 32 X= 4.216127277396D+00 Y= -3.213430319138D+00 Z= -3.216460090594D+00
I= 33 X= 4.969698870137D+00 Y= -2.723785701749D+00 Z= 1.767106531869D+00
I= 34 X= 2.023879797578D+00 Y= -4.689532500306D+00 Z= 2.068758699306D+00
I= 35 X= 9.196531551391D-01 Y= 4.115916794135D-02 Z= -2.320370140219D-01
I= 36 X= 3.996216338573D+00 Y= 2.137287377507D+00 Z= 1.743029886622D+00

I= 37 X= 4.970254486695D+00 Y= 6.987440447808D-01 Z= 2.967091944386D+00

I= 38 X= 3.338885001088D+00 Y= 3.695848007181D+00 Z= 2.686439577001D+00

Forward Direction:

Total Energy: -651.6049930 Hartrees

Potential Energy: -651.7806958 Hartress

Kinetic Energy: 0.1757029 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 3.369054222997D+12 Y= 1.036762521643D+13 Z= 9.356373009073D+12

I= 1 X= 1.005222016003D+13 Y= -1.107329685090D+13 Z= 1.161466297135D+12

I= 2 X= 1.008504658946D+13 Y= 2.805242850432D+13 Z= -5.562955198935D+12

I= 3 X= -6.450739869472D+10 Y= 1.820814641735D+13 Z= 3.956381395861D+12

I= 4 X= 1.772373816407D+13 Y= -6.536235290630D+12 Z= -1.363220413371D+13

I= 5 X= 2.706304459301D+13 Y= -1.035036029113D+13 Z= 9.868222305722D+11

I= 6 X= -9.150134147649D+13 Y= -1.482229458667D+12 Z= 5.953445727986D+13

I= 7 X= -9.485716752568D+13 Y= 2.253826298345D+13 Z= -4.767392997559D+13

I= 8 X= 5.153215855231D+13 Y= -9.021051236672D+13 Z= -1.436125632421D+13

I= 9 X= 8.932873602226D+12 Y= -2.298436848485D+13 Z= 7.228247973184D+12

I= 10 X= -3.144477222968D+12 Y= 6.360357241755D+13 Z= 2.898826722359D+13

I= 11 X= 4.272094554858D+13 Y= 6.970935752104D+13 Z= 2.807168044012D+13

I= 12 X= -3.580428883377D+13 Y= -3.774775201651D+13 Z= 2.056734929911D+13

I= 13 X= -1.766593328670D+13 Y= 2.264295687199D+12 Z= -1.715053311795D+13

I= 14 X= -8.531763954797D+13 Y= 2.461294814211D+13 Z= -1.041704270129D+12

I= 15 X= 1.098346000213D+14 Y= -8.337965882664D+13 Z= 5.181999483828D+13

I= 16 X= -3.607599042625D+13 Y= -3.497769110993D+12 Z= 3.047488228632D+13

I= 17 X= -4.154935406852D+12 Y= 1.848755901517D+13 Z= 5.388161738990D+11

I= 18 X= -4.853869591502D+13 Y= 5.364394972311D+13 Z= 4.353295945789D+13

I= 19 X= -9.570835870549D+13 Y= -1.121631725102D+14 Z= -5.720102577021D+13

I= 20 X= 2.444792042136D+13 Y= 5.116062448994D+13 Z= -2.124347003429D+13

I= 21 X= -2.304716163107D+12 Y= -2.934672366981D+12 Z= 2.825273353254D+12

I= 22 X= -6.198502887576D+13 Y= -6.416190838687D+13 Z= -5.154861641662D+12

I= 23 X= 1.063388575961D+13 Y= 4.644823006088D+13 Z= -5.165160275888D+13
I= 24 X= -1.283926745810D+13 Y= -9.114981948084D+13 Z= -4.462169282692D+13
I= 25 X= -1.192843744445D+13 Y= -3.687548933591D+13 Z= -2.530852743554D+12
I= 26 X= 2.917172399806D+12 Y= 5.417316858746D+12 Z= 3.457261685530D+12
I= 27 X= 7.497333534292D+13 Y= -7.564679236490D+12 Z= 4.311979215921D+13
I= 28 X= 9.004808456656D+13 Y= 1.501929963325D+14 Z= -3.718862939716D+13
I= 29 X= 2.092543717034D+12 Y= 1.564648140455D+13 Z= -6.831582332335D+12
I= 30 X= 2.430051351533D+13 Y= 6.012519825790D+12 Z= 2.329455589064D+12
I= 31 X= -4.558958270285D+13 Y= -6.461724210598D+13 Z= -2.843391101461D+13
I= 32 X= 4.235500691828D+13 Y= -1.541837417405D+13 Z= 9.905834703622D+13
I= 33 X= -1.932394319212D+13 Y= -1.633873226126D+13 Z= -3.583510996737D+13
I= 34 X= -9.455021623380D+13 Y= -5.347296700498D+13 Z= 8.951849819063D+13
I= 35 X= -2.372566409690D+12 Y= -7.898367029488D+11 Z= 3.947934193212D+11
I= 36 X= -9.737968489619D+12 Y= 1.010289214197D+13 Z= 6.586830782808D+12
I= 37 X= 4.316314185392D+10 Y= 7.315134117855D+13 Z= -9.251944699165D+13
I= 38 X= 4.222471815172D+13 Y= 1.301524762832D+13 Z= -8.944990501184D+12

Backward Direction:

Total Energy: -651.6050436 Hartrees

Potential Energy: -651.7806958 Hartress

Kinetic Energy: 0.1756522 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.892498082804D+12 Y= 1.022742442716D+13 Z= 9.345899590233D+12
I= 1 X= 1.028977179222D+13 Y= -1.158175067972D+13 Z= 3.158883602838D+11
I= 2 X= 9.775873014014D+12 Y= 2.851833335319D+13 Z= -6.291252125231D+12
I= 3 X= -2.586125458483D+11 Y= 1.825106629458D+13 Z= 2.935947733017D+12
I= 4 X= 1.923482347539D+13 Y= -6.659269020005D+12 Z= -1.460010550016D+13
I= 5 X= 2.716635768293D+13 Y= -1.105639333091D+13 Z= -5.343851086073D+12
I= 6 X= -4.966633781983D+13 Y= 3.701533836610D+13 Z= 7.771555360958D+13
I= 7 X= -8.626891424271D+13 Y= 3.065582714098D+13 Z= -4.688627046665D+13
I= 8 X= 6.316358114310D+13 Y= -8.069260525953D+13 Z= -1.218663301054D+13

I= 9 X= 9.461074868985D+12 Y= -2.275610931651D+13 Z= 6.653525586502D+12
I= 10 X= -2.967436565943D+12 Y= 6.476607405511D+13 Z= 2.764088273510D+13
I= 11 X= 4.259761396347D+13 Y= 6.971776152689D+13 Z= 2.798749929623D+13
I= 12 X= -3.544174351491D+13 Y= -3.765406940879D+13 Z= 2.022056944057D+13
I= 13 X= -1.756424304761D+13 Y= 2.194148836774D+12 Z= -1.740213323077D+13
I= 14 X= -8.517344896137D+13 Y= 2.418139805527D+13 Z= -1.016604613246D+12
I= 15 X= 1.101878765748D+14 Y= -8.373555928531D+13 Z= 5.122097772500D+13
I= 16 X= -3.614462329266D+13 Y= -3.401447960060D+12 Z= 3.054534924390D+13
I= 17 X= -3.983886450066D+12 Y= 1.833358458397D+13 Z= 4.713703757717D+11
I= 18 X= -4.835679189627D+13 Y= 5.355023633788D+13 Z= 4.313117147226D+13
I= 19 X= -9.570874047155D+13 Y= -1.123121912424D+14 Z= -5.703112903660D+13
I= 20 X= 2.464960164714D+13 Y= 5.090584174206D+13 Z= -2.132658759115D+13
I= 21 X= -2.650413617583D+12 Y= -2.928810501230D+12 Z= 2.298321361654D+12
I= 22 X= -6.221519953429D+13 Y= -6.366138224751D+13 Z= -6.402305188818D+12
I= 23 X= 1.085303756591D+13 Y= 4.625615316451D+13 Z= -5.209337661865D+13
I= 24 X= -1.329580496292D+13 Y= -9.116299314074D+13 Z= -4.524350332583D+13
I= 25 X= -1.193087389733D+13 Y= -3.694102220437D+13 Z= -2.677186451734D+12
I= 26 X= 2.651606863952D+12 Y= 5.040722371740D+12 Z= 3.352422856838D+12
I= 27 X= 7.520586480077D+13 Y= -7.348559792338D+12 Z= 4.303448334241D+13
I= 28 X= 9.010307772700D+13 Y= 1.501841034057D+14 Z= -3.692055750155D+13
I= 29 X= 1.186235722048D+12 Y= 1.618159774195D+13 Z= -7.526623279378D+12
I= 30 X= 2.437110356054D+13 Y= 6.164837644741D+12 Z= 1.795059343998D+12
I= 31 X= -4.551772364705D+13 Y= -6.511128146514D+13 Z= -2.876508689551D+13
I= 32 X= 4.120252109435D+13 Y= -1.437510318018D+13 Z= 9.798186023824D+13
I= 33 X= -1.916410210060D+13 Y= -1.640952403837D+13 Z= -3.637962674459D+13
I= 34 X= -9.400940898338D+13 Y= -5.355478934776D+13 Z= 8.916849416031D+13
I= 35 X= -2.590702299514D+12 Y= -8.786105821496D+11 Z= 1.243401047850D+12
I= 36 X= -1.237884331269D+13 Y= 6.947284710344D+12 Z= 5.002954429603D+12
I= 37 X= 3.112182508949D+12 Y= 7.512819005136D+13 Z= -9.641794561643D+13
I= 38 X= 4.408328853300D+13 Y= 1.288981431400D+13 Z= -1.146264961546D+13

Seed: 40191278813

CM Start Point Coordinates: bohr

I= 0 X= -2.711520250140D+00 Y= 2.245114963823D+00 Z= -6.368781280563D-01
I= 1 X= -3.236984678812D+00 Y= -6.979260138037D-02 Z= -1.958042760253D+00
I= 2 X= -2.190915377972D+00 Y= 1.749627676694D+00 Z= 1.909631321551D+00
I= 3 X= -2.858739407651D+00 Y= -1.960117804936D+00 Z= -6.110746859026D-02
I= 4 X= -2.282688286513D+00 Y= -7.909004303381D-01 Z= 2.499764795590D+00
I= 5 X= 4.378265017649D+00 Y= 2.160398902841D+00 Z= -1.133943600516D+00
I= 6 X= 2.556352934331D+00 Y= 7.388828031037D-01 Z= -2.996407891348D+00
I= 7 X= 6.057649990611D+00 Y= 1.238072998095D+00 Z= -1.222017248326D+00
I= 8 X= 4.123124081880D+00 Y= 4.092791509914D+00 Z= -2.078145213382D+00
I= 9 X= -2.599124128512D+00 Y= -2.460969728468D+00 Z= 4.707825936096D+00
I= 10 X= -4.552081424306D+00 Y= -1.903994435368D+00 Z= 5.573985546778D+00
I= 11 X= -2.458132737140D+00 Y= -4.360717365052D+00 Z= 4.267530815487D+00
I= 12 X= -1.239312850206D+00 Y= -1.754333266373D+00 Z= 6.147047884346D+00
I= 13 X= -2.342810068579D+00 Y= 3.740991905222D+00 Z= 3.842651507478D+00
I= 14 X= -4.401281997920D+00 Y= 4.248683933356D+00 Z= 4.515049039535D+00
I= 15 X= -1.024203938103D+00 Y= 3.514116049212D+00 Z= 5.683040198870D+00
I= 16 X= -1.971070459841D+00 Y= 5.545769673680D+00 Z= 2.898707439315D+00
I= 17 X= -2.885388187360D+00 Y= 4.991053909268D+00 Z= -1.652636055920D+00
I= 18 X= -4.974942930748D+00 Y= 5.955873518341D+00 Z= -1.351329321565D+00
I= 19 X= -1.404987018728D+00 Y= 6.232517243657D+00 Z= -7.640243548181D-01
I= 20 X= -2.448317522972D+00 Y= 5.051614132568D+00 Z= -3.580143654183D+00
I= 21 X= -3.531321813543D+00 Y= -4.891870658230D-01 Z= -4.573426084185D+00
I= 22 X= -5.739628658136D+00 Y= -6.978583578730D-01 Z= -5.199449544533D+00
I= 23 X= -2.806644350805D+00 Y= 1.242732808426D+00 Z= -5.606869299393D+00
I= 24 X= -2.389276813913D+00 Y= -2.040117531299D+00 Z= -5.559691555715D+00
I= 25 X= -3.541309489768D+00 Y= -4.642893413650D+00 Z= -6.278243122224D-01
I= 26 X= -3.251719473360D+00 Y= -4.908490747257D+00 Z= -2.520097570740D+00

I= 27 X= -2.135771046715D+00 Y= -6.165956467219D+00 Z= 4.001077133489D-02
I= 28 X= -5.590506727080D+00 Y= -4.728045025001D+00 Z= 7.578777577497D-02
I= 29 X= 2.833632942490D+00 Y= -3.530171996848D+00 Z= -1.604318393679D+00
I= 30 X= 3.273526673282D+00 Y= -3.304614759201D+00 Z= 1.124231200575D+00
I= 31 X= 1.702764703686D+00 Y= -4.982066914623D+00 Z= -2.634030556110D+00
I= 32 X= 4.068791132176D+00 Y= -2.706767816694D+00 Z= -3.032719763469D+00
I= 33 X= 5.347213770611D+00 Y= -2.680966613037D+00 Z= 1.631209509397D+00
I= 34 X= 2.078120904472D+00 Y= -4.556643539169D+00 Z= 2.146330033311D+00
I= 35 X= 9.433724758123D-01 Y= -1.017672109386D-02 Z= -2.194356507360D-01
I= 36 X= 3.582465068889D+00 Y= 2.363539392479D+00 Z= 1.579278931825D+00
I= 37 X= 4.975664923146D+00 Y= 1.499581604388D+00 Z= 2.652043180426D+00
I= 38 X= 2.895334637519D+00 Y= 4.049054811516D+00 Z= 2.264164755272D+00

Forward Direction:

Total Energy: -651.6173018 Hartrees

Potential Energy: -651.8266478 Hartress

Kinetic Energy: 0.2093461 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.667818201702D+12 Y= 3.068020392065D+13 Z= -3.714864321720D+12
I= 1 X= -8.973163389742D+12 Y= 9.950315524153D+11 Z= -2.587682913210D+12
I= 2 X= 1.037732645091D+13 Y= -1.364662565677D+13 Z= 1.219934768280D+13
I= 3 X= -9.563046204783D+12 Y= -1.410535746114D+13 Z= 1.010350040802D+13
I= 4 X= -1.687038396241D+13 Y= 1.861249371735D+13 Z= 3.563074316330D+13
I= 5 X= 1.158256784132D+13 Y= -3.790817732144D+12 Z= -2.508102312445D+12
I= 6 X= -1.724996388840D+13 Y= 4.987026737873D+13 Z= -8.136293693211D+13
I= 7 X= -2.974680409128D+13 Y= -3.666391286075D+12 Z= 6.069920892492D+13
I= 8 X= -1.428418357068D+13 Y= -8.613861672149D+13 Z= 5.226399923299D+13
I= 9 X= -8.295088330016D+12 Y= -1.048825468087D+13 Z= -1.702631613381D+13
I= 10 X= 1.907098846766D+13 Y= 6.126488860877D+13 Z= -3.076356183528D+13
I= 11 X= 8.273636217440D+12 Y= -1.039046062286D+14 Z= -4.040579878218D+13
I= 12 X= 2.043498641592D+14 Y= 9.061654749322D+13 Z= 1.343752603234D+14

I= 13 X= 1.589199976237D+13 Y= -1.169594498208D+12 Z= 3.313446621819D+12
I= 14 X= -7.599993951378D+11 Y= -3.625772345065D+13 Z= -6.744786881935D+13
I= 15 X= -8.586314785224D+13 Y= -6.704374486266D+11 Z= -5.352827952761D+13
I= 16 X= -3.709697117774D+13 Y= 3.377964783200D+13 Z= -6.714354920223D+13
I= 17 X= -1.691983509006D+13 Y= -1.170183191288D+13 Z= 5.611273686142D+12
I= 18 X= -3.697549739782D+13 Y= 1.101912227815D+14 Z= 8.989527719310D+13
I= 19 X= -2.168651502051D+13 Y= -4.045003279808D+13 Z= -8.874971828163D+09
I= 20 X= 8.334978197589D+13 Y= -3.659922038061D+13 Z= -8.369425410525D+13
I= 21 X= -1.813915313532D+13 Y= -1.219081055409D+13 Z= -3.411536899898D+12
I= 22 X= 7.396242974689D+13 Y= -7.365683870403D+10 Z= 4.371612141797D+13
I= 23 X= 3.865285473965D+13 Y= 6.602743057180D+13 Z= -9.726128250457D+13
I= 24 X= 8.457639050115D+12 Y= -1.730453608696D+13 Z= 1.171593559436D+14
I= 25 X= 1.021623961923D+13 Y= 1.566566249002D+13 Z= 3.722181473368D+12
I= 26 X= -9.803689951998D+12 Y= -5.230447589231D+13 Z= -9.404833793420D+13
I= 27 X= 2.094990896292D+13 Y= -3.393917130292D+13 Z= -3.967865039305D+13
I= 28 X= -2.444027523834D+13 Y= 2.713558091039D+13 Z= 7.245963966966D+12
I= 29 X= -6.820714177080D+12 Y= -2.589935183186D+12 Z= -8.179929800841D+12
I= 30 X= 1.441441406486D+13 Y= -6.197775377449D+11 Z= 1.748022303353D+13
I= 31 X= 9.844795871494D+12 Y= 4.801733470349D+13 Z= 2.748175231951D+13
I= 32 X= -1.090048485655D+12 Y= -1.392027322477D+13 Z= 7.057706162832D+13
I= 33 X= 1.210538648053D+13 Y= -6.364909244096D+13 Z= 5.626347507799D+13
I= 34 X= 6.559731849616D+13 Y= -4.108557522591D+12 Z= -1.204464325967D+14
I= 35 X= 4.363522176906D+11 Y= 8.900156227050D+11 Z= -1.541648459273D+12
I= 36 X= 9.558284959302D+12 Y= -1.477049032923D+13 Z= -1.403179820204D+12
I= 37 X= 5.499810116302D+11 Y= -4.410103601127D+12 Z= -1.727105303953D+14
I= 38 X= -1.090961048732D+14 Y= 6.774686375249D+13 Z= -2.167777612098D+12

Backward Direction:

Total Energy: -651.6173069 Hartrees

Potential Energy: -651.8266478 Hartress

Kinetic Energy: 0.2093410 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -6.982065242645D+12 Y= 3.058775377763D+13 Z= -3.721770625956D+12
I= 1 X= -8.816518892788D+12 Y= 6.597507784947D+11 Z= -3.145267513867D+12
I= 2 X= 1.017345355320D+13 Y= -1.333940220970D+13 Z= 1.171909963787D+13
I= 3 X= -9.691041549992D+12 Y= -1.407705556177D+13 Z= 9.430613771502D+12
I= 4 X= -1.587395553289D+13 Y= 1.853136374789D+13 Z= 3.499249697506D+13
I= 5 X= 1.165069377864D+13 Y= -4.256384694035D+12 Z= -6.682626962782D+12
I= 6 X= 1.033655734487D+13 Y= 7.525604195499D+13 Z= -6.937409610269D+13
I= 7 X= -2.408360316218D+13 Y= 1.686431379935D+12 Z= 6.121860139019D+13
I= 8 X= -6.614278985643D+12 Y= -7.986239051246D+13 Z= 5.369797286289D+13
I= 9 X= -7.946785856870D+12 Y= -1.033773774855D+13 Z= -1.740529521770D+13
I= 10 X= 1.918773126976D+13 Y= 6.203145663705D+13 Z= -3.165204391494D+13
I= 11 X= 8.192309829204D+12 Y= -1.038990645239D+14 Z= -4.046130887701D+13
I= 12 X= 2.045889310388D+14 Y= 9.067832296218D+13 Z= 1.341465893797D+14
I= 13 X= 1.595905556888D+13 Y= -1.215850204162D+12 Z= 3.147538380511D+12
I= 14 X= -6.649183278924D+11 Y= -3.654229293906D+13 Z= -6.743131779042D+13
I= 15 X= -8.563019290289D+13 Y= -9.051226372844D+11 Z= -5.392327886165D+13
I= 16 X= -3.714222853941D+13 Y= 3.384316319080D+13 Z= -6.709708241454D+13
I= 17 X= -1.680704328465D+13 Y= -1.180336456462D+13 Z= 5.566799091428D+12
I= 18 X= -3.685554763547D+13 Y= 1.101294270056D+14 Z= 8.963033319363D+13
I= 19 X= -2.168676677564D+13 Y= -4.054829759603D+13 Z= 1.031570605936D+11
I= 20 X= 8.348277309647D+13 Y= -3.676722727975D+13 Z= -8.374906284997D+13
I= 21 X= -1.836711033424D+13 Y= -1.218694516429D+13 Z= -3.759015592404D+12
I= 22 X= 7.381065235264D+13 Y= 2.563963299257D+11 Z= 4.289354164203D+13
I= 23 X= 3.879736616789D+13 Y= 6.590077267905D+13 Z= -9.755259367947D+13
I= 24 X= 8.156592537806D+12 Y= -1.731322296071D+13 Z= 1.167493263706D+14
I= 25 X= 1.021463299743D+13 Y= 1.562244929874D+13 Z= 3.625687211596D+12
I= 26 X= -9.978807162309D+12 Y= -5.255280698290D+13 Z= -9.411746995297D+13
I= 27 X= 2.110324178090D+13 Y= -3.379665945185D+13 Z= -3.973490408448D+13
I= 28 X= -2.440401205820D+13 Y= 2.712971679877D+13 Z= 7.422733915502D+12

I= 29 X= -7.418344931184D+12 Y= -2.237072821364D+12 Z= -8.638248438759D+12
I= 30 X= 1.446096201872D+13 Y= -5.193372761415D+11 Z= 1.712783550757D+13
I= 31 X= 9.892180622652D+12 Y= 4.769155901229D+13 Z= 2.726337082680D+13
I= 32 X= -1.850011962839D+12 Y= -1.323232736773D+13 Z= 6.986721285764D+13
I= 33 X= 1.221078768277D+13 Y= -6.369577342048D+13 Z= 5.590441394584D+13
I= 34 X= 6.595393351799D+13 Y= -4.162512194501D+12 Z= -1.206772296034D+14
I= 35 X= 2.925107016854D+11 Y= 8.314770241432D+11 Z= -9.820660438289D+11
I= 36 X= 7.816859289315D+12 Y= -1.685133708091D+13 Z= -2.447607570281D+12
I= 37 X= 2.573730517800D+12 Y= -3.106544891394D+12 Z= -1.752812488350D+14
I= 38 X= -1.078705404656D+14 Y= 6.766415146649D+13 Z= -3.827953322024D+12

Seed: 40972791204

CM Start Point Coordinates: bohr

I= 0 X= -2.481937098610D+00 Y= 2.431836099870D+00 Z= -4.694319015911D-01
I= 1 X= -3.010744195235D+00 Y= 4.636583608284D-02 Z= -1.962043391604D+00
I= 2 X= -2.326488733288D+00 Y= 1.687325826650D+00 Z= 2.102770755116D+00
I= 3 X= -2.865965079697D+00 Y= -2.165252243342D+00 Z= -2.409477634540D-01
I= 4 X= -2.529463068331D+00 Y= -1.054086089797D+00 Z= 2.272518208295D+00
I= 5 X= 4.192809625048D+00 Y= 2.174076935523D+00 Z= -1.519527206006D+00
I= 6 X= 2.273186141769D+00 Y= 1.137139981421D+00 Z= -3.125606941859D+00
I= 7 X= 5.813105551060D+00 Y= 8.969651667289D-01 Z= -1.927478311928D+00
I= 8 X= 4.048291644825D+00 Y= 3.540071942540D+00 Z= -2.747657329011D+00
I= 9 X= -2.642413437675D+00 Y= -2.578739131978D+00 Z= 4.773399045819D+00
I= 10 X= -4.279689515727D+00 Y= -2.192721938579D+00 Z= 5.568013961619D+00
I= 11 X= -2.457292443696D+00 Y= -4.621960843289D+00 Z= 4.549534478547D+00
I= 12 X= -1.171881050350D+00 Y= -2.112457539309D+00 Z= 6.258713762861D+00
I= 13 X= -1.814352604968D+00 Y= 3.485635741348D+00 Z= 4.098616361045D+00
I= 14 X= -3.453383216712D+00 Y= 4.023359174162D+00 Z= 4.992349786750D+00
I= 15 X= -5.332365082481D-01 Y= 2.585118628646D+00 Z= 5.647709020767D+00
I= 16 X= -7.664806443941D-01 Y= 5.374580262572D+00 Z= 3.798204099707D+00

I= 17 X= -2.521282498826D+00 Y= 5.049127425328D+00 Z= -1.874874778457D+00
I= 18 X= -4.625628644550D+00 Y= 5.465860315720D+00 Z= -2.127261846846D+00
I= 19 X= -1.975655153227D+00 Y= 6.474546103091D+00 Z= -5.777254651330D-01
I= 20 X= -1.288765587411D+00 Y= 4.968915152096D+00 Z= -3.422259942073D+00
I= 21 X= -3.738287301524D+00 Y= -3.783388360861D-01 Z= -4.561179964558D+00
I= 22 X= -5.884521848840D+00 Y= -7.062957123297D-01 Z= -4.814933647578D+00
I= 23 X= -3.401838782696D+00 Y= 1.381557613047D+00 Z= -5.761676250035D+00
I= 24 X= -3.183877443652D+00 Y= -2.079571785203D+00 Z= -5.105455547661D+00
I= 25 X= -3.512062956162D+00 Y= -4.635612668835D+00 Z= -1.075779024049D+00
I= 26 X= -2.817169162377D+00 Y= -4.953550295313D+00 Z= -3.344968126122D+00
I= 27 X= -2.308388059470D+00 Y= -6.410249763816D+00 Z= -4.564956854335D-01
I= 28 X= -5.347651360289D+00 Y= -5.610217807584D+00 Z= -5.498749602605D-01
I= 29 X= 3.093591962002D+00 Y= -3.525013785182D+00 Z= -1.109332786608D+00
I= 30 X= 3.088794757974D+00 Y= -2.839885611362D+00 Z= 1.652204810071D+00
I= 31 X= 1.702984075869D+00 Y= -4.666496448507D+00 Z= -1.691458841568D+00
I= 32 X= 4.671995394631D+00 Y= -2.993499402157D+00 Z= -2.322054027729D+00
I= 33 X= 4.946735512001D+00 Y= -1.712379067561D+00 Z= 2.647061024800D+00
I= 34 X= 2.267739280463D+00 Y= -4.030310352138D+00 Z= 3.091298095080D+00
I= 35 X= 8.828661521045D-01 Y= -2.031134080628D-02 Z= -2.183748004324D-01
I= 36 X= 3.727272767071D+00 Y= 2.651155579673D+00 Z= 1.177896804872D+00
I= 37 X= 5.179700157552D+00 Y= 1.614994158886D+00 Z= 2.469196636280D+00
I= 38 X= 2.397063419687D+00 Y= 4.364853070187D+00 Z= 1.896642684386D+00

Forward Direction:

Total Energy: -651.6094877 Hartrees

Potential Energy: -651.7859967 Hartress

Kinetic Energy: 0.1765090 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.630625295930D+13 Y= -8.907628481417D+12 Z= 7.513443317441D+12

I= 1 X= 2.400856811128D+13 Y= 2.264711198759D+13 Z= 2.475680351692D+13

I= 2 X= 5.553517094042D+12 Y= -6.634471867623D+12 Z= -1.648074630493D+13

I= 3 X= -1.009904903505D+13 Y= 1.220716828765D+13 Z= -8.570756414490D+12
I= 4 X= 8.136568128273D+12 Y= -8.126404524308D+12 Z= -1.685735349077D+13
I= 5 X= -9.997548130422D+12 Y= 5.250670890053D+12 Z= 1.646789653607D+13
I= 6 X= -3.283025065821D+13 Y= -6.783878262682D+12 Z= -1.255664208379D+13
I= 7 X= -6.945561225484D+13 Y= -1.006972221606D+14 Z= 5.280405786725D+12
I= 8 X= -4.294414359443D+13 Y= 2.546475159753D+13 Z= -1.107837125808D+14
I= 9 X= 4.445769878105D+12 Y= 1.261025775395D+11 Z= 1.949478553462D+13
I= 10 X= 1.887161420567D+13 Y= 1.809406138414D+13 Z= -2.408895043642D+13
I= 11 X= 2.364011358648D+13 Y= 1.020525386554D+14 Z= -1.657280214742D+12
I= 12 X= 6.831333575765D+11 Y= -3.707749023312D+13 Z= -3.963755856720D+13
I= 13 X= -1.240721855412D+12 Y= 2.548501157268D+12 Z= 9.510375352649D+12
I= 14 X= -2.729459917429D+13 Y= -3.247304713337D+13 Z= -2.134278178163D+13
I= 15 X= 7.458117391790D+13 Y= -9.907976041283D+13 Z= 1.326008861533D+14
I= 16 X= -5.840588161885D+13 Y= 3.848899476204D+13 Z= 3.199661989254D+13
I= 17 X= 7.398129723167D+12 Y= -5.885518597909D+12 Z= 2.757295107337D+13
I= 18 X= -2.249813869829D+13 Y= -3.707290900374D+12 Z= -5.598541836395D+13
I= 19 X= 3.715566960822D+13 Y= 7.817414916000D+12 Z= -9.476514909946D+13
I= 20 X= 5.092237662052D+13 Y= 1.286264955761D+13 Z= -1.059103581026D+14
I= 21 X= -5.709655748830D+12 Y= 1.338674790774D+13 Z= -3.183785056959D+13
I= 22 X= -1.376812086931D+14 Y= -1.471024782462D+13 Z= -1.069201313193D+14
I= 23 X= 9.920498238019D+12 Y= 6.928935750301D+13 Z= -7.293031876435D+13
I= 24 X= -1.950779865552D+13 Y= 4.741892742407D+13 Z= 3.864181583603D+13
I= 25 X= -1.255316993525D+13 Y= 5.469294239754D+12 Z= -1.050832482117D+13
I= 26 X= 4.535439619832D+12 Y= 1.124196853759D+14 Z= 8.194931454430D+13
I= 27 X= -4.324083321481D+13 Y= -2.074161681712D+13 Z= 1.548433509837D+13
I= 28 X= 6.337737838026D+12 Y= -7.802977702706D+13 Z= -2.665749730159D+13
I= 29 X= 1.199425945348D+13 Y= 3.558275044620D+12 Z= -1.243819117281D+13
I= 30 X= -1.528072098194D+13 Y= -1.403835579454D+13 Z= -1.067809085598D+13
I= 31 X= -9.384051788862D+13 Y= -1.072256588044D+14 Z= -1.425746730713D+13
I= 32 X= -6.865056762009D+13 Y= 1.336058356496D+12 Z= -5.671956910324D+13

I= 33 X= -3.476612537390D+13 Y= 5.451769862521D+12 Z= 8.777505807144D+13
I= 34 X= 5.882779311503D+13 Y= 1.220130510810D+13 Z= 1.390001069257D+13
I= 35 X= -2.618231343805D+11 Y= -8.412673972704D+11 Z= 1.891567817948D+12
I= 36 X= 9.993244466777D+12 Y= -1.231330373868D+13 Z= -2.441942835146D+12
I= 37 X= -1.500910609126D+13 Y= 4.924681964651D+13 Z= 4.103909496487D+12
I= 38 X= 3.838439494997D+13 Y= 4.886210812360D+13 Z= 2.385632020053D+13

Backward Direction:

Total Energy: -651.6093764 Hartrees

Potential Energy: -651.7859967 Hartress

Kinetic Energy: 0.1766203 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.555272750114D+13 Y= -9.129312467838D+12 Z= 7.496882857207D+12
I= 1 X= 2.438418220231D+13 Y= 2.184315024520D+13 Z= 2.341978474860D+13
I= 2 X= 5.064655150728D+12 Y= -5.897788116813D+12 Z= -1.763232159669D+13
I= 3 X= -1.040596601057D+13 Y= 1.227503273417D+13 Z= -1.018425518061D+13
I= 4 X= 1.052588001931D+13 Y= -8.320944138636D+12 Z= -1.838778875408D+13
I= 5 X= -9.834190579614D+12 Y= 4.134299015440D+12 Z= 6.457903769254D+12
I= 6 X= 3.331880853488D+13 Y= 5.408806318312D+13 Z= 1.619111248111D+13
I= 7 X= -5.587595825395D+13 Y= -8.786181676330D+13 Z= 6.525844557954D+12
I= 8 X= -2.455266291138D+13 Y= 4.051436425478D+13 Z= -1.073452215166D+14
I= 9 X= 5.280956056314D+12 Y= 4.870235268375D+11 Z= 1.858604065932D+13
I= 10 X= 1.915154899446D+13 Y= 1.993219650795D+13 Z= -2.621942034431D+13
I= 11 X= 2.344510300530D+13 Y= 1.020658269799D+14 Z= -1.790386538648D+12
I= 12 X= 1.256386124374D+12 Y= -3.692936029923D+13 Z= -4.018588315850D+13
I= 13 X= -1.079930339425D+12 Y= 2.437585708501D+12 Z= 9.112547948421D+12
I= 14 X= -2.706660655952D+13 Y= -3.315540949342D+13 Z= -2.130309446985D+13
I= 15 X= 7.513977102093D+13 Y= -9.964250640696D+13 Z= 1.316537267090D+14
I= 16 X= -5.851440316269D+13 Y= 3.864129672968D+13 Z= 3.210804148714D+13
I= 17 X= 7.668590504232D+12 Y= -6.128981318176D+12 Z= 2.746630650317D+13
I= 18 X= -2.221051400604D+13 Y= -3.855469492024D+12 Z= -5.662072120399D+13

I= 19 X= 3.715506597250D+13 Y= 7.581788091691D+12 Z= -9.449651020400D+13
I= 20 X= 5.124127281731D+13 Y= 1.245978981278D+13 Z= -1.060417826903D+14
I= 21 X= -6.256268858941D+12 Y= 1.339601663201D+13 Z= -3.267106141129D+13
I= 22 X= -1.380451520736D+14 Y= -1.391882127046D+13 Z= -1.088925756807D+14
I= 23 X= 1.026701871446D+13 Y= 6.898564758693D+13 Z= -7.362884685215D+13
I= 24 X= -2.022967085489D+13 Y= 4.739809738430D+13 Z= 3.765861573656D+13
I= 25 X= -1.255702242303D+13 Y= 5.365674366832D+12 Z= -1.073970610695D+13
I= 26 X= 4.115530249303D+12 Y= 1.118242181958D+14 Z= 8.178354452202D+13
I= 27 X= -4.287316012998D+13 Y= -2.039989107173D+13 Z= 1.534944572627D+13
I= 28 X= 6.424692438008D+12 Y= -7.804383842858D+13 Z= -2.623362489356D+13
I= 29 X= 1.056121497036D+13 Y= 4.404395259662D+12 Z= -1.353718246649D+13
I= 30 X= -1.516910475930D+13 Y= -1.379751249269D+13 Z= -1.152307246968D+13
I= 31 X= -9.372689512147D+13 Y= -1.080068285395D+14 Z= -1.478111906158D+13
I= 32 X= -7.047286584792D+13 Y= 2.985667266501D+12 Z= -5.842169848661D+13
I= 33 X= -3.451338635457D+13 Y= 5.339834664112D+12 Z= 8.691407398101D+13
I= 34 X= 5.968291174088D+13 Y= 1.207192849478D+13 Z= 1.334658807210D+13
I= 35 X= -6.067372650567D+11 Y= -9.816357026196D+11 Z= 3.233377101290D+12
I= 36 X= 5.817521514456D+12 Y= -1.730291637174D+13 Z= -4.946351141926D+12
I= 37 X= -1.015640557721D+13 Y= 5.237259188750D+13 Z= -2.060354726140D+12
I= 38 X= 4.132314650855D+13 Y= 4.866377431396D+13 Z= 1.987542460194D+13

Seed: 42986769806

CM Start Point Coordinates: bohr

I= 0 X= -2.193315807889D+00 Y= 2.391670715703D+00 Z= -5.164165917110D-01
I= 1 X= -3.032945502482D+00 Y= 4.420606157951D-02 Z= -2.023979370266D+00
I= 2 X= -2.213052308024D+00 Y= 1.607736351178D+00 Z= 2.112073507543D+00
I= 3 X= -2.965067572566D+00 Y= -1.932600110291D+00 Z= -2.190643615551D-01
I= 4 X= -2.420825156913D+00 Y= -9.034917404355D-01 Z= 2.272870651721D+00
I= 5 X= 3.911067803848D+00 Y= 2.254662699735D+00 Z= -1.971911343425D+00
I= 6 X= 2.139373783641D+00 Y= -1.255005933041D-01 Z= -3.139396738491D+00

I= 7 X= 5.672504378473D+00 Y= 1.267130040930D+00 Z= -2.085860428840D+00
I= 8 X= 3.594622425612D+00 Y= 3.398217666298D+00 Z= -3.617982906885D+00
I= 9 X= -2.778228838891D+00 Y= -2.487843855110D+00 Z= 4.664415339946D+00
I= 10 X= -4.792333220511D+00 Y= -2.533518978974D+00 Z= 5.236807212328D+00
I= 11 X= -2.076919277565D+00 Y= -4.392943445009D+00 Z= 4.254323299010D+00
I= 12 X= -1.539437048797D+00 Y= -1.379293876405D+00 Z= 6.420215073433D+00
I= 13 X= -2.033131706273D+00 Y= 3.276361572461D+00 Z= 4.312884625138D+00
I= 14 X= -3.748489901769D+00 Y= 3.172986148027D+00 Z= 5.933251789055D+00
I= 15 X= 1.054814658179D-02 Y= 2.765603626126D+00 Z= 5.405822141940D+00
I= 16 X= -2.152061900074D+00 Y= 5.316015375752D+00 Z= 3.751982635317D+00
I= 17 X= -2.356692962518D+00 Y= 5.077597038262D+00 Z= -1.621509448113D+00
I= 18 X= -4.375045520066D+00 Y= 5.449538299142D+00 Z= -2.181737962112D+00
I= 19 X= -1.597596176897D+00 Y= 6.506478801053D+00 Z= -3.429552369145D-01
I= 20 X= -1.497535904317D+00 Y= 4.930662352526D+00 Z= -3.675878973511D+00
I= 21 X= -3.340335015173D+00 Y= 2.291105431398D-01 Z= -4.852858444758D+00
I= 22 X= -5.337816197943D+00 Y= 8.724146555241D-01 Z= -5.574816136814D+00
I= 23 X= -2.093904964186D+00 Y= 1.608167531344D+00 Z= -5.779454711321D+00
I= 24 X= -3.144109860474D+00 Y= -1.566268690544D+00 Z= -5.512596069539D+00
I= 25 X= -3.310046209297D+00 Y= -4.615884167289D+00 Z= -9.142839469107D-01
I= 26 X= -1.821224479846D+00 Y= -5.104403096616D+00 Z= -2.705530741964D+00
I= 27 X= -2.395885344234D+00 Y= -5.658319129153D+00 Z= 7.874900445153D-01
I= 28 X= -5.587564424186D+00 Y= -5.155185454373D+00 Z= -1.147692767786D+00
I= 29 X= 3.083870226940D+00 Y= -3.516326817389D+00 Z= -7.955871409682D-01
I= 30 X= 3.675296555580D+00 Y= -2.684229250828D+00 Z= 1.589631633952D+00
I= 31 X= 1.802055794384D+00 Y= -5.145930962240D+00 Z= -1.156089158331D+00
I= 32 X= 3.951196035945D+00 Y= -2.817140350668D+00 Z= -2.480843218171D+00
I= 33 X= 5.496064798434D+00 Y= -1.596706191343D+00 Z= 1.740296392138D+00
I= 34 X= 2.803078802811D+00 Y= -3.715924904127D+00 Z= 2.950964047885D+00
I= 35 X= 8.166503455766D-01 Y= -1.158266909355D-01 Z= -1.676944156400D-01
I= 36 X= 3.592182477698D+00 Y= 2.835514725300D+00 Z= 6.540045663724D-01

I= 37 X= 5.260329263223D+00 Y= 2.446790946049D+00 Z= 2.122276846157D+00

I= 38 X= 2.491240657215D+00 Y= 4.862974689878D+00 Z= 8.724500529155D-01

Forward Direction:

Total Energy: -651.6172332 Hartrees

Potential Energy: -651.7968385 Hartress

Kinetic Energy: 0.1796053 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -3.615778895809D+10 Y= -1.293706074968D+13 Z= -8.736706921786D+12

I= 1 X= -1.544241215029D+13 Y= 5.823464708634D+11 Z= -4.624532907713D+12

I= 2 X= 3.889010502798D+12 Y= 3.813889145568D+12 Z= 3.854951998177D+13

I= 3 X= 1.376990622893D+13 Y= 2.434941803676D+12 Z= 8.270922976570D+12

I= 4 X= -8.505389370449D+12 Y= -1.199494808940D+13 Z= -2.622706785480D+13

I= 5 X= 5.189845961487D+12 Y= 1.596372770891D+10 Z= -8.170492639856D+12

I= 6 X= -1.415861260543D+13 Y= 1.470013524307D+13 Z= -1.012338186789D+14

I= 7 X= -2.687887374872D+13 Y= -7.885287993863D+12 Z= 3.444799943067D+13

I= 8 X= -1.260056249074D+14 Y= 9.216187434693D+13 Z= 3.430331963649D+13

I= 9 X= 1.337162466406D+13 Y= 3.660437918509D+12 Z= 8.380771766982D+12

I= 10 X= -2.751128363732D+13 Y= -1.510268586808D+13 Z= -2.642690798172D+13

I= 11 X= -3.175816669289D+13 Y= 5.895970662431D+13 Z= 1.077026869000D+13

I= 12 X= 4.638837047217D+13 Y= 3.678287408106D+13 Z= -4.735263873047D+13

I= 13 X= -1.809062430059D+13 Y= 1.084714862791D+13 Z= 2.003074692822D+13

I= 14 X= 7.628369871139D+13 Y= -2.601045226090D+13 Z= -8.926981141637D+13

I= 15 X= 5.334941507717D+13 Y= 4.721110408348D+12 Z= -6.165374652843D+13

I= 16 X= 5.152933172373D+12 Y= -6.327515720322D+13 Z= 7.872939223017D+13

I= 17 X= 2.586748154237D+13 Y= 1.348282599385D+13 Z= -1.427008781005D+12

I= 18 X= -3.234895273491D+13 Y= -3.071133408133D+13 Z= -8.620101675512D+13

I= 19 X= -2.942661845440D+13 Y= 2.307908497090D+13 Z= -5.158106587499D+13

I= 20 X= -4.624162010306D+13 Y= -7.959831547635D+13 Z= 1.084181011815D+14

I= 21 X= 2.452862406705D+13 Y= -3.357104585127D+12 Z= 2.172949938398D+13

I= 22 X= -1.090913204648D+14 Y= 4.076565590974D+13 Z= -2.225499545001D+13

I= 23 X= -5.629785100399D+12 Y= 1.016830696111D+14 Z= -4.198761408731D+13
I= 24 X= -6.422284763180D+13 Y= 3.421602391470D+13 Z= 1.396994165572D+12
I= 25 X= 1.471327323581D+13 Y= -3.077242755374D+12 Z= -9.646234237023D+12
I= 26 X= -6.377237352752D+13 Y= 2.616337717757D+13 Z= 1.537719617946D+13
I= 27 X= -9.850168477176D+13 Y= 3.607886276411D+13 Z= -6.592265732745D+13
I= 28 X= -7.806486325467D+13 Y= -5.055825973978D+13 Z= -9.451690961718D+12
I= 29 X= -6.318772100395D+12 Y= -5.059443711419D+12 Z= 1.753302804476D+13
I= 30 X= 2.501974014229D+13 Y= 5.609622917904D+12 Z= -1.793506370861D+13
I= 31 X= -9.489435849560D+12 Y= -2.718934821879D+13 Z= -2.251651121697D+13
I= 32 X= -2.674039712763D+13 Y= -6.585722692636D+11 Z= -1.953394940607D+13
I= 33 X= -6.526118941000D+13 Y= -1.063255500787D+14 Z= 3.169378596157D+13
I= 34 X= 1.979265256921D+13 Y= -2.663493372635D+12 Z= -2.139852386322D+13
I= 35 X= -1.534701815411D+12 Y= -5.661328326276D+11 Z= -2.204986652057D+11
I= 36 X= -6.758160413531D+12 Y= 1.754916075957D+13 Z= -1.493837027003D+13
I= 37 X= 7.524115432632D+13 Y= -1.085456118021D+14 Z= 7.556826984976D+13
I= 38 X= 2.499496149090D+13 Y= -9.922973241569D+13 Z= 4.695255764770D+13

Backward Direction:

Total Energy: -651.6172791 Hartrees

Potential Energy: -651.7968385 Hartress

Kinetic Energy: 0.1795594 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.398101526947D+11 Y= -1.308523313177D+13 Z= -8.747775843392D+12
I= 1 X= -1.519135371206D+13 Y= 4.498276767807D+10 Z= -5.518189057677D+12
I= 2 X= 3.562257811563D+12 Y= 4.306284599974D+12 Z= 3.777981325427D+13
I= 3 X= 1.356476457437D+13 Y= 2.480302035203D+12 Z= 7.192469084344D+12
I= 4 X= -6.908386160819D+12 Y= -1.212497732089D+13 Z= -2.725000254865D+13
I= 5 X= 5.299033272128D+12 Y= -7.302132273841D+11 Z= -1.486111793864D+13
I= 6 X= 3.005506258597D+13 Y= 5.538661332891D+13 Z= -8.201897423070D+13
I= 7 X= -1.780230609049D+13 Y= 6.938278977171D+11 Z= 3.528044400229D+13
I= 8 X= -1.137128581892D+14 Y= 1.022209544576D+14 Z= 3.660158855952D+13

I= 9 X= 1.392985860516D+13 Y= 3.901675538921D+12 Z= 7.773371582694D+12
I= 10 X= -2.732417673359D+13 Y= -1.387408623740D+13 Z= -2.785090260422D+13
I= 11 X= -3.188851072702D+13 Y= 5.896858846529D+13 Z= 1.068130114174D+13
I= 12 X= 4.677152953065D+13 Y= 3.688188332760D+13 Z= -4.771913593175D+13
I= 13 X= -1.798315211601D+13 Y= 1.077301333775D+13 Z= 1.976484123436D+13
I= 14 X= 7.643608775175D+13 Y= -2.646653959312D+13 Z= -8.924328463060D+13
I= 15 X= 5.372277837575D+13 Y= 4.344974012141D+12 Z= -6.228682280097D+13
I= 16 X= 5.080397960104D+12 Y= -6.317335939016D+13 Z= 7.880386582563D+13
I= 17 X= 2.604825606508D+13 Y= 1.332009682138D+13 Z= -1.498289440476D+12
I= 18 X= -3.215670595682D+13 Y= -3.081037587642D+13 Z= -8.662564978445D+13
I= 19 X= -2.942702194944D+13 Y= 2.292159327876D+13 Z= -5.140150907337D+13
I= 20 X= -4.602847158644D+13 Y= -7.986758475906D+13 Z= 1.083302576980D+14
I= 21 X= 2.416327080321D+13 Y= -3.350909419118D+12 Z= 2.117258574146D+13
I= 22 X= -1.093345782640D+14 Y= 4.129464116043D+13 Z= -2.357336664340D+13
I= 23 X= -5.398172680477D+12 Y= 1.014800715381D+14 Z= -4.245450650144D+13
I= 24 X= -6.470534312927D+13 Y= 3.420210122960D+13 Z= 7.398285073772D+11
I= 25 X= 1.471069825488D+13 Y= -3.146501721283D+12 Z= -9.800888244388D+12
I= 26 X= -6.405303869426D+13 Y= 2.576537012150D+13 Z= 1.526639638439D+13
I= 27 X= -9.825593405735D+13 Y= 3.630727041015D+13 Z= -6.601281666506D+13
I= 28 X= -7.800674326745D+13 Y= -5.056765830700D+13 Z= -9.168376923870D+12
I= 29 X= -7.276611324067D+12 Y= -4.493901514669D+12 Z= 1.679846817867D+13
I= 30 X= 2.509434382467D+13 Y= 5.770601283715D+12 Z= -1.849984487201D+13
I= 31 X= -9.413491007111D+12 Y= -2.771147786484D+13 Z= -2.286651722880D+13
I= 32 X= -2.795841145994D+13 Y= 4.440174462025D+11 Z= -2.067164352737D+13
I= 33 X= -6.509226000780D+13 Y= -1.064003669642D+14 Z= 3.111830882768D+13
I= 34 X= 2.036420925874D+13 Y= -2.749968003269D+12 Z= -2.176842856287D+13
I= 35 X= -1.765240563286D+12 Y= -6.599542519921D+11 Z= 6.763594391388D+11
I= 36 X= -9.549191159539D+12 Y= 1.421413052530D+13 Z= -1.661230330595D+13
I= 37 X= 7.848467323932D+13 Y= -1.064563624608D+14 Z= 7.144810881400D+13
I= 38 X= 2.695920722213D+13 Y= -9.936229766678D+13 Z= 4.429174845125D+13

Seed: 4485029639

CM Start Point Coordinates: bohr

I= 0 X= -2.338910441240D+00 Y= 2.341740550506D+00 Z= -6.055713610706D-01
I= 1 X= -2.807228166751D+00 Y= 5.630280910615D-02 Z= -1.992898872778D+00
I= 2 X= -2.304024805118D+00 Y= 1.657607489941D+00 Z= 2.057315705596D+00
I= 3 X= -2.827813265484D+00 Y= -1.974251574106D+00 Z= -1.923536766655D-01
I= 4 X= -2.545646775397D+00 Y= -1.116687658769D+00 Z= 2.276772087413D+00
I= 5 X= 3.911190378418D+00 Y= 2.440623866127D+00 Z= -1.667652296851D+00
I= 6 X= 2.373657703006D+00 Y= 6.415091989756D-01 Z= -3.095481812765D+00
I= 7 X= 6.013525589274D+00 Y= 1.571089459242D+00 Z= -2.254555376693D+00
I= 8 X= 3.227686558512D+00 Y= 3.979821961411D+00 Z= -2.791706205351D+00
I= 9 X= -2.592076553881D+00 Y= -2.552163215044D+00 Z= 4.688291792733D+00
I= 10 X= -4.670547881545D+00 Y= -3.064784276877D+00 Z= 5.315821320703D+00
I= 11 X= -1.393810493079D+00 Y= -4.419762798341D+00 Z= 4.604538979312D+00
I= 12 X= -2.440220599616D+00 Y= -1.329173965534D+00 Z= 6.556386756302D+00
I= 13 X= -1.820939904478D+00 Y= 3.557432447074D+00 Z= 4.226746154227D+00
I= 14 X= -3.425623506464D+00 Y= 3.720304573085D+00 Z= 5.268816116573D+00
I= 15 X= -4.660268615283D-01 Y= 2.742618793111D+00 Z= 5.537737164992D+00
I= 16 X= -1.272721973789D+00 Y= 5.305495047139D+00 Z= 3.925939817284D+00
I= 17 X= -2.304094831076D+00 Y= 4.957746102776D+00 Z= -1.390701177673D+00
I= 18 X= -4.064372384900D+00 Y= 5.647613340496D+00 Z= -1.533328551642D+00
I= 19 X= -1.148820338731D+00 Y= 6.339527056262D+00 Z= -2.668059955899D-01
I= 20 X= -2.169180582440D+00 Y= 5.404545027207D+00 Z= -3.527191784737D+00
I= 21 X= -3.398723789720D+00 Y= 1.474351339931D-01 Z= -4.753242478606D+00
I= 22 X= -5.455908956800D+00 Y= 5.357102825239D-01 Z= -5.211151472848D+00
I= 23 X= -2.465170643311D+00 Y= 1.636112600831D+00 Z= -5.499597339660D+00
I= 24 X= -2.701593644855D+00 Y= -1.661176006780D+00 Z= -5.245973452001D+00
I= 25 X= -3.209421893342D+00 Y= -4.751464096731D+00 Z= -8.404543359000D-01
I= 26 X= -2.317905508547D+00 Y= -5.611521199469D+00 Z= -2.647344424501D+00

I= 27 X= -2.371982444634D+00 Y= -5.883138941922D+00 Z= 8.877286025851D-01
I= 28 X= -5.532212892654D+00 Y= -4.909334883196D+00 Z= -1.023708106463D+00
I= 29 X= 2.683656334659D+00 Y= -3.830847020317D+00 Z= -6.817224652740D-01
I= 30 X= 3.309604396822D+00 Y= -2.990806137021D+00 Z= 1.643287674663D+00
I= 31 X= 1.666568250096D+00 Y= -5.318842304115D+00 Z= -9.841134907731D-01
I= 32 X= 3.956967524785D+00 Y= -3.178635438195D+00 Z= -2.266561800077D+00
I= 33 X= 5.182175569509D+00 Y= -1.846195976932D+00 Z= 2.205863279537D+00
I= 34 X= 2.505493712591D+00 Y= -3.703104060919D+00 Z= 3.444926158923D+00
I= 35 X= 8.552884575232D-01 Y= -8.163794678533D-02 Z= -2.511452760899D-01
I= 36 X= 3.303977824784D+00 Y= 3.030608346271D+00 Z= 8.622042149595D-01
I= 37 X= 4.969886427631D+00 Y= 2.516225621400D+00 Z= 2.233856268643D+00
I= 38 X= 2.322003816742D+00 Y= 4.927269829046D+00 Z= 1.229417859329D+00

Forward Direction:

Total Energy: -651.6135610 Hartrees

Potential Energy: -651.7902729 Hartress

Kinetic Energy: 0.1767119 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -2.136546125974D+11 Y= -8.666974054238D+12 Z= 5.180274503278D+12
I= 1 X= 4.901423011518D+12 Y= 2.404194898089D+13 Z= 4.139578471266D+13
I= 2 X= 7.015228924277D+12 Y= -6.903373312614D+12 Z= -4.392195954653D+12
I= 3 X= 2.307527630581D+13 Y= 1.459433313730D+13 Z= -5.061970985496D+12
I= 4 X= -8.500351181015D+12 Y= -2.490222208141D+13 Z= 4.137127397005D+12
I= 5 X= -1.339231335367D+13 Y= 5.965935045459D+12 Z= -2.719549814446D+12
I= 6 X= 5.670621314960D+13 Y= -9.259825452883D+13 Z= -7.505963797080D+13
I= 7 X= -4.197708996446D+13 Y= 3.594559333252D+13 Z= 5.257498123678D+12
I= 8 X= 4.639932758788D+13 Y= -7.684150693360D+13 Z= -2.313282543965D+13
I= 9 X= 1.298896299386D+12 Y= -4.515447446289D+12 Z= -1.669070456345D+13
I= 10 X= 9.095326520944D+13 Y= -6.283445753933D+12 Z= -4.529715140012D+13
I= 11 X= 1.439461267378D+13 Y= 7.356153768364D+13 Z= 4.743799983352D+13
I= 12 X= 3.087105105314D+12 Y= 8.300306522976D+13 Z= 8.852495363331D+13

I= 13 X= -3.066178643590D+12 Y= -4.117112347228D+12 Z= 3.077805358750D+11
I= 14 X= -2.472339117166D+13 Y= -3.027516953441D+13 Z= 7.216755697032D+12
I= 15 X= -6.223730870990D+13 Y= 3.884710303511D+11 Z= -1.028986147800D+14
I= 16 X= -6.861579605470D+13 Y= -3.555227084276D+13 Z= -3.175519258414D+13
I= 17 X= -6.286684630193D+12 Y= -5.748737854336D+11 Z= 4.792870419865D+12
I= 18 X= -8.616960014764D+13 Y= 6.324109131999D+13 Z= -6.534449598685D+13
I= 19 X= -3.032136205120D+13 Y= -6.895004954601D+13 Z= -8.272168049659D+12
I= 20 X= 1.818984977393D+13 Y= 2.266617468636D+13 Z= -1.026827614803D+14
I= 21 X= -6.948917799156D+12 Y= -6.927849498148D+12 Z= -2.335854722892D+12
I= 22 X= 1.126344577196D+14 Y= -9.147712038088D+12 Z= 2.476939393723D+13
I= 23 X= 7.725937528873D+13 Y= -6.230159168781D+11 Z= -9.118777334392D+12
I= 24 X= -2.201038475472D+13 Y= 1.140966812709D+14 Z= -6.020190900917D+13
I= 25 X= 7.297090722039D+12 Y= 1.739106928697D+13 Z= 4.855856970255D+12
I= 26 X= 1.810318143531D+13 Y= 2.318894934681D+11 Z= 3.823236730105D+13
I= 27 X= -3.320465389779D+13 Y= -5.020857984607D+12 Z= -4.590111066154D+13
I= 28 X= -1.087611390217D+14 Y= -8.060958030519D+13 Z= 1.100186082504D+13
I= 29 X= -6.792855865790D+12 Y= 7.282164152012D+12 Z= -1.038870101035D+13
I= 30 X= -9.353476068727D+12 Y= 7.863990665231D+12 Z= 3.850549002182D+11
I= 31 X= -5.509693930623D+13 Y= -5.503981381642D+12 Z= 2.932196820114D+13
I= 32 X= 9.878562961907D+13 Y= -3.096990392312D+13 Z= -6.120187570727D+13
I= 33 X= 9.291774108115D+12 Y= 2.759584355344D+13 Z= -8.295698770336D+13
I= 34 X= -4.048819931383D+13 Y= -1.148432049205D+14 Z= 1.290240460412D+14
I= 35 X= 3.581438000701D+11 Y= -4.813878813737D+10 Z= -1.208150864707D+11
I= 36 X= 5.236533059874D+12 Y= -1.151194285088D+13 Z= 1.547293526181D+13
I= 37 X= 1.862739716581D+13 Y= -6.917964074225D+13 Z= 1.931385645127D+13
I= 38 X= 8.827580211996D+12 Y= 1.074897657157D+14 Z= -7.915452628054D+13

Backward Direction:

Total Energy: -651.6135696 Hartrees

Potential Energy: -651.7902729 Hartress

Kinetic Energy: 0.1767033 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -8.125072692147D+11 Y= -8.843153959708D+12 Z= 5.167113334037D+12
I= 1 X= 5.199936478183D+12 Y= 2.340301287041D+13 Z= 4.033320980885D+13
I= 2 X= 6.626713488175D+12 Y= -6.317905341707D+12 Z= -5.307392535874D+12
I= 3 X= 2.283135880284D+13 Y= 1.464826735282D+13 Z= -6.344274074641D+12
I= 4 X= -6.601482657034D+12 Y= -2.505682941926D+13 Z= 2.920837737476D+12
I= 5 X= -1.326248747932D+13 Y= 5.078715838624D+12 Z= -1.067483612453D+13
I= 6 X= 1.092771507467D+14 Y= -4.422122431380D+13 Z= -5.221280643985D+13
I= 7 X= -3.118487081988D+13 Y= 4.614633246584D+13 Z= 6.247291247532D+12
I= 8 X= 6.101567126179D+13 Y= -6.488106096577D+13 Z= -2.040013805664D+13
I= 9 X= 1.962647551719D+12 Y= -4.228611126508D+12 Z= -1.741291544280D+13
I= 10 X= 9.117573904351D+13 Y= -4.822616411899D+12 Z= -4.699030927589D+13
I= 11 X= 1.423963104916D+13 Y= 7.357209837355D+13 Z= 4.733221564971D+13
I= 12 X= 3.542688843646D+12 Y= 8.312078919432D+13 Z= 8.808918117941D+13
I= 13 X= -2.938392079432D+12 Y= -4.205260678448D+12 Z= -8.386615092689D+09
I= 14 X= -2.454219757361D+13 Y= -3.081746642387D+13 Z= 7.248296580462D+12
I= 15 X= -6.179337232417D+13 Y= -5.876261265394D+10 Z= -1.036513550492D+14
I= 16 X= -6.870204186255D+13 Y= -3.543123122166D+13 Z= -3.166664200745D+13
I= 17 X= -6.071740123343D+12 Y= -7.683620025526D+11 Z= 4.708116300788D+12
I= 18 X= -8.594101489258D+13 Y= 6.312332867912D+13 Z= -6.584939307219D+13
I= 19 X= -3.032184178568D+13 Y= -6.913731030291D+13 Z= -8.058671457962D+12
I= 20 X= 1.844328758418D+13 Y= 2.234600815663D+13 Z= -1.027872091320D+14
I= 21 X= -7.383330077797D+12 Y= -6.920483325070D+12 Z= -2.998036100574D+12
I= 22 X= 1.123452193724D+14 Y= -8.518738079809D+12 Z= 2.320182440730D+13
I= 23 X= 7.753476705407D+13 Y= -8.643846546081D+11 Z= -9.673921684392D+12
I= 24 X= -2.258408146562D+13 Y= 1.140801269227D+14 Z= -6.098329202357D+13
I= 25 X= 7.294029013695D+12 Y= 1.730871900257D+13 Z= 4.671970284788D+12
I= 26 X= 1.776946497848D+13 Y= -2.413487967834D+11 Z= 3.810062414667D+13
I= 27 X= -3.291245143135D+13 Y= -4.749276755051D+12 Z= -4.600831189655D+13
I= 28 X= -1.086920332088D+14 Y= -8.062075537575D+13 Z= 1.133872683268D+13

I= 29 X= -7.931745715407D+12 Y= 7.954605054110D+12 Z= -1.126210727392D+13
I= 30 X= -9.264770811097D+12 Y= 8.055397138595D+12 Z= -2.864811142697D+11
I= 31 X= -5.500663937592D+13 Y= -6.124803896258D+12 Z= 2.890580410160D+13
I= 32 X= 9.733738640232D+13 Y= -2.965890285543D+13 Z= -6.255461660082D+13
I= 33 X= 9.492634515382D+12 Y= 2.750688479451D+13 Z= -8.364124143458D+13
I= 34 X= -3.980860706659D+13 Y= -1.149460249727D+14 Z= 1.285842220094D+14
I= 35 X= 8.402865024693D+10 Y= -1.596943193054D+11 Z= 9.455670051578D+11
I= 36 X= 1.917942085490D+12 Y= -1.547736000950D+13 Z= 1.348259565165D+13
I= 37 X= 2.248400554080D+13 Y= -6.669548179456D+13 Z= 1.441490318283D+13
I= 38 X= 1.116310737296D+13 Y= 1.073321429966D+14 Z= -8.231828123262D+13

Seed: 53753451982

CM Start Point Coordinates: bohr

I= 0 X= -2.481308621442D+00 Y= 2.480975458008D+00 Z= -5.928567299715D-01
I= 1 X= -2.860050843254D+00 Y= 1.362593883036D-01 Z= -2.106530462267D+00
I= 2 X= -2.405517205038D+00 Y= 1.590447770603D+00 Z= 2.112578676530D+00
I= 3 X= -2.967404715978D+00 Y= -1.830797662429D+00 Z= -1.799061079914D-01
I= 4 X= -2.691334658356D+00 Y= -9.921080987421D-01 Z= 2.236560199975D+00
I= 5 X= 3.960659160326D+00 Y= 2.690634137808D+00 Z= -1.791664238760D+00
I= 6 X= 2.584317576837D+00 Y= 8.047683606235D-02 Z= -2.972751927097D+00
I= 7 X= 5.602667580346D+00 Y= 1.736300655511D+00 Z= -3.073397738190D+00
I= 8 X= 2.748058252887D+00 Y= 4.161558218614D+00 Z= -3.051938501718D+00
I= 9 X= -2.661650628921D+00 Y= -2.512749650944D+00 Z= 4.605479020344D+00
I= 10 X= -4.345759565304D+00 Y= -2.552091760569D+00 Z= 5.665407597250D+00
I= 11 X= -2.014251121590D+00 Y= -4.448842730391D+00 Z= 4.231256895146D+00
I= 12 X= -9.161528517319D-01 Y= -2.297427782478D+00 Z= 5.982124751629D+00
I= 13 X= -2.158872593129D+00 Y= 3.650848178743D+00 Z= 4.205725776484D+00
I= 14 X= -3.903585910596D+00 Y= 3.788224485851D+00 Z= 4.688390134071D+00
I= 15 X= -8.489653435181D-01 Y= 3.197940781556D+00 Z= 5.776326745476D+00
I= 16 X= -1.716003473679D+00 Y= 5.469646256200D+00 Z= 3.290524138987D+00

I= 17 X= -2.596919156574D+00 Y= 5.107258253377D+00 Z= -1.613177966470D+00
I= 18 X= -4.294619611178D+00 Y= 6.372819940684D+00 Z= -7.798743582942D-01
I= 19 X= -7.769037072603D-01 Y= 5.993748135203D+00 Z= -7.642549609763D-01
I= 20 X= -2.635436151952D+00 Y= 4.911427251828D+00 Z= -3.626139740755D+00
I= 21 X= -3.319694664271D+00 Y= -3.690171969169D-01 Z= -4.737707477225D+00
I= 22 X= -5.371449959315D+00 Y= -1.036092104080D+00 Z= -4.891979416982D+00
I= 23 X= -3.306596874527D+00 Y= 1.588758564294D+00 Z= -5.870381841766D+00
I= 24 X= -2.009772182248D+00 Y= -1.684421138156D+00 Z= -5.335495916998D+00
I= 25 X= -3.542267671592D+00 Y= -4.576309736057D+00 Z= -8.534230578524D-01
I= 26 X= -3.470305968870D+00 Y= -4.749072076284D+00 Z= -3.203763247194D+00
I= 27 X= -2.405267780504D+00 Y= -5.829728538507D+00 Z= 1.838176041823D-01
I= 28 X= -5.452515312999D+00 Y= -5.007208971623D+00 Z= -3.976641109108D-02
I= 29 X= 2.928435607578D+00 Y= -3.334638799982D+00 Z= -1.067841840132D+00
I= 30 X= 3.325859306182D+00 Y= -2.947094952862D+00 Z= 1.507281010208D+00
I= 31 X= 1.850428328911D+00 Y= -5.150845997358D+00 Z= -1.691957175188D+00
I= 32 X= 4.247274046848D+00 Y= -2.977544663188D+00 Z= -2.378317833841D+00
I= 33 X= 5.163798500357D+00 Y= -1.938486890062D+00 Z= 2.138182779754D+00
I= 34 X= 2.374114500398D+00 Y= -3.935316566385D+00 Z= 3.165498753490D+00
I= 35 X= 8.952944955903D-01 Y= -1.056928034641D-01 Z= -1.729535667340D-01
I= 36 X= 3.953550243600D+00 Y= 2.503063959755D+00 Z= 9.725573574837D-01
I= 37 X= 5.340502758830D+00 Y= 1.431112885803D+00 Z= 1.799267523690D+00
I= 38 X= 3.077638108784D+00 Y= 4.099066907614D+00 Z= 1.760190590813D+00

Forward Direction:

Total Energy: -651.6178600 Hartrees

Potential Energy: -651.8052799 Hartress

Kinetic Energy: 0.1874199 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.435407416819D+13 Y= -2.015788934448D+12 Z= 1.235419235337D+13

I= 1 X= -3.101886599324D+12 Y= -9.936560279508D+12 Z= 5.050879915637D+12

I= 2 X= 1.540494541797D+13 Y= 1.974395113377D+13 Z= 2.632693284402D+12

I= 3 X= 4.373204663824D+12 Y= 1.216626096634D+13 Z= -1.881063129138D+13
I= 4 X= 9.893108995612D+12 Y= -5.496235975150D+12 Z= -1.723779960577D+13
I= 5 X= -6.804252951793D+12 Y= -1.135638630540D+12 Z= 5.614376425220D+12
I= 6 X= -1.519383758272D+13 Y= -7.130115588021D+13 Z= 5.657678605032D+13
I= 7 X= 1.987830222628D+13 Y= -9.946665258090D+12 Z= -3.384020716877D+13
I= 8 X= 7.042365821413D+13 Y= -8.980137357990D+13 Z= 7.918898158258D+13
I= 9 X= -2.475514645287D+13 Y= 5.035893626799D+12 Z= 1.362790778373D+13
I= 10 X= 2.511065974002D+13 Y= 5.371321284282D+12 Z= -1.202929961143D+13
I= 11 X= 1.184979183609D+12 Y= 1.166593005187D+14 Z= -1.931324919091D+12
I= 12 X= 1.284524623477D+13 Y= -1.790434284036D+13 Z= -1.039017269897D+14
I= 13 X= -4.394760992808D+12 Y= -9.495815528180D+12 Z= -6.400932105195D+12
I= 14 X= 1.207903048368D+12 Y= -2.833669627177D+13 Z= 1.438486076509D+13
I= 15 X= -1.272602828840D+12 Y= -3.680366665923D+13 Z= -2.359240687552D+13
I= 16 X= 2.947801798277D+13 Y= 9.443280330095D+13 Z= -1.539794197216D+14
I= 17 X= -2.012866798696D+12 Y= -1.979287035415D+13 Z= -7.423648923797D+12
I= 18 X= -1.353068831786D+14 Y= 6.561628436391D+13 Z= -3.356407593254D+13
I= 19 X= -1.619543226455D+12 Y= -1.547873055038D+12 Z= 8.654958017432D+13
I= 20 X= -1.029748935637D+14 Y= 8.851762931173D+13 Z= 2.842231338393D+13
I= 21 X= -1.403155579234D+12 Y= -1.232582191059D+13 Z= -1.355949217887D+13
I= 22 X= -5.974409665490D+13 Y= 2.730397855319D+13 Z= -1.657788862321D+13
I= 23 X= 5.322509255087D+13 Y= 2.550918840168D+13 Z= 9.947050463024D+13
I= 24 X= -6.362229286524D+13 Y= 5.235271814511D+13 Z= 7.530394200274D+13
I= 25 X= -4.571680893653D+12 Y= -1.778627205970D+13 Z= -3.189608475773D+12
I= 26 X= -4.460731102917D+12 Y= 5.555075963402D+13 Z= 1.000478877607D+14
I= 27 X= -7.978137313571D+13 Y= 6.783331681797D+13 Z= -9.545134588319D+12
I= 28 X= -7.166215634479D+13 Y= -1.229961975968D+13 Z= 1.031337251065D+14
I= 29 X= 1.300931885961D+12 Y= -5.322913960346D+12 Z= -1.353956870778D+13
I= 30 X= -3.897178761713D+12 Y= -3.475023328978D+12 Z= 2.471940506193D+13
I= 31 X= 3.536470253389D+13 Y= -9.157293325312D+13 Z= 2.795974120282D+13
I= 32 X= 6.573465571088D+13 Y= 8.345722890245D+12 Z= -1.190311912865D+14

I= 33 X= 7.128612238730D+13 Y= 4.699555258596D+13 Z= 3.236211765921D+13
I= 34 X= -2.189602857813D+13 Y= 1.005846519881D+14 Z= -9.856544745336D+13
I= 35 X= 7.439070593457D+11 Y= 2.289127023612D+11 Z= 6.044243961531D+11
I= 36 X= 1.798266283268D+12 Y= 1.599355938298D+13 Z= 4.877931081675D+12
I= 37 X= 2.988483757217D+12 Y= -9.888740057589D+12 Z= -8.906550092605D+13
I= 38 X= 7.181558421876D+13 Y= -2.653286405823D+13 Z= 1.085719049476D+13

Backward Direction:

Total Energy: -651.6178319 Hartrees

Potential Energy: -651.8052799 Hartress

Kinetic Energy: 0.1874480 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.391067467434D+13 Y= -2.146235178720D+12 Z= 1.234444762663D+13
I= 1 X= -2.880862748182D+12 Y= -1.040963816511D+13 Z= 4.264133508750D+12
I= 2 X= 1.511728275457D+13 Y= 2.017744040811D+13 Z= 1.955068000250D+12
I= 3 X= 4.192604485064D+12 Y= 1.220619467007D+13 Z= -1.976006774158D+13
I= 4 X= 1.129905974989D+13 Y= -5.610709568177D+12 Z= -1.813835872373D+13
I= 5 X= -6.708127926564D+12 Y= -1.792549044897D+12 Z= -2.758369506674D+11
I= 6 X= 2.373047357477D+13 Y= -3.548207669032D+13 Z= 7.349292298948D+13
I= 7 X= 2.786902324633D+13 Y= -2.393884912890D+12 Z= -3.310734948844D+13
I= 8 X= 8.124581842155D+13 Y= -8.094567988690D+13 Z= 8.121230433125D+13
I= 9 X= -2.426369506534D+13 Y= 5.248271543868D+12 Z= 1.309317200973D+13
I= 10 X= 2.527538270914D+13 Y= 6.452941256947D+12 Z= -1.328293910991D+13
I= 11 X= 1.070228464192D+12 Y= 1.166671198123D+14 Z= -2.009649121507D+12
I= 12 X= 1.318256728051D+13 Y= -1.781717825084D+13 Z= -1.042243794536D+14
I= 13 X= -4.300145909388D+12 Y= -9.561081874382D+12 Z= -6.635027009044D+12
I= 14 X= 1.342061498343D+12 Y= -2.873822102822D+13 Z= 1.440821409731D+13
I= 15 X= -9.439056832291D+11 Y= -3.713480515638D+13 Z= -2.414974705524D+13
I= 16 X= 2.941416028566D+13 Y= 9.452242285649D+13 Z= -1.539138555411D+14
I= 17 X= -1.853718663164D+12 Y= -1.993613193296D+13 Z= -7.486402143260D+12
I= 18 X= -1.351376352319D+14 Y= 6.552909113196D+13 Z= -3.393790930506D+13

I= 19 X= -1.619898434583D+12 Y= -1.686523727929D+12 Z= 8.670765625859D+13
I= 20 X= -1.027872444137D+14 Y= 8.828057321844D+13 Z= 2.834497877570D+13
I= 21 X= -1.724800949184D+12 Y= -1.232036788452D+13 Z= -1.404978120860D+13
I= 22 X= -5.995825306776D+13 Y= 2.776968032040D+13 Z= -1.773854062368D+13
I= 23 X= 5.342899674875D+13 Y= 2.533047536350D+13 Z= 9.905946741894D+13
I= 24 X= -6.404706652649D+13 Y= 5.234046105631D+13 Z= 7.472539429054D+13
I= 25 X= -4.573947832720D+12 Y= -1.784724544413D+13 Z= -3.325760937089D+12
I= 26 X= -4.707819767044D+12 Y= 5.520036690453D+13 Z= 9.995034315508D+13
I= 27 X= -7.956502205329D+13 Y= 6.803439963785D+13 Z= -9.624507987635D+12
I= 28 X= -7.161098937052D+13 Y= -1.230789395137D+13 Z= 1.033831457448D+14
I= 29 X= 4.576807476729D+11 Y= -4.825028627468D+12 Z= -1.418625181333D+13
I= 30 X= -3.831500055006D+12 Y= -3.333303103792D+12 Z= 2.422218971665D+13
I= 31 X= 3.543156195503D+13 Y= -9.203259956365D+13 Z= 2.765160706160D+13
I= 32 X= 6.466235469384D+13 Y= 9.316407749126D+12 Z= -1.200327809492D+14
I= 33 X= 7.143484245125D+13 Y= 4.692968618762D+13 Z= 3.185548592156D+13
I= 34 X= -2.139284827563D+13 Y= 1.005085224802D+14 Z= -9.889109976514D+13
I= 35 X= 5.409480896999D+11 Y= 1.463153121564D+11 Z= 1.393989700860D+12
I= 36 X= -6.588682771530D+11 Y= 1.305750500863D+13 Z= 3.404253763466D+12
I= 37 X= 5.843974479575D+12 Y= -8.049431493192D+12 Z= -9.269275944991D+13
I= 38 X= 7.354484357761D+13 Y= -2.664957028610D+13 Z= 8.514698846754D+12

Seed: 5613632441

CM Start Point Coordinates: bohr

I= 0 X= -2.838471736764D+00 Y= 2.438754869254D+00 Z= -6.650509048430D-01
I= 1 X= -3.106880770473D+00 Y= 1.812272899803D-01 Z= -1.986480569720D+00
I= 2 X= -2.408158102548D+00 Y= 1.813926310692D+00 Z= 2.105318600304D+00
I= 3 X= -2.979304975125D+00 Y= -1.960459139629D+00 Z= -3.987700879525D-01
I= 4 X= -2.386550883531D+00 Y= -7.702075178291D-01 Z= 2.171288402410D+00
I= 5 X= 4.175898694514D+00 Y= 2.049676445998D+00 Z= -1.593975177504D+00
I= 6 X= 2.590515678709D+00 Y= 2.013849200138D-01 Z= -2.765650822980D+00

I= 7 X= 5.759249151228D+00 Y= 8.370389334738D-01 Z= -2.298003557364D+00
I= 8 X= 3.791531031597D+00 Y= 3.279059846674D+00 Z= -3.030910845700D+00
I= 9 X= -2.180276345244D+00 Y= -2.566883801846D+00 Z= 4.671997760370D+00
I= 10 X= -4.286931828462D+00 Y= -2.958848622830D+00 Z= 5.431676059972D+00
I= 11 X= -1.460321224414D+00 Y= -4.566168348687D+00 Z= 4.355551233394D+00
I= 12 X= -9.398185876961D-01 Y= -1.843701931003D+00 Z= 6.192587855234D+00
I= 13 X= -2.233869098128D+00 Y= 3.680042070598D+00 Z= 4.071715296979D+00
I= 14 X= -4.360686001300D+00 Y= 4.371557484314D+00 Z= 4.411602725651D+00
I= 15 X= -1.243406523361D+00 Y= 3.144827869350D+00 Z= 5.967287245859D+00
I= 16 X= -1.480282407483D+00 Y= 5.706189877297D+00 Z= 3.082956866715D+00
I= 17 X= -3.012164918915D+00 Y= 5.060002520476D+00 Z= -1.547465634389D+00
I= 18 X= -5.251031278383D+00 Y= 5.648907604634D+00 Z= -2.113994550548D+00
I= 19 X= -1.855601563154D+00 Y= 6.418993143197D+00 Z= -2.595410089261D-01
I= 20 X= -1.638877741070D+00 Y= 5.139678009851D+00 Z= -3.137431442472D+00
I= 21 X= -3.868022111764D+00 Y= 1.688142086095D-02 Z= -4.707757602401D+00
I= 22 X= -6.083010844624D+00 Y= 5.775573180741D-01 Z= -4.879183155815D+00
I= 23 X= -2.921512866429D+00 Y= 1.359986918982D+00 Z= -6.000721822474D+00
I= 24 X= -3.608185332501D+00 Y= -1.934480878963D+00 Z= -5.534674986523D+00
I= 25 X= -3.248890599008D+00 Y= -4.600116906413D+00 Z= -1.063004564553D+00
I= 26 X= -2.866837195911D+00 Y= -5.275518085980D+00 Z= -2.985395941675D+00
I= 27 X= -2.113146373171D+00 Y= -5.995085837333D+00 Z= 5.018715481657D-01
I= 28 X= -5.480384984825D+00 Y= -4.866442234906D+00 Z= -1.116516910899D+00
I= 29 X= 3.169918224859D+00 Y= -3.456060544572D+00 Z= -8.892225976892D-01
I= 30 X= 3.077602144063D+00 Y= -3.208781943054D+00 Z= 1.809295960330D+00
I= 31 X= 1.718454341771D+00 Y= -4.768910454542D+00 Z= -1.383684054825D+00
I= 32 X= 4.682688445911D+00 Y= -2.840041347003D+00 Z= -2.110029684018D+00
I= 33 X= 4.802676800366D+00 Y= -2.532721300039D+00 Z= 2.775350920236D+00
I= 34 X= 1.983350999522D+00 Y= -4.376629300468D+00 Z= 2.612991413888D+00
I= 35 X= 9.332733889243D-01 Y= -8.189029246742D-02 Z= -1.938483669982D-01
I= 36 X= 3.850740371763D+00 Y= 2.522779880760D+00 Z= 1.015274398078D+00

I= 37 X= 5.233725018690D+00 Y= 1.943575863253D+00 Z= 2.358801414800D+00

I= 38 X= 2.896420464026D+00 Y= 4.711428791451D+00 Z= 1.401172122616D+00

Forward Direction:

Total Energy: -651.6131070 Hartrees

Potential Energy: -651.7818965 Hartress

Kinetic Energy: 0.1687894 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 9.454607459446D+12 Y= -2.949266618406D+12 Z= -1.931491906461D+13

I= 1 X= 2.687242172819D+12 Y= -4.140174842296D+12 Z= -1.198156604634D+13

I= 2 X= -7.836431841873D+12 Y= 3.049219256812D+12 Z= 8.629486302061D+12

I= 3 X= -1.179684904830D+13 Y= -1.451245020438D+13 Z= -3.341773598352D+12

I= 4 X= -1.301409378668D+12 Y= 7.121426971693D+12 Z= 3.490752481789D+13

I= 5 X= -5.880782225465D+12 Y= -9.811879369498D+12 Z= 2.281495593361D+13

I= 6 X= -1.228805743995D+13 Y= -1.698457288424D+13 Z= -9.929971818368D+13

I= 7 X= -7.498818226869D+13 Y= 3.160738905807D+13 Z= -2.174061320359D+13

I= 8 X= 4.064245924699D+13 Y= -4.426434209411D+13 Z= 9.586534988362D+13

I= 9 X= -1.484958272717D+12 Y= -1.596549976983D+13 Z= -8.423651780838D+12

I= 10 X= -6.858574058547D+13 Y= 3.604667367679D+13 Z= -9.378757108790D+13

I= 11 X= 2.806432379661D+13 Y= 1.249844044383D+12 Z= 5.477529346580D+12

I= 12 X= 6.277005001979D+13 Y= 3.715297691376D+13 Z= -7.208270171627D+09

I= 13 X= 5.322983272565D+11 Y= -7.030320201980D+12 Z= 9.513090226767D+12

I= 14 X= -5.686012132463D+13 Y= -2.903383906766D+12 Z= 3.895458095790D+13

I= 15 X= -3.829657741531D+13 Y= 5.991745108793D+13 Z= -3.318955020565D+13

I= 16 X= 1.082243519970D+14 Y= 4.694256289013D+13 Z= 3.770244135668D+13

I= 17 X= -1.763262017168D+13 Y= -1.926530688797D+13 Z= -1.010101209216D+13

I= 18 X= 9.636848741029D+13 Y= 9.286437599683D+12 Z= -3.769718998851D+13

I= 19 X= -3.036805588473D+13 Y= -8.464389215760D+12 Z= -3.390629605285D+13

I= 20 X= -4.511554383819D+12 Y= 1.538229267328D+13 Z= -5.475873606448D+13

I= 21 X= -2.871531582246D+13 Y= 3.050548891759D+12 Z= 5.924819018917D+12

I= 22 X= 1.974926757650D+13 Y= -3.194474992737D+13 Z= -9.234365588423D+13

I= 23 X= 5.273188022664D+13 Y= 1.046274050985D+14 Z= -9.223179343874D+13
I= 24 X= 1.272154040662D+13 Y= 1.417431865746D+13 Z= -4.031741054623D+13
I= 25 X= -4.747421602652D+12 Y= 2.432283002938D+13 Z= -4.576698814895D+12
I= 26 X= -8.156882708107D+13 Y= 5.407939162137D+13 Z= 5.223682058987D+13
I= 27 X= 7.957622071186D+13 Y= -3.178080933106D+13 Z= 1.423398098018D+14
I= 28 X= 6.698639061832D+13 Y= -2.427140940033D+13 Z= -7.356826975522D+13
I= 29 X= -3.653229139201D+12 Y= -2.200328959145D+13 Z= -9.480989481827D+12
I= 30 X= 4.151504368172D+12 Y= -7.680996179259D+12 Z= 1.168095946822D+13
I= 31 X= -3.001252985735D+13 Y= 6.221266472151D+13 Z= 4.281544356023D+13
I= 32 X= -4.834254399599D+12 Y= -1.189756979973D+13 Z= -2.211803982338D+13
I= 33 X= 6.213084004553D+12 Y= 2.306947347463D+13 Z= -7.692279611091D+12
I= 34 X= -5.474018726822D+13 Y= -3.354865320257D+13 Z= -1.491351377764D+13
I= 35 X= 3.540112097149D+12 Y= 3.153865369443D+12 Z= 7.374885696882D+11
I= 36 X= -1.587930165543D+13 Y= -2.144784164807D+12 Z= -2.130435843637D+13
I= 37 X= 7.657717189370D+13 Y= -7.843019548386D+13 Z= 9.841241729633D+12
I= 38 X= 1.062034024470D+14 Y= -5.926496473892D+12 Z= 9.224573740035D+13

Backward Direction:

Total Energy: -651.6131292 Hartrees

Potential Energy: -651.7818965 Hartress

Kinetic Energy: 0.1687672 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 8.700740428599D+12 Y= -3.171051092821D+12 Z= -1.933148703152D+13
I= 1 X= 3.063026528139D+12 Y= -4.944501018647D+12 Z= -1.331919088286D+13
I= 2 X= -8.325515386533D+12 Y= 3.786236944574D+12 Z= 7.477389004081D+12
I= 3 X= -1.210390514972D+13 Y= -1.444455499401D+13 Z= -4.956003760337D+12
I= 4 X= 1.088985584519D+12 Y= 6.926799172650D+12 Z= 3.337639581114D+13
I= 5 X= -5.717350624071D+12 Y= -1.092875729119D+13 Z= 1.280042565347D+13
I= 6 X= 5.389098702273D+13 Y= 4.391496171835D+13 Z= -7.053893230500D+13
I= 7 X= -6.140237262880D+13 Y= 4.444861273037D+13 Z= -2.049460987470D+13
I= 8 X= 5.904227675856D+13 Y= -2.920790746786D+13 Z= 9.930539961187D+13

I= 9 X= -6.493935017211D+11 Y= -1.560441521720D+13 Z= -9.332808589717D+12
I= 10 X= -6.830567889946D+13 Y= 3.788564202692D+13 Z= -9.591900672693D+13
I= 11 X= 2.786922482123D+13 Y= 1.263138395147D+12 Z= 5.344362682841D+12
I= 12 X= 6.334356264834D+13 Y= 3.730117399177D+13 Z= -5.557814182402D+11
I= 13 X= 6.931627368354D+11 Y= -7.141285930259D+12 Z= 9.115082488822D+12
I= 14 X= -5.663202535409D+13 Y= -3.586055581841D+12 Z= 3.899428625806D+13
I= 15 X= -3.773772709821D+13 Y= 5.935445000068D+13 Z= -3.413713899629D+13
I= 16 X= 1.081157812655D+14 Y= 4.709493389055D+13 Z= 3.781391345854D+13
I= 17 X= -1.736203679425D+13 Y= -1.950887997165D+13 Z= -1.020770500717D+13
I= 18 X= 9.665624247638D+13 Y= 9.138191829557D+12 Z= -3.833278082594D+13
I= 19 X= -3.036865980734D+13 Y= -8.700122843152D+12 Z= -3.363753538358D+13
I= 20 X= -4.192513626675D+12 Y= 1.497925030917D+13 Z= -5.489022022764D+13
I= 21 X= -2.926217670738D+13 Y= 3.059821816043D+12 Z= 5.091230483435D+12
I= 22 X= 1.938515922590D+13 Y= -3.115296461680D+13 Z= -9.431699435480D+13
I= 23 X= 5.307855778678D+13 Y= 1.043235575092D+14 Z= -9.293063816806D+13
I= 24 X= 1.199934098617D+13 Y= 1.415347917307D+13 Z= -4.130105632732D+13
I= 25 X= -4.751275839583D+12 Y= 2.421916318834D+13 Z= -4.808184987520D+12
I= 26 X= -8.198892680234D+13 Y= 5.348365452691D+13 Z= 5.207097542108D+13
I= 27 X= 7.994406046179D+13 Y= -3.143892868107D+13 Z= 1.422048592731D+14
I= 28 X= 6.707338463398D+13 Y= -2.428547717319D+13 Z= -7.314420520372D+13
I= 29 X= -5.086923220407D+12 Y= -2.115678583288D+13 Z= -1.058047894405D+13
I= 30 X= 4.263171185574D+12 Y= -7.440043704387D+12 Z= 1.083559482766D+13
I= 31 X= -2.989885558417D+13 Y= 6.143114088251D+13 Z= 4.229155443882D+13
I= 32 X= -6.657378672368D+12 Y= -1.024721312966D+13 Z= -2.382094077846D+13
I= 33 X= 6.465937588418D+12 Y= 2.295748754141D+13 Z= -8.553653983635D+12
I= 34 X= -5.388468102049D+13 Y= -3.367808845673D+13 Z= -1.546718726116D+13
I= 35 X= 3.195041617137D+12 Y= 3.013433435443D+12 Z= 2.079906092973D+12
I= 36 X= -2.005691745797D+13 Y= -7.136658581338D+12 Z= -2.380990198671D+13
I= 37 X= 8.143207212244D+13 Y= -7.530300633789D+13 Z= 3.674183256802D+12
I= 38 X= 1.091434861294D+14 Y= -6.124920190905D+12 Z= 8.826303727045D+13

Seed: 7377033437

CM Start Point Coordinates: bohr

I= 0 X= -2.564145288641D+00 Y= 2.346758711477D+00 Z= -5.759063288728D-01
I= 1 X= -2.890341813980D+00 Y= 7.006255427072D-02 Z= -1.950789692481D+00
I= 2 X= -2.265640173197D+00 Y= 1.803002024441D+00 Z= 1.978856734851D+00
I= 3 X= -2.957814783303D+00 Y= -1.935188348564D+00 Z= -1.333080050370D-01
I= 4 X= -2.488951490366D+00 Y= -8.429741545769D-01 Z= 2.152659484733D+00
I= 5 X= 4.223101401500D+00 Y= 2.588376603249D+00 Z= -9.419996424516D-01
I= 6 X= 2.089642373281D+00 Y= 1.081052922648D+00 Z= -2.601631234662D+00
I= 7 X= 5.955355221324D+00 Y= 1.558396274634D+00 Z= -1.719511717017D+00
I= 8 X= 3.638652465695D+00 Y= 4.468448282367D+00 Z= -1.824739446378D+00
I= 9 X= -2.463968974567D+00 Y= -2.288816289149D+00 Z= 4.781940951880D+00
I= 10 X= -4.509848784317D+00 Y= -2.704049299115D+00 Z= 5.578133386296D+00
I= 11 X= -1.888354713606D+00 Y= -4.382885993300D+00 Z= 4.484292376403D+00
I= 12 X= -1.043026381876D+00 Y= -1.562197926227D+00 Z= 6.074968129770D+00
I= 13 X= -2.131278196196D+00 Y= 3.801223026717D+00 Z= 3.975942308595D+00
I= 14 X= -4.247066384076D+00 Y= 4.523332102896D+00 Z= 4.334869105291D+00
I= 15 X= -1.089830481704D+00 Y= 2.821588946430D+00 Z= 5.656928855701D+00
I= 16 X= -7.338808479177D-01 Y= 5.608711546325D+00 Z= 3.386334903579D+00
I= 17 X= -2.610698949854D+00 Y= 4.712972480909D+00 Z= -1.974496316855D+00
I= 18 X= -4.707727322349D+00 Y= 5.313028763626D+00 Z= -2.208498161431D+00
I= 19 X= -1.891286284646D+00 Y= 6.722444887005D+00 Z= -8.403491461881D-01
I= 20 X= -2.027145725599D+00 Y= 4.529331670579D+00 Z= -3.890824345423D+00
I= 21 X= -3.541800855261D+00 Y= -3.453110195635D-01 Z= -4.794473203741D+00
I= 22 X= -5.423304500748D+00 Y= 8.693457559422D-02 Z= -5.484043240107D+00
I= 23 X= -2.097719467967D+00 Y= 7.333500906167D-01 Z= -6.051703978597D+00
I= 24 X= -3.215305647742D+00 Y= -2.689889924666D+00 Z= -5.149372346640D+00
I= 25 X= -3.589096091044D+00 Y= -4.673689113621D+00 Z= -4.653178246117D-01
I= 26 X= -3.755613843599D+00 Y= -5.099089648815D+00 Z= -2.726539806304D+00

I= 27 X= -1.876913435574D+00 Y= -5.798865150562D+00 Z= 1.732145365189D-01
I= 28 X= -5.592458859033D+00 Y= -5.319056157699D+00 Z= 2.981556012283D-01
I= 29 X= 2.731822653917D+00 Y= -3.400228156389D+00 Z= -1.675933779644D+00
I= 30 X= 3.583127806760D+00 Y= -2.972025611757D+00 Z= 7.104182690372D-01
I= 31 X= 1.261182300418D+00 Y= -4.969940193743D+00 Z= -2.321716329631D+00
I= 32 X= 4.213596313512D+00 Y= -3.039396507694D+00 Z= -3.113716103290D+00
I= 33 X= 5.453606564359D+00 Y= -2.055228068875D+00 Z= 1.104368835300D+00
I= 34 X= 3.066230515753D+00 Y= -4.240095159632D+00 Z= 2.593325340630D+00
I= 35 X= 8.880406960980D-01 Y= -7.172629948921D-02 Z= -1.769461527228D-01
I= 36 X= 3.630761104844D+00 Y= 2.264532071500D+00 Z= 1.623704206933D+00
I= 37 X= 4.755930244210D+00 Y= 1.030101241451D+00 Z= 2.936358689448D+00
I= 38 X= 2.413155563846D+00 Y= 3.677878997613D+00 Z= 2.907754483246D+00

Forward Direction:

Total Energy: -651.6239351 Hartrees

Potential Energy: -651.8074526 Hartress

Kinetic Energy: 0.1835175 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.463622727479D+12 Y= 1.593491209161D+13 Z= 3.578034172808D+11
I= 1 X= 1.179793700471D+13 Y= 3.718201108213D+12 Z= -1.063342925917D+13
I= 2 X= -2.850833340298D+12 Y= -2.513308236847D+13 Z= -1.708494489984D+13
I= 3 X= -1.950696903473D+13 Y= -1.914557436927D+13 Z= -7.228103027009D+12
I= 4 X= -7.353093218059D+12 Y= -5.909438616251D+12 Z= 2.112840174703D+13
I= 5 X= 1.139878041744D+13 Y= -1.170960900868D+13 Z= -1.231962744062D+13
I= 6 X= -6.445689987720D+12 Y= -4.335592363951D+13 Z= 3.260853797309D+13
I= 7 X= -1.309304809948D+14 Y= 6.859267502073D+13 Z= 4.018427355863D+13
I= 8 X= -2.431984476378D+13 Y= -1.238673588291D+13 Z= -8.416929773183D+13
I= 9 X= -1.393013292969D+12 Y= -3.557269026164D+12 Z= -5.135496164985D+12
I= 10 X= 4.934079201303D+13 Y= 6.453301973329D+12 Z= 5.055961334166D+13
I= 11 X= -5.961120198978D+13 Y= 1.186771136560D+14 Z= 4.199264862640D+13
I= 12 X= -5.342361523964D+12 Y= -3.283591335740D+13 Z= 7.257454050197D+13

I= 13 X= 1.279430283697D+13 Y= 2.855978073578D+13 Z= -4.281971556043D+12
I= 14 X= 2.111746289643D+13 Y= -2.335650429388D+13 Z= 8.129907101114D+12
I= 15 X= 4.242701430208D+13 Y= -8.738146647308D+12 Z= 1.742735798319D+14
I= 16 X= -5.667585621741D+13 Y= 3.141421676213D+12 Z= 1.507619179328D+13
I= 17 X= 4.700705893488D+12 Y= -7.294780265151D+12 Z= 1.106350753412D+13
I= 18 X= -4.141938322799D+13 Y= 7.881573880308D+13 Z= -3.362492428149D+13
I= 19 X= -3.020452089383D+13 Y= -1.388609692464D+12 Z= -4.673349285885D+13
I= 20 X= 2.627728946330D+13 Y= 9.942167959645D+12 Z= 1.145037425443D+14
I= 21 X= 6.842661303574D+12 Y= 5.680893079621D+12 Z= 2.086732564797D+12
I= 22 X= -1.066406759806D+14 Y= -3.776011947905D+13 Z= -1.006417068275D+13
I= 23 X= 2.341652677748D+13 Y= 1.193267063924D+13 Z= 4.910560353541D+13
I= 24 X= 2.628393560745D+13 Y= -7.716105660734D+13 Z= -7.987700726659D+12
I= 25 X= 2.750227211875D+13 Y= 4.979626996664D+11 Z= -3.098260832081D+12
I= 26 X= -7.209393993429D+13 Y= 4.770410976972D+13 Z= 2.691301862685D+13
I= 27 X= -7.003348934233D+13 Y= 1.734855932336D+14 Z= -2.424112328555D+13
I= 28 X= -4.687100252897D+13 Y= 9.575831461219D+12 Z= 3.852485655052D+13
I= 29 X= -1.433474691376D+13 Y= -1.272223090602D+13 Z= -6.978485874740D+12
I= 30 X= 1.082401105862D+13 Y= -5.621800743928D+12 Z= -9.934996045866D+12
I= 31 X= 2.689641763991D+13 Y= 2.665591598381D+13 Z= 5.762036379720D+13
I= 32 X= 7.258577170539D+13 Y= -2.290236463095D+13 Z= -3.499938083511D+13
I= 33 X= -1.282199485430D+14 Y= 3.396779910575D+13 Z= 2.422976323520D+13
I= 34 X= 3.063707394467D+13 Y= 5.633660617153D+12 Z= 3.339249132488D+13
I= 35 X= 1.144994573114D+11 Y= 1.862428114620D+12 Z= -1.308802488983D+12
I= 36 X= 2.449683255674D+12 Y= -2.737409145184D+13 Z= 2.994934455676D+13
I= 37 X= -4.312822261310D+13 Y= 5.411258548132D+13 Z= -5.132945360989D+13
I= 38 X= -5.876820905735D+13 Y= 1.754830701608D+13 Z= -9.176357455776D+13

Backward Direction:

Total Energy: -651.6239184 Hartrees

Potential Energy: -651.8074526 Hartress

Kinetic Energy: 0.1835343 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 2.223657995615D+12 Y= 1.586431548780D+13 Z= 3.525296386419D+11
I= 1 X= 1.191755358046D+13 Y= 3.462174636926D+12 Z= -1.105921095849D+13
I= 2 X= -3.006514377358D+12 Y= -2.489848097997D+13 Z= -1.745167100357D+13
I= 3 X= -1.960470859874D+13 Y= -1.912396252694D+13 Z= -7.741931451378D+12
I= 4 X= -6.592202417957D+12 Y= -5.971390930650D+12 Z= 2.064102539685D+13
I= 5 X= 1.145080261416D+13 Y= -1.206512437217D+13 Z= -1.550737007945D+13
I= 6 X= 1.461987732809D+13 Y= -2.397088633340D+13 Z= 4.176343399674D+13
I= 7 X= -1.266059581836D+14 Y= 7.268018737335D+13 Z= 4.058089105454D+13
I= 8 X= -1.846296669373D+13 Y= -7.594095859605D+12 Z= -8.307428949009D+13
I= 9 X= -1.127043209204D+12 Y= -3.442331570121D+12 Z= -5.424891457400D+12
I= 10 X= 4.942993894020D+13 Y= 7.038667199258D+12 Z= 4.988115234039D+13
I= 11 X= -5.967330428126D+13 Y= 1.186813454051D+14 Z= 4.195026011244D+13
I= 12 X= -5.159805716493D+12 Y= -3.278874048325D+13 Z= 7.239992322277D+13
I= 13 X= 1.284550786449D+13 Y= 2.852445904112D+13 Z= -4.408662094351D+12
I= 14 X= 2.119006851858D+13 Y= -2.357380670979D+13 Z= 8.142545764873D+12
I= 15 X= 4.260490292012D+13 Y= -8.917356503972D+12 Z= 1.739719511900D+14
I= 16 X= -5.671041556261D+13 Y= 3.189923158312D+12 Z= 1.511167467404D+13
I= 17 X= 4.786835764435D+12 Y= -7.372312438782D+12 Z= 1.102954592607D+13
I= 18 X= -4.132778740733D+13 Y= 7.876855043195D+13 Z= -3.382724031437D+13
I= 19 X= -3.020471312799D+13 Y= -1.463646476496D+12 Z= -4.664794317850D+13
I= 20 X= 2.637884389184D+13 Y= 9.813874839904D+12 Z= 1.144618895923D+14
I= 21 X= 6.668589060567D+12 Y= 5.683844761527D+12 Z= 1.821391540970D+12
I= 22 X= -1.067565759449D+14 Y= -3.750808491507D+13 Z= -1.069230750033D+13
I= 23 X= 2.352687831735D+13 Y= 1.183595238363D+13 Z= 4.888315304714D+13
I= 24 X= 2.605405105107D+13 Y= -7.716769005660D+13 Z= -8.300806737949D+12
I= 25 X= 2.750104526909D+13 Y= 4.649643257670D+11 Z= -3.171945598954D+12
I= 26 X= -7.222766261257D+13 Y= 4.751447965145D+13 Z= 2.686022815995D+13
I= 27 X= -6.991640163240D+13 Y= 1.735944178589D+14 Z= -2.428407962230D+13
I= 28 X= -4.684331131356D+13 Y= 9.571353526686D+12 Z= 3.865984127795D+13

I= 29 X= -1.479110858222D+13 Y= -1.245277881377D+13 Z= -7.328466288163D+12
I= 30 X= 1.085955591855D+13 Y= -5.545102740715D+12 Z= -1.020408554270D+13
I= 31 X= 2.693260149733D+13 Y= 2.640714776465D+13 Z= 5.745360373243D+13
I= 32 X= 7.200544983151D+13 Y= -2.237703671351D+13 Z= -3.554143421490D+13
I= 33 X= -1.281394622785D+14 Y= 3.393215266833D+13 Z= 2.395557765307D+13
I= 34 X= 3.090939163215D+13 Y= 5.592459855047D+12 Z= 3.321625054977D+13
I= 35 X= 4.659469530415D+09 Y= 1.817726980078D+12 Z= -8.814952207658D+11
I= 36 X= 1.119899067728D+12 Y= -2.896306372291D+13 Z= 2.915180060928D+13
I= 37 X= -4.158285083561D+13 Y= 5.510800652223D+13 Z= -5.329250077292D+13
I= 38 X= -5.783234588384D+13 Y= 1.748514641437D+13 Z= -9.303131479769D+13

Seed: 7632425560

CM Start Point Coordinates: bohr

I= 0 X= -2.421888367681D+00 Y= 2.312938828694D+00 Z= -4.651866093532D-01
I= 1 X= -3.164148115791D+00 Y= 6.366572581329D-02 Z= -1.993417463084D+00
I= 2 X= -2.411643749182D+00 Y= 1.477306921766D+00 Z= 2.187850165034D+00
I= 3 X= -3.049855132908D+00 Y= -2.036626842226D+00 Z= -4.341646617531D-01
I= 4 X= -2.440134344910D+00 Y= -1.079686654851D+00 Z= 2.171657533748D+00
I= 5 X= 4.270457617040D+00 Y= 2.146307980279D+00 Z= -2.101230588113D+00
I= 6 X= 2.169517427631D+00 Y= 3.934342289912D-01 Z= -3.196347925283D+00
I= 7 X= 5.978473334357D+00 Y= 9.297930135729D-01 Z= -2.808876326678D+00
I= 8 X= 3.859449347718D+00 Y= 3.512920578592D+00 Z= -3.681640492347D+00
I= 9 X= -2.651311369064D+00 Y= -2.804215856338D+00 Z= 4.468144614525D+00
I= 10 X= -4.540815571194D+00 Y= -2.704636716027D+00 Z= 4.916609137170D+00
I= 11 X= -1.837462538374D+00 Y= -4.539809307176D+00 Z= 3.810459090869D+00
I= 12 X= -1.777019786900D+00 Y= -1.982265916336D+00 Z= 6.118228518485D+00
I= 13 X= -2.256725586012D+00 Y= 3.281638091851D+00 Z= 4.255002728106D+00
I= 14 X= -4.151064209939D+00 Y= 3.225425330177D+00 Z= 5.111371277560D+00
I= 15 X= -9.272079669725D-01 Y= 2.892171711581D+00 Z= 5.914702628708D+00
I= 16 X= -1.991323882012D+00 Y= 5.348719352411D+00 Z= 3.752777737023D+00

I= 17 X= -2.545210459752D+00 Y= 4.952694310926D+00 Z= -1.197066244007D+00
I= 18 X= -4.467031860436D+00 Y= 5.912839271686D+00 Z= -1.024012089289D+00
I= 19 X= -1.288283266046D+00 Y= 5.998371273494D+00 Z= -2.060367930816D-01
I= 20 X= -2.544109372086D+00 Y= 5.218211195629D+00 Z= -3.241789158513D+00
I= 21 X= -4.054517478312D+00 Y= 1.203736885797D-01 Z= -4.768539496717D+00
I= 22 X= -6.171706695571D+00 Y= 3.078113936646D-01 Z= -4.356844541291D+00
I= 23 X= -3.535431402846D+00 Y= 1.761066630998D+00 Z= -5.973877886974D+00
I= 24 X= -4.000253358052D+00 Y= -2.051440854298D+00 Z= -5.528034148478D+00
I= 25 X= -3.828469421901D+00 Y= -4.666006443605D+00 Z= -1.125241261929D+00
I= 26 X= -2.766137054340D+00 Y= -5.615347476216D+00 Z= -3.034595760720D+00
I= 27 X= -3.258086465553D+00 Y= -5.580171827655D+00 Z= 5.192113005280D-01
I= 28 X= -6.256773737575D+00 Y= -4.761526458254D+00 Z= -1.261655244976D+00
I= 29 X= 3.083429403510D+00 Y= -3.753705842460D+00 Z= -1.585733047918D-01
I= 30 X= 3.236062500112D+00 Y= -2.498510288844D+00 Z= 2.371171630890D+00
I= 31 X= 1.416309589396D+00 Y= -5.349110899509D+00 Z= -2.663220862592D-01
I= 32 X= 4.394879914318D+00 Y= -3.660469523372D+00 Z= -1.913554785856D+00
I= 33 X= 4.759617995778D+00 Y= -1.384680817300D+00 Z= 2.876949611722D+00
I= 34 X= 1.829215742629D+00 Y= -3.106854910720D+00 Z= 3.896245121722D+00
I= 35 X= 9.938575026982D-01 Y= -2.558628282400D-02 Z= -2.543144270727D-01
I= 36 X= 3.718279676272D+00 Y= 2.735761011546D+00 Z= 5.719247395774D-01
I= 37 X= 4.629947089973D+00 Y= 2.294330838343D+00 Z= 2.320512365944D+00
I= 38 X= 3.021944346783D+00 Y= 4.840357063931D+00 Z= 9.132759032744D-01

Forward Direction:

Total Energy: -651.6036976 Hartrees

Potential Energy: -651.8067583 Hartress

Kinetic Energy: 0.2030607 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.623538182075D+13 Y= -2.298800841153D+12 Z= -3.619102861929D+11

I= 1 X= -2.291961772133D+13 Y= -2.806836483604D+12 Z= -2.809555369987D+13

I= 2 X= -2.848558111126D+11 Y= 7.238917597565D+12 Z= -1.581158056015D+12

I= 3 X= -6.755092474158D+12 Y= -1.604841477886D+13 Z= 1.781055474508D+13
I= 4 X= 4.592243735760D+12 Y= 1.181799952832D+13 Z= 5.515704220229D+12
I= 5 X= -3.626484992235D+12 Y= -1.618829601924D+13 Z= 1.305829178551D+13
I= 6 X= -5.657024024482D+13 Y= -3.925211020403D+13 Z= 7.077873320722D+13
I= 7 X= -4.713426655830D+13 Y= -3.681057045214D+13 Z= -7.144510292258D+13
I= 8 X= -1.022484617124D+13 Y= 1.645258463606D+14 Z= 2.435772737926D+13
I= 9 X= 9.106590475445D+12 Y= -1.073717437639D+13 Z= -9.345680269669D+12
I= 10 X= 8.097011146419D+13 Y= 9.833951774956D+13 Z= -5.843481668010D+13
I= 11 X= 2.193142708010D+13 Y= -4.370349967717D+13 Z= -5.448308329160D+13
I= 12 X= -1.074156005049D+14 Y= -5.592303069060D+12 Z= 7.883674936080D+13
I= 13 X= 3.160954240845D+12 Y= 3.135216786626D+13 Z= -1.608610773122D+12
I= 14 X= -1.461282328139D+14 Y= -4.934754581800D+13 Z= 4.005276477634D+13
I= 15 X= 9.392674328639D+13 Y= -5.607567821640D+13 Z= 3.562792264205D+13
I= 16 X= 2.121564172358D+13 Y= -6.737142201008D+13 Z= -3.286610841480D+13
I= 17 X= 1.367661301095D+13 Y= -1.029843518139D+12 Z= -1.738713180282D+13
I= 18 X= -2.770700244540D+13 Y= 3.738578598107D+13 Z= -8.757345561972D+13
I= 19 X= 8.983287627151D+13 Y= 1.286849019072D+14 Z= 3.543217096341D+13
I= 20 X= 3.080881974710D+12 Y= 3.389899856672D+13 Z= -9.100615763882D+12
I= 21 X= -6.996689326868D+12 Y= 6.308494618618D+12 Z= -2.145262037735D+12
I= 22 X= -2.719426589545D+13 Y= -1.713919360554D+13 Z= 4.607833738350D+13
I= 23 X= -5.204866968560D+12 Y= 4.579949093693D+13 Z= -3.341477356298D+12
I= 24 X= 1.485007260554D+14 Y= -1.106077780189D+14 Z= -3.374271187749D+13
I= 25 X= -1.267008068050D+13 Y= -1.443199157034D+12 Z= 2.431805904225D+13
I= 26 X= 5.284756081913D+13 Y= -6.821619527672D+13 Z= -3.095447549940D+13
I= 27 X= -1.398029789129D+13 Y= 4.392952487539D+12 Z= -9.530066802333D+13
I= 28 X= 5.410313722016D+13 Y= 4.870967955026D+13 Z= -6.101693062718D+13
I= 29 X= -3.294882610541D+12 Y= -1.962936082088D+13 Z= 2.789600792692D+13
I= 30 X= -5.712739940271D+12 Y= 1.356232719892D+12 Z= -2.299223684457D+13
I= 31 X= 8.010753772774D+13 Y= 5.299471420685D+13 Z= -2.767547589780D+13
I= 32 X= 1.045384303966D+14 Y= 1.753305902432D+13 Z= -4.586682797016D+13

I= 33 X= 1.058883985717D+13 Y= 2.367424665103D+13 Z= -1.146727676911D+13
I= 34 X= -8.851736514695D+13 Y= 1.556367364959D+13 Z= 4.689342299780D+13
I= 35 X= 1.743920968552D+12 Y= -8.311540272605D+11 Z= 1.210395401650D+12
I= 36 X= 1.709092139289D+12 Y= 4.386997907909D+12 Z= -1.093314011732D+13
I= 37 X= 5.628601759057D+13 Y= 1.284880342769D+13 Z= 2.351493947439D+13
I= 38 X= -7.105813795249D+13 Y= 6.083559918194D+13 Z= 5.962735668300D+13

Backward Direction:

Total Energy: -651.6036918 Hartrees

Potential Energy: -651.8067583 Hartress

Kinetic Energy: 0.2030665 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -1.675460172630D+13 Y= -2.451553131247D+12 Z= -3.733213407867D+11
I= 1 X= -2.266079924183D+13 Y= -3.360809725569D+12 Z= -2.901683214285D+13
I= 2 X= -6.217082001743D+11 Y= 7.746532654217D+12 Z= -2.374655884350D+12
I= 3 X= -6.966574918216D+12 Y= -1.600165249382D+13 Z= 1.669876659026D+13
I= 4 X= 6.238609211170D+12 Y= 1.168395118360D+13 Z= 4.461151323241D+12
I= 5 X= -3.513922784473D+12 Y= -1.695753677931D+13 Z= 6.160863892508D+12
I= 6 X= -1.098995096882D+13 Y= 2.691958749423D+12 Z= 9.058749519201D+13
I= 7 X= -3.777714848032D+13 Y= -2.796628001189D+13 Z= -7.058692806528D+13
I= 8 X= 2.447881443002D+12 Y= 1.748958456823D+14 Z= 2.672703420778D+13
I= 9 X= 9.682079044087D+12 Y= -1.048848026617D+13 Z= -9.971854772956D+12
I= 10 X= 8.116300170833D+13 Y= 9.960609253377D+13 Z= -5.990282599424D+13
I= 11 X= 2.179705421812D+13 Y= -4.369434329820D+13 Z= -5.457480076382D+13
I= 12 X= -1.070205982719D+14 Y= -5.490233504713D+12 Z= 7.845892398380D+13
I= 13 X= 3.271748319767D+12 Y= 3.127574110764D+13 Z= -1.882735428447D+12
I= 14 X= -1.459711335349D+14 Y= -4.981773050324D+13 Z= 4.008011149101D+13
I= 15 X= 9.431164699724D+13 Y= -5.646344071738D+13 Z= 3.497527841428D+13
I= 16 X= 2.114086448187D+13 Y= -6.726647768880D+13 Z= -3.278933289578D+13
I= 17 X= 1.386297515905D+13 Y= -1.197602540219D+12 Z= -1.746061569843D+13
I= 18 X= -2.750881343272D+13 Y= 3.728368288973D+13 Z= -8.801121373590D+13

I= 19 X= 8.983246034080D+13 Y= 1.285225422430D+14 Z= 3.561727772214D+13
I= 20 X= 3.300618748016D+12 Y= 3.362140634539D+13 Z= -9.191174436811D+12
I= 21 X= -7.373335405779D+12 Y= 6.314881274922D+12 Z= -2.719389496191D+12
I= 22 X= -2.744504262333D+13 Y= -1.659385776665D+13 Z= 4.471921624569D+13
I= 23 X= -4.966095554470D+12 Y= 4.559021832502D+13 Z= -3.822801097143D+12
I= 24 X= 1.480033169399D+14 Y= -1.106221310514D+14 Z= -3.442019006899D+13
I= 25 X= -1.267273525590D+13 Y= -1.514598869022D+12 Z= 2.415862478792D+13
I= 26 X= 5.255822048917D+13 Y= -6.862650445737D+13 Z= -3.106870003424D+13
I= 27 X= -1.372695120348D+13 Y= 4.628420055018D+12 Z= -9.539361411458D+13
I= 28 X= 5.416305365170D+13 Y= 4.869999049127D+13 Z= -6.072485955209D+13
I= 29 X= -4.282327974498D+12 Y= -1.904633810259D+13 Z= 2.713874332292D+13
I= 30 X= -5.635830308530D+12 Y= 1.522186816605D+12 Z= -2.357447500309D+13
I= 31 X= 8.018582998384D+13 Y= 5.245644589426D+13 Z= -2.803630035912D+13
I= 32 X= 1.032827680939D+14 Y= 1.866972902913D+13 Z= -4.703968742716D+13
I= 33 X= 1.076299074721D+13 Y= 2.359711723336D+13 Z= -1.206054150170D+13
I= 34 X= -8.792814203805D+13 Y= 1.547452614740D+13 Z= 4.651208479553D+13
I= 35 X= 1.506256426826D+12 Y= -9.278754030868D+11 Z= 2.134974768755D+12
I= 36 X= -1.168207441684D+12 Y= 9.488842000608D+11 Z= -1.265881326064D+13
I= 37 X= 5.962979142087D+13 Y= 1.500263002118D+13 Z= 1.926742711472D+13
I= 38 X= -6.903317875826D+13 Y= 6.069893642799D+13 Z= 5.688430372439D+13

Seed: 834740114

CM Start Point Coordinates: bohr

I= 0 X= -2.893572103813D+00 Y= 2.365631778755D+00 Z= -6.831395148087D-01
I= 1 X= -3.024982943033D+00 Y= -1.156944698954D-01 Z= -2.025042305816D+00
I= 2 X= -2.445782366052D+00 Y= 1.892426116778D+00 Z= 2.042246629062D+00
I= 3 X= -2.915973704714D+00 Y= -2.008179821366D+00 Z= -1.260697574466D-01
I= 4 X= -2.434090170839D+00 Y= -6.736954767186D-01 Z= 2.384944318300D+00
I= 5 X= 4.180345533315D+00 Y= 2.377056683017D+00 Z= -9.242577412912D-01
I= 6 X= 2.260649347324D+00 Y= 9.084086553423D-01 Z= -2.572619470723D+00

I= 7 X= 5.844663213360D+00 Y= 1.468428755454D+00 Z= -1.562287388675D+00
I= 8 X= 4.101255853806D+00 Y= 4.190192047118D+00 Z= -1.942835324303D+00
I= 9 X= -2.411659541065D+00 Y= -2.252903212374D+00 Z= 4.767203135928D+00
I= 10 X= -3.907438459251D+00 Y= -1.000254339087D+00 Z= 6.140305651291D+00
I= 11 X= -2.686064874587D+00 Y= -4.423680229821D+00 Z= 4.640892268082D+00
I= 12 X= -4.978145916025D-01 Y= -1.874465434883D+00 Z= 5.836773368589D+00
I= 13 X= -2.176509312859D+00 Y= 3.835800393010D+00 Z= 4.086311182977D+00
I= 14 X= -3.845350349832D+00 Y= 3.589866498402D+00 Z= 5.419054163645D+00
I= 15 X= -2.578898962605D-01 Y= 3.583866392213D+00 Z= 5.225651293169D+00
I= 16 X= -2.197644568474D+00 Y= 6.123226952192D+00 Z= 3.596034657536D+00
I= 17 X= -2.728697073071D+00 Y= 4.852761099082D+00 Z= -1.840536605044D+00
I= 18 X= -4.659155700188D+00 Y= 6.008580590917D+00 Z= -1.679025581106D+00
I= 19 X= -1.131322449463D+00 Y= 6.189430938391D+00 Z= -1.108880478403D+00
I= 20 X= -2.497237771479D+00 Y= 4.912184356762D+00 Z= -3.896757453303D+00
I= 21 X= -3.451727551720D+00 Y= -6.906832079121D-01 Z= -4.703338529066D+00
I= 22 X= -5.612116139981D+00 Y= 4.217114105693D-01 Z= -5.246279158327D+00
I= 23 X= -1.886397419370D+00 Y= 4.660957721325D-01 Z= -6.036282406056D+00
I= 24 X= -3.666229466511D+00 Y= -2.750572940192D+00 Z= -5.299499274005D+00
I= 25 X= -3.312309212040D+00 Y= -4.687189580804D+00 Z= -6.267984985291D-01
I= 26 X= -2.463538680505D+00 Y= -5.136178135788D+00 Z= -2.576809657046D+00
I= 27 X= -2.477816585223D+00 Y= -5.768606601083D+00 Z= 1.003006460199D+00
I= 28 X= -5.216220163382D+00 Y= -5.217555328182D+00 Z= -8.211919916380D-01
I= 29 X= 3.047627689473D+00 Y= -3.315431220818D+00 Z= -1.799255722367D+00
I= 30 X= 3.144470705152D+00 Y= -3.277043150450D+00 Z= 8.669640765655D-01
I= 31 X= 1.647589433571D+00 Y= -4.364410897572D+00 Z= -2.997254898963D+00
I= 32 X= 4.360070323846D+00 Y= -2.671901194559D+00 Z= -3.062891808481D+00
I= 33 X= 4.831973387111D+00 Y= -2.771256759764D+00 Z= 1.981761258454D+00
I= 34 X= 1.633394685691D+00 Y= -4.435664475245D+00 Z= 2.077722227430D+00
I= 35 X= 8.978690847494D-01 Y= -2.775735400564D-02 Z= -2.062941832669D-01
I= 36 X= 3.826086427668D+00 Y= 2.007215758742D+00 Z= 1.645846655700D+00

I= 37 X= 5.337689837918D+00 Y= 9.694275159236D-01 Z= 2.710347868057D+00

I= 38 X= 2.968829477218D+00 Y= 3.205719956175D+00 Z= 3.173847281442D+00

Forward Direction:

Total Energy: -651.6095807 Hartrees

Potential Energy: -651.8139111 Hartress

Kinetic Energy: 0.2043304 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.625388254172D+12 Y= -4.154148848825D+12 Z= -2.673694654038D+13

I= 1 X= -9.047308643530D+12 Y= 2.825234031740D+13 Z= 7.451023930670D+12

I= 2 X= -1.836694867994D+12 Y= -7.021650951200D+12 Z= 5.930126501082D+12

I= 3 X= -4.471743623636D+11 Y= -4.347677353560D+12 Z= -4.723204285403D+12

I= 4 X= 4.719034394152D+12 Y= 1.139797201321D+13 Z= -4.480188158085D+12

I= 5 X= -1.213189177117D+13 Y= 1.796356420684D+13 Z= 1.607231869883D+13

I= 6 X= 3.672844810158D+13 Y= 3.398462904581D+13 Z= 3.236060332546D+13

I= 7 X= -3.112020792950D+12 Y= -3.055017551296D+13 Z= 5.994943451143D+13

I= 8 X= -7.564405879896D+13 Y= -1.940652595130D+14 Z= 7.936696143086D+13

I= 9 X= 7.969070984623D+10 Y= -5.392195332465D+12 Z= 6.612001459837D+12

I= 10 X= 1.564622090697D+14 Y= -3.399313591975D+13 Z= -7.667148522237D+12

I= 11 X= -5.284398229332D+13 Y= 8.472205494798D+13 Z= 8.420482092963D+13

I= 12 X= 5.182303794842D+13 Y= 1.034487355085D+13 Z= 4.279805983903D+13

I= 13 X= 2.832522315365D+13 Y= -3.734732502352D+12 Z= -1.724667357009D+13

I= 14 X= -6.676708105245D+13 Y= 1.803784586091D+13 Z= 5.847930576531D+13

I= 15 X= -3.979199297454D+13 Y= -4.250116523667D+13 Z= 1.077947402878D+14

I= 16 X= -7.374532601339D+13 Y= -1.019987835372D+14 Z= -6.930555270680D+13

I= 17 X= -8.355155399662D+12 Y= -1.755687373776D+12 Z= -6.409549146264D+12

I= 18 X= -1.572355552235D+13 Y= 2.877850716175D+13 Z= -6.080239531065D+13

I= 19 X= -4.548695646996D+13 Y= -1.639438465900D+13 Z= -4.181598663605D+13

I= 20 X= -9.780006333186D+13 Y= -5.846118962349D+13 Z= 1.403719160392D+14

I= 21 X= 1.876911364196D+13 Y= 4.696693187591D+12 Z= 7.876835628042D+12

I= 22 X= 1.234311461209D+13 Y= -3.871632029811D+13 Z= -4.026259777760D+13

I= 23 X= 2.307223997002D+13 Y= 1.011775944731D+14 Z= -5.148841127688D+13
I= 24 X= 3.021021638170D+12 Y= -6.784796221772D+13 Z= 3.809558312438D+12
I= 25 X= 8.394568910177D+12 Y= -1.546097934053D+12 Z= -2.884288010758D+12
I= 26 X= -6.732073284534D+13 Y= -2.775264227901D+13 Z= 2.326041943283D+13
I= 27 X= 8.108981610695D+12 Y= 7.537140843996D+13 Z= -8.025302870354D+13
I= 28 X= -4.740351379318D+13 Y= -7.410333922932D+13 Z= -6.358286661390D+13
I= 29 X= 2.506675786762D+12 Y= 1.083468471407D+13 Z= 1.493187772173D+13
I= 30 X= 3.789433607631D+12 Y= 2.624086713086D+12 Z= -8.280584748767D+12
I= 31 X= -1.191291916825D+13 Y= -9.114416111915D+12 Z= 5.977403404886D+13
I= 32 X= 4.826660547323D+13 Y= -3.002353766738D+13 Z= -8.595119139195D+13
I= 33 X= 6.533130217557D+13 Y= -9.229053681751D+12 Z= -4.381177878243D+13
I= 34 X= -4.784773653622D+13 Y= -1.774941003176D+14 Z= 8.160940220702D+13
I= 35 X= -1.393164953143D+12 Y= -1.461053119421D+11 Z= -4.028918871331D+11
I= 36 X= 9.427295657166D+11 Y= 4.893779801455D+12 Z= -4.490847942630D+12
I= 37 X= 1.186110881560D+14 Y= -2.039391348893D+13 Z= 3.504866676364D+13
I= 38 X= 3.018291163387D+13 Y= -1.942348716680D+13 Z= 8.263973295999D+12

Backward Direction:

Total Energy: -651.6095866 Hartrees

Potential Energy: -651.8139111 Hartress

Kinetic Energy: 0.2043244 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= -5.801178080046D+12 Y= -4.205865468877D+12 Z= -2.674080992792D+13
I= 1 X= -8.959681692780D+12 Y= 2.806478421603D+13 Z= 7.139111043974D+12
I= 2 X= -1.950741388803D+12 Y= -6.849790121219D+12 Z= 5.661475692381D+12
I= 3 X= -5.187749750785D+11 Y= -4.331845267191D+12 Z= -5.099617143499D+12
I= 4 X= 5.276436569729D+12 Y= 1.135258789965D+13 Z= -4.837223145402D+12
I= 5 X= -1.209378212171D+13 Y= 1.770312600482D+13 Z= 1.373708915196D+13
I= 6 X= 5.216035112541D+13 Y= 4.818543414947D+13 Z= 3.906716220978D+13
I= 7 X= 5.597442751777D+10 Y= -2.755580590940D+13 Z= 6.023998271489D+13
I= 8 X= -7.135351333765D+13 Y= -1.905543378699D+14 Z= 8.016912644385D+13

I= 9 X= 2.745311652660D+11 Y= -5.307996143085D+12 Z= 6.400000520443D+12
I= 10 X= 1.565275150236D+14 Y= -3.356431768526D+13 Z= -8.164165486551D+12
I= 11 X= -5.288947626518D+13 Y= 8.472515498017D+13 Z= 8.417376857830D+13
I= 12 X= 5.195677200489D+13 Y= 1.037943076256D+13 Z= 4.267014128496D+13
I= 13 X= 2.836273417386D+13 Y= -3.760607945234D+12 Z= -1.733948266130D+13
I= 14 X= -6.671389269897D+13 Y= 1.787865766458D+13 Z= 5.848856440676D+13
I= 15 X= -3.966167795856D+13 Y= -4.263244815059D+13 Z= 1.075737776187D+14
I= 16 X= -7.377064298608D+13 Y= -1.019632530363D+14 Z= -6.927955918642D+13
I= 17 X= -8.292059640566D+12 Y= -1.812484748652D+12 Z= -6.434428235933D+12
I= 18 X= -1.565645558449D+13 Y= 2.874393863447D+13 Z= -6.095060495932D+13
I= 19 X= -4.548709724141D+13 Y= -1.644935401982D+13 Z= -4.175331593024D+13
I= 20 X= -9.772566811947D+13 Y= -5.855517271093D+13 Z= 1.403412560114D+14
I= 21 X= 1.864159436512D+13 Y= 4.698855484858D+12 Z= 7.682456008804D+12
I= 22 X= 1.225821032804D+13 Y= -3.853168851901D+13 Z= -4.072274900681D+13
I= 23 X= 2.315307969333D+13 Y= 1.011067420278D+14 Z= -5.165137077899D+13
I= 24 X= 2.852616194241D+12 Y= -6.785282165953D+13 Z= 3.580187728686D+12
I= 25 X= 8.393670157126D+12 Y= -1.570271395153D+12 Z= -2.938266911714D+12
I= 26 X= -6.741869343245D+13 Y= -2.789155871783D+13 Z= 2.322174697332D+13
I= 27 X= 8.194755988868D+12 Y= 7.545112958615D+13 Z= -8.028449701733D+13
I= 28 X= -4.738322817514D+13 Y= -7.410661960276D+13 Z= -6.348398149771D+13
I= 29 X= 2.172361083256D+12 Y= 1.103207596092D+13 Z= 1.467549422460D+13
I= 30 X= 3.815472537848D+12 Y= 2.680273007577D+12 Z= -8.477710368381D+12
I= 31 X= -1.188641212216D+13 Y= -9.296655068313D+12 Z= 5.965187141378D+13
I= 32 X= 4.784148183054D+13 Y= -2.963870067185D+13 Z= -8.634828087143D+13
I= 33 X= 6.539026361829D+13 Y= -9.255167024988D+12 Z= -4.401263761262D+13
I= 34 X= -4.764824605433D+13 Y= -1.775242825698D+14 Z= 8.148029433201D+13
I= 35 X= -1.473629914244D+12 Y= -1.788518122150D+11 Z= -8.986142302150D+10
I= 36 X= -3.142415465501D+10 Y= 3.729753901289D+12 Z= -5.075100938284D+12
I= 37 X= 1.197431738506D+14 Y= -1.966470259799D+13 Z= 3.361060658746D+13
I= 38 X= 3.086849248663D+13 Y= -1.946975642784D+13 Z= 7.335270828424D+12

Seed: 8789762236

CM Start Point Coordinates: bohr

I= 0 X= -2.448083940088D+00 Y= 2.391059836569D+00 Z= -5.699677762583D-01
I= 1 X= -3.312378156539D+00 Y= 2.022682221744D-01 Z= -2.027611342512D+00
I= 2 X= -2.289100792946D+00 Y= 1.535345565574D+00 Z= 2.094544258594D+00
I= 3 X= -2.975072949998D+00 Y= -2.012936546260D+00 Z= -4.520264760387D-01
I= 4 X= -2.415054599414D+00 Y= -1.081533269451D+00 Z= 2.159914626933D+00
I= 5 X= 4.234204888170D+00 Y= 1.996377748924D+00 Z= -1.843341064059D+00
I= 6 X= 2.526145338153D+00 Y= 1.545448889599D-01 Z= -2.766231182147D+00
I= 7 X= 6.002370266320D+00 Y= 1.100130743466D+00 Z= -2.361765129950D+00
I= 8 X= 3.630283929082D+00 Y= 3.388255475423D+00 Z= -3.555722844725D+00
I= 9 X= -2.307470441903D+00 Y= -2.647782413826D+00 Z= 4.555121090674D+00
I= 10 X= -4.357923556388D+00 Y= -3.156005053208D+00 Z= 4.891046698551D+00
I= 11 X= -7.616126010542D-01 Y= -4.287029039641D+00 Z= 4.772784849286D+00
I= 12 X= -1.738949952180D+00 Y= -1.121653011512D+00 Z= 6.210375837779D+00
I= 13 X= -1.888134142239D+00 Y= 3.252001051404D+00 Z= 4.278972444360D+00
I= 14 X= -3.591320598669D+00 Y= 3.621996765565D+00 Z= 5.485375405000D+00
I= 15 X= -2.019902983713D-01 Y= 2.782879407297D+00 Z= 5.533556174175D+00
I= 16 X= -1.422087320179D+00 Y= 5.384668781283D+00 Z= 3.789357906974D+00
I= 17 X= -2.580702512155D+00 Y= 5.021920059464D+00 Z= -1.521608783302D+00
I= 18 X= -4.327116128757D+00 Y= 6.191003242676D+00 Z= -1.219631081256D+00
I= 19 X= -9.132644251285D-01 Y= 6.251167363861D+00 Z= -7.564534796242D-01
I= 20 X= -2.384864688065D+00 Y= 4.516890428751D+00 Z= -3.701836831111D+00
I= 21 X= -3.911201098759D+00 Y= 2.271141810668D-01 Z= -4.698043348544D+00
I= 22 X= -5.946150706049D+00 Y= 1.389601129512D+00 Z= -5.199182462277D+00
I= 23 X= -2.306018888551D+00 Y= 1.369638966091D+00 Z= -5.714183693414D+00
I= 24 X= -4.228511869912D+00 Y= -2.072812791803D+00 Z= -5.676663370353D+00
I= 25 X= -3.292183658099D+00 Y= -4.654771945792D+00 Z= -1.197241434849D+00
I= 26 X= -1.777956445863D+00 Y= -5.359876249372D+00 Z= -3.068982909489D+00

I= 27 X= -3.049937056329D+00 Y= -6.053393602688D+00 Z= 6.718518525866D-01
I= 28 X= -5.478422095701D+00 Y= -5.105483464959D+00 Z= -1.827286903697D+00
I= 29 X= 3.066103452203D+00 Y= -3.708485049188D+00 Z= -3.435389461086D-01
I= 30 X= 3.177214211479D+00 Y= -2.712168240656D+00 Z= 2.175057605377D+00
I= 31 X= 1.816947769023D+00 Y= -5.618119276070D+00 Z= -7.167141447144D-01
I= 32 X= 4.479469450695D+00 Y= -3.310177927859D+00 Z= -1.812259013859D+00
I= 33 X= 4.892129851862D+00 Y= -1.957148796553D+00 Z= 3.050162381434D+00
I= 34 X= 2.198497569404D+00 Y= -3.365564504121D+00 Z= 3.748636796930D+00
I= 35 X= 8.810203779534D-01 Y= -5.921016118449D-02 Z= -2.264485040950D-01
I= 36 X= 3.608676959095D+00 Y= 2.971151717182D+00 Z= 7.554941003376D-01
I= 37 X= 4.699623576862D+00 Y= 2.523634929416D+00 Z= 2.493639984148D+00
I= 38 X= 2.311945308064D+00 Y= 4.787431521017D+00 Z= 1.011995577288D+00

Forward Direction:

Total Energy: -651.6030950 Hartrees

Potential Energy: -651.7782806 Hartress

Kinetic Energy: 0.1751857 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.674178177281D+13 Y= -9.896728986174D+11 Z= 7.790796099432D+12
I= 1 X= 3.246892656566D+12 Y= 2.975508931952D+13 Z= -1.363285169441D+13
I= 2 X= 9.707928627154D+11 Y= 1.596489332693D+13 Z= 4.219699618470D+12
I= 3 X= -1.320277371716D+13 Y= -2.235894957112D+13 Z= 2.384085694157D+13
I= 4 X= -4.284416338844D+12 Y= -3.954449600044D+11 Z= -2.308182296457D+13
I= 5 X= 6.618048898645D+12 Y= -1.611020551107D+13 Z= -3.743120279726D+12
I= 6 X= -2.030795151519D+13 Y= -4.899411705728D+13 Z= -5.635930386785D+13
I= 7 X= 4.980898775961D+13 Y= 2.476036977653D+13 Z= 2.687755921496D+13
I= 8 X= -7.046828848409D+13 Y= 8.191469285177D+13 Z= -6.792428205084D+13
I= 9 X= -9.043193180571D+12 Y= 5.843526190473D+12 Z= 9.362547746145D+12
I= 10 X= -6.138346677668D+12 Y= 7.178216488412D+12 Z= 4.267563179999D+12
I= 11 X= 3.258792885539D+13 Y= -7.661439238552D+13 Z= -8.283812761469D+13
I= 12 X= -5.372886086530D+13 Y= 9.229198152557D+12 Z= 1.917371873143D+13

I= 13 X= -3.653537383763D+12 Y= 1.056917987599D+13 Z= 4.956145723804D+12
I= 14 X= -1.188510924466D+14 Y= 1.677902890748D+13 Z= 9.599621625191D+13
I= 15 X= 3.372046370177D+13 Y= -6.181889706578D+13 Z= 2.844224736908D+13
I= 16 X= -1.525085853312D+13 Y= -4.377233538899D+13 Z= -4.478996037170D+13
I= 17 X= 1.208776790817D+13 Y= -5.383500211615D+12 Z= -3.388428412404D+12
I= 18 X= 1.178257977774D+14 Y= -1.132853746220D+14 Z= 1.969341878110D+13
I= 19 X= 5.160816542170D+13 Y= 4.721084390250D+13 Z= 2.602835275865D+13
I= 20 X= -2.859593419570D+13 Y= -1.040313261009D+14 Z= 8.347475413873D+13
I= 21 X= -7.120441880442D+12 Y= -1.049340410303D+13 Z= -2.443875734311D+11
I= 22 X= 5.952502194314D+13 Y= 3.815366913999D+12 Z= -1.042462703984D+13
I= 23 X= 2.218533850916D+13 Y= 6.364662739347D+13 Z= -3.215816932930D+13
I= 24 X= 2.045907940523D+13 Y= -8.795947179154D+13 Z= 1.775393741487D+13
I= 25 X= -2.436566276703D+13 Y= 1.394743895128D+13 Z= -3.476909381252D+12
I= 26 X= 7.096966374359D+12 Y= -5.076562567903D+13 Z= -2.269837289975D+13
I= 27 X= -5.859533543797D+13 Y= -2.592150399147D+13 Z= 6.888180324976D+12
I= 28 X= 1.985480526945D+14 Y= 3.418311775518D+13 Z= 3.840807901178D+12
I= 29 X= -1.670935872206D+13 Y= -6.892590253367D+12 Z= -4.988682168975D+12
I= 30 X= -1.507306337251D+13 Y= 8.816757553928D+12 Z= -1.446417923881D+13
I= 31 X= 5.099339862650D+13 Y= 8.487680018991D+13 Z= 1.756902424177D+13
I= 32 X= 2.288950912270D+13 Y= 3.899314678724D+13 Z= 3.149423642718D+13
I= 33 X= 3.932059405620D+12 Y= -7.498469278053D+12 Z= -7.754444544096D+13
I= 34 X= 6.372951168683D+13 Y= 3.832337559761D+13 Z= -1.063291516134D+14
I= 35 X= 2.642064748119D+12 Y= -1.193208480743D+12 Z= 1.263153230154D+12
I= 36 X= -1.495848146462D+13 Y= 7.872099717324D+12 Z= 2.166877350172D+12
I= 37 X= -2.039657394563D+13 Y= 9.828923509539D+13 Z= 1.142428896114D+11
I= 38 X= -2.989756352245D+13 Y= -5.901468858586D+13 Z= 5.243586883368D+13

Backward Direction:

Total Energy: -651.6031318 Hartrees

Potential Energy: -651.7782806 Hartress

Kinetic Energy: 0.1751489 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.625274101182D+13 Y= -1.133546611307D+12 Z= 7.780048301744D+12
I= 1 X= 3.490667566971D+12 Y= 2.923331522709D+13 Z= -1.450058173181D+13
I= 2 X= 6.535196854515D+11 Y= 1.644300375743D+13 Z= 3.472323070443D+12
I= 3 X= -1.340196394890D+13 Y= -2.231490529928D+13 Z= 2.279369038015D+13
I= 4 X= -2.733744240005D+12 Y= -5.217018762139D+11 Z= -2.407508101075D+13
I= 5 X= 6.724068544501D+12 Y= -1.683473491381D+13 Z= -1.023964195738D+13
I= 6 X= 2.262302825735D+13 Y= -9.488005878896D+12 Z= -3.770190669924D+13
I= 7 X= 5.862223255044D+13 Y= 3.309059451833D+13 Z= 2.768585350223D+13
I= 8 X= -5.853215069237D+13 Y= 9.168194614861D+13 Z= -6.569268885851D+13
I= 9 X= -8.501154317203D+12 Y= 6.077765197148D+12 Z= 8.772769019548D+12
I= 10 X= -5.956667983954D+12 Y= 8.371172859011D+12 Z= 2.884880461984D+12
I= 11 X= 3.246136628003D+13 Y= -7.660576821695D+13 Z= -8.292451410175D+13
I= 12 X= -5.335681774073D+13 Y= 9.325335018115D+12 Z= 1.881785408276D+13
I= 13 X= -3.549183105719D+12 Y= 1.049719534605D+13 Z= 4.697954294874D+12
I= 14 X= -1.187031244114D+14 Y= 1.633617325093D+13 Z= 9.602197346084D+13
I= 15 X= 3.408299525139D+13 Y= -6.218412125998D+13 Z= 2.782753745119D+13
I= 16 X= -1.532128940957D+13 Y= -4.367349085879D+13 Z= -4.471764735126D+13
I= 17 X= 1.226329793696D+13 Y= -5.541508403329D+12 Z= -3.457641128657D+12
I= 18 X= 1.180124672469D+14 Y= -1.133815430669D+14 Z= 1.928110492467D+13
I= 19 X= 5.160777366048D+13 Y= 4.705792123747D+13 Z= 2.620270037193D+13
I= 20 X= -2.838896940743D+13 Y= -1.042927835449D+14 Z= 8.338945910055D+13
I= 21 X= -7.475195775258D+12 Y= -1.048738866722D+13 Z= -7.851444359166D+11
I= 22 X= 5.928882136575D+13 Y= 4.329005611085D+12 Z= -1.170475059378D+13
I= 23 X= 2.241023154121D+13 Y= 6.344951856533D+13 Z= -3.261151659216D+13
I= 24 X= 1.999058174331D+13 Y= -8.797299055387D+13 Z= 1.711583697395D+13
I= 25 X= -2.436816304691D+13 Y= 1.388018927715D+13 Z= -3.627076677041D+12
I= 26 X= 6.824443662736D+12 Y= -5.115208603961D+13 Z= -2.280595824833D+13
I= 27 X= -5.835671426862D+13 Y= -2.569972274129D+13 Z= 6.800636629439D+12
I= 28 X= 1.986044865451D+14 Y= 3.417399185409D+13 Z= 4.115902633923D+12

I= 29 X= -1.763940979952D+13 Y= -6.343455159768D+12 Z= -5.701931510773D+12
I= 30 X= -1.500062403989D+13 Y= 8.973065731662D+12 Z= -1.501257537536D+13
I= 31 X= 5.106714021519D+13 Y= 8.436981819380D+13 Z= 1.722917235150D+13
I= 32 X= 2.170683095165D+13 Y= 4.006374896302D+13 Z= 3.038954827412D+13
I= 33 X= 4.096087947041D+12 Y= -7.571115629377D+12 Z= -7.810322724303D+13
I= 34 X= 6.428448677943D+13 Y= 3.823940970649D+13 Z= -1.066883249048D+14
I= 35 X= 2.418214224257D+12 Y= -1.284308020520D+12 Z= 2.133992330375D+12
I= 36 X= -1.766854083269D+13 Y= 4.633822987000D+12 Z= 5.415072578063D+11
I= 37 X= -1.724715367997D+13 Y= 1.003178726366D+14 Z= -3.886386988115D+12
I= 38 X= -2.799030308114D+13 Y= -5.914340794916D+13 Z= 4.985225312612D+13

Seed: 9370370777

CM Start Point Coordinates: bohr

I= 0 X= -2.518084978858D+00 Y= 2.350863025673D+00 Z= -7.427067208807D-01
I= 1 X= -3.041074674891D+00 Y= -4.588745436743D-02 Z= -2.086268180309D+00
I= 2 X= -2.501193812089D+00 Y= 1.660932656249D+00 Z= 2.045605803130D+00
I= 3 X= -3.081331155878D+00 Y= -1.987640773007D+00 Z= -2.530638556574D-01
I= 4 X= -2.561382518099D+00 Y= -8.758291091198D-01 Z= 2.394385376096D+00
I= 5 X= 4.218617520447D+00 Y= 2.258102246660D+00 Z= -1.306923843836D+00
I= 6 X= 2.393992760469D+00 Y= 6.602654323810D-01 Z= -2.933224055390D+00
I= 7 X= 5.856991929623D+00 Y= 1.326165698105D+00 Z= -2.078486245661D+00
I= 8 X= 3.213431166184D+00 Y= 3.565540706860D+00 Z= -2.647437550453D+00
I= 9 X= -2.249054032014D+00 Y= -2.359751981987D+00 Z= 4.759301792534D+00
I= 10 X= -3.831776615240D+00 Y= -1.683004492935D+00 Z= 6.086988624288D+00
I= 11 X= -2.638290822287D+00 Y= -4.452501650838D+00 Z= 4.313666081629D+00
I= 12 X= -1.391136059566D-01 Y= -2.041411040532D+00 Z= 5.343893726887D+00
I= 13 X= -2.388618343966D+00 Y= 3.558226856508D+00 Z= 4.227625418343D+00
I= 14 X= -4.072109305281D+00 Y= 3.334390299641D+00 Z= 5.602670169690D+00
I= 15 X= -5.863515758517D-01 Y= 3.269364553889D+00 Z= 5.605699398911D+00
I= 16 X= -2.498772716765D+00 Y= 5.643658185964D+00 Z= 3.699908695481D+00

I= 17 X= -2.295840496660D+00 Y= 4.856474946978D+00 Z= -2.010431779951D+00
I= 18 X= -4.094536336309D+00 Y= 5.846774944071D+00 Z= -2.460548942828D+00
I= 19 X= -1.683264260597D+00 Y= 6.054777123372D+00 Z= -6.792524228704D-01
I= 20 X= -1.289222938717D+00 Y= 4.655560912378D+00 Z= -3.847233507755D+00
I= 21 X= -3.815348327641D+00 Y= -8.167089773132D-02 Z= -4.868990016782D+00
I= 22 X= -5.999909317196D+00 Y= 3.643831769463D-01 Z= -4.395649438444D+00
I= 23 X= -2.761771697721D+00 Y= 1.144272830766D+00 Z= -5.855203689262D+00
I= 24 X= -3.498661044542D+00 Y= -1.793513621467D+00 Z= -6.152066970620D+00
I= 25 X= -3.514279767222D+00 Y= -4.670969367531D+00 Z= -8.427482527068D-01
I= 26 X= -2.817603547760D+00 Y= -5.338236938774D+00 Z= -2.841625377776D+00
I= 27 X= -2.239663714176D+00 Y= -5.415453193420D+00 Z= 6.749694744796D-01
I= 28 X= -5.249930130064D+00 Y= -5.051994504791D+00 Z= -8.752131038390D-01
I= 29 X= 2.818645757793D+00 Y= -3.388665504968D+00 Z= -1.373824953379D+00
I= 30 X= 3.517465314129D+00 Y= -3.092233776989D+00 Z= 1.136310564571D+00
I= 31 X= 1.095396960664D+00 Y= -4.815795035075D+00 Z= -2.128742966503D+00
I= 32 X= 4.235580559404D+00 Y= -2.775262607162D+00 Z= -2.483065022787D+00
I= 33 X= 5.175557720539D+00 Y= -1.861880277824D+00 Z= 1.776001632726D+00
I= 34 X= 2.867031810816D+00 Y= -4.192616573975D+00 Z= 2.819444415358D+00
I= 35 X= 9.109150971925D-01 Y= -6.963650859605D-02 Z= -1.438177089064D-01
I= 36 X= 3.684473405322D+00 Y= 2.690088928135D+00 Z= 1.151080547896D+00
I= 37 X= 4.753116488387D+00 Y= 1.995054322256D+00 Z= 2.662067288054D+00
I= 38 X= 2.846556769927D+00 Y= 4.511192959468D+00 Z= 1.783997729283D+00

Forward Direction:

Total Energy: -651.6189702 Hartrees

Potential Energy: -651.7880888 Hartress

Kinetic Energy: 0.1691186 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.898912613336D+13 Y= 1.992830134854D+13 Z= -2.130126961745D+13

I= 1 X= -2.119817126040D+13 Y= -7.658373177672D+12 Z= -1.555355688668D+13

I= 2 X= 1.749471825316D+13 Y= -4.132702980729D+12 Z= -2.351838619511D+12

I= 3 X= 2.292558832791D+13 Y= 1.331176952597D+13 Z= 7.579013118602D+12
I= 4 X= 1.485923819987D+12 Y= -2.385633025436D+13 Z= -9.600777959496D+12
I= 5 X= 6.401476513363D+12 Y= 1.249281747831D+12 Z= 1.751748564344D+13
I= 6 X= -3.887378783853D+13 Y= -3.404649416891D+13 Z= 2.997307521865D+13
I= 7 X= -1.217614681437D+14 Y= 1.011159387245D+14 Z= 2.116797871065D+13
I= 8 X= 2.339734158667D+13 Y= -6.337380530028D+13 Z= -7.907096040992D+13
I= 9 X= -5.032047183536D+12 Y= 1.051123843299D+13 Z= -3.623303940820D+12
I= 10 X= 1.228544281056D+14 Y= 2.209564961858D+13 Z= -1.392963490029D+12
I= 11 X= -3.370467954841D+13 Y= 2.437208564646D+13 Z= -4.884949581963D+13
I= 12 X= 3.216183566784D+13 Y= 6.146095227558D+13 Z= -4.632250199786D+13
I= 13 X= -2.604585555640D+12 Y= 1.608697000793D+13 Z= 3.286190988832D+12
I= 14 X= -1.307646217893D+14 Y= 6.507558198975D+13 Z= 2.253779097442D+13
I= 15 X= 4.747373508225D+13 Y= -6.393171832848D+13 Z= -4.051748209200D+12
I= 16 X= -1.346933435127D+13 Y= -5.920156072089D+13 Z= -1.053687084368D+13
I= 17 X= 7.687622013688D+10 Y= -6.290866110410D+11 Z= -4.249150981098D+11
I= 18 X= -4.337020792799D+13 Y= 7.177031795440D+13 Z= -2.546477368057D+13
I= 19 X= -4.359196192967D+13 Y= -2.458191686445D+13 Z= 4.117878495369D+13
I= 20 X= -3.592864621219D+13 Y= -1.897943694053D+13 Z= 8.123867141555D+13
I= 21 X= 8.623135154274D+12 Y= 7.046038117046D+11 Z= -3.427532836708D+12
I= 22 X= -1.282883076967D+14 Y= 8.757683954720D+12 Z= -1.597040079369D+13
I= 23 X= -1.943476626003D+13 Y= 2.690248425378D+13 Z= -1.048111881447D+14
I= 24 X= -1.838211918839D+13 Y= 3.713477308803D+13 Z= 7.553937199654D+13
I= 25 X= -1.827594658694D+13 Y= -4.580762171518D+11 Z= 4.050181986289D+12
I= 26 X= -5.337906638625D+11 Y= -7.054741617027D+13 Z= -9.877673657148D+13
I= 27 X= 2.245118913753D+13 Y= 8.268885372032D+13 Z= 5.078042851794D+13
I= 28 X= 4.447567916304D+13 Y= 1.388466219593D+13 Z= -3.194436735805D+13
I= 29 X= -4.008552846615D+12 Y= -5.322351442239D+12 Z= 2.523484190068D+13
I= 30 X= -1.563394285421D+13 Y= 1.142495787004D+13 Z= -1.186544558803D+13
I= 31 X= -1.013042534573D+14 Y= -5.577618019337D+13 Z= -5.598950722137D+13
I= 32 X= 4.323703091825D+13 Y= 4.161135109875D+13 Z= -5.591492721964D+13

I= 33 X= -8.599807418318D+13 Y= -3.267889774000D+13 Z= 3.819891813008D+13
I= 34 X= 7.814138239199D+13 Y= -1.157810789872D+13 Z= -3.426533888361D+13
I= 35 X= 1.652239198742D+12 Y= -1.969082259092D+12 Z= 1.065707325221D+12
I= 36 X= -8.006827289719D+12 Y= -6.021632735931D+12 Z= 8.086173375707D+12
I= 37 X= 8.951265919492D+13 Y= -5.778144050918D+13 Z= 4.232999624969D+13
I= 38 X= -1.937138873680D+13 Y= 1.329649311690D+13 Z= 3.488494752885D+13

Backward Direction:

Total Energy: -651.6189699 Hartrees

Potential Energy: -651.7880888 Hartress

Kinetic Energy: 0.1691189 Hartress

CM Start Point Velocity: bohr/s

I= 0 X= 1.822726920891D+13 Y= 1.970416628037D+13 Z= -2.131801318015D+13
I= 1 X= -2.081840413902D+13 Y= -8.471224042025D+12 Z= -1.690535859905D+13
I= 2 X= 1.700045113849D+13 Y= -3.387873978585D+12 Z= -3.516146473159D+12
I= 3 X= 2.261527787795D+13 Y= 1.338038432585D+13 Z= 5.947674467223D+12
I= 4 X= 3.901653489268D+12 Y= -2.405302082492D+13 Z= -1.114813470512D+13
I= 5 X= 6.566640248434D+12 Y= 1.205665462090D+11 Z= 7.396815920637D+12
I= 6 X= 2.800665815911D+13 Y= 2.749848685059D+13 Z= 5.903868356153D+13
I= 7 X= -1.080316687016D+14 Y= 1.140932606756D+14 Z= 2.242718786029D+13
I= 8 X= 4.199217037386D+13 Y= -4.815779438374D+13 Z= -7.559445116020D+13
I= 9 X= -4.187626645596D+12 Y= 1.087614995822D+13 Z= -4.542096488491D+12
I= 10 X= 1.231374580308D+14 Y= 2.395410835491D+13 Z= -3.546989253844D+12
I= 11 X= -3.390184629118D+13 Y= 2.438552089385D+13 Z= -4.898407385141D+13
I= 12 X= 3.274142668117D+13 Y= 6.161072002967D+13 Z= -4.687688922152D+13
I= 13 X= -2.442016220547D+12 Y= 1.597482820674D+13 Z= 2.883964946541D+12
I= 14 X= -1.305341083382D+14 Y= 6.438567499237D+13 Z= 2.257791709084D+13
I= 15 X= 4.803850839685D+13 Y= -6.450068640585D+13 Z= -5.009380062560D+12
I= 16 X= -1.357905577039D+13 Y= -5.904757480832D+13 Z= -1.042421730413D+13
I= 17 X= 3.503273906541D+11 Y= -8.752412139419D+11 Z= -5.327388011540D+11
I= 18 X= -4.307940307253D+13 Y= 7.162050100313D+13 Z= -2.610710085183D+13

I= 19 X= -4.359257224178D+13 Y= -2.482014893220D+13 Z= 4.145039409638D+13
I= 20 X= -3.560622408563D+13 Y= -1.938675096691D+13 Z= 8.110579371169D+13
I= 21 X= 8.070478335785D+12 Y= 7.139750156193D+11 Z= -4.269956196028D+12
I= 22 X= -1.286562750696D+14 Y= 9.557861038347D+12 Z= -1.796465378130D+13
I= 23 X= -1.908441442435D+13 Y= 2.659541632131D+13 Z= -1.055174396102D+14
I= 24 X= -1.911197287333D+13 Y= 3.711371273713D+13 Z= 7.454530100050D+13
I= 25 X= -1.827984167229D+13 Y= -5.628417773043D+11 Z= 3.816242397807D+12
I= 26 X= -9.583428234284D+11 Y= -7.114946721212D+13 Z= -9.894433945618D+13
I= 27 X= 2.282292744928D+13 Y= 8.303435780824D+13 Z= 5.064404771891D+13
I= 28 X= 4.456359518933D+13 Y= 1.387044532345D+13 Z= -3.151580834761D+13
I= 29 X= -5.457441996433D+12 Y= -4.466875975078D+12 Z= 2.412369944794D+13
I= 30 X= -1.552109252837D+13 Y= 1.166846409007D+13 Z= -1.271976986549D+13
I= 31 X= -1.011893744023D+14 Y= -5.656598704625D+13 Z= -5.651894880802D+13
I= 32 X= 4.139458418232D+13 Y= 4.327919915082D+13 Z= -5.763587644880D+13
I= 33 X= -8.574254071836D+13 Y= -3.279207056092D+13 Z= 3.732841444162D+13
I= 34 X= 7.900595576455D+13 Y= -1.170891497897D+13 Z= -3.482488050170D+13
I= 35 X= 1.303511474335D+12 Y= -2.111002567274D+12 Z= 2.422352520341D+12
I= 36 X= -1.222871973794D+13 Y= -1.106641375458D+13 Z= 5.554074711804D+12
I= 37 X= 9.441901430066D+13 Y= -5.462110771164D+13 Z= 3.609757593460D+13
I= 38 X= -1.640014444856D+13 Y= 1.309596639655D+13 Z= 3.086003657667D+13