Electronic Supplementary Information

DFT rationalization of mechanism and selectivity in gold-catalyzed oxidative cyclization of diynones with alcohols

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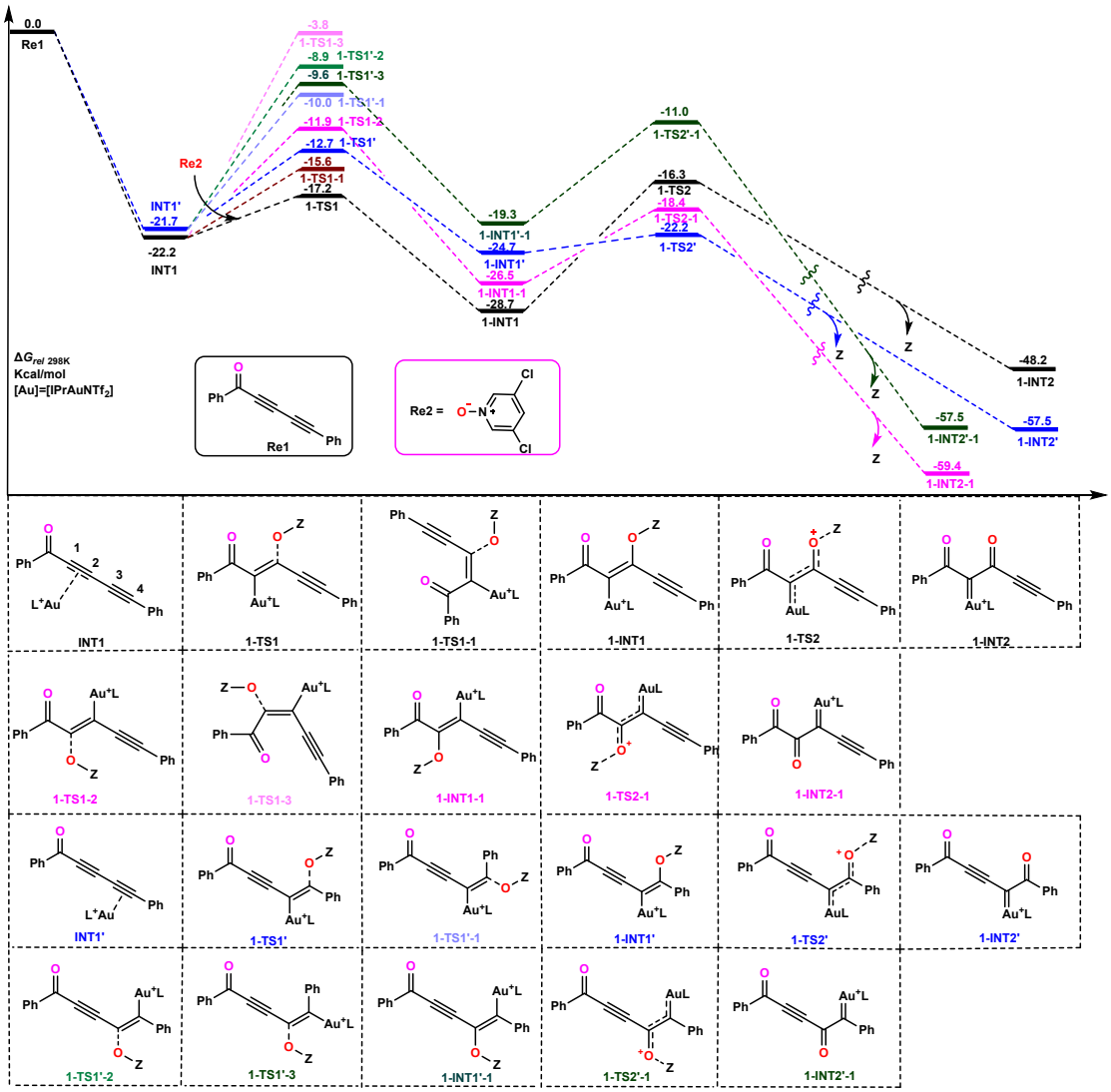

Figure S1. Different conformers and configurations of the transition states for **Re2** attacking **Re1**. Energies are in kcal/mol.

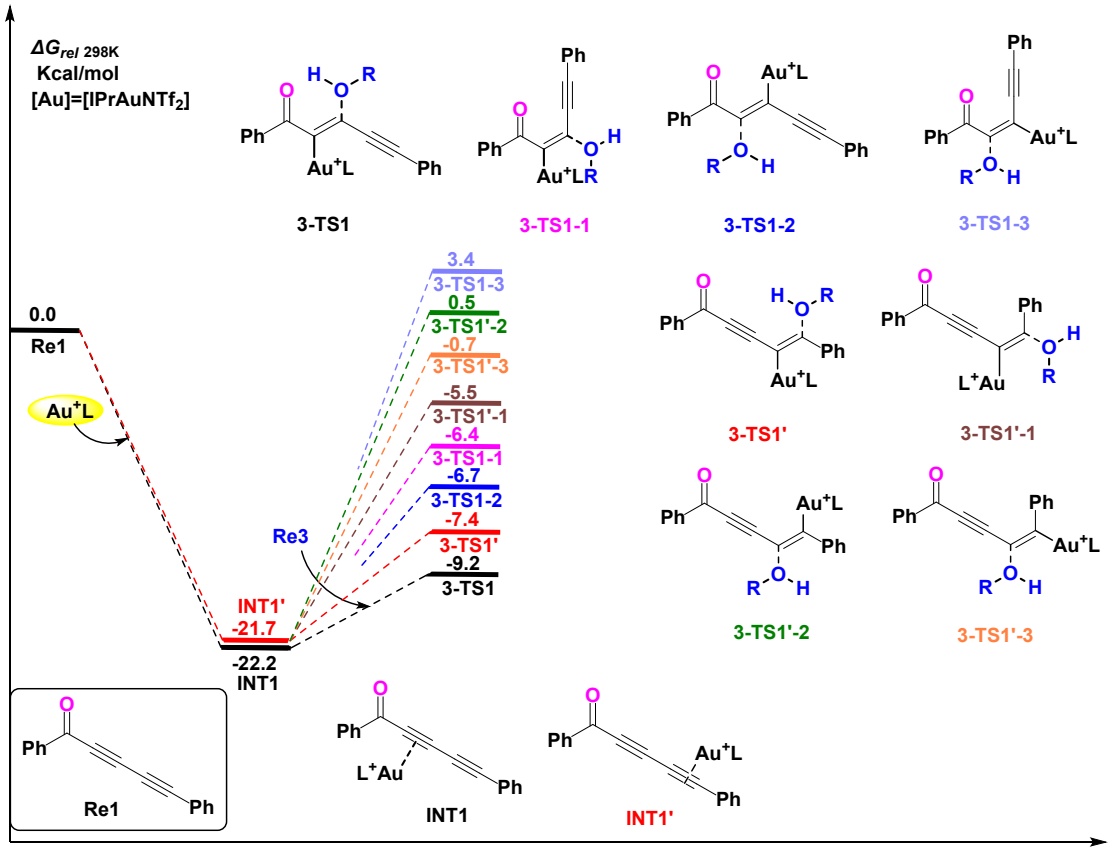

Figure S2. Different conformers and configurations of the transition states for **Re3** attacking **Re1**. Energies are in kcal/mol.

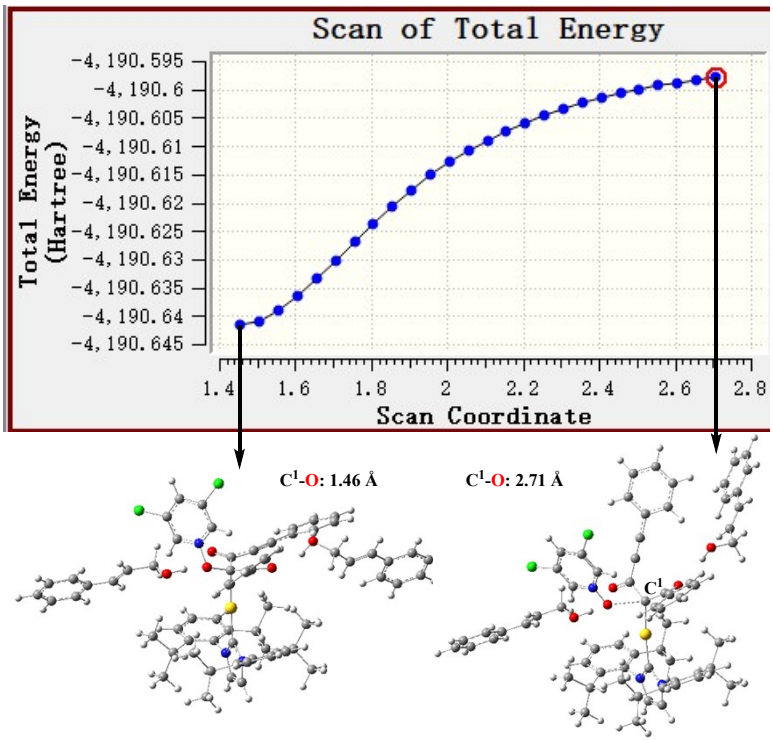

Figure S3. C^1-O key scan results for intermediate **1-INT3**.

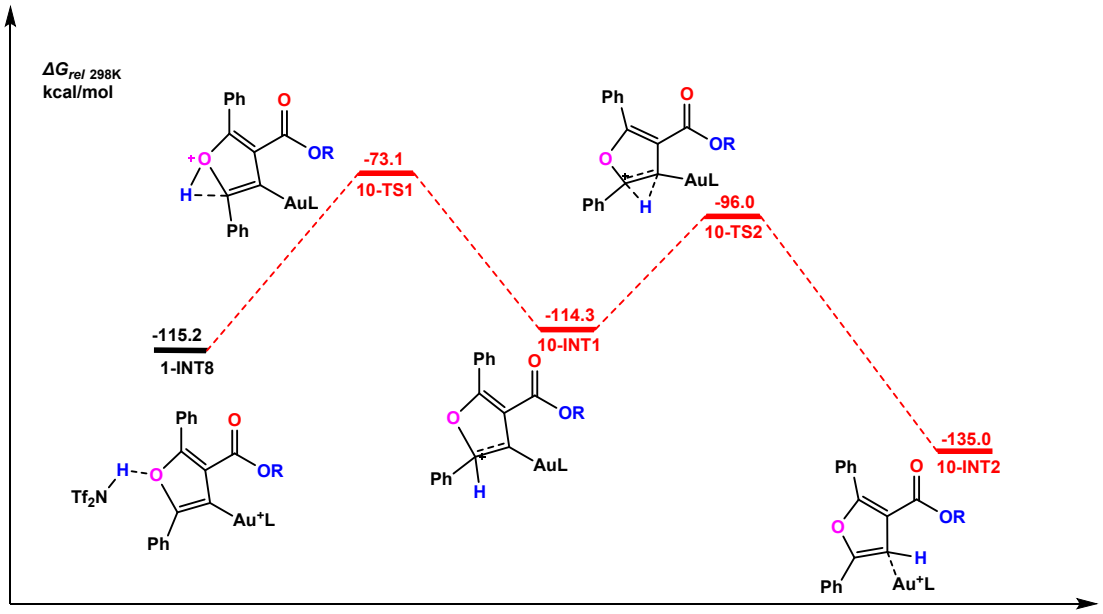

Figure S4. Direct proton migration. Relative energies are expressed in kcal/mol.

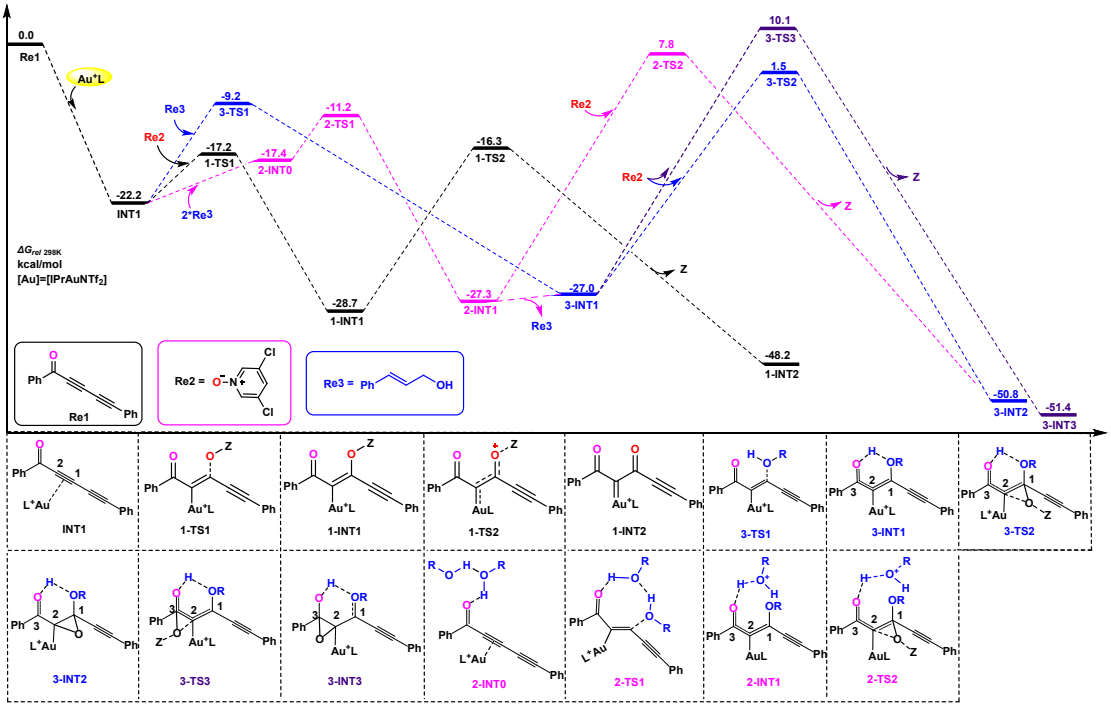

Figure S5. Full energy profile calculated for **Re1** (additions). Relative energies are expressed in kcal/mol.

Cartesian coordinates of the stationary points

Re1

C	2.88242426	-1.41476115	-0.00005942
O	3.10283726	-2.62434715	0.00010058
C	4.01115526	-0.43299615	-0.00008242
C	5.31835126	-0.95202215	-0.00046742
C	3.87354026	0.96145785	0.00031458
C	6.42841726	-0.11757015	-0.00046542
H	5.42052826	-2.03168815	-0.00075942
C	4.97126926	1.81535785	0.00037158
C	6.25308126	1.27062885	-0.00002942
H	7.42733226	-0.54137815	-0.00078342
H	4.80101526	2.88623385	0.00072658
C	1.48348476	-0.93505974	-0.00029197
C	0.28881276	-0.67957374	-0.00015497
C	-1.15621422	-0.34302850	-0.00012435
C	-2.34693222	-0.06641050	-0.00005435
C	-3.79748900	0.26797700	-0.00002500
C	-4.77334600	-0.76361500	0.00020200
C	-4.19702400	1.62004300	-0.00034100
C	-6.11981000	-0.39302300	0.00014100
C	-5.54525000	1.95795500	-0.00042700
H	-3.43350000	2.39091300	-0.00050800
C	-6.50869400	0.94777300	-0.00018000
H	-6.87800400	-1.17127300	0.00032900
H	-5.84309100	3.00178400	-0.00068900
H	-7.56451600	1.20208800	-0.00025000
H	7.11483826	1.93117785	0.00000058
H	2.90105604	1.40774734	0.00067544
H	-4.48207474	-1.79320765	0.00038236

Zero-point correction= 0.212084 (Hartree/Particle)
Thermal correction to Energy= 0.226893
Thermal correction to Enthalpy= 0.227837
Thermal correction to Gibbs Free Energy= 0.166334
Sum of electronic and zero-point Energies= -728.745923
Sum of electronic and thermal Energies= -728.731114
Sum of electronic and thermal Enthalpies= -728.730170
Sum of electronic and thermal Free Energies= -728.791673

Re2

C	1.18532000	1.04715300	-0.00021100
C	1.18346800	-0.33641600	-0.00015600
C	0.00003900	-1.07403100	0.00003500
C	-1.18336900	-0.33657700	0.00017600
C	-1.18535600	1.04708900	0.00012900
H	0.00018700	-2.15521000	0.00008100
H	2.07132700	1.66426300	-0.00036000
H	-2.07157100	1.66390800	0.00023900
Cl	-2.72185900	-1.16370300	0.00043400
Cl	2.72193400	-1.16359600	-0.00035300
N	-0.00013300	1.74368800	-0.00006700
O	-0.00011200	3.01275000	-0.00008700

Zero-point correction= 0.073627 (Hartree/Particle)
Thermal correction to Energy= 0.081071
Thermal correction to Enthalpy= 0.082015
Thermal correction to Gibbs Free Energy= 0.040487
Sum of electronic and zero-point Energies= -1242.560937
Sum of electronic and thermal Energies= -1242.553493
Sum of electronic and thermal Enthalpies= -1242.552549
Sum of electronic and thermal Free Energies= -1242.594077

Re3

C	-0.84344000	-0.58676900	-0.20941100
C	-1.89086300	0.24754200	-0.29389800
H	-1.04927500	-1.65812600	-0.22463000
H	-1.75381400	1.32739500	-0.26704100
C	0.58094400	-0.23984100	-0.09601400
C	1.52089100	-1.27483800	0.04999600
C	1.05725900	1.08430900	-0.12501700
C	2.88286800	-1.00342200	0.16889200
H	1.17304900	-2.30467300	0.07158700
C	2.41632600	1.35663800	-0.00521700
H	0.35978000	1.90715800	-0.24672600
C	3.33700300	0.31501900	0.14292700
H	3.58820300	-1.82173600	0.28132700
H	2.76146100	2.38631000	-0.03054800
H	4.39718900	0.53146200	0.23436600
C	-3.31563000	-0.21135100	-0.40208200
H	-3.35749200	-1.31197300	-0.42602500
H	-3.76700800	0.15061500	-1.33378800
O	-4.13684400	0.32490500	0.63569000
H	-3.72948600	0.07060000	1.47490100

Zero-point correction= 0.167017 (Hartree/Particle)

Thermal correction to Energy=	0.176294
Thermal correction to Enthalpy=	0.177238
Thermal correction to Gibbs Free Energy=	0.131392
Sum of electronic and zero-point Energies=	-424.023905
Sum of electronic and thermal Energies=	-424.014628
Sum of electronic and thermal Enthalpies=	-424.013684
Sum of electronic and thermal Free Energies=	-424.059531

Z

C	1.14896200	1.38661000	0.00056900
C	1.18767300	-0.00990500	0.00041100
C	-0.00001000	-0.73666800	0.00013200
C	-1.18778600	-0.00961800	-0.00021100
C	-1.14903000	1.38662200	-0.00046900
H	-0.00025700	-1.81994200	0.00012400
H	2.07090200	1.96147700	0.00028400
H	-2.07071700	1.96186700	-0.00059900
Cl	-2.72660400	-0.84328200	0.00008800
Cl	2.72662000	-0.84326400	-0.00020100
N	0.00013600	2.06651900	-0.00006900

Zero-point correction=	0.069636 (Hartree/Particle)
Thermal correction to Energy=	0.076196
Thermal correction to Enthalpy=	0.077140
Thermal correction to Gibbs Free Energy=	0.037651
Sum of electronic and zero-point Energies=	-1167.407808
Sum of electronic and thermal Energies=	-1167.401248
Sum of electronic and thermal Enthalpies=	-1167.400304
Sum of electronic and thermal Free Energies=	-1167.439793

NTf_2^-

S	1.30418300	-0.88778000	-0.24023900
S	-1.51040900	-0.86896600	0.31234500
O	1.02739500	-0.76681700	-1.67846000
O	2.27537700	-1.89240300	0.21150800
O	-2.32107900	-1.06049200	1.52017000
O	-1.81679800	-1.65794000	-0.88687400
C	2.11755800	0.73655400	0.20701900
C	-1.90661600	0.89422200	-0.18550800
F	3.24097400	0.88821700	-0.51893600
F	2.45209900	0.78395000	1.50407500
F	1.30853200	1.77422100	-0.05922700
F	-1.60555700	1.75088700	0.80349500

F	-3.22301100	1.00594700	-0.44478600
F	-1.23376700	1.26503000	-1.28250600
N	0.03733900	-0.83853800	0.76678000

Zero-point correction= 0.053449 (Hartree/Particle)
Thermal correction to Energy= 0.067858
Thermal correction to Enthalpy= 0.068802
Thermal correction to Gibbs Free Energy= 0.010132
Sum of electronic and zero-point Energies= -1827.150632
Sum of electronic and thermal Energies= -1827.136224
Sum of electronic and thermal Enthalpies= -1827.135279
Sum of electronic and thermal Free Energies= -1827.193949

$Au^{+}L$

Au	-0.00009300	-0.00218500	-1.68981400
C	0.00001800	0.00021000	0.28785300
C	0.68019200	0.00276400	2.41295000
C	-0.68010400	0.00256000	2.41297100
H	-1.39236100	0.00334800	3.22242800
H	1.39247500	0.00372100	3.22238500
N	1.08957200	0.00124400	1.08721600
N	-1.08951700	0.00104100	1.08724700
C	2.47528900	0.00096700	0.64667200
C	3.11408600	-1.24105600	0.45693700
C	3.11389100	1.24280200	0.45492100
C	4.45114500	-1.20707100	0.04249900
C	4.45097200	1.20836600	0.04061100
C	5.11211100	0.00053100	-0.16533400
H	4.98175300	-2.14050700	-0.11502800
H	4.98145800	2.14163100	-0.11834300
H	6.14979300	0.00035900	-0.48462800
C	-2.47524100	0.00062000	0.64673100
C	-3.11416500	1.24237400	0.45553900
C	-3.11370100	-1.24148800	0.45642300
C	-4.45124100	1.20776300	0.04121700
C	-4.45076300	-1.20767700	0.04199300
C	-5.11205200	-0.00015300	-0.16528600
H	-4.98198000	2.14095300	-0.11733000
H	-4.98112300	-2.14118200	-0.11595900
H	-6.14973300	-0.00045400	-0.48458200
C	-2.42741000	2.58520700	0.68839300
C	-3.09519900	3.36160100	1.84131100
C	-2.38592700	3.43243800	-0.59840000
H	-1.39018400	2.39680200	0.98442300

H	-3.09624900	2.78190800	2.76971500
H	-2.56188100	4.29911800	2.02695100
H	-4.13415800	3.61166800	1.60525600
H	-1.88320700	2.90039000	-1.41346900
H	-3.39177300	3.69246800	-0.94237900
H	-1.84628500	4.36751900	-0.41893000
C	-2.42642300	-2.58389900	0.69016700
C	-2.38275100	-3.43087600	-0.59671700
C	-3.09517900	-3.36083600	1.84213600
H	-1.38970900	-2.39483000	0.98757900
H	-1.87893300	-2.89846900	-1.41088100
H	-1.84311700	-4.36585800	-0.41667700
H	-3.38801400	-3.69105200	-0.94228900
H	-3.09789500	-2.78115800	2.77054100
H	-4.13362300	-3.61173000	1.60469900
H	-2.56139400	-4.29795100	2.02844500
C	2.42680200	2.58555800	0.68723100
C	2.38533500	3.43236700	-0.59983500
C	3.09424700	3.36245800	1.84000300
H	1.38956900	2.39701900	0.98315700
H	1.88283600	2.89995300	-1.41480200
H	1.84548000	4.36739800	-0.42074200
H	3.39117500	3.69248700	-0.94376500
H	3.09520100	2.78308900	2.76860800
H	4.13321300	3.61260100	1.60405900
H	2.56075200	4.29996100	2.02520800
C	2.42716900	-2.58356600	0.69120800
C	3.09632100	-3.36003500	1.84326800
C	2.38348500	-3.43092700	-0.59541900
H	1.39047300	-2.39465900	0.98878700
H	3.09914100	-2.78007800	2.77149700
H	2.56273000	-4.29718300	2.02997400
H	4.13475400	-3.61083600	1.60568700
H	1.87941100	-2.89889500	-1.40967100
H	3.38876800	-3.69093100	-0.94106400
H	1.84412000	-4.36599300	-0.41502400

Zero-point correction= 0.572657 (Hartree/Particle)
Thermal correction to Energy= 0.605223
Thermal correction to Enthalpy= 0.606167
Thermal correction to Gibbs Free Energy= 0.504559
Sum of electronic and zero-point Energies= -1294.803490
Sum of electronic and thermal Energies= -1294.770924
Sum of electronic and thermal Enthalpies= -1294.769980
Sum of electronic and thermal Free Energies= -1294.871588

INT1

C	0.44612800	-2.45346100	-2.34026400
O	0.15936700	-1.96631100	-3.41609600
C	0.17363900	-3.85830300	-1.95779700
C	-0.41106200	-4.69765300	-2.92272500
C	0.48085700	-4.36301100	-0.68478200
C	-0.68022900	-6.02623500	-2.61361000
H	-0.63993900	-4.28862500	-3.90090000
C	0.20629700	-5.69449200	-0.38013200
C	-0.37179600	-6.52535600	-1.34328800
H	-1.12883900	-6.67556800	-3.35884100
H	0.44398100	-6.08504200	0.60434100
C	1.13146700	-1.56883200	-1.31637600
C	2.31473300	-1.29246400	-0.97643400
C	3.55171900	-0.96864300	-0.59104600
C	4.70348900	-0.69280300	-0.25517200
C	6.02261300	-0.37650100	0.11783700
C	6.74746900	0.60266300	-0.60331100
C	6.63183800	-1.03903800	1.21039900
C	8.05069200	0.90710100	-0.23318400
C	7.93604700	-0.72372200	1.56762400
H	6.07130100	-1.79008800	1.75673200
C	8.64407100	0.24643100	0.84872600
H	8.60881700	1.65596400	-0.78555600
H	8.40566700	-1.23157500	2.40366800
H	9.66402000	0.48766800	1.13217200
H	-0.58180100	-7.56386800	-1.10512500
H	0.93081600	-3.71626400	0.06177500
H	6.27518300	1.10344100	-1.44169600
Au	-0.10647200	-0.15598700	-0.30611600
C	-1.46227200	1.12549700	0.48867900
C	-2.79041000	2.92356500	0.77752500
C	-3.10031300	2.02527900	1.74884700
H	-3.82032500	2.06269200	2.55034500
H	-3.18490400	3.90334900	0.56172300
N	-1.78278900	2.35584300	0.01099900
N	-2.27636500	0.92482500	1.55689500
C	-1.16442000	3.00144500	-1.13179100
C	-0.04632300	3.82936100	-0.90704000
C	-1.72279600	2.78963600	-2.40824900
C	0.52028900	4.45418300	-2.02446300
C	-1.11330500	3.44363700	-3.48630800

C	-0.00543900	4.26513300	-3.29962700
H	1.38253700	5.10033000	-1.89199800
H	-1.51437400	3.30658000	-4.48534100
H	0.44862800	4.76236800	-4.15153800
C	-2.30259300	-0.26532100	2.38453100
C	-3.17075000	-1.31473500	2.02266000
C	-1.47862900	-0.30584300	3.52673600
C	-3.18815600	-2.44282400	2.85242400
C	-1.53937700	-1.46037100	4.31682800
C	-2.38269100	-2.51728000	3.98529100
H	-3.84523700	-3.27170200	2.60864500
H	-0.92099700	-1.52943000	5.20639200
H	-2.41643200	-3.40072000	4.61594600
C	-4.07663800	-1.26178500	0.79628100
C	-5.56512600	-1.27389500	1.19787000
C	-3.75916200	-2.40018100	-0.19250500
H	-3.89053100	-0.31929700	0.27244300
H	-5.80587600	-0.44740600	1.87395900
H	-6.19919500	-1.18123600	0.31034800
H	-5.83625000	-2.20620200	1.70368500
H	-2.70727300	-2.38458400	-0.49543900
H	-3.96630800	-3.38234400	0.24443900
H	-4.37478700	-2.30276600	-1.09250300
C	-0.54787500	0.83600100	3.92420200
C	0.92852500	0.39589300	3.88373400
C	-0.91927800	1.41424200	5.30388600
H	-0.66229600	1.64326600	3.19455500
H	1.20319400	0.02627000	2.89026600
H	1.58316600	1.23881900	4.12858400
H	1.12920800	-0.40142500	4.60673400
H	-1.95753200	1.75991200	5.32711900
H	-0.79940700	0.67043900	6.09801700
H	-0.27338500	2.26430500	5.54608800
C	-2.94466200	1.90858600	-2.65074600
C	-2.64582900	0.77745300	-3.65415300
C	-4.15313900	2.75005200	-3.10845800
H	-3.21961200	1.43552400	-1.70290500
H	-1.79681100	0.16383300	-3.33781300
H	-3.52000900	0.12588300	-3.75522100
H	-2.41631400	1.17218200	-4.64908200
H	-4.40152700	3.52883700	-2.38022500
H	-3.95589900	3.24187700	-4.06641600
H	-5.03365700	2.11248200	-3.23715100
C	0.55203400	4.06482700	0.47684700

C	0.47333000	5.54996000	0.88147700
C	1.99954400	3.54188000	0.56032400
H	-0.03532600	3.49932600	1.20659600
H	-0.55738800	5.91743000	0.85878200
H	0.86075900	5.68949200	1.89592000
H	1.06498100	6.18125200	0.21092100
H	2.05103100	2.47656400	0.31229800
H	2.65977600	4.07910500	-0.12827700
H	2.39457000	3.67730400	1.57258000

Zero-point correction= 0.785448 (Hartree/Particle)
Thermal correction to Energy= 0.834686
Thermal correction to Enthalpy= 0.835630
Thermal correction to Gibbs Free Energy= 0.692389
Sum of electronic and zero-point Energies= -2023.592678
Sum of electronic and thermal Energies= -2023.543440
Sum of electronic and thermal Enthalpies= -2023.542496
Sum of electronic and thermal Free Energies= -2023.685737

INT1'

C	-4.84215600	0.55314500	0.00036900
O	-4.49551400	1.73169300	0.00103400
C	-6.24526900	0.09657000	0.00012100
C	-7.26395000	1.06519100	0.00069900
C	-6.57441600	-1.26851100	-0.00066500
C	-8.59576500	0.66798100	0.00049300
H	-6.98678800	2.11389500	0.00130400
C	-7.91038300	-1.66109900	-0.00086700
C	-8.91936000	-0.69411800	-0.00028800
H	-9.38467500	1.41345300	0.00093900
H	-8.16692400	-2.71567800	-0.00147400
C	-3.77546000	-0.44822000	-0.00021600
C	-2.76324800	-1.13494600	-0.00060800
C	-1.63669000	-1.88981300	-0.00102700
C	-0.62489500	-2.62750100	-0.00146500
C	0.08387000	-3.87511900	-0.00212500
C	1.48969100	-3.94052400	-0.00246300
C	-0.66933600	-5.06957700	-0.00243200
C	2.12890800	-5.17620600	-0.00309800
C	-0.01921600	-6.29823100	-0.00306200
H	-1.75308900	-5.01926200	-0.00217000
C	1.37802600	-6.35475500	-0.00339700
H	3.21317100	-5.22129600	-0.00335900
H	-0.60219700	-7.21364200	-0.00329400

H	1.88045100	-7.31700200	-0.00389400
H	-9.96088300	-1.00145200	-0.00044500
H	-5.78643900	-2.01632400	-0.00111400
H	2.06883600	-3.02316700	-0.00222600
Au	0.34605200	-0.58764000	-0.00035200
C	1.53071600	1.04760800	0.00055900
C	2.71858100	2.83353900	0.68150100
C	2.71848100	2.83436800	-0.67838400
H	3.16415100	3.51039800	-1.39007300
H	3.16435600	3.50869900	1.39395000
N	1.98652300	1.72805500	1.08397700
N	1.98637300	1.72936600	-1.08209600
C	1.75727200	1.37212300	2.47280100
C	0.60366700	1.86833300	3.11208300
C	2.72231600	0.57829900	3.12547800
C	0.43147100	1.53309400	4.46115900
C	2.49519400	0.28014700	4.47437200
C	1.36378600	0.75033900	5.13570700
H	-0.44452500	1.89535700	4.98964700
H	3.21648700	-0.32468300	5.01460700
H	1.21010500	0.50804700	6.18297600
C	1.75696800	1.37508100	-2.47131700
C	2.72193800	0.58202700	-3.12504000
C	0.60328900	1.87204200	-3.10988400
C	2.49465800	0.28546000	-4.47425600
C	0.43093100	1.53838200	-4.45933200
C	1.36316800	0.75642100	-5.13490500
H	3.21589700	-0.31871900	-5.01529100
H	-0.44512500	1.90126600	-4.98729300
H	1.20937200	0.51536400	-6.18244300
C	3.98315500	0.06741400	-2.43720300
C	5.24612100	0.73651000	-3.01607700
C	4.08989600	-1.46767500	-2.51125800
H	3.92928200	0.33445400	-1.37713000
H	5.20007000	1.82663000	-2.92902000
H	6.13917400	0.39153800	-2.48513400
H	5.37371800	0.49428900	-4.07600700
H	3.20010700	-1.95012200	-2.09413500
H	4.20337100	-1.81639500	-3.54240600
H	4.96441700	-1.81303800	-1.95018900
C	-0.43635800	2.73934100	-2.40655900
C	-1.82274000	2.06702800	-2.40974300
C	-0.49988700	4.15172100	-3.02063800
H	-0.13724600	2.85480600	-1.36029000

H	-1.77277900	1.05732800	-1.99035600
H	-2.53357700	2.64131200	-1.80891500
H	-2.22695700	1.98728100	-3.42428100
H	0.47275100	4.65258300	-2.98108900
H	-0.81403200	4.11821300	-4.06874600
H	-1.22234000	4.76867000	-2.47708500
C	3.98342500	0.06442800	2.43688400
C	4.08998500	-1.47076800	2.50899200
C	5.24651600	0.73264200	3.01650200
H	3.92950900	0.33281800	1.37715400
H	3.20013000	-1.95258900	2.09128600
H	4.96445200	-1.81553100	1.94746900
H	4.20344000	-1.82079100	3.53970200
H	5.20056700	1.82287800	2.93085800
H	5.37420100	0.48903700	4.07610300
H	6.13947800	0.38826200	2.48502300
C	-0.43608400	2.73641200	2.40987500
C	-0.49970200	4.14804100	3.02566700
C	-1.82240700	2.06396800	2.41229600
H	-0.13703100	2.85317000	1.36373300
H	0.47290300	4.64901300	2.98672500
H	-1.22219600	4.76560100	2.48286300
H	-0.81384800	4.11324400	4.07373200
H	-1.77236100	1.05478300	1.99168000
H	-2.22657300	1.98294400	3.42675200
H	-2.53332900	2.63890800	1.81219500

Zero-point correction= 0.786085 (Hartree/Particle)
Thermal correction to Energy= 0.835093
Thermal correction to Enthalpy= 0.836037
Thermal correction to Gibbs Free Energy= 0.696082
Sum of electronic and zero-point Energies= -2023.587049
Sum of electronic and thermal Energies= -2023.538041
Sum of electronic and thermal Enthalpies= -2023.537097
Sum of electronic and thermal Free Energies= -2023.677051

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C	-0.51472200	2.38833400	-1.40691300
O	-0.14629500	2.49464000	-2.56246100
C	-0.77205700	3.56804200	-0.52979500
C	-0.66890100	4.84570500	-1.10136600
C	-1.10517500	3.44021400	0.82771700
C	-0.90672800	5.97871200	-0.32815200
H	-0.40544200	4.92293100	-2.15080400

C	-1.33985400	4.57808400	1.60079700
C	-1.24357800	5.84702800	1.02268200
H	-0.82982700	6.96515800	-0.77519300
H	-1.58956800	4.47693000	2.65284600
C	-0.67953200	1.01167100	-0.81167000
C	-1.77072100	0.32809100	-0.72161500
C	-2.50692400	-0.77021700	-0.41122200
C	-3.21800300	-1.73020400	-0.13558600
C	-4.00609500	-2.86672000	0.17878500
C	-4.24151700	-3.85944400	-0.79779600
C	-4.56254800	-3.01487000	1.46816500
C	-5.01740400	-4.97064000	-0.48589700
C	-5.33646500	-4.13073500	1.76766500
H	-4.37647500	-2.25309600	2.21823800
C	-5.56546600	-5.10743800	0.79335200
H	-5.19693900	-5.73164100	-1.23875400
H	-5.76193200	-4.24213100	2.76001200
H	-6.17107000	-5.97656300	1.03149800
H	-1.42645500	6.73191600	1.62515300
H	-1.17039900	2.45406000	1.27744600
H	-3.80960100	-3.74489700	-1.78656700
Au	1.10006500	0.07271300	-0.25738800
C	2.91052300	-0.74596200	0.18611700
C	5.12636700	-0.96095900	0.57113500
C	4.58145800	-2.20366600	0.62182400
H	5.02519500	-3.16964600	0.80099900
H	6.14217900	-0.62338000	0.69828100
N	4.08883700	-0.07782600	0.30443800
N	3.22110700	-2.05490400	0.38259300
C	4.25990900	1.35527300	0.16760800
C	4.48382300	1.88620200	-1.11887500
C	4.22490600	2.14848100	1.33186200
C	4.68109400	3.26954400	-1.21229000
C	4.42934100	3.52470000	1.17459100
C	4.65601600	4.08038500	-0.08133400
H	4.86002400	3.71562100	-2.18532000
H	4.41217400	4.16862900	2.04823000
H	4.81515300	5.15018900	-0.17909900
C	2.28308500	-3.15772500	0.33641900
C	1.63510400	-3.54066400	1.52758700
C	2.08244900	-3.81633500	-0.89318400
C	0.75283900	-4.62566700	1.45602000
C	1.18855500	-4.89434900	-0.90259900
C	0.53104500	-5.29634800	0.25649700

H	0.23749500	-4.95175200	2.35414100
H	1.00960800	-5.42719200	-1.83120500
H	-0.15350200	-6.13901000	0.22616900
C	1.85652400	-2.83137200	2.85994100
C	2.44984600	-3.78330700	3.91708000
C	0.55784900	-2.17528100	3.36806300
H	2.58219900	-2.02791800	2.70339700
H	3.39060300	-4.22571100	3.57478400
H	2.64862800	-3.24191100	4.84764600
H	1.76308200	-4.60322200	4.15104900
H	0.15195900	-1.47829400	2.62775400
H	-0.21128000	-2.92455100	3.58338500
H	0.74912300	-1.62109100	4.29296600
C	2.78541300	-3.40519300	-2.18356600
C	1.77648200	-2.91369200	-3.24023000
C	3.66200300	-4.54517800	-2.73874800
H	3.45119500	-2.56674700	-1.95926100
H	1.18712400	-2.07058100	-2.86579900
H	2.30226800	-2.58685600	-4.14325600
H	1.08224800	-3.70924600	-3.53048400
H	4.40194000	-4.87757200	-2.00374000
H	3.06083300	-5.41534000	-3.02175000
H	4.19816100	-4.20958100	-3.63213700
C	3.98097400	1.57419100	2.72450800
C	2.72461900	2.18468000	3.37505800
C	5.21640200	1.74957400	3.62963700
H	3.80057900	0.49954100	2.62610800
H	1.84346600	2.04510200	2.74097800
H	2.53056700	1.71060800	4.34302900
H	2.84375100	3.25855100	3.55161800
H	6.10387300	1.28097100	3.19258000
H	5.44676000	2.80752100	3.79152200
H	5.04003600	1.29374800	4.60934900
C	4.54389900	1.02563300	-2.37734500
C	5.98525900	0.94742200	-2.92099000
C	3.56796900	1.51822100	-3.46332000
H	4.23974400	0.00904200	-2.11046400
H	6.67792600	0.54774500	-2.17307300
H	6.02649200	0.29883300	-3.80214500
H	6.35103600	1.93608300	-3.21712800
H	2.54068300	1.57919700	-3.09171500
H	3.84693200	2.50815000	-3.83855700
H	3.58219400	0.83201700	-4.31645300
C	-4.61400800	2.39887100	0.02878100

C	-5.87236800	2.41335000	0.61122500
C	-6.87821400	1.54706100	0.17486200
C	-6.56883100	0.67075500	-0.86415500
C	-5.30360200	0.66508800	-1.43937400
H	-7.86346200	1.56024300	0.62417400
H	-3.79138300	3.04186000	0.31244700
H	-5.00032200	0.03012700	-2.25867800
Cl	-7.76026800	-0.43579000	-1.46690600
Cl	-6.18117900	3.53218000	1.90078400
N	-4.35886500	1.53226300	-0.98977100
O	-3.17769100	1.53253400	-1.55617100

Zero-point correction= 0.859544 (Hartree/Particle)
Thermal correction to Energy= 0.917391
Thermal correction to Enthalpy= 0.918335
Thermal correction to Gibbs Free Energy= 0.752937
Sum of electronic and zero-point Energies= -3266.145081
Sum of electronic and thermal Energies= -3266.087235
Sum of electronic and thermal Enthalpies= -3266.086291
Sum of electronic and thermal Free Energies= -3266.251689

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C	-0.37060800	-2.89633400	-0.39468800
O	-0.76376100	-3.51108400	0.60370400
C	0.44939200	-3.57074300	-1.43522100
C	0.85003500	-4.89947800	-1.21786500
C	0.78061000	-2.93514100	-2.64275800
C	1.57639600	-5.57833700	-2.19088300
H	0.57722300	-5.37718100	-0.28300300
C	1.49993900	-3.62156900	-3.61956700
C	1.90044300	-4.94075700	-3.39317700
H	1.88741000	-6.60433600	-2.01900500
H	1.74786900	-3.13036900	-4.55549000
C	-0.69592400	-1.44474600	-0.53719400
C	-1.94152100	-1.07277100	-0.85852700
C	-2.55468200	0.19330400	-0.98000600
C	-3.17800200	1.23310000	-1.10513200
C	-3.89061300	2.45954300	-1.26670800
C	-4.46426300	3.10595000	-0.15386300
C	-4.03860500	3.03171600	-2.54625200
C	-5.16986700	4.29471200	-0.32170400
C	-4.74390200	4.22202100	-2.70350200
H	-3.59696700	2.53506700	-3.40418700
C	-5.31136400	4.85500500	-1.59434900

H	-5.61273100	4.78471800	0.54025000
H	-4.85348600	4.65586000	-3.69272900
H	-5.86372200	5.78110500	-1.72140200
H	2.46248900	-5.47400200	-4.15442900
H	0.47029200	-1.90927900	-2.81517600
H	-4.34733300	2.66894000	0.83253900
Au	0.81818700	-0.12946700	-0.06197900
C	2.34406900	1.13599900	0.46477700
C	3.52524000	2.96783700	1.07930600
C	4.39198900	1.92480800	1.02281400
H	5.45137500	1.86803400	1.21377900
H	3.67420100	4.00584900	1.32907300
N	2.27549200	2.46848700	0.73535300
N	3.65415300	0.81073800	0.64483800
C	1.07447300	3.27676000	0.69734000
C	0.72331600	3.90666200	-0.51284000
C	0.32949600	3.42589000	1.88399500
C	-0.42896200	4.70210200	-0.51028700
C	-0.81184000	4.23497800	1.82601800
C	-1.18913300	4.86606500	0.64399900
H	-0.73394100	5.20018800	-1.42519900
H	-1.40979200	4.37474300	2.72143900
H	-2.07966900	5.48658000	0.62039400
C	4.22672100	-0.50783500	0.46566300
C	4.23171400	-1.39638500	1.55914600
C	4.78733000	-0.82964600	-0.78685400
C	4.81911100	-2.65219800	1.36063200
C	5.36484500	-2.09758000	-0.92369600
C	5.37958000	-3.00086600	0.13539300
H	4.84072800	-3.36421100	2.17978200
H	5.80981300	-2.37981800	-1.87254300
H	5.83329600	-3.97905700	0.00633100
C	3.64804100	-1.04327300	2.92399300
C	4.74472000	-0.99974300	4.00673900
C	2.51130700	-2.00444400	3.32170100
H	3.21403900	-0.04118400	2.86221700
H	5.53483100	-0.28691800	3.74982800
H	4.31756400	-0.70001100	4.96931100
H	5.21344100	-1.97977900	4.14238800
H	1.71546200	-2.01121200	2.57056600
H	2.87377200	-3.03112300	3.43666800
H	2.07640600	-1.69918400	4.27929400
C	4.80783000	0.14557100	-1.96052500
C	4.17866300	-0.46221000	-3.22807200

C	6.23962000	0.64550000	-2.24021300
H	4.20320000	1.01662600	-1.69089900
H	3.16185700	-0.81598200	-3.03476400
H	4.13812600	0.28794000	-4.02478300
H	4.76234600	-1.30847600	-3.60438200
H	6.67837200	1.12447400	-1.35905100
H	6.89828600	-0.17966600	-2.53048100
H	6.23808700	1.37527900	-3.05651500
C	0.71291600	2.74966900	3.19676700
C	-0.35274300	1.72319400	3.62907000
C	0.97772500	3.78020300	4.31153700
H	1.64452400	2.19843100	3.03889600
H	-0.50679800	0.96475100	2.85482600
H	-0.04137400	1.21658500	4.54865900
H	-1.31556500	2.20676800	3.82619100
H	1.75505600	4.49396600	4.02113500
H	0.07645400	4.35201700	4.55539200
H	1.30579500	3.27481100	5.22562700
C	1.53494700	3.75241800	-1.79509100
C	2.07953600	5.10700100	-2.28857700
C	0.71547800	3.04721100	-2.89323200
H	2.39831800	3.11637700	-1.57820800
H	2.68849900	5.59766300	-1.52270800
H	2.70283700	4.96446300	-3.17732900
H	1.26999900	5.79280400	-2.55918400
H	0.35352200	2.07287400	-2.55030700
H	-0.15417300	3.64406600	-3.18804500
H	1.33052300	2.89248500	-3.78605400
C	-3.63454100	-2.78563400	0.90505700
C	-4.70034800	-2.95718700	1.78450100
C	-6.00222400	-2.63011400	1.39599400
C	-6.21391200	-2.12355700	0.11140200
C	-5.13875700	-1.95105700	-0.75360200
H	-6.83357700	-2.76779300	2.07789500
H	-2.58352100	-3.02500700	1.10169200
H	-5.20234900	-1.56400900	-1.76086100
Cl	-7.79986900	-1.69472100	-0.42393200
Cl	-4.38885500	-3.59216600	3.36097100
N	-3.91264100	-2.29603700	-0.31843800
O	-2.88130500	-2.16590100	-1.23267500

Zero-point correction= 0.862227 (Hartree/Particle)
Thermal correction to Energy= 0.919476
Thermal correction to Enthalpy= 0.920421
Thermal correction to Gibbs Free Energy= 0.758243

Sum of electronic and zero-point Energies=	-3266.161367
Sum of electronic and thermal Energies=	-3266.104118
Sum of electronic and thermal Enthalpies=	-3266.103173
Sum of electronic and thermal Free Energies=	-3266.265351

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C	-0.94501300	-2.62659300	-0.33760900
O	-1.39642200	-3.08369100	0.71636600
C	-0.35893500	-3.49002000	-1.38952100
C	-0.21778500	-4.86310000	-1.12943100
C	0.01600300	-2.97576800	-2.64123900
C	0.29849900	-5.70755600	-2.10688600
H	-0.51914800	-5.24237600	-0.15874800
C	0.52689800	-3.82612500	-3.62014500
C	0.67043000	-5.19009700	-3.35244500
H	0.40978800	-6.76831700	-1.90411800
H	0.80997800	-3.42869300	-4.58987800
C	-0.94702800	-1.13726400	-0.47620100
C	-2.14523300	-0.52849200	-0.81857700
C	-2.45648800	0.85628600	-0.67999800
C	-2.83281500	2.00717800	-0.55483100
C	-3.26705200	3.35923700	-0.41672200
C	-3.36146500	3.95319900	0.85756800
C	-3.61459900	4.11293100	-1.55528100
C	-3.79132300	5.27164900	0.98460100
C	-4.03745900	5.43268900	-1.41794700
H	-3.54476500	3.65572800	-2.53695600
C	-4.12698900	6.01475200	-0.15057800
H	-3.86814000	5.72029300	1.97048200
H	-4.30240500	6.00713200	-2.30040200
H	-4.46196400	7.04239600	-0.04744700
H	1.06957900	-5.85158300	-4.11576900
H	-0.09805200	-1.91614900	-2.84925500
H	-3.10035800	3.37124100	1.73529800
Au	0.80967300	-0.18636200	-0.09517400
C	2.60446100	0.71751300	0.33920200
C	4.23560900	2.25386400	0.64767200
C	4.74620700	1.04227600	0.98953600
H	5.72141500	0.75610200	1.34897900
H	4.67534400	3.23814100	0.64813900
N	2.92294900	2.03755600	0.25351100
N	3.73582500	0.11195800	0.79331600
C	2.02349300	3.09023600	-0.17214400

C	1.94446600	3.39681400	-1.54489500
C	1.28839800	3.77944100	0.81279800
C	1.07427900	4.42776400	-1.92048600
C	0.43587900	4.80063300	0.37675700
C	0.32562500	5.12041200	-0.97357000
H	0.98584800	4.69229400	-2.96955000
H	-0.15254700	5.35140800	1.10346600
H	-0.34660800	5.91308700	-1.28755300
C	3.89376700	-1.30915700	1.03061800
C	3.50529300	-1.83378700	2.27950900
C	4.46404000	-2.09704000	0.01040500
C	3.69728700	-3.20588900	2.48396600
C	4.63691900	-3.46082100	0.27574400
C	4.25721500	-4.01142900	1.49662700
H	3.40831100	-3.64644400	3.43300700
H	5.07588600	-4.09855200	-0.48500100
H	4.40171600	-5.07189900	1.68066600
C	2.91045800	-0.98040300	3.39565700
C	3.83223500	-0.95209000	4.63116700
C	1.49149200	-1.44965400	3.77097500
H	2.82492000	0.04776000	3.03181700
H	4.83189000	-0.58488800	4.37797300
H	3.41516600	-0.29589800	5.40205400
H	3.94567400	-1.94862200	5.07008500
H	0.82755900	-1.44723200	2.90062500
H	1.49978600	-2.46451500	4.18167200
H	1.06326700	-0.78862000	4.53185700
C	4.90150800	-1.52586300	-1.33559100
C	4.19371300	-2.22520700	-2.51163500
C	6.43386800	-1.58850600	-1.49574700
H	4.61273300	-0.47113800	-1.37004600
H	3.10556400	-2.16524300	-2.41577100
H	4.48245900	-1.75505700	-3.45762400
H	4.46504900	-3.28392200	-2.57463400
H	6.94557800	-1.05611500	-0.68759500
H	6.79247600	-2.62289600	-1.48942800
H	6.73775800	-1.13604200	-2.44526400
C	1.39292200	3.46155300	2.30181400
C	0.04750400	2.97546300	2.87412300
C	1.93294700	4.66611400	3.09771500
H	2.10764100	2.64328900	2.42890100
H	-0.31936500	2.09863200	2.33116600
H	0.16033900	2.70437400	3.92910900
H	-0.71776400	3.75619000	2.81260100

H	2.90723700	4.99256800	2.72035900
H	1.25233500	5.52180800	3.04129000
H	2.04930700	4.40358000	4.15420700
C	2.76225900	2.67092600	-2.60890700
C	3.73119400	3.63215300	-3.32549100
C	1.85545500	1.93933900	-3.61736900
H	3.37035800	1.90930100	-2.11216600
H	4.40430200	4.12465600	-2.61662300
H	4.34312500	3.08539900	-4.05032100
H	3.19254400	4.41460500	-3.86976900
H	1.19164900	1.23220400	-3.10938100
H	1.23177500	2.64160700	-4.18003400
H	2.46244100	1.38325400	-4.33940400
C	-4.29478100	-2.06375200	0.83853300
C	-5.44158000	-2.31696300	1.59836100
C	-6.70443700	-2.07104800	1.05466500
C	-6.79499000	-1.57054100	-0.24731200
C	-5.62837600	-1.32345200	-0.97311600
H	-7.60049800	-2.26695900	1.63208600
H	-3.27245000	-2.26025400	1.16850800
H	-5.60660800	-0.93051900	-1.98281300
Cl	-8.33610400	-1.24442800	-0.96702200
Cl	-5.28034500	-2.94586700	3.20372000
N	-4.46666600	-1.58272000	-0.38517600
O	-3.06398500	-1.30705100	-1.40030500

Zero-point correction= 0.859782 (Hartree/Particle)
Thermal correction to Energy= 0.917258
Thermal correction to Enthalpy= 0.918202
Thermal correction to Gibbs Free Energy= 0.755656
Sum of electronic and zero-point Energies= -3266.149725
Sum of electronic and thermal Energies= -3266.092249
Sum of electronic and thermal Enthalpies= -3266.091305
Sum of electronic and thermal Free Energies= -3266.253851

1-INT2

C	-1.15455900	2.88658800	-0.23097200
O	-1.65783900	2.63102700	-1.33340800
C	-0.67056500	4.15623800	0.27451600
C	-0.70755300	5.28524500	-0.56568500
C	-0.18317900	4.25567400	1.59052200
C	-0.25305000	6.50717800	-0.08713300
H	-1.09211300	5.18310900	-1.57543700
C	0.26620500	5.48592900	2.06037400

C	0.23283400	6.60565500	1.22308400
H	-0.27594700	7.38430700	-0.72561600
H	0.63835200	5.57610500	3.07558900
C	-1.19786800	1.56277800	0.40186000
C	-2.36983100	1.31118300	1.27948800
C	-3.65860700	1.01572700	0.79744700
C	-4.77391500	0.78120400	0.35923300
C	-6.07010600	0.51230300	-0.14059100
C	-6.30261600	0.49654900	-1.53328100
C	-7.13478800	0.26282300	0.75286300
C	-7.57925200	0.23443200	-2.01647000
C	-8.40611000	0.00173700	0.25506900
H	-6.94874100	0.27871200	1.82152300
C	-8.62904200	-0.01277000	-1.12566000
H	-7.75988500	0.22351700	-3.08653500
H	-9.22529100	-0.18933500	0.94073300
H	-9.62444000	-0.21599500	-1.50872600
H	0.58533700	7.56366000	1.59358000
H	-0.17640300	3.38066200	2.23354000
H	-5.48008300	0.69278700	-2.21304800
Au	0.21426700	0.15720800	0.11707500
C	1.65363600	-1.27214300	-0.13765600
C	2.71850400	-3.25858800	-0.21709500
C	3.61321400	-2.29902400	-0.57667400
H	4.65097300	-2.36453600	-0.86143100
H	2.82017500	-4.32810600	-0.12697200
N	1.52191500	-2.61161700	0.04849900
N	2.94365600	-1.08667200	-0.52272900
C	0.30191300	-3.28334300	0.45428000
C	0.05413900	-3.45397700	1.83115600
C	-0.56879900	-3.75224800	-0.54984500
C	-1.12248000	-4.12430900	2.18842500
C	-1.72871200	-4.41482700	-0.13000300
C	-2.00398000	-4.60017800	1.22194100
H	-1.34833500	-4.27765600	3.23887500
H	-2.42273400	-4.79326500	-0.87375100
H	-2.90802100	-5.12056000	1.52384200
C	3.54752700	0.19664800	-0.82508000
C	3.48116500	0.67568900	-2.14879100
C	4.18777200	0.89638200	0.21733400
C	4.08201800	1.91362600	-2.40929800
C	4.77000900	2.12844300	-0.10516000
C	4.71825800	2.63307400	-1.40160800
H	4.05374700	2.31643100	-3.41687600

H	5.27370900	2.69747700	0.66988500
H	5.18024200	3.58921800	-1.62886400
C	2.80478800	-0.09140400	-3.28114400
C	3.82371200	-0.50927500	-4.36030800
C	1.64089500	0.71069200	-3.89527000
H	2.37802200	-1.00974400	-2.86669900
H	4.63469600	-1.10965400	-3.93596900
H	3.33271200	-1.10360800	-5.13751900
H	4.27505900	0.36254100	-4.84466000
H	0.89878200	0.98319300	-3.13785000
H	1.99268800	1.63360800	-4.36737300
H	1.13802700	0.11759900	-4.66600600
C	4.26483200	0.37407400	1.64935200
C	3.49374400	1.28909200	2.62102900
C	5.72470400	0.18273400	2.10522600
H	3.78483500	-0.60859000	1.68417100
H	2.44389000	1.38586300	2.32481000
H	3.52503600	0.87892600	3.63565500
H	3.92828000	2.29353300	2.65488500
H	6.26871300	-0.49146300	1.43630000
H	6.26640300	1.13344300	2.13093000
H	5.75444800	-0.24235600	3.11346800
C	-0.29963200	-3.57078700	-2.04103000
C	-1.39142900	-2.71257200	-2.70991400
C	-0.14521100	-4.92838600	-2.75505200
H	0.64692100	-3.03439100	-2.15784300
H	-1.47979500	-1.73350400	-2.22777000
H	-1.15334700	-2.55222500	-3.76651900
H	-2.37038100	-3.20037500	-2.66153200
H	0.65301100	-5.52886900	-2.30745000
H	-1.06836800	-5.51469700	-2.70625600
H	0.09588300	-4.77687100	-3.81204200
C	1.00102900	-2.95461400	2.91836400
C	1.60297000	-4.12777100	3.71741500
C	0.30977100	-1.94198600	3.85221100
H	1.83193700	-2.43138200	2.43530400
H	2.12951700	-4.83107500	3.06438700
H	2.31577900	-3.75648200	4.46067100
H	0.82818000	-4.68739200	4.25118000
H	-0.10333700	-1.09631500	3.29330300
H	-0.50975000	-2.40432400	4.41154200
H	1.02622100	-1.55111200	4.58210100
O	-1.99776400	1.42232800	2.45119700

Zero-point correction= 0.789081 (Hartree/Particle)

Thermal correction to Energy=	0.839411
Thermal correction to Enthalpy=	0.840355
Thermal correction to Gibbs Free Energy=	0.694667
Sum of electronic and zero-point Energies=	-2098.789801
Sum of electronic and thermal Energies=	-2098.739472
Sum of electronic and thermal Enthalpies=	-2098.738527
Sum of electronic and thermal Free Energies=	-2098.884215

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C	-0.12247300	2.33109400	0.48751200
O	-0.64342600	2.70411000	-0.56079000
C	0.32141800	3.28096900	1.53354700
C	0.13659400	4.65534000	1.30569700
C	0.89461400	2.84518900	2.73883200
C	0.52524700	5.57891700	2.27000400
H	-0.31188300	4.97257600	0.37059000
C	1.27972400	3.77420100	3.70343400
C	1.09650800	5.13955200	3.46920600
H	0.38337100	6.64049200	2.09247100
H	1.71893600	3.43602700	4.63681500
C	0.12647100	0.86713700	0.69960100
C	-0.68758000	-0.04889700	1.08806700
C	-1.12435200	-1.28439500	1.41111800
C	-1.57733500	-2.38201300	1.71970400
C	-2.09124700	-3.65688000	2.05381500
C	-2.80558600	-4.40556500	1.09139700
C	-1.90394600	-4.18542600	3.35063800
C	-3.31869300	-5.65345800	1.42570100
C	-2.42188500	-5.43500100	3.67107500
H	-1.35672600	-3.60613500	4.08689300
C	-3.12840200	-6.16847300	2.71220200
H	-3.86971700	-6.22606900	0.68646500
H	-2.27903500	-5.83899500	4.66826100
H	-3.53300800	-7.14283900	2.96869500
H	1.39683300	5.86230300	4.22216100
H	1.03221500	1.78381500	2.91900300
H	-2.94935900	-3.99352900	0.09809300
Au	2.00577900	0.17790500	0.07611200
C	3.82417900	-0.40231800	-0.62798500
C	5.61668200	-1.63809800	-1.23002400
C	5.83002400	-0.36970300	-1.66546600
H	6.65471300	0.06977100	-2.20284600
H	6.21835500	-2.52906100	-1.30953500

N	4.38127600	-1.64199600	-0.59511800
N	4.72186400	0.37659100	-1.28767200
C	3.78722400	-2.81611900	0.01141500
C	4.08636800	-3.09878500	1.35921600
C	2.96421600	-3.63966100	-0.78236700
C	3.52243700	-4.25601400	1.91045200
C	2.42965200	-4.78324700	-0.17604600
C	2.70414800	-5.08988800	1.15366500
H	3.73235400	-4.50883700	2.94512100
H	1.79362800	-5.44413700	-0.75647000
H	2.28265900	-5.98544800	1.60065600
C	4.56785600	1.79207300	-1.56105200
C	3.89354300	2.18271100	-2.73522800
C	5.13014200	2.71295400	-0.65393700
C	3.79098600	3.55675400	-2.98562200
C	4.99808100	4.07281500	-0.95989600
C	4.33705600	4.49188600	-2.11122000
H	3.27861100	3.89657400	-3.88015400
H	5.42076300	4.81263900	-0.28752000
H	4.24911900	5.55214300	-2.32900900
C	3.29693200	1.18707500	-3.72510000
C	4.02709000	1.24222900	-5.08184300
C	1.78062800	1.39970500	-3.89979500
H	3.43651300	0.17927800	-3.32278900
H	5.09903100	1.05083000	-4.96918800
H	3.61828500	0.49082900	-5.76520600
H	3.91307700	2.22136400	-5.55836800
H	1.25618000	1.34649300	-2.94038300
H	1.55971100	2.37434300	-4.34691000
H	1.36555400	0.63198700	-4.56116600
C	5.87212000	2.28832000	0.60996700
C	5.24655200	2.90415500	1.87618300
C	7.37364400	2.62656100	0.51473900
H	5.78830200	1.20171600	0.70687800
H	4.18324800	2.65907100	1.95760600
H	5.75549900	2.52615500	2.76906100
H	5.33935600	3.99491300	1.88305100
H	7.83906900	2.15312900	-0.35576900
H	7.53323000	3.70628200	0.42908800
H	7.90075400	2.28148400	1.41012600
C	2.65326400	-3.34331700	-2.24638500
C	1.13984100	-3.17476700	-2.48219100
C	3.24380200	-4.42380000	-3.17408500
H	3.12684700	-2.39351600	-2.51162100

H	0.72342500	-2.38727400	-1.84612700
H	0.94756200	-2.90769600	-3.52644600
H	0.59458400	-4.10104300	-2.27272900
H	4.32532500	-4.52284200	-3.03749800
H	2.79434700	-5.40396000	-2.98436500
H	3.05638800	-4.16952400	-4.22231700
C	4.98812200	-2.21431100	2.21472000
C	6.26176500	-2.96450000	2.65208000
C	4.23230800	-1.64510200	3.43090500
H	5.30692900	-1.36185500	1.60782700
H	6.82222100	-3.33988300	1.79004100
H	6.91949000	-2.29856900	3.21991600
H	6.02462100	-3.82076900	3.29172800
H	3.34388700	-1.08729800	3.11811700
H	3.90936100	-2.43945100	4.11181200
H	4.88050000	-0.96812100	3.99694200
C	-5.99515200	1.00329700	1.72697100
C	-4.79281000	1.44673400	2.12878300
H	-6.07848000	-0.04671500	1.44419200
H	-4.64140800	2.48290800	2.42342800
C	-7.24905800	1.76363200	1.63174900
C	-8.42489900	1.08172900	1.26934600
C	-7.33561400	3.14529200	1.88862900
C	-9.64462000	1.75070200	1.17028300
H	-8.37783400	0.01485100	1.06648900
C	-8.55194900	3.81346500	1.78734300
H	-6.44682100	3.70264100	2.16836200
C	-9.71251700	3.12020600	1.42879800
H	-10.54074600	1.20200700	0.89559800
H	-8.59785000	4.87960900	1.98933800
H	-10.66002400	3.64505600	1.35334100
C	-3.57991900	0.57079000	2.21193100
H	-3.82792700	-0.46680500	1.95078300
H	-3.15747500	0.57451400	3.22293800
O	-2.53341500	1.07103000	1.36108000
H	-2.82731900	1.03892000	0.40775400
C	-6.07219700	0.52549600	-2.28766700
C	-4.75071700	0.54181700	-2.51811800
H	-6.49406500	1.33753800	-1.69471200
H	-4.26698000	-0.24667800	-3.09172800
C	-7.05152400	-0.46997300	-2.74908900
C	-8.39800100	-0.31657000	-2.37350800
C	-6.71056900	-1.57331900	-3.55431700
C	-9.36887600	-1.23104900	-2.78066000

H	-8.68089600	0.53116200	-1.75487100
C	-7.67881700	-2.48692000	-3.95964800
H	-5.68201400	-1.71441600	-3.87241100
C	-9.01322500	-2.32136300	-3.57497200
H	-10.40326900	-1.08960500	-2.48082800
H	-7.39515600	-3.32951200	-4.58396600
H	-9.76688900	-3.03378200	-3.89695800
C	-3.84191600	1.63358900	-2.05041400
H	-4.39588600	2.36774500	-1.44989100
H	-3.41305100	2.16272900	-2.91337900
O	-2.76260600	1.06057100	-1.28387900
H	-1.98613100	1.65337100	-1.32164900

Zero-point correction= 1.122684 (Hartree/Particle)
Thermal correction to Energy= 1.192684
Thermal correction to Enthalpy= 1.193628
Thermal correction to Gibbs Free Energy= 0.997306
Sum of electronic and zero-point Energies= -2871.648411
Sum of electronic and thermal Energies= -2871.578411
Sum of electronic and thermal Enthalpies= -2871.577466
Sum of electronic and thermal Free Energies= -2871.773789

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C	-0.38555900	-2.19784400	-0.96011900
O	-1.24442100	-2.83081100	-0.22423200
C	0.37745100	-3.05686100	-1.87549100
C	0.27462900	-4.45875600	-1.77715700
C	1.14625400	-2.49121000	-2.91123000
C	0.93609000	-5.27296900	-2.68981600
H	-0.32407900	-4.89312400	-0.98515700
C	1.79525700	-3.31138500	-3.82824800
C	1.69467700	-4.70167900	-3.71680600
H	0.85840500	-6.35239900	-2.60679500
H	2.37802800	-2.86980600	-4.63034700
C	-0.16787800	-0.77522600	-0.86429200
C	-1.18399200	0.11207000	-1.06055900
C	-1.06225200	1.52511300	-0.98732000
C	-1.10560000	2.74334900	-1.00481100
C	-1.16390900	4.16629100	-1.03077700
C	-2.30646200	4.83645600	-0.54719800
C	-0.09495500	4.91858200	-1.55845600
C	-2.37308900	6.22594200	-0.58981400
C	-0.17498100	6.30787900	-1.59953400
H	0.78494600	4.40494100	-1.93024000

C	-1.31013900	6.96464800	-1.11625000
H	-3.25551400	6.73416300	-0.21344800
H	0.64847900	6.88202600	-2.01377900
H	-1.36704900	8.04833200	-1.15119800
H	2.20463600	-5.34028100	-4.43201900
H	1.21770100	-1.41232900	-2.99110600
H	-3.12908600	4.25879100	-0.13805600
Au	1.72610000	-0.28726100	-0.15554700
C	3.56580200	0.10517600	0.66292700
C	5.57283000	1.01211300	1.19476700
C	5.42514000	-0.11092600	1.94099800
H	6.07061100	-0.57083000	2.67167300
H	6.37283000	1.73270300	1.14198800
N	4.42517000	1.13309400	0.42000900
N	4.19346300	-0.65619800	1.60309200
C	4.20457800	2.23895900	-0.48815600
C	4.56103800	2.08440000	-1.84300000
C	3.70419700	3.44511600	0.04102500
C	4.39681300	3.19490700	-2.67979000
C	3.56501000	4.52266000	-0.84317500
C	3.90817400	4.40207000	-2.18724100
H	4.66770300	3.11615500	-3.72790300
H	3.18789600	5.46946900	-0.46994800
H	3.80257400	5.25405500	-2.85276500
C	3.67151900	-1.87575300	2.18512900
C	2.79630200	-1.77910300	3.28550100
C	4.09306500	-3.10819500	1.64654600
C	2.32486400	-2.97789500	3.83509000
C	3.59163600	-4.27279800	2.24084300
C	2.71509900	-4.21100500	3.32044900
H	1.64987700	-2.94327400	4.68452500
H	3.89596300	-5.24036100	1.85383600
H	2.34092200	-5.12735000	3.76753000
C	2.37578200	-0.44849000	3.90262400
C	2.92767300	-0.30219800	5.33515100
C	0.84696600	-0.26139700	3.87430300
H	2.80799800	0.35820600	3.30389700
H	4.01849700	-0.39101800	5.35638400
H	2.65889600	0.67554000	5.74811000
H	2.51933100	-1.06848400	6.00215300
H	0.45849200	-0.32816100	2.85332200
H	0.33711200	-1.01676800	4.48141800
H	0.58034100	0.72087800	4.27818600
C	5.06728800	-3.21532000	0.47660000

C	4.45102500	-3.97091600	-0.71579900
C	6.39537500	-3.86345700	0.91665000
H	5.29827200	-2.20391900	0.12973700
H	3.53173300	-3.48913900	-1.06088400
H	5.15854400	-3.99535900	-1.55135400
H	4.21205400	-5.00770300	-0.45743500
H	6.86146000	-3.30919100	1.73759200
H	6.24348700	-4.89287500	1.25705300
H	7.10260500	-3.88984500	0.08129600
C	3.32459700	3.61648200	1.50922900
C	1.81845600	3.89739200	1.67230700
C	4.17247900	4.70936800	2.18920400
H	3.53312500	2.67661800	2.02814700
H	1.21578100	3.10089100	1.22574200
H	1.56105000	3.96806600	2.73447200
H	1.53047700	4.84067800	1.19765300
H	5.24350500	4.49955200	2.10407000
H	3.99120800	5.69420100	1.74650200
H	3.92344700	4.77506400	3.25323200
C	5.13975400	0.78999800	-2.40510400
C	6.62975600	0.95859900	-2.76447100
C	4.33221700	0.27779400	-3.61234800
H	5.07319700	0.02235200	-1.62919500
H	7.21815500	1.27515400	-1.89741500
H	7.04522600	0.01308200	-3.12820300
H	6.76716100	1.70830000	-3.55059500
H	3.27531300	0.15873300	-3.35435500
H	4.39598800	0.96079500	-4.46565200
H	4.71921900	-0.69296000	-3.93964900
C	-5.76677000	-0.03506300	-2.13152100
C	-4.53737200	-0.43765400	-2.49255800
H	-5.85579200	0.92730100	-1.62596600
H	-4.37948000	-1.39031000	-2.99308600
C	-7.04114100	-0.73592600	-2.33841800
C	-8.21524000	-0.16607500	-1.81372500
C	-7.14749000	-1.95289400	-3.03827500
C	-9.45202300	-0.79013200	-1.97440600
H	-8.15303200	0.77559600	-1.27424800
C	-8.38130300	-2.57613700	-3.19769100
H	-6.26273000	-2.41182600	-3.46883000
C	-9.53902400	-1.99889100	-2.66605000
H	-10.34669400	-0.32940300	-1.56610800
H	-8.44396200	-3.51303600	-3.74328200
H	-10.50045700	-2.48620700	-2.79660700

C	-3.31458900	0.38280800	-2.25153800
H	-3.55897400	1.35050000	-1.80356700
H	-2.75246900	0.55967500	-3.17702700
O	-2.45213000	-0.37305300	-1.34735100
H	-3.15463300	-0.84627300	0.45972100
C	-6.15956100	-0.97881800	2.07550600
C	-4.87461800	-1.12694500	2.43764300
H	-6.53174100	-1.60211900	1.26136900
H	-4.43831400	-0.52894200	3.23484000
C	-7.15694900	-0.06601000	2.65047700
C	-8.44463000	-0.03454400	2.08588300
C	-6.88830000	0.78020600	3.74303100
C	-9.42937200	0.81508700	2.58843300
H	-8.66952200	-0.68291500	1.24290600
C	-7.87080900	1.62849700	4.24387800
H	-5.90804200	0.77097800	4.20975800
C	-9.14575300	1.65068400	3.66906400
H	-10.41832500	0.82137600	2.13956500
H	-7.64582200	2.27204700	5.08935500
H	-9.91103700	2.31117200	4.06548600
C	-3.95303400	-2.10750900	1.78808600
H	-4.48260600	-2.71648300	1.04487200
H	-3.49642000	-2.77945500	2.52168800
O	-2.82431100	-1.43136800	1.16640200
H	-1.83189800	-2.23401000	0.38487500

Zero-point correction= 1.125233 (Hartree/Particle)
Thermal correction to Energy= 1.194573
Thermal correction to Enthalpy= 1.195518
Thermal correction to Gibbs Free Energy= 1.004115
Sum of electronic and zero-point Energies= -2871.678946
Sum of electronic and thermal Energies= -2871.609605
Sum of electronic and thermal Enthalpies= -2871.608661
Sum of electronic and thermal Free Energies= -2871.800064

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C	1.52933800	-2.20544800	0.47394500
O	2.56274600	-2.41369500	-0.16865900
C	0.75862100	-3.32076200	1.06726400
C	1.15591400	-4.63462600	0.75529500
C	-0.29410800	-3.11168500	1.97421900
C	0.49794600	-5.71694600	1.32737800
H	1.98058400	-4.77913200	0.06609800
C	-0.94139000	-4.20010800	2.55568400

C	-0.54987300	-5.50066800	2.22978200
H	0.80176000	-6.72902200	1.07884400
H	-1.75209600	-4.03199900	3.25664000
C	1.05754700	-0.79131600	0.65137700
C	1.79719300	0.22857400	0.97102200
C	1.92777500	1.53884000	1.31201200
C	2.11619100	2.70355100	1.64211700
C	2.31673000	4.05169800	2.02838000
C	2.84461000	4.98410400	1.10810500
C	1.99998600	4.46888400	3.34001100
C	3.04824500	6.30331900	1.49726100
C	2.21044000	5.79080900	3.71633200
H	1.59782500	3.74888700	4.04493000
C	2.73302700	6.70738400	2.79855000
H	3.45574700	7.01805800	0.78935300
H	1.96954400	6.10894000	4.72564400
H	2.89667700	7.73795600	3.09841200
H	-1.05682400	-6.34810600	2.68209000
H	-0.59700800	-2.10243400	2.23238000
H	3.08840000	4.65906300	0.10204100
Au	-0.87253000	-0.24025200	0.02688300
C	-2.71209900	0.24143300	-0.71176400
C	-4.33560100	1.15554900	-1.99249400
C	-4.93581300	0.31601400	-1.11058900
H	-5.97253000	0.06040700	-0.96247200
H	-4.74245200	1.78236800	-2.76949700
N	-2.97260200	1.10040500	-1.73402200
N	-3.92708400	-0.23776100	-0.33269000
C	-1.98241200	1.87706900	-2.45248100
C	-1.72656100	3.19406700	-2.02077800
C	-1.34313900	1.29467600	-3.56506700
C	-0.78025100	3.93149600	-2.74274100
C	-0.40633100	2.08129900	-4.24712200
C	-0.12573900	3.38325200	-3.84238900
H	-0.55873200	4.95070200	-2.44156100
H	0.10512600	1.66860100	-5.11092600
H	0.60073300	3.97550400	-4.39105100
C	-4.17010500	-1.19715400	0.72560100
C	-4.26889300	-2.56067600	0.38367700
C	-4.34413300	-0.71953800	2.04025400
C	-4.54875200	-3.46099000	1.41909400
C	-4.61605400	-1.66816900	3.03425800
C	-4.72152600	-3.02268000	2.72916500
H	-4.63635000	-4.51889400	1.19281600

H	-4.75914000	-1.33854500	4.05857600
H	-4.94755400	-3.73808000	3.51466400
C	-4.09762100	-3.07755600	-1.04200600
C	-5.40277400	-3.70459400	-1.57153500
C	-2.92215300	-4.06813800	-1.14848000
H	-3.86164300	-2.22752400	-1.68921800
H	-6.23572000	-2.99531700	-1.53227400
H	-5.27667900	-4.02204200	-2.61156900
H	-5.69012100	-4.58569800	-0.98867200
H	-1.98599800	-3.61378200	-0.81086500
H	-3.09464800	-4.96441900	-0.54409800
H	-2.79324900	-4.38989500	-2.18710800
C	-4.26945500	0.75970900	2.40743400
C	-3.13619900	1.03692400	3.41394100
C	-5.62277200	1.27412200	2.93738400
H	-4.03836300	1.32672400	1.50087900
H	-2.16804800	0.71403700	3.01773400
H	-3.07585100	2.10854300	3.63056100
H	-3.30333200	0.51678600	4.36275500
H	-6.42570300	1.11093600	2.21167500
H	-5.90751500	0.77037800	3.86661300
H	-5.56686500	2.34748100	3.14555900
C	-1.64257600	-0.11937300	-4.05368000
C	-0.37872500	-1.00053100	-4.06152900
C	-2.31294700	-0.09742700	-5.44224300
H	-2.35021700	-0.57952200	-3.35762900
H	0.08357400	-1.04127000	-3.07002700
H	-0.63257900	-2.02201800	-4.36261300
H	0.37053300	-0.62632500	-4.76659300
H	-3.23358300	0.49482100	-5.43522900
H	-1.64851600	0.33051500	-6.19992100
H	-2.56659200	-1.11428600	-5.75871300
C	-2.43275300	3.83130100	-0.82739600
C	-3.25142800	5.06709200	-1.25007600
C	-1.43829300	4.17955600	0.29673500
H	-3.13819200	3.10279200	-0.41682900
H	-3.98195500	4.81792300	-2.02614000
H	-3.79438900	5.47502600	-0.39142200
H	-2.60876300	5.86144400	-1.64320200
H	-0.88969500	3.29285200	0.62886200
H	-0.70632400	4.92518800	-0.03069300
H	-1.97088900	4.59551900	1.15849500
C	6.74404700	-0.49751700	-0.45415800
C	6.06004400	-0.27410100	0.68133000

H	6.32191100	-0.10812500	-1.38186300
H	6.41851500	-0.63655900	1.64157300
C	8.02131500	-1.20138400	-0.61507300
C	8.57592300	-1.30137000	-1.90341500
C	8.72025700	-1.78537600	0.45871200
C	9.78524200	-1.96028700	-2.11721400
H	8.04911500	-0.85598800	-2.74373800
C	9.92685600	-2.44370500	0.24562100
H	8.31943400	-1.72572300	1.46588400
C	10.46507700	-2.53402100	-1.04241300
H	10.19552700	-2.02532900	-3.12046000
H	10.45236200	-2.88858800	1.08541900
H	11.40774000	-3.04812500	-1.20380100
C	4.76502900	0.47042300	0.70826000
H	4.52560900	0.89190700	-0.27539600
H	4.76982600	1.27824400	1.44433400
O	3.69789200	-0.42146000	1.14069900
H	3.61890700	-1.16218800	0.49430500

Zero-point correction= 0.954301 (Hartree/Particle)
Thermal correction to Energy= 1.013216
Thermal correction to Enthalpy= 1.014160
Thermal correction to Gibbs Free Energy= 0.847083
Sum of electronic and zero-point Energies= -2447.609871
Sum of electronic and thermal Energies= -2447.550956
Sum of electronic and thermal Enthalpies= -2447.550012
Sum of electronic and thermal Free Energies= -2447.717089

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C	-2.35818900	3.63241500	-1.38165300
O	-1.87755400	4.14412600	-2.38664400
C	-3.30020600	4.34330100	-0.47783900
C	-3.72805900	5.63047000	-0.84078200
C	-3.75745100	3.76838900	0.71745500
C	-4.60733700	6.32836100	-0.01940300
H	-3.36000700	6.05719700	-1.76772800
C	-4.63412700	4.47263000	1.54095800
C	-5.06075700	5.75080400	1.17174600
H	-4.94105300	7.32194100	-0.30227900
H	-4.98156200	4.02969000	2.46942300
C	-1.99149600	2.25845700	-1.05672100
C	-1.62079700	1.10452100	-0.91812800
C	-1.08658900	-0.16789800	-0.72091200
C	-1.47566700	-1.37979600	-0.85932300

C	-1.41232300	-2.80034700	-0.75801600
C	-1.29837000	-3.59728600	-1.91890000
C	-1.48033100	-3.41855100	0.50932800
C	-1.23852600	-4.98110300	-1.80505700
C	-1.41095600	-4.80582000	0.61047200
H	-1.56927600	-2.80175000	1.39782400
C	-1.29241500	-5.58601000	-0.54282100
H	-1.14696000	-5.59272100	-2.69703900
H	-1.45413800	-5.27877500	1.58638800
H	-1.24313000	-6.66756200	-0.46054100
H	-5.74519300	6.29891000	1.81255800
H	-3.41470200	2.77801100	1.00373600
H	-1.26723300	-3.11521000	-2.88971300
Au	0.96796300	-0.14303400	-0.13734000
C	2.91910700	0.14243500	0.33944100
C	4.84427400	0.44475300	1.47766000
C	5.11088600	0.64689100	0.16113300
H	6.02539500	0.90259400	-0.34905400
H	5.47851500	0.49010300	2.34812700
N	3.49347700	0.13621100	1.57094900
N	3.91910100	0.45793100	-0.52465100
C	2.80633500	-0.14003600	2.81633000
C	2.20120900	0.93200900	3.50217800
C	2.80109200	-1.46376300	3.29988600
C	1.55916400	0.63525400	4.71103300
C	2.14765200	-1.69757700	4.51613500
C	1.53114000	-0.66241300	5.21375600
H	1.08137600	1.43461400	5.26871500
H	2.12639000	-2.70331900	4.92409700
H	1.03301900	-0.86673100	6.15694700
C	3.77936600	0.58553000	-1.96310200
C	4.02548300	-0.54905500	-2.76179000
C	3.43232900	1.84315200	-2.49713300
C	3.91254500	-0.39134100	-4.14846000
C	3.33442600	1.93810600	-3.89090900
C	3.57152000	0.83662800	-4.70826200
H	4.09750000	-1.24167700	-4.79747800
H	3.07010300	2.88946100	-4.34090900
H	3.49173500	0.93655000	-5.78662500
C	4.40972800	-1.90773400	-2.18327200
C	5.82949600	-2.32209700	-2.61791100
C	3.37806800	-2.99168100	-2.55108100
H	4.41440200	-1.82715000	-1.09201600
H	6.57334900	-1.57490900	-2.32359800

H	6.10625100	-3.27601200	-2.15739300
H	5.89556400	-2.44544000	-3.70365700
H	2.37448200	-2.71504700	-2.21237500
H	3.33443800	-3.15478600	-3.63278200
H	3.64692900	-3.94484100	-2.08370500
C	3.19760400	3.07970300	-1.63426500
C	1.84889300	3.75810000	-1.93960000
C	4.36454500	4.07805400	-1.78062000
H	3.16706400	2.76315000	-0.58704600
H	1.01075500	3.06393500	-1.83345300
H	1.68753100	4.59433800	-1.25170100
H	1.81515700	4.16388900	-2.95519300
H	5.32362400	3.62119800	-1.51541700
H	4.44458300	4.44392300	-2.80950700
H	4.21006600	4.94423200	-1.12906800
C	3.48513200	-2.61694400	2.57158200
C	2.49837100	-3.75300000	2.24292100
C	4.69105100	-3.14483700	3.37465000
H	3.86777900	-2.24061600	1.61843200
H	1.65148700	-3.38555900	1.65516600
H	3.00142500	-4.53472400	1.66447100
H	2.10314700	-4.21948200	3.15133800
H	5.41944700	-2.35236200	3.57371800
H	4.37842600	-3.55680200	4.33974000
H	5.19992200	-3.94093600	2.82148700
C	2.23572900	2.37180700	2.99788500
C	3.01615100	3.28402300	3.96550200
C	0.81874200	2.91933600	2.74004200
H	2.76548500	2.38793600	2.04094500
H	4.03436400	2.91739900	4.12950600
H	3.08238600	4.29875400	3.56018200
H	2.52497700	3.34812700	4.94183600
H	0.28010200	2.30289100	2.01323100
H	0.22648500	2.95216100	3.66050000
H	0.87376300	3.93927200	2.34591200
C	-4.97471200	-2.66163300	-1.09679000
C	-6.13213700	-2.85977600	-0.35592200
C	-6.73929200	-1.80591400	0.32669900
C	-6.13585400	-0.55040000	0.23278500
C	-4.97871300	-0.36305300	-0.50896700
H	-7.64474800	-1.95401300	0.90153900
H	-4.46439500	-3.43026900	-1.65845000
H	-4.46443800	0.58038300	-0.63041200
Cl	-6.82970500	0.81604600	1.04827500

Cl	-6.81668200	-4.45375900	-0.29690100
N	-4.41847400	-1.41987500	-1.16303200
O	-3.34422000	-1.23430500	-1.88043900

Zero-point correction= 0.859278 (Hartree/Particle)
Thermal correction to Energy= 0.917420
Thermal correction to Enthalpy= 0.918364
Thermal correction to Gibbs Free Energy= 0.751915
Sum of electronic and zero-point Energies= -3266.133769
Sum of electronic and thermal Energies= -3266.075627
Sum of electronic and thermal Enthalpies= -3266.074683
Sum of electronic and thermal Free Energies= -3266.241132

2-TS1'

C	2.39777500	2.48656400	-1.41427600
O	3.38893300	2.50853200	-0.67549200
C	2.21144000	3.44625000	-2.52206900
C	3.18699900	4.43700500	-2.72760800
C	1.09286900	3.37931100	-3.36820700
C	3.03976000	5.34997400	-3.76566500
H	4.04536400	4.46911900	-2.06538700
C	0.95162800	4.29424800	-4.40877200
C	1.92320900	5.27911600	-4.60667000
H	3.79220100	6.11587100	-3.92538400
H	0.08970400	4.24022700	-5.06646100
C	1.38479600	1.47470800	-1.17488700
C	0.70146600	0.52898800	-0.82344800
C	-0.09897300	-0.52407900	-0.39765900
C	0.03411400	-1.76220300	-0.13398300
C	-0.22894300	-3.13464500	0.08569100
C	0.39602500	-3.83118200	1.14525900
C	-1.12847900	-3.81368900	-0.77023800
C	0.11343200	-5.17638800	1.34338000
C	-1.40914700	-5.15674000	-0.55038000
H	-1.60429700	-3.27299300	-1.58140700
C	-0.78832800	-5.83807600	0.50171400
H	0.59814100	-5.71513400	2.15107600
H	-2.10610300	-5.67422900	-1.20134500
H	-1.00274800	-6.89027200	0.66344100
H	1.81252900	5.99171500	-5.41869400
H	0.34415900	2.60889400	-3.20964700
H	1.11677600	-3.31106500	1.76313400
Au	-2.16294400	-0.14398200	0.04881000
C	-4.08453400	0.39721400	0.40715200

C	-6.34085600	0.44165100	0.43558800
C	-5.90115800	1.56005400	1.06851400
H	-6.43612300	2.37356900	1.53129200
H	-7.33698100	0.08157100	0.23492400
N	-5.21296800	-0.26260600	0.03510300
N	-4.51381200	1.51808000	1.04278000
C	-5.25313800	-1.52930800	-0.66794700
C	-5.24584300	-1.51762100	-2.07730600
C	-5.32595800	-2.71405300	0.09176000
C	-5.30566500	-2.75723600	-2.72662000
C	-5.38640800	-3.92253200	-0.61360000
C	-5.37611600	-3.94642700	-2.00566100
H	-5.30667200	-2.78938000	-3.81163700
H	-5.44935800	-4.85561400	-0.06252700
H	-5.43332500	-4.89489700	-2.53190000
C	-3.65910200	2.53649200	1.62227200
C	-3.26217800	2.39391000	2.96672500
C	-3.28555100	3.63367100	0.82056400
C	-2.45058400	3.40164000	3.50223000
C	-2.47464900	4.60972100	1.41245200
C	-2.05984800	4.49640900	2.73645300
H	-2.12303100	3.32760300	4.53435700
H	-2.16595000	5.47076800	0.82802600
H	-1.43239300	5.26678500	3.17460100
C	-3.67667500	1.21299300	3.83931200
C	-4.52542800	1.67150700	5.04164100
C	-2.45244100	0.39795500	4.30058400
H	-4.30107000	0.54440200	3.23873900
H	-5.41627900	2.21922900	4.71834300
H	-4.85269400	0.80664500	5.62768500
H	-3.95635500	2.32708200	5.70842900
H	-1.86608200	0.04452600	3.44617400
H	-1.79040900	0.99355000	4.93724100
H	-2.77334200	-0.47363900	4.88037500
C	-3.72803000	3.79430600	-0.63075100
C	-2.52062300	3.83289300	-1.58746200
C	-4.62115600	5.03775900	-0.81196500
H	-4.32790900	2.92140400	-0.90547600
H	-1.90180200	2.93625000	-1.48015100
H	-2.86280200	3.89320000	-2.62598800
H	-1.88439800	4.70303700	-1.39757400
H	-5.50106100	4.99863100	-0.16202500
H	-4.07759100	5.95891700	-0.57879600
H	-4.96819300	5.11005900	-1.84779400

C	-5.35062800	-2.72567800	1.61765000
C	-4.14499500	-3.48908900	2.19892300
C	-6.67928600	-3.29577400	2.15305800
H	-5.27601800	-1.69239400	1.96918300
H	-3.19860400	-3.06826100	1.84579800
H	-4.15636000	-3.43629100	3.29244300
H	-4.16574300	-4.54734200	1.91944300
H	-7.53946900	-2.73414800	1.77528000
H	-6.81310700	-4.34264900	1.86189600
H	-6.69875000	-3.25064400	3.24659200
C	-5.19143500	-0.23407300	-2.90047400
C	-6.46902000	-0.05493100	-3.74468900
C	-3.92956200	-0.18060300	-3.78365800
H	-5.13706100	0.61369600	-2.21120700
H	-7.36689500	-0.05518800	-3.11875900
H	-6.43503100	0.89452100	-4.28846900
H	-6.57851000	-0.85602900	-4.48272500
H	-3.01939400	-0.26231700	-3.18018600
H	-3.91949400	-0.98952100	-4.52133800
H	-3.89137200	0.76635600	-4.33190500
C	5.39569400	-3.26926100	-1.36085900
C	4.59307200	-2.21700100	-1.14115500
H	4.93060400	-4.22001300	-1.62524700
H	5.00446600	-1.25494000	-0.84184800
C	6.86349600	-3.30142400	-1.27901900
C	7.65099500	-2.13837200	-1.18147800
C	7.51949800	-4.54448600	-1.30522000
C	9.03818900	-2.22150400	-1.09641300
H	7.17807300	-1.16105300	-1.19308200
C	8.90842900	-4.62896700	-1.21813500
H	6.92897700	-5.45345000	-1.38972000
C	9.67383500	-3.46721400	-1.11140900
H	9.62520700	-1.31015800	-1.02840100
H	9.39229000	-5.60111600	-1.23727500
H	10.75626900	-3.52917900	-1.05028100
C	3.10092700	-2.25925500	-1.28538500
H	2.77284800	-3.24895800	-1.61898600
H	2.77669500	-1.52733500	-2.04267400
O	2.42190100	-1.99929000	-0.04504600
H	2.79122500	-1.16982100	0.34682800
C	6.51275100	1.44899300	2.31652300
C	5.73049200	0.41513800	1.96916200
H	6.03548800	2.30533600	2.79571700
H	6.14444700	-0.45682100	1.46536100

C	7.96441300	1.58257300	2.12712800
C	8.78767000	0.51419800	1.72360900
C	8.56776800	2.82926500	2.36847800
C	10.15763000	0.69598000	1.55656700
H	8.35903100	-0.46826700	1.55208300
C	9.93945800	3.01218400	2.19891400
H	7.94886300	3.66365300	2.68940000
C	10.74065300	1.94538700	1.79075400
H	10.77689000	-0.14409500	1.25482400
H	10.38214300	3.98551400	2.38947800
H	11.81053700	2.08153600	1.66399000
C	4.25670000	0.37099700	2.24228000
H	3.94809600	1.25324400	2.81981000
H	4.00085000	-0.51615700	2.83340500
O	3.46723700	0.26243300	1.04730200
H	3.56367800	1.07582100	0.51199500

Zero-point correction= 1.122559 (Hartree/Particle)
Thermal correction to Energy= 1.192814
Thermal correction to Enthalpy= 1.193758
Thermal correction to Gibbs Free Energy= 0.997993
Sum of electronic and zero-point Energies= -2871.639453
Sum of electronic and thermal Energies= -2871.569197
Sum of electronic and thermal Enthalpies= -2871.568253
Sum of electronic and thermal Free Energies= -2871.764019

3-TS1'

C	-4.00939000	1.84831500	0.57941300
O	-4.99954600	1.27633700	1.03146800
C	-3.94638300	3.31281500	0.36894900
C	-5.06584800	4.08826900	0.71595600
C	-2.80752500	3.93114300	-0.17058300
C	-5.04361600	5.46516900	0.52523200
H	-5.93513900	3.58990800	1.13111000
C	-2.79206700	5.31087900	-0.36295400
C	-3.90723900	6.07758400	-0.01555900
H	-5.90778000	6.06461300	0.79399000
H	-1.91371200	5.78729300	-0.78712500
C	-2.84136700	1.04176100	0.23458000
C	-1.98026000	0.21328400	-0.00374800
C	-0.98151500	-0.73262100	-0.26607800
C	-1.05989100	-1.96980700	-0.61705200
C	-0.57889200	-3.28499700	-0.87024300
C	-0.79133600	-3.90703100	-2.12006900

C	0.11583600	-3.97401400	0.14851900
C	-0.30584100	-5.18910000	-2.34331900
C	0.60681500	-5.25270900	-0.09371600
H	0.27547900	-3.49142200	1.10676400
C	0.39383400	-5.86119100	-1.33393500
H	-0.47182100	-5.66930900	-3.30224100
H	1.14940500	-5.77618100	0.68645700
H	0.76911600	-6.86394200	-1.51496200
H	-3.89340900	7.15299400	-0.16670700
H	-1.94236700	3.33238000	-0.43902800
H	-1.34984000	-3.38169200	-2.88610700
Au	1.05188700	-0.15806300	-0.09016600
C	2.95641500	0.51538100	0.13454300
C	5.15276500	0.64220400	0.64547700
C	4.78171900	1.84500400	0.13608500
H	5.34230600	2.74979700	-0.03491300
H	6.10271800	0.28442100	1.00844400
N	4.02115000	-0.16305600	0.63811000
N	3.43077600	1.75160100	-0.17180000
C	3.99839900	-1.53285900	1.11117100
C	3.67844900	-1.77035700	2.46322100
C	4.32651300	-2.56102800	0.20504000
C	3.68579200	-3.10234000	2.89652100
C	4.31942100	-3.87230100	0.69723200
C	4.00362300	-4.14191100	2.02627400
H	3.45011800	-3.32526500	3.93237400
H	4.57132800	-4.69076200	0.03013700
H	4.01596500	-5.16573500	2.38908800
C	2.65264100	2.83654700	-0.73688000
C	2.57247100	2.94634800	-2.13984600
C	2.03789500	3.74933100	0.14320900
C	1.83617100	4.01988400	-2.65585200
C	1.31881900	4.80499800	-0.43207400
C	1.21844700	4.94074300	-1.81413500
H	1.75269000	4.13915900	-3.73140700
H	0.83916300	5.53379800	0.21392700
H	0.66436000	5.77291200	-2.23883800
C	3.24655100	1.96470900	-3.09417100
C	4.29341400	2.66830600	-3.98041700
C	2.20878200	1.21141300	-3.94936800
H	3.77717000	1.21633600	-2.49808800
H	5.05215700	3.17778200	-3.37810300
H	4.80108500	1.93909400	-4.61987600
H	3.83067600	3.41511300	-4.63325600

H	1.49201200	0.67399400	-3.31985900
H	1.64504600	1.89592600	-4.59128400
H	2.70822600	0.48430400	-4.59794300
C	2.13282100	3.63960200	1.66243500
C	0.74332400	3.45568400	2.30311900
C	2.86948800	4.85096500	2.26809800
H	2.71957100	2.74891000	1.90638100
H	0.23791400	2.56874600	1.90802200
H	0.83881900	3.33915000	3.38755500
H	0.09634000	4.31941500	2.11934400
H	3.87164500	4.96601300	1.84305000
H	2.32404400	5.78308600	2.08906700
H	2.97225200	4.73024800	3.35123100
C	4.68177800	-2.30103200	-1.25605200
C	3.64196900	-2.92563000	-2.20686500
C	6.10494800	-2.79054900	-1.58912500
H	4.66468300	-1.22036400	-1.42548700
H	2.63781700	-2.53841100	-2.00720600
H	3.89554500	-2.69840600	-3.24754900
H	3.60808700	-4.01507600	-2.10354500
H	6.85181000	-2.32935800	-0.93537600
H	6.19416000	-3.87621700	-1.48077800
H	6.35924800	-2.54009300	-2.62392800
C	3.34676600	-0.65466000	3.44996200
C	4.37959100	-0.58941600	4.59265100
C	1.91444400	-0.79363400	4.00135600
H	3.39417400	0.29918000	2.91629300
H	5.39559100	-0.45572900	4.20808800
H	4.15538600	0.25004500	5.25835500
H	4.37065000	-1.50247200	5.19655400
H	1.17625300	-0.78950400	3.19254800
H	1.78940700	-1.72116900	4.56969000
H	1.68509300	0.03872300	4.67451200
C	-6.41089200	-2.71921600	-0.08775500
C	-5.22528600	-2.19410100	0.27164500
H	-6.41146400	-3.72659300	-0.50705900
H	-5.15699300	-1.19947500	0.71024200
C	-7.73776800	-2.10617000	0.02983400
C	-7.93741200	-0.78451900	0.47619900
C	-8.86321300	-2.87146500	-0.32499800
C	-9.22274500	-0.25924400	0.56405800
H	-7.08945700	-0.16353800	0.74775700
C	-10.14950100	-2.34323800	-0.23438700
H	-8.72314000	-3.89191100	-0.67304500

C	-10.33300000	-1.03398400	0.21168400
H	-9.36236800	0.76109600	0.90910900
H	-11.00527800	-2.95156400	-0.51130800
H	-11.33324300	-0.61731500	0.28383800
C	-3.93741900	-2.92522600	0.09169900
H	-4.09447000	-3.96658900	-0.19966300
H	-3.32674600	-2.90093000	1.00219300
O	-3.13670100	-2.32238300	-0.98854400
H	-3.48184100	-1.42581100	-1.12577100

Zero-point correction= 0.953370 (Hartree/Particle)
Thermal correction to Energy= 1.012906
Thermal correction to Enthalpy= 1.013850
Thermal correction to Gibbs Free Energy= 0.845902
Sum of electronic and zero-point Energies= -2447.598929
Sum of electronic and thermal Energies= -2447.539394
Sum of electronic and thermal Enthalpies= -2447.538450
Sum of electronic and thermal Free Energies= -2447.706398

4-TS1

C	-1.07112800	-1.71773100	-1.60976300
O	-1.73294400	-2.25811500	-0.72028100
C	-0.68359900	-2.40539400	-2.85478300
C	-1.22623300	-3.68772900	-3.06715100
C	0.19914200	-1.85215300	-3.79966000
C	-0.89631200	-4.40009400	-4.21331000
H	-1.90176200	-4.10055000	-2.32591200
C	0.52755900	-2.57669600	-4.94338200
C	-0.01881100	-3.84528800	-5.15189700
H	-1.31935400	-5.38579000	-4.37915500
H	1.20785100	-2.15031900	-5.67365300
C	-0.64954100	-0.31120900	-1.28273000
C	-1.35754300	0.79733000	-1.94413400
C	-2.51207200	1.49347900	-1.54277200
C	-3.51103400	2.17188200	-1.35581700
C	-4.66022100	2.98104100	-1.17886300
C	-5.56082800	2.75171200	-0.11553600
C	-4.90524100	4.03208500	-2.09127500
C	-6.68142500	3.56257700	0.02512300
C	-6.02800100	4.83609000	-1.93562700
H	-4.21061500	4.20054700	-2.90741200
C	-6.91533600	4.60284800	-0.87992100
H	-7.37587400	3.38380800	0.83971700
H	-6.21510600	5.64328700	-2.63645500

H	-7.79259800	5.23194200	-0.76362900
H	0.23852900	-4.40402200	-6.04686900
H	0.61506900	-0.86436500	-3.64563100
H	-5.37899200	1.93713200	0.57751500
Au	1.05575100	0.00875800	-0.25687200
C	2.81027500	0.31927200	0.74675800
C	4.62665200	1.30224700	1.65429800
C	4.70726600	-0.02983800	1.91688500
H	5.44707700	-0.60698600	2.44774000
H	5.28280600	2.11880900	1.90925700
N	3.45615400	1.49951400	0.93796700
N	3.58604600	-0.61790600	1.35257400
C	2.98751700	2.79265900	0.47849100
C	3.36013600	3.22507400	-0.80975500
C	2.19503400	3.56482000	1.35154300
C	2.90346500	4.48486200	-1.21646700
C	1.76590800	4.81423100	0.88694700
C	2.11535500	5.27096300	-0.38076100
H	3.17074500	4.85451700	-2.20138300
H	1.15266100	5.43834800	1.52926300
H	1.77467900	6.24541300	-0.71792100
C	3.28103000	-2.03436200	1.41567500
C	2.51120700	-2.50648400	2.49777300
C	3.78208000	-2.87421000	0.40102600
C	2.23322900	-3.87869800	2.53073700
C	3.47386800	-4.23716900	0.49106200
C	2.70545000	-4.73477000	1.53985900
H	1.64328200	-4.28128800	3.34804900
H	3.84314200	-4.91728900	-0.27001800
H	2.47912800	-5.79570800	1.58879500
C	2.01165600	-1.60581100	3.62434100
C	2.68666100	-1.97378000	4.96149900
C	0.47628800	-1.63308000	3.75264700
H	2.29547500	-0.57486900	3.39194900
H	3.77786800	-1.92557600	4.88827100
H	2.36864700	-1.28486300	5.75067800
H	2.42059600	-2.98748500	5.27811600
H	-0.01360800	-1.29262300	2.83524200
H	0.10918000	-2.63868300	3.98255000
H	0.15981500	-0.97476400	4.56877200
C	4.64333100	-2.36578400	-0.75140500
C	4.01141800	-2.67942800	-2.12099700
C	6.07738900	-2.92572900	-0.66331500
H	4.71439800	-1.27669900	-0.67266300

H	3.00278500	-2.26233200	-2.20129500
H	4.62255700	-2.25437800	-2.92405000
H	3.94181200	-3.75774000	-2.29638700
H	6.55065500	-2.67209400	0.29054700
H	6.08596100	-4.01639500	-0.75793700
H	6.69639000	-2.51674700	-1.46834500
C	1.79262000	3.09688200	2.74735600
C	0.27055000	2.87122100	2.84457600
C	2.28211100	4.07137700	3.83642600
H	2.27307700	2.13274600	2.93983200
H	-0.07046900	2.13043800	2.11438700
H	0.00542900	2.51078200	3.84414500
H	-0.28164700	3.80060300	2.66943200
H	3.36557100	4.21844900	3.78654200
H	1.80893600	5.05382800	3.74162500
H	2.03790700	3.68235500	4.83005300
C	4.22797700	2.39520900	-1.75092000
C	5.58699900	3.07766700	-2.00558700
C	3.49957500	2.09415200	-3.07534100
H	4.43328800	1.43365600	-1.27078800
H	6.12806000	3.25576500	-1.07078700
H	6.21459400	2.44990300	-2.64629900
H	5.46235600	4.04339900	-2.50579400
H	2.53872800	1.59957200	-2.89974900
H	3.30395000	3.00865900	-3.64439500
H	4.11396900	1.44088900	-3.70370000
O	-0.71091800	1.00012000	-2.98260800
C	-5.08246800	-1.07009400	2.06095000
C	-4.22328200	-0.43633300	1.24444600
H	-4.84225700	-1.09276400	3.12492300
H	-4.39353700	-0.40209800	0.17000200
C	-6.33116000	-1.75607000	1.70338600
C	-7.03568300	-2.43944800	2.71022200
C	-6.86120200	-1.76447300	0.39902100
C	-8.22195200	-3.11497100	2.42811700
H	-6.64321500	-2.44067000	3.72407800
C	-8.04498300	-2.43868500	0.11655900
H	-6.34843200	-1.23646600	-0.39942100
C	-8.73075800	-3.11767700	1.12907500
H	-8.74796400	-3.63732700	3.22160300
H	-8.43861900	-2.43376400	-0.89573200
H	-9.65531700	-3.64108400	0.90499500
C	-2.98119700	0.24780600	1.72869200
H	-2.86710400	0.10895300	2.81283900

H	-3.01721000	1.32739400	1.53793900
O	-1.79681600	-0.21729500	1.05686100
H	-1.91804100	-1.15204700	0.80988600

Zero-point correction= 0.957770 (Hartree/Particle)
Thermal correction to Energy= 1.017953
Thermal correction to Enthalpy= 1.018898
Thermal correction to Gibbs Free Energy= 0.850186
Sum of electronic and zero-point Energies= -2522.811924
Sum of electronic and thermal Energies= -2522.751740
Sum of electronic and thermal Enthalpies= -2522.750796
Sum of electronic and thermal Free Energies= -2522.919508

4-INT1

C	-1.95780200	-0.58756800	-1.61528600
O	-2.95672200	-0.98520900	-0.84325800
C	-1.73462700	-1.45923200	-2.77329300
C	-2.82365900	-2.25015800	-3.20163600
C	-0.51347400	-1.54595900	-3.46920700
C	-2.70045700	-3.07594000	-4.31301500
H	-3.76548900	-2.19626800	-2.66947500
C	-0.39567500	-2.38643900	-4.57101800
C	-1.48681100	-3.14596800	-5.00130400
H	-3.55075400	-3.66444000	-4.64227500
H	0.55149000	-2.44701600	-5.09705900
C	-1.29502700	0.61879500	-1.19084200
C	-0.52949300	1.55131600	-2.10922500
C	-0.17907500	2.82919100	-1.54167500
C	0.16216100	3.93720200	-1.16770200
C	0.56224600	5.23408800	-0.74373400
C	0.19707700	5.71752800	0.52992900
C	1.32541900	6.05220300	-1.60272400
C	0.59012000	6.99064000	0.93123400
C	1.71340700	7.32348600	-1.19071500
H	1.59985900	5.67947800	-2.58401800
C	1.34782100	7.79420800	0.07382000
H	0.30349200	7.36045900	1.91086000
H	2.29761300	7.95081500	-1.85671900
H	1.65002700	8.78803500	0.38985300
H	-1.39005200	-3.79259900	-5.86824300
H	0.33845000	-0.96502200	-3.14662300
H	-0.39390700	5.08882200	1.18789500
Au	0.41348700	-0.42233200	-0.18456200
C	1.97017300	-1.18654600	0.86203700

C	3.98357800	-1.40541000	1.85208200
C	3.26273800	-2.52003200	2.14024300
H	3.50674100	-3.39660900	2.71828700
H	4.98264800	-1.11113900	2.13016400
N	3.17479900	-0.59444700	1.06784000
N	2.02746900	-2.37119800	1.52393300
C	3.56752900	0.71353600	0.57939500
C	4.19062000	0.80395300	-0.68102600
C	3.33347500	1.83179800	1.40475200
C	4.58985800	2.07719600	-1.10562800
C	3.74955400	3.07896700	0.92337900
C	4.37260000	3.20204100	-0.31532100
H	5.07633500	2.18700700	-2.06955700
H	3.58336100	3.96492000	1.52786700
H	4.68885700	4.17971200	-0.66632200
C	0.95788000	-3.34732500	1.59315000
C	-0.02390000	-3.19750700	2.59318400
C	0.96490900	-4.41600800	0.67412700
C	-1.04195200	-4.15798300	2.63646600
C	-0.07727000	-5.34646000	0.77005600
C	-1.07229000	-5.21828600	1.73514200
H	-1.81678500	-4.07747600	3.39233500
H	-0.10693000	-6.18470900	0.08131500
H	-1.87007200	-5.95291800	1.79048100
C	-0.00252100	-2.07295000	3.62483000
C	0.20233000	-2.63016300	5.04810600
C	-1.27030100	-1.20020700	3.54978800
H	0.84943500	-1.42211300	3.40685000
H	1.12078700	-3.22125300	5.11901400
H	0.26905500	-1.81094300	5.77129000
H	-0.63040500	-3.27332900	5.35027300
H	-1.39049900	-0.75578300	2.55642600
H	-2.17201800	-1.77983000	3.77276000
H	-1.21162600	-0.38677600	4.28035000
C	2.05710500	-4.60532900	-0.37455100
C	1.48175700	-4.67023900	-1.80136600
C	2.91024400	-5.85189100	-0.06363400
H	2.72299600	-3.73772400	-0.33784800
H	0.89745000	-3.77620300	-2.03713000
H	2.29447900	-4.75028600	-2.53081900
H	0.83243500	-5.54097200	-1.93765700
H	3.35698600	-5.79616000	0.93424500
H	2.30918100	-6.76601100	-0.10610600
H	3.72090300	-5.95156700	-0.79264100

C	2.65522300	1.73434300	2.76816500
C	1.30881900	2.48472400	2.77641800
C	3.57728000	2.23185400	3.89841900
H	2.43874900	0.68078300	2.96978100
H	0.63826200	2.10832800	1.99728000
H	0.81331300	2.36412700	3.74569300
H	1.45076000	3.55699800	2.60590600
H	4.52326700	1.68160500	3.91622100
H	3.81394000	3.29468200	3.78641100
H	3.09103200	2.10187200	4.87059900
C	4.44387500	-0.40631300	-1.57431000
C	5.95077300	-0.71161000	-1.68921300
C	3.80627100	-0.22587400	-2.96577300
H	3.96861500	-1.27777300	-1.11359900
H	6.39993200	-0.89543400	-0.70795500
H	6.11427500	-1.59944100	-2.30854700
H	6.49120800	0.12110200	-2.15091200
H	2.74224400	0.01964700	-2.88969300
H	4.28934500	0.57723900	-3.53133400
H	3.91057700	-1.14588500	-3.55025700
O	-0.19835500	1.25491900	-3.25138200
C	-5.20549400	1.78235600	0.64482500
C	-4.37755400	1.68804200	-0.41329100
H	-4.82643800	2.29099200	1.53265600
H	-4.70527200	1.20425800	-1.33097600
C	-6.58181700	1.29060300	0.76594400
C	-7.24660900	1.45280500	1.99471400
C	-7.27254600	0.66424600	-0.28946100
C	-8.55312400	1.00083400	2.17000500
H	-6.72940300	1.93917500	2.81800400
C	-8.57675900	0.21390500	-0.11495900
H	-6.79194800	0.53561500	-1.25456000
C	-9.22214700	0.37894300	1.11529200
H	-9.04849000	1.13629400	3.12661500
H	-9.09649500	-0.26363300	-0.94020000
H	-10.24123600	0.02810200	1.24651900
C	-2.99252100	2.25072400	-0.39678100
H	-2.87315600	2.97813200	0.40834600
H	-2.73876800	2.73605400	-1.34232800
O	-1.95956400	1.22627100	-0.10281300
H	-3.06415800	-0.30782800	-0.13672300

Zero-point correction= 0.961089 (Hartree/Particle)
Thermal correction to Energy= 1.020662
Thermal correction to Enthalpy= 1.021607

Thermal correction to Gibbs Free Energy=	0.854604
Sum of electronic and zero-point Energies=	-2522.856837
Sum of electronic and thermal Energies=	-2522.797263
Sum of electronic and thermal Enthalpies=	-2522.796319
Sum of electronic and thermal Free Energies=	-2522.963322

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C	0.20835600	2.22097200	0.88032100
O	0.89938600	1.95038000	1.86029800
C	0.38100200	1.28991000	-0.26877100
C	1.31557400	1.66371900	-1.40271900
Au	-0.47671700	-0.51695000	-0.07870100
C	-1.34147500	-2.37332200	0.09584000
C	-1.77557200	-4.57057600	-0.17149400
C	-2.70770200	-4.06787400	0.68323200
H	-3.53452400	-4.53860600	1.19038300
H	-1.62633200	-5.56729900	-0.55461200
N	-0.94557600	-3.51736300	-0.52167600
N	-2.42606100	-2.71960000	0.83613600
C	0.20319700	-3.62203400	-1.40038500
C	0.02947700	-3.34396300	-2.77201900
C	1.44063000	-3.99997000	-0.84015700
C	1.16181800	-3.44437100	-3.59092800
C	2.53575600	-4.08200100	-1.70995800
C	2.40076700	-3.80662000	-3.06805700
H	1.06909500	-3.24133500	-4.65297900
H	3.50618400	-4.36856600	-1.31708500
H	3.26334200	-3.88040000	-3.72356700
C	-3.18665800	-1.80682200	1.66914900
C	-2.77674500	-1.61779200	3.00425100
C	-4.30584200	-1.16133800	1.10609900
C	-3.53453100	-0.73486500	3.78364600
C	-5.02209500	-0.28901500	1.93481100
C	-4.64269600	-0.07700600	3.25744800
H	-3.25232700	-0.56347900	4.81752400
H	-5.88992900	0.22859200	1.53825600
H	-5.21586600	0.60127300	3.88246700
C	-1.57779500	-2.33304600	3.61974100
C	-2.02108900	-3.30171100	4.73478300
C	-0.52168100	-1.33688300	4.13724200
H	-1.09921300	-2.93335800	2.83998700
H	-2.74476500	-4.03607400	4.36672400
H	-1.15795500	-3.84536900	5.13197800

H	-2.48704500	-2.76503600	5.56741100
H	-0.18066600	-0.66095900	3.34662200
H	-0.91339800	-0.72247700	4.95414000
H	0.34871000	-1.87807700	4.52217000
C	-4.75200200	-1.37175600	-0.33809200
C	-4.64355000	-0.06882300	-1.15467800
C	-6.17643300	-1.95615600	-0.41072500
H	-4.08093600	-2.10052500	-0.80304300
H	-3.62158200	0.32467000	-1.14274700
H	-4.92857000	-0.24835700	-2.19656600
H	-5.30552900	0.70793500	-0.75845900
H	-6.25279300	-2.89663600	0.14385100
H	-6.91653000	-1.26502000	0.00476500
H	-6.45408200	-2.15188200	-1.45136300
C	1.62519700	-4.31745500	0.64128400
C	2.57957700	-3.31518000	1.31915700
C	2.10120100	-5.76855900	0.85154000
H	0.65474300	-4.22270400	1.13773500
H	2.20797200	-2.28906200	1.22829600
H	2.67729700	-3.54470100	2.38504000
H	3.58152400	-3.35218600	0.87958300
H	1.41331100	-6.48701500	0.39478900
H	3.09214000	-5.93552600	0.41759400
H	2.16680200	-5.99371300	1.92063100
C	-1.31888300	-2.97409600	-3.38390500
C	-1.84629200	-4.11268400	-4.28098000
C	-1.25629600	-1.64469000	-4.16074600
H	-2.03829000	-2.83804900	-2.57083100
H	-1.94098500	-5.05133700	-3.72596300
H	-2.83125400	-3.85593000	-4.68382100
H	-1.17565800	-4.29340000	-5.12718100
H	-0.87667300	-0.82911900	-3.53687600
H	-0.60908000	-1.71940400	-5.04028100
H	-2.25529400	-1.36813700	-4.51278600
O	1.31686500	0.73583900	-2.44043500
O	2.53828400	1.71961600	-0.65395600
H	1.20022600	-0.15701700	-2.07896800
C	5.78093800	0.82990600	0.01473100
C	4.48264000	0.82747700	0.35931700
H	6.02698500	0.63740100	-1.03031200
H	4.15973800	1.02956000	1.37765300
C	6.94112100	1.05915800	0.88342200
C	6.83186800	1.31677400	2.26362700
C	8.22621700	1.02427800	0.31318300

C	7.96718600	1.53390000	3.03734400
H	5.85445500	1.34943000	2.73514500
C	9.36405100	1.24058500	1.08837700
H	8.32884300	0.82746800	-0.75110900
C	9.23823300	1.49651700	2.45419600
H	7.86371700	1.73305200	4.09995500
H	10.34641100	1.21008200	0.62669500
H	10.12179900	1.66601400	3.06212800
C	3.39157700	0.54196000	-0.61570500
H	3.78540000	0.34961200	-1.61858900
H	2.79762400	-0.32577000	-0.29649500
C	-0.76226800	3.25438500	0.79565800
C	-1.60586200	4.13385400	0.72244800
C	-2.57841300	5.16146600	0.64416000
C	-3.11882400	5.71489900	1.82491700
C	-3.00710700	5.63775800	-0.61370100
C	-4.07325800	6.72255100	1.74220700
H	-2.78081800	5.34765200	2.78817300
C	-3.96095900	6.64723800	-0.68096000
H	-2.57672100	5.21557700	-1.51563700
C	-4.49502000	7.18846200	0.49283600
H	-4.48773800	7.14878900	2.65021100
H	-4.28927900	7.01602800	-1.64759000
H	-5.23903200	7.97705700	0.43399800
C	1.01232100	3.03026900	-1.99101300
C	1.66468600	4.17607000	-1.51783600
C	0.04526800	3.14060500	-3.00065300
C	1.35970300	5.42163700	-2.06493200
H	2.41989400	4.08345500	-0.74620800
C	-0.25985000	4.39064800	-3.53808100
H	-0.44052900	2.24813200	-3.37909600
C	0.39622900	5.53271300	-3.07092200
H	1.87902800	6.30595200	-1.70881000
H	-0.99527300	4.47043000	-4.33320500
H	0.16510100	6.50488400	-3.49611100

Zero-point correction=	0.958332 (Hartree/Particle)
Thermal correction to Energy=	1.017832
Thermal correction to Enthalpy=	1.018776
Thermal correction to Gibbs Free Energy=	0.851259
Sum of electronic and zero-point Energies=	-2522.798471
Sum of electronic and thermal Energies=	-2522.738971
Sum of electronic and thermal Enthalpies=	-2522.738026
Sum of electronic and thermal Free Energies=	-2522.905544

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C	-1.97994600	0.37766700	-0.58187700
O	-2.13771400	-0.25167800	-1.63204800
C	-1.04656000	-0.43226200	0.23193600
C	-1.64645100	-1.47972000	1.11570400
Au	0.93865400	-0.26447800	-0.13047700
C	2.93714100	-0.14114000	-0.57489100
C	5.19079900	-0.21420800	-0.43739500
C	4.86887400	0.10770800	-1.71771500
H	5.48700200	0.30885500	-2.57781500
H	6.14577200	-0.34634000	0.04512000
N	3.99458500	-0.36434200	0.25049400
N	3.48398600	0.14981400	-1.78449800
C	3.90790500	-0.69316200	1.65944900
C	3.92709800	0.36055600	2.59501700
C	3.84190300	-2.05147100	2.03135800
C	3.87847200	0.01297300	3.95136600
C	3.79304600	-2.33700700	3.40183900
C	3.81375600	-1.31904400	4.35232900
H	3.90165700	0.79751000	4.70153700
H	3.74795300	-3.37110000	3.72823200
H	3.78806000	-1.56638100	5.40964300
C	2.73671700	0.46401100	-2.98735400
C	2.36081500	-0.59248500	-3.84052900
C	2.44220700	1.81506700	-3.25936200
C	1.65703300	-0.25487300	-5.00299200
C	1.73770400	2.09036400	-4.43773700
C	1.34799700	1.06932700	-5.30007000
H	1.34827400	-1.04108000	-5.68473600
H	1.49301500	3.11897200	-4.68360200
H	0.80290900	1.30675700	-6.20867100
C	2.68841100	-2.05437300	-3.55243100
C	3.62854200	-2.64208700	-4.62339200
C	1.40867600	-2.90146300	-3.41065800
H	3.21640200	-2.10541100	-2.59528800
H	4.55580700	-2.06583800	-4.70282200
H	3.89145100	-3.67511800	-4.37389700
H	3.15640100	-2.64921500	-5.61094700
H	0.74826100	-2.49540600	-2.63739200
H	0.84147000	-2.93455700	-4.34626600
H	1.66419400	-3.93198800	-3.14240100
C	2.86115500	2.95976200	-2.34153200
C	1.64240800	3.75267200	-1.83139400

C	3.87902700	3.88862400	-3.03259200
H	3.35610900	2.53171800	-1.46440500
H	0.92917600	3.09968700	-1.31817400
H	1.96262400	4.52938000	-1.12906300
H	1.11244600	4.24762700	-2.65143300
H	4.76745400	3.33856500	-3.35871300
H	3.44599600	4.37098800	-3.91470900
H	4.20221200	4.67849000	-2.34679300
C	3.84884100	-3.19158400	1.01779900
C	2.63672700	-4.12588800	1.19514400
C	5.17176300	-3.98166700	1.08191900
H	3.77523900	-2.75740300	0.01635800
H	1.69477600	-3.57019100	1.15863000
H	2.62532900	-4.87963100	0.40106600
H	2.67265500	-4.66010400	2.15008300
H	6.03687300	-3.33367800	0.90892500
H	5.30334500	-4.45769400	2.05910100
H	5.18225600	-4.76999800	0.32245000
C	4.00589400	1.83004900	2.19197200
C	5.30631000	2.48417500	2.69893800
C	2.76644600	2.61223200	2.66816800
H	4.01959200	1.88529800	1.09948400
H	6.19128200	1.95403300	2.33316800
H	5.36791400	3.52237400	2.35742500
H	5.35226600	2.49154000	3.79270800
H	1.84335900	2.16105800	2.29063800
H	2.70476600	2.64015900	3.76109100
H	2.81298500	3.64721500	2.31393500
O	-0.89065900	-2.65466500	1.22717800
O	-2.97614000	-1.71081100	0.76490500
H	-0.83708800	-3.04928300	0.34332300
C	-5.57567400	-2.22096100	-0.05325400
C	-5.10121100	-2.78811000	1.06445700
H	-4.89456200	-1.61011800	-0.64143000
H	-5.72840300	-3.42962400	1.68058800
C	-6.93533700	-2.34229100	-0.60112000
C	-7.99128200	-2.98052600	0.07610600
C	-7.19998500	-1.79076200	-1.86696100
C	-9.25590000	-3.07048800	-0.49774300
H	-7.82738200	-3.40356600	1.06282900
C	-8.46630700	-1.88073300	-2.44332700
H	-6.39701900	-1.29172300	-2.40402300
C	-9.50013000	-2.52241200	-1.76093800
H	-10.05694200	-3.56689500	0.04239100

H	-8.64497800	-1.45037200	-3.42449700
H	-10.48840400	-2.59373700	-2.20519500
C	-3.70501700	-2.63991300	1.58686700
H	-3.72087300	-2.28180900	2.62751100
H	-3.18250600	-3.60555100	1.59370700
C	-2.51622800	1.64514400	-0.26254500
C	-2.98118500	2.74397300	-0.00827200
C	-3.53073500	4.01724300	0.28458000
C	-4.40163600	4.63821300	-0.63627100
C	-3.21390800	4.66713700	1.49679500
C	-4.94277400	5.88510900	-0.34323100
H	-4.64226100	4.13286600	-1.56556000
C	-3.76032200	5.91461800	1.77624200
H	-2.54490600	4.18278000	2.20069400
C	-4.62353200	6.52331100	0.85931800
H	-5.61399700	6.36137400	-1.05062100
H	-3.51642400	6.41516200	2.70792200
H	-5.04869900	7.49696400	1.08299500
C	-1.47536900	-0.64363300	2.39793300
C	-2.51018600	0.22343700	2.79615600
C	-0.29981300	-0.73841300	3.16741000
C	-2.38279400	0.95804700	3.97100600
H	-3.40954500	0.29137100	2.19466700
C	-0.18256900	0.00221200	4.33974000
H	0.49289600	-1.40740500	2.85525400
C	-1.22021900	0.84940900	4.74180500
H	-3.19120000	1.60770400	4.29150100
H	0.71883700	-0.08232700	4.93764100
H	-1.12494600	1.42362000	5.65864300

Zero-point correction= 0.959348 (Hartree/Particle)
Thermal correction to Energy= 1.019353
Thermal correction to Enthalpy= 1.020298
Thermal correction to Gibbs Free Energy= 0.852092
Sum of electronic and zero-point Energies= -2522.809604
Sum of electronic and thermal Energies= -2522.749598
Sum of electronic and thermal Enthalpies= -2522.748654
Sum of electronic and thermal Free Energies= -2522.916860

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C	0.00395800	2.65660900	0.20372900
O	-0.73485900	2.46168100	-0.87394100
C	0.25823000	3.94697300	0.85916700
C	0.22177200	4.03761600	2.25867600

C	0.51423700	5.08275600	0.07511500
C	0.44060000	5.27156300	2.87117300
H	-0.00612800	3.15786800	2.85282100
C	0.73520700	6.30820200	0.69653200
C	0.69981400	6.40155000	2.09241100
H	0.40176900	5.35135700	3.95277500
H	0.92866900	7.19201900	0.09697600
C	-0.88049900	1.52442700	0.39436000
C	-2.12477500	1.81446300	1.21233800
C	-3.22542500	2.44866700	0.55807800
C	-4.16540400	2.99643200	0.00892600
C	-5.26465500	3.63659000	-0.62275900
C	-5.17714500	4.02931000	-1.97470400
C	-6.45113700	3.88510100	0.09856000
C	-6.25706100	4.65638600	-2.58736100
C	-7.52441100	4.51310700	-0.52492900
H	-6.51338800	3.58246500	1.13861000
C	-7.42972700	4.89869000	-1.86544600
H	-6.18693000	4.95785500	-3.62786000
H	-8.43586600	4.70366900	0.03296600
H	-8.27005100	5.38896900	-2.34766200
H	0.86798300	7.36077500	2.57263500
H	0.53013200	4.99840500	-1.00702500
H	-4.26175800	3.83672200	-2.52459900
Au	-0.46894600	-0.49373500	0.18023600
C	-0.23750100	-2.52489000	0.00736900
C	-0.80217900	-4.70466600	-0.20071100
C	0.54355600	-4.64714000	-0.03102700
H	1.29046500	-5.42326200	0.01172800
H	-1.46744700	-5.54198500	-0.33649500
N	-1.26495100	-3.39690900	-0.17507600
N	0.87442200	-3.30278100	0.09385000
C	-2.65889100	-3.02475900	-0.32450100
C	-3.46516500	-2.96227000	0.83021300
C	-3.14816500	-2.76846800	-1.62115300
C	-4.81262400	-2.62703500	0.64878100
C	-4.50284300	-2.43430300	-1.73769300
C	-5.32704900	-2.36553100	-0.61797600
H	-5.46689100	-2.57069300	1.51277600
H	-4.91691900	-2.22732700	-2.71948400
H	-6.37566400	-2.10787500	-0.73319100
C	2.22994100	-2.83059100	0.27883200
C	3.03355500	-2.64419400	-0.86425100
C	2.70323600	-2.63102500	1.59191600

C	4.35927800	-2.24036800	-0.65631100
C	4.03375900	-2.21649500	1.73631400
C	4.85578300	-2.02807400	0.62801200
H	5.01291100	-2.10512500	-1.51293600
H	4.43492400	-2.05430700	2.73173700
H	5.88872100	-1.72222100	0.76646500
C	2.52742600	-2.87787200	-2.28499800
C	3.29839600	-4.01955300	-2.97700900
C	2.57857600	-1.58674100	-3.12472400
H	1.47850200	-3.18197900	-2.22875200
H	3.24403700	-4.94801900	-2.40007800
H	2.87992700	-4.21278200	-3.96979100
H	4.35664700	-3.77065600	-3.10629600
H	1.97979600	-0.79134700	-2.66841100
H	3.60307500	-1.21736800	-3.23774800
H	2.18119200	-1.77024000	-4.12796600
C	1.84255000	-2.85924500	2.83124400
C	1.62242400	-1.55058900	3.61510800
C	2.43675000	-3.95621200	3.73706600
H	0.85872700	-3.20782900	2.50458000
H	1.13411000	-0.79267300	2.99325600
H	0.98219000	-1.73226200	4.48420400
H	2.56872300	-1.13829800	3.98141800
H	2.57306000	-4.89594100	3.19293600
H	3.40979200	-3.66248200	4.14391300
H	1.76954900	-4.14784200	4.58322000
C	-2.27701600	-2.84160800	-2.87178500
C	-2.18018900	-1.47123500	-3.57084800
C	-2.77492000	-3.92926200	-3.84386500
H	-1.26316600	-3.11943200	-2.56785600
H	-1.79199900	-0.70537500	-2.89148300
H	-1.51198300	-1.53280600	-4.43624700
H	-3.15778700	-1.13483200	-3.93106100
H	-2.81389000	-4.91115100	-3.36161500
H	-3.77809000	-3.70420000	-4.21987600
H	-2.10666000	-4.00216900	-4.70808700
C	-2.93902800	-3.26200600	2.23094400
C	-3.50924500	-4.59427400	2.75925500
C	-3.22066700	-2.11098900	3.21579800
H	-1.85199800	-3.37372000	2.17007600
H	-3.27111900	-5.42939200	2.09242600
H	-3.09607600	-4.82108000	3.74739300
H	-4.59889700	-4.54783900	2.85584400
H	-2.81412100	-1.15966900	2.86018300

H	-4.29417900	-1.97548500	3.38219000
H	-2.76755500	-2.33306300	4.18759300
O	-2.12773900	1.46404800	2.38863100
C	4.92981100	2.68199000	-0.02434700
C	3.99817600	1.72127500	0.11693000
H	4.69232000	3.67426200	0.36131800
H	4.17279600	0.70596500	-0.22895400
C	6.25931100	2.56694700	-0.62976900
C	7.09684000	3.69670800	-0.63059800
C	6.73950700	1.37868700	-1.21379200
C	8.37121700	3.64579700	-1.19237800
H	6.74118300	4.62198900	-0.18451400
C	8.01109500	1.32774000	-1.77437000
H	6.11324900	0.49196300	-1.23227500
C	8.83246800	2.46045400	-1.76561400
H	9.00223500	4.52915500	-1.18241200
H	8.36710800	0.40461400	-2.22211700
H	9.82454200	2.41639900	-2.20446100
C	2.69124600	1.98405500	0.77488000
H	2.39412000	1.20006600	1.47790200
H	2.66376800	2.95458100	1.26841500
O	1.60887100	2.07391900	-0.25452700
H	1.40460100	1.17313100	-0.58128900

Zero-point correction=	0.958274 (Hartree/Particle)
Thermal correction to Energy=	1.018062
Thermal correction to Enthalpy=	1.019006
Thermal correction to Gibbs Free Energy=	0.850353
Sum of electronic and zero-point Energies=	-2522.794103
Sum of electronic and thermal Energies=	-2522.734314
Sum of electronic and thermal Enthalpies=	-2522.733370
Sum of electronic and thermal Free Energies=	-2522.902024

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C	1.22463900	-2.32131500	-0.10307200
O	1.65231300	-2.41596700	1.04571100
C	0.94705100	-3.51122900	-0.94662800
C	0.35865800	-3.42373200	-2.21980000
C	1.29065800	-4.77196100	-0.42761700
C	0.12085200	-4.58211100	-2.95791900
H	0.08767500	-2.45888500	-2.63162000
C	1.05550500	-5.92401400	-1.16968200
C	0.47034900	-5.83008400	-2.43696300
H	-0.33403800	-4.51129700	-3.94117000

H	1.32410900	-6.89507400	-0.76499800
C	0.88931400	-0.93332400	-0.59627200
C	1.99317800	-0.03636800	-0.90147100
C	2.26010100	1.34522400	-0.70664700
C	2.49659500	2.52678800	-0.54501500
C	2.76317300	3.91386700	-0.36271500
C	2.87180100	4.76544900	-1.48036300
C	2.92057800	4.44231300	0.93460600
C	3.13141800	6.12063400	-1.29726800
C	3.18176700	5.79883800	1.10449800
H	2.83631200	3.78441700	1.79339100
C	3.28685700	6.63857100	-0.00825400
H	3.21609500	6.77376100	-2.16013400
H	3.30556800	6.20253700	2.10453700
H	3.49217100	7.69579200	0.12918400
H	0.28701900	-6.72973600	-3.01723900
H	1.73629600	-4.82051400	0.56024700
H	2.74973300	4.35542700	-2.47745200
Au	-1.01356500	-0.26364200	-0.14119900
C	-2.90372700	0.36513200	0.33310600
C	-4.72626300	1.66236800	0.67282200
C	-5.05076000	0.39714900	1.04385700
H	-5.96593100	-0.01780800	1.43427500
H	-5.30047100	2.57474900	0.67405100
N	-3.40672400	1.62583300	0.24050400
N	-3.92406900	-0.38563000	0.82829800
C	-2.67661500	2.78152800	-0.23717600
C	-1.97749400	3.56827100	0.69967100
C	-2.71432300	3.08014500	-1.61356700
C	-1.28890400	4.68549800	0.21170100
C	-2.00854800	4.21118100	-2.04274400
C	-1.30209800	5.00458100	-1.14332300
H	-0.73568900	5.31306000	0.90344700
H	-2.01624700	4.47326300	-3.09620000
H	-0.76094000	5.87656700	-1.49861400
C	-3.86727100	-1.80965000	1.09403700
C	-4.29023400	-2.69680800	0.08411100
C	-3.41933500	-2.24269900	2.35788000
C	-4.25501200	-4.06526700	0.37793900
C	-3.40649900	-3.62300300	2.59331800
C	-3.81986100	-4.52534100	1.61754700
H	-4.57342200	-4.77896100	-0.37538500
H	-3.06924600	-3.99423000	3.55585900
H	-3.80348300	-5.59134100	1.82417900

C	-4.76762600	-2.22992700	-1.28769500
C	-6.23490900	-2.62693700	-1.54276400
C	-3.84709100	-2.75206400	-2.40805500
H	-4.71825500	-1.13736600	-1.31476400
H	-6.89885200	-2.22998000	-0.76825200
H	-6.57214100	-2.23925500	-2.50958300
H	-6.35938700	-3.71451600	-1.56067500
H	-2.80901800	-2.44849500	-2.24049600
H	-3.86978700	-3.84502600	-2.46899900
H	-4.16913400	-2.35871800	-3.37808300
C	-2.96622000	-1.28458900	3.45505400
C	-1.50811400	-1.55419200	3.87577900
C	-3.91393400	-1.33639700	4.67002700
H	-3.00290200	-0.26635800	3.05672800
H	-0.82840600	-1.50880200	3.01910600
H	-1.18467000	-0.81025700	4.61158800
H	-1.39877100	-2.54117100	4.33697800
H	-4.94506800	-1.10268000	4.38617800
H	-3.91401200	-2.32794800	5.13421800
H	-3.59934600	-0.61372200	5.43003100
C	-3.48056200	2.23615600	-2.62781100
C	-2.53473800	1.62096200	-3.67766000
C	-4.60575300	3.04774900	-3.29953600
H	-3.95294800	1.40615100	-2.09429500
H	-1.75748800	1.01307700	-3.20373900
H	-3.09722700	0.98155500	-4.36596200
H	-2.04006000	2.39426800	-4.27466000
H	-5.30288800	3.45525500	-2.56053100
H	-4.20539800	3.88737400	-3.87699100
H	-5.17356900	2.41325400	-3.98765600
C	-1.94767100	3.25269000	2.19228600
C	-2.58701500	4.38454900	3.02039400
C	-0.51563200	2.94991600	2.67443800
H	-2.54130200	2.35021200	2.36415100
H	-3.61779900	4.57719000	2.70664700
H	-2.60013900	4.11908700	4.08246000
H	-2.02927600	5.32122000	2.91883200
H	-0.07886300	2.11766100	2.11313800
H	0.13780900	3.82039400	2.55228300
H	-0.52074600	2.68327500	3.73652200
O	1.48033000	-0.57131500	-2.01278800
C	6.65643900	-0.55554900	0.54633300
C	5.51911300	-1.27939300	0.58656800
H	6.56133000	0.53122600	0.57769100

H	5.53303500	-2.36550400	0.56868100
C	8.03480600	-1.04196800	0.48175300
C	9.07622000	-0.09724600	0.43099800
C	8.36819100	-2.41070600	0.46828900
C	10.40780500	-0.50126800	0.36556200
H	8.83439500	0.96255400	0.44401800
C	9.69734000	-2.81312400	0.40334500
H	7.58735200	-3.16344400	0.51360900
C	10.72148500	-1.86093700	0.35137000
H	11.19794700	0.24213900	0.32747000
H	9.93979900	-3.87135800	0.39543800
H	11.75792500	-2.18052100	0.30228300
C	4.18712800	-0.63871500	0.68047700
H	4.23870500	0.43769200	0.85818100
H	3.49478700	-1.12087800	1.37075700
O	3.47365800	-0.82900900	-0.64624600
H	4.07672100	-0.56054300	-1.36544200

Zero-point correction= 0.958843 (Hartree/Particle)
Thermal correction to Energy= 1.018180
Thermal correction to Enthalpy= 1.019124
Thermal correction to Gibbs Free Energy= 0.853511
Sum of electronic and zero-point Energies= -2522.792338
Sum of electronic and thermal Energies= -2522.733000
Sum of electronic and thermal Enthalpies= -2522.732056
Sum of electronic and thermal Free Energies= -2522.897669

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C	-2.46666300	2.00392000	-1.35165900
O	-3.56065300	1.95528300	-0.74640300
C	-2.19498000	2.41299600	-2.70304700
C	-0.89976000	2.30185300	-3.24485100
C	-3.26603800	2.91109100	-3.47588300
C	-0.68795000	2.69624000	-4.56305400
H	-0.08877600	1.91519000	-2.63217500
C	-3.03546800	3.30533000	-4.78543500
C	-1.74664300	3.19725500	-5.32674300
H	0.30322100	2.61514800	-4.99727300
H	-3.84864300	3.69438900	-5.38938500
C	-1.78549300	1.45038800	-0.19630400
C	-1.42187300	2.40701800	0.92258100
C	-2.25333400	3.53295900	1.16755500
C	-2.95376700	4.49574300	1.43482000
C	-3.76175100	5.61738500	1.74348000

C	-4.92031500	5.88883000	0.98376200
C	-3.41264800	6.46744000	2.81523600
C	-5.70902800	6.99057700	1.29409700
C	-4.20978300	7.56636900	3.11459900
H	-2.52172800	6.25298800	3.39591000
C	-5.35544100	7.82884000	2.35660200
H	-6.60066400	7.19829700	0.71115400
H	-3.94088400	8.21991400	3.93824600
H	-5.97493000	8.68810600	2.59486100
H	-1.57016700	3.50619600	-6.35293900
H	-4.25541100	2.98095600	-3.03497000
H	-5.18501700	5.22769500	0.16527000
Au	-1.53552000	-0.55737000	-0.04394800
C	-1.32299400	-2.59142300	0.06766500
C	-1.36581100	-4.72645700	0.80076100
C	-0.91522200	-4.74293400	-0.48078900
H	-0.61790900	-5.55844700	-1.11987700
H	-1.53782400	-5.52415700	1.50504800
N	-1.60833000	-3.39932800	1.12431100
N	-0.89807200	-3.42619600	-0.91803800
C	-2.14774100	-2.96305000	2.39824500
C	-1.26957300	-2.84471800	3.49416200
C	-3.53295500	-2.71343000	2.49376500
C	-1.82153900	-2.43903500	4.71549100
C	-4.02373200	-2.30469400	3.74005100
C	-3.18056600	-2.16577400	4.83842300
H	-1.17686100	-2.33932900	5.58270000
H	-5.08421300	-2.10275600	3.85230900
H	-3.58549800	-1.85203000	5.79594600
C	-0.57864700	-3.03655000	-2.27930700
C	-1.61068700	-3.09049900	-3.23825200
C	0.74451800	-2.66101500	-2.59099600
C	-1.27918100	-2.75316800	-4.55650900
C	1.01421900	-2.34086500	-3.92745100
C	0.01831900	-2.38715600	-4.89945000
H	-2.04806800	-2.78267000	-5.32226800
H	2.02004300	-2.05119900	-4.21003900
H	0.25635900	-2.13770000	-5.92941800
C	-3.04616200	-3.48676500	-2.90250400
C	-3.50112000	-4.71828700	-3.70964800
C	-4.01230000	-2.30233200	-3.10160900
H	-3.09018800	-3.76309100	-1.84512200
H	-2.83397600	-5.57110500	-3.54957100
H	-4.51084600	-5.01682400	-3.40999100

H	-3.52324700	-4.51175400	-4.78436900
H	-3.72160800	-1.44722900	-2.48264900
H	-4.03061700	-1.97260500	-4.14555400
H	-5.03199800	-2.59179600	-2.82651700
C	1.86106800	-2.62957200	-1.55053500
C	2.83362200	-1.45430500	-1.75426900
C	2.62904000	-3.96874900	-1.53296700
H	1.40195900	-2.49403000	-0.56589400
H	2.30541900	-0.50077400	-1.84058700
H	3.51153200	-1.38289300	-0.89989000
H	3.45157900	-1.58871500	-2.64866900
H	1.97229600	-4.81557200	-1.30912900
H	3.10020700	-4.15966600	-2.50310600
H	3.41891700	-3.94416400	-0.77534300
C	-4.50417900	-2.90923800	1.33288700
C	-5.28880500	-1.62306700	1.01007600
C	-5.46149900	-4.08637700	1.61094600
H	-3.92669600	-3.16493600	0.44004700
H	-4.61634000	-0.79006200	0.78117200
H	-5.93690100	-1.78521700	0.14254700
H	-5.92787100	-1.31910400	1.84527900
H	-4.91241900	-5.01409800	1.80086100
H	-6.09246200	-3.88926600	2.48359800
H	-6.12156800	-4.25223400	0.75321600
C	0.21866700	-3.17137500	3.40932900
C	0.54133400	-4.46279600	4.18918900
C	1.09534100	-2.00170400	3.89152800
H	0.47307400	-3.34788000	2.35981500
H	-0.04577900	-5.31301000	3.82684300
H	1.60149600	-4.71597200	4.08644900
H	0.32750100	-4.34612000	5.25669100
H	0.92750900	-1.11007800	3.28228400
H	0.90128700	-1.74930800	4.93863800
H	2.15361500	-2.27114600	3.81230600
O	-0.41097700	2.16786000	1.58272800
C	4.20623500	3.70161700	-0.23932000
C	3.36239200	3.10923700	-1.09910000
H	3.77272700	4.22691800	0.61347900
H	3.73221100	2.55772700	-1.96189400
C	5.67574200	3.73309200	-0.29327100
C	6.38046900	4.29894700	0.78461100
C	6.41908600	3.21894300	-1.37315500
C	7.77397900	4.34284000	0.79347700
H	5.82432000	4.70832200	1.62445000

C	7.81059700	3.26270200	-1.36549900
H	5.90632100	2.79111500	-2.22910600
C	8.49550700	3.82320600	-0.28179300
H	8.29486800	4.78453500	1.63780300
H	8.36500900	2.86629800	-2.21132500
H	9.58070800	3.85990800	-0.28160700
C	1.86856400	3.16029000	-0.96424400
H	1.43564200	3.76014900	-1.77657500
H	1.58887800	3.64624400	-0.01754600
O	1.25787900	1.87206900	-1.08038800
H	1.58889500	1.30173200	-0.35051700
C	5.24708700	-0.02734600	1.41881900
C	3.99271100	-0.30181200	1.80969300
H	5.49709000	1.01055300	1.19879100
H	3.67940400	-1.32436700	2.01228300
C	6.35233300	-0.97981700	1.23349400
C	7.52942200	-0.53490300	0.60580600
C	6.29181000	-2.32117000	1.65647200
C	8.60121600	-1.40073800	0.39197100
H	7.59762300	0.49974300	0.27927300
C	7.36148100	-3.18556900	1.44243400
H	5.40907300	-2.68557000	2.17369100
C	8.52110800	-2.73043300	0.80709900
H	9.50037700	-1.03558400	-0.09584600
H	7.29740600	-4.21580700	1.78112200
H	9.35635800	-3.40562400	0.64662800
C	2.94477600	0.74397000	2.02122300
H	3.33894500	1.73433700	1.76049000
H	2.64504100	0.76637700	3.07925100
O	1.78496500	0.43377700	1.21894600
H	1.02139500	0.93828600	1.55341600

Zero-point correction= 1.127258 (Hartree/Particle)
Thermal correction to Energy= 1.198129
Thermal correction to Enthalpy= 1.199074
Thermal correction to Gibbs Free Energy= 1.004924
Sum of electronic and zero-point Energies= -2946.843324
Sum of electronic and thermal Energies= -2946.772452
Sum of electronic and thermal Enthalpies= -2946.771508
Sum of electronic and thermal Free Energies= -2946.965657

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C	-2.81271200	4.04614000	-0.18947000
O	-3.67697200	4.37060100	-0.99554500

C	-2.05032100	5.08578100	0.57042300
C	-1.56738200	4.86292600	1.87358600
C	-1.90964700	6.35902000	-0.00967800
C	-0.93996600	5.89432700	2.57382800
H	-1.71406800	3.89613500	2.34677800
C	-1.27095600	7.37928400	0.68755000
C	-0.78606900	7.14857400	1.97977800
H	-0.58561700	5.72244300	3.58544600
H	-1.15740200	8.35787500	0.23146800
C	-2.53693400	2.58614400	0.02194700
C	-1.27798200	2.05685100	0.16929400
C	-1.11953900	0.63526500	0.12392700
C	-1.46228500	-0.56209600	0.13156000
C	-2.06773700	-1.85289800	0.08071300
C	-1.48827900	-2.98396900	0.68853700
C	-3.31491100	-1.96212100	-0.57347100
C	-2.15013900	-4.20655800	0.63528100
C	-3.96997900	-3.18936900	-0.60166700
H	-3.75843100	-1.08251900	-1.02627000
C	-3.38882100	-4.31175600	-0.00398100
H	-1.69919000	-5.07758900	1.09958200
H	-4.93674700	-3.26719600	-1.08820800
H	-3.90250100	-5.26776100	-0.03500800
H	-0.29738000	7.94980500	2.52602100
H	-2.31476600	6.52490600	-1.00235200
H	-0.53212500	-2.89786500	1.19377300
Au	0.89364000	-0.30472500	-0.02322000
C	2.86643800	-0.74697100	-0.15222400
C	5.07796100	-0.58923900	-0.55314500
C	4.84793000	-1.81225300	-0.00919300
H	5.51592500	-2.62535600	0.22493100
H	5.98780100	-0.11841500	-0.88858900
N	3.85030200	0.05361700	-0.63463000
N	3.48301100	-1.89375100	0.23309200
C	3.67149000	1.39565700	-1.15658500
C	3.39864300	1.55017900	-2.53038700
C	3.81535000	2.48273600	-0.27112300
C	3.26871700	2.85915900	-3.01083100
C	3.68109500	3.76706500	-0.81222200
C	3.41106100	3.95526300	-2.16488200
H	3.05871000	3.02026400	-4.06347000
H	3.79312800	4.63066200	-0.16423700
H	3.31473600	4.96108600	-2.56292500
C	2.82772000	-3.04986300	0.81210100

C	2.67160000	-3.10137200	2.21247000
C	2.40480000	-4.08209600	-0.04951900
C	2.05439000	-4.24089100	2.74423500
C	1.79921000	-5.19836000	0.54174100
C	1.62556700	-5.27927400	1.92104100
H	1.91925700	-4.31943700	3.81837000
H	1.46503100	-6.01695800	-0.08773200
H	1.16250400	-6.15925700	2.35799000
C	3.15139100	-1.99537800	3.14780800
C	4.24536200	-2.50621000	4.10649600
C	1.97997200	-1.36433700	3.92530300
H	3.59891500	-1.20258100	2.54114300
H	5.09559400	-2.92414400	3.55845400
H	4.61438200	-1.68669500	4.73122300
H	3.86452400	-3.28587500	4.77387800
H	1.22083400	-0.96434700	3.24499600
H	1.49310400	-2.09244400	4.58223000
H	2.34061100	-0.54302500	4.55298600
C	2.57911300	-4.02705700	-1.56447300
C	1.21760100	-4.01794000	-2.28664900
C	3.47109400	-5.17645700	-2.07370400
H	3.08476700	-3.09007200	-1.81689700
H	0.59342900	-3.18294500	-1.95326800
H	1.36304700	-3.92581700	-3.36777100
H	0.66125300	-4.94313900	-2.10518400
H	4.45174200	-5.17053900	-1.58756800
H	3.01432000	-6.15386000	-1.88827500
H	3.62715500	-5.08446200	-3.15315400
C	4.12337800	2.31307300	1.21373300
C	3.07920300	3.01792800	2.10112200
C	5.54951200	2.79750300	1.54429800
H	4.07649400	1.24626300	1.45354800
H	2.06450300	2.68677700	1.86181000
H	3.27676100	2.80182000	3.15625400
H	3.11645200	4.10551500	1.97921800
H	6.30362900	2.26441400	0.95653800
H	5.66298000	3.86637200	1.33608000
H	5.77159300	2.63825700	2.60440200
C	3.24680400	0.37434100	-3.49070200
C	4.33452700	0.39455900	-4.58295500
C	1.83618300	0.33369500	-4.11053800
H	3.37555400	-0.55263700	-2.92363800
H	5.33959500	0.38691500	-4.14933100
H	4.23836200	-0.48207100	-5.23154700

H	4.25250300	1.28458000	-5.21495400
H	1.06313900	0.28788700	-3.33654000
H	1.64163900	1.21825500	-4.72534900
H	1.72907900	-0.54616100	-4.75317700
O	-0.10192200	2.74242000	0.25496100
C	-6.71661200	0.46478100	-0.40402100
C	-5.66422700	0.77574100	0.37018500
H	-6.99286200	1.17240100	-1.18632900
H	-5.32637700	0.10571400	1.15804900
C	-7.56192200	-0.73497800	-0.33519100
C	-8.54532800	-0.92372200	-1.32243200
C	-7.43659700	-1.71054400	0.67278900
C	-9.36940900	-2.04810400	-1.31343100
H	-8.66094900	-0.17727200	-2.10419600
C	-8.25931900	-2.83321500	0.68223900
H	-6.70216100	-1.58471200	1.46254700
C	-9.22859200	-3.00829700	-0.31091900
H	-10.12262300	-2.17158500	-2.08582100
H	-8.15301100	-3.57105800	1.47235500
H	-9.87230100	-3.88266900	-0.29677800
C	-4.89788400	2.04654600	0.21295200
H	-4.84031400	2.59581400	1.16233100
H	-5.33901800	2.70034100	-0.54160300
O	-3.54074100	1.69748700	-0.19829700
H	-0.27428500	3.69280300	0.35464400

Zero-point correction= 0.960376 (Hartree/Particle)
Thermal correction to Energy= 1.020334
Thermal correction to Enthalpy= 1.021278
Thermal correction to Gibbs Free Energy= 0.854108
Sum of electronic and zero-point Energies= -2522.861644
Sum of electronic and thermal Energies= -2522.801686
Sum of electronic and thermal Enthalpies= -2522.800742
Sum of electronic and thermal Free Energies= -2522.967912

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C	-0.32855700	-3.16459800	-0.09695600
O	-0.23788000	-3.58427500	1.05462800
C	-1.00643500	-3.85787100	-1.20477900
C	-0.93019900	-3.36991400	-2.51938300
C	-1.72540800	-5.03206200	-0.92691000
C	-1.57359300	-4.05139200	-3.54925100
H	-0.35730900	-2.47268100	-2.73955400
C	-2.36499400	-5.70896500	-1.95965200

C	-2.28988600	-5.21863300	-3.26847800
H	-1.51132000	-3.68215200	-4.56788700
H	-2.91993200	-6.61829700	-1.75136100
C	0.29597300	-1.81940000	-0.29662000
C	1.77860900	-1.85095800	-0.63695800
C	2.18937700	-0.77870600	-1.53885700
C	2.57570800	0.04684600	-2.34100600
C	3.06044700	0.99028100	-3.29548900
C	3.30361300	0.58327500	-4.62227900
C	3.31880300	2.32326500	-2.92026400
C	3.78866800	1.49765200	-5.55306500
C	3.81021300	3.22679300	-3.85881200
H	3.13325300	2.63523400	-1.89780300
C	4.04374300	2.81838800	-5.17489900
H	3.97327700	1.17836000	-6.57401100
H	4.01633600	4.25132200	-3.56391500
H	4.42737200	3.52664800	-5.90282300
H	-2.78805800	-5.75131800	-4.07311700
H	-1.76501200	-5.39230800	0.09591700
H	3.11229600	-0.44594700	-4.90770400
Au	-0.84988600	-0.23931700	0.15186600
C	-2.14859100	1.26291600	0.68748200
C	-3.07410800	3.23344100	1.29032500
C	-4.05926200	2.29623300	1.30719000
H	-5.10825300	2.37112500	1.54448600
H	-3.09119800	4.28857400	1.51122000
N	-1.91049300	2.58327500	0.90968000
N	-3.47611300	1.09573200	0.93610300
C	-0.62372100	3.23530600	0.77788600
C	0.20236500	3.32232500	1.91678600
C	-0.27158700	3.77571000	-0.47431100
C	1.44050100	3.95750700	1.75940600
C	0.97631000	4.40555400	-0.56829900
C	1.82555400	4.49159300	0.53213400
H	2.10586900	4.04586700	2.61259600
H	1.28065600	4.83977300	-1.51538500
H	2.78595600	4.99009200	0.43791300
C	-4.20330100	-0.15530000	0.82573200
C	-4.84444400	-0.44974600	-0.39437000
C	-4.26423200	-1.00014900	1.95225800
C	-5.57257900	-1.64397700	-0.46091800
C	-5.00778200	-2.17997200	1.82394900
C	-5.65650000	-2.49891000	0.63438400
H	-6.08218500	-1.90511000	-1.38300100

H	-5.08193100	-2.85476000	2.67058000
H	-6.23183100	-3.41702000	0.56132600
C	-4.77493800	0.46263300	-1.61545000
C	-6.16595800	1.01168900	-1.98925900
C	-4.11772000	-0.24927400	-2.81395900
H	-4.14368500	1.32143500	-1.36796500
H	-6.62146800	1.55367200	-1.15439700
H	-6.08874300	1.69906200	-2.83779400
H	-6.85125000	0.20726200	-2.27521300
H	-3.12173200	-0.62379500	-2.55664100
H	-4.71664000	-1.10018400	-3.15399600
H	-4.01706700	0.44238600	-3.65683300
C	-3.58577400	-0.67347500	3.27922800
C	-2.65347300	-1.80865800	3.74491500
C	-4.62790200	-0.33041700	4.36338000
H	-2.96243200	0.21430600	3.13517300
H	-1.90801000	-2.05963300	2.98391600
H	-2.12532000	-1.50941400	4.65606500
H	-3.21213500	-2.72072100	3.97794600
H	-5.26289200	0.50889100	4.06161100
H	-5.28242000	-1.18338200	4.57028900
H	-4.12919600	-0.05847600	5.29930100
C	-1.18702100	3.71460800	-1.69371700
C	-0.55639000	2.89545600	-2.83611700
C	-1.58019800	5.12626100	-2.17268200
H	-2.10994900	3.20413400	-1.40280300
H	-0.30976100	1.88030600	-2.50922800
H	-1.25227400	2.82419100	-3.67853100
H	0.36421500	3.35856100	-3.20471500
H	-2.05546900	5.70452300	-1.37409000
H	-0.70856800	5.69099600	-2.51855900
H	-2.28392100	5.06018200	-3.00851300
C	-0.20785300	2.78618100	3.28610400
C	-0.30805500	3.92262000	4.32332400
C	0.74013200	1.67376600	3.77298700
H	-1.20373200	2.34226000	3.19620700
H	-1.00308600	4.70296500	3.99790200
H	-0.66242400	3.53083900	5.28196500
H	0.66375900	4.39542900	4.49722300
H	0.75714900	0.83352500	3.07162900
H	1.76501900	2.04145400	3.88938900
H	0.41189700	1.29504600	4.74626100
O	2.22748000	-3.05864300	-1.17924100
O	2.20305100	-1.77547200	0.72595300

H	2.32125900	-3.68252200	-0.44146900
C	2.96188300	-0.61463900	1.21372900
H	2.59381400	0.27908900	0.70095200
H	2.70351000	-0.55572900	2.27223200
C	5.25573300	-1.11970600	2.02829500
C	4.42280100	-0.83266400	1.01109900
H	4.82439200	-1.19120300	3.02763100
H	4.78265200	-0.75648700	-0.01167800
C	6.70316900	-1.34189500	1.97178000
C	7.38958100	-1.60791500	3.17069400
C	7.44291900	-1.30433500	0.77354100
C	8.76509000	-1.83028300	3.17760200
H	6.83322000	-1.64137700	4.10407900
C	8.81565900	-1.52643600	0.78044900
H	6.94284600	-1.10268200	-0.16870100
C	9.48293300	-1.78992800	1.98166000
H	9.27509300	-2.03497000	4.11401900
H	9.37061200	-1.49525600	-0.15246800
H	10.55487800	-1.96269500	1.98222200

Zero-point correction= 0.958158 (Hartree/Particle)
Thermal correction to Energy= 1.017871
Thermal correction to Enthalpy= 1.018815
Thermal correction to Gibbs Free Energy= 0.849792
Sum of electronic and zero-point Energies= -2522.796862
Sum of electronic and thermal Energies= -2522.737149
Sum of electronic and thermal Enthalpies= -2522.736205
Sum of electronic and thermal Free Energies= -2522.905228

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C	1.70857500	0.10431300	1.60901900
O	1.74150000	-1.03518500	2.08429300
C	2.16736700	1.32868800	2.25590600
C	2.91106300	1.21533700	3.44427400
C	1.86174300	2.59481800	1.72927700
C	3.35585800	2.36239400	4.09110700
H	3.13368600	0.22756200	3.83432500
C	2.30220600	3.73912400	2.38926700
C	3.05106100	3.62270400	3.56430200
H	3.93782200	2.28034100	5.00343600
H	2.06139800	4.72013800	1.99202600
C	1.05028000	-0.12699800	0.30920600
C	1.96953500	-0.49511700	-0.83387200
C	1.89158400	0.84982200	-1.43851600

C	1.86145900	1.99488000	-1.86020300
C	1.84378000	3.31994900	-2.36677500
C	0.93976000	3.67961600	-3.38948400
C	2.74166900	4.28343000	-1.85767100
C	0.93932500	4.97759200	-3.88844100
C	2.72827200	5.57878000	-2.36346500
H	3.43777200	4.00102700	-1.07463400
C	1.83045200	5.92687400	-3.37763100
H	0.24791900	5.25131600	-4.67902500
H	3.42105600	6.31767200	-1.97334300
H	1.82758000	6.93810300	-3.77280600
H	3.39690600	4.51723400	4.07379400
H	1.27375900	2.67690100	0.82178700
H	0.25775300	2.93332200	-3.78276500
Au	-0.95604800	-0.32651200	0.16124200
C	-2.97678200	-0.64333700	0.02351100
C	-4.95900500	-1.61969000	-0.44354100
C	-5.22083300	-0.42897900	0.15717700
H	-6.15232800	0.05131700	0.40994600
H	-5.61647100	-2.38807600	-0.81719600
N	-3.57867800	-1.73582800	-0.51747100
N	-3.99425200	0.15653800	0.43788400
C	-2.88604900	-2.88657400	-1.06495000
C	-2.54672800	-2.88238200	-2.43297200
C	-2.60650200	-3.96859300	-0.20559400
C	-1.90762800	-4.02264600	-2.93572200
C	-1.96171000	-5.07884000	-0.76541700
C	-1.61834400	-5.10899600	-2.11423200
H	-1.63483500	-4.05934600	-3.98546300
H	-1.73074700	-5.93235800	-0.13581400
H	-1.12552300	-5.98394300	-2.52782800
C	-3.83459700	1.43800000	1.09592900
C	-3.72740800	1.46201500	2.50111400
C	-3.81759000	2.60264700	0.30322100
C	-3.58098000	2.71526900	3.10878100
C	-3.67201500	3.82660600	0.96779400
C	-3.55200900	3.88431900	2.35361600
H	-3.49439800	2.77474200	4.18915300
H	-3.65653600	4.74639400	0.39140500
H	-3.44275800	4.84508500	2.84797800
C	-3.77715100	0.20403000	3.36324800
C	-4.98963500	0.22382700	4.31528500
C	-2.46323000	-0.00292300	4.14152900
H	-3.89980400	-0.65989100	2.70320500

H	-5.92964100	0.33805300	3.76627100
H	-5.04021500	-0.71022300	4.88387100
H	-4.92339100	1.04601200	5.03509700
H	-1.60607700	-0.07391500	3.46433300
H	-2.27503500	0.82028900	4.83843500
H	-2.51125000	-0.92714200	4.72641600
C	-3.95576400	2.57717700	-1.21623000
C	-2.69922800	3.14145600	-1.90703600
C	-5.22488300	3.31955000	-1.67914700
H	-4.05594400	1.53531200	-1.53446400
H	-1.80239700	2.58679600	-1.61308000
H	-2.80394000	3.07292100	-2.99513700
H	-2.54043900	4.19515500	-1.65529200
H	-6.12467600	2.90308500	-1.21567300
H	-5.18335900	4.38358100	-1.42501100
H	-5.33636400	3.24193600	-2.76545600
C	-2.97167700	-3.97495500	1.27621100
C	-1.71661600	-4.06678000	2.16625600
C	-3.97141100	-5.10147700	1.60470900
H	-3.46401500	-3.02686900	1.51268600
H	-1.02507300	-3.24141100	1.96910900
H	-1.99934700	-4.02850400	3.22328900
H	-1.17562800	-5.00460600	2.00374900
H	-4.88150100	-5.01972400	1.00192800
H	-3.53842700	-6.08968600	1.41955900
H	-4.25850200	-5.05851500	2.66020600
C	-2.85636900	-1.71345900	-3.36290900
C	-3.97693600	-2.07725100	-4.35754500
C	-1.59626500	-1.21880500	-4.09912900
H	-3.21805800	-0.88029400	-2.75265800
H	-4.89303000	-2.37933100	-3.83979900
H	-4.21552400	-1.22005600	-4.99565700
H	-3.67611100	-2.90445600	-5.00875200
H	-0.78636100	-0.99132000	-3.39957800
H	-1.22407600	-1.96431300	-4.80943800
H	-1.82843900	-0.31433600	-4.67136900
O	1.44586700	-1.43217900	-1.73688400
C	6.67284600	-0.92944500	-0.70011300
C	5.48070500	-1.54524000	-0.72348900
H	6.73964600	0.05989900	-1.15476200
H	5.34349700	-2.52944500	-0.28156000
C	7.93442400	-1.42761700	-0.13626700
C	9.07255800	-0.60480700	-0.20181700
C	8.06266800	-2.69110400	0.47121400

C	10.29548200	-1.02240500	0.32088300
H	8.99290300	0.37330200	-0.66998000
C	9.28255700	-3.10832100	0.99406500
H	7.20506900	-3.35400800	0.53385000
C	10.40480100	-2.27667400	0.92183000
H	11.16128600	-0.36993200	0.25751100
H	9.36186100	-4.08711200	1.45809300
H	11.35558800	-2.60716700	1.32903600
C	4.27444400	-0.95361200	-1.37224000
H	3.88851600	-1.59556900	-2.17301800
H	4.49202400	0.03546100	-1.79367200
O	3.23636500	-0.82642900	-0.35918200
H	1.27980900	-2.24873700	-1.23999200

Zero-point correction= 0.958993 (Hartree/Particle)
Thermal correction to Energy= 1.019238
Thermal correction to Enthalpy= 1.020182
Thermal correction to Gibbs Free Energy= 0.850479
Sum of electronic and zero-point Energies= -2522.811434
Sum of electronic and thermal Energies= -2522.751189
Sum of electronic and thermal Enthalpies= -2522.750245
Sum of electronic and thermal Free Energies= -2522.919948

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C	1.05041400	0.36633800	1.42810600
O	1.61519800	-0.73061400	1.33454400
C	1.13796100	1.26579800	2.57956300
C	2.08796900	0.97810800	3.57569200
C	0.28842400	2.37606000	2.71592200
C	2.19494400	1.80382500	4.68891000
H	2.72826500	0.11031600	3.45604300
C	0.39477900	3.19341400	3.83861300
C	1.34894200	2.91082000	4.82029800
H	2.93200000	1.58884500	5.45604100
H	-0.26539000	4.04770100	3.95100000
C	0.24038100	0.48673300	0.20206700
C	0.88207900	1.02146400	-1.06450700
C	0.31081300	2.36831300	-0.86179000
C	-0.24984800	3.44238800	-0.69637200
C	-0.87115900	4.70232100	-0.50706600
C	-2.07247700	5.01002300	-1.18257200
C	-0.28425400	5.66043700	0.34872200
C	-2.66665100	6.25427200	-1.00145500
C	-0.89063300	6.89982300	0.52108200

H	0.64029900	5.41901100	0.86298000
C	-2.07918000	7.19839600	-0.15277800
H	-3.58672300	6.49459300	-1.52497600
H	-0.43654100	7.63685500	1.17576600
H	-2.54670900	8.16908900	-0.01862900
H	1.43230000	3.55244000	5.69248000
H	-0.45428600	2.58643600	1.95477800
H	-2.51848400	4.26936300	-1.83823600
Au	-1.59931400	-0.33940900	0.06653300
C	-3.41578800	-1.26726600	-0.14869000
C	-5.44439900	-1.86540800	-0.94289700
C	-5.11402300	-2.74498500	0.03876000
H	-5.64060200	-3.59619700	0.43919200
H	-6.31977700	-1.79172700	-1.56779100
N	-4.39261500	-0.96589400	-1.04550800
N	-3.86822000	-2.36342800	0.51580300
C	-4.37512100	0.15911300	-1.96012500
C	-4.97870500	1.36259500	-1.54441100
C	-3.78419400	-0.00906300	-3.22909100
C	-4.97764900	2.42662900	-2.45565600
C	-3.81595200	1.08941600	-4.09683500
C	-4.40524300	2.29272000	-3.71810800
H	-5.44174300	3.36705000	-2.17435300
H	-3.37648700	0.99855200	-5.08439900
H	-4.42508600	3.12654300	-4.41394300
C	-3.15869000	-3.05198800	1.57625900
C	-2.29187000	-4.10767000	1.23082800
C	-3.38928500	-2.65115300	2.90740400
C	-1.63478600	-4.76409700	2.27878100
C	-2.70459700	-3.34579000	3.91210400
C	-1.83620700	-4.38916400	3.60397900
H	-0.95945100	-5.58305900	2.05227600
H	-2.85783300	-3.06725500	4.94998100
H	-1.31789700	-4.91517300	4.40014400
C	-2.05429800	-4.55467100	-0.20849700
C	-2.53464900	-6.00192200	-0.43424900
C	-0.57657300	-4.38869400	-0.61294100
H	-2.64237600	-3.91138100	-0.86980100
H	-3.59413100	-6.11640200	-0.18415300
H	-2.40078600	-6.28837700	-1.48236400
H	-1.97057500	-6.71221700	0.17880300
H	-0.24451400	-3.35444100	-0.47626800
H	0.07747300	-5.03365300	-0.01697900
H	-0.44051200	-4.65955700	-1.66532800

C	-4.34833300	-1.52574700	3.28465200
C	-3.63179400	-0.39758600	4.05133300
C	-5.55079600	-2.06447800	4.08557200
H	-4.74195400	-1.08672100	2.36301400
H	-2.79698600	0.00869500	3.47159800
H	-4.33103400	0.41802800	4.26303900
H	-3.23553100	-0.74884000	5.00941400
H	-6.09057800	-2.83715800	3.52885000
H	-5.23277800	-2.50314800	5.03687500
H	-6.25343800	-1.25555400	4.31071300
C	-3.16738500	-1.32701000	-3.68762400
C	-1.77190100	-1.13948600	-4.31230200
C	-4.11549700	-2.06105200	-4.65899300
H	-3.04025400	-1.96489300	-2.80744600
H	-1.09228800	-0.60856600	-3.63946400
H	-1.33755500	-2.11863500	-4.54053000
H	-1.82006200	-0.58419400	-5.25491800
H	-5.09328300	-2.25341000	-4.20514900
H	-4.28109900	-1.47219500	-5.56727200
H	-3.68639300	-3.02310600	-4.95727400
C	-5.61338500	1.54471500	-0.16810600
C	-7.09641100	1.95059500	-0.27050100
C	-4.81715100	2.55301000	0.68362700
H	-5.57843700	0.58518200	0.35604400
H	-7.67179900	1.22389300	-0.85240600
H	-7.54113800	2.01459800	0.72773600
H	-7.21697300	2.92818300	-0.74800600
H	-3.77776400	2.23149300	0.80638400
H	-4.80853300	3.54717400	0.22487900
H	-5.26544700	2.64896900	1.67812900
O	0.78593500	0.43842500	-2.19819700
O	2.51207600	1.18929200	-0.65677500
H	1.95225100	-0.55730300	-2.22918000
O	2.89445200	-0.81833300	-1.89345000
H	2.89098000	0.09691500	-1.13136800
C	5.45489900	-1.98849900	-1.51502100
C	4.34062600	-2.65962400	-1.19513800
H	5.35238600	-0.98309200	-1.91772600
H	4.39697300	-3.65535100	-0.75857900
C	6.83793900	-2.46771900	-1.35826200
C	7.15960600	-3.82183400	-1.14998700
C	7.89060500	-1.53889800	-1.42735900
C	8.48305400	-4.22569600	-0.99940500
H	6.37107100	-4.56838300	-1.12641900

C	9.21638400	-1.94270500	-1.27423100
H	7.66397100	-0.48851600	-1.58788700
C	9.51825800	-3.28759100	-1.05830000
H	8.71051800	-5.27664600	-0.84538700
H	10.01178000	-1.20499200	-1.32368200
H	10.55025700	-3.60606800	-0.94474100
C	2.93695100	-2.17360300	-1.37556400
H	2.40509900	-2.80055700	-2.10287300
H	2.38210600	-2.21115700	-0.43104400
C	5.23806300	1.71671200	-0.05210100
C	4.63612100	2.29856600	-1.09959000
H	4.62851500	1.11188000	0.61664400
H	5.20074200	2.91717500	-1.79479600
C	6.66216700	1.79705100	0.30863700
C	7.60731200	2.53690500	-0.42779500
C	7.10896400	1.09990400	1.44457500
C	8.94321600	2.57438300	-0.03903000
H	7.29931800	3.08967500	-1.31028200
C	8.44661200	1.13727400	1.83543000
H	6.39542900	0.51809400	2.02264400
C	9.37004700	1.87524800	1.09470400
H	9.65555100	3.15242000	-0.62057500
H	8.76744900	0.58775700	2.71544500
H	10.41293300	1.90744200	1.39533100
C	3.17724400	2.21135800	-1.43370700
H	2.67806800	3.16550000	-1.22462900
H	3.03256100	1.99850400	-2.50187900

Zero-point correction= 1.122268 (Hartree/Particle)
Thermal correction to Energy= 1.192545
Thermal correction to Enthalpy= 1.193489
Thermal correction to Gibbs Free Energy= 0.999814
Sum of electronic and zero-point Energies= -2946.808999
Sum of electronic and thermal Energies= -2946.738721
Sum of electronic and thermal Enthalpies= -2946.737777
Sum of electronic and thermal Free Energies= -2946.931452

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C	1.29938500	0.43272300	0.57649600
O	1.74924500	-0.68950700	0.84247100
C	0.31956600	0.28601800	-0.51521200
C	0.74808100	0.25466500	-1.96625700
Au	-1.59726200	-0.14496200	-0.04773000
C	-3.52914200	-0.67528500	0.40519700

C	-5.75378800	-1.03639500	0.25227400
C	-5.34198400	-1.52361900	1.45223100
H	-5.88442300	-2.00762100	2.24833200
H	-6.72831700	-1.00636100	-0.20769000
N	-4.63030700	-0.51995000	-0.37715600
N	-3.97600300	-1.29435900	1.53004300
C	-4.65149600	0.10500000	-1.68484400
C	-4.96702600	1.47607900	-1.76515600
C	-4.39185800	-0.69318600	-2.81749400
C	-5.02140700	2.04638900	-3.04325400
C	-4.45752200	-0.06592800	-4.06842600
C	-4.77172300	1.28596900	-4.18282500
H	-5.27058900	3.09817900	-3.14535200
H	-4.26873500	-0.64813900	-4.96457900
H	-4.82888900	1.74631900	-5.16496900
C	-3.14686600	-1.68342500	2.65395700
C	-2.59251800	-2.97913300	2.66181300
C	-2.94720500	-0.75533300	3.69506800
C	-1.79565400	-3.32650300	3.75954400
C	-2.14303400	-1.16106800	4.76724300
C	-1.57038000	-2.42941700	4.79985100
H	-1.34748800	-4.31423500	3.79959900
H	-1.96558700	-0.47345000	5.58824200
H	-0.94998600	-2.72199100	5.64168200
C	-2.82052100	-3.99011500	1.54177000
C	-3.48227900	-5.27994800	2.06543900
C	-1.50876500	-4.30168000	0.79517000
H	-3.50859600	-3.54918200	0.81427500
H	-4.42571800	-5.06741600	2.57806200
H	-3.69380800	-5.96146400	1.23529600
H	-2.83338000	-5.80975000	2.77008300
H	-1.06528400	-3.38942700	0.38285500
H	-0.77147200	-4.76481600	1.45914600
H	-1.69679300	-4.99552800	-0.03100500
C	-3.56705100	0.63879000	3.69946500
C	-2.48666100	1.73760300	3.71283800
C	-4.55116200	0.81230200	4.87317000
H	-4.13956900	0.76268500	2.77535100
H	-1.80643000	1.63611800	2.86111100
H	-2.95239300	2.72752500	3.66372600
H	-1.88617400	1.69976900	4.62760200
H	-5.34141900	0.05539000	4.84897100
H	-4.04232300	0.72986300	5.83892600
H	-5.02435100	1.79862900	4.83042800

C	-4.07819700	-2.18381800	-2.73186100
C	-2.75990100	-2.53949500	-3.44588700
C	-5.25195500	-3.02358200	-3.27587000
H	-3.95129500	-2.44453700	-1.67688500
H	-1.91942500	-1.94914600	-3.06853100
H	-2.53301100	-3.60060300	-3.29655300
H	-2.82852500	-2.37348900	-4.52606100
H	-6.18240000	-2.81445700	-2.73789300
H	-5.42845300	-2.81809900	-4.33676200
H	-5.03488900	-4.09185400	-3.17483800
C	-5.24199300	2.34094900	-0.53815300
C	-6.67062600	2.91883600	-0.55938800
C	-4.19048500	3.45814600	-0.39346700
H	-5.16238600	1.70951300	0.35169400
H	-7.42327200	2.12652900	-0.62117200
H	-6.86030500	3.49628300	0.35110800
H	-6.82237700	3.58728600	-1.41293300
H	-3.17781700	3.04541500	-0.34721100
H	-4.22969500	4.15738000	-1.23526400
H	-4.37088100	4.03157500	0.52180600
O	0.30632600	-0.65398400	-2.75399600
O	2.41794600	0.16348500	-1.87982700
H	1.25574800	-1.89840900	-2.46178700
O	2.18958400	-2.18961600	-2.15511600
H	2.47898700	-1.06767700	-1.84742900
C	4.32964400	-4.38208500	-0.64442300
C	3.50274200	-3.33858400	-0.47027200
H	4.00798800	-5.17379100	-1.32233500
H	3.76059900	-2.51169300	0.18722300
C	5.64314600	-4.60430600	-0.02711900
C	6.38270100	-5.73774200	-0.40808500
C	6.20172100	-3.73606100	0.92988900
C	7.63873200	-5.99529200	0.13869800
H	5.96532500	-6.42030100	-1.14419400
C	7.45508800	-3.99271600	1.47613700
H	5.65140700	-2.85761200	1.25271800
C	8.17992100	-5.12253400	1.08302400
H	8.19290700	-6.87598600	-0.17187700
H	7.87030900	-3.31174400	2.21340200
H	9.15753100	-5.31977400	1.51252400
C	2.17183700	-3.24692400	-1.13668300
H	1.92288700	-4.17367200	-1.66034200
H	1.38314900	-3.00803400	-0.41621900
C	4.97705800	1.31098600	-1.57043000

C	4.45808200	1.13096900	-2.79321200
H	4.37847500	1.00029700	-0.71652400
H	5.01551900	1.41146300	-3.68547300
C	6.28936100	1.88403000	-1.23361000
C	7.21667800	2.32207900	-2.19761000
C	6.64134500	2.00287500	0.12223900
C	8.44343300	2.85673700	-1.81601600
H	6.98163400	2.24255700	-3.25471800
C	7.87005200	2.53832400	0.50614700
H	5.93823600	1.66769200	0.88115000
C	8.77707000	2.96827800	-0.46253800
H	9.14503100	3.18695200	-2.57653300
H	8.11960900	2.61772400	1.56034900
H	9.73603200	3.38463200	-0.16916700
C	3.11255300	0.54090600	-3.09417600
H	2.49321400	1.25841200	-3.64428000
H	3.21093000	-0.34595500	-3.73401000
C	1.59189000	1.63166700	1.27100200
C	1.82997900	2.65339800	1.89354000
C	2.10867600	3.84461700	2.61068100
C	3.02591000	3.82797900	3.68287800
C	1.47043500	5.05208400	2.25491500
C	3.29590900	4.99991500	4.38105300
H	3.51284000	2.89672700	3.95246200
C	1.74857800	6.21654600	2.96201800
H	0.76738700	5.05851700	1.42831500
C	2.65951500	6.19233300	4.02288000
H	4.00216600	4.98629800	5.20500400
H	1.25769000	7.14507500	2.68824300
H	2.87394300	7.10457000	4.57119000
C	0.40803000	1.72417000	-2.26277200
C	1.19769400	2.80922500	-1.83726100
C	-0.78101900	1.96086700	-2.97972100
C	0.81545400	4.11061700	-2.15612200
H	2.12182900	2.63027400	-1.30051800
C	-1.15586900	3.26347700	-3.28930600
H	-1.37034700	1.11106200	-3.30499200
C	-0.36071900	4.33912800	-2.87620400
H	1.44052300	4.94499200	-1.85307200
H	-2.06614000	3.44137100	-3.85283300
H	-0.65467500	5.35527900	-3.12248700

Zero-point correction= 1.122634 (Hartree/Particle)
Thermal correction to Energy= 1.192771
Thermal correction to Enthalpy= 1.193715

Thermal correction to Gibbs Free Energy=	0.999441
Sum of electronic and zero-point Energies=	-2946.805764
Sum of electronic and thermal Energies=	-2946.735628
Sum of electronic and thermal Enthalpies=	-2946.734684
Sum of electronic and thermal Free Energies=	-2946.928957

1-INT3

C	1.27299200	1.44075600	1.39192200
O	2.33399200	1.27123900	0.79061700
C	1.28654800	1.71235800	2.86983800
C	2.39899500	2.40980000	3.37879600
C	0.28362100	1.27522700	3.75311800
C	2.48527400	2.68940000	4.74145500
H	3.18645600	2.72876200	2.70135800
C	0.39186900	1.53709400	5.11803400
C	1.48478200	2.25265200	5.61329700
H	3.33865400	3.24115100	5.12369100
H	-0.37770300	1.18058700	5.79601600
C	-0.01349600	1.33887000	0.61753500
C	-0.06417000	1.76523300	-0.82895200
C	1.12927600	1.83623500	-1.60576000
C	2.07439900	2.02074900	-2.35398700
C	3.21203100	2.21758100	-3.18005000
C	4.48099500	2.42848700	-2.59792900
C	3.07958700	2.20038000	-4.58493100
C	5.59218300	2.60606900	-3.41705600
C	4.20028400	2.37395200	-5.38981200
H	2.09962300	2.04584500	-5.02480300
C	5.45613700	2.57482900	-4.80801000
H	6.56727500	2.76074500	-2.96661600
H	4.09717000	2.35567200	-6.47042400
H	6.32900600	2.70943300	-5.43992700
H	1.55878400	2.46440100	6.67589300
H	-0.56455800	0.71429000	3.37956300
H	4.58286300	2.46999100	-1.51736800
Au	-0.27868000	-0.82268800	0.48411100
C	-0.44430500	-2.84486700	0.36812900
C	-0.87529400	-4.94496100	-0.33980400
C	-0.17246000	-5.04202300	0.81777900
H	0.16530500	-5.89926000	1.37724000
H	-1.27387900	-5.70114000	-0.99634000
N	-1.03546900	-3.59097900	-0.60205900
N	0.08260700	-3.74514000	1.24101100

C	-1.74374000	-3.07796700	-1.75876500
C	-3.13857900	-2.90080200	-1.66218100
C	-1.01277000	-2.82874600	-2.93771200
C	-3.80407700	-2.45118100	-2.80937700
C	-1.73304300	-2.37637900	-4.05017700
C	-3.11159600	-2.19107900	-3.98912000
H	-4.87900500	-2.30782200	-2.77572500
H	-1.20785900	-2.17611700	-4.97852600
H	-3.64953500	-1.84896600	-4.86857700
C	0.80447100	-3.41871800	2.45401000
C	2.19941800	-3.23275300	2.37871800
C	0.08120900	-3.33725000	3.66076800
C	2.86987900	-2.94195500	3.57330100
C	0.80633500	-3.04222700	4.82182000
C	2.18373600	-2.84497100	4.78063700
H	3.94520800	-2.79590500	3.55705700
H	0.28466600	-2.97322600	5.77135900
H	2.72611500	-2.62142500	5.69451700
C	2.98710400	-3.37080000	1.07900100
C	3.85873000	-4.64308400	1.09928500
C	3.83666900	-2.12168200	0.77846800
H	2.27348200	-3.47588700	0.25628900
H	3.25566100	-5.54223400	1.26174600
H	4.38900800	-4.75806400	0.14838500
H	4.60804000	-4.59753800	1.89636000
H	3.22497800	-1.21533500	0.74870900
H	4.62214900	-1.97736600	1.52776600
H	4.32972600	-2.23385200	-0.19304300
C	-1.42433800	-3.57382500	3.74657100
C	-2.17149200	-2.32641200	4.25584700
C	-1.74822300	-4.80618400	4.61464000
H	-1.79811200	-3.78020300	2.73935400
H	-1.99111500	-1.46479400	3.60513400
H	-3.25003700	-2.51330700	4.27819500
H	-1.86120000	-2.05712600	5.27084400
H	-1.25084900	-5.70495200	4.23651900
H	-1.42837200	-4.66215800	5.65171900
H	-2.82683800	-4.99329100	4.62250400
C	0.48906400	-3.07417800	-3.05175600
C	1.24630900	-1.83834900	-3.57178700
C	0.77536800	-4.30862200	-3.93143700
H	0.87725000	-3.28865700	-2.05141800
H	1.06627700	-0.96156600	-2.94298700
H	2.32327500	-2.03509800	-3.57933300

H	0.95445200	-1.58494000	-4.59613300
H	0.28336900	-5.20530200	-3.54089000
H	0.42000100	-4.15540800	-4.95572200
H	1.85159600	-4.50496100	-3.97621500
C	-3.92645600	-3.21783900	-0.39441900
C	-4.67473100	-4.55972800	-0.53779400
C	-4.89576500	-2.08739200	-0.00292200
H	-3.21201100	-3.32671400	0.42763900
H	-3.99087400	-5.38800300	-0.75055600
H	-5.21497400	-4.79600900	0.38479300
H	-5.40606300	-4.51565400	-1.35170700
H	-4.39605300	-1.11562900	0.02997800
H	-5.72969500	-2.00316800	-0.70732100
H	-5.32849400	-2.29639100	0.98125600
O	-1.15816400	2.06976300	-1.33488000
C	-6.98070900	0.77254900	-2.26754900
C	-6.03297200	1.44854600	-1.60116200
H	-6.66718500	0.17783100	-3.12686500
H	-6.28606500	2.06161500	-0.73767200
C	-8.42540800	0.73700000	-1.99612100
C	-9.25441500	-0.01467600	-2.84704300
C	-9.02606900	1.41782000	-0.92030900
C	-10.63080000	-0.08645700	-2.63677700
H	-8.81011600	-0.54611100	-3.68524400
C	-10.39929500	1.34560400	-0.70807400
H	-8.41544300	2.00711100	-0.24286700
C	-11.20938100	0.59390400	-1.56516500
H	-11.24999300	-0.67230800	-3.30975000
H	-10.84272100	1.87820300	0.12840100
H	-12.28090500	0.54149800	-1.39748300
C	-4.58954300	1.46179600	-1.99631300
H	-4.31839300	2.45181800	-2.39937700
H	-4.40466100	0.72407900	-2.78847900
O	-3.77604400	1.17703100	-0.84650500
H	-2.84129500	1.27758400	-1.11119000
C	7.89032500	1.28851000	-0.19825800
C	6.65664900	1.07828900	0.28621800
H	8.46588900	2.11169700	0.22753700
H	6.04434500	0.25982800	-0.09213400
C	8.59395700	0.52519600	-1.24075000
C	7.97703000	-0.47995800	-2.00973500
C	9.94776400	0.81069600	-1.49168500
C	8.69196400	-1.17509800	-2.98064700
H	6.92782100	-0.71245600	-1.85402700

C	10.66528700	0.11390900	-2.46309700
H	10.44083300	1.58642400	-0.91098400
C	10.04018200	-0.88398800	-3.21136600
H	8.19661300	-1.94604800	-3.56431000
H	11.71119200	0.35079500	-2.63502400
H	10.59485600	-1.42864500	-3.96960800
C	6.03056900	1.91796400	1.36378200
H	6.72539700	2.70427200	1.67582900
H	5.81891700	1.29896000	2.25111800
O	4.83707600	2.58123600	0.93384800
H	4.11617200	1.93122200	0.87600400
C	-2.73515400	3.45264000	0.77077900
C	-3.13153900	4.78750800	0.73501900
C	-2.25651900	5.80229600	1.12236000
C	-0.97926800	5.44569400	1.55947800
C	-0.60512900	4.10760900	1.61233800
H	-2.55870700	6.84244200	1.08440800
H	-3.33204900	2.60806100	0.41152100
H	0.34982800	3.76576300	1.98505300
Cl	0.15082200	6.65141200	2.06866900
Cl	-4.72254100	5.16881000	0.17310700
N	-1.49466500	3.18021200	1.20989900
O	-1.20453500	1.80255000	1.31656100

Zero-point correction= 1.203924 (Hartree/Particle)
Thermal correction to Energy= 1.284178
Thermal correction to Enthalpy= 1.285122
Thermal correction to Gibbs Free Energy= 1.066669
Sum of electronic and zero-point Energies= -4189.437789
Sum of electronic and thermal Energies= -4189.357536
Sum of electronic and thermal Enthalpies= -4189.356592
Sum of electronic and thermal Free Energies= -4189.575044

1-TS3

C	1.44856000	-0.88940100	-0.81154300
O	1.43718100	-0.17938000	-1.92566600
C	1.58535100	-0.07351700	2.89989900
C	2.75409200	0.70315500	2.82919100
C	0.96223800	-0.25941100	4.14428800
C	3.27482700	1.29136400	3.98271800
H	3.26685400	0.81401200	1.88099800
C	1.46979900	0.35317600	5.28882700
C	2.62821400	1.12962800	5.21052100
H	4.19095800	1.87221800	3.92438300

H	0.97092900	0.21390100	6.24328100
C	0.75930900	-0.18438800	0.37712400
C	1.01565900	-0.83326200	1.73066900
C	1.18104300	-2.30856900	-0.97369100
C	1.07772700	-3.49074100	-1.23175000
C	0.97980000	-4.89129300	-1.48442600
C	1.05825000	-5.80804700	-0.41740200
C	0.82857700	-5.37534700	-2.79885700
C	0.98815600	-7.17665200	-0.66546700
C	0.75162000	-6.74571500	-3.03562100
H	0.77889600	-4.66955700	-3.62174800
C	0.83222500	-7.64881900	-1.97192400
H	1.05825600	-7.87760400	0.16112700
H	0.63739400	-7.11111400	-4.05181100
H	0.77974500	-8.71684000	-2.16116500
H	3.03205300	1.59683100	6.10385600
H	0.08096300	-0.88988600	4.20118200
H	1.17335700	-5.43195800	0.59375900
Au	-1.38040000	-0.29461400	0.19162800
C	-3.42040100	-0.54706500	0.19902900
C	-5.65664500	-0.20355400	0.37179000
C	-5.44919700	-1.54307500	0.36608300
H	-6.13695900	-2.37103700	0.42232800
H	-6.56132100	0.37903700	0.43551400
N	-4.40600400	0.39315900	0.26582900
N	-4.07875600	-1.73811900	0.26099100
C	-4.23024700	1.82466700	0.17752400
C	-3.96035300	2.55163300	1.35406300
C	-4.41090400	2.43670700	-1.08018400
C	-3.83556600	3.94178100	1.23256400
C	-4.27190500	3.82930700	-1.14115500
C	-3.98518600	4.57441700	0.00046700
H	-3.63912300	4.53758700	2.11846200
H	-4.41022200	4.33619600	-2.09127200
H	-3.90417000	5.65604600	-0.06484700
C	-3.49048000	-3.06246700	0.20302500
C	-3.30714000	-3.65819200	-1.06074400
C	-3.20951900	-3.72520700	1.41439200
C	-2.82356300	-4.97165400	-1.08331600
C	-2.73381800	-5.03852300	1.32764100
C	-2.54485100	-5.65699200	0.09527400
H	-2.66296400	-5.46458200	-2.03659700
H	-2.50995800	-5.58344900	2.23890000
H	-2.17034100	-6.67465400	0.05109700

C	-3.62995200	-2.94821900	-2.37250700
C	-4.80266600	-3.63261000	-3.10250300
C	-2.39185300	-2.84437900	-3.28349100
H	-3.94276900	-1.92574500	-2.14073300
H	-5.70010400	-3.66898200	-2.47639100
H	-5.05136600	-3.08988400	-4.02055100
H	-4.55202100	-4.66108000	-3.38184900
H	-1.56196500	-2.34652100	-2.77342500
H	-2.04406400	-3.83295800	-3.60033700
H	-2.63458100	-2.27487000	-4.18705100
C	-3.43364200	-3.08373800	2.78033000
C	-2.20302600	-3.22198000	3.69658000
C	-4.69362300	-3.65794800	3.46016400
H	-3.59972600	-2.01239100	2.62743500
H	-1.29566500	-2.86102300	3.20457500
H	-2.35941800	-2.64850400	4.61701500
H	-2.03264000	-4.26216600	3.99311300
H	-5.58872200	-3.51279300	2.84654900
H	-4.58661900	-4.73276600	3.64020300
H	-4.86456800	-3.17190300	4.42652600
C	-4.78713800	1.65304600	-2.33585700
C	-3.71064400	1.76122000	-3.43065400
C	-6.16629000	2.08865300	-2.87061600
H	-4.86431900	0.59602000	-2.06798100
H	-2.74336200	1.39515000	-3.07368100
H	-3.99790300	1.16388300	-4.30201400
H	-3.57996600	2.79465000	-3.76713300
H	-6.94503200	1.98529700	-2.10842200
H	-6.15995100	3.13337200	-3.19818400
H	-6.45016500	1.47387000	-3.73064200
C	-3.86328300	1.89684500	2.72914300
C	-5.02077900	2.35502900	3.63955900
C	-2.49954000	2.14867200	3.39810300
H	-3.95951100	0.81550600	2.59848500
H	-5.99442000	2.14474800	3.18606600
H	-4.97612300	1.83473900	4.60168300
H	-4.97298600	3.43039500	3.84011900
H	-1.68349200	1.75087400	2.78660600
H	-2.31956100	3.21614300	3.56535700
H	-2.45914900	1.65204800	4.37271800
O	0.68185100	-2.00192600	1.89017300
C	0.33993500	2.38993500	-1.27429800
C	-0.21721100	3.60153400	-1.67233700
C	-0.43317900	4.62609600	-0.75197100

C	-0.08288900	4.40630700	0.58168900
C	0.47670100	3.19700300	0.96658700
H	-0.84919300	5.57530300	-1.06519800
H	0.59670600	1.52935700	-1.89640400
H	0.80190900	2.94695000	1.96697000
Cl	-0.32287900	5.63767200	1.77509900
Cl	-0.58777000	3.83803200	-3.34652300
N	0.66610000	2.25203600	0.02378700
O	1.39008500	1.16422400	0.42747200
C	6.26397300	-2.17813300	0.03659900
C	5.16812400	-1.68536800	0.63691200
H	6.11638500	-2.86171000	-0.80057000
H	5.25013500	-0.98560000	1.46617300
C	7.67013400	-1.90799600	0.36747100
C	8.06741000	-1.17895500	1.50441300
C	8.67206600	-2.40040000	-0.48735000
C	9.41386100	-0.94306200	1.76446000
H	7.31907900	-0.80672100	2.19757000
C	10.02122400	-2.16386000	-0.22806500
H	8.38451600	-2.97340900	-1.36544800
C	10.39739300	-1.43214200	0.89875900
H	9.70080500	-0.38219900	2.64934200
H	10.77736200	-2.55345300	-0.90325600
H	11.44731800	-1.24921400	1.10683800
C	3.77581700	-2.04793400	0.22078900
H	3.18086600	-2.39142100	1.07247700
H	3.78867800	-2.84798600	-0.52759800
O	3.14469800	-0.86047000	-0.32660300
H	3.66790500	-0.61930900	-1.48532700
C	3.74667500	3.15484000	-2.71309600
C	4.07167900	1.97268700	-2.16761400
H	3.69238200	3.21975000	-3.80037500
H	4.11341100	1.84712300	-1.08722000
C	3.44306200	4.40784000	-2.00278700
C	2.88052700	5.47876200	-2.72062800
C	3.69783000	4.59297600	-0.62936700
C	2.56308100	6.68245100	-2.09083900
H	2.69452400	5.36273300	-3.78519400
C	3.38348400	5.79545100	-0.00055000
H	4.17480500	3.80194000	-0.05841700
C	2.81025200	6.84511300	-0.72634600
H	2.13763100	7.49750800	-2.66922100
H	3.60524900	5.92471000	1.05505600
H	2.58056700	7.78643300	-0.23619900

C	4.44498300	0.76283100	-2.97297600
H	5.50236100	0.51369000	-2.82211500
H	4.29138200	0.93566900	-4.04264500
O	3.70023300	-0.41842800	-2.60635700
H	2.57293700	-0.27160700	-2.52582300

Zero-point correction= 1.198741 (Hartree/Particle)
Thermal correction to Energy= 1.276630
Thermal correction to Enthalpy= 1.277575
Thermal correction to Gibbs Free Energy= 1.069627
Sum of electronic and zero-point Energies= -4189.396579
Sum of electronic and thermal Energies= -4189.318689
Sum of electronic and thermal Enthalpies= -4189.317745
Sum of electronic and thermal Free Energies= -4189.525692

1-TS3-1

C	1.14625600	-1.34425100	-1.59806900
O	1.23168600	-0.43420600	-2.56457900
C	0.44822300	-2.61800500	-2.06292500
C	0.42971800	-2.84447600	-3.44997600
C	-0.10192300	-3.59115400	-1.21690800
C	-0.10294900	-4.01941600	-3.97602800
H	0.84139900	-2.08634900	-4.10493900
C	-0.63566100	-4.76705100	-1.74812800
C	-0.63416300	-4.99004900	-3.12450100
H	-0.09823100	-4.17797700	-5.05067500
H	-1.04699800	-5.51407500	-1.07657500
C	0.75021300	-0.67591800	-0.23050100
C	1.29942500	-1.32792100	1.02967800
C	1.95126100	-0.48031800	2.01117800
C	2.56292600	0.08764000	2.89911000
C	3.26613100	0.72848400	3.96037300
C	3.91895500	1.96087800	3.75507600
C	3.31833000	0.12630600	5.23434400
C	4.60319000	2.57462700	4.79996300
C	4.00033000	0.75052800	6.27460700
H	2.82261400	-0.82614100	5.38993800
C	4.64291200	1.97319400	6.06092600
H	5.10931500	3.52038000	4.63239500
H	4.03587900	0.28117300	7.25285600
H	5.17783000	2.45421500	6.87412900
H	-1.04141100	-5.91141200	-3.53092300
H	-0.06988700	-3.45097000	-0.14449300
H	3.89747800	2.41833900	2.77059000

Au	-1.36044200	-0.55104600	0.13612200
C	-3.36418700	-0.52273200	0.63017100
C	-5.32442100	-0.03081000	1.66301900
C	-5.56045100	-1.05537500	0.80877200
H	-6.46060100	-1.60360900	0.58378700
H	-5.97712200	0.50170700	2.33516300
N	-3.97833200	0.28970600	1.54029400
N	-4.35306900	-1.34982000	0.18880600
C	-3.36881500	1.38120400	2.27013300
C	-2.60918700	1.09131200	3.42365100
C	-3.62624800	2.69638900	1.83127000
C	-2.05457800	2.17814700	4.11103800
C	-3.05308100	3.74226500	2.56623400
C	-2.26796000	3.48768000	3.68690400
H	-1.46183000	1.99788000	5.00122900
H	-3.23724600	4.76889600	2.26500500
H	-1.83599700	4.31352200	4.24450600
C	-4.24228000	-2.43363600	-0.76775700
C	-4.27331700	-2.13309200	-2.14381100
C	-4.22231200	-3.75270100	-0.26939900
C	-4.28391300	-3.21435300	-3.03345700
C	-4.24835600	-4.79096200	-1.20748900
C	-4.28152800	-4.52735200	-2.57369600
H	-4.30765400	-3.02289800	-4.10148600
H	-4.24398100	-5.81979000	-0.86112100
H	-4.30484200	-5.34887400	-3.28337300
C	-4.32925800	-0.70889400	-2.68776100
C	-5.66698400	-0.43718000	-3.40455400
C	-3.13267600	-0.40732700	-3.61042800
H	-4.26537600	-0.01685700	-1.84293900
H	-6.52016200	-0.60727000	-2.74008800
H	-5.70974800	0.60007800	-3.75320500
H	-5.79113200	-1.08616700	-4.27740700
H	-2.18128700	-0.60141100	-3.10597200
H	-3.15731100	-1.02119400	-4.51656300
H	-3.15304000	0.64207500	-3.92416100
C	-4.19080600	-4.08112600	1.22182200
C	-2.95388500	-4.92028300	1.59619300
C	-5.48771500	-4.78390500	1.67060600
H	-4.11878200	-3.14215400	1.77867500
H	-2.02739300	-4.41265300	1.31310900
H	-2.92932000	-5.09492100	2.67681000
H	-2.96776900	-5.89971000	1.10676100
H	-6.37361500	-4.17987800	1.44931700

H	-5.61286800	-5.74874300	1.16848900
H	-5.46704700	-4.97087000	2.74912400
C	-4.53875800	3.01529600	0.64801000
C	-3.85081400	3.89274200	-0.41216100
C	-5.84899600	3.67292400	1.12910400
H	-4.80473700	2.07629400	0.15486900
H	-2.95500600	3.40425900	-0.80455300
H	-4.53055600	4.07334200	-1.25082000
H	-3.56174600	4.86904200	-0.00864700
H	-6.37409200	3.04541700	1.85595200
H	-5.65598400	4.63855400	1.60782300
H	-6.52245600	3.84688100	0.28375500
C	-2.46411200	-0.32603800	3.97252300
C	-3.56238400	-0.60062800	5.02314300
C	-1.07214600	-0.61662200	4.55762400
H	-2.61353500	-1.02673300	3.14617800
H	-4.56605400	-0.46788300	4.60726200
H	-3.48485900	-1.62701000	5.39621400
H	-3.46251100	0.07743400	5.87737300
H	-0.27687200	-0.38770700	3.84323600
H	-0.88430300	-0.04710800	5.47403800
H	-0.99682500	-1.67693400	4.81766500
O	1.17556100	-2.52489900	1.27023100
C	0.20439600	1.99593600	-1.65920900
C	-0.31354600	3.26464800	-1.90500100
C	-0.19215100	4.28155600	-0.95914500
C	0.42490500	3.98552400	0.25900500
C	0.91864000	2.71201800	0.50134300
H	-0.56147900	5.27889900	-1.16463400
H	0.24697400	1.14418900	-2.34132000
H	1.40593000	2.38618500	1.41022200
Cl	0.60413100	5.20403400	1.47658500
Cl	-1.08082200	3.56839000	-3.42658500
N	0.80567700	1.78616300	-0.47364800
O	1.49210800	0.62749200	-0.24413100
C	5.30848700	-3.64768900	-0.02037000
C	4.65707500	-3.22826900	-1.11696900
H	4.70705700	-3.93289400	0.84333900
H	5.20220200	-2.91844400	-2.00737300
C	6.75944700	-3.77763500	0.16999200
C	7.69441300	-3.57157000	-0.86220800
C	7.24394600	-4.12866700	1.44241000
C	9.05893700	-3.70245500	-0.62365400
H	7.35238500	-3.31934400	-1.86138900

C	8.61084500	-4.25997700	1.68242300
H	6.53583200	-4.29869600	2.24968500
C	9.52429700	-4.04589000	0.64978800
H	9.76426800	-3.54318600	-1.43418000
H	8.96158800	-4.53240700	2.67353800
H	10.58976300	-4.15111200	0.83111500
C	3.16416200	-3.18062600	-1.20576900
H	2.69818500	-3.62252100	-0.32325700
H	2.80519300	-3.70839100	-2.09644600
O	2.74597200	-1.78509900	-1.27961800
H	3.37975100	-1.13252600	-2.12426200
C	3.67153400	3.18352700	-2.33364100
C	3.84889600	2.07165900	-3.06490400
H	3.88906100	3.12289100	-1.26566800
H	3.68251100	2.06949800	-4.14068700
C	3.24142900	4.51251300	-2.79456900
C	3.24167300	5.57934800	-1.87741600
C	2.81803800	4.77280500	-4.11205600
C	2.84150900	6.86015200	-2.25798500
H	3.57794600	5.40213200	-0.85832500
C	2.41651100	6.05033000	-4.49214400
H	2.80333800	3.97234100	-4.84533300
C	2.42619100	7.10061200	-3.56845600
H	2.86325400	7.67025000	-1.53478100
H	2.09781400	6.23043800	-5.51460900
H	2.11838100	8.09681600	-3.87132900
C	4.34428700	0.78058400	-2.48713800
H	4.32283900	0.81241700	-1.39027500
H	5.38027800	0.59623400	-2.79782700
O	3.57475400	-0.34043200	-2.96832500
H	2.45306700	-0.19758300	-2.90843300

Zero-point correction= 1.198568 (Hartree/Particle)
Thermal correction to Energy= 1.276440
Thermal correction to Enthalpy= 1.277384
Thermal correction to Gibbs Free Energy= 1.068407
Sum of electronic and zero-point Energies= -4189.389503
Sum of electronic and thermal Energies= -4189.311631
Sum of electronic and thermal Enthalpies= -4189.310687
Sum of electronic and thermal Free Energies= -4189.519664

1-INT4

C	0.21025300	2.31884500	1.60154200
O	0.01922100	1.99951600	2.77858600

C	-0.26651100	3.67910500	1.17585100
C	-1.19364800	4.28802200	2.04874300
C	0.18882200	4.41205700	0.06666700
C	-1.65881400	5.57654600	1.81544600
H	-1.52771600	3.73214900	2.91663500
C	-0.27043900	5.71172800	-0.15427300
C	-1.19382500	6.29716000	0.71101800
H	-2.37540700	6.02409400	2.49770700
H	0.10520200	6.26873400	-1.00739500
C	0.79469600	1.20921000	0.70275600
C	1.77997600	1.50154800	-0.48391400
C	2.87975800	2.38855900	-0.06635000
C	3.77703600	3.10054200	0.33358000
C	4.82452200	3.95132300	0.80410900
C	4.74911000	4.52406500	2.08854500
C	5.93985700	4.22827300	-0.00966400
C	5.76970500	5.35438200	2.54409800
C	6.95558800	5.05920200	0.45563200
H	5.99786600	3.79028800	-1.00092300
C	6.87375200	5.62336500	1.73120100
H	5.70366800	5.79339600	3.53498400
H	7.81201700	5.26830000	-0.17816400
H	7.66748100	6.27154100	2.09014600
H	-1.54600800	7.30893900	0.53155300
H	0.89965400	3.98768100	-0.62422600
H	3.88823200	4.31366200	2.71493200
Au	-0.97479000	0.23899700	-0.02498500
C	-2.72863900	-0.50719100	-0.80995500
C	-4.71678400	-1.54714900	-1.11694800
C	-4.50284400	-0.75366600	-2.19651700
H	-5.09594000	-0.57627600	-3.07905500
H	-5.53295000	-2.20538900	-0.86662500
N	-3.61898600	-1.38924400	-0.27913000
N	-3.28285000	-0.12341100	-1.99315700
C	-3.45725900	-2.12188000	0.95873400
C	-2.98478000	-3.44832800	0.88519000
C	-3.82890500	-1.50435500	2.17012200
C	-2.87061900	-4.15576100	2.08869900
C	-3.69396400	-2.26250000	3.34057500
C	-3.22087200	-3.57141300	3.30334900
H	-2.51972700	-5.18313600	2.07038100
H	-3.97703300	-1.82390800	4.29204000
H	-3.13825200	-4.14245500	4.22343200
C	-2.69426900	0.82068200	-2.92067100

C	-3.11460600	2.16491700	-2.86616400
C	-1.74686800	0.34673900	-3.85225200
C	-2.51996600	3.05669400	-3.76790900
C	-1.18209000	1.28767200	-4.72279000
C	-1.55837500	2.62801700	-4.67846800
H	-2.81415500	4.10119500	-3.75368300
H	-0.44725100	0.96407200	-5.45336300
H	-1.10754000	3.33870100	-5.36452100
C	-4.18909200	2.66173400	-1.90341300
C	-5.45922000	3.08439600	-2.66979200
C	-3.67905300	3.80237200	-1.00480300
H	-4.46729600	1.83431200	-1.24362800
H	-5.85340800	2.26769500	-3.28335400
H	-6.24236400	3.39013900	-1.96869200
H	-5.25891000	3.93067100	-3.33490200
H	-2.79673300	3.49990800	-0.43489900
H	-3.41215900	4.69004700	-1.58653600
H	-4.45926200	4.09762400	-0.29575700
C	-1.36739500	-1.12663500	-3.97525000
C	0.14562700	-1.35678500	-3.80445300
C	-1.86799800	-1.71020400	-5.31247300
H	-1.86793100	-1.67668700	-3.17315400
H	0.50165400	-0.98624000	-2.83822400
H	0.37169500	-2.42695400	-3.86180400
H	0.71927300	-0.85868100	-4.59325500
H	-2.94956800	-1.58527400	-5.42466100
H	-1.38750100	-1.22138000	-6.16615700
H	-1.64229800	-2.77999100	-5.37041200
C	-4.40532400	-0.09363700	2.24393100
C	-3.61065600	0.81032200	3.20516600
C	-5.89871300	-0.13338900	2.62873900
H	-4.33663600	0.35676000	1.24966100
H	-2.55462700	0.87113100	2.92499600
H	-4.02186800	1.82474900	3.18824600
H	-3.66807700	0.45338700	4.23881100
H	-6.47982800	-0.73743100	1.92466600
H	-6.04202100	-0.55776500	3.62795100
H	-6.31689700	0.87825800	2.63307600
C	-2.61260100	-4.12715000	-0.43079900
C	-3.46091300	-5.38959100	-0.68022000
C	-1.10794000	-4.44896300	-0.49134300
H	-2.82322000	-3.43157200	-1.24778200
H	-4.53163200	-5.16360300	-0.66439500
H	-3.22004200	-5.82063200	-1.65713300

H	-3.27348800	-6.15915400	0.07537800
H	-0.50667200	-3.54231900	-0.37056900
H	-0.81674300	-5.15801700	0.29063200
H	-0.85192400	-4.89905300	-1.45597200
O	1.13808700	2.10632100	-1.57926000
C	0.67661900	-0.84508000	3.24029200
C	0.49989500	-2.10377500	3.80351400
C	0.99562200	-3.24023500	3.16053800
C	1.66413100	-3.08569100	1.94347700
C	1.83312600	-1.82080700	1.39107600
H	0.87785600	-4.22173700	3.60463600
H	0.34528700	0.11085700	3.63568100
H	2.33805800	-1.58383300	0.46098100
Cl	2.32968800	-4.45505500	1.12150800
Cl	-0.30040600	-2.23410900	5.33193900
N	1.33730400	-0.76741000	2.06912000
O	1.69594400	0.48049900	1.64003500
C	4.39541700	-2.03489400	-2.27173200
C	4.25466100	-0.91256000	-1.54729800
H	3.75551000	-2.15284500	-3.14738800
H	4.85555800	-0.74046400	-0.65580800
C	5.32044300	-3.15189900	-2.03268100
C	6.32848600	-3.12002600	-1.05021000
C	5.19817000	-4.31056000	-2.81986900
C	7.16997200	-4.21164900	-0.85835600
H	6.46620500	-2.23051900	-0.44292200
C	6.04048000	-5.40475000	-2.62800200
H	4.43225700	-4.34868000	-3.59072000
C	7.02903900	-5.35994800	-1.64430700
H	7.94583600	-4.16563600	-0.09966700
H	5.92850700	-6.28842900	-3.24929400
H	7.69125800	-6.20746700	-1.49537500
C	3.28687400	0.17539900	-1.88956100
H	2.81173400	-0.00288900	-2.85996700
H	3.79086100	1.14740100	-1.92541000
O	2.26543300	0.21059500	-0.86043400
H	0.35835500	1.56833500	-1.79768900

Zero-point correction=	1.036883 (Hartree/Particle)
Thermal correction to Energy=	1.104709
Thermal correction to Enthalpy=	1.105653
Thermal correction to Gibbs Free Energy=	0.921356
Sum of electronic and zero-point Energies=	-3765.391493
Sum of electronic and thermal Energies=	-3765.323668
Sum of electronic and thermal Enthalpies=	-3765.322723

Sum of electronic and thermal Free Energies= -3765.507020

1-TS4

C	0.64503100	-0.05511200	-2.08916900
O	1.23048700	1.00270600	-2.30035400
C	-0.10942500	-0.72833900	-3.18753300
C	0.22147700	-0.33637500	-4.49786600
C	-1.12232300	-1.68101900	-2.98894300
C	-0.44025200	-0.89415900	-5.58626200
H	0.99928100	0.40578100	-4.63834300
C	-1.79194500	-2.22681000	-4.08287400
C	-1.45054100	-1.83914300	-5.38042400
H	-0.17389300	-0.59129100	-6.59420900
H	-2.58671500	-2.94697400	-3.91767400
C	0.65545900	-0.66726100	-0.71150000
C	1.80308200	-1.61164900	-0.36748100
C	1.35243200	-2.89183200	-0.93863900
C	1.02065000	-3.94375600	-1.45178200
C	0.64621500	-5.17971100	-2.05045100
C	0.29216400	-6.28166600	-1.24486200
C	0.63838200	-5.31471500	-3.45408800
C	-0.06026500	-7.49098800	-1.83605000
C	0.28024600	-6.52818100	-4.03347000
H	0.91045700	-4.46560200	-4.07191500
C	-0.06762000	-7.61664300	-3.22835900
H	-0.32616400	-8.33856500	-1.21203000
H	0.27641100	-6.62828200	-5.11444300
H	-0.34125600	-8.56281600	-3.68530000
H	-1.97299900	-2.26828000	-6.23046400
H	-1.40452300	-1.98375700	-1.98788700
H	0.30691000	-6.17681200	-0.16508300
Au	-1.01701000	-0.65203100	0.46312000
C	-2.62544400	-0.66332300	1.74186100
C	-4.68543300	-0.86299300	2.64901100
C	-3.82891900	-0.53908400	3.65209500
H	-3.99525700	-0.37703500	4.70456600
H	-5.74789800	-1.04523300	2.65083900
N	-3.93150300	-0.93571200	1.48563000
N	-2.56989200	-0.42088200	3.08068200
C	-4.47566400	-1.27858000	0.18724400
C	-4.96629100	-0.24160300	-0.63037000
C	-4.51497300	-2.63793900	-0.18388800
C	-5.48590100	-0.60724100	-1.87885800

C	-5.04851700	-2.94149300	-1.44272400
C	-5.52408300	-1.93833100	-2.28378600
H	-5.87169800	0.16329800	-2.53865300
H	-5.10262400	-3.97801400	-1.76149700
H	-5.93846900	-2.19647200	-3.25402800
C	-1.36400200	-0.08209300	3.81102000
C	-0.52806400	-1.13265100	4.24811200
C	-1.09381800	1.27744500	4.06576800
C	0.63862500	-0.77441200	4.93447200
C	0.08625900	1.57221600	4.76278500
C	0.94602700	0.56203900	5.18574600
H	1.30644500	-1.55115100	5.29099900
H	0.32425000	2.60674600	4.98810600
H	1.84857300	0.81424000	5.73595600
C	-0.89617200	-2.60369200	4.06683600
C	-1.60058500	-3.13339200	5.33501200
C	0.30313700	-3.49438300	3.69882900
H	-1.60840900	-2.67325700	3.23907000
H	-2.49815500	-2.55476000	5.57523800
H	-1.89939900	-4.17790000	5.19842500
H	-0.93215200	-3.08492600	6.20116500
H	0.82653600	-3.12197200	2.81438800
H	1.02282400	-3.57210500	4.52050400
H	-0.04756500	-4.51002200	3.48812400
C	-2.05400500	2.40275800	3.68714100
C	-1.36980700	3.55203100	2.92455700
C	-2.77300400	2.92936100	4.94799900
H	-2.81773300	1.99125800	3.02040700
H	-0.96399400	3.21470600	1.96696600
H	-2.10455800	4.33557400	2.71206400
H	-0.56896900	4.01220300	3.51328000
H	-3.29427600	2.13016200	5.48525400
H	-2.06276400	3.38576600	5.64561000
H	-3.50996100	3.69106700	4.67439900
C	-4.04312100	-3.76488200	0.73107000
C	-2.91467500	-4.59365600	0.08957000
C	-5.22154600	-4.66629900	1.15173500
H	-3.63539600	-3.31835100	1.64271300
H	-2.05189900	-3.96851400	-0.16017800
H	-2.57871700	-5.37309300	0.78169000
H	-3.24868700	-5.09089000	-0.82679700
H	-6.01347000	-4.08996700	1.64035200
H	-5.66515500	-5.17315000	0.28867500
H	-4.88169800	-5.43635500	1.85184700

C	-4.98589300	1.22234500	-0.20047600
C	-6.43513500	1.72897400	-0.04995800
C	-4.18011300	2.11764700	-1.15974500
H	-4.51137300	1.29757200	0.78247600
H	-7.00720100	1.11703800	0.65528500
H	-6.43851400	2.76105100	0.31443000
H	-6.96532400	1.71372900	-1.00773400
H	-3.12618800	1.82947100	-1.18806400
H	-4.58179200	2.07687200	-2.17801800
H	-4.22533900	3.15952600	-0.82834800
O	1.95295600	-1.76495400	1.02082400
C	3.34545800	1.49253200	1.87219600
C	4.61625800	2.03621700	1.98973300
C	5.29069800	2.53011400	0.87247300
C	4.63472000	2.45435900	-0.35478100
C	3.36542300	1.89826100	-0.46238400
H	6.28558100	2.94943300	0.95465000
H	2.75879200	1.12082800	2.70157500
H	2.80114600	1.77770100	-1.37813200
Cl	5.39299200	3.05760200	-1.79218500
Cl	5.35327500	2.09571700	3.56156100
N	2.75297200	1.43607100	0.65186300
O	1.51758200	0.93211800	0.59374900
C	6.37273800	-0.99133000	-0.36267000
C	5.35288100	-1.20884100	-1.20839000
H	6.28209100	-1.38554100	0.65049400
H	5.37369200	-0.82409700	-2.22610700
C	7.62069700	-0.26147100	-0.62694400
C	8.02157800	0.13618100	-1.91675900
C	8.45726000	0.06171600	0.45713300
C	9.20467500	0.84389900	-2.10738900
H	7.41283900	-0.12445200	-2.77704500
C	9.64172700	0.77247600	0.26667300
H	8.17323200	-0.25339000	1.45847200
C	10.01857000	1.16855300	-1.01730900
H	9.50009800	1.13667400	-3.11065000
H	10.27307600	1.00889100	1.11815400
H	10.94352300	1.71596900	-1.17131000
C	4.13916100	-1.99233100	-0.82631700
H	4.20453500	-2.33883400	0.20962000
H	4.00410400	-2.86602200	-1.47842300
O	2.98074700	-1.13005400	-0.97573800
H	1.77269800	-0.87938600	1.38433900
C	-1.72653700	5.77310600	-1.49582700

C	-1.35415700	4.50651400	-1.73237700
H	-1.16472500	6.33580100	-0.74901100
H	-1.89400600	3.88802900	-2.44665300
C	-2.82990600	6.51692200	-2.12230400
C	-3.56804400	6.02486700	-3.21545100
C	-3.17136400	7.78140600	-1.61121300
C	-4.61282300	6.76440400	-3.76193900
H	-3.31396400	5.06246600	-3.64932900
C	-4.21747700	8.52336200	-2.15797600
H	-2.60825900	8.18230500	-0.77188400
C	-4.94468400	8.01670600	-3.23547100
H	-5.16719300	6.36778400	-4.60788000
H	-4.46231900	9.49734600	-1.74425900
H	-5.75764900	8.59297400	-3.66699900
C	-0.18968200	3.84354600	-1.06545500
H	0.30375500	4.55723200	-0.38663100
H	0.54421000	3.54329400	-1.82969100
O	-0.63963400	2.68476800	-0.35420800
H	0.13941800	2.16002700	-0.10408300

Zero-point correction=	1.202852 (Hartree/Particle)
Thermal correction to Energy=	1.282034
Thermal correction to Enthalpy=	1.282978
Thermal correction to Gibbs Free Energy=	1.067953
Sum of electronic and zero-point Energies=	-4189.395977
Sum of electronic and thermal Energies=	-4189.316795
Sum of electronic and thermal Enthalpies=	-4189.315851
Sum of electronic and thermal Free Energies=	-4189.530876

1-INT5

C	1.19334600	1.20111600	-2.81279800
O	1.28953800	0.38827400	-3.82841700
C	2.33612700	2.10868600	-2.64236700
C	3.15635300	2.34337900	-3.76587700
C	2.65024700	2.73507400	-1.41990700
C	4.24600400	3.20210700	-3.67286400
H	2.92064500	1.85980300	-4.70627500
C	3.75354900	3.57763000	-1.33230500
C	4.54731000	3.82084500	-2.45686900
H	4.86070500	3.38808900	-4.54766900
H	3.99655600	4.04180200	-0.38206100
C	-0.00119900	1.16818600	-1.98211100
C	-1.13978500	0.36058700	-2.54627500
C	-0.36757300	2.29949800	-1.17303100

C	-0.72529300	3.24259200	-0.49474500
C	-1.12283000	4.36137900	0.29576300
C	-2.22325700	4.26229000	1.17062200
C	-0.42073600	5.58029800	0.20842900
C	-2.60703800	5.35898300	1.93761700
C	-0.81124300	6.66925100	0.98285300
H	0.42185300	5.66095200	-0.47099500
C	-1.90367300	6.56307000	1.84765700
H	-3.45833800	5.27526900	2.60645400
H	-0.26603500	7.60524300	0.90768900
H	-2.20752800	7.41610800	2.44662700
H	5.40072900	4.48844000	-2.38470200
H	2.05028700	2.54979100	-0.53865100
H	-2.76833400	3.32602200	1.23494800
Au	0.79424100	-0.27981600	-0.45842400
C	1.36347200	-1.60055400	0.95609700
C	1.44928700	-3.44820200	2.24426900
C	2.45133500	-2.62281400	2.64425000
H	3.19766200	-2.72976400	3.41475700
H	1.14453700	-4.42097600	2.59504500
N	0.78895200	-2.80534300	1.20589800
N	2.38516200	-1.49052200	1.84300200
C	-0.36161800	-3.34712800	0.50905800
C	-1.64405200	-3.08490100	1.03162500
C	-0.14365000	-4.12817000	-0.64360300
C	-2.73537000	-3.64021700	0.35125800
C	-1.27396300	-4.65368400	-1.28187500
C	-2.55513500	-4.41598200	-0.79133100
H	-3.73833100	-3.46859800	0.72951200
H	-1.14667400	-5.26145000	-2.17210900
H	-3.41547200	-4.84375000	-1.29775300
C	3.27867100	-0.35476500	1.96239000
C	4.48172800	-0.36792900	1.22884800
C	2.91232900	0.69646800	2.82700900
C	5.33362700	0.73285100	1.38217300
C	3.80457200	1.77068300	2.93689800
C	5.00099200	1.78997900	2.22494900
H	6.27149000	0.75891400	0.83652200
H	3.56134400	2.59790300	3.59632600
H	5.68199100	2.62894600	2.33488000
C	4.88399300	-1.51527600	0.30691800
C	6.14643300	-2.23316800	0.82500100
C	5.07462000	-1.03639100	-1.14535300
H	4.07326100	-2.25005900	0.30007200

H	6.00564600	-2.61087900	1.84271100
H	6.39327100	-3.08215400	0.17955200
H	7.01172500	-1.56271600	0.83693200
H	4.17107800	-0.55141300	-1.52778300
H	5.89877000	-0.32057200	-1.22833300
H	5.30826900	-1.88540400	-1.79583600
C	1.62139700	0.69666800	3.64039600
C	0.71935600	1.89276500	3.27942100
C	1.91417700	0.65898500	5.15381800
H	1.06281200	-0.21230000	3.39701000
H	0.47199200	1.90320700	2.21336200
H	-0.21727700	1.84253000	3.84408600
H	1.19772100	2.84690500	3.52303900
H	2.52438400	-0.20850900	5.42442600
H	2.44890700	1.55632600	5.48118400
H	0.97860100	0.60575600	5.71962100
C	1.24480200	-4.41515100	-1.20706100
C	1.40351400	-3.84197000	-2.62923000
C	1.56544900	-5.92252400	-1.17600200
H	1.98253300	-3.91385600	-0.57333900
H	1.19932600	-2.76654800	-2.65065300
H	2.42403100	-4.00394800	-2.99086900
H	0.72124600	-4.32538600	-3.33581100
H	1.49040100	-6.32838600	-0.16225100
H	0.88154800	-6.49180200	-1.81354800
H	2.58258600	-6.10150800	-1.53889700
C	-1.88090100	-2.23586100	2.27759400
C	-2.58266400	-3.04192100	3.38835100
C	-2.66499400	-0.95194700	1.94116500
H	-0.90816800	-1.92580500	2.67097200
H	-2.01565200	-3.93973100	3.65385600
H	-2.69067900	-2.43024300	4.28966200
H	-3.58484500	-3.35985000	3.08365300
H	-2.15452700	-0.35759800	1.17664700
H	-3.66920600	-1.17881500	1.56922300
H	-2.77729500	-0.33289900	2.83735500
O	-1.00223300	-0.41049900	-3.50988600
C	-5.50532800	-0.45235100	-1.07597800
C	-4.67340800	0.31731600	-1.79588700
H	-5.23022600	-1.49907300	-0.93870800
H	-4.88568200	1.36830400	-1.97652200
C	-6.77435600	-0.06595500	-0.44648400
C	-7.48863900	-1.03562300	0.27894900
C	-7.31423600	1.23137600	-0.53344500

C	-8.69723300	-0.72577300	0.90042000
H	-7.09041600	-2.04501900	0.35027500
C	-8.52000300	1.54163700	0.08713300
H	-6.79256100	2.00186600	-1.09280600
C	-9.21696800	0.56550100	0.80687500
H	-9.23308000	-1.49143200	1.45336500
H	-8.92244700	2.54713500	0.00727900
H	-10.15944400	0.81145000	1.28656600
C	-3.44591300	-0.21993000	-2.44428300
H	-3.45173000	-0.09098300	-3.53078200
H	-3.28177200	-1.27700000	-2.21857400
O	-2.28928500	0.53804900	-1.92803200
H	0.39200300	-0.10851000	-3.91353900

Zero-point correction= 0.961282 (Hartree/Particle)
Thermal correction to Energy= 1.020737
Thermal correction to Enthalpy= 1.021681
Thermal correction to Gibbs Free Energy= 0.854475
Sum of electronic and zero-point Energies= -2522.910313
Sum of electronic and thermal Energies= -2522.850858
Sum of electronic and thermal Enthalpies= -2522.849914
Sum of electronic and thermal Free Energies= -2523.017120

6-TS1

C	-0.04642000	1.62483100	-0.96959200
O	0.57962300	1.34065000	-1.99450900
C	0.49426800	2.66283800	-0.04052200
C	-0.28908500	3.71819700	0.44840000
C	1.87150700	2.62853600	0.24116100
C	0.29974400	4.72572300	1.21311600
H	-1.34231400	3.76119000	0.20219800
C	2.44357400	3.61913500	1.03627500
C	1.66131000	4.67222900	1.51923000
H	-0.30594200	5.55440000	1.56740500
H	3.50366200	3.57432300	1.26564800
C	-1.33094300	0.83487600	-0.70213700
C	-2.47412500	1.18701200	0.32448600
C	-2.05147300	1.34712100	1.72343000
C	-1.88045200	1.65122200	2.88684300
C	-1.68425100	2.02641300	4.25153200
C	-2.56150800	1.55853900	5.24991000
C	-0.63452900	2.89537100	4.60917300
C	-2.38107200	1.94186500	6.57634200
C	-0.46415400	3.27309100	5.93890300

H	0.03079000	3.27044100	3.83872200
C	-1.33226400	2.79673900	6.92470500
H	-3.06290600	1.57789200	7.33890900
H	0.34579400	3.94481200	6.20700600
H	-1.19600800	3.09571500	7.95957900
H	2.11412000	5.45517200	2.12083500
H	2.48823100	1.83861200	-0.17398700
H	-3.38308500	0.90683200	4.97209500
Au	-0.26115500	-0.89993000	0.29291100
C	0.70377900	-2.46942400	1.15505400
C	2.28300000	-3.71697400	2.17879000
C	1.13984400	-4.44644200	2.15803700
H	0.92011300	-5.43797200	2.51903900
H	3.26414200	-3.94063300	2.56442500
N	2.00173200	-2.50586000	1.56173400
N	0.17940100	-3.67203400	1.51993700
C	3.00382700	-1.47830000	1.34927300
C	3.62997200	-1.40342900	0.08781000
C	3.35211400	-0.64839800	2.43370600
C	4.60469000	-0.41221700	-0.08212500
C	4.35429200	0.30373100	2.21046600
C	4.96495900	0.43033800	0.96546100
H	5.08228400	-0.29222200	-1.04730200
H	4.65810500	0.95464000	3.02417400
H	5.73044900	1.18395300	0.80604400
C	-1.14172700	-4.16656000	1.18793900
C	-2.23202100	-3.81875900	2.01076500
C	-1.26030700	-5.02019600	0.07195400
C	-3.48629300	-4.32983000	1.65456700
C	-2.54031900	-5.49971400	-0.23408700
C	-3.64221200	-5.15416400	0.54299300
H	-4.35138100	-4.08704000	2.26154100
H	-2.67219100	-6.16002800	-1.08555100
H	-4.62515900	-5.54138300	0.29119900
C	-2.06466900	-2.99029800	3.28075600
C	-1.87586000	-3.91834300	4.50040600
C	-3.22228300	-2.00702200	3.51908400
H	-1.15490500	-2.39110500	3.17657200
H	-1.01361700	-4.58165800	4.37833100
H	-1.71979200	-3.32730500	5.40868600
H	-2.76024300	-4.54585400	4.65379100
H	-3.38659900	-1.36079300	2.65272800
H	-4.15938100	-2.52385700	3.75127600
H	-2.98471400	-1.37315700	4.37845800

C	-0.06838900	-5.45497600	-0.77892300
C	-0.18511400	-4.95097500	-2.22857700
C	0.12211300	-6.98430700	-0.73863300
H	0.83773900	-5.00771700	-0.36186200
H	-0.24360100	-3.85855000	-2.25823800
H	0.68995900	-5.25904700	-2.81010700
H	-1.07326700	-5.35818000	-2.72331700
H	0.23436100	-7.34771700	0.28759400
H	-0.72932300	-7.50930100	-1.18333400
H	1.01786600	-7.27040300	-1.29906500
C	2.71864700	-0.77654500	3.81638400
C	2.17659000	0.56722000	4.33454500
C	3.71420500	-1.38865200	4.82345400
H	1.86502700	-1.45736000	3.74028500
H	1.47530100	1.01349800	3.62533300
H	1.65222300	0.42269600	5.28416000
H	2.98157400	1.28795100	4.51169700
H	4.07122200	-2.37141300	4.49852700
H	4.59138700	-0.74537200	4.94852600
H	3.24266600	-1.50764100	5.80434700
C	3.33478300	-2.37215100	-1.05464100
C	4.59174500	-3.18843700	-1.41961700
C	2.76446400	-1.65545300	-2.29271600
H	2.57847600	-3.08612300	-0.71332500
H	4.98989600	-3.72367200	-0.55165000
H	4.35331200	-3.92549000	-2.19362000
H	5.38743800	-2.54554000	-1.80867300
H	1.82761900	-1.14260100	-2.05339500
H	3.44870700	-0.89611200	-2.67974900
H	2.56936200	-2.38371400	-3.08838000
O	-3.43976900	0.14315000	0.29004900
C	-0.92235700	-0.83817000	-3.68707000
C	-0.98994400	-1.80592400	-4.69232600
C	-2.00180300	-2.76895200	-4.65737300
C	-2.90467800	-2.76433700	-3.59032000
C	-2.79043900	-1.79612500	-2.59145100
H	-2.08664500	-3.50741000	-5.44622500
H	-0.20287300	-0.02375600	-3.62815300
H	-3.43848100	-1.73517600	-1.72484300
Cl	-4.17667100	-3.93975500	-3.50647800
Cl	0.16122800	-1.78166100	-5.98531900
N	-1.81052000	-0.90420100	-2.70300000
O	-1.93687100	0.60904500	-1.87811600
C	-6.20142700	3.79217700	-0.55442000

C	-4.88521900	3.89672500	-0.31518700
H	-6.73669800	2.96559200	-0.08479900
H	-4.29522400	4.69719000	-0.75644400
C	-7.04179400	4.67092900	-1.37959500
C	-6.54548200	5.80036500	-2.05778300
C	-8.40969800	4.37115800	-1.50454500
C	-7.38768600	6.59246900	-2.83174700
H	-5.49510500	6.06373900	-1.97919700
C	-9.25457300	5.16476400	-2.27891700
H	-8.81165100	3.50467300	-0.98496100
C	-8.74594400	6.27909700	-2.94654800
H	-6.98595400	7.46010600	-3.34702900
H	-10.30812800	4.91384800	-2.35930500
H	-9.40004700	6.90113000	-3.55010500
C	-4.14254900	2.95647800	0.57750300
H	-4.79727700	2.16424500	0.95417800
H	-3.70168500	3.47673500	1.43821600
O	-3.06121200	2.36993000	-0.19992000
H	-3.88047500	0.26478700	-0.56569100
C	6.32706300	3.44500500	-1.94036100
C	5.52815700	2.70046100	-2.71948900
H	5.85416400	4.18104400	-1.28839300
H	5.93980000	1.93860300	-3.37959100
C	7.79436400	3.39663800	-1.84625300
C	8.43641800	4.17734600	-0.86891700
C	8.59552000	2.60100700	-2.68712300
C	9.82315500	4.15961000	-0.72538900
H	7.83569100	4.80581600	-0.21561600
C	9.97969400	2.58170800	-2.54444700
H	8.13355000	2.00062000	-3.46494600
C	10.60129800	3.35926400	-1.56222500
H	10.29517300	4.77279300	0.03686500
H	10.57931400	1.96288700	-3.20594000
H	11.68195000	3.34464300	-1.45668500
C	4.03718100	2.84351000	-2.76390300
H	3.73029100	3.20363800	-3.76102100
H	3.71111200	3.59742700	-2.03141200
O	3.44993500	1.57008100	-2.49785700
H	2.48240300	1.66205200	-2.48675500

Zero-point correction= 1.202805 (Hartree/Particle)
Thermal correction to Energy= 1.280932
Thermal correction to Enthalpy= 1.281876
Thermal correction to Gibbs Free Energy= 1.075094

Sum of electronic and zero-point Energies=	-4189.389062
Sum of electronic and thermal Energies=	-4189.310935
Sum of electronic and thermal Enthalpies=	-4189.309991
Sum of electronic and thermal Free Energies=	-4189.516773

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C	1.49494900	-2.28468800	0.81484900
O	0.32451700	-2.06021700	1.19624000
C	2.17703500	-3.51367800	1.19157000
C	1.57820200	-4.36841600	2.14223900
C	3.39915500	-3.87798500	0.59322400
C	2.20292200	-5.55557200	2.49491000
H	0.63590500	-4.07803600	2.59311200
C	4.01173400	-5.07689600	0.94408800
C	3.41861600	-5.91084900	1.89529000
H	1.74978800	-6.20916000	3.23323500
H	4.94980700	-5.36028600	0.47849000
C	2.13475600	-1.23570200	-0.11971800
C	3.14251100	-0.25580600	0.57473400
C	4.50756200	-0.68321700	0.24880600
C	5.61875500	-1.04653700	-0.07937600
C	6.93007100	-1.47692900	-0.44231600
C	7.84247400	-1.88311800	0.55169300
C	7.32177100	-1.49984400	-1.79547100
C	9.11983400	-2.30377200	0.19275800
C	8.60195300	-1.92242200	-2.14214300
H	6.61869200	-1.18449400	-2.55963100
C	9.50178300	-2.32465700	-1.15146000
H	9.82018000	-2.61342800	0.96230900
H	8.89933700	-1.93692400	-3.18610300
H	10.49981200	-2.65210700	-1.42627200
H	3.90246300	-6.84304000	2.17125400
H	3.86339400	-3.23331800	-0.14418900
H	7.54015000	-1.86058000	1.59362300
Au	-1.27736900	-0.88506200	0.42630700
C	-2.90792300	0.01068700	-0.25203100
C	-4.90911700	0.32118500	-1.23716500
C	-4.52120100	1.51141400	-0.71018500
H	-4.99685500	2.47869200	-0.70667100
H	-5.79323200	0.03843700	-1.78528000
N	-3.90649800	-0.59345700	-0.94708900
N	-3.28726300	1.30493900	-0.10810300
C	-3.93044100	-1.99033700	-1.33740700

C	-3.35557500	-2.35016100	-2.57300800
C	-4.53861500	-2.91838500	-0.46866300
C	-3.39575900	-3.70573700	-2.92232100
C	-4.54698900	-4.25891800	-0.87318800
C	-3.98141200	-4.64998200	-2.08374800
H	-2.96399900	-4.02375600	-3.86599100
H	-5.00531800	-5.00506800	-0.23171800
H	-4.00156800	-5.69532100	-2.37727600
C	-2.51885600	2.34695300	0.54480500
C	-2.68360300	2.53789100	1.93094700
C	-1.66645300	3.13944000	-0.24958900
C	-1.94313100	3.56875900	2.52287800
C	-0.95409800	4.15601700	0.39817800
C	-1.08923100	4.36793000	1.76742500
H	-2.04301800	3.74990900	3.58860000
H	-0.28383300	4.78950700	-0.17338500
H	-0.52699700	5.16557300	2.24370800
C	-3.62410900	1.69243400	2.78483400
C	-4.75993200	2.54636500	3.38254800
C	-2.85998100	0.93484700	3.88789600
H	-4.08878600	0.93879900	2.14168200
H	-5.33037100	3.05874800	2.60142400
H	-5.45218200	1.91611200	3.95010900
H	-4.37108500	3.30976000	4.06409600
H	-2.07942400	0.29602000	3.46143700
H	-2.38292400	1.62327200	4.59305800
H	-3.54625500	0.30038900	4.45816400
C	-1.50803200	2.94021000	-1.75406300
C	-0.05465300	2.59819000	-2.13284900
C	-2.00842100	4.17180000	-2.53537300
H	-2.12852900	2.09114100	-2.05655200
H	0.31099500	1.71762200	-1.59674900
H	0.01625700	2.39869800	-3.20733600
H	0.61851800	3.42999600	-1.90418300
H	-3.05143100	4.40446000	-2.29744000
H	-1.40937500	5.05905300	-2.30660000
H	-1.93870200	3.99193400	-3.61310100
C	-5.17260600	-2.52412200	0.86233000
C	-4.43568000	-3.17250700	2.05065800
C	-6.67686800	-2.85915300	0.89200900
H	-5.08083700	-1.43988400	0.97873000
H	-3.37505700	-2.90030500	2.05608200
H	-4.87760700	-2.84370900	2.99692900
H	-4.50200100	-4.26477600	2.01529400

H	-7.21167000	-2.37833300	0.06693500
H	-6.84956600	-3.93730000	0.81596600
H	-7.12353300	-2.51756500	1.83121800
C	-2.72152600	-1.34053700	-3.52531600
C	-3.50697200	-1.25794400	-4.84990000
C	-1.23348200	-1.65015300	-3.78009400
H	-2.76896900	-0.35177400	-3.05896100
H	-4.55757200	-1.00161700	-4.67970100
H	-3.07220700	-0.49376600	-5.50207300
H	-3.48094600	-2.20950200	-5.39048800
H	-0.65591100	-1.65789100	-2.85066300
H	-1.10332900	-2.62230300	-4.26664100
H	-0.79959700	-0.89158300	-4.43963500
O	2.96722400	-0.37550100	1.98051300
O	1.78496200	-1.16279400	-1.27178300
C	2.99025600	4.44651700	0.56123700
C	3.24126000	3.34371700	-0.16067200
H	3.13000600	4.38860100	1.64128100
H	3.11154700	3.33061200	-1.24012500
C	2.53060200	5.75418700	0.07226400
C	2.38109200	6.05846000	-1.29508000
C	2.21151800	6.75205900	1.01111900
C	1.91648200	7.30687900	-1.70024300
H	2.64421400	5.32063700	-2.04696000
C	1.74769500	8.00312000	0.60542300
H	2.33634300	6.54129800	2.07056500
C	1.59550000	8.28439200	-0.75269200
H	1.81392600	7.52399400	-2.75950300
H	1.51102900	8.75848800	1.34889100
H	1.23889900	9.25856000	-1.07307600
C	3.74202700	2.07473500	0.44176800
H	3.83735500	2.15677900	1.53041000
H	4.72149000	1.79880800	0.03086100
O	2.80157700	1.01448000	0.10931800
H	2.18970600	0.16075500	2.20417800

Zero-point correction=	0.964440 (Hartree/Particle)
Thermal correction to Energy=	1.025639
Thermal correction to Enthalpy=	1.026583
Thermal correction to Gibbs Free Energy=	0.855030
Sum of electronic and zero-point Energies=	-2598.078305
Sum of electronic and thermal Energies=	-2598.017105
Sum of electronic and thermal Enthalpies=	-2598.016161
Sum of electronic and thermal Free Energies=	-2598.187715

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C	0.12424600	-2.44393000	0.24792000
O	-1.05383600	-2.72511800	0.46221600
C	1.01419300	-3.40988200	-0.45326900
C	0.60907000	-4.75727600	-0.43325300
C	2.16998000	-3.04626700	-1.16495700
C	1.35556700	-5.72611100	-1.09595800
H	-0.29174600	-5.02337700	0.10878800
C	2.90657600	-4.02065300	-1.83723700
C	2.50525200	-5.35863700	-1.80131700
H	1.04189000	-6.76492000	-1.06678600
H	3.79183000	-3.73479100	-2.39720600
C	0.60983700	-1.07834500	0.65716100
C	0.53635000	-0.73548200	2.12255000
C	1.38557300	0.32387600	2.65486900
C	2.03051500	1.18038400	3.22231400
C	2.81153400	2.17713000	3.88228500
C	4.21692300	2.09133700	3.87945000
C	2.18630500	3.24788100	4.54989300
C	4.97710500	3.05948100	4.53053100
C	2.95529600	4.21119900	5.19814400
H	1.10297400	3.31148700	4.55539400
C	4.34997200	4.12014700	5.19037600
H	6.06042300	2.98512400	4.52823800
H	2.46671400	5.03177100	5.71473800
H	4.94581200	4.87022900	5.70159700
H	3.08537300	-6.11316300	-2.32442900
H	2.48941100	-2.01204000	-1.18772000
H	4.69570100	1.26479400	3.36484500
Au	0.80502700	0.33575400	-0.78139600
C	0.87032700	1.77080000	-2.24604500
C	0.46973100	2.90550300	-4.15830500
C	1.24554500	3.69447400	-3.36957800
H	1.64617700	4.68305500	-3.52558400
H	0.05273600	3.07071800	-5.13847700
N	0.25095200	1.72944300	-3.45706500
N	1.48039100	2.98496400	-2.20090800
C	-0.54536200	0.62101600	-3.94659200
C	0.07619300	-0.33629600	-4.77516000
C	-1.90542800	0.56062500	-3.58511200
C	-0.71454900	-1.39918100	-5.22636100
C	-2.64076300	-0.53587800	-4.05431200
C	-2.05499500	-1.50465700	-4.86284600

H	-0.27578700	-2.15462800	-5.87009400
H	-3.68777400	-0.62569400	-3.78416700
H	-2.64711100	-2.34227800	-5.21955600
C	2.26105700	3.49837400	-1.09322000
C	1.60599300	4.26833200	-0.11166600
C	3.64577400	3.23932400	-1.06955800
C	2.39553800	4.79497200	0.91779100
C	4.38215500	3.79272000	-0.01540300
C	3.76715700	4.56434700	0.96640800
H	1.92745900	5.39159200	1.69409600
H	5.45241900	3.61762300	0.03475800
H	4.35634500	4.97997700	1.77789100
C	0.10493900	4.54218400	-0.13017300
C	-0.18998000	6.04568000	-0.29978700
C	-0.58650800	3.97682000	1.12595700
H	-0.32840500	4.02694400	-0.99244400
H	0.26522800	6.44483800	-1.21194100
H	-1.26964400	6.21749900	-0.35647000
H	0.19508800	6.62684900	0.54448200
H	-0.40864300	2.90260700	1.23251400
H	-0.22634000	4.47077600	2.03485300
H	-1.66773800	4.13860200	1.06728700
C	4.35299600	2.40020200	-2.12941600
C	5.03851100	1.16805800	-1.50578200
C	5.35508500	3.24371400	-2.94149400
H	3.59994700	2.02600600	-2.82905300
H	4.32387200	0.56276000	-0.93854700
H	5.48011500	0.54557400	-2.29177300
H	5.84533600	1.46282900	-0.82611400
H	4.86381900	4.09477200	-3.42367800
H	6.15379100	3.63887200	-2.30533700
H	5.82220300	2.63530200	-3.72282300
C	-2.59761300	1.62747000	-2.74077700
C	-3.02908200	1.07640300	-1.36827100
C	-3.79307400	2.24622000	-3.49334000
H	-1.88398900	2.43765500	-2.55931500
H	-2.16423600	0.76953200	-0.77221100
H	-3.56722900	1.84477200	-0.80324900
H	-3.68311400	0.20444400	-1.45917000
H	-3.49382300	2.64667900	-4.46731900
H	-4.58763000	1.51292100	-3.66403700
H	-4.22243700	3.06411900	-2.90613200
C	1.53156500	-0.22072500	-5.22094500
C	1.61707900	0.28803800	-6.67522300

C	2.30931100	-1.53955600	-5.06160200
H	2.02452700	0.51996800	-4.58322200
H	1.12173700	1.25666400	-6.79536600
H	2.66191400	0.40232100	-6.98229100
H	1.13843700	-0.41523200	-7.36462400
H	2.23512400	-1.92858900	-4.04212600
H	1.94316500	-2.31453700	-5.74247900
H	3.36743200	-1.37956800	-5.29374200
O	0.57853100	-1.87768700	2.93215400
C	3.45556100	-3.29093200	2.27036200
C	4.29476700	-4.31950500	2.67357600
C	5.61873400	-4.39571000	2.24343500
C	6.05680400	-3.38700300	1.38553000
C	5.21260500	-2.36418300	0.98163100
H	6.27443100	-5.19641000	2.56000400
H	2.42604800	-3.17700600	2.57894600
H	5.49753100	-1.55785600	0.32186800
Cl	7.69164300	-3.39179100	0.79123600
Cl	3.65523200	-5.53030100	3.74651600
N	3.92266100	-2.32074200	1.43051600
O	3.15597300	-1.34985300	1.05102200
C	-4.08448300	0.47052500	2.36914000
C	-2.87514100	0.35335400	2.94879800
H	-4.35948500	-0.28681900	1.63517800
H	-2.52154200	1.06743400	3.68931800
C	-5.10183000	1.49683400	2.62139700
C	-4.87631900	2.63213300	3.42384100
C	-6.36925300	1.33967900	2.03043000
C	-5.88382000	3.56935500	3.62833100
H	-3.90555400	2.78547100	3.88582500
C	-7.37947800	2.27747100	2.23787200
H	-6.55989300	0.46554800	1.41333400
C	-7.14013000	3.39592700	3.03739700
H	-5.69269900	4.43948300	4.24988800
H	-8.35222500	2.13249600	1.77742500
H	-7.92453200	4.12893100	3.20115600
C	-1.96699700	-0.78061800	2.62336600
H	-2.44309100	-1.50293700	1.96435200
H	-1.59325600	-1.29273600	3.51265300
O	-0.80499300	-0.21204300	1.90462200
H	0.77502200	-1.59320800	3.83684000
C	-7.17576100	-2.79542900	0.67878400
C	-6.16977300	-2.61021200	-0.18936300
H	-6.95603700	-3.33479100	1.60104400

H	-6.32282400	-2.06096600	-1.11677200
C	-8.57164700	-2.35039800	0.54667500
C	-9.44692400	-2.53889000	1.63072300
C	-9.08021300	-1.74044100	-0.61591800
C	-10.77731900	-2.12741100	1.56479200
H	-9.07413900	-3.01277700	2.53543400
C	-10.40784400	-1.32838300	-0.68252200
H	-8.43590100	-1.59686000	-1.47806300
C	-11.26336300	-1.51866100	0.40734100
H	-11.43355500	-2.28419900	2.41589200
H	-10.78120600	-0.86270400	-1.59019600
H	-12.29984000	-1.19981100	0.35012900
C	-4.78068700	-3.12792900	0.02144200
H	-4.53688300	-3.86443200	-0.76232400
H	-4.71496100	-3.64692600	0.98965400
O	-3.86908200	-2.02724300	-0.04460500
H	-2.96186400	-2.36939200	-0.04070000

Zero-point correction= 1.201807 (Hartree/Particle)
Thermal correction to Energy= 1.281697
Thermal correction to Enthalpy= 1.282641
Thermal correction to Gibbs Free Energy= 1.064396
Sum of electronic and zero-point Energies= -4189.379375
Sum of electronic and thermal Energies= -4189.299484
Sum of electronic and thermal Enthalpies= -4189.298540
Sum of electronic and thermal Free Energies= -4189.516785

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C	-2.81271200	4.04614000	-0.18947000
O	-3.67697200	4.37060100	-0.99554500
C	-2.05032100	5.08578100	0.57042300
C	-1.56738200	4.86292600	1.87358600
C	-1.90964700	6.35902000	-0.00967800
C	-0.93996600	5.89432700	2.57382800
H	-1.71406800	3.89613500	2.34677800
C	-1.27095600	7.37928400	0.68755000
C	-0.78606900	7.14857400	1.97977800
H	-0.58561700	5.72244300	3.58544600
H	-1.15740200	8.35787500	0.23146800
C	-2.53693400	2.58614400	0.02194700
C	-1.27798200	2.05685100	0.16929400
C	-1.11953900	0.63526500	0.12392700
C	-1.46228500	-0.56209600	0.13156000
C	-2.06773700	-1.85289800	0.08071300

C	-1.48827900	-2.98396900	0.68853700
C	-3.31491100	-1.96212100	-0.57347100
C	-2.15013900	-4.20655800	0.63528100
C	-3.96997900	-3.18936900	-0.60166700
H	-3.75843100	-1.08251900	-1.02627000
C	-3.38882100	-4.31175600	-0.00398100
H	-1.69919000	-5.07758900	1.09958200
H	-4.93674700	-3.26719600	-1.08820800
H	-3.90250100	-5.26776100	-0.03500800
H	-0.29738000	7.94980500	2.52602100
H	-2.31476600	6.52490600	-1.00235200
H	-0.53212500	-2.89786500	1.19377300
Au	0.89364000	-0.30472500	-0.02322000
C	2.86643800	-0.74697100	-0.15222400
C	5.07796100	-0.58923900	-0.55314500
C	4.84793000	-1.81225300	-0.00919300
H	5.51592500	-2.62535600	0.22493100
H	5.98780100	-0.11841500	-0.88858900
N	3.85030200	0.05361700	-0.63463000
N	3.48301100	-1.89375100	0.23309200
C	3.67149000	1.39565700	-1.15658500
C	3.39864300	1.55017900	-2.53038700
C	3.81535000	2.48273600	-0.27112300
C	3.26871700	2.85915900	-3.01083100
C	3.68109500	3.76706500	-0.81222200
C	3.41106100	3.95526300	-2.16488200
H	3.05871000	3.02026400	-4.06347000
H	3.79312800	4.63066200	-0.16423700
H	3.31473600	4.96108600	-2.56292500
C	2.82772000	-3.04986300	0.81210100
C	2.67160000	-3.10137200	2.21247000
C	2.40480000	-4.08209600	-0.04951900
C	2.05439000	-4.24089100	2.74423500
C	1.79921000	-5.19836000	0.54174100
C	1.62556700	-5.27927400	1.92104100
H	1.91925700	-4.31943700	3.81837000
H	1.46503100	-6.01695800	-0.08773200
H	1.16250400	-6.15925700	2.35799000
C	3.15139100	-1.99537800	3.14780800
C	4.24536200	-2.50621000	4.10649600
C	1.97997200	-1.36433700	3.92530300
H	3.59891500	-1.20258100	2.54114300
H	5.09559400	-2.92414400	3.55845400
H	4.61438200	-1.68669500	4.73122300

H	3.86452400	-3.28587500	4.77387800
H	1.22083400	-0.96434700	3.24499600
H	1.49310400	-2.09244400	4.58223000
H	2.34061100	-0.54302500	4.55298600
C	2.57911300	-4.02705700	-1.56447300
C	1.21760100	-4.01794000	-2.28664900
C	3.47109400	-5.17645700	-2.07370400
H	3.08476700	-3.09007200	-1.81689700
H	0.59342900	-3.18294500	-1.95326800
H	1.36304700	-3.92581700	-3.36777100
H	0.66125300	-4.94313900	-2.10518400
H	4.45174200	-5.17053900	-1.58756800
H	3.01432000	-6.15386000	-1.88827500
H	3.62715500	-5.08446200	-3.15315400
C	4.12337800	2.31307300	1.21373300
C	3.07920300	3.01792800	2.10112200
C	5.54951200	2.79750300	1.54429800
H	4.07649400	1.24626300	1.45354800
H	2.06450300	2.68677700	1.86181000
H	3.27676100	2.80182000	3.15625400
H	3.11645200	4.10551500	1.97921800
H	6.30362900	2.26441400	0.95653800
H	5.66298000	3.86637200	1.33608000
H	5.77159300	2.63825700	2.60440200
C	3.24680400	0.37434100	-3.49070200
C	4.33452700	0.39455900	-4.58295500
C	1.83618300	0.33369500	-4.11053800
H	3.37555400	-0.55263700	-2.92363800
H	5.33959500	0.38691500	-4.14933100
H	4.23836200	-0.48207100	-5.23154700
H	4.25250300	1.28458000	-5.21495400
H	1.06313900	0.28788700	-3.33654000
H	1.64163900	1.21825500	-4.72534900
H	1.72907900	-0.54616100	-4.75317700
O	-0.10192200	2.74242000	0.25496100
C	-6.71661200	0.46478100	-0.40402100
C	-5.66422700	0.77574100	0.37018500
H	-6.99286200	1.17240100	-1.18632900
H	-5.32637700	0.10571400	1.15804900
C	-7.56192200	-0.73497800	-0.33519100
C	-8.54532800	-0.92372200	-1.32243200
C	-7.43659700	-1.71054400	0.67278900
C	-9.36940900	-2.04810400	-1.31343100
H	-8.66094900	-0.17727200	-2.10419600

C	-8.25931900	-2.83321500	0.68223900
H	-6.70216100	-1.58471200	1.46254700
C	-9.22859200	-3.00829700	-0.31091900
H	-10.12262300	-2.17158500	-2.08582100
H	-8.15301100	-3.57105800	1.47235500
H	-9.87230100	-3.88266900	-0.29677800
C	-4.89788400	2.04654600	0.21295200
H	-4.84031400	2.59581400	1.16233100
H	-5.33901800	2.70034100	-0.54160300
O	-3.54074100	1.69748700	-0.19829700
H	-0.27428500	3.69280300	0.35464400

Zero-point correction= 0.960376 (Hartree/Particle)
Thermal correction to Energy= 1.020334
Thermal correction to Enthalpy= 1.021278
Thermal correction to Gibbs Free Energy= 0.854108
Sum of electronic and zero-point Energies= -2522.861644
Sum of electronic and thermal Energies= -2522.801686
Sum of electronic and thermal Enthalpies= -2522.800742
Sum of electronic and thermal Free Energies= -2522.967912

8-TS1

C	0.49470200	-1.54541000	-2.15241900
O	-0.55110800	-1.63378000	-2.79287600
C	1.41021900	-2.71057600	-2.01582600
C	1.11077800	-3.83250600	-2.81148300
C	2.50760100	-2.75595900	-1.13967500
C	1.90192000	-4.97318800	-2.74125200
H	0.25956500	-3.78384300	-3.48127700
C	3.29217900	-3.90552200	-1.06929200
C	2.99469200	-5.01110900	-1.86892200
H	1.67143000	-5.83098000	-3.36543000
H	4.13757800	-3.93377500	-0.39006800
C	0.77899800	-0.23870500	-1.45061800
C	1.68720200	0.71603600	-2.25839200
C	1.76931900	2.11370200	-1.77683400
C	2.07259600	3.26008300	-1.50701700
C	2.40451700	4.61994500	-1.21467000
C	2.91860200	4.98052800	0.04607100
C	2.24009200	5.61434500	-2.19951600
C	3.25223400	6.30569700	0.31325800
C	2.57614000	6.93705500	-1.92241900
H	1.85886100	5.33823200	-3.17750400
C	3.08082800	7.28624700	-0.66744500

H	3.65165500	6.57486500	1.28643600
H	2.44873300	7.69570100	-2.68849500
H	3.34463000	8.31796700	-0.45598100
H	3.61372000	-5.90199900	-1.81445800
H	2.75782200	-1.90097700	-0.52507700
H	3.05573300	4.21353800	0.80089500
Au	0.34218400	-0.13807900	0.50608900
C	0.04892900	-0.18415000	2.55304400
C	-0.75711300	0.09131100	4.64636300
C	0.39152000	-0.62467600	4.74436300
H	0.90672400	-1.03297200	5.59865000
H	-1.44656600	0.43978200	5.39801300
N	-0.95367300	0.35279600	3.29667700
N	0.87186200	-0.78873900	3.45248200
C	-2.09821500	1.08538300	2.79135100
C	-2.02455700	2.49115000	2.74868200
C	-3.25455100	0.35962800	2.43312900
C	-3.16688800	3.17821700	2.31816200
C	-4.36379100	1.10215700	2.01066900
C	-4.32340400	2.49353100	1.95709600
H	-3.15065700	4.26304200	2.27918700
H	-5.27336300	0.58398000	1.72778300
H	-5.20339400	3.04481800	1.63898100
C	2.06322700	-1.55387400	3.14103400
C	1.94133200	-2.95297800	3.01826600
C	3.29499900	-0.87736400	3.03318500
C	3.11531600	-3.67823000	2.77953800
C	4.43317900	-1.65610600	2.78918100
C	4.34780200	-3.04043000	2.66831000
H	3.06164800	-4.75802300	2.68392800
H	5.40051900	-1.17139400	2.70483200
H	5.24680100	-3.62431500	2.49329000
C	0.61045200	-3.68997600	3.14299800
C	0.60399500	-4.63437400	4.36158400
C	0.26015300	-4.44985300	1.84907900
H	-0.17899100	-2.94976500	3.30264400
H	0.81546200	-4.09532700	5.29064600
H	-0.37397100	-5.11531100	4.46409400
H	1.35352800	-5.42566500	4.25929900
H	0.22575000	-3.77528300	0.98856500
H	0.99269400	-5.23301900	1.62963200
H	-0.71869900	-4.93029900	1.94780400
C	3.43474600	0.63215200	3.20308100
C	4.10343900	1.28720200	1.97952200

C	4.19570700	0.97314300	4.50052400
H	2.43221400	1.06172200	3.28959800
H	3.55185500	1.07778100	1.05772500
H	4.14835400	2.37321500	2.11444900
H	5.13160800	0.93567600	1.84449900
H	3.70136500	0.54771500	5.37961100
H	5.21935100	0.58533100	4.47556900
H	4.25313500	2.05811300	4.63625300
C	-3.34653200	-1.15923500	2.55671200
C	-4.06842500	-1.82247900	1.37034500
C	-4.02368400	-1.54826300	3.88914000
H	-2.32686700	-1.55777600	2.57474400
H	-3.63744600	-1.54191000	0.40539000
H	-4.00230800	-2.91117100	1.46836300
H	-5.13419600	-1.57277000	1.34876200
H	-3.49051600	-1.14309000	4.75509800
H	-5.05215900	-1.17406800	3.92625000
H	-4.05913900	-2.63746300	3.99462100
C	-0.78093500	3.27390000	3.15925500
C	-1.07309900	4.22017300	4.34056400
C	-0.18099600	4.04225200	1.96668100
H	-0.02200400	2.56148900	3.49619200
H	-1.47078400	3.67582400	5.20289900
H	-0.15619000	4.72924000	4.65467100
H	-1.80229800	4.99023400	4.06932900
H	0.09499300	3.36286700	1.15397800
H	-0.88423700	4.78006600	1.56638600
H	0.71909400	4.58306500	2.27541400
O	1.37022800	0.66825700	-3.61961600
C	-3.19563200	1.62718900	-2.02359200
C	-4.12716000	2.62416300	-1.77067700
C	-3.75127000	3.96056100	-1.64162200
C	-2.39483100	4.25336600	-1.77354000
C	-1.46761800	3.25601400	-2.03633600
H	-4.48047700	4.73822700	-1.45227800
H	-3.42343200	0.56581500	-2.12934200
H	-0.40546500	3.41652100	-2.15028000
Cl	-1.83424100	5.89232300	-1.61913700
Cl	-5.80113000	2.17622900	-1.62411700
N	-1.88407100	1.96645200	-2.16558800
O	-1.02778100	1.02648900	-2.49335800
C	5.98129800	-1.12784800	-2.96487600
C	5.26309100	-0.13544900	-2.41323800
H	5.57140500	-1.61550100	-3.84970800

H	5.60259300	0.37376500	-1.51392100
C	7.27700600	-1.65354900	-2.51767600
C	8.04463800	-1.04912900	-1.50364000
C	7.78239200	-2.81438100	-3.13015100
C	9.26257500	-1.59592400	-1.11184500
H	7.69452700	-0.13647300	-1.03094400
C	9.00166900	-3.36353100	-2.73696800
H	7.20754000	-3.28824400	-3.92190700
C	9.74598100	-2.75676100	-1.72449300
H	9.84444700	-1.11173500	-0.33284600
H	9.37248200	-4.26041400	-3.22420800
H	10.69955100	-3.17749600	-1.41993300
C	3.98047600	0.34861600	-2.99416900
H	3.74316500	-0.14716100	-3.93827900
H	3.99766400	1.43290700	-3.15776000
O	2.91611800	0.06718900	-2.02387000
H	0.43583200	0.94835700	-3.68237300
C	-6.13623000	-3.29880800	-1.95178500
C	-5.38095500	-2.33689800	-2.50257500
H	-5.63361000	-4.20512100	-1.61127900
H	-5.82540500	-1.40017100	-2.83560400
C	-7.59067100	-3.28419700	-1.73512000
C	-8.17002100	-4.30074200	-0.95554600
C	-8.43944100	-2.29840900	-2.27288100
C	-9.54142900	-4.32695600	-0.70617700
H	-7.53219500	-5.07686800	-0.53949500
C	-9.80874000	-2.32342000	-2.02474600
H	-8.02786100	-1.51564200	-2.90294400
C	-10.36700800	-3.33605900	-1.23839400
H	-9.96494600	-5.12263400	-0.10015700
H	-10.44680300	-1.55586900	-2.45353500
H	-11.43645900	-3.35532700	-1.05110900
C	-3.90474400	-2.45976000	-2.71673600
H	-3.67953800	-2.42281100	-3.79473200
H	-3.54823200	-3.42903100	-2.33997500
O	-3.23597800	-1.38095200	-2.05055000
H	-2.30934200	-1.35823500	-2.35385100

Zero-point correction=	1.202298 (Hartree/Particle)
Thermal correction to Energy=	1.281671
Thermal correction to Enthalpy=	1.282615
Thermal correction to Gibbs Free Energy=	1.067369
Sum of electronic and zero-point Energies=	-4189.383221
Sum of electronic and thermal Energies=	-4189.303848
Sum of electronic and thermal Enthalpies=	-4189.302904

Sum of electronic and thermal Free Energies= -4189.518150

8-TS2

C	1.67616300	0.14374300	1.59839800
O	1.78781000	-0.95692600	2.13142500
C	2.01946900	1.41847200	2.24959300
C	2.84871200	1.37046900	3.38366400
C	1.51308500	2.64981400	1.80351800
C	3.18276800	2.54441200	4.05043700
H	3.22267500	0.40859000	3.71826700
C	1.83819100	3.82055600	2.48591500
C	2.67724400	3.76942500	3.60256600
H	3.83239400	2.50853100	4.91923800
H	1.43556700	4.77132000	2.15038300
C	1.05645800	-0.05768700	0.25089200
C	1.97237200	-0.49836200	-0.83343400
C	1.82804600	0.92638100	-1.23989300
C	1.85496500	2.10214400	-1.59109100
C	1.87664300	3.45466500	-1.99254800
C	0.97890200	3.91726700	-2.98253000
C	2.80956500	4.34875700	-1.41712200
C	1.02048100	5.24633600	-3.38469800
C	2.83565200	5.67625300	-1.82646300
H	3.49408800	3.98669900	-0.65760900
C	1.94538500	6.12458500	-2.80864800
H	0.33681800	5.60174900	-4.14887200
H	3.55143100	6.36340000	-1.38695500
H	1.97426900	7.16181600	-3.12837100
H	2.93394400	4.68451400	4.12809100
H	0.84932100	2.68576500	0.94718800
H	0.27112500	3.22393700	-3.42404600
Au	-0.96325700	-0.30290300	0.10392200
C	-2.96091400	-0.74346400	0.01017800
C	-4.86101300	-1.94031800	-0.23879000
C	-5.21684900	-0.67269800	0.09677600
H	-6.18410200	-0.21926600	0.24194500
H	-5.45577200	-2.81595400	-0.44306800
N	-3.47460300	-1.96629500	-0.28866200
N	-4.03924100	0.04829200	0.24607500
C	-2.68685000	-3.13989000	-0.61234600
C	-2.37216900	-3.38434500	-1.96488900
C	-2.28311400	-3.98896700	0.43768400
C	-1.62461800	-4.53433000	-2.24923900

C	-1.53618400	-5.12226600	0.09108400
C	-1.21121500	-5.39459700	-1.23490400
H	-1.36841900	-4.76095700	-3.27943100
H	-1.20750100	-5.80090000	0.87182900
H	-0.63643700	-6.28299700	-1.47962700
C	-3.98463500	1.45273400	0.59718800
C	-3.93297300	1.80344800	1.96078900
C	-4.00996700	2.40455000	-0.44158300
C	-3.89354500	3.16945800	2.26764000
C	-3.96770700	3.75488900	-0.07326100
C	-3.90933900	4.13493300	1.26493700
H	-3.85388700	3.47944300	3.30721400
H	-3.98727400	4.51773700	-0.84553800
H	-3.88316300	5.18834300	1.52789500
C	-3.92383800	0.77333000	3.08610600
C	-5.16542200	0.91424100	3.98905800
C	-2.62441900	0.85115400	3.91102600
H	-3.96195500	-0.22399400	2.63795800
H	-6.09266600	0.82741300	3.41385800
H	-5.16723700	0.13239300	4.75516800
H	-5.18232200	1.88090600	4.50266600
H	-1.74242300	0.71236800	3.27775900
H	-2.52706800	1.81750500	4.41643000
H	-2.61675500	0.07254800	4.68058000
C	-4.08387100	2.02254000	-1.91714400
C	-2.80885800	2.44899200	-2.67099200
C	-5.34656500	2.59609500	-2.58927000
H	-4.14818200	0.93264500	-1.98700700
H	-1.91785000	1.99534300	-2.22417500
H	-2.86490900	2.13546500	-3.71892500
H	-2.68097900	3.53665500	-2.65346400
H	-6.25596300	2.27238000	-2.07359500
H	-5.33984600	3.69075800	-2.59423200
H	-5.40903800	2.26068700	-3.62946800
C	-2.62314800	-3.72682100	1.90162000
C	-1.35186200	-3.55906000	2.75700300
C	-3.53566100	-4.83146900	2.47068800
H	-3.17827700	-2.78580400	1.96104500
H	-0.70917400	-2.75987600	2.37454600
H	-1.62230300	-3.31415900	3.78933700
H	-0.75985200	-4.47975700	2.78287500
H	-4.45806700	-4.93043600	1.88949900
H	-3.03536500	-5.80519300	2.46841200
H	-3.80947700	-4.60202300	3.50544500

C	-2.82097400	-2.47033000	-3.10149700
C	-3.88720000	-3.15883800	-3.97705300
C	-1.63176300	-1.98626500	-3.95352600
H	-3.28277600	-1.58157100	-2.66103500
H	-4.75959400	-3.45977600	-3.38815900
H	-4.22884600	-2.48223900	-4.76714500
H	-3.48595200	-4.05714800	-4.45744600
H	-0.86523700	-1.50381700	-3.33948600
H	-1.15879300	-2.81354400	-4.49266500
H	-1.97604200	-1.26576700	-4.70283400
O	1.45107200	-1.33875200	-1.82078100
C	6.67365100	-0.83186300	-0.82091900
C	5.49783500	-1.47864000	-0.82858200
H	6.70336500	0.16858000	-1.25481700
H	5.39726400	-2.47578200	-0.40654100
C	7.96169700	-1.30869400	-0.30026400
C	9.07762400	-0.45736100	-0.38083100
C	8.13592700	-2.57916900	0.28048800
C	10.32371700	-0.85445700	0.10157500
H	8.96213600	0.52675800	-0.82854500
C	9.37893400	-2.97590200	0.76316800
H	7.29586700	-3.26296300	0.35437100
C	10.47873100	-2.11613400	0.67638800
H	11.17180800	-0.18021500	0.02750600
H	9.49381300	-3.96029900	1.20741600
H	11.44764500	-2.43052100	1.05241100
C	4.26147600	-0.90610200	-1.43593800
H	3.87772900	-1.53523300	-2.24747700
H	4.44083300	0.10178400	-1.83136500
O	3.23985300	-0.83836400	-0.39966300
H	1.17158500	-2.15783300	-1.38254400

Zero-point correction=	0.958586 (Hartree/Particle)
Thermal correction to Energy=	1.018151
Thermal correction to Enthalpy=	1.019095
Thermal correction to Gibbs Free Energy=	0.852285
Sum of electronic and zero-point Energies=	-2522.811353
Sum of electronic and thermal Energies=	-2522.751788
Sum of electronic and thermal Enthalpies=	-2522.750844
Sum of electronic and thermal Free Energies=	-2522.917654

8-TS3

C	1.67434200	-1.89446300	-0.77405700
O	1.71354800	-2.21966700	-1.96635400
C	2.07975600	-2.73854800	0.35144400
C	2.51526600	-4.04902200	0.09291300
C	2.06597600	-2.24308500	1.66599700
C	2.92691400	-4.85733000	1.14652300
H	2.52571900	-4.40698200	-0.93128900
C	2.48341000	-3.05587700	2.71599700
C	2.91111300	-4.36139300	2.45526100
H	3.26443900	-5.87062700	0.95365100
H	2.48113700	-2.67597400	3.73249200
C	1.09297900	-0.53043600	-0.58550700
C	2.03108800	0.57975900	-1.01180700
C	1.73198700	1.89954400	-0.46087500
C	1.59056300	3.00039800	0.02882200
C	1.42782700	4.30619900	0.58368300
C	1.18519000	5.40770200	-0.25959100
C	1.52277400	4.50721600	1.97437900
C	1.03800500	6.68168400	0.28334300
C	1.36909100	5.78494200	2.50707400
H	1.72100000	3.66049100	2.62356100
C	1.12638700	6.87337500	1.66485800
H	0.85992400	7.52833000	-0.37276400
H	1.44683000	5.93346200	3.57978300
H	1.01384800	7.86895200	2.08317600
H	3.23715300	-4.99438100	3.27517000
H	1.73863700	-1.22555100	1.86520400
H	1.11947600	5.25292200	-1.33141500
Au	-0.86327400	-0.35121700	-0.25146000
C	-2.89935500	-0.25920300	-0.00700100
C	-5.03362700	0.46549300	0.08994700
C	-5.05229000	-0.88587200	0.24766700
H	-5.86938500	-1.57345500	0.39539000
H	-5.83066000	1.19134500	0.07489800
N	-3.70747100	0.83249700	-0.06468300
N	-3.73703900	-1.31419200	0.18550500
C	-3.26749800	2.19989900	-0.26701100
C	-2.99380400	2.98865000	0.86813900
C	-3.17111100	2.68476900	-1.58630700
C	-2.59618700	4.31182400	0.64361600
C	-2.77787800	4.01927600	-1.74617500
C	-2.49228800	4.82337700	-0.64689000
H	-2.36341400	4.94978600	1.48987100
H	-2.69531900	4.43171700	-2.74678900

H	-2.18529200	5.85407000	-0.79450200
C	-3.33425200	-2.70310200	0.30104000
C	-3.24298400	-3.47562500	-0.87453400
C	-3.09298500	-3.22552300	1.58750000
C	-2.89483400	-4.82392900	-0.72519100
C	-2.75178800	-4.58083500	1.67239400
C	-2.65468400	-5.37255600	0.53139200
H	-2.81674500	-5.45286100	-1.60630700
H	-2.56282900	-5.02154200	2.64607900
H	-2.39258900	-6.42248000	0.62199900
C	-3.52476000	-2.91548800	-2.26581400
C	-4.81840200	-3.51605600	-2.85244200
C	-2.33475400	-3.12363300	-3.22247300
H	-3.67793500	-1.83572100	-2.17612300
H	-5.67907700	-3.33319900	-2.20112000
H	-5.03404700	-3.07517900	-3.83096800
H	-4.72856200	-4.59882200	-2.98694500
H	-1.41290100	-2.69182900	-2.82025900
H	-2.15020300	-4.18543200	-3.41417300
H	-2.54111000	-2.64849900	-4.18687500
C	-3.20281300	-2.38965700	2.85917800
C	-1.89630500	-2.41711500	3.67555900
C	-4.40182400	-2.83654000	3.71956600
H	-3.37764700	-1.34874800	2.57044100
H	-1.04021500	-2.10550700	3.06875700
H	-1.97381300	-1.74211100	4.53405800
H	-1.68287700	-3.41825200	4.06353100
H	-5.34201600	-2.77605400	3.16226200
H	-4.28423300	-3.87060200	4.05943100
H	-4.49283500	-2.20193400	4.60698400
C	-3.48015200	1.83443800	-2.81475900
C	-2.25554000	1.71495700	-3.74313400
C	-4.70518800	2.37633100	-3.57824400
H	-3.73018300	0.82329800	-2.47902300
H	-1.38464200	1.31769000	-3.21244000
H	-2.48073300	1.04719000	-4.58114400
H	-1.97460700	2.68610000	-4.16337300
H	-5.58946800	2.42946400	-2.93511200
H	-4.51953200	3.38132100	-3.97070300
H	-4.94197600	1.72730600	-4.42742100
C	-3.10548300	2.46111900	2.29586100
C	-4.08732200	3.29704200	3.13970600
C	-1.72115900	2.38192300	2.96902900
H	-3.50350900	1.44248600	2.25605300

H	-5.07711900	3.34384100	2.67500900
H	-4.20041800	2.85639300	4.13541200
H	-3.73338600	4.32422500	3.27265100
H	-1.04292700	1.73717300	2.40050400
H	-1.25651900	3.37034000	3.04227100
H	-1.81245700	1.97660800	3.98237300
O	1.66830700	0.55546500	-2.40213100
C	6.72328300	0.63924000	-0.37706100
C	5.68834600	0.31610100	-1.16839300
H	6.59033300	1.47488400	0.31126800
H	5.74901000	-0.51384600	-1.86872200
C	8.04538900	0.00269400	-0.31706400
C	8.96490800	0.45007600	0.64785600
C	8.44032200	-1.03714000	-1.17990200
C	10.23128900	-0.12222100	0.75628600
H	8.67887100	1.25577100	1.31949700
C	9.70399600	-1.60903100	-1.07218800
H	7.75913700	-1.39649900	-1.94520800
C	10.60518400	-1.15535900	-0.10345800
H	10.92516200	0.23975700	1.50913600
H	9.99177400	-2.40856800	-1.74859200
H	11.59167600	-1.60221600	-0.02478300
C	4.40480800	1.07572900	-1.16746800
H	4.16728300	1.46734300	-2.16418300
H	4.43110000	1.91029300	-0.45952600
O	3.33708800	0.15666800	-0.77902000
H	1.90182900	-0.33574000	-2.73760800

Zero-point correction= 0.959148 (Hartree/Particle)
Thermal correction to Energy= 1.018400
Thermal correction to Enthalpy= 1.019344
Thermal correction to Gibbs Free Energy= 0.853073
Sum of electronic and zero-point Energies= -2522.804787
Sum of electronic and thermal Energies= -2522.745536
Sum of electronic and thermal Enthalpies= -2522.744591
Sum of electronic and thermal Free Energies= -2522.910862

8-TS4

C	-0.32855700	-3.16459800	-0.09695600
O	-0.23788000	-3.58427500	1.05462800
C	-1.00643500	-3.85787100	-1.20477900
C	-0.93019900	-3.36991400	-2.51938300
C	-1.72540800	-5.03206200	-0.92691000

C	-1.57359300	-4.05139200	-3.54925100
H	-0.35730900	-2.47268100	-2.73955400
C	-2.36499400	-5.70896500	-1.95965200
C	-2.28988600	-5.21863300	-3.26847800
H	-1.51132000	-3.68215200	-4.56788700
H	-2.91993200	-6.61829700	-1.75136100
C	0.29597300	-1.81940000	-0.29662000
C	1.77860900	-1.85095800	-0.63695800
C	2.18937700	-0.77870600	-1.53885700
C	2.57570800	0.04684600	-2.34100600
C	3.06044700	0.99028100	-3.29548900
C	3.30361300	0.58327500	-4.62227900
C	3.31880300	2.32326500	-2.92026400
C	3.78866800	1.49765200	-5.55306500
C	3.81021300	3.22679300	-3.85881200
H	3.13325300	2.63523400	-1.89780300
C	4.04374300	2.81838800	-5.17489900
H	3.97327700	1.17836000	-6.57401100
H	4.01633600	4.25132200	-3.56391500
H	4.42737200	3.52664800	-5.90282300
H	-2.78805800	-5.75131800	-4.07311700
H	-1.76501200	-5.39230800	0.09591700
H	3.11229600	-0.44594700	-4.90770400
Au	-0.84988600	-0.23931700	0.15186600
C	-2.14859100	1.26291600	0.68748200
C	-3.07410800	3.23344100	1.29032500
C	-4.05926200	2.29623300	1.30719000
H	-5.10825300	2.37112500	1.54448600
H	-3.09119800	4.28857400	1.51122000
N	-1.91049300	2.58327500	0.90968000
N	-3.47611300	1.09573200	0.93610300
C	-0.62372100	3.23530600	0.77788600
C	0.20236500	3.32232500	1.91678600
C	-0.27158700	3.77571000	-0.47431100
C	1.44050100	3.95750700	1.75940600
C	0.97631000	4.40555400	-0.56829900
C	1.82555400	4.49159300	0.53213400
H	2.10586900	4.04586700	2.61259600
H	1.28065600	4.83977300	-1.51538500
H	2.78595600	4.99009200	0.43791300
C	-4.20330100	-0.15530000	0.82573200
C	-4.84444400	-0.44974600	-0.39437000
C	-4.26423200	-1.00014900	1.95225800
C	-5.57257900	-1.64397700	-0.46091800

C	-5.00778200	-2.17997200	1.82394900
C	-5.65650000	-2.49891000	0.63438400
H	-6.08218500	-1.90511000	-1.38300100
H	-5.08193100	-2.85476000	2.67058000
H	-6.23183100	-3.41702000	0.56132600
C	-4.77493800	0.46263300	-1.61545000
C	-6.16595800	1.01168900	-1.98925900
C	-4.11772000	-0.24927400	-2.81395900
H	-4.14368500	1.32143500	-1.36796500
H	-6.62146800	1.55367200	-1.15439700
H	-6.08874300	1.69906200	-2.83779400
H	-6.85125000	0.20726200	-2.27521300
H	-3.12173200	-0.62379500	-2.55664100
H	-4.71664000	-1.10018400	-3.15399600
H	-4.01706700	0.44238600	-3.65683300
C	-3.58577400	-0.67347500	3.27922800
C	-2.65347300	-1.80865800	3.74491500
C	-4.62790200	-0.33041700	4.36338000
H	-2.96243200	0.21430600	3.13517300
H	-1.90801000	-2.05963300	2.98391600
H	-2.12532000	-1.50941400	4.65606500
H	-3.21213500	-2.72072100	3.97794600
H	-5.26289200	0.50889100	4.06161100
H	-5.28242000	-1.18338200	4.57028900
H	-4.12919600	-0.05847600	5.29930100
C	-1.18702100	3.71460800	-1.69371700
C	-0.55639000	2.89545600	-2.83611700
C	-1.58019800	5.12626100	-2.17268200
H	-2.10994900	3.20413400	-1.40280300
H	-0.30976100	1.88030600	-2.50922800
H	-1.25227400	2.82419100	-3.67853100
H	0.36421500	3.35856100	-3.20471500
H	-2.05546900	5.70452300	-1.37409000
H	-0.70856800	5.69099600	-2.51855900
H	-2.28392100	5.06018200	-3.00851300
C	-0.20785300	2.78618100	3.28610400
C	-0.30805500	3.92262000	4.32332400
C	0.74013200	1.67376600	3.77298700
H	-1.20373200	2.34226000	3.19620700
H	-1.00308600	4.70296500	3.99790200
H	-0.66242400	3.53083900	5.28196500
H	0.66375900	4.39542900	4.49722300
H	0.75714900	0.83352500	3.07162900
H	1.76501900	2.04145400	3.88938900

H	0.41189700	1.29504600	4.74626100
O	2.22748000	-3.05864300	-1.17924100
O	2.20305100	-1.77547200	0.72595300
H	2.32125900	-3.68252200	-0.44146900
C	2.96188300	-0.61463900	1.21372900
H	2.59381400	0.27908900	0.70095200
H	2.70351000	-0.55572900	2.27223200
C	5.25573300	-1.11970600	2.02829500
C	4.42280100	-0.83266400	1.01109900
H	4.82439200	-1.19120300	3.02763100
H	4.78265200	-0.75648700	-0.01167800
C	6.70316900	-1.34189500	1.97178000
C	7.38958100	-1.60791500	3.17069400
C	7.44291900	-1.30433500	0.77354100
C	8.76509000	-1.83028300	3.17760200
H	6.83322000	-1.64137700	4.10407900
C	8.81565900	-1.52643600	0.78044900
H	6.94284600	-1.10268200	-0.16870100
C	9.48293300	-1.78992800	1.98166000
H	9.27509300	-2.03497000	4.11401900
H	9.37061200	-1.49525600	-0.15246800
H	10.55487800	-1.96269500	1.98222200

Zero-point correction= 0.958158 (Hartree/Particle)
Thermal correction to Energy= 1.017871
Thermal correction to Enthalpy= 1.018815
Thermal correction to Gibbs Free Energy= 0.849792
Sum of electronic and zero-point Energies= -2522.796862
Sum of electronic and thermal Energies= -2522.737149
Sum of electronic and thermal Enthalpies= -2522.736205
Sum of electronic and thermal Free Energies= -2522.905228

8-INT1

C	2.97017500	-2.89634100	-0.05909400
O	3.86816900	-2.69795900	-0.86549200
C	2.82642900	-4.20241600	0.65001900
C	3.50411800	-5.31354900	0.11846900
C	2.10593900	-4.34131800	1.84962200
C	3.44431600	-6.54520100	0.76169500
H	4.07463000	-5.18318600	-0.79507500
C	2.06153200	-5.57476400	2.49887000
C	2.72273400	-6.67738700	1.95310000
H	3.96475400	-7.40131900	0.34354100
H	1.52040700	-5.67345600	3.43506200

C	1.93404600	-1.82490600	0.18053000
C	2.25541200	-0.50724300	0.25120000
C	1.27335800	0.55185600	0.36246000
C	1.02272800	1.76789100	0.50986500
C	0.83612600	3.16132600	0.74317600
C	0.72321100	4.06125300	-0.33771200
C	0.82337900	3.65121100	2.06666100
C	0.60225400	5.42467400	-0.09279300
C	0.70450800	5.01757400	2.29754900
H	0.91839500	2.95497600	2.89325800
C	0.59325900	5.90308100	1.22131700
H	0.52139200	6.11715900	-0.92460000
H	0.70344400	5.39415500	3.31541500
H	0.50362600	6.96917200	1.40672600
H	2.68379400	-7.63744200	2.45925600
H	1.60110100	-3.48589700	2.28598300
H	0.73816100	3.68072700	-1.35372300
Au	-0.90685800	0.35371800	0.04984500
C	-2.85101100	-0.12710300	-0.28928300
C	-5.09634800	-0.02098000	-0.49744300
C	-4.71922200	-1.28830400	-0.80408900
H	-5.29343500	-2.15063800	-1.10195300
H	-6.06675100	0.44784500	-0.47355500
N	-3.93864700	0.68001200	-0.18530400
N	-3.33745700	-1.33913200	-0.67033100
C	-3.92050900	2.08213900	0.18314300
C	-3.98197100	2.41980400	1.54965500
C	-3.87526000	3.04249200	-0.84709200
C	-3.98584600	3.78314600	1.86956300
C	-3.88192700	4.38956600	-0.46486500
C	-3.93547800	4.75750200	0.87666200
H	-4.03569000	4.08448100	2.91124200
H	-3.85025200	5.15936200	-1.22965700
H	-3.94509300	5.80855100	1.14954200
C	-2.54452400	-2.52941300	-0.90299800
C	-1.97754500	-2.72152700	-2.17938200
C	-2.38920200	-3.44797600	0.15466200
C	-1.20881600	-3.87669500	-2.37090300
C	-1.61367900	-4.58872300	-0.09719200
C	-1.02441300	-4.80005600	-1.34361000
H	-0.75539600	-4.05861500	-3.33995300
H	-1.47257600	-5.32189700	0.69047300
H	-0.43076500	-5.69279300	-1.51718500
C	-2.17845700	-1.74924900	-3.33759200

C	-2.97237500	-2.40786600	-4.48381200
C	-0.83808000	-1.18233400	-3.84414100
H	-2.77048500	-0.90389900	-2.97513500
H	-3.94215100	-2.78038000	-4.13923000
H	-3.15208500	-1.68392900	-5.28489700
H	-2.42605800	-3.25235300	-4.91611200
H	-0.28181300	-0.69543300	-3.03681100
H	-0.20107700	-1.96652300	-4.26584000
H	-1.01462600	-0.44335200	-4.63215400
C	-3.02308100	-3.25211400	1.52864500
C	-1.96521800	-3.23405600	2.64918000
C	-4.10280400	-4.31869900	1.80046300
H	-3.51755500	-2.27641000	1.53982000
H	-1.19615200	-2.48081000	2.45590700
H	-2.43897100	-3.00821900	3.60980100
H	-1.46902400	-4.20512900	2.75008200
H	-4.88276200	-4.30847400	1.03254600
H	-3.67266500	-5.32523700	1.82276300
H	-4.57884600	-4.13896200	2.76955300
C	-3.82514900	2.67538500	-2.32766200
C	-2.52158400	3.16756900	-2.98549200
C	-5.06194300	3.20082400	-3.08281300
H	-3.83428700	1.58455200	-2.41193500
H	-1.64439900	2.75891400	-2.47369900
H	-2.48292800	2.85517400	-4.03407400
H	-2.44814700	4.25972200	-2.96253000
H	-5.99113100	2.82572700	-2.64241300
H	-5.10661600	4.29443400	-3.06918000
H	-5.03073200	2.88374100	-4.13010100
C	-4.05764200	1.38023900	2.66386600
C	-5.39398800	1.47391000	3.42708700
C	-2.85937400	1.49159600	3.62619800
H	-4.01227300	0.38610600	2.20919200
H	-6.24948200	1.35502600	2.75476800
H	-5.45159000	0.69202100	4.19112100
H	-5.50030800	2.43952500	3.93174300
H	-1.90971800	1.39227100	3.09019400
H	-2.85200200	2.45288800	4.15007500
H	-2.90788300	0.70305600	4.38409000
O	0.63142000	-2.19645300	0.33772500
C	6.25151800	1.79502900	-0.63819200
C	5.60609600	0.61876500	-0.62966600
H	5.65730400	2.69862400	-0.78219100
H	6.13188600	-0.32018500	-0.47565700

C	7.69203300	2.03189300	-0.47390400
C	8.15719600	3.35766200	-0.42471000
C	8.63491700	0.99286900	-0.35979800
C	9.51200600	3.64109800	-0.25939000
H	7.44349000	4.17308200	-0.51488400
C	9.98730100	1.27482200	-0.19444300
H	8.30984800	-0.04188800	-0.40616500
C	10.43281200	2.59956800	-0.14248600
H	9.84779600	4.67331500	-0.22317800
H	10.69958900	0.45933500	-0.10893900
H	11.48942600	2.81515400	-0.01518200
C	4.13652700	0.49341700	-0.84640600
H	3.91543100	-0.16922900	-1.69161700
H	3.67213000	1.47344300	-1.01717400
O	3.55881200	-0.11782400	0.34505700
H	0.47554700	-3.09851000	0.01584100

Zero-point correction= 0.959776 (Hartree/Particle)
Thermal correction to Energy= 1.020007
Thermal correction to Enthalpy= 1.020951
Thermal correction to Gibbs Free Energy= 0.851074
Sum of electronic and zero-point Energies= -2522.859960
Sum of electronic and thermal Energies= -2522.799729
Sum of electronic and thermal Enthalpies= -2522.798785
Sum of electronic and thermal Free Energies= -2522.968662

1-INT6

C	0.36921200	-1.57927300	0.94694600
O	0.68747800	-2.52769100	0.12686800
C	0.05573600	-2.04639100	2.30975300
C	0.72145900	-3.20412400	2.75548900
C	-0.85630900	-1.39739400	3.16117300
C	0.48489100	-3.69104800	4.03846700
H	1.43768300	-3.68852000	2.10223400
C	-1.10085600	-1.90572900	4.43378900
C	-0.42731800	-3.04777000	4.87714700
H	1.01604400	-4.57306200	4.38225200
H	-1.82049700	-1.41032100	5.07851900
C	0.36695000	-0.18746400	0.52465300
C	1.09368800	0.07121400	-0.77509000
C	0.43684900	0.85697400	1.51230100
C	0.50639100	1.77120500	2.30877800
C	0.60047300	2.84245400	3.24441400

C	0.98594600	4.12894000	2.81618900
C	0.31435700	2.63354700	4.60848400
C	1.07608700	5.17454600	3.73126900
C	0.40715400	3.68653500	5.51483900
H	0.03191800	1.64039500	4.94343500
C	0.78621200	4.95957500	5.08125300
H	1.38002400	6.15996700	3.39009400
H	0.18917900	3.51205400	6.56473500
H	0.86172500	5.77736800	5.79198300
H	-0.61363300	-3.43392300	5.87529600
H	-1.38414200	-0.51282300	2.82616500
H	1.22283400	4.28789400	1.76917100
Au	-1.74293800	-0.12233600	-0.17203900
C	-3.62497600	0.04256500	-0.88699400
C	-5.37374200	0.15964300	-2.30776700
C	-5.86054500	0.30954900	-1.04858000
H	-6.86444000	0.45954900	-0.68589700
H	-5.86746100	0.15163900	-3.26596500
N	-3.99972700	-0.00220100	-2.19195700
N	-4.77367500	0.23458200	-0.18654200
C	-3.09582600	-0.18932100	-3.31125800
C	-2.54939600	0.95320200	-3.92882400
C	-2.80389700	-1.50336200	-3.72746800
C	-1.68146500	0.74267200	-5.00684900
C	-1.92369800	-1.65006100	-4.80655900
C	-1.36812900	-0.54259400	-5.43995100
H	-1.23725200	1.59792300	-5.50644400
H	-1.66184700	-2.64660900	-5.14713800
H	-0.68255700	-0.68247600	-6.27020800
C	-4.86183600	0.33764200	1.25557000
C	-5.12695000	-0.83252700	1.99480000
C	-4.69084100	1.60278700	1.85265100
C	-5.22278200	-0.70227700	3.38579600
C	-4.79429500	1.66967900	3.24762900
C	-5.05852300	0.53299500	4.00672700
H	-5.42731200	-1.58168700	3.98840500
H	-4.66597600	2.62643800	3.74375700
H	-5.13770600	0.61081400	5.08727000
C	-5.31514200	-2.20081200	1.34628100
C	-6.75897100	-2.71011400	1.52913600
C	-4.29335700	-3.22784600	1.87033700
H	-5.14136500	-2.09648000	0.27137600
H	-7.48977800	-2.00376600	1.12174900
H	-6.89225600	-3.66914800	1.01794100

H	-6.99811600	-2.86115300	2.58708400
H	-3.26655200	-2.88287600	1.72002400
H	-4.42694000	-3.42151200	2.93965700
H	-4.41388600	-4.18078900	1.34481400
C	-4.42099500	2.87261400	1.05144800
C	-3.10853900	3.55467300	1.48280800
C	-5.61255400	3.84716900	1.14205100
H	-4.30759300	2.59474100	-0.00052400
H	-2.25637200	2.87412800	1.40035600
H	-2.91185700	4.42562400	0.84895500
H	-3.15553600	3.90657700	2.51840700
H	-6.54158500	3.38117600	0.79733400
H	-5.77277400	4.18628800	2.17089400
H	-5.42774200	4.73258900	0.52497900
C	-3.39218000	-2.74166100	-3.05826200
C	-2.29178500	-3.62980500	-2.44499100
C	-4.27206900	-3.54326100	-4.03820600
H	-4.03951300	-2.41307400	-2.23917000
H	-1.68920700	-3.07964400	-1.71652900
H	-2.73966200	-4.48993400	-1.93605800
H	-1.61095800	-4.01502700	-3.21021400
H	-5.07587900	-2.92694500	-4.45451200
H	-3.68494000	-3.93434200	-4.87531800
H	-4.72833000	-4.39739200	-3.52706800
C	-2.85778700	2.37614100	-3.47170000
C	-3.62936000	3.15781300	-4.55347600
C	-1.57858300	3.12636000	-3.05160100
H	-3.50312800	2.32112200	-2.58977500
H	-4.56246500	2.65333400	-4.82502500
H	-3.87822500	4.16209800	-4.19471000
H	-3.03475500	3.26854700	-5.46628900
H	-1.03040800	2.58462200	-2.27491100
H	-0.90349400	3.26953800	-3.90184800
H	-1.83165300	4.11814200	-2.66199200
O	1.35755900	-0.82624400	-1.57625600
C	3.25930300	3.99388700	-2.09246400
C	3.19623900	2.77653000	-1.53323900
H	2.60356600	4.20333500	-2.93913900
H	3.80575000	2.49648900	-0.67820700
C	4.12759100	5.11216700	-1.69596300
C	3.94792900	6.36395200	-2.31030200
C	5.13821300	4.99090700	-0.72315300
C	4.73617700	7.45993900	-1.96194900
H	3.17690200	6.47409700	-3.06936000

C	5.92481000	6.08481800	-0.37455500
H	5.31667900	4.03251700	-0.24607300
C	5.72807700	7.32515500	-0.98998100
H	4.57731300	8.41696200	-2.45126200
H	6.70117100	5.96827400	0.37637600
H	6.34752700	8.17487300	-0.71764600
C	2.31555000	1.68833400	-2.04615100
H	2.88689100	0.79061900	-2.29266200
H	1.72205200	2.00016300	-2.91072700
O	1.37510800	1.34838900	-0.96735400
H	1.09006600	-2.13283700	-0.72164300
S	3.88574300	-3.59561400	-1.04346500
S	4.48749700	-0.94677500	-0.13018000
O	5.06063400	-3.57757100	-1.91753700
O	2.57442200	-3.95623100	-1.60434600
O	3.71741300	0.03851500	0.65262000
O	4.94543700	-0.55351700	-1.46922300
C	4.23215400	-4.94114700	0.20292600
C	6.04987200	-1.19494100	0.86335400
F	4.39080400	-6.10513500	-0.43945100
F	3.21175300	-5.07884400	1.07109600
F	5.34456900	-4.67600400	0.89530300
F	5.75299400	-1.48979800	2.13489800
F	6.77628300	-0.06808800	0.84453400
F	6.77917100	-2.18893900	0.34851500
N	3.70689300	-2.34813100	-0.01529200

Zero-point correction= 1.015981 (Hartree/Particle)
Thermal correction to Energy= 1.091854
Thermal correction to Enthalpy= 1.092798
Thermal correction to Gibbs Free Energy= 0.885857
Sum of electronic and zero-point Energies= -4350.124602
Sum of electronic and thermal Energies= -4350.048729
Sum of electronic and thermal Enthalpies= -4350.047785
Sum of electronic and thermal Free Energies= -4350.254726

1-INT7

C	-1.81576100	2.27101400	-0.14512400
O	-2.15750900	1.02973900	-0.03617500
C	-2.80145600	3.32703300	0.12127900
C	-3.77024200	3.14483800	1.12462500
C	-2.83324800	4.48530900	-0.67641900
C	-4.74720600	4.11571400	1.32856200
H	-3.74790300	2.25971800	1.75163200

C	-3.82634400	5.43718200	-0.48177900
C	-4.78048600	5.25652500	0.52466900
H	-5.48947600	3.96974800	2.10637000
H	-3.85834600	6.32050500	-1.11195800
C	-0.45254800	2.50020400	-0.53774800
C	0.28720500	3.73662900	-0.15795700
C	0.20121300	1.50018900	-1.20655500
C	0.78987000	0.55296700	-1.82303000
C	1.06988800	0.33401300	-3.25232900
C	1.27372300	1.43637600	-4.10258500
C	1.14358700	-0.95966400	-3.79328400
C	1.53747500	1.24627200	-5.45683200
C	1.39612600	-1.14414600	-5.15228900
H	0.98456700	-1.81726000	-3.14722300
C	1.59693300	-0.04459800	-5.98826800
H	1.69425800	2.10795200	-6.09975800
H	1.43693700	-2.15140800	-5.55680100
H	1.79926800	-0.19112200	-7.04529700
H	-5.55201300	6.00564700	0.67857900
H	-2.09702200	4.61898200	-1.46050900
H	1.23447900	2.43814800	-3.68542300
O	-0.14666500	4.66123000	0.50093300
C	4.83827000	4.52898100	0.12485000
C	3.78539700	4.52182600	-0.70570600
H	4.65216400	4.75394200	1.17558300
H	3.90489500	4.30766900	-1.76571800
C	6.24833500	4.27586500	-0.20765900
C	7.21810100	4.42574000	0.79948000
C	6.68113500	3.88237000	-1.48828300
C	8.56953200	4.19861900	0.54166700
H	6.90324600	4.73007700	1.79480800
C	8.02941000	3.65428900	-1.74628800
H	5.95779200	3.74730400	-2.28645100
C	8.98133900	3.81211100	-0.73390800
H	9.29933900	4.32484400	1.33637000
H	8.34111000	3.35021400	-2.74156400
H	10.03270000	3.63388100	-0.93987000
C	2.39279200	4.82344700	-0.25611400
H	1.98908500	5.71975700	-0.74437200
H	2.33535600	4.98263400	0.82428400
O	1.55871800	3.69735500	-0.62560100
H	-3.17588200	0.77995100	0.02853900
Au	1.31632800	-0.82455500	-0.31164700
C	1.79512800	-2.27742700	1.03476300

C	2.06604600	-4.31735900	1.97547800
C	2.41554100	-3.39082600	2.90383700
H	2.76137000	-3.49396000	3.91949500
H	2.04602300	-5.39430500	2.01507800
N	1.69079500	-3.61941700	0.83475500
N	2.24582400	-2.14514100	2.31146100
C	1.29190500	-4.24789400	-0.40825800
C	-0.07623300	-4.49193800	-0.63870800
C	2.30146100	-4.60000900	-1.32781300
C	-0.41725100	-5.11610700	-1.84636800
C	1.89957700	-5.22279200	-2.51513500
C	0.55511000	-5.47899800	-2.77304800
H	-1.46212500	-5.31473700	-2.06152600
H	2.65000400	-5.50751100	-3.24651500
H	0.26386700	-5.96190800	-3.70144600
C	2.52609900	-0.89074200	2.97864900
C	3.80519300	-0.31897600	2.82511800
C	1.51706800	-0.31295200	3.77343500
C	4.05615700	0.87988100	3.50304100
C	1.82747900	0.88551400	4.42895800
C	3.08057400	1.47604200	4.29738900
H	5.02940800	1.35125400	3.40568700
H	1.07263300	1.36251300	5.04600400
H	3.29743900	2.40593500	4.81547700
C	4.90049500	-0.94451300	1.96701100
C	6.13379300	-1.31934500	2.81202100
C	5.28838400	-0.02646900	0.79137100
H	4.50972500	-1.87122100	1.53668600
H	5.86962500	-1.99949400	3.62841500
H	6.88633000	-1.81334500	2.18824200
H	6.60135700	-0.43361500	3.25477200
H	4.41820300	0.21088700	0.17204300
H	5.71878600	0.91782800	1.14026700
H	6.03568900	-0.51720500	0.15852200
C	0.12787800	-0.92283400	3.93080500
C	-0.95951700	0.01359200	3.37168700
C	-0.16032400	-1.30068400	5.39708700
H	0.09101700	-1.84690900	3.34623600
H	-0.78108700	0.23977200	2.31659000
H	-1.94947800	-0.44342000	3.44836800
H	-0.98893600	0.96167900	3.92005200
H	0.59184400	-1.99212800	5.79224500
H	-0.17297600	-0.41746800	6.04461600
H	-1.14052400	-1.78138300	5.47560200

C	3.78255600	-4.32445300	-1.08365800
C	4.35743900	-3.36345700	-2.14232600
C	4.59695000	-5.63138600	-1.01698200
H	3.88436200	-3.83008500	-0.11332900
H	3.79248800	-2.42718500	-2.17561200
H	5.40193000	-3.12597700	-1.91308800
H	4.33035300	-3.80688600	-3.14329200
H	4.21696700	-6.30172100	-0.23913200
H	4.56253700	-6.17353000	-1.96778600
H	5.64765400	-5.41562000	-0.79571200
C	-1.17318500	-4.11877000	0.35305400
C	-1.85812000	-5.37863100	0.92040000
C	-2.20508100	-3.15952200	-0.27021800
H	-0.70945800	-3.59400900	1.19399800
H	-1.13851300	-6.04763700	1.40526300
H	-2.61434500	-5.09406300	1.65848500
H	-2.36302000	-5.94666900	0.13206800
H	-1.73656600	-2.23143200	-0.61055800
H	-2.71091600	-3.61002900	-1.13002500
H	-2.97698800	-2.90738200	0.46224300
S	-5.05651700	-0.38677200	-1.48740300
S	-5.07155300	-0.52800600	1.42420500
O	-6.06086100	-1.44671500	-1.47323600
O	-3.86620600	-0.47942600	-2.33321800
O	-4.24456000	0.11229600	2.45811500
O	-5.22635900	-1.98114300	1.41194300
C	-5.93630900	1.15147600	-2.08102300
C	-6.78792500	0.15758800	1.72390100
F	-6.37487200	0.94788900	-3.32650500
F	-5.09611800	2.19410800	-2.08003000
F	-6.97769600	1.43261800	-1.29174400
F	-6.75869600	1.49694600	1.67974700
F	-7.19184500	-0.22518400	2.93924500
F	-7.65021300	-0.28952400	0.81334700
N	-4.58106200	0.13813300	0.00926000

Zero-point correction=	1.014501 (Hartree/Particle)
Thermal correction to Energy=	1.090347
Thermal correction to Enthalpy=	1.091291
Thermal correction to Gibbs Free Energy=	0.884618
Sum of electronic and zero-point Energies=	-4350.144882
Sum of electronic and thermal Energies=	-4350.069036
Sum of electronic and thermal Enthalpies=	-4350.068092
Sum of electronic and thermal Free Energies=	-4350.274765

1-TS5

C	-1.73763700	1.95812400	-0.42006200
O	-2.51639600	1.18248500	0.34036000
C	-2.35836900	3.15349900	-1.02653700
C	-3.18000200	3.98183600	-0.24661300
C	-2.19004300	3.43443400	-2.39203900
C	-3.79750100	5.09214500	-0.82082800
H	-3.34678100	3.75262300	0.79957200
C	-2.81812400	4.53810400	-2.96100900
C	-3.61749600	5.37334200	-2.17550400
H	-4.43248300	5.72501700	-0.20875600
H	-2.69793400	4.73811500	-4.02171800
C	-0.44545200	1.47663500	-0.54154500
C	0.71109600	2.15288600	-1.14501300
C	-0.27800300	0.16006100	0.05979100
C	-1.26940100	-0.38903700	0.68426900
C	-2.02208900	-1.31434600	1.46594800
C	-1.70078600	-1.53036700	2.82275900
C	-3.10759600	-2.00432300	0.88893300
C	-2.43544700	-2.44200100	3.57433400
C	-3.85349600	-2.89257600	1.65673000
H	-3.36553200	-1.81293600	-0.14604600
C	-3.51334600	-3.11785000	2.99353400
H	-2.18319800	-2.61252500	4.61656900
H	-4.70411100	-3.40032600	1.21438600
H	-4.09628400	-3.81478300	3.58912300
H	-4.11180700	6.23051600	-2.62366700
H	-1.59089400	2.77018500	-3.00515900
H	-0.87595300	-0.98046400	3.26386100
O	1.75276400	1.58514000	-1.45214700
C	2.97563300	5.85704800	-0.56827800
C	2.67459300	4.58775900	-0.87920800
H	2.44627700	6.65278900	-1.09400200
H	3.18858900	3.75183300	-0.41098700
C	3.97587000	6.31907200	0.40643000
C	4.38599200	7.66322000	0.38090000
C	4.53608200	5.47435000	1.38334000
C	5.33581100	8.14559400	1.28069800
H	3.95517800	8.33339800	-0.35893900
C	5.48175600	5.95645600	2.28430400
H	4.21331400	4.43995000	1.44865800
C	5.89029000	7.29302100	2.23580000
H	5.63882900	9.18791600	1.23811700

H	5.89379500	5.29165600	3.03896800
H	6.62513000	7.66644100	2.94304700
C	1.63891900	4.21861600	-1.89617300
H	2.06899600	3.60255800	-2.69167700
H	1.17015300	5.10520700	-2.32875300
O	0.54278600	3.48485500	-1.29203200
H	-3.58089400	1.18171000	0.18740500
Au	1.41958000	-1.04786300	-0.03532500
C	3.06296700	-2.24870800	-0.18610600
C	4.38061100	-4.05525400	-0.56642300
C	5.19248900	-3.02661400	-0.21678800
H	6.26304000	-2.96974200	-0.10658800
H	4.59764800	-5.07833000	-0.82712200
N	3.08091100	-3.56447400	-0.54193700
N	4.37310800	-1.92651600	0.00891000
C	1.91611800	-4.36532400	-0.85336100
C	1.36488000	-5.16846900	0.16459000
C	1.39999200	-4.33030600	-2.16398400
C	0.25578500	-5.95576600	-0.16705100
C	0.28800800	-5.13685900	-2.43622300
C	-0.27905300	-5.94101400	-1.45204300
H	-0.19689600	-6.58449800	0.59363900
H	-0.13884500	-5.13263500	-3.43421400
H	-1.14219600	-6.55703200	-1.68696200
C	4.88121100	-0.62274900	0.38251000
C	5.36778000	0.22262500	-0.63541400
C	4.90511400	-0.27048900	1.74627200
C	5.89959000	1.45677700	-0.24334400
C	5.44370300	0.97924600	2.07754700
C	5.93924300	1.83336400	1.09655100
H	6.28531300	2.13344500	-0.99882100
H	5.47667200	1.28322200	3.11937800
H	6.35507000	2.79782300	1.37325300
C	5.35953600	-0.16749000	-2.11087500
C	6.77826000	-0.54053500	-2.58820300
C	4.74871000	0.92965900	-3.00279000
H	4.72923100	-1.05490000	-2.22206900
H	7.20294400	-1.36354400	-2.00373600
H	6.75955700	-0.84758400	-3.63929100
H	7.45896800	0.31317200	-2.50048900
H	3.75470200	1.21482700	-2.65080600
H	5.37831500	1.82591700	-3.02895700
H	4.66589100	0.56441200	-4.03229700
C	4.38880300	-1.18594000	2.85206800

C	3.23573300	-0.52941900	3.63535600
C	5.52706300	-1.62283200	3.79525700
H	3.98606300	-2.08970300	2.38661000
H	2.41613700	-0.25060600	2.96599900
H	2.84522000	-1.22348100	4.38753100
H	3.56748100	0.37361000	4.15862900
H	6.32969600	-2.12749500	3.24762000
H	5.96776200	-0.76597700	4.31556200
H	5.14817000	-2.31398700	4.55564700
C	2.00461200	-3.47738300	-3.27507400
C	0.97782400	-2.48806100	-3.85930100
C	2.61887000	-4.36002100	-4.37991000
H	2.81451200	-2.88148100	-2.84527300
H	0.56977600	-1.83540600	-3.08192000
H	1.45319400	-1.85784600	-4.61812300
H	0.14155200	-3.00849200	-4.33777200
H	3.38170400	-5.03528200	-3.97826800
H	1.85618900	-4.97406200	-4.87049600
H	3.08787900	-3.73627900	-5.14820200
C	1.92241400	-5.20632600	1.58443400
C	2.47117500	-6.60322200	1.93592100
C	0.87595500	-4.74384000	2.61582900
H	2.76007600	-4.50515900	1.64125000
H	3.24553700	-6.92058300	1.22974800
H	2.90849400	-6.60017800	2.93999100
H	1.67947100	-7.35964300	1.92086900
H	0.50922100	-3.73977100	2.38546300
H	0.01205800	-5.41614100	2.64319000
H	1.31532500	-4.72845900	3.61931000
S	-6.02560400	1.67565300	1.19062400
S	-5.49283900	0.68387900	-1.51245100
O	-7.40618200	1.87753200	0.76281200
O	-5.28481100	2.72829300	1.88874100
O	-4.25161600	0.27924800	-2.18003200
O	-6.39107800	1.66126900	-2.11491000
C	-6.06640100	0.26893400	2.42122600
C	-6.49442800	-0.89606800	-1.40648100
F	-6.85993600	0.60771400	3.44133300
F	-4.83558200	0.02826200	2.88833600
F	-6.54080600	-0.84756200	1.85499900
F	-7.61874400	-0.71751700	-0.71594700
F	-5.77598900	-1.86986000	-0.82000200
F	-6.79712700	-1.28445000	-2.64862600
N	-5.04088300	1.01528900	0.03868200

Zero-point correction=	1.013669 (Hartree/Particle)
Thermal correction to Energy=	1.088391
Thermal correction to Enthalpy=	1.089335
Thermal correction to Gibbs Free Energy=	0.887873
Sum of electronic and zero-point Energies=	-4350.127344
Sum of electronic and thermal Energies=	-4350.052622
Sum of electronic and thermal Enthalpies=	-4350.051678
Sum of electronic and thermal Free Energies=	-4350.253140

1-INT8

C	2.17233200	0.15270300	-0.94101700
O	1.98916900	-1.18248600	-1.21657600
C	3.52058700	0.65724000	-1.21619900
C	4.33282100	-0.02072200	-2.14889500
C	4.04168900	1.80277100	-0.58527400
C	5.61527200	0.43677000	-2.44127400
H	3.95274300	-0.90458400	-2.64779200
C	5.32078800	2.26058100	-0.89393000
C	6.11567400	1.58299500	-1.82056700
H	6.22130300	-0.10310500	-3.16328000
H	5.69980400	3.15002000	-0.39834500
C	0.94939100	0.67594000	-0.57775700
C	0.60580400	2.08818900	-0.28193400
C	-0.05370800	-0.36939500	-0.63383300
C	0.64142600	-1.48941300	-1.02118900
C	0.30355000	-2.88871700	-1.27882200
C	-0.85281100	-3.47185900	-0.72998600
C	1.14006200	-3.69264800	-2.07889000
C	-1.16071400	-4.80725600	-0.97556500
C	0.83135700	-5.03131600	-2.31305000
H	2.03301300	-3.26778600	-2.52323900
C	-0.32075100	-5.59692000	-1.76460600
H	-2.05776500	-5.23377300	-0.53719000
H	1.49544700	-5.63086600	-2.92923000
H	-0.55864900	-6.64134700	-1.94551000
H	7.11367100	1.94248900	-2.05442200
H	3.44622200	2.32220200	0.15296600
H	-1.49872700	-2.87223000	-0.09802300
O	-0.26086200	2.72287000	-0.85228500
C	2.67383600	5.81500900	0.69535300
C	1.74549500	4.96167500	0.23643500
H	2.92474100	5.77021300	1.75629600
H	1.44897000	4.95267200	-0.80935000

C	3.41226400	6.83469600	-0.06429100
C	4.34247200	7.64205900	0.61367100
C	3.23857500	7.04327300	-1.44580000
C	5.07422700	8.62089000	-0.05732200
H	4.49078900	7.49527100	1.68082000
C	3.96913700	8.01928400	-2.11657700
H	2.52971400	6.43574500	-1.99974300
C	4.89053600	8.81371500	-1.42675700
H	5.78733200	9.23149500	0.48928500
H	3.82092600	8.16187900	-3.18329500
H	5.45878500	9.57447400	-1.95398000
C	1.03567700	3.97929600	1.11461200
H	-0.04830000	4.11276800	1.06310200
H	1.36986500	4.05914700	2.15146600
O	1.33352000	2.60237300	0.74274200
H	3.18566000	-2.33728200	-0.27127200
Au	-2.04106100	-0.10902500	-0.22977000
C	-4.03594500	0.23036500	0.15233800
C	-6.29127800	-0.00718200	0.33076900
C	-5.99109900	1.26958500	0.67260200
H	-6.61621000	2.09055600	0.98412600
H	-7.23213800	-0.53068500	0.28040600
N	-5.08777800	-0.62951400	0.01805600
N	-4.61149600	1.39987400	0.55914500
C	-5.00620000	-2.01891600	-0.37372600
C	-5.04095400	-2.34041100	-1.74495700
C	-4.95159800	-2.99724100	0.63930400
C	-5.02369300	-3.69813400	-2.08688600
C	-4.94177800	-4.33909800	0.23818400
C	-4.98045400	-4.68767700	-1.10923300
H	-5.04400900	-3.98272100	-3.13436900
H	-4.90190900	-5.11935100	0.99238600
H	-4.97297900	-5.73459400	-1.39879100
C	-3.92085300	2.63649100	0.85570900
C	-3.47618600	2.85913500	2.17386800
C	-3.77865200	3.59093200	-0.17059300
C	-2.89022600	4.10001500	2.45317800
C	-3.19135100	4.81561100	0.16801800
C	-2.75808800	5.07286500	1.46559600
H	-2.53824300	4.30701000	3.45934600
H	-3.06777900	5.57469000	-0.59760800
H	-2.31047900	6.03308600	1.70670000
C	-3.60407700	1.81660600	3.28011900
C	-4.48391600	2.32211100	4.43981900

C	-2.21955800	1.36412400	3.78379100
H	-4.09549000	0.93443800	2.86054900
H	-5.48009800	2.61296100	4.09042200
H	-4.60487100	1.53855700	5.19539400
H	-4.03842400	3.19174900	4.93445000
H	-1.61451800	0.96322300	2.96512300
H	-1.66819900	2.19385000	4.23950900
H	-2.32800900	0.58147900	4.54244200
C	-4.24711600	3.34013400	-1.60052300
C	-3.13057000	3.60837400	-2.62741800
C	-5.51185500	4.16181400	-1.92123400
H	-4.51063900	2.28221100	-1.68709900
H	-2.22190100	3.05663700	-2.37551300
H	-3.46424300	3.30596700	-3.62610000
H	-2.87656100	4.67298000	-2.67836100
H	-6.33129000	3.93008300	-1.23232100
H	-5.31271900	5.23684500	-1.85140700
H	-5.85675500	3.95147200	-2.93931400
C	-4.90084700	-2.65157300	2.12508400
C	-3.57903500	-3.11779200	2.76584000
C	-6.11764200	-3.21963000	2.88142400
H	-4.93835500	-1.56314700	2.22332400
H	-2.71602700	-2.66877700	2.26577800
H	-3.54774200	-2.83002800	3.82223800
H	-3.46957900	-4.20626000	2.71547400
H	-7.05999600	-2.86101300	2.45425900
H	-6.13512900	-4.31414300	2.85187300
H	-6.08565600	-2.91809000	3.93376300
C	-5.10039100	-1.28400400	-2.84369600
C	-6.40148600	-1.39747700	-3.66241100
C	-3.85865000	-1.34774800	-3.75375300
H	-5.10018200	-0.29880500	-2.36921000
H	-7.28697700	-1.31493600	-3.02337800
H	-6.44892200	-0.60086500	-4.41240100
H	-6.46146500	-2.35444400	-4.19162600
H	-2.93918200	-1.22325700	-3.17461100
H	-3.79832400	-2.30374700	-4.28465400
H	-3.90037700	-0.55167100	-4.50486900
S	3.32198000	-3.03747600	1.95410900
S	4.88750900	-3.88271100	-0.52916400
O	4.07794700	-4.10209600	2.58799700
O	1.87318400	-2.93136800	1.99828400
O	4.66725300	-3.52521400	-1.92463900
O	4.86862600	-5.24963300	-0.04556700

C	3.98012000	-1.41443000	2.62179600
C	6.54523700	-3.15842200	-0.03790300
F	3.67666700	-1.35036600	3.91726500
F	3.41030800	-0.40114000	1.97376300
F	5.30212900	-1.36075900	2.46793300
F	6.55697400	-1.85096600	-0.27594500
F	7.47897000	-3.76028300	-0.77378900
F	6.77280500	-3.38554000	1.25283700
N	3.81632800	-2.88755800	0.33557200

Zero-point correction= 1.018378 (Hartree/Particle)
Thermal correction to Energy= 1.093282
Thermal correction to Enthalpy= 1.094226
Thermal correction to Gibbs Free Energy= 0.891095
Sum of electronic and zero-point Energies= -4350.169121
Sum of electronic and thermal Energies= -4350.094217
Sum of electronic and thermal Enthalpies= -4350.093273
Sum of electronic and thermal Free Energies= -4350.296404

1-INT9

C	-1.88499800	2.15378100	-1.72744600
O	-0.75486800	2.59972200	-2.33615200
C	-3.09813100	2.89822700	-2.07897200
C	-2.99829000	4.26473600	-2.40278100
C	-4.35924000	2.28179900	-2.15384000
C	-4.12647600	4.99246100	-2.77347700
H	-2.03020300	4.75066000	-2.35210000
C	-5.48451500	3.01454400	-2.52287500
C	-5.37594600	4.37205700	-2.83317100
H	-4.02925000	6.04748400	-3.01406700
H	-6.44934600	2.51836300	-2.57711800
C	-1.55369700	1.06116500	-0.94504100
C	-2.42877000	0.29375000	-0.03819000
C	-0.13203900	0.79733000	-1.09764400
C	0.30118400	1.79001200	-1.95688000
C	1.57978300	2.15656300	-2.57210700
C	2.76914700	1.46598900	-2.27351100
C	1.64418700	3.22462000	-3.49004100
C	3.97341500	1.83231800	-2.86933400
C	2.85184700	3.58520100	-4.08286900
H	0.73857900	3.76501400	-3.74014900
C	4.02498700	2.89261700	-3.77710800
H	4.87487400	1.27998500	-2.62092700

H	2.87436900	4.41113200	-4.78881800
H	4.96631900	3.17517700	-4.24016100
H	-6.25578900	4.93958900	-3.12261400
H	-4.45848300	1.22779100	-1.92683100
H	2.74737100	0.64440100	-1.56677100
O	-2.22626300	-0.85515700	0.32025600
C	-6.66448800	-0.34734000	0.69311000
C	-5.33987500	-0.56124600	0.68936800
H	-7.03230600	0.55205900	1.18891200
H	-4.90639400	-1.43342300	0.20658200
C	-7.71296500	-1.19216700	0.10173900
C	-9.04955800	-0.76139800	0.17145100
C	-7.44746300	-2.41866700	-0.53674300
C	-10.08344700	-1.51900900	-0.37717400
H	-9.27507000	0.18225800	0.66224600
C	-8.47844600	-3.17544900	-1.08525800
H	-6.42701300	-2.78340100	-0.60293400
C	-9.80211000	-2.73053200	-1.00915800
H	-11.10760100	-1.16286600	-0.31039000
H	-8.25049900	-4.11864900	-1.57402500
H	-10.60405800	-3.32468200	-1.43755200
C	-4.36157900	0.35847000	1.35377200
H	-3.73491200	-0.18584900	2.06628700
H	-4.87060700	1.17930200	1.86314000
O	-3.48822000	1.01400400	0.39785300
H	0.79733900	1.93665400	0.76867400
Au	0.81520900	-0.88113900	-0.38334600
C	1.66642100	-2.66360200	0.20349300
C	2.97287400	-4.52485800	0.26818700
C	1.97945900	-4.69609300	1.17354400
H	1.75772200	-5.51075800	1.84339800
H	3.79409100	-5.16133600	-0.01756200
N	2.77390200	-3.27741400	-0.31300300
N	1.18841000	-3.55459700	1.12175900
C	3.64227900	-2.74980500	-1.34278600
C	3.23511200	-2.84102100	-2.68977300
C	4.89272400	-2.22129300	-0.95929700
C	4.12368900	-2.36879500	-3.66362800
C	5.74300200	-1.77442700	-1.97851500
C	5.36407400	-1.84327300	-3.31611700
H	3.83950800	-2.41961200	-4.70991100
H	6.71543400	-1.36812300	-1.71842100
H	6.03830100	-1.48789200	-4.09012700
C	-0.00451300	-3.40421900	1.92939300

C	0.09656900	-2.75508200	3.17473800
C	-1.20417700	-3.97484700	1.46088200
C	-1.05835300	-2.69675400	3.96436200
C	-2.32539500	-3.88931500	2.29378600
C	-2.25553900	-3.25994000	3.53292600
H	-1.01691600	-2.20292700	4.93036000
H	-3.26676600	-4.31771400	1.96380900
H	-3.13811400	-3.20605000	4.16419400
C	1.39412300	-2.13765400	3.68458800
C	1.94880900	-2.91671400	4.89361100
C	1.21665700	-0.64488400	4.01704400
H	2.13734300	-2.20146700	2.88527100
H	2.12595000	-3.96898400	4.64676800
H	2.89743000	-2.48165400	5.22597300
H	1.25385200	-2.88633200	5.73977800
H	0.79417500	-0.10636800	3.16461000
H	0.54628700	-0.49586900	4.87011300
H	2.17876900	-0.18873800	4.26974700
C	-1.31304500	-4.68028000	0.11240400
C	-2.43641300	-4.08614300	-0.75770100
C	-1.49086400	-6.20105600	0.29269200
H	-0.37624900	-4.52153200	-0.42928500
H	-2.31995500	-3.00427600	-0.85332500
H	-2.41767300	-4.53896700	-1.75533000
H	-3.42436900	-4.28578700	-0.32729300
H	-0.66574600	-6.64003300	0.86365600
H	-2.42039500	-6.43024600	0.82512700
H	-1.53145900	-6.70118500	-0.68110500
C	5.35722200	-2.15877400	0.49390100
C	5.86862800	-0.76185600	0.89020400
C	6.43239400	-3.22988600	0.77253900
H	4.49795300	-2.37705900	1.13462900
H	5.11231000	0.00541500	0.71372000
H	6.12155300	-0.74842700	1.95581300
H	6.77502400	-0.48863000	0.33905900
H	6.07260700	-4.23923500	0.54774300
H	7.32681500	-3.05545400	0.16449800
H	6.73291600	-3.20551200	1.82543300
C	1.91024500	-3.46297600	-3.12235900
C	2.14774300	-4.80458300	-3.84526500
C	1.07430300	-2.50345600	-3.98987300
H	1.32261700	-3.67345600	-2.22535100
H	2.69776900	-5.50983600	-3.21328500
H	1.19231500	-5.26625400	-4.11670700

H	2.72422100	-4.66385200	-4.76597400
H	0.88674000	-1.56154100	-3.46685400
H	1.57186200	-2.27520900	-4.93849800
H	0.10721300	-2.95991600	-4.22668400
S	-0.22982700	3.13091800	2.50221500
S	2.71841500	2.56707200	1.91322600
O	0.28099000	3.64814200	3.75787800
O	-1.30043900	2.15260200	2.40567000
O	3.29725800	1.58814900	1.00580000
O	2.95016700	2.55847700	3.34519500
C	-0.76807500	4.61148700	1.48372100
C	3.24614800	4.25347400	1.28169800
F	-1.89420700	5.08385900	2.01015200
F	-0.97398400	4.24309900	0.22187300
F	0.17683100	5.54963500	1.52412000
F	2.75002600	4.45426900	0.06522700
F	4.57674400	4.26624800	1.23790300
F	2.81397900	5.20004500	2.11072100
N	1.05846300	2.56127100	1.55275500

Zero-point correction= 1.018131 (Hartree/Particle)
Thermal correction to Energy= 1.093052
Thermal correction to Enthalpy= 1.093996
Thermal correction to Gibbs Free Energy= 0.890865
Sum of electronic and zero-point Energies= -4350.171784
Sum of electronic and thermal Energies= -4350.096863
Sum of electronic and thermal Enthalpies= -4350.095919
Sum of electronic and thermal Free Energies= -4350.299050

1-TS6

C	-1.37688000	2.52020800	-1.82496400
O	-0.15396900	2.69063300	-2.43190100
C	-2.46575900	3.26642700	-2.46249800
C	-2.18850500	4.51305700	-3.05332900
C	-3.77106700	2.75343100	-2.54566300
C	-3.19340300	5.23119100	-3.69693200
H	-1.18400800	4.91777200	-2.99137700
C	-4.77160600	3.47587700	-3.19108500
C	-4.48922100	4.71608100	-3.76828000
H	-2.96429400	6.19617700	-4.13987300
H	-5.77494400	3.06388300	-3.24936500
C	-1.21440600	1.65196100	-0.77083100
C	-2.18258400	1.24588800	0.26982700
C	0.19146700	1.24772000	-0.71278100

C	0.77394200	1.94167300	-1.77330100
C	2.14075600	2.07116400	-2.27357300
C	3.21291900	1.43189200	-1.62362000
C	2.40898200	2.86123600	-3.40878000
C	4.51323400	1.58601600	-2.09675800
C	3.71167500	3.00532100	-3.87794600
H	1.59065700	3.35810700	-3.91721000
C	4.77002600	2.37006400	-3.22419000
H	5.32732100	1.08607500	-1.58124300
H	3.90089900	3.61749700	-4.75516100
H	5.78633100	2.48608900	-3.58999800
H	-5.27274200	5.27588200	-4.27088600
H	-3.99906000	1.79183900	-2.10333400
H	3.02936800	0.82126500	-0.74690500
O	-1.99065900	0.33474400	1.05621900
C	-6.49757600	0.85700200	0.96463800
C	-5.17380000	0.67103900	1.07973800
H	-6.88259500	1.86928000	1.09510200
H	-4.72575900	-0.31510000	0.98487500
C	-7.52544300	-0.16140800	0.70116700
C	-8.88067500	0.19187900	0.82289700
C	-7.21886100	-1.48226200	0.32210300
C	-9.89377900	-0.73762000	0.59074100
H	-9.13766500	1.20893600	1.10868300
C	-8.22956000	-2.41046100	0.08874500
H	-6.18159600	-1.77741400	0.19762700
C	-9.57261500	-2.04477500	0.22396600
H	-10.93331700	-0.43985300	0.69500800
H	-7.97161900	-3.42414000	-0.20598500
H	-10.35855400	-2.77134800	0.03957200
C	-4.21975100	1.78629500	1.37690400
H	-3.63173200	1.57948000	2.27517700
H	-4.74165800	2.73855100	1.49090600
O	-3.29352900	2.01002700	0.28073600
H	0.79294300	1.65105000	0.54115200
Au	0.64834800	-0.79003000	-0.30956600
C	0.98145900	-2.78543800	-0.08223200
C	1.90335800	-4.85898000	-0.14218700
C	0.66836300	-4.98066600	0.40109800
H	0.12976600	-5.84060600	0.76437800
H	2.66182900	-5.59329500	-0.35632300
N	2.08727300	-3.51031400	-0.42704500
N	0.11446800	-3.70623300	0.42811200
C	3.29358500	-3.00241500	-1.04738700

C	3.29263600	-2.78049800	-2.43955300
C	4.43922600	-2.81500500	-0.24472100
C	4.48845600	-2.34330100	-3.02251900
C	5.60713900	-2.38417300	-0.88619200
C	5.63390200	-2.14832500	-2.25786900
H	4.52073700	-2.15851800	-4.09157800
H	6.50759400	-2.23184400	-0.30055900
H	6.55216200	-1.81417700	-2.73257400
C	-1.23599800	-3.46554000	0.89391300
C	-1.43748900	-3.07449100	2.23160300
C	-2.29669500	-3.70587400	-0.00190100
C	-2.76177900	-2.96533800	2.67302900
C	-3.59916100	-3.57980700	0.49547600
C	-3.83171800	-3.22460100	1.82173400
H	-2.95494800	-2.66721800	3.69828500
H	-4.44014000	-3.76624100	-0.16598200
H	-4.85063600	-3.13964600	2.18913500
C	-0.28905200	-2.77568300	3.18891700
C	-0.11177500	-3.90997400	4.21807600
C	-0.46874700	-1.41166300	3.88258500
H	0.63169300	-2.71450100	2.60243000
H	0.08476500	-4.87209500	3.73221200
H	0.72772600	-3.68938700	4.88569600
H	-1.00917400	-4.02559400	4.83590100
H	-0.69152400	-0.62896800	3.15338600
H	-1.28476100	-1.43522000	4.61366600
H	0.44468500	-1.13420600	4.41654700
C	-2.07829900	-4.06370800	-1.46926800
C	-2.56926600	-2.92841800	-2.38983200
C	-2.73256500	-5.40760100	-1.84210000
H	-1.00324300	-4.17107000	-1.63873800
H	-2.06402900	-1.98686600	-2.15454200
H	-2.36914300	-3.17399800	-3.43870500
H	-3.64778400	-2.76846400	-2.28478700
H	-2.36495500	-6.22224100	-1.20950400
H	-3.82180700	-5.37051100	-1.73587200
H	-2.51217300	-5.66166100	-2.88440100
C	4.45926700	-3.10961000	1.25376500
C	5.17875500	-2.02181500	2.07186200
C	5.09833300	-4.48798200	1.53003400
H	3.42332500	-3.14120100	1.60461800
H	4.75173300	-1.03500600	1.88729600
H	5.07535900	-2.23953500	3.14005600
H	6.25183300	-1.99077600	1.85315000

H	4.57817700	-5.29855600	1.01045700
H	6.14403400	-4.50363900	1.20349300
H	5.07818000	-4.70931800	2.60237600
C	2.07676600	-3.03513500	-3.32601800
C	2.31488000	-4.24916600	-4.24696000
C	1.68280900	-1.78856300	-4.13972500
H	1.22745400	-3.27536700	-2.68164500
H	2.54678100	-5.15085200	-3.67044200
H	1.42336200	-4.45203000	-4.85022200
H	3.14905400	-4.07037400	-4.93399700
H	1.50139600	-0.93241400	-3.48432500
H	2.46223700	-1.50832200	-4.85601300
H	0.76770600	-1.98524300	-4.70867500
S	0.36406200	3.53657000	2.20940700
S	2.40048800	1.44132000	2.48354200
O	0.81362500	3.93387800	3.53701400
O	-1.04879800	3.34808800	1.89777500
O	2.78275900	0.29496500	1.65368600
O	2.07554600	1.26888200	3.89273600
C	0.93602600	4.88565700	1.04474100
C	3.90533400	2.56436700	2.42420400
F	0.32715500	6.02232600	1.38397400
F	0.61710100	4.57655000	-0.21732300
F	2.25731700	5.04719300	1.13504200
F	4.16911100	2.90816500	1.16121700
F	4.93905700	1.87000900	2.91300600
F	3.72319300	3.66024500	3.15396600
N	1.23321700	2.23798600	1.60549400

Zero-point correction= 1.013195 (Hartree/Particle)
Thermal correction to Energy= 1.087289
Thermal correction to Enthalpy= 1.088233
Thermal correction to Gibbs Free Energy= 0.890553
Sum of electronic and zero-point Energies= -4350.162174
Sum of electronic and thermal Energies= -4350.088080
Sum of electronic and thermal Enthalpies= -4350.087136
Sum of electronic and thermal Free Energies= -4350.284815

P

C	1.40538600	0.41695100	2.85027300
O	0.15958300	0.18724900	3.42107800
C	2.54514000	0.01732900	3.67384400
C	2.34076200	-0.35688300	5.01618500
C	3.85423700	-0.01358800	3.15775700

C	3.41259200	-0.74579200	5.81510600
H	1.33965500	-0.33649400	5.43063400
C	4.92034000	-0.40158200	3.96461200
C	4.70771200	-0.77040800	5.29464100
H	3.23420200	-1.02745600	6.84878800
H	5.92327100	-0.41527900	3.54830000
C	1.21033200	0.92377300	1.59033200
C	2.14994000	1.35633700	0.52099300
C	-0.22588700	0.98448300	1.35901600
C	-0.81124200	0.56889100	2.56185300
C	-2.18444900	0.59090900	3.05153800
C	-3.21836100	1.04048800	2.20870000
C	-2.48154900	0.21005700	4.37233400
C	-4.52185400	1.11063800	2.68918800
C	-3.79145800	0.27717900	4.83972600
H	-1.68510900	-0.12684300	5.02660700
C	-4.81399000	0.72959800	4.00203400
H	-5.30751700	1.47193100	2.03312200
H	-4.01280800	-0.01563000	5.86184300
H	-5.83331000	0.78939800	4.37255300
H	5.54321200	-1.07217100	5.91934900
H	4.04572000	0.28210100	2.13464000
H	-3.00783100	1.32371600	1.18295000
O	2.00395900	1.03483900	-0.64193700
C	6.34393500	1.97084200	-0.26373200
C	5.03505300	1.79680100	-0.50441800
H	6.64904800	2.86432600	0.28253600
H	4.67172800	0.94495200	-1.07369300
C	7.44919900	1.09483800	-0.68174100
C	8.76856900	1.57279900	-0.59952600
C	7.24877200	-0.21659900	-1.15256200
C	9.84833300	0.78213000	-0.99093300
H	8.94380200	2.58048300	-0.23096700
C	8.32638100	-1.00746200	-1.54105400
H	6.24273600	-0.62249600	-1.19757300
C	9.63179300	-0.51175200	-1.46598400
H	10.85823200	1.17652600	-0.92305300
H	8.15081500	-2.01873000	-1.89800200
H	10.47050600	-1.13195100	-1.76845900
C	3.98720900	2.75805400	-0.03797900
H	3.34017800	3.10133200	-0.84828900
H	4.42568500	3.61855000	0.46971400
O	3.12213500	2.15531400	0.98012100
H	-0.68242200	1.66903700	0.63859500

Au	-0.65881200	-0.88734900	0.16998000
C	-0.98530900	-2.49436800	-1.00790400
C	-1.93941400	-4.27488200	-2.02183100
C	-0.69326900	-4.13201800	-2.53714000
H	-0.16105400	-4.69767400	-3.28422900
H	-2.71454300	-4.99521700	-2.22359600
N	-2.10970200	-3.25936400	-1.08917700
N	-0.11802300	-3.03816700	-1.90370000
C	-3.31296900	-3.09850400	-0.29684400
C	-3.33253800	-3.63564200	1.00621200
C	-4.42493300	-2.45411900	-0.87946400
C	-4.51406300	-3.48922200	1.74328300
C	-5.57942000	-2.34575700	-0.09495500
C	-5.62452700	-2.85019900	1.20167300
H	-4.56267400	-3.88614200	2.75249400
H	-6.45336500	-1.85308700	-0.50671300
H	-6.53124300	-2.74735900	1.79088500
C	1.24310000	-2.61038400	-2.16500100
C	1.46525600	-1.60498700	-3.12630800
C	2.28606500	-3.27213900	-1.48618500
C	2.79807300	-1.29322400	-3.42225900
C	3.59718900	-2.91469300	-1.82188800
C	3.85162300	-1.94451700	-2.78784900
H	3.00913300	-0.52404600	-4.15711900
H	4.42673000	-3.40568300	-1.32183000
H	4.87623300	-1.69005700	-3.04478500
C	0.33346200	-0.87885500	-3.84620800
C	0.12470600	-1.45531900	-5.26187200
C	0.55683000	0.64422500	-3.89381300
H	-0.58905900	-1.04643900	-3.28267000
H	-0.10771300	-2.52595900	-5.23859800
H	-0.70174600	-0.93972600	-5.76159200
H	1.02306400	-1.32190900	-5.87481400
H	0.81084800	1.03668000	-2.90629100
H	1.36310100	0.91314100	-4.58565700
H	-0.35231400	1.14827100	-4.23100300
C	2.04245600	-4.33026700	-0.41410400
C	2.55555900	-3.85853600	0.96050000
C	2.65604500	-5.68980000	-0.80157600
H	0.96330900	-4.47995700	-0.31844400
H	2.08246800	-2.91723300	1.25571300
H	2.33490000	-4.60865600	1.72780400
H	3.63911200	-3.70104600	0.95158100
H	2.26691700	-6.04697900	-1.76070100

H	3.74598300	-5.62980600	-0.88815200
H	2.42567100	-6.44295600	-0.04054100
C	-4.42275700	-1.93411100	-2.31551900
C	-5.11114400	-0.56624500	-2.46646300
C	-5.07534000	-2.96391300	-3.26374400
H	-3.38100700	-1.80100400	-2.62387300
H	-4.66519500	0.17939200	-1.80759000
H	-4.99281200	-0.21158400	-3.49530000
H	-6.18715800	-0.62665100	-2.26881800
H	-4.57643300	-3.93758300	-3.23001500
H	-6.12672900	-3.12227700	-2.99926900
H	-5.03949400	-2.60406100	-4.29723000
C	-2.15485500	-4.38907400	1.61833300
C	-2.50847400	-5.87242500	1.84821600
C	-1.65901500	-3.72907200	2.91867600
H	-1.32292700	-4.36134800	0.90958900
H	-2.81961600	-6.35824900	0.91768300
H	-1.64212800	-6.41502700	2.24156300
H	-3.32571200	-5.98226200	2.56889100
H	-1.36223000	-2.69049200	2.74563600
H	-2.43196500	-3.73400000	3.69423700
H	-0.79201000	-4.27188900	3.31044100
S	-0.33054200	4.54542300	-0.90020700
S	-2.32892200	2.61243200	-1.67554800
O	-0.62929400	5.32039700	-2.10459000
O	1.06262000	4.23457500	-0.55407300
O	-2.64263700	1.25811400	-1.16738200
O	-2.08145900	2.79062700	-3.10702600
C	-0.92797500	5.57953000	0.53555400
C	-3.91276800	3.54856800	-1.33500200
F	-0.27581100	6.74747400	0.54011000
F	-0.69602200	4.95210100	1.69617900
F	-2.24086300	5.81781300	0.43008500
F	-4.22694300	3.46770000	-0.03096600
F	-4.91092700	2.99916000	-2.04314900
F	-3.79647500	4.83276000	-1.67220200
N	-1.24189900	3.21296000	-0.65483900

Zero-point correction=	1.018677 (Hartree/Particle)
Thermal correction to Energy=	1.093392
Thermal correction to Enthalpy=	1.094336
Thermal correction to Gibbs Free Energy=	0.893020
Sum of electronic and zero-point Energies=	-4350.181069
Sum of electronic and thermal Energies=	-4350.106354

Sum of electronic and thermal Enthalpies= -4350.105410
Sum of electronic and thermal Free Energies= -4350.306726

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C	-0.11061400	2.73353500	-1.36539500
O	0.02164800	2.58797700	-2.56483800
C	0.16104600	4.01370700	-0.65901200
C	0.56765400	5.11332500	-1.43410400
C	0.01870300	4.15481800	0.72966700
C	0.82258100	6.33775200	-0.82579400
H	0.67064900	4.98389500	-2.50613900
C	0.27865400	5.38326600	1.33484600
C	0.67875900	6.47379300	0.55906700
H	1.13209800	7.18741100	-1.42666800
H	0.16876000	5.49105400	2.40959100
C	-0.55138900	1.52414700	-0.52621000
C	-1.80769200	1.40057000	-0.26303100
C	-3.11323900	1.74537500	-0.28712800
C	-4.30722900	2.03425700	-0.30790800
C	-5.66948000	2.41342800	-0.37515900
C	-6.43022200	2.12161600	-1.52998000
C	-6.27596300	3.09463100	0.70414800
C	-7.76473600	2.50492800	-1.59702100
C	-7.61206100	3.46993200	0.62530600
H	-5.68717500	3.32507900	1.58590900
C	-8.35624900	3.17654500	-0.52212700
H	-8.34558800	2.28486200	-2.48704100
H	-8.07516900	3.99530400	1.45440000
H	-9.39849700	3.47514500	-0.58015500
H	0.87845800	7.43061100	1.03260400
H	-0.29222200	3.30715400	1.33108000
H	-5.95878600	1.60645300	-2.36038400
Au	1.01446200	0.21995300	-0.14218100
C	2.60931600	-1.01882600	0.12660300
C	3.91970000	-2.85574300	0.28829400
C	4.72265800	-1.76852200	0.41503200
H	5.78631800	-1.68302800	0.56787800
H	4.14078900	-3.91067200	0.30438700
N	2.62616100	-2.37908000	0.11165000
N	3.90495800	-0.65091700	0.31364900
C	1.47259900	-3.23501100	-0.06766300
C	0.78377200	-3.68156000	1.07821200
C	1.11366500	-3.61495700	-1.37661700

C	-0.29435000	-4.55320300	0.87884400
C	0.02129900	-4.48214000	-1.51445300
C	-0.67082000	-4.95307900	-0.40114500
H	-0.83823100	-4.93093000	1.73915300
H	-0.27914000	-4.80438900	-2.50657200
H	-1.50266400	-5.63907600	-0.53224300
C	4.38632500	0.71349800	0.40408300
C	4.77122500	1.37168700	-0.78110400
C	4.47249800	1.30877800	1.67816300
C	5.25980700	2.67795000	-0.65497400
C	4.96421200	2.61836600	1.74005500
C	5.35495000	3.29605800	0.58866700
H	5.57148000	3.21635900	-1.54424200
H	5.04364700	3.11195700	2.70353100
H	5.73748400	4.30984800	0.66090400
C	4.69945600	0.71674100	-2.15726500
C	6.11222200	0.41502800	-2.69769400
C	3.89110200	1.56032000	-3.16153800
H	4.17853400	-0.23965000	-2.05183800
H	6.67702500	-0.22761500	-2.01442900
H	6.05050300	-0.09169800	-3.66627600
H	6.68835500	1.33543000	-2.83899600
H	2.87712700	1.75823100	-2.80168800
H	4.37208000	2.52324000	-3.36167600
H	3.81359500	1.03094700	-4.11683500
C	4.04674600	0.59718000	2.95915600
C	2.81761400	1.27866300	3.59250100
C	5.20682000	0.49301900	3.96822100
H	3.75133700	-0.42444800	2.70161000
H	1.97733200	1.30750600	2.89125700
H	2.49950300	0.73327200	4.48737200
H	3.04253800	2.30762700	3.89208900
H	6.07345500	-0.01420100	3.53264500
H	5.53604300	1.47989600	4.30867400
H	4.89149600	-0.07179800	4.85152500
C	1.85899100	-3.13372300	-2.61830300
C	0.94450500	-2.29943000	-3.53654800
C	2.49495500	-4.31078600	-3.38415100
H	2.67287500	-2.47851200	-2.29537400
H	0.53659500	-1.43098100	-3.00921600
H	1.50827500	-1.93419200	-4.40082600
H	0.10693200	-2.89392900	-3.91674000
H	3.17548100	-4.88395400	-2.74658700
H	1.73530900	-5.00118000	-3.76470000

H	3.06491400	-3.94013800	-4.24193200
C	1.17530400	-3.26765500	2.49301200
C	1.75603000	-4.45752400	3.28299200
C	-0.00352200	-2.62020400	3.24486600
H	1.96028800	-2.50986900	2.41878100
H	2.62627900	-4.88958000	2.77866100
H	2.06923600	-4.13549000	4.28135400
H	1.01534600	-5.25449800	3.40720600
H	-0.42138700	-1.78157400	2.67967800
H	-0.80662900	-3.34139000	3.43223000
H	0.33190800	-2.24803600	4.21838800
C	-4.12299500	-0.81752300	1.42230600
C	-5.29473100	-1.53773000	1.22353800
C	-5.37241500	-2.51759600	0.23596800
C	-4.23044700	-2.74704400	-0.53611400
C	-3.06470900	-2.02665100	-0.32467100
H	-6.28172700	-3.08310700	0.07491200
H	-3.98929700	-0.05554800	2.17563800
H	-2.14388200	-2.16306200	-0.87379400
Cl	-4.25570300	-3.95007000	-1.78751800
Cl	-6.66401200	-1.19090100	2.23080900
N	-3.03200400	-1.07963800	0.65423600
O	-1.93722800	-0.38986500	0.84631800

Zero-point correction= 0.859545 (Hartree/Particle)
Thermal correction to Energy= 0.917267
Thermal correction to Enthalpy= 0.918211
Thermal correction to Gibbs Free Energy= 0.754124
Sum of electronic and zero-point Energies= -3266.140921
Sum of electronic and thermal Energies= -3266.083199
Sum of electronic and thermal Enthalpies= -3266.082255
Sum of electronic and thermal Free Energies= -3266.246342

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C	1.63836800	-2.29592400	0.50132800
O	1.79142000	-2.61427700	-0.67361100
C	1.43178700	-3.26862600	1.59698200
C	1.36458500	-4.63359100	1.26848500
C	1.31381200	-2.86509300	2.93647700
C	1.18408300	-5.58094100	2.27006300
H	1.45634000	-4.92431900	0.22740600
C	1.13553800	-3.81848300	3.93639200
C	1.07071900	-5.17433500	3.60450800
H	1.13516900	-6.63570600	2.01745600

H	1.05176400	-3.50678800	4.97273900
C	1.69164200	-0.85211600	0.84501000
C	1.31002500	0.35754400	0.91321500
C	1.71994300	1.63399400	1.26216200
C	2.02162700	2.77942800	1.55607000
C	2.39795500	4.10540500	1.90890400
C	1.66876300	5.20617100	1.41333400
C	3.50159500	4.33168800	2.75727400
C	2.04224200	6.50099000	1.76052500
C	3.86325500	5.63094600	3.09956500
H	4.05929700	3.48405600	3.14219100
C	3.13706300	6.71662000	2.60225600
H	1.47917800	7.34569800	1.37550200
H	4.71229500	5.79848300	3.75494300
H	3.42339800	7.72884700	2.87093500
H	0.93414900	-5.91604000	4.38600200
H	1.37334300	-1.81161400	3.19109800
H	0.81854400	5.03044100	0.76186000
Au	-0.69146900	0.09925500	0.13931300
C	-2.58689600	0.10929100	-0.57833800
C	-4.65639200	-0.51542500	-1.22195600
C	-4.52930600	0.81028600	-1.48744000
H	-5.21706800	1.52028400	-1.91746500
H	-5.47865800	-1.19593500	-1.37304600
N	-3.45478200	-0.93179300	-0.66358200
N	-3.25238500	1.17955500	-1.08561000
C	-3.18987800	-2.29061700	-0.23241800
C	-2.68751000	-3.20858900	-1.17686200
C	-3.48306200	-2.63875400	1.10124900
C	-2.48202600	-4.52312400	-0.74030200
C	-3.24924100	-3.96639700	1.48019600
C	-2.75757600	-4.89896500	0.57162100
H	-2.10272500	-5.26156100	-1.43915800
H	-3.46237800	-4.27359000	2.49929700
H	-2.59101800	-5.92472500	0.88675600
C	-2.72490000	2.52585700	-1.19118900
C	-2.96032400	3.42219400	-0.12936800
C	-2.02653000	2.88512100	-2.36164700
C	-2.46559000	4.72495500	-0.27158000
C	-1.55529700	4.20103600	-2.44575600
C	-1.77289500	5.11236500	-1.41578600
H	-2.63323400	5.44597500	0.52236600
H	-1.01637100	4.51663800	-3.33348800
H	-1.40796000	6.13110300	-1.50926700

C	-3.71744100	3.03477600	1.13729100
C	-5.00863200	3.86152000	1.29816500
C	-2.82154300	3.15252000	2.38586200
H	-4.01384300	1.98511100	1.05261900
H	-5.66440300	3.75651300	0.42802300
H	-5.56329400	3.53169000	2.18241400
H	-4.79068000	4.92707100	1.42290800
H	-1.92066300	2.53848100	2.28802200
H	-2.50554000	4.18649800	2.55808200
H	-3.36638400	2.82103800	3.27578100
C	-1.77883200	1.91804600	-3.51538800
C	-0.27232500	1.71676100	-3.76996300
C	-2.50479100	2.37481100	-4.79624200
H	-2.19019600	0.94250600	-3.23965200
H	0.23835900	1.36462400	-2.86780300
H	-0.11799200	0.97583300	-4.56100900
H	0.21048300	2.64623000	-4.08896900
H	-3.58159900	2.48173700	-4.63116500
H	-2.12599900	3.33915800	-5.15023500
H	-2.35564700	1.64495300	-5.59839300
C	-4.03721200	-1.64700700	2.12000700
C	-3.05034900	-1.42576100	3.28299300
C	-5.42099300	-2.08433300	2.63977400
H	-4.17051700	-0.68176900	1.62236800
H	-2.08301700	-1.06427400	2.91903200
H	-3.44947800	-0.68615400	3.98489600
H	-2.87459600	-2.35183400	3.83982700
H	-6.13443400	-2.21461600	1.82001600
H	-5.36551900	-3.03161700	3.18548500
H	-5.82449300	-1.33154400	3.32455400
C	-2.39909200	-2.83302300	-2.62759300
C	-3.48068000	-3.40550200	-3.56701500
C	-0.99283300	-3.27143500	-3.07823400
H	-2.43588900	-1.74211400	-2.70994500
H	-4.48165700	-3.05570700	-3.29448300
H	-3.28711300	-3.10446200	-4.60170200
H	-3.49164100	-4.49994500	-3.53286900
H	-0.21417800	-2.89445900	-2.40910000
H	-0.90246200	-4.36187800	-3.11826100
H	-0.79202900	-2.89455100	-4.08639100
C	4.73234000	0.22451200	-0.21459400
C	5.55744400	0.34871000	-1.32332000
C	6.12739800	-0.77328200	-1.92668400
C	5.83314500	-2.02021300	-1.37473900

C	5.00259700	-2.13255200	-0.26829100
H	6.77447300	-0.67948700	-2.78978000
H	4.25959900	1.04948300	0.30070900
H	4.73664900	-3.06366200	0.20987100
Cl	6.50162000	-3.46512900	-2.06254000
Cl	5.87514100	1.93605900	-1.94959200
N	4.47431600	-1.01174000	0.29234800
O	3.70832800	-1.12971900	1.35079400

Zero-point correction= 0.859607 (Hartree/Particle)
Thermal correction to Energy= 0.917575
Thermal correction to Enthalpy= 0.918519
Thermal correction to Gibbs Free Energy= 0.754145
Sum of electronic and zero-point Energies= -3266.133992
Sum of electronic and thermal Energies= -3266.076023
Sum of electronic and thermal Enthalpies= -3266.075079
Sum of electronic and thermal Free Energies= -3266.239453

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C	1.86057500	3.00057800	-1.19226000
O	2.64479300	2.52143300	-2.00114700
C	1.77070300	4.46720600	-0.92790700
C	2.40014000	5.32641900	-1.84532500
C	1.11334400	5.00262600	0.19216000
C	2.36644900	6.70204000	-1.64518700
H	2.90649700	4.89387200	-2.70120300
C	1.08966200	6.38192900	0.38997000
C	1.71149600	7.23151700	-0.52798800
H	2.85031900	7.36406800	-2.35652400
H	0.59333100	6.79373400	1.26330700
C	0.87668300	2.20813600	-0.45315800
C	-0.31458200	1.91227300	-0.11486900
C	-1.51833500	2.52818300	0.18174200
C	-2.57911000	3.06868600	0.45649100
C	-3.77992500	3.76153400	0.76332200
C	-3.76017700	5.16191500	0.93984500
C	-4.99980600	3.06490200	0.89354400
C	-4.93308000	5.84313000	1.24692100
C	-6.16756700	3.75811900	1.19555000
H	-5.01419200	1.98991000	0.74752500
C	-6.13709000	5.14422000	1.37531200
H	-4.91196700	6.91984700	1.38329500
H	-7.10532500	3.21960900	1.29268700

H	-7.05118300	5.67978800	1.61296600
H	1.68963000	8.30595800	-0.37217700
H	0.63787300	4.34827000	0.91528100
H	-2.82169600	5.69566700	0.83126000
Au	-0.56279600	-0.25409300	-0.10976500
C	-1.08427300	-2.21209100	-0.11521500
C	-1.01469700	-4.46788000	-0.02112200
C	-2.29527800	-4.11028400	-0.29389100
H	-3.18171100	-4.70248800	-0.45382600
H	-0.55620700	-5.43516700	0.10629800
N	-0.28296900	-3.29204900	0.08638700
N	-2.32265800	-2.72309700	-0.34733000
C	1.13576500	-3.26220700	0.38108900
C	2.04679100	-3.31119000	-0.69198900
C	1.53762600	-3.23268900	1.73118400
C	3.41047700	-3.33549100	-0.37211600
C	2.91404500	-3.25497500	1.98945300
C	3.84106400	-3.31069000	0.95171400
H	4.14216700	-3.38381900	-1.17266400
H	3.26216500	-3.24135200	3.01766000
H	4.90328200	-3.34439100	1.17663700
C	-3.52418400	-1.95743600	-0.61315100
C	-4.35049900	-1.61048400	0.47407200
C	-3.83582500	-1.63774100	-1.94992300
C	-5.53250400	-0.91779700	0.18195100
C	-5.02667100	-0.93736600	-2.17873100
C	-5.86817000	-0.58354100	-1.12779500
H	-6.20263500	-0.64691300	0.99227100
H	-5.30163500	-0.67382900	-3.19509300
H	-6.79240400	-0.05084300	-1.33133200
C	-4.01583600	-1.96140400	1.92074700
C	-5.05044500	-2.93547600	2.51823800
C	-3.87448300	-0.69726200	2.79077700
H	-3.04672700	-2.46896500	1.93381900
H	-5.12540100	-3.85409900	1.92771100
H	-4.76835900	-3.21107600	3.53946300
H	-6.04772100	-2.48570700	2.55971400
H	-3.12574800	-0.01242000	2.38041300
H	-4.82146300	-0.15280000	2.86722800
H	-3.57001900	-0.96910700	3.80677300
C	-2.95094800	-2.03239000	-3.12830700
C	-2.46218700	-0.79762400	-3.90974700
C	-3.66941700	-3.03144600	-4.05701000
H	-2.06287100	-2.53593700	-2.73484800

H	-1.92365800	-0.10283000	-3.25764400
H	-1.78664000	-1.10299700	-4.71535300
H	-3.29499000	-0.25309000	-4.36623400
H	-3.98138900	-3.93054200	-3.51598600
H	-4.56340500	-2.58849100	-4.50758000
H	-3.00539000	-3.33918600	-4.87112200
C	0.55043400	-3.17920700	2.89331700
C	0.68388300	-1.85925300	3.67844600
C	0.69869600	-4.39831900	3.82461700
H	-0.46350300	-3.20756700	2.48360800
H	0.52828500	-0.99414900	3.02523200
H	-0.05876500	-1.81662000	4.48182100
H	1.67340100	-1.76642700	4.13898000
H	0.57768000	-5.33836500	3.27730100
H	1.67987500	-4.42007600	4.30964100
H	-0.05891100	-4.36576900	4.61400600
C	1.61010600	-3.34029300	-2.15317600
C	2.02517500	-4.65505800	-2.84217500
C	2.14229000	-2.11415200	-2.92083700
H	0.51786600	-3.28808500	-2.18416400
H	1.61642200	-5.52794300	-2.32331700
H	1.66184800	-4.67359400	-3.87459300
H	3.11397600	-4.76633200	-2.87213400
H	1.85463700	-1.18257100	-2.42427300
H	3.23502500	-2.13777500	-2.99746500
H	1.74391300	-2.10294100	-3.94049900
C	4.36018500	0.50673700	-0.88693000
C	5.71591500	0.56699800	-0.59633000
C	6.17143600	0.64113800	0.72054000
C	5.20838700	0.64906200	1.72981200
C	3.85626100	0.58500100	1.42769300
H	7.22849100	0.69212300	0.94957200
H	3.93961200	0.48516000	-1.87999600
H	3.06197400	0.57337400	2.15952800
Cl	5.68512100	0.73465300	3.39872100
Cl	6.84822500	0.54781100	-1.91291300
N	3.45503000	0.51531100	0.12872500
O	2.17505400	0.43751800	-0.13734400

Zero-point correction= 0.859307 (Hartree/Particle)
Thermal correction to Energy= 0.917125
Thermal correction to Enthalpy= 0.918069
Thermal correction to Gibbs Free Energy= 0.754518
Sum of electronic and zero-point Energies= -3266.119107
Sum of electronic and thermal Energies= -3266.061289

Sum of electronic and thermal Enthalpies= -3266.060345
Sum of electronic and thermal Free Energies= -3266.223896

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C	-0.34554100	-3.27874400	-0.88403200
O	-0.63993300	-4.17663000	-0.08799900
C	0.87075500	-3.37562400	-1.72414500
C	1.79443000	-4.39694400	-1.43449100
C	1.06013100	-2.57430900	-2.86374000
C	2.88737000	-4.60823700	-2.26600400
H	1.62339700	-5.02032300	-0.56384400
C	2.15300600	-2.79709800	-3.69963200
C	3.06621200	-3.81069200	-3.40195000
H	3.59488400	-5.40023400	-2.04079500
H	2.28561100	-2.18827300	-4.58844200
C	-1.30217200	-2.13608600	-1.06289800
C	-1.10503600	-0.80299400	-0.93921600
C	-2.18882500	0.07914700	-1.15311000
C	-3.07224100	0.89320700	-1.38199500
C	-4.11087400	1.83209800	-1.64503500
C	-5.06700700	1.58156900	-2.65238300
C	-4.20087400	3.02523800	-0.89801400
C	-6.08405100	2.49898400	-2.90100700
C	-5.22833200	3.93044900	-1.14764200
H	-3.46019300	3.22622400	-0.13102100
C	-6.17083200	3.67226900	-2.14702400
H	-6.80868300	2.30066300	-3.68486000
H	-5.29337000	4.84449100	-0.56491900
H	-6.96677300	4.38470200	-2.34106100
H	3.91224900	-3.98735300	-4.05979300
H	0.34262200	-1.79867800	-3.10415700
H	-4.98768200	0.67793100	-3.24980100
Au	0.60776200	0.12140600	-0.23000100
C	2.15072500	1.19442700	0.60085100
C	4.12731100	1.86909300	1.47924400
C	3.25755400	2.90291400	1.59967000
H	3.37701200	3.89098800	2.01377300
H	5.16173900	1.77044100	1.76568300
N	3.43606000	0.83158100	0.86569100
N	2.05198700	2.47480300	1.05973800
C	4.05525900	-0.43977200	0.55373900
C	3.94239900	-1.49396100	1.48158600
C	4.80736800	-0.53905300	-0.63398900

C	4.61389600	-2.68535600	1.18042800
C	5.45851700	-1.75367500	-0.87985300
C	5.36530500	-2.81482500	0.01601200
H	4.55367400	-3.51903600	1.87319400
H	6.05103500	-1.86596300	-1.78238600
H	5.88590500	-3.74519800	-0.19105500
C	0.86501300	3.30431400	1.02838300
C	0.62479700	4.09773400	-0.11127700
C	0.03153500	3.32217900	2.16479500
C	-0.49459900	4.93878500	-0.08191800
C	-1.07398000	4.18140900	2.13614300
C	-1.33204500	4.98615400	1.02930700
H	-0.70760300	5.57001700	-0.93885400
H	-1.73490200	4.22739000	2.99628700
H	-2.18525500	5.65857000	1.03555000
C	1.52875900	4.08373600	-1.33978700
C	2.25712000	5.43135900	-1.51374200
C	0.74823200	3.70387300	-2.61304300
H	2.29327400	3.31556700	-1.19157500
H	2.84818500	5.68646900	-0.62830000
H	2.93475800	5.38998800	-2.37265900
H	1.54959600	6.24865700	-1.68787700
H	0.23793500	2.74308400	-2.49359600
H	-0.00633900	4.45649400	-2.86398100
H	1.43142600	3.62671300	-3.46513000
C	0.28366100	2.45559100	3.39537800
C	-0.85473600	1.43752300	3.60312500
C	0.50576800	3.30987500	4.65861700
H	1.19913900	1.88102500	3.22840400
H	-0.97605000	0.80055100	2.72100500
H	-0.63699100	0.79611000	4.46364200
H	-1.80996900	1.93766300	3.79484700
H	1.33726900	4.00975400	4.52888100
H	-0.38391300	3.89539900	4.91182200
H	0.73409500	2.66811600	5.51568800
C	4.94944900	0.61319300	-1.62485900
C	4.42904300	0.23101000	-3.02306000
C	6.40492300	1.11667900	-1.69374500
H	4.33285500	1.44501600	-1.27209900
H	3.38845200	-0.10302100	-2.97967300
H	4.48792900	1.09245200	-3.69656300
H	5.02207800	-0.57553000	-3.46673300
H	6.77115200	1.42807400	-0.71026000
H	7.07955600	0.33914300	-2.06675000

H	6.48031200	1.97443200	-2.36997300
C	3.15185600	-1.37838500	2.78110800
C	4.07284100	-1.49742400	4.01145200
C	2.00668000	-2.40760300	2.84200600
H	2.69241300	-0.38648400	2.81347900
H	4.86460100	-0.74180800	3.99409700
H	3.49669700	-1.36358200	4.93288300
H	4.55270300	-2.48020500	4.06037100
H	1.33147900	-2.30036200	1.98726700
H	2.38669600	-3.43449400	2.84403400
H	1.42403100	-2.26983100	3.75911500
C	-3.26647700	-3.26646600	0.79733100
C	-4.24568800	-3.26954500	1.78688500
C	-5.47080000	-2.63342300	1.57471700
C	-5.68850200	-1.98826400	0.35494400
C	-4.69234300	-1.97683700	-0.61567200
H	-6.23896300	-2.64157800	2.33943600
H	-2.28952700	-3.75791500	0.83328800
H	-4.75965400	-1.48228900	-1.57374100
Cl	-7.18043600	-1.17727100	0.03470300
Cl	-3.92953700	-4.09710900	3.27170500
N	-3.54043500	-2.61479000	-0.34655900
O	-2.61576600	-2.64795300	-1.39682300

Zero-point correction= 0.862135 (Hartree/Particle)
Thermal correction to Energy= 0.919332
Thermal correction to Enthalpy= 0.920276
Thermal correction to Gibbs Free Energy= 0.759646
Sum of electronic and zero-point Energies= -3266.156472
Sum of electronic and thermal Energies= -3266.099276
Sum of electronic and thermal Enthalpies= -3266.098331
Sum of electronic and thermal Free Energies= -3266.258962

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C	-1.65080700	-2.24911200	0.04880800
O	-0.72304300	-2.33494900	0.85077200
C	-2.47144500	-3.45760600	-0.28020100
C	-2.54021100	-4.47290800	0.68914400
C	-3.09423600	-3.65585100	-1.52473800
C	-3.24383600	-5.64650500	0.43466800
H	-2.02985600	-4.32304400	1.63483000
C	-3.78032200	-4.84171600	-1.78407200
C	-3.86581700	-5.83282400	-0.80335000

H	-3.30095700	-6.41986700	1.19463700
H	-4.24160900	-4.99673000	-2.75488000
C	-1.98781300	-0.92707600	-0.57143700
C	-1.12085900	0.16021000	-0.64531400
C	-1.60954900	1.37698100	-1.12160300
C	-1.98088000	2.46894300	-1.54022700
C	-2.39805300	3.73226400	-2.02992700
C	-3.70686100	3.91158200	-2.53065500
C	-1.50664700	4.82844800	-2.03053800
C	-4.10818900	5.15031200	-3.01778300
C	-1.91911800	6.06488000	-2.51501600
H	-0.50060300	4.69033800	-1.64875900
C	-3.21698300	6.22812600	-3.00940900
H	-5.11366100	5.27981200	-3.40606700
H	-1.22982800	6.90350200	-2.51198000
H	-3.53349900	7.19453100	-3.38999100
H	-4.40739700	-6.75195300	-1.00664000
H	-3.01869800	-2.90047200	-2.29890600
H	-4.38941000	3.06789900	-2.53734800
Au	0.87732300	0.06747800	-0.15978100
C	2.88232200	0.01241400	0.26874300
C	5.09844300	-0.44014000	0.17031300
C	4.89753500	0.37582500	1.23614300
H	5.58424500	0.78632600	1.95868100
H	5.99658700	-0.88492700	-0.22659500
N	3.85442500	-0.65521800	-0.41012800
N	3.53463000	0.64410100	1.28242300
C	3.63458800	-1.49150300	-1.57262700
C	3.46529000	-2.87742200	-1.37856300
C	3.62021500	-0.88714100	-2.84547000
C	3.26395800	-3.66255100	-2.52053300
C	3.41240900	-1.72331300	-3.94929200
C	3.23447800	-3.09468800	-3.79110000
H	3.13152600	-4.73427100	-2.41108200
H	3.39420400	-1.29313700	-4.94580400
H	3.07787900	-3.72442600	-4.66201900
C	2.90544000	1.47831200	2.28444700
C	2.80120000	2.86188800	2.03907700
C	2.44350000	0.87338100	3.47029900
C	2.19470000	3.64554500	3.02827000
C	1.84577000	1.70780500	4.42339700
C	1.71980500	3.07699100	4.20691300
H	2.09759300	4.71571900	2.87364000
H	1.47996900	1.27737600	5.35047700

H	1.25650000	3.70467300	4.96263000
C	3.31755400	3.52015600	0.76306000
C	4.42494900	4.54851800	1.06611400
C	2.16998300	4.15860100	-0.04386500
H	3.75945000	2.74388200	0.13195000
H	5.25683100	4.09205600	1.61167200
H	4.81974200	4.96820200	0.13505900
H	4.04789900	5.37976200	1.67081200
H	1.40772400	3.41401200	-0.29497000
H	1.68669800	4.96492300	0.51840200
H	2.55588900	4.58647800	-0.97553400
C	2.58204700	-0.61971300	3.75346300
C	1.20820500	-1.30021300	3.91035600
C	3.47433100	-0.87215900	4.98532500
H	3.07467700	-1.08679500	2.89590000
H	0.60603900	-1.19873700	3.00282900
H	1.33966300	-2.36933400	4.10750600
H	0.64596500	-0.87620500	4.74955300
H	4.46275600	-0.41690600	4.86613600
H	3.02774900	-0.46139100	5.89678600
H	3.61254800	-1.94717700	5.13977000
C	3.83337800	0.60823500	-3.06049800
C	2.60963100	1.26507600	-3.72754400
C	5.12029300	0.87975700	-3.86470000
H	3.95646000	1.08031000	-2.08152600
H	1.70512900	1.10829300	-3.13133700
H	2.76933200	2.34355000	-3.83245800
H	2.43048600	0.85887100	-4.72850100
H	5.99829700	0.44805800	-3.37374900
H	5.06139600	0.45531000	-4.87224200
H	5.28488800	1.95739700	-3.96781400
C	3.52633100	-3.53996200	-0.00500100
C	4.79187500	-4.41254800	0.12507100
C	2.25733100	-4.35490500	0.30773300
H	3.59416800	-2.75249300	0.75138600
H	5.70322800	-3.83186400	-0.05143900
H	4.85521200	-4.84579600	1.12863400
H	4.78169100	-5.23792100	-0.59453500
H	1.36072100	-3.72966300	0.28377400
H	2.12208600	-5.17987400	-0.39964000
H	2.33553300	-4.79356900	1.30827800
C	-4.00190100	0.00365100	1.17463600
C	-5.02334200	0.34217200	2.06317900
C	-6.35702800	0.21480600	1.66912900

C	-6.63799300	-0.25276200	0.38077600
C	-5.59321900	-0.58148500	-0.48074300
H	-7.16092400	0.47245600	2.34890300
H	-2.93691800	0.06512600	1.38904200
H	-5.71396600	-0.95446300	-1.49046500
Cl	-8.27062500	-0.43765900	-0.15697000
Cl	-4.61790900	0.92256400	3.64075800
N	-4.34767300	-0.43359200	-0.02989600
O	-3.24186300	-0.80426000	-1.09384900

Zero-point correction= 0.859872 (Hartree/Particle)
Thermal correction to Energy= 0.917170
Thermal correction to Enthalpy= 0.918114
Thermal correction to Gibbs Free Energy= 0.755642
Sum of electronic and zero-point Energies= -3266.154259
Sum of electronic and thermal Energies= -3266.096961
Sum of electronic and thermal Enthalpies= -3266.096017
Sum of electronic and thermal Free Energies= -3266.258488

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C	1.78067100	3.15571200	-0.41459800
O	1.22779800	2.82313000	-1.46256300
C	3.07450300	3.84891000	-0.34855600
C	3.70791300	4.15753400	-1.57018300
C	3.69053600	4.20628600	0.86705700
C	4.93295400	4.81038500	-1.57560800
H	3.21758500	3.87658900	-2.49609000
C	4.92043500	4.86034400	0.85071700
C	5.54059300	5.16233300	-0.36391400
H	5.41757900	5.04929300	-2.51706800
H	5.39494300	5.13720900	1.78679300
C	0.94382000	2.78858000	0.82578500
C	-0.29556000	2.01256600	0.45218500
C	-1.48167200	2.65363600	0.43047900
C	-2.58501000	3.22042800	0.39730500
C	-3.83058400	3.85276400	0.36409600
C	-3.92485800	5.25803700	0.54673300
C	-5.01074500	3.09137600	0.15086200
C	-5.16570500	5.87615700	0.51870400
C	-6.24383700	3.72440800	0.12124600
H	-4.92724200	2.01846700	0.01279800
C	-6.32070900	5.11171200	0.30584100
H	-5.24292000	6.94905900	0.65984500
H	-7.14857500	3.14835300	-0.04235300

H	-7.28968000	5.60149800	0.28364400
H	6.49832100	5.67449400	-0.36908400
H	3.20664900	3.97645300	1.80775300
H	-3.01799200	5.83067300	0.70864900
Au	-0.10131200	0.00829900	0.20357200
C	0.10281700	-2.00790500	-0.08068300
C	0.99313000	-4.07226000	-0.28163300
C	-0.34594500	-4.18244600	-0.49059500
H	-0.96313600	-5.03738900	-0.71523300
H	1.77702900	-4.81235900	-0.28684300
N	1.25111300	-2.73290100	-0.03212700
N	-0.87664700	-2.90732900	-0.36415100
C	2.56830600	-2.19025600	0.23856200
C	3.35385700	-1.76151000	-0.85052400
C	3.00979500	-2.13747000	1.57569000
C	4.62855800	-1.26041800	-0.55877500
C	4.29181200	-1.62249000	1.80421300
C	5.09344300	-1.18988900	0.75159000
H	5.26606100	-0.92460900	-1.37052400
H	4.66736200	-1.56359800	2.82090700
H	6.08656300	-0.79946100	0.95306000
C	-2.28150400	-2.58700300	-0.52110000
C	-3.11272800	-2.63698100	0.61579000
C	-2.75431200	-2.25875400	-1.80759300
C	-4.46761100	-2.33516400	0.42961400
C	-4.11830500	-1.96589600	-1.93079400
C	-4.96636700	-2.00341600	-0.82727200
H	-5.14062900	-2.36761100	1.28062000
H	-4.52073600	-1.71160700	-2.90631100
H	-6.02298100	-1.78293900	-0.94922600
C	-2.60275000	-3.00432900	2.00610400
C	-3.26733500	-4.29350800	2.52883100
C	-2.78847200	-1.84138500	3.00026600
H	-1.52854800	-3.19990200	1.93665200
H	-3.11226500	-5.13240100	1.84308100
H	-2.84728300	-4.56862300	3.50149300
H	-4.34684800	-4.16585200	2.65865700
H	-2.28383400	-0.93488400	2.65065000
H	-3.84727700	-1.60330400	3.14621600
H	-2.37223600	-2.10768900	3.97719300
C	-1.85755600	-2.22051100	-3.04134800
C	-1.80676100	-0.80980500	-3.65991600
C	-2.29056800	-3.27078500	-4.08354100
H	-0.83860900	-2.47272600	-2.73298800

H	-1.45810900	-0.06879000	-2.93346400
H	-1.12280400	-0.79533700	-4.51460700
H	-2.79118800	-0.49286100	-4.01969800
H	-2.29574000	-4.27969500	-3.65896800
H	-3.29549200	-3.06678300	-4.46701400
H	-1.60368500	-3.26499900	-4.93584100
C	2.16493600	-2.61460100	2.75358600
C	1.85447300	-1.46332700	3.73006300
C	2.83458500	-3.79660700	3.48227300
H	1.20735500	-2.97448500	2.36499300
H	1.33875800	-0.63991100	3.22562800
H	1.21431400	-1.81949800	4.54377600
H	2.76757100	-1.06068200	4.18022600
H	3.02630300	-4.63186200	2.80127500
H	3.79132300	-3.50436900	3.92675800
H	2.19098000	-4.15842700	4.29053900
C	2.88358200	-1.83905500	-2.30053000
C	3.71493900	-2.86375500	-3.09859500
C	2.90051400	-0.45872500	-2.98536100
H	1.84632600	-2.18736600	-2.30595700
H	3.66972000	-3.85940400	-2.64575100
H	3.34205600	-2.94064400	-4.12501300
H	4.76843500	-2.56999500	-3.14806600
H	2.28959700	0.27013100	-2.44403100
H	3.91683800	-0.05811900	-3.05784900
H	2.50776100	-0.54027700	-4.00414800
O	1.17058700	3.02371400	1.99229700

Zero-point correction= 0.789994 (Hartree/Particle)
Thermal correction to Energy= 0.840055
Thermal correction to Enthalpy= 0.840999
Thermal correction to Gibbs Free Energy= 0.696334
Sum of electronic and zero-point Energies= -2098.812636
Sum of electronic and thermal Energies= -2098.762575
Sum of electronic and thermal Enthalpies= -2098.761631
Sum of electronic and thermal Free Energies= -2098.906295

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C	3.98712700	3.21011300	0.28089800
O	4.72955800	2.84866400	1.18860500
C	4.44456700	4.06986200	-0.84378700
C	5.78557100	4.48562200	-0.86091800
C	3.57869100	4.46917900	-1.87232500
C	6.25167000	5.29057000	-1.89507400

H	6.43662800	4.16722100	-0.05372300
C	4.04908300	5.27445500	-2.90792400
C	5.38427300	5.68536900	-2.91962100
H	7.28813200	5.61377300	-1.90649100
H	3.37791900	5.58335300	-3.70359500
C	2.59672300	2.77889500	0.29601500
C	1.46492200	2.34070900	0.40883600
C	0.19048400	1.75335300	0.54147600
C	-0.89326600	2.34940700	0.88667000
C	-1.75939600	3.36662400	1.35256700
C	-1.93758400	3.56500400	2.74344200
C	-2.39495000	4.23800900	0.43738400
C	-2.71790400	4.62013200	3.19829300
C	-3.16921700	5.29502100	0.90685000
H	-2.24740800	4.08883900	-0.62742500
C	-3.33087600	5.48541600	2.28233300
H	-2.84360600	4.78011500	4.26435000
H	-3.64148700	5.97412500	0.20428400
H	-3.93285400	6.31333000	2.64438600
H	5.74987900	6.31447900	-3.72594800
H	2.54097500	4.14901400	-1.85506000
H	-1.44782800	2.89197800	3.43916600
Au	0.39235800	-0.34120600	0.25284300
C	0.84610100	-2.30971200	0.03787500
C	2.01370100	-4.24097200	0.12403400
C	0.80576400	-4.51999300	-0.43029600
H	0.38472600	-5.44325700	-0.79419600
H	2.85910100	-4.87305300	0.34313900
N	2.02314800	-2.88199200	0.40507300
N	0.09965500	-3.32328300	-0.47593300
C	3.13512700	-2.17441300	1.01142000
C	4.11295000	-1.60982800	0.16805800
C	3.18637000	-2.08421800	2.41644800
C	5.16321900	-0.91803500	0.78275400
C	4.26157200	-1.38042700	2.97238300
C	5.23552200	-0.79733700	2.16736500
H	5.93180600	-0.46026500	0.16843400
H	4.33287500	-1.28427800	4.05122000
H	6.05257700	-0.24379900	2.61899700
C	-1.23873600	-3.19693700	-1.01187700
C	-2.33300300	-3.39338300	-0.14586500
C	-1.38720600	-2.91701600	-2.38566400
C	-3.61513100	-3.30885800	-0.70467200
C	-2.69349000	-2.83739100	-2.88595600

C	-3.79589100	-3.03700300	-2.05825900
H	-4.48154100	-3.46737000	-0.06999400
H	-2.84721100	-2.62965800	-3.94023900
H	-4.79871800	-2.98628600	-2.47226900
C	-2.17303400	-3.69963200	1.33973000
C	-2.63868600	-5.13226200	1.66793500
C	-2.90232700	-2.66136200	2.21417800
H	-1.11003100	-3.63500300	1.58863000
H	-2.08959100	-5.87815000	1.08459000
H	-2.48134400	-5.34982800	2.72915800
H	-3.70477000	-5.26391400	1.45527800
H	-2.57561900	-1.64410300	1.97754300
H	-3.98808800	-2.71369800	2.07760500
H	-2.69821800	-2.85310200	3.27266300
C	-0.20332000	-2.70672000	-3.32535200
C	-0.17979700	-1.27038300	-3.88429700
C	-0.18964800	-3.74709100	-4.46265000
H	0.71802500	-2.84248900	-2.75202900
H	-0.12504000	-0.53292300	-3.07635400
H	0.69274500	-1.12819800	-4.52996800
H	-1.07237300	-1.05731300	-4.48226400
H	-0.17533400	-4.76897600	-4.07100500
H	-1.06764400	-3.65125300	-5.10956300
H	0.69825800	-3.61155000	-5.08818600
C	2.13739100	-2.70878400	3.33210100
C	1.38509600	-1.63396200	4.14120400
C	2.76023800	-3.76937000	4.26140500
H	1.39702200	-3.22041700	2.70935200
H	0.90860800	-0.90298000	3.47979500
H	0.60784000	-2.09721000	4.75825200
H	2.06087500	-1.09082900	4.80949200
H	3.26696000	-4.55436500	3.69112900
H	3.49520100	-3.32575200	4.94056700
H	1.98523900	-4.24118400	4.87432700
C	4.07019200	-1.72580900	-1.35277200
C	5.26470400	-2.54233700	-1.88476100
C	3.99901000	-0.34206600	-2.02659400
H	3.15936700	-2.26543200	-1.63043500
H	5.29686400	-3.54261200	-1.44105700
H	5.19658700	-2.65520800	-2.97174600
H	6.21626600	-2.04964000	-1.66078200
H	3.13939300	0.23076400	-1.66544300
H	4.89988000	0.24789300	-1.83020300
H	3.90844100	-0.45384800	-3.11232900

C	-4.52530000	1.57689500	1.00227200
C	-5.72148100	1.84685100	0.34937200
C	-5.89158500	1.52614700	-0.99629400
C	-4.81725600	0.92241400	-1.65390200
C	-3.62937600	0.65118200	-0.99056900
H	-6.82155500	1.73274400	-1.51119600
H	-4.33109800	1.79534300	2.04196600
H	-2.76988600	0.16643800	-1.43150200
Cl	-4.95440000	0.49867500	-3.33182600
Cl	-7.00527100	2.59589500	1.24433800
N	-3.50344100	0.98583900	0.32495600
O	-2.37931300	0.74341400	0.94633800

Zero-point correction= 0.859309 (Hartree/Particle)
Thermal correction to Energy= 0.917217
Thermal correction to Enthalpy= 0.918162
Thermal correction to Gibbs Free Energy= 0.754277
Sum of electronic and zero-point Energies= -3266.122745
Sum of electronic and thermal Energies= -3266.064837
Sum of electronic and thermal Enthalpies= -3266.063893
Sum of electronic and thermal Free Energies= -3266.227777

1-INT1'

C	-2.60798000	3.43111200	-1.60799100
O	-2.48964600	3.84674800	-2.75524200
C	-3.24584900	4.23263700	-0.52405600
C	-3.81168700	5.47267000	-0.85937400
C	-3.28942900	3.78578600	0.80500800
C	-4.41846200	6.25030200	0.12209500
H	-3.76215900	5.80102400	-1.89213900
C	-3.89506600	4.56853300	1.78701100
C	-4.46155600	5.79928500	1.44579300
H	-4.85728200	7.20831100	-0.13954300
H	-3.92031600	4.22482900	2.81688500
C	-2.12789400	2.09823800	-1.27584800
C	-1.69062700	0.96806000	-1.10586100
C	-1.12428900	-0.29804900	-0.84365600
C	-1.79929600	-1.43361200	-1.10558900
C	-1.46662200	-2.84517600	-0.85473800
C	-1.65584800	-3.81399100	-1.86086500
C	-0.97759300	-3.25706100	0.39684000
C	-1.36008800	-5.15443100	-1.61935800
C	-0.68578900	-4.60080500	0.63389100
H	-0.83450300	-2.51797600	1.17872600

C	-0.87759500	-5.55257800	-0.36946300
H	-1.49536500	-5.88675200	-2.40968300
H	-0.31664200	-4.90529100	1.60830800
H	-0.65218200	-6.59761400	-0.18041900
H	-4.93313200	6.40932600	2.21070800
H	-2.83417200	2.83486000	1.06748400
H	-2.00724200	-3.50427100	-2.84113600
Au	0.84231600	-0.15196700	-0.19107600
C	2.79836300	0.17599300	0.32779300
C	4.71385200	0.54056200	1.47933900
C	4.98243000	0.74925400	0.16541300
H	5.89113100	1.03485500	-0.33934700
H	5.34065600	0.60692700	2.35386800
N	3.37205500	0.18783600	1.56230200
N	3.79983700	0.52301900	-0.52618100
C	2.69654900	-0.12410000	2.80360600
C	1.99230700	0.90006200	3.46780200
C	2.80563900	-1.43376200	3.31303000
C	1.36173300	0.56570600	4.67298500
C	2.15609700	-1.70793200	4.52299100
C	1.43823800	-0.72246300	5.19488400
H	0.81200400	1.32921100	5.21444700
H	2.22055700	-2.70512700	4.94749800
H	0.94594400	-0.95651400	6.13431400
C	3.66628400	0.65873400	-1.96310300
C	3.90498200	-0.47148300	-2.76997700
C	3.33046900	1.92157500	-2.49059800
C	3.78701800	-0.30573800	-4.15528900
C	3.22309200	2.02502400	-3.88304400
C	3.44752600	0.92622700	-4.70740400
H	3.96599800	-1.15343100	-4.80947400
H	2.96132000	2.98075300	-4.32613700
H	3.36108000	1.03151200	-5.78479700
C	4.29125200	-1.83300900	-2.20015600
C	5.71523500	-2.23665900	-2.63133600
C	3.26619700	-2.91857700	-2.58035000
H	4.29035500	-1.75928600	-1.10852200
H	6.45415000	-1.48884800	-2.32603800
H	5.99408600	-3.19371300	-2.17839800
H	5.78731800	-2.34949200	-3.71795700
H	2.26007500	-2.64679500	-2.24639500
H	3.23034800	-3.07663400	-3.66319500
H	3.53574500	-3.87317200	-2.11620000
C	3.09822700	3.15429700	-1.62155300

C	1.67159800	3.71064500	-1.79255300
C	4.15585700	4.24091300	-1.90095100
H	3.20667900	2.85980900	-0.57318700
H	0.91771300	2.95468600	-1.55341200
H	1.51964400	4.56882400	-1.12928400
H	1.48983400	4.04986000	-2.81717800
H	5.17184100	3.86231200	-1.74933700
H	4.08916000	4.60964000	-2.92958300
H	4.00890800	5.09547400	-1.23246900
C	3.61277200	-2.52952300	2.62194900
C	2.74364400	-3.75185500	2.27379200
C	4.83120900	-2.94104400	3.47263300
H	3.99376500	-2.13146900	1.67719800
H	1.91073700	-3.47139000	1.62271200
H	3.34343900	-4.50501300	1.75222300
H	2.33241900	-4.22381100	3.17270900
H	5.47661400	-2.08453800	3.69184900
H	4.52243400	-3.37586100	4.42895900
H	5.42989400	-3.68977100	2.94391800
C	1.92531100	2.33494200	2.95233700
C	2.68751100	3.29356400	3.88960000
C	0.47380000	2.80458000	2.73991800
H	2.41888700	2.37195800	1.97727900
H	3.73101000	2.98722500	4.01373600
H	2.67873600	4.31032600	3.48366400
H	2.23118900	3.32787600	4.88440900
H	-0.05273800	2.15063700	2.03781500
H	-0.08736700	2.81882100	3.68016100
H	0.46126700	3.82079800	2.33295000
C	-4.78698300	-2.68228600	-1.08469300
C	-5.94875800	-2.85703800	-0.33705000
C	-6.46746000	-1.79793200	0.41087700
C	-5.79970300	-0.56984300	0.39140900
C	-4.63971300	-0.41521400	-0.36085800
H	-7.37423200	-1.92414600	0.99135600
H	-4.31447900	-3.44699600	-1.68463000
H	-4.06134300	0.49786900	-0.45090900
Cl	-6.40408900	0.77889600	1.28380800
Cl	-6.73197800	-4.39573800	-0.35626300
N	-4.18725400	-1.47732200	-1.05654400
O	-3.06504200	-1.29050200	-1.85298500

Zero-point correction= 0.861742 (Hartree/Particle)
Thermal correction to Energy= 0.919239
Thermal correction to Enthalpy= 0.920183

Thermal correction to Gibbs Free Energy=	0.755804
Sum of electronic and zero-point Energies=	-3266.148617
Sum of electronic and thermal Energies=	-3266.091120
Sum of electronic and thermal Enthalpies=	-3266.090176
Sum of electronic and thermal Free Energies=	-3266.254555

1-TS2'

C	-2.87416900	3.42990800	-0.77435000
O	-2.94336000	3.95866400	-1.87914300
C	-3.37559300	4.07685200	0.46836700
C	-4.00686000	5.32603000	0.36042300
C	-3.23181200	3.47529800	1.72725900
C	-4.49008000	5.96203800	1.49958700
H	-4.10488200	5.77347500	-0.62302500
C	-3.71491900	4.11597200	2.86687400
C	-4.34476000	5.35801300	2.75331200
H	-4.97927800	6.92763700	1.41560600
H	-3.59974300	3.65173600	3.84173300
C	-2.28099300	2.10696900	-0.67229400
C	-1.77723900	0.99129600	-0.72397500
C	-1.12576200	-0.25046700	-0.72181300
C	-1.81883500	-1.37210900	-1.14781500
C	-1.42641600	-2.79417700	-1.04681500
C	-1.93629000	-3.72498600	-1.97144900
C	-0.58360100	-3.25765100	-0.02087300
C	-1.60217000	-5.07418800	-1.87959100
C	-0.25049200	-4.60823000	0.06677600
H	-0.19468500	-2.55931500	0.71315100
C	-0.75849300	-5.52120100	-0.86019700
H	-1.99518100	-5.77636200	-2.60871100
H	0.40397800	-4.94371400	0.86489400
H	-0.50116600	-6.57360700	-0.78799500
H	-4.72131200	5.85697200	3.64146700
H	-2.73674400	2.51162900	1.80925300
H	-2.57858700	-3.38069400	-2.77515000
Au	0.87494500	-0.09106800	-0.25206600
C	2.86224900	0.22429000	0.14718100
C	4.98314000	0.06179800	0.92054400
C	4.89974900	1.20719500	0.19632000
H	5.63602800	1.96126900	-0.03047500
H	5.80571800	-0.38529200	1.45494100
N	3.72671300	-0.52991000	0.87925300
N	3.59519900	1.29268600	-0.26968000

C	3.40870200	-1.78266900	1.53120100
C	2.87945500	-1.74799200	2.83727200
C	3.68056100	-2.98331900	0.84550600
C	2.60737500	-2.97681200	3.45153700
C	3.39770100	-4.18126300	1.51460800
C	2.86552200	-4.18089600	2.80133600
H	2.20148000	-2.98944300	4.45833800
H	3.60341400	-5.12606400	1.02120900
H	2.66124200	-5.12201200	3.30385400
C	3.10237900	2.37810500	-1.09547200
C	3.20465200	2.25618100	-2.49562900
C	2.56743600	3.51691700	-0.46090800
C	2.73737000	3.32743000	-3.26683600
C	2.11801700	4.55616400	-1.28457200
C	2.19913300	4.46428700	-2.67110200
H	2.79769800	3.26910200	-4.34907500
H	1.69850500	5.44979300	-0.83338400
H	1.84212200	5.28231900	-3.28946300
C	3.79757400	1.03122000	-3.18538700
C	5.07160100	1.39316400	-3.97437200
C	2.76209700	0.33520100	-4.08956500
H	4.08784600	0.31041600	-2.41509000
H	5.82461400	1.85764000	-3.32968400
H	5.51230400	0.49478300	-4.41866600
H	4.85452200	2.09285300	-4.78802900
H	1.87102000	0.04781600	-3.52257800
H	2.44205700	0.98593100	-4.90979600
H	3.19270300	-0.56878500	-4.53298100
C	2.46749500	3.65587900	1.05513800
C	1.00723200	3.83968300	1.51093000
C	3.36097500	4.79965100	1.57456900
H	2.83080200	2.72859700	1.50823400
H	0.37585300	3.02034900	1.15373100
H	0.95202400	3.86696500	2.60442500
H	0.58231900	4.77655800	1.13656300
H	4.40748300	4.65362700	1.28847700
H	3.04119600	5.76854900	1.17778100
H	3.31290800	4.85575100	2.66698500
C	4.26933500	-3.02306300	-0.56200400
C	3.33258000	-3.74356600	-1.55068000
C	5.67393200	-3.65866800	-0.56307700
H	4.37788200	-1.99399900	-0.91656200
H	2.33992800	-3.28418400	-1.56696100
H	3.74839000	-3.69997700	-2.56259800

H	3.20808300	-4.80008000	-1.29153300
H	6.35841200	-3.12438700	0.10351500
H	5.64097500	-4.70316900	-0.23653600
H	6.09920400	-3.63936400	-1.57161800
C	2.61625400	-0.44974100	3.59462800
C	3.47287000	-0.36140800	4.87314500
C	1.11894600	-0.27535400	3.91524900
H	2.90620400	0.38597600	2.95150600
H	4.53990700	-0.45227700	4.64725800
H	3.31297700	0.59987600	5.37212700
H	3.21568200	-1.15158400	5.58600100
H	0.51713100	-0.28304400	3.00035800
H	0.75276500	-1.07296100	4.57035900
H	0.94960900	0.67787800	4.42683000
C	-4.25995200	-1.54972900	0.34824500
C	-5.45294900	-1.77424400	1.03626300
C	-6.65543000	-1.85354800	0.33035300
C	-6.63322500	-1.70439700	-1.06043600
C	-5.42022500	-1.48805100	-1.71423800
H	-7.59057600	-2.02543400	0.85071900
H	-3.28041400	-1.46211700	0.81183600
H	-5.30772900	-1.36033000	-2.78450300
Cl	-8.09225500	-1.78787200	-1.98277100
Cl	-5.42247500	-1.94365200	2.75791300
N	-4.31757200	-1.42881600	-0.97103300
O	-2.97910700	-1.12712100	-1.81707300

Zero-point correction= 0.859578 (Hartree/Particle)
Thermal correction to Energy= 0.917119
Thermal correction to Enthalpy= 0.918063
Thermal correction to Gibbs Free Energy= 0.753447
Sum of electronic and zero-point Energies= -3266.148204
Sum of electronic and thermal Energies= -3266.090663
Sum of electronic and thermal Enthalpies= -3266.089719
Sum of electronic and thermal Free Energies= -3266.254335

1-INT2'

C	-4.95503500	0.24222500	1.35437400
O	-4.98012800	-0.15784900	2.51476500
C	-6.07290100	0.23114700	0.40415500
C	-7.30723000	-0.29443300	0.82149700
C	-5.92108400	0.73580200	-0.89668200
C	-8.37965100	-0.31319800	-0.06286100
H	-7.40090800	-0.67654700	1.83265500

C	-6.99827000	0.71419000	-1.77782000
C	-8.22544400	0.19013200	-1.35996100
H	-9.33641400	-0.71651700	0.25285400
H	-6.88708600	1.10444400	-2.78429900
C	-3.64951000	0.75923600	0.97233800
C	-2.46988000	1.12172800	0.87176000
C	-1.17107200	1.49225700	0.73215600
C	-0.75956400	2.84541000	1.25226700
C	-0.79197600	4.06256100	0.43779800
C	-0.37633700	5.27339200	1.01871800
C	-1.23701200	4.03266800	-0.89386800
C	-0.41085400	6.44352200	0.26906400
C	-1.26765400	5.20780100	-1.63969400
H	-1.55597300	3.09584100	-1.34342100
C	-0.85572000	6.41054700	-1.05765500
H	-0.09461900	7.38203600	0.71288400
H	-1.61124200	5.19056500	-2.66895000
H	-0.88206200	7.32672500	-1.63992900
H	-9.06594100	0.17487400	-2.04728100
H	-4.96516000	1.14643600	-1.21355200
H	-0.03885600	5.27306500	2.05001700
Au	0.26997500	0.17436100	0.20973700
C	1.75761700	-1.17120000	-0.18347400
C	3.79266900	-2.09421000	-0.48460500
C	2.87651600	-3.10014400	-0.51854000
H	2.99247300	-4.16310300	-0.65679500
H	4.86577200	-2.10562100	-0.58786400
N	3.08989000	-0.91863200	-0.27801800
N	1.63397700	-2.51670500	-0.33243500
C	3.70065300	0.39430700	-0.18781700
C	3.88199600	1.12833300	-1.37739500
C	4.10402300	0.86377000	1.07823000
C	4.48693600	2.38599300	-1.26468800
C	4.70539100	2.12799900	1.12584300
C	4.89477900	2.88134500	-0.02909300
H	4.64337900	2.98322300	-2.15750500
H	5.03111400	2.52495800	2.08199800
H	5.36577000	3.85782900	0.03339600
C	0.38161800	-3.24845400	-0.30392100
C	-0.08891300	-3.72799900	0.93495200
C	-0.29513500	-3.46199600	-1.52153300
C	-1.29405600	-4.44173300	0.92522600
C	-1.49524700	-4.18122600	-1.46644400
C	-1.99056400	-4.66578500	-0.25890000

H	-1.68898200	-4.82966600	1.85873600
H	-2.04543000	-4.36848000	-2.38330500
H	-2.92097100	-5.22549000	-0.24128800
C	0.65487200	-3.51673600	2.25047100
C	1.15780900	-4.85594600	2.82597300
C	-0.20691800	-2.76006400	3.27980200
H	1.53471700	-2.89698700	2.05194600
H	1.80424200	-5.38191000	2.11619600
H	1.72979500	-4.68478300	3.74342900
H	0.32495200	-5.52227300	3.07268700
H	-0.54496200	-1.79532000	2.88805700
H	-1.09387400	-3.33428300	3.56577700
H	0.37112900	-2.57271200	4.19029600
C	0.22037300	-2.95133400	-2.86400400
C	-0.74006200	-1.91238800	-3.47494500
C	0.48603400	-4.10929000	-3.84618700
H	1.17559300	-2.44479600	-2.69628900
H	-0.89137700	-1.06748700	-2.79477500
H	-0.33431200	-1.52544400	-4.41545500
H	-1.71992100	-2.35034400	-3.69128200
H	1.19043100	-4.83557500	-3.42880800
H	-0.43518100	-4.64571900	-4.09480600
H	0.90807000	-3.72565900	-4.78054700
C	3.92581700	0.06227400	2.36438300
C	3.06461700	0.82086500	3.39317900
C	5.28884900	-0.33503200	2.96597800
H	3.39622100	-0.86411700	2.12177800
H	2.08707600	1.09083200	2.98168900
H	2.90156100	0.19924300	4.27944000
H	3.55287200	1.74286100	3.72461800
H	5.89071400	-0.91078600	2.25556500
H	5.86968800	0.54675100	3.25462700
H	5.14473900	-0.94632600	3.86250900
C	3.45211900	0.61413900	-2.74831200
C	4.65225900	0.47995500	-3.70608300
C	2.34983000	1.50168200	-3.35871100
H	3.02622300	-0.38601800	-2.62248700
H	5.42685700	-0.17158600	-3.28971700
H	4.32963900	0.05540200	-4.66217400
H	5.11213700	1.45119900	-3.91414400
H	1.47742300	1.55811500	-2.69910100
H	2.70662500	2.52237100	-3.53032100
H	2.02513700	1.09654200	-4.32272800
O	-0.39665700	2.75839600	2.41895400

Zero-point correction=	0.789068 (Hartree/Particle)
Thermal correction to Energy=	0.839274
Thermal correction to Enthalpy=	0.840218
Thermal correction to Gibbs Free Energy=	0.694521
Sum of electronic and zero-point Energies=	-2098.801040
Sum of electronic and thermal Energies=	-2098.750834
Sum of electronic and thermal Enthalpies=	-2098.749890
Sum of electronic and thermal Free Energies=	-2098.895588

1-TS1'-2

C	-3.04811000	3.04070300	-0.72261100
O	-2.40878800	3.53341900	-1.64862300
C	-4.33459700	3.59332400	-0.22749800
C	-4.93772500	4.63381500	-0.95177400
C	-4.94556400	3.10875200	0.94142400
C	-6.14348600	5.17435500	-0.51632500
H	-4.44533800	4.99729100	-1.84740000
C	-6.15105600	3.65683700	1.37581400
C	-6.75118700	4.68636900	0.64573300
H	-6.61219300	5.97634800	-1.07804900
H	-6.61785900	3.29087500	2.28510100
C	-2.54596700	1.84240900	-0.07072800
C	-2.05924300	0.84124100	0.43679500
C	-1.59585000	-0.29283000	1.03966500
C	-0.61862300	-1.08498300	1.35688900
C	-0.47260500	-2.24500500	2.23195900
C	-1.22358700	-2.36057600	3.42205300
C	0.45369100	-3.25834500	1.91412200
C	-1.04926400	-3.46202600	4.25702500
C	0.60380500	-4.36772100	2.74245000
H	1.04146100	-3.17197300	1.00574800
C	-0.14248300	-4.47053100	3.91881000
H	-1.62259100	-3.53220000	5.17647900
H	1.31129500	-5.14675000	2.47567400
H	-0.01394500	-5.32820100	4.57198300
H	-7.69060300	5.11278800	0.98466800
H	-4.46315700	2.32487200	1.51992900
H	-1.93146000	-1.58339400	3.68158900
Au	1.06083500	-0.26720000	0.33521800
C	2.72823300	0.48518900	-0.55799600
C	4.57409300	1.72521600	-0.95379400
C	4.35159400	0.96143000	-2.05407000
H	4.88490300	0.88443800	-2.98767000

H	5.34081800	2.45005000	-0.73292200
N	3.57003800	1.42161700	-0.04495400
N	3.21770600	0.20289000	-1.79465700
C	3.44897200	2.04139500	1.26006300
C	2.75245600	3.26238900	1.35898500
C	4.06330800	1.41405500	2.36233500
C	2.67535200	3.85227700	2.62672700
C	3.94968600	2.05050900	3.60445500
C	3.26399700	3.25460000	3.73755300
H	2.14823500	4.79384900	2.74282500
H	4.41009600	1.59862700	4.47744900
H	3.19238600	3.73169600	4.71048000
C	2.66985600	-0.75980900	-2.72961700
C	3.23520300	-2.05085600	-2.76374700
C	1.63430200	-0.35090100	-3.59367400
C	2.72629900	-2.94801600	-3.71057500
C	1.16680700	-1.29290400	-4.51897100
C	1.70515900	-2.57490500	-4.58010600
H	3.13972500	-3.94989500	-3.77055900
H	0.37360800	-1.01306700	-5.20501400
H	1.33013900	-3.28546700	-5.31084400
C	4.36872400	-2.48775800	-1.83966800
C	5.67332500	-2.71877200	-2.62860300
C	3.99261000	-3.73583800	-1.01893800
H	4.55827600	-1.68181100	-1.12445800
H	5.97458600	-1.82169300	-3.17876100
H	6.48832000	-2.98895300	-1.94936400
H	5.56146900	-3.53009100	-3.35523900
H	3.08243900	-3.56587300	-0.43493400
H	3.82358100	-4.60799100	-1.65844700
H	4.80035700	-3.98867000	-0.32449700
C	1.03370000	1.05123500	-3.57184900
C	-0.49898700	1.01632900	-3.41921100
C	1.44846200	1.85188700	-4.82256600
H	1.42937000	1.57924300	-2.69956600
H	-0.79539400	0.39789300	-2.56607300
H	-0.89101900	2.02347600	-3.25160700
H	-0.98399200	0.61029300	-4.31353800
H	2.53702000	1.93505900	-4.90514700
H	1.08134200	1.37535300	-5.73761500
H	1.03230200	2.86352200	-4.78172100
C	4.84878800	0.11098500	2.24827200
C	4.26053300	-0.99345500	3.14710100
C	6.34405100	0.33491700	2.55072400

H	4.77595300	-0.24306400	1.21556600
H	3.20838200	-1.18190100	2.91127700
H	4.81499200	-1.92750700	3.00842200
H	4.32419700	-0.72778600	4.20714000
H	6.77962600	1.08781900	1.88618300
H	6.49743600	0.67310000	3.58064700
H	6.90314100	-0.59727500	2.41989600
C	2.10802400	3.95342500	0.16071500
C	2.83374500	5.27032800	-0.17990300
C	0.60192500	4.19014800	0.38051000
H	2.20540900	3.29487800	-0.70760600
H	3.89541500	5.10339800	-0.38907100
H	2.38347000	5.73596800	-1.06246100
H	2.76751800	5.98651700	0.64562100
H	0.09004500	3.25791500	0.63662000
H	0.42015200	4.90735300	1.18791500
H	0.14028200	4.58709300	-0.52851900
C	-5.10080200	-0.92215400	0.34261100
C	-5.88874900	-1.65678600	-0.53464700
C	-5.65375000	-3.01624000	-0.74160200
C	-4.60391100	-3.60550900	-0.03508100
C	-3.82593100	-2.86106200	0.84108000
H	-6.26592200	-3.59414700	-1.42287200
H	-5.23097800	0.13019900	0.55013800
H	-3.00754300	-3.25491600	1.42754100
Cl	-4.25086100	-5.29134300	-0.23344100
Cl	-7.17393400	-0.85007800	-1.37203000
N	-4.09100100	-1.53825700	1.01204000
O	-3.36480300	-0.83353000	1.85574500

Zero-point correction= 0.859754 (Hartree/Particle)
Thermal correction to Energy= 0.917479
Thermal correction to Enthalpy= 0.918423
Thermal correction to Gibbs Free Energy= 0.755341
Sum of electronic and zero-point Energies= -3266.135644
Sum of electronic and thermal Energies= -3266.077920
Sum of electronic and thermal Enthalpies= -3266.076975
Sum of electronic and thermal Free Energies= -3266.240057

1-TS1'-3

C	5.62063500	-1.06946000	0.10356000
O	5.99629500	0.10256700	0.07863500
C	6.52672100	-2.23134200	0.21027300
C	6.04365100	-3.54882100	0.16710900

C	7.90393800	-1.99282400	0.35328800
C	6.93006600	-4.61798700	0.26740400
H	4.97958700	-3.73299900	0.04787400
C	8.78471800	-3.06364800	0.45506800
C	8.29881400	-4.37551500	0.41232100
H	6.55858500	-5.63717900	0.23109600
H	9.84899000	-2.88227300	0.56727100
C	4.18810300	-1.30191700	0.02765000
C	2.95950400	-1.36800500	0.00026200
C	1.62175500	-1.44764900	-0.01772300
C	0.41242900	-1.89315700	0.05921000
C	0.04036200	-3.30588700	0.29206600
C	-1.23331000	-3.78308200	-0.06900900
C	0.95944700	-4.20369000	0.87406600
C	-1.56954700	-5.12081100	0.13021300
C	0.61156600	-5.53304900	1.08686700
H	1.93958100	-3.84777800	1.17596400
C	-0.65286800	-5.99795000	0.71137400
H	-2.55384700	-5.47203300	-0.16301900
H	1.32626900	-6.20940400	1.54584600
H	-0.92058100	-7.03728000	0.87554200
H	8.98924400	-5.20997300	0.49100800
H	8.25548000	-0.96709000	0.38227600
H	-1.95097200	-3.10586300	-0.51873700
Au	-1.14243900	-0.45610400	-0.00129600
C	-2.78684600	0.75008100	0.02558100
C	-4.19768100	2.50200300	0.25901300
C	-4.93704200	1.43402800	-0.13477000
H	-5.99254900	1.33116900	-0.32821800
H	-4.47722000	3.51933200	0.48035300
N	-2.88113700	2.06693600	0.35232300
N	-4.05857400	0.36751800	-0.27161900
C	-1.78548200	2.92375200	0.75664500
C	-1.44338700	2.97883200	2.12260700
C	-1.14282300	3.69982200	-0.22854900
C	-0.40945100	3.85084600	2.48898300
C	-0.12310300	4.55969800	0.19876500
C	0.24038600	4.63743100	1.54105100
H	-0.12218200	3.92546800	3.53313700
H	0.38580900	5.18343700	-0.52968700
H	1.02808900	5.31805000	1.85103900
C	-4.46192200	-0.96698500	-0.66617000
C	-4.43704400	-1.30170700	-2.03530500
C	-4.88774800	-1.86194800	0.33633700

C	-4.84886100	-2.59388300	-2.38558900
C	-5.29271400	-3.13810000	-0.07551100
C	-5.27323400	-3.50247600	-1.41941800
H	-4.84416100	-2.88800100	-3.43038300
H	-5.63267000	-3.85281200	0.66757600
H	-5.59810300	-4.49545300	-1.71625300
C	-4.00339200	-0.32492600	-3.12441600
C	-5.17165200	0.00597700	-4.07446800
C	-2.78220000	-0.84901700	-3.90468900
H	-3.69990400	0.60998800	-2.64398100
H	-6.03040500	0.41076500	-3.52960100
H	-4.85995600	0.74852100	-4.81597700
H	-5.51152800	-0.88217400	-4.61682600
H	-1.93599900	-1.03802500	-3.23640100
H	-3.00979100	-1.78089700	-4.43239600
H	-2.46798800	-0.11433500	-4.65324100
C	-4.93019500	-1.49616600	1.81714900
C	-4.02272400	-2.41606300	2.65656900
C	-6.37551700	-1.50012200	2.35379500
H	-4.54561500	-0.47826700	1.92954300
H	-2.98910000	-2.39039600	2.29832700
H	-4.03049900	-2.09925700	3.70461600
H	-4.36323300	-3.45608000	2.62485900
H	-7.01820700	-0.82137000	1.78410400
H	-6.82020400	-2.49924500	2.30194800
H	-6.39272700	-1.18369700	3.40164600
C	-1.52226200	3.64888100	-1.70556300
C	-0.32266300	3.25147800	-2.58747600
C	-2.13856600	4.98330100	-2.17097500
H	-2.28347500	2.87416200	-1.83496700
H	0.10454000	2.29828900	-2.26200700
H	-0.63952700	3.15259400	-3.63085300
H	0.46566800	4.01157600	-2.55721000
H	-3.01831300	5.25079200	-1.57688100
H	-1.42024300	5.80557400	-2.08796500
H	-2.44646700	4.91554700	-3.21934200
C	-2.14994900	2.15352000	3.19411300
C	-2.85918200	3.05500900	4.22389000
C	-1.17743100	1.17695200	3.88359000
H	-2.92034700	1.54860600	2.70741200
H	-3.57244900	3.73077500	3.74169500
H	-3.40703500	2.44398000	4.94822300
H	-2.14477400	3.66848400	4.78215400
H	-0.71454500	0.50208300	3.15631300

H	-0.37824300	1.70935500	4.41007900
H	-1.71022000	0.56832700	4.62139700
C	3.32596300	1.53150500	-1.68738100
C	4.46092800	2.32988900	-1.67262100
C	4.79859400	3.07407300	-0.54380100
C	3.95343300	2.98246000	0.56138800
C	2.82051100	2.18273300	0.53430100
H	5.68809500	3.69071000	-0.52241500
H	3.00411700	0.93547100	-2.52882600
H	2.11517300	2.08362700	1.34635300
Cl	4.30378400	3.87735700	2.00850800
Cl	5.46075200	2.37802800	-3.08877300
N	2.51969600	1.48147900	-0.59230200
O	1.44785100	0.73341500	-0.61999100

Zero-point correction= 0.859195 (Hartree/Particle)
Thermal correction to Energy= 0.916907
Thermal correction to Enthalpy= 0.917851
Thermal correction to Gibbs Free Energy= 0.754891
Sum of electronic and zero-point Energies= -3266.128066
Sum of electronic and thermal Energies= -3266.070355
Sum of electronic and thermal Enthalpies= -3266.069411
Sum of electronic and thermal Free Energies= -3266.232370

1-INT1'-1

C	3.04612200	2.86093700	0.87234900
O	2.39762700	3.26999900	1.83157400
C	4.32685100	3.49078700	0.44297800
C	4.93090900	4.42361700	1.30024100
C	4.92658900	3.19110800	-0.79073700
C	6.12665400	5.03419500	0.93393500
H	4.44603200	4.65106800	2.24360800
C	6.11980400	3.81078400	-1.15861400
C	6.72291300	4.72805300	-0.29392600
H	6.59527800	5.75141900	1.60073400
H	6.57329300	3.59075200	-2.12042200
C	2.59202900	1.70379400	0.12054800
C	2.16647300	0.71970500	-0.46238800
C	1.81241400	-0.44754000	-1.16600300
C	0.61954100	-1.07154400	-1.28182300
C	0.45571900	-2.30139400	-2.09135700
C	-0.19530300	-3.41857100	-1.52970700
C	0.90650600	-2.39201200	-3.42379100
C	-0.35535000	-4.59504200	-2.26163200

C	0.71186500	-3.55841800	-4.16296900
H	1.38749000	-1.53580800	-3.88492000
C	0.09138800	-4.66743300	-3.58327800
H	-0.84775300	-5.44867200	-1.80523300
H	1.04773400	-3.60071900	-5.19493300
H	-0.05275500	-5.57601900	-4.15983400
H	7.65294700	5.21040800	-0.57968200
H	4.43306800	2.50448100	-1.47352800
H	-0.57308400	-3.35327000	-0.51349800
Au	-1.03780500	-0.25677900	-0.35634700
C	-2.70592700	0.54848200	0.53083300
C	-4.51173300	1.84896600	0.94786500
C	-4.35152400	1.02281400	2.01236800
H	-4.91334500	0.92135200	2.92673900
H	-5.24156100	2.61570700	0.74424800
N	-3.49643500	1.54612800	0.04950300
N	-3.24335500	0.22980400	1.74020800
C	-3.33120800	2.21138200	-1.22689500
C	-2.60263100	3.41663300	-1.26655100
C	-3.93843100	1.64382300	-2.36500500
C	-2.48811600	4.05486900	-2.50781800
C	-3.78626300	2.32519300	-3.57887200
C	-3.07052000	3.51680600	-3.65183600
H	-1.93533600	4.98654900	-2.57708500
H	-4.23999000	1.91844800	-4.47727000
H	-2.96979000	4.03034200	-4.60352300
C	-2.76973200	-0.81297600	2.62687000
C	-3.38017200	-2.08166300	2.55021500
C	-1.75109800	-0.50762600	3.55109400
C	-2.93271800	-3.06409700	3.44197400
C	-1.34772300	-1.52979400	4.41988400
C	-1.92982300	-2.79301200	4.36882500
H	-3.38096800	-4.05248200	3.41263900
H	-0.56893900	-1.32797300	5.14856700
H	-1.60448900	-3.56813100	5.05670000
C	-4.48868200	-2.41420500	1.55492100
C	-5.79551900	-2.80289300	2.27377100
C	-4.04867000	-3.51347000	0.56885700
H	-4.69915200	-1.51865400	0.96335700
H	-6.12975300	-2.01209100	2.95278300
H	-6.59204600	-2.98260500	1.54453200
H	-5.67418400	-3.71696900	2.86403500
H	-3.15365800	-3.21242400	0.01552300
H	-3.82800700	-4.45255400	1.08727000

H	-4.84446800	-3.71471300	-0.15598400
C	-1.09143000	0.86453900	3.64081100
C	0.43384000	0.77201700	3.44407700
C	-1.44151500	1.57091600	4.96538800
H	-1.48120000	1.48419600	2.82863500
H	0.67570400	0.23516900	2.52138000
H	0.87460800	1.76998100	3.36965800
H	0.91462500	0.24894600	4.27833800
H	-2.52345000	1.68826000	5.08533000
H	-1.07063600	1.00833000	5.82868400
H	-0.98640300	2.56604700	4.99562200
C	-4.74877900	0.35201600	-2.31954800
C	-4.13213300	-0.73644400	-3.21926500
C	-6.22576600	0.60393500	-2.68250500
H	-4.72730500	-0.02914400	-1.29446400
H	-3.09453100	-0.94193900	-2.93777200
H	-4.70186200	-1.66752500	-3.13125600
H	-4.14333400	-0.44131200	-4.27363000
H	-6.68062100	1.34671800	-2.01939900
H	-6.32999300	0.96785500	-3.70979500
H	-6.80176300	-0.32346100	-2.59887700
C	-1.95693100	4.03825900	-0.03214900
C	-2.64418600	5.36390600	0.35112400
C	-0.44082600	4.23165700	-0.22174800
H	-2.08897300	3.34858900	0.80659800
H	-3.71347100	5.22373400	0.54069400
H	-2.19133100	5.78019900	1.25683600
H	-2.54406900	6.10919700	-0.44481300
H	0.04090200	3.29241600	-0.50851300
H	-0.22355900	4.97483800	-0.99648100
H	0.02006200	4.57472700	0.70931100
C	3.58723700	-2.89727500	-0.68065900
C	4.49890900	-3.56761100	0.12845400
C	5.67464100	-2.93265000	0.53994300
C	5.91093400	-1.61958800	0.12729000
C	4.98542400	-0.96491000	-0.68178900
H	6.39071800	-3.45087400	1.16748700
H	2.65449700	-3.30811700	-1.04876600
H	5.08440700	0.05043700	-1.04002600
Cl	7.34128900	-0.78261300	0.60850100
Cl	4.16068300	-5.19207700	0.60479200
N	3.87482300	-1.63201700	-1.04696500
O	2.99786400	-0.98512000	-1.89606300

Zero-point correction= 0.861666 (Hartree/Particle)

Thermal correction to Energy=	0.919130
Thermal correction to Enthalpy=	0.920074
Thermal correction to Gibbs Free Energy=	0.757584
Sum of electronic and zero-point Energies=	-3266.144719
Sum of electronic and thermal Energies=	-3266.087255
Sum of electronic and thermal Enthalpies=	-3266.086311
Sum of electronic and thermal Free Energies=	-3266.248801

1-TS2'-1

C	2.42039300	3.31370700	0.76989500
O	1.52645800	3.71262600	1.51300000
C	3.68647000	4.06684800	0.56360900
C	3.89402500	5.23702600	1.31215800
C	4.66083400	3.64672700	-0.35476200
C	5.06257900	5.97255700	1.14552100
H	3.12663500	5.54586300	2.01376600
C	5.82866500	4.38805700	-0.52181000
C	6.03090600	5.54920100	0.22851500
H	5.22256000	6.87594300	1.72595500
H	6.57901700	4.06671400	-1.23789900
C	2.25750200	2.05457300	0.05761900
C	2.04957100	0.99673800	-0.50908800
C	1.94205200	-0.25655800	-1.18455900
C	0.80021800	-1.06063000	-1.18335600
C	0.81174300	-2.37888500	-1.83076800
C	0.11782300	-3.44254400	-1.20902000
C	1.44742600	-2.63650700	-3.06790700
C	0.11155900	-4.71814600	-1.76456400
C	1.39438400	-3.90278400	-3.64391800
H	1.94110500	-1.82894800	-3.59438100
C	0.74304200	-4.95156300	-2.98931500
H	-0.40704300	-5.52492700	-1.25566700
H	1.86105800	-4.07226400	-4.60973500
H	0.71254200	-5.93931300	-3.43921400
H	6.94140500	6.12649700	0.09748500
H	4.49291500	2.74779000	-0.94029400
H	-0.39942300	-3.25493300	-0.27324400
Au	-0.94673300	-0.35397900	-0.36926900
C	-2.72005200	0.36277200	0.39539900
C	-4.65380900	1.51413700	0.63214400
C	-4.44678100	0.82650400	1.78364400
H	-5.02505800	0.76624700	2.69137500
H	-5.45037800	2.17465900	0.33052300

N	-3.58795900	1.21939100	-0.20854900
N	-3.26011600	0.12218300	1.62111900
C	-3.47298400	1.72720100	-1.56185000
C	-2.87349000	2.98696000	-1.76192000
C	-4.00831800	0.95648100	-2.61396000
C	-2.82332600	3.47014400	-3.07534700
C	-3.92114600	1.48863100	-3.90623200
C	-3.33916000	2.73165600	-4.13650600
H	-2.37317700	4.43861100	-3.26776900
H	-4.32227400	0.92320500	-4.74147400
H	-3.28937800	3.12758700	-5.14659500
C	-2.73133300	-0.79338300	2.61140400
C	-3.22226400	-2.11554800	2.62301200
C	-1.78453500	-0.31936100	3.54046800
C	-2.72239900	-2.97738700	3.60688800
C	-1.32534700	-1.22647300	4.50439500
C	-1.78553600	-2.53951900	4.53895100
H	-3.07858500	-4.00216600	3.64746400
H	-0.60079700	-0.89479100	5.24135100
H	-1.41817300	-3.22272900	5.29926500
C	-4.26639700	-2.62581600	1.63355400
C	-5.56194300	-3.05035000	2.35328600
C	-3.71513200	-3.77257300	0.76452900
H	-4.52567600	-1.80788900	0.95553800
H	-5.97598500	-2.23186700	2.95047400
H	-6.31987200	-3.35513500	1.62444800
H	-5.38903400	-3.89676500	3.02582400
H	-2.83438900	-3.45152800	0.19986100
H	-3.43299400	-4.63899200	1.37189000
H	-4.47410000	-4.10411300	0.04821700
C	-1.27072600	1.11637500	3.54606900
C	0.26702700	1.17577900	3.49290100
C	-1.81440400	1.89511000	4.76078000
H	-1.63876800	1.61567300	2.64548300
H	0.65062600	0.60296100	2.64258400
H	0.59973600	2.20942600	3.36988400
H	0.71932800	0.77623000	4.40731000
H	-2.90909300	1.90983900	4.77286900
H	-1.47813000	1.44846800	5.70257200
H	-1.46136300	2.93098800	4.73611900
C	-4.68025300	-0.39718900	-2.40238200
C	-3.93704200	-1.52200100	-3.14887900
C	-6.16842200	-0.35312900	-2.80280900
H	-4.63952800	-0.63853000	-1.33636700

H	-2.89157900	-1.58517500	-2.83088400
H	-4.41372700	-2.48778000	-2.95032900
H	-3.95081000	-1.36328800	-4.23216300
H	-6.70932300	0.42209000	-2.25086600
H	-6.29123900	-0.14682000	-3.87098300
H	-6.64785800	-1.31515100	-2.59394800
C	-2.31070400	3.82649900	-0.61961900
C	-3.24143300	5.01258400	-0.29325400
C	-0.88088900	4.31687700	-0.91133700
H	-2.25548400	3.19499500	0.27210200
H	-4.24721400	4.67688600	-0.02033600
H	-2.83994600	5.59291800	0.54370700
H	-3.33812100	5.68457900	-1.15258500
H	-0.22870300	3.48545700	-1.19394500
H	-0.86249500	5.05446000	-1.72064200
H	-0.45656500	4.78728400	-0.02026900
C	3.79529800	-1.79506400	0.34883700
C	4.75371800	-2.44001000	1.13335700
C	6.04816600	-2.61400900	0.63827000
C	6.35438400	-2.13361000	-0.63950300
C	5.37011500	-1.49167400	-1.39124300
H	6.80370400	-3.11333400	1.23379700
H	2.76303600	-1.61652900	0.64540600
H	5.51658300	-1.08669000	-2.38564900
Cl	7.94098700	-2.32094300	-1.29957400
Cl	4.32079200	-3.01779700	2.70470600
N	4.16244700	-1.36564000	-0.84828600
O	3.06936600	-0.64074400	-1.83334500

Zero-point correction= 0.859993 (Hartree/Particle)
Thermal correction to Energy= 0.917264
Thermal correction to Enthalpy= 0.918208
Thermal correction to Gibbs Free Energy= 0.756656
Sum of electronic and zero-point Energies= -3266.139337
Sum of electronic and thermal Energies= -3266.082067
Sum of electronic and thermal Enthalpies= -3266.081122
Sum of electronic and thermal Free Energies= -3266.242674

1-INT2'-1

C	4.61742700	-0.44737300	0.85145700
O	4.04384200	-0.79124100	1.87894200
C	6.08193100	-0.32432100	0.71319400
C	6.88257600	-0.56664000	1.84332400
C	6.68025200	0.02048300	-0.50983200

C	8.26491400	-0.46196500	1.74700700
H	6.39970400	-0.83355500	2.77724400
C	8.06614900	0.12250400	-0.60089000
C	8.85700400	-0.11752300	0.52583000
H	8.88554900	-0.64800900	2.61784200
H	8.53027700	0.38489300	-1.54625000
C	3.77840300	-0.13727000	-0.31526700
C	2.97871200	0.08355800	-1.20558400
C	1.98603800	0.38957700	-2.21019100
C	0.88318700	1.27910500	-1.74179100
C	0.89294400	2.64053200	-2.13566500
C	-0.13114900	3.52128800	-1.67281300
C	1.91257600	3.17249800	-2.98499000
C	-0.12766500	4.85835100	-2.02985900
C	1.89956000	4.50718100	-3.34760300
H	2.68612300	2.51573400	-3.36724200
C	0.88414600	5.34903500	-2.86800600
H	-0.90485200	5.52394500	-1.66988800
H	2.66996200	4.90415300	-4.00004300
H	0.88099600	6.39716800	-3.15325400
H	9.93759900	-0.03798200	0.45345500
H	6.06191000	0.19906400	-1.38453000
H	-0.90605500	3.12262400	-1.02631300
Au	-0.49010900	0.31454800	-0.60915900
C	-1.84365900	-0.68431300	0.56918400
C	-3.34048200	-1.15477100	2.19227400
C	-3.12928100	-2.29646200	1.48453100
H	-3.54369800	-3.28606400	1.59067300
H	-3.97254100	-0.95033500	3.04142100
N	-2.54737900	-0.17477700	1.61469000
N	-2.20688900	-1.99145600	0.49554600
C	-2.48048000	1.19951100	2.07027600
C	-1.46479300	1.55986200	2.97919300
C	-3.44799100	2.10837200	1.59492200
C	-1.43497000	2.89436100	3.40458500
C	-3.36577100	3.42811700	2.05623300
C	-2.37153300	3.81852800	2.94989400
H	-0.66941500	3.21026300	4.10619500
H	-4.09585700	4.15640000	1.71675900
H	-2.33139100	4.84599600	3.29953300
C	-1.70520500	-2.94721600	-0.47408100
C	-2.35669200	-3.04514800	-1.72011100
C	-0.60396000	-3.74958800	-0.11385500
C	-1.85310200	-3.98207000	-2.63073700

C	-0.14926200	-4.67084800	-1.06560500
C	-0.76228100	-4.78512900	-2.31003500
H	-2.32497600	-4.08577400	-3.60266500
H	0.69691900	-5.30736700	-0.82690200
H	-0.39074100	-5.50611400	-3.03199000
C	-3.56695000	-2.19689200	-2.09974100
C	-4.81034800	-3.07257400	-2.35335600
C	-3.26570200	-1.29496400	-3.31245700
H	-3.80320100	-1.53843800	-1.25819500
H	-5.04762300	-3.69394700	-1.48406500
H	-5.68030700	-2.44379100	-2.56885600
H	-4.66443800	-3.73969500	-3.20882300
H	-2.40473700	-0.64596800	-3.12054400
H	-3.04394400	-1.88569600	-4.20691500
H	-4.12969100	-0.66158800	-3.53914900
C	0.09113100	-3.65706500	1.24167600
C	1.57240700	-3.26100700	1.09291500
C	-0.05607300	-4.96960700	2.03692800
H	-0.39493000	-2.86912600	1.82524500
H	1.68055900	-2.31512500	0.55465900
H	2.03737800	-3.13895400	2.07560000
H	2.13840300	-4.02449100	0.54916300
H	-1.10752100	-5.23759800	2.18252500
H	0.43032800	-5.80490000	1.52301800
H	0.40893600	-4.87047300	3.02299100
C	-4.55764400	1.71242300	0.62417300
C	-4.44245000	2.47450500	-0.71047300
C	-5.95193000	1.90601300	1.25244500
H	-4.44995500	0.64793800	0.39587800
H	-3.47519200	2.29257300	-1.19093400
H	-5.22714700	2.15100100	-1.40187600
H	-4.55298700	3.55463300	-0.56815300
H	-6.05249500	1.34428500	2.18629000
H	-6.14983000	2.95923000	1.47603800
H	-6.73001900	1.56160500	0.56391700
C	-0.42793700	0.57283700	3.50759800
C	-0.56400700	0.37805100	5.03085100
C	1.00374600	0.99786300	3.12610600
H	-0.61157100	-0.39901200	3.04011300
H	-1.56695800	0.03505500	5.30407900
H	0.15740000	-0.36615600	5.38260500
H	-0.37147500	1.30898100	5.57374200
H	1.10176200	1.13427300	2.04416900
H	1.28424300	1.93891900	3.61105900

H	1.72725400	0.23554600	3.42911700
O	1.97565600	-0.06508300	-3.34453400

Zero-point correction= 0.789593 (Hartree/Particle)
Thermal correction to Energy= 0.839818
Thermal correction to Enthalpy= 0.840762
Thermal correction to Gibbs Free Energy= 0.696013
Sum of electronic and zero-point Energies= -2098.794890
Sum of electronic and thermal Energies= -2098.744665
Sum of electronic and thermal Enthalpies= -2098.743721
Sum of electronic and thermal Free Energies= -2098.888471

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C	0.25064800	-3.15600100	-1.49901300
O	0.17454900	-3.73820700	-2.58205600
C	-0.29747200	-3.74490700	-0.25240800
C	-1.16321200	-4.84622700	-0.38083000
C	0.10328200	-3.31753400	1.02528100
C	-1.62558700	-5.50319300	0.75370400
H	-1.44737800	-5.17377800	-1.37475500
C	-0.35716900	-3.98619100	2.15808500
C	-1.22114900	-5.07601300	2.02396000
H	-2.29315500	-6.35316500	0.65297600
H	-0.03309100	-3.66490500	3.14285400
C	0.97037000	-1.87377800	-1.42656800
C	1.21467200	-0.66026200	-1.12365000
C	2.14958900	0.33605900	-1.31932400
C	2.95286600	1.24617500	-1.45440000
C	3.92681100	2.26233500	-1.63898000
C	4.78015600	2.23053200	-2.76289800
C	4.05633400	3.30688700	-0.69876000
C	5.73718900	3.22465000	-2.93868100
C	5.02087800	4.29217900	-0.88339800
H	3.39987400	3.32672600	0.16514200
C	5.86036800	4.25433600	-2.00103800
H	6.38934400	3.19760900	-3.80599100
H	5.12155700	5.09213500	-0.15632000
H	6.61034100	5.02684700	-2.14107100
H	-1.57510100	-5.59791100	2.90804800
H	0.79549600	-2.48894900	1.12877800
H	4.67650200	1.42736100	-3.48510600
Au	-0.64189400	0.02318500	-0.24671400
C	-2.26090000	1.05591700	0.41185800
C	-4.34800300	1.87689700	0.65365600

C	-3.51656000	2.65208200	1.39624100
H	-3.70871100	3.51334000	2.01539100
H	-5.41310600	1.92400800	0.49519400
N	-3.56342700	0.89936800	0.05658400
N	-2.23783000	2.13697400	1.23562000
C	-4.08734200	-0.13584400	-0.81336200
C	-3.99022400	0.03885300	-2.20880900
C	-4.70555300	-1.25446400	-0.21772300
C	-4.51552200	-0.97828200	-3.01598300
C	-5.21836200	-2.23304900	-1.07767000
C	-5.11955000	-2.10207600	-2.46011500
H	-4.45927500	-0.88163600	-4.09550000
H	-5.70438900	-3.10804500	-0.65815900
H	-5.52402300	-2.87458500	-3.10729600
C	-1.05194200	2.71400800	1.83695900
C	-0.60636200	2.20577900	3.07357500
C	-0.41894800	3.78150200	1.16874200
C	0.53310600	2.79674400	3.63326500
C	0.71127900	4.33687300	1.78226400
C	1.18543100	3.84956100	2.99754400
H	0.90811200	2.43367900	4.58498400
H	1.22038600	5.16810900	1.30427300
H	2.06103800	4.29873000	3.45692600
C	-1.31698600	1.07790500	3.81548400
C	-1.87046100	1.56143700	5.17077400
C	-0.40161200	-0.14841700	3.99379800
H	-2.17146100	0.75572700	3.21279900
H	-2.54839900	2.41158900	5.04623600
H	-2.42363700	0.75605500	5.66456300
H	-1.06679600	1.87381100	5.84529700
H	-0.04580500	-0.51827700	3.02672300
H	0.47406400	0.08703300	4.60732800
H	-0.94734100	-0.95740100	4.49067600
C	-0.92081500	4.35354600	-0.15444400
C	0.14871800	4.26386900	-1.25947600
C	-1.42137000	5.80168700	0.01926800
H	-1.77400400	3.75422500	-0.48626700
H	0.48902800	3.23388800	-1.40260500
H	-0.25951700	4.62445300	-2.20920100
H	1.02536200	4.87658000	-1.02616400
H	-2.21112000	5.86709700	0.77451500
H	-0.61160000	6.47044900	0.32830900
H	-1.82357700	6.18111300	-0.92547300
C	-4.86762700	-1.41101300	1.29230700

C	-4.32075000	-2.75576400	1.80397000
C	-6.34218600	-1.22606500	1.70679200
H	-4.28736700	-0.62381800	1.78368600
H	-3.26893400	-2.88877100	1.53839800
H	-4.40663300	-2.80272900	2.89461300
H	-4.88046300	-3.60377500	1.39659600
H	-6.73464100	-0.25401600	1.39109700
H	-6.97708700	-1.99805200	1.26002600
H	-6.44564100	-1.29530700	2.79446200
C	-3.39465300	1.28477800	-2.85877500
C	-4.48987600	2.10846900	-3.56720400
C	-2.24725900	0.94138300	-3.82761300
H	-2.97230200	1.91602800	-2.07140500
H	-5.28908000	2.39266200	-2.87532700
H	-4.06451400	3.02457900	-3.98965800
H	-4.94555600	1.54379100	-4.38694700
H	-1.45521200	0.37749700	-3.32432400
H	-2.59786500	0.34416400	-4.67522800
H	-1.80760500	1.85892600	-4.23173900
C	4.71918100	-3.16076800	-0.32420800
C	4.43040200	-2.67266000	-1.54094300
H	4.24917200	-4.10061500	-0.03067500
H	4.87852100	-1.74939300	-1.90056500
C	5.62913100	-2.59345300	0.68090800
C	5.88626800	-3.33096800	1.84988200
C	6.25808000	-1.34260500	0.53255900
C	6.74598200	-2.84558600	2.83418800
H	5.41050100	-4.29988100	1.98050800
C	7.11458400	-0.85681600	1.51558900
H	6.07403500	-0.74294100	-0.35365600
C	7.36437500	-1.60581100	2.67010200
H	6.93443800	-3.43610500	3.72589300
H	7.59234000	0.10949700	1.38218200
H	8.03647000	-1.22462400	3.43305700
C	3.51823800	-3.36224100	-2.50096600
H	3.08249600	-4.26383700	-2.05220300
H	4.06124300	-3.66395000	-3.40847900
O	2.47259100	-2.44665700	-2.91377600
H	1.80248400	-2.95507700	-3.40685400

Zero-point correction=	0.953387 (Hartree/Particle)
Thermal correction to Energy=	1.012813
Thermal correction to Enthalpy=	1.013757
Thermal correction to Gibbs Free Energy=	0.845889
Sum of electronic and zero-point Energies=	-2447.592368

Sum of electronic and thermal Energies= -2447.532942
Sum of electronic and thermal Enthalpies= -2447.531998
Sum of electronic and thermal Free Energies= -2447.699865

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C	0.90603100	3.02304000	-0.97092800
O	1.20247300	2.97474400	-2.14989500
C	1.45592800	4.03287100	-0.02902100
C	2.32526700	5.00635800	-0.55164200
C	1.13782900	4.04622000	1.33806800
C	2.86018600	5.98252300	0.28172700
H	2.55878900	4.97973400	-1.61057200
C	1.68040700	5.02422600	2.17000300
C	2.53863900	5.99221300	1.64332300
H	3.52601800	6.73736400	-0.12522200
H	1.43353900	5.03279400	3.22721000
C	-0.05869400	1.95602100	-0.42506100
C	-1.29233300	2.33370400	-0.27994700
C	-2.25190000	3.29233500	-0.32208100
C	-3.13623400	4.14147300	-0.35830700
C	-4.13261700	5.14501900	-0.41102000
C	-4.78841200	5.43084400	-1.62949900
C	-4.47707400	5.86674900	0.75371200
C	-5.76614900	6.41780100	-1.67486100
C	-5.45762100	6.85014400	0.69443500
H	-3.96885300	5.64535300	1.68627900
C	-6.10146000	7.12604700	-0.51627900
H	-6.26774400	6.63814900	-2.61168600
H	-5.72132200	7.40439700	1.58947700
H	-6.86573200	7.89614300	-0.55725100
H	2.95757100	6.75518200	2.29291200
H	0.47117000	3.29509300	1.74789800
H	-4.51753000	4.87690000	-2.52214900
Au	0.88183700	0.12437000	-0.22096400
C	1.92453700	-1.62715500	-0.09295400
C	2.57681000	-3.78475700	-0.24864300
C	3.63068800	-3.07315200	0.22801300
H	4.62594100	-3.37659900	0.50991200
H	2.46730400	-4.83417900	-0.46935500
N	1.53773900	-2.88299400	-0.43984800
N	3.21455900	-1.75217500	0.31728600
C	0.23309700	-3.25283200	-0.94828800
C	-0.73858800	-3.70491500	-0.03202000

C	0.00906100	-3.18437000	-2.33833500
C	-1.97850800	-4.09372100	-0.55445000
C	-1.25144600	-3.58344300	-2.80121400
C	-2.23213400	-4.03478700	-1.92244000
H	-2.75401700	-4.44956100	0.11579100
H	-1.46119000	-3.55012100	-3.86573700
H	-3.19776000	-4.35205600	-2.30547800
C	4.05495900	-0.66371500	0.77682500
C	4.83927600	0.02454100	-0.17120700
C	4.06705700	-0.36083300	2.15298100
C	5.65865300	1.05432400	0.30736100
C	4.90399700	0.68148300	2.57005300
C	5.69156900	1.38099600	1.66014000
H	6.28113900	1.60556400	-0.38997400
H	4.94081000	0.94584500	3.62220200
H	6.33631300	2.18295400	2.00718200
C	4.84951400	-0.32795200	-1.65615300
C	6.18215400	-0.99745400	-2.05081800
C	4.56036000	0.89252800	-2.55060500
H	4.05197400	-1.05461400	-1.83911900
H	6.37511200	-1.89604200	-1.45579500
H	6.16590300	-1.28702500	-3.10648700
H	7.02639600	-0.31564100	-1.90453900
H	3.60679500	1.36644700	-2.29995000
H	5.34590800	1.65060500	-2.46814500
H	4.51737600	0.58322900	-3.59995600
C	3.21974400	-1.10868400	3.17818300
C	2.18764200	-0.17529800	3.84093900
C	4.09569600	-1.80925200	4.23521500
H	2.65802700	-1.88876400	2.65536500
H	1.53725100	0.28986100	3.09295800
H	1.55894800	-0.73830200	4.53886700
H	2.67583100	0.62526000	4.40636500
H	4.81084200	-2.49621400	3.77196500
H	4.66545800	-1.08696300	4.82852800
H	3.47057800	-2.38441400	4.92580300
C	1.07009400	-2.72366800	-3.33360400
C	0.62154000	-1.46639600	-4.10342400
C	1.45951300	-3.86017300	-4.29985200
H	1.96965200	-2.45301300	-2.77309700
H	0.39390400	-0.64099200	-3.42154600
H	1.41517800	-1.13472500	-4.78045300
H	-0.26916300	-1.66115600	-4.70985900
H	1.81213600	-4.74420900	-3.75911500

H	0.61239900	-4.16710900	-4.92176900
H	2.25998900	-3.53066500	-4.96985000
C	-0.47989800	-3.80869700	1.46860500
C	-0.44918100	-5.28149700	1.92453000
C	-1.50145500	-2.99946900	2.28994300
H	0.50589300	-3.38227400	1.67633100
H	0.30422400	-5.85643200	1.37675400
H	-0.21415900	-5.34595500	2.99186700
H	-1.41725600	-5.76777800	1.76587200
H	-1.51215900	-1.94676300	1.98997300
H	-2.51736000	-3.39066500	2.17672200
H	-1.24696900	-3.04433200	3.35393200
C	-4.80060600	-1.69138200	-0.02548600
C	-4.34568000	-0.57488600	0.56734100
H	-4.64350200	-1.79281400	-1.09984900
H	-4.47903300	-0.40054900	1.63231500
C	-5.51466200	-2.81345400	0.59696800
C	-5.72178200	-2.91943900	1.98611900
C	-6.01497300	-3.83599400	-0.22950000
C	-6.40493400	-4.00707800	2.52167400
H	-5.34698900	-2.14846400	2.65229000
C	-6.70099700	-4.92491000	0.30683200
H	-5.87367500	-3.76516500	-1.30531900
C	-6.89808000	-5.01404300	1.68527400
H	-6.55628800	-4.07124100	3.59510200
H	-7.08365500	-5.69981400	-0.35052400
H	-7.43247000	-5.85968300	2.10721900
C	-3.65979300	0.51618600	-0.18571200
H	-4.15899700	1.47986900	-0.05230900
H	-3.59847900	0.29881800	-1.25781700
O	-2.32051700	0.74429000	0.35180100
H	-1.73112900	0.00792300	0.10517700

Zero-point correction= 0.953716 (Hartree/Particle)
Thermal correction to Energy= 1.012853
Thermal correction to Enthalpy= 1.013797
Thermal correction to Gibbs Free Energy= 0.847297
Sum of electronic and zero-point Energies= -2447.601851
Sum of electronic and thermal Energies= -2447.542714
Sum of electronic and thermal Enthalpies= -2447.541770
Sum of electronic and thermal Free Energies= -2447.708270

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C	4.98989300	1.69882400	0.84940700

O	5.33586200	1.30586500	1.95876000
C	5.95673700	2.02605000	-0.23217700
C	7.32821000	1.89067000	0.03768300
C	5.53557600	2.46071400	-1.49780200
C	8.26409500	2.18624500	-0.94790300
H	7.63152000	1.55765100	1.02458100
C	6.47601200	2.75445000	-2.48363700
C	7.83904400	2.61768200	-2.20940900
H	9.32440400	2.08452500	-0.73768200
H	6.14913500	3.09149000	-3.46262100
C	3.56789500	1.84935000	0.56880800
C	2.35860500	1.91963000	0.43874000
C	0.94913500	1.91441600	0.29723200
C	0.25849500	3.00321900	0.31153300
C	-0.04023600	4.37572900	0.44415700
C	-0.04455200	4.96488000	1.73133800
C	-0.26988900	5.17911400	-0.69901400
C	-0.25110300	6.33321100	1.86375300
C	-0.48711600	6.54181800	-0.55036400
H	-0.27328400	4.71533600	-1.67943700
C	-0.47508600	7.11752300	0.72732700
H	-0.24042800	6.79027200	2.84777300
H	-0.65965400	7.16236600	-1.42364500
H	-0.64038600	8.18521000	0.83602000
H	8.57134200	2.84907800	-2.97736600
H	4.47477400	2.56927700	-1.70367000
H	0.13183400	4.34137600	2.60157200
Au	0.36972600	-0.10483900	0.09906700
C	0.07614300	-2.11216200	-0.07733100
C	0.52560900	-4.32304100	-0.02076400
C	-0.72248400	-4.17230900	-0.53567500
H	-1.44358700	-4.89596800	-0.87993200
H	1.11409800	-5.20519000	0.17356200
N	1.00284500	-3.04984600	0.25454200
N	-0.98368300	-2.80806400	-0.56320300
C	2.31329100	-2.76051300	0.80605600
C	3.39115300	-2.58095500	-0.08419500
C	2.44843200	-2.66918200	2.20590700
C	4.63871600	-2.28143100	0.47630200
C	3.71986700	-2.36342800	2.70568900
C	4.80211400	-2.16418200	1.85365900
H	5.49202000	-2.13006600	-0.17735000
H	3.86264300	-2.27281200	3.77767800
H	5.77387300	-1.91059200	2.26466300

C	-2.22184200	-2.22465800	-1.03574500
C	-3.28341000	-2.08021000	-0.11955100
C	-2.31739800	-1.84854400	-2.39018300
C	-4.46819700	-1.50853500	-0.59868200
C	-3.52965400	-1.28744000	-2.81230500
C	-4.59095000	-1.11400200	-1.92854600
H	-5.30642900	-1.36755400	0.07574000
H	-3.64185200	-0.98611300	-3.84916800
H	-5.52088200	-0.67173600	-2.27275900
C	-3.18419300	-2.51452400	1.34061200
C	-4.28149100	-3.53247100	1.70778400
C	-3.21320300	-1.30055600	2.28946100
H	-2.22171500	-3.01350700	1.48677800
H	-4.25369700	-4.40578900	1.04884100
H	-4.14645600	-3.87975200	2.73711900
H	-5.28166400	-3.09372300	1.63557900
H	-2.38304000	-0.61695900	2.08010700
H	-4.14910900	-0.74148200	2.18864800
H	-3.12734600	-1.62710500	3.33099400
C	-1.18069000	-2.03720200	-3.39033300
C	-0.68968100	-0.68795700	-3.95032300
C	-1.58729100	-2.99525000	-4.52788000
H	-0.33612200	-2.49597900	-2.86779000
H	-0.35956400	-0.02122000	-3.14699500
H	0.15331100	-0.84374500	-4.63140000
H	-1.47821500	-0.17550600	-4.51116900
H	-1.90753000	-3.96688300	-4.13888400
H	-2.41117100	-2.58704400	-5.12206600
H	-0.74239300	-3.16208900	-5.20361300
C	1.28829200	-2.88751800	3.17262100
C	0.99337800	-1.61945900	3.99751500
C	1.54374300	-4.09937500	4.09091300
H	0.38981000	-3.10883000	2.58806000
H	0.77826000	-0.76479400	3.34779000
H	0.12817100	-1.78264400	4.64874200
H	1.84165500	-1.34847000	4.63387400
H	1.71910400	-5.01171400	3.51205100
H	2.41704700	-3.93966000	4.73120100
H	0.68133800	-4.27180200	4.74307400
C	3.25105500	-2.69828100	-1.59932900
C	4.07946700	-3.87647700	-2.14906900
C	3.62263300	-1.38053100	-2.30655400
H	2.20172200	-2.90388800	-1.83266700
H	3.79452100	-4.82230700	-1.67739600

H	3.92971100	-3.97709400	-3.22894700
H	5.14991100	-3.72822400	-1.97445000
H	3.01655500	-0.54738100	-1.93690600
H	4.67437100	-1.12093800	-2.14978100
H	3.46139700	-1.47097200	-3.38591800
C	-5.18589400	1.97685800	0.82213300
C	-4.22597700	2.53128000	0.06407800
H	-4.96218900	1.80634800	1.87627600
H	-4.37848800	2.72465900	-0.99536000
C	-6.53280600	1.56117500	0.40902600
C	-7.35064200	0.89988500	1.34311000
C	-7.04846300	1.78949700	-0.88161800
C	-8.63231300	0.46909100	1.00143000
H	-6.97544300	0.72785800	2.34913900
C	-8.32783700	1.36027300	-1.22256100
H	-6.45243800	2.31886000	-1.61875500
C	-9.12478100	0.69602900	-0.28394700
H	-9.24657700	-0.03761200	1.73968000
H	-8.71101100	1.55138800	-2.22064200
H	-10.12375200	0.36668100	-0.55275900
C	-2.89973900	2.95258200	0.61190400
H	-2.80761700	2.69189300	1.67403300
H	-2.75671100	4.03355400	0.51285600
O	-1.80567500	2.38314300	-0.14853500
H	-1.81176400	1.41493300	-0.05448900

Zero-point correction= 0.952939 (Hartree/Particle)
Thermal correction to Energy= 1.012514
Thermal correction to Enthalpy= 1.013458
Thermal correction to Gibbs Free Energy= 0.845230
Sum of electronic and zero-point Energies= -2447.586373
Sum of electronic and thermal Energies= -2447.526798
Sum of electronic and thermal Enthalpies= -2447.525853
Sum of electronic and thermal Free Energies= -2447.694082

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C	5.61151300	-1.11547100	-1.44447900
O	5.91276500	-0.01744900	-1.91507700
C	6.53839200	-2.25584300	-1.32096000
C	6.11097200	-3.49670000	-0.82178700
C	7.87430200	-2.07957800	-1.71920700
C	7.01328200	-4.55213200	-0.72010400
H	5.07578400	-3.63363700	-0.52096700
C	8.77107600	-3.13670300	-1.61534900

C	8.34159000	-4.37183300	-1.11600900
H	6.68501400	-5.51301700	-0.33679200
H	9.80385700	-3.00436800	-1.92180500
C	4.23965300	-1.26101500	-0.99023600
C	3.06403600	-1.20418900	-0.63547300
C	1.77494400	-1.13498300	-0.26675100
C	0.63398500	-1.52835800	0.22033200
C	0.52737500	-2.80690700	0.97078300
C	-0.69821900	-3.49614700	1.03456700
C	1.64444000	-3.35288400	1.63647000
C	-0.79515200	-4.70546100	1.71979700
C	1.53590700	-4.55061200	2.33554800
H	2.58996400	-2.82027500	1.62785800
C	0.31789700	-5.23550900	2.37427500
H	-1.74773000	-5.22495400	1.75147900
H	2.40201300	-4.94956500	2.85481000
H	0.23659900	-6.17091100	2.91939900
H	9.04440900	-5.19584700	-1.03691700
H	8.18134300	-1.11288500	-2.10384600
H	-1.57137600	-3.08719000	0.53771700
Au	-1.10668400	-0.38204000	-0.03814300
C	-2.88013700	0.60226800	-0.25849700
C	-4.46214400	2.15108100	-0.72045100
C	-5.09569700	1.05414000	-0.23184100
H	-6.14050900	0.85439800	-0.05658200
H	-4.84207700	3.10157200	-1.05875900
N	-3.10417800	1.85780700	-0.73158400
N	-4.11287100	0.11347300	0.04530700
C	-2.08625300	2.77800400	-1.19554600
C	-1.53069800	3.68659700	-0.27297300
C	-1.72466800	2.74827100	-2.55756500
C	-0.57247100	4.58595300	-0.75836100
C	-0.75635200	3.66720600	-2.98362200
C	-0.18740900	4.57820800	-2.09646400
H	-0.12817800	5.30762200	-0.07999900
H	-0.45892600	3.68156900	-4.02777900
H	0.55025600	5.29192400	-2.45150700
C	-4.38506400	-1.20756900	0.57670100
C	-4.64195200	-2.25518400	-0.33116400
C	-4.40672200	-1.37878400	1.97532800
C	-4.92212400	-3.51625100	0.21055000
C	-4.69553100	-2.66170700	2.45742600
C	-4.95051500	-3.71890200	1.58812500
H	-5.12767700	-4.34727600	-0.45692000

H	-4.72409200	-2.83240100	3.52893800
H	-5.18037700	-4.70310900	1.98581600
C	-4.63511500	-2.06691700	-1.84573800
C	-6.02682200	-2.33584000	-2.45205800
C	-3.55754600	-2.93858000	-2.51940600
H	-4.38377100	-1.02382200	-2.05960600
H	-6.79140400	-1.69388300	-2.00334600
H	-6.01486800	-2.14636900	-3.53016300
H	-6.33628700	-3.37504900	-2.30169500
H	-2.56210500	-2.71742400	-2.12076800
H	-3.75080500	-4.00574100	-2.37002600
H	-3.54148300	-2.75488100	-3.59868100
C	-4.13945400	-0.24327800	2.95867100
C	-2.90497900	-0.53354400	3.83485100
C	-5.37951600	0.05297000	3.82543100
H	-3.92115100	0.66236800	2.38488100
H	-2.01498200	-0.71191100	3.22283200
H	-2.70165200	0.31581900	4.49516400
H	-3.05887400	-1.41370100	4.46747800
H	-6.25229200	0.29379100	3.21023000
H	-5.64290900	-0.80307600	4.45486500
H	-5.18572700	0.90327900	4.48703100
C	-2.34755700	1.78530200	-3.56511300
C	-1.30473800	0.79640500	-4.12271100
C	-3.05533000	2.54178500	-4.70684900
H	-3.10838200	1.19250500	-3.04914900
H	-0.87746400	0.18028400	-3.32236800
H	-1.76782100	0.11764700	-4.84587900
H	-0.48916200	1.31787000	-4.63509900
H	-3.80985100	3.23373500	-4.32040100
H	-2.34771000	3.12288500	-5.30678500
H	-3.55486200	1.83537400	-5.37739900
C	-1.93594700	3.73131000	1.19711800
C	-2.62416900	5.06533900	1.54845000
C	-0.73499600	3.46357400	2.12489900
H	-2.66267000	2.93339700	1.37567700
H	-3.50380300	5.24122200	0.92122200
H	-2.94862400	5.06131400	2.59385100
H	-1.94602700	5.91432600	1.41451500
H	-0.25705800	2.50690900	1.89171300
H	0.02103300	4.25162800	2.03938800
H	-1.06242000	3.43637500	3.16921300
C	4.25014400	2.40766400	0.24192100
C	2.97178200	2.42090400	-0.17225500

H	4.96803600	1.85002800	-0.35982200
H	2.19926300	2.96540600	0.36550900
C	4.82006200	3.07849100	1.41696000
C	6.20783800	2.99523900	1.62807500
C	4.04780000	3.79885800	2.34793600
C	6.80739300	3.61135500	2.72544400
H	6.81814600	2.44300300	0.91792300
C	4.64507100	4.41209300	3.44445100
H	2.97251800	3.87575600	2.21683600
C	6.02761700	4.32235900	3.63799900
H	7.88144700	3.53673900	2.86705700
H	4.03349100	4.96290700	4.15321000
H	6.49033900	4.80364300	4.49432100
C	2.53083200	1.74468700	-1.42437800
H	3.35561000	1.19294600	-1.89095200
H	2.13334900	2.46480800	-2.15165800
O	1.42918400	0.83093500	-1.12120300
H	0.96065900	0.62743800	-1.94630200

Zero-point correction= 0.953023 (Hartree/Particle)
Thermal correction to Energy= 1.012125
Thermal correction to Enthalpy= 1.013069
Thermal correction to Gibbs Free Energy= 0.847521
Sum of electronic and zero-point Energies= -2447.586404
Sum of electronic and thermal Energies= -2447.527301
Sum of electronic and thermal Enthalpies= -2447.526357
Sum of electronic and thermal Free Energies= -2447.691905

3-TS1'-2

C	-1.62779200	4.29358000	0.88832800
O	-0.74429300	4.38480300	1.73663700
C	-2.61055100	5.36414100	0.60444300
C	-2.61544700	6.49993300	1.43129700
C	-3.51874000	5.27139500	-0.46214300
C	-3.52443600	7.52527200	1.19549100
H	-1.90288700	6.55275100	2.24741700
C	-4.42473900	6.30295700	-0.69706000
C	-4.42950600	7.42748700	0.13247000
H	-3.53165800	8.40172300	1.83585600
H	-5.12281600	6.23508800	-1.52557000
C	-1.71920400	3.05414400	0.12481700
C	-1.68449800	1.96723200	-0.43374300
C	-1.69318300	0.75302200	-1.07184000
C	-1.03137000	-0.34275600	-1.33461500

C	-1.40522600	-1.46597100	-2.20813200
C	-1.33840100	-2.78767300	-1.73145200
C	-1.81478700	-1.24170700	-3.53911300
C	-1.71283100	-3.85095900	-2.55016600
C	-2.16551800	-2.31538000	-4.35938000
H	-1.81185800	-0.23133900	-3.93941500
C	-2.12549300	-3.62019400	-3.86517900
H	-1.67279700	-4.86469500	-2.16353900
H	-2.46463800	-2.12929200	-5.38643500
H	-2.40314300	-4.45314300	-4.50333900
H	-5.13717400	8.23058000	-0.05047200
H	-3.50231900	4.40212000	-1.11358700
H	-1.00560300	-2.96950500	-0.71433700
Au	0.83123800	-0.34143500	-0.36506800
C	2.65924100	-0.38618000	0.53828900
C	4.30477800	-0.70455700	2.05372800
C	4.84152100	-0.03220200	1.00330700
H	5.84139900	0.32841300	0.82384500
H	4.74122500	-1.04915700	2.97723500
N	2.96623300	-0.91741100	1.75182000
N	3.82016900	0.15409000	0.08134300
C	2.04951700	-1.63244700	2.61683900
C	1.27206300	-0.89695400	3.53345500
C	2.00335300	-3.03835200	2.52338600
C	0.42083100	-1.62368100	4.37558800
C	1.13056000	-3.70902300	3.38892100
C	0.34844100	-3.01188900	4.30580200
H	-0.19005700	-1.09225600	5.09858800
H	1.06896700	-4.79211800	3.34826500
H	-0.31614600	-3.55352300	4.97256000
C	4.00035600	0.82506100	-1.19118300
C	4.36985700	0.05206700	-2.31030000
C	3.84081200	2.22408900	-1.24226500
C	4.57581200	0.73178200	-3.51705300
C	4.06332600	2.84800200	-2.47617900
C	4.42609300	2.11322400	-3.60120400
H	4.86354500	0.17112600	-4.40088500
H	3.95235900	3.92490700	-2.55380700
H	4.59649300	2.61945400	-4.54677200
C	4.56827200	-1.45963200	-2.25087700
C	6.04115300	-1.83991500	-2.50196400
C	3.63137200	-2.19741100	-3.22657000
H	4.31302800	-1.79921400	-1.24262000
H	6.70988300	-1.35108300	-1.78639400

H	6.17661600	-2.92229500	-2.40806000
H	6.36345300	-1.55080400	-3.50758600
H	2.58240100	-1.95181500	-3.03338400
H	3.85004200	-1.94081400	-4.26813400
H	3.75401600	-3.28048300	-3.12195500
C	3.44860500	3.06248500	-0.02989200
C	2.15660900	3.86006800	-0.28920800
C	4.59873900	3.99219200	0.40522300
H	3.24376300	2.38506800	0.80445600
H	1.34835300	3.20067400	-0.61979000
H	1.82639200	4.36256500	0.62444200
H	2.30361900	4.62506100	-1.05914300
H	5.50670300	3.42746700	0.64052500
H	4.84969900	4.71063900	-0.38202600
H	4.31213300	4.56053500	1.29587000
C	2.86120000	-3.83801800	1.54619200
C	1.99778100	-4.65252700	0.56405400
C	3.85853800	-4.74692200	2.29212000
H	3.44814300	-3.13429100	0.94868600
H	1.32620200	-4.00272100	-0.00604400
H	2.63581000	-5.18825300	-0.14643700
H	1.38724400	-5.39691400	1.08557300
H	4.50378500	-4.16987600	2.96204200
H	3.34079000	-5.49802500	2.89737300
H	4.49822200	-5.27725600	1.57937400
C	1.32494700	0.62379800	3.64053600
C	1.90703200	1.07208100	4.99569400
C	-0.05835300	1.25452100	3.39129800
H	1.99343400	0.99850000	2.86008200
H	2.91237100	0.66906000	5.15520900
H	1.96791400	2.16417700	5.03909700
H	1.27997900	0.74026200	5.82981700
H	-0.48130300	0.90742700	2.44322800
H	-0.76459800	1.00040900	4.18915100
H	0.01738300	2.34435700	3.34136100
C	-6.05606200	-1.01542300	-0.67442500
C	-4.94484200	-0.31976400	-0.36914400
H	-6.68947100	-0.62464300	-1.47251300
H	-4.27025200	-0.64845400	0.41818900
C	-6.54971300	-2.25029500	-0.05817000
C	-7.70381700	-2.85046400	-0.59270100
C	-5.92701800	-2.86308200	1.04618900
C	-8.21796100	-4.02694700	-0.05101600
H	-8.19977300	-2.38644800	-1.44148300

C	-6.44103100	-4.03654800	1.58757700
H	-5.04330000	-2.41566300	1.49113500
C	-7.58727800	-4.62384000	1.04104300
H	-9.11021300	-4.47425000	-0.47814400
H	-5.95223500	-4.49459600	2.44226800
H	-7.98693000	-5.53809800	1.46912700
C	-4.58679000	0.94328900	-1.07105800
H	-4.31912300	1.75338100	-0.38854500
H	-5.39024800	1.28886900	-1.72832800
O	-3.39317500	0.79980100	-1.93303800
H	-3.43706200	-0.07046700	-2.37290600

Zero-point correction= 0.953925 (Hartree/Particle)
Thermal correction to Energy= 1.012906
Thermal correction to Enthalpy= 1.013850
Thermal correction to Gibbs Free Energy= 0.847898
Sum of electronic and zero-point Energies= -2447.594638
Sum of electronic and thermal Energies= -2447.535658
Sum of electronic and thermal Enthalpies= -2447.534714
Sum of electronic and thermal Free Energies= -2447.700665

3-TS1-3

C	2.63061000	-0.73367500	-2.48510000
O	2.10323200	-1.49761000	-3.28057700
C	3.91718800	-0.03312400	-2.72343300
C	4.41126000	0.00589000	-4.03851200
C	4.64499200	0.56204100	-1.68001000
C	5.61955000	0.64029900	-4.30408100
H	3.83592700	-0.46686500	-4.82723300
C	5.85745100	1.19245300	-1.95334300
C	6.34202300	1.23468200	-3.26290700
H	6.00290000	0.67253100	-5.31913500
H	6.42918700	1.63885700	-1.14577800
C	1.95260800	-0.35921600	-1.23272800
C	1.29016500	0.53213600	-0.57594100
C	1.52835100	1.87200400	-0.28499100
C	1.69785200	3.04655900	0.00362800
C	1.94696800	4.41094700	0.30918000
C	3.15130100	5.02004700	-0.10394700
C	0.99815500	5.17030800	1.02614900
C	3.39700900	6.35546400	0.19737500
C	1.25406400	6.50576000	1.32003800
H	0.07071200	4.70153600	1.33943200
C	2.45098500	7.09971500	0.90846400

H	4.32499200	6.81908900	-0.12244800
H	0.52198600	7.08726900	1.87201000
H	2.64616000	8.14213700	1.14128600
H	7.28731100	1.72598600	-3.47361000
H	4.28162500	0.50525800	-0.65855100
H	3.87712100	4.43375000	-0.65800100
Au	-0.71970200	-0.04554900	-0.14543400
C	-2.69211700	-0.45954500	0.08625900
C	-4.66618900	-1.55463700	0.06675100
C	-4.92513600	-0.24535200	0.31980300
H	-5.85268900	0.27577000	0.49378800
H	-5.32238800	-2.40550300	-0.02006700
N	-3.28914700	-1.67104700	-0.07289200
N	-3.70260300	0.41378500	0.32753300
C	-2.57962200	-2.91094300	-0.31422800
C	-2.18120200	-3.21676200	-1.63590300
C	-2.31702400	-3.75308000	0.78420500
C	-1.46443200	-4.40631700	-1.82437500
C	-1.61154500	-4.93822800	0.52855200
C	-1.18193900	-5.25777800	-0.75568600
H	-1.13811900	-4.67836300	-2.82200800
H	-1.39702100	-5.61639100	1.34849400
H	-0.63397900	-6.17881600	-0.93077400
C	-3.54367200	1.83617000	0.56290600
C	-3.36189400	2.27855300	1.88852100
C	-3.59917600	2.71024900	-0.54127200
C	-3.22724700	3.65834400	2.08808500
C	-3.45720400	4.07836200	-0.27883400
C	-3.27413400	4.54909900	1.01868200
H	-3.09168600	4.03804700	3.09600600
H	-3.49503600	4.78393300	-1.10255700
H	-3.17603000	5.61579900	1.19766000
C	-3.31424200	1.33285400	3.08483100
C	-4.47794700	1.59979300	4.06033300
C	-1.95523700	1.40610200	3.80835600
H	-3.42780600	0.30839100	2.71753400
H	-5.44849200	1.51282300	3.56174900
H	-4.45461900	0.88082900	4.88548400
H	-4.41612800	2.60320300	4.49350500
H	-1.12874100	1.18029100	3.12667300
H	-1.77839600	2.40009800	4.23175900
H	-1.92531800	0.68623800	4.63280800
C	-3.81267500	2.23331900	-1.97493600
C	-2.61729300	2.59934000	-2.87632000

C	-5.13355800	2.77641200	-2.55563200
H	-3.88802500	1.14172700	-1.96610700
H	-1.68228000	2.18441800	-2.48625800
H	-2.77086900	2.20657800	-3.88660900
H	-2.49318800	3.68386700	-2.95902300
H	-5.99156300	2.49179800	-1.93839100
H	-5.12209700	3.86885000	-2.62467200
H	-5.29545900	2.38244000	-3.56401400
C	-2.76586700	-3.43472000	2.20827700
C	-1.56583800	-3.27191600	3.16101100
C	-3.75233800	-4.49634100	2.73477800
H	-3.29657200	-2.47835500	2.19595200
H	-0.88979700	-2.48261100	2.81763400
H	-1.91325100	-3.00667900	4.16458800
H	-0.98921700	-4.19861500	3.24701600
H	-4.62474700	-4.59474100	2.08115900
H	-3.28177600	-5.48186500	2.80984500
H	-4.10603800	-4.22165200	3.73342300
C	-2.56925500	-2.34869500	-2.83111900
C	-3.89427000	-2.85555300	-3.44235700
C	-1.47596900	-2.26041400	-3.91060900
H	-2.74170000	-1.33153500	-2.46611500
H	-4.70660200	-2.86089000	-2.70881200
H	-4.19769000	-2.21546200	-4.27693000
H	-3.78169200	-3.87578000	-3.82383100
H	-0.50794500	-1.94866800	-3.50675900
H	-1.33222900	-3.21444100	-4.42802500
H	-1.77251800	-1.53049600	-4.67007600
C	3.60124700	-2.00066200	1.91438400
C	3.01947500	-2.74029200	0.95587400
H	2.98023200	-1.27005500	2.43499200
H	3.58177300	-3.47895100	0.38900100
C	4.99640100	-2.04957300	2.36953300
C	5.93883300	-2.96861500	1.86994200
C	5.41586100	-1.13525300	3.35218200
C	7.25027000	-2.96428700	2.33411200
H	5.64500500	-3.69552300	1.11897300
C	6.72950500	-1.13120200	3.81835000
H	4.69971400	-0.42206900	3.75330500
C	7.65211300	-2.04598000	3.30975400
H	7.96282400	-3.68194200	1.93838600
H	7.03099600	-0.41720900	4.57897800
H	8.67575700	-2.04867200	3.67181100
C	1.56975400	-2.63603400	0.61849200

H	1.07834500	-1.85016400	1.20868100
H	1.04084400	-3.57970700	0.80030100
O	1.43154100	-2.34695200	-0.79724600
H	0.53699400	-2.57599500	-1.10231600

Zero-point correction= 0.952972 (Hartree/Particle)
Thermal correction to Energy= 1.012197
Thermal correction to Enthalpy= 1.013141
Thermal correction to Gibbs Free Energy= 0.846960
Sum of electronic and zero-point Energies= -2447.578164
Sum of electronic and thermal Energies= -2447.518940
Sum of electronic and thermal Enthalpies= -2447.517996
Sum of electronic and thermal Free Energies= -2447.684177

9-TS1

C	1.28443800	0.78384000	1.17655200
O	1.44275100	1.58905000	0.25685600
C	2.30854300	0.49525200	2.20135500
C	3.35733000	1.42042900	2.36399700
C	2.27946300	-0.66763100	2.99241400
C	4.35755800	1.17742400	3.30022500
H	3.36920400	2.33403200	1.77880800
C	3.28963500	-0.90729500	3.91919000
C	4.32870300	0.01455000	4.07486600
H	5.16087000	1.89646200	3.42479500
H	3.26804400	-1.81072900	4.52061500
C	-0.03998500	0.07912200	1.12566000
C	-1.18635400	0.78856200	1.78000300
C	-1.06590300	2.21812700	2.01066700
C	-0.96039400	3.41559600	2.17872700
C	-0.86173600	4.82442200	2.38595400
C	-1.89214800	5.50512700	3.06563700
C	0.25828600	5.53829700	1.91490900
C	-1.80294300	6.87886900	3.26857700
C	0.33203600	6.91329000	2.12670100
H	1.05994800	5.02144300	1.39448100
C	-0.69178400	7.58494700	2.79928600
H	-2.59741800	7.39872200	3.79513100
H	1.19641800	7.46217800	1.76561300
H	-0.62382300	8.65667700	2.96063900
H	5.11365300	-0.17255900	4.80171800
H	1.47724700	-1.38578000	2.87308800
H	-2.74823700	4.94882300	3.43441800
Au	-0.22965900	-1.78279200	0.33566100

C	-0.47232600	-3.67329800	-0.41934200
C	-0.23374300	-5.59635800	-1.58027200
C	-1.33623600	-5.72781400	-0.79701600
H	-2.03095100	-6.54345700	-0.67706300
H	0.22499000	-6.27359900	-2.28248800
N	0.28365400	-4.33155500	-1.33690700
N	-1.46892700	-4.53953200	-0.09228400
C	1.45272600	-3.78585400	-1.99830600
C	1.27362200	-3.10540900	-3.21956000
C	2.71416100	-3.97582300	-1.39995200
C	2.41961700	-2.58167600	-3.83111000
C	3.82269400	-3.43076800	-2.05960700
C	3.67870400	-2.73671000	-3.25770000
H	2.32358300	-2.05327800	-4.77443200
H	4.81152200	-3.55673400	-1.63003400
H	4.55307200	-2.32458000	-3.75281100
C	-2.53460200	-4.25641400	0.84780400
C	-2.35199700	-4.61245600	2.19950900
C	-3.71093500	-3.64868900	0.36481900
C	-3.39919600	-4.32629500	3.08447000
C	-4.72542400	-3.39207200	1.29639800
C	-4.57318300	-3.72288700	2.64027600
H	-3.29691400	-4.58968600	4.13267500
H	-5.65066700	-2.93489300	0.95964500
H	-5.37634000	-3.52014700	3.34280700
C	-1.08810500	-5.29306600	2.71769400
C	-1.39605600	-6.69423900	3.28210100
C	-0.36376900	-4.42196100	3.76221500
H	-0.40015400	-5.42452500	1.87757600
H	-1.87921000	-7.32983500	2.53351600
H	-0.47238500	-7.18775900	3.60083900
H	-2.06064200	-6.64031200	4.15022700
H	-0.09260800	-3.44746800	3.34146700
H	-0.98613700	-4.24916900	4.64627000
H	0.55571400	-4.91363300	4.09599300
C	-3.92228400	-3.29013100	-1.10326900
C	-4.18714200	-1.78428700	-1.29640500
C	-5.05076700	-4.13949100	-1.72233000
H	-3.00351700	-3.52550200	-1.64821400
H	-3.37295500	-1.17270900	-0.89719600
H	-4.29210600	-1.55908600	-2.36288800
H	-5.11681500	-1.47571500	-0.80598600
H	-4.84638400	-5.21095800	-1.62916200
H	-6.01259500	-3.94226900	-1.23761000

H	-5.16116300	-3.90653400	-2.78626800
C	2.91173200	-4.75956400	-0.10599400
C	3.60002700	-3.91106200	0.97922400
C	3.68873900	-6.06647500	-0.36360100
H	1.92619300	-5.03742000	0.27975100
H	3.04393000	-2.99036500	1.17848300
H	3.67049200	-4.47831100	1.91333600
H	4.61761500	-3.63074200	0.68888400
H	3.18179500	-6.69774100	-1.10033500
H	4.69675100	-5.86292100	-0.73912900
H	3.78812500	-6.64058900	0.56334100
C	-0.08354300	-2.95605200	-3.90185800
C	-0.11374800	-3.72608500	-5.23797400
C	-0.47359900	-1.47916500	-4.10159700
H	-0.84464900	-3.40200900	-3.25475100
H	0.13004400	-4.78434100	-5.09934200
H	-1.10875800	-3.66335800	-5.69032900
H	0.60332800	-3.31244100	-5.95446800
H	-0.53756200	-0.94833100	-3.14661600
H	0.24584700	-0.95842500	-4.74295700
H	-1.45115800	-1.41571400	-4.59156700
O	-0.77553200	0.07036000	3.01830200
C	0.34554000	2.07375200	-2.58176100
C	0.48552800	3.27789900	-3.25340800
C	-0.51845900	4.24485400	-3.23544400
C	-1.66947000	3.93959000	-2.50889700
C	-1.80590100	2.73199300	-1.84173200
H	-0.41154700	5.18508600	-3.76035900
H	1.09080400	1.29402000	-2.55404600
H	-2.67380900	2.43589400	-1.26981400
Cl	-2.98072500	5.08022400	-2.43285600
Cl	1.95858100	3.56466200	-4.13906000
N	-0.80016900	1.80823700	-1.88839300
O	-0.94476300	0.67731600	-1.28495000
C	-5.47296400	1.83788300	0.70942300
C	-4.26069400	1.97079900	1.27349700
H	-5.95553000	0.86128000	0.77110500
H	-3.72155800	2.91327100	1.23002600
C	-6.25410900	2.86323800	0.00453100
C	-5.91183100	4.22882200	0.01162500
C	-7.40316800	2.46922700	-0.70341200
C	-6.68473600	5.15815600	-0.67843700
H	-5.04715000	4.56931500	0.57309400
C	-8.17587900	3.39926000	-1.39665600

H	-7.68767900	1.41990600	-0.71103800
C	-7.81801500	4.74790300	-1.38779800
H	-6.41030500	6.20880500	-0.65520600
H	-9.05814600	3.07224200	-1.93870900
H	-8.42088700	5.47675800	-1.92094600
C	-3.59784800	0.86182800	2.02624500
H	-4.26063000	-0.00293000	2.10921800
H	-3.30915200	1.17650400	3.03552300
O	-2.41093200	0.34207200	1.34101600
H	-1.22160900	-0.79461900	2.96059000
C	6.31231300	3.71237700	-0.12919200
C	5.06865700	3.44222100	-0.55447200
H	6.50887800	4.71781100	0.24530900
H	4.81529500	2.45044300	-0.92982200
C	7.47451300	2.81185300	-0.09892400
C	8.67276100	3.27461100	0.47300900
C	7.45196900	1.50273300	-0.61613700
C	9.80465600	2.46303100	0.53560400
H	8.71225800	4.28493300	0.87263300
C	8.58104500	0.69164700	-0.55410900
H	6.54693600	1.11905500	-1.07767200
C	9.76336400	1.16636900	0.02256400
H	10.71826800	2.84455000	0.98204100
H	8.54372000	-0.31460100	-0.96221500
H	10.64364400	0.53197500	0.06576100
C	3.95185000	4.44675000	-0.55095600
H	3.56806400	4.59005300	-1.57348800
H	4.31820300	5.41638000	-0.20068800
O	2.87760700	4.09031400	0.32831700
H	2.48586200	3.24999000	0.03940100

Zero-point correction= 1.202351 (Hartree/Particle)
Thermal correction to Energy= 1.282161
Thermal correction to Enthalpy= 1.283106
Thermal correction to Gibbs Free Energy= 1.066188
Sum of electronic and zero-point Energies= -4189.386178
Sum of electronic and thermal Energies= -4189.306367
Sum of electronic and thermal Enthalpies= -4189.305423
Sum of electronic and thermal Free Energies= -4189.522341

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C	1.95682500	3.37051900	0.09880500
O	1.14158400	4.28664400	-0.33442400
C	3.39152500	3.67210600	-0.07947200

C	3.79837000	5.01637200	0.01933800
C	4.34435000	2.68394400	-0.38554100
C	5.13674300	5.35667100	-0.14742700
H	3.06111700	5.77926300	0.24326600
C	5.67963300	3.03406200	-0.56603800
C	6.07917900	4.36689200	-0.43873800
H	5.44542400	6.39292100	-0.05242400
H	6.40634900	2.26483400	-0.80800100
C	1.43038500	2.12648300	0.55682800
C	2.31457900	1.08499900	1.17369200
C	0.06077400	1.93755300	0.34684500
C	-0.74035300	2.96129300	-0.04437300
C	-1.83793900	3.66979400	0.53881800
C	-2.48968200	4.67338300	-0.21675500
C	-2.24079600	3.44525200	1.88050400
C	-3.50873500	5.42932400	0.34909000
C	-3.25508000	4.20723800	2.44026300
H	-1.74168600	2.67490500	2.45951400
C	-3.88816600	5.19791200	1.67558800
H	-4.00369800	6.20022800	-0.23229700
H	-3.55734700	4.04050900	3.46915400
H	-4.68091000	5.79287300	2.11953800
H	7.12288300	4.63493200	-0.57264300
H	4.04805700	1.65022200	-0.52052200
H	-2.17578500	4.84588200	-1.24148400
O	2.95286800	1.29412400	2.18365700
C	5.32119500	-1.54613000	-0.07538600
C	4.60476800	-0.89170600	0.85391100
H	4.80419200	-2.28316500	-0.69185000
H	5.05655000	-0.13560100	1.48886000
C	6.74899800	-1.38606800	-0.38244300
C	7.28553700	-2.07754500	-1.48265200
C	7.61056600	-0.56688900	0.37314500
C	8.63042100	-1.95108800	-1.82719600
H	6.63614100	-2.71827900	-2.07417700
C	8.95344800	-0.44087200	0.02958500
H	7.23228400	-0.03728000	1.24213900
C	9.46939500	-1.13058400	-1.07264200
H	9.02268600	-2.49425800	-2.68178300
H	9.60421900	0.19040100	0.62762400
H	10.51841000	-1.03229900	-1.33501000
C	3.14837400	-1.14588800	1.07556400
H	2.90805600	-1.21794100	2.13943100
H	2.80747000	-2.04286000	0.56092400

O	2.30369400	-0.08068600	0.50560400
H	0.12659100	3.74120600	-0.69948500
Au	-1.02607200	0.16582000	0.10309100
C	-2.15429600	-1.52453800	-0.17699800
C	-3.85204600	-2.86844800	-0.83423900
C	-2.95029300	-3.64117300	-0.17812400
H	-2.94228900	-4.69607200	0.04336200
H	-4.79201000	-3.11186900	-1.30252700
N	-3.35225200	-1.57383900	-0.82320000
N	-1.91338200	-2.80470500	0.21497400
C	-4.03579600	-0.44932400	-1.43011500
C	-5.05831100	0.18527100	-0.69606100
C	-3.68156900	-0.07011100	-2.74067600
C	-5.72297000	1.25122600	-1.31449000
C	-4.37822000	1.00645100	-3.30394300
C	-5.38580500	1.66148000	-2.60144700
H	-6.51909400	1.76221700	-0.78206100
H	-4.13473200	1.32699100	-4.31199500
H	-5.91812300	2.48791300	-3.06313700
C	-0.73528800	-3.29757600	0.90016100
C	0.27360300	-3.90505000	0.12443500
C	-0.68485200	-3.22504900	2.30628800
C	1.36185100	-4.45876700	0.81037800
C	0.43538900	-3.78462500	2.93514500
C	1.44372100	-4.40082000	2.19970000
H	2.15166400	-4.94716600	0.24787800
H	0.50921000	-3.75090900	4.01750200
H	2.29437600	-4.84163800	2.71100400
C	0.22245700	-3.97856900	-1.39964500
C	0.19645100	-5.43678000	-1.89792900
C	1.38453300	-3.19246400	-2.03813100
H	-0.70458900	-3.50518700	-1.73577400
H	-0.65064800	-5.99000800	-1.48011500
H	0.11351400	-5.46418600	-2.98908100
H	1.11018100	-5.97286400	-1.62186300
H	1.39246200	-2.15064500	-1.70254300
H	2.35329300	-3.63837700	-1.78763800
H	1.29315900	-3.20012600	-3.12921800
C	-1.79194400	-2.60011300	3.14942600
C	-1.27117000	-1.40751400	3.97453300
C	-2.46753400	-3.64975300	4.05410600
H	-2.55880400	-2.21298500	2.47203400
H	-0.82119100	-0.64526200	3.32993000
H	-2.09321800	-0.94527500	4.53096200

H	-0.51485800	-1.71851300	4.70232200
H	-2.87482500	-4.48058600	3.46944800
H	-1.76276000	-4.06800800	4.77989300
H	-3.29004700	-3.19444200	4.61495400
C	-2.61749300	-0.79212600	-3.56262400
C	-1.47591800	0.15369700	-3.98240200
C	-3.24276900	-1.48711800	-4.78921200
H	-2.17420600	-1.57374000	-2.93897200
H	-0.99909100	0.61317300	-3.11053000
H	-0.71116300	-0.40022200	-4.53642200
H	-1.83637900	0.95733500	-4.63261500
H	-4.02618700	-2.19250600	-4.49446100
H	-3.69036300	-0.76202200	-5.47643000
H	-2.47818400	-2.04137300	-5.34293900
C	-5.46862200	-0.25222400	0.70728700
C	-6.90564800	-0.81095100	0.72055000
C	-5.30816500	0.88714300	1.73063400
H	-4.80251000	-1.06041000	1.02354200
H	-7.01798400	-1.65087900	0.02756700
H	-7.16888600	-1.16229700	1.72339200
H	-7.63469500	-0.04625700	0.43355400
H	-4.28145500	1.26457000	1.74407400
H	-5.97104200	1.72911700	1.50589600
H	-5.55726300	0.53020100	2.73542000

Zero-point correction= 0.956991 (Hartree/Particle)
Thermal correction to Energy= 1.015715
Thermal correction to Enthalpy= 1.016659
Thermal correction to Gibbs Free Energy= 0.852824
Sum of electronic and zero-point Energies= -2522.861991
Sum of electronic and thermal Energies= -2522.803267
Sum of electronic and thermal Enthalpies= -2522.802323
Sum of electronic and thermal Free Energies= -2522.966158

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C	-2.19687800	2.70208000	0.88415900
O	-1.26227900	3.61029900	1.05834000
C	-3.56729700	3.15710500	1.02583300
C	-3.81048000	4.40382200	1.64676700
C	-4.65390700	2.41311000	0.52086700
C	-5.10848700	4.87832200	1.77374900
H	-2.97679600	4.98012600	2.03050800
C	-5.94883300	2.90391500	0.64095200
C	-6.17908300	4.13018500	1.27067700

H	-5.29006300	5.83060100	2.26112600
H	-6.77772800	2.32688600	0.24431100
C	-1.62220000	1.42971100	0.55268500
C	-2.31615500	0.12172000	0.33125000
C	-0.24645200	1.55137900	0.51464100
C	0.06372300	2.97459200	0.83974700
C	0.82811100	3.78612600	-0.18260600
C	1.88439700	4.60355000	0.23072400
C	0.46209100	3.75443800	-1.53540500
C	2.57393900	5.38282200	-0.69985000
C	1.14634300	4.53960800	-2.46084200
H	-0.35499500	3.11902600	-1.86504400
C	2.20373000	5.35377900	-2.04450300
H	3.39233100	6.01599100	-0.37162500
H	0.85626600	4.51549200	-3.50672800
H	2.73493000	5.96508500	-2.76775500
H	-7.19321600	4.50589400	1.36786400
H	-4.49741500	1.46467300	0.02668900
H	2.16723800	4.63519400	1.27946600
O	-2.07594900	-0.60723700	-0.60890300
C	-6.30724200	-1.31779800	0.56627300
C	-5.01227800	-1.37519100	0.21079100
H	-6.53890200	-1.30486300	1.63239600
H	-4.70881300	-1.38879300	-0.83267300
C	-7.48269400	-1.26904800	-0.31298200
C	-8.75355300	-1.11733000	0.27030400
C	-7.40096400	-1.36634500	-1.71552800
C	-9.90358900	-1.05669900	-0.51526000
H	-8.83591300	-1.04951100	1.35233500
C	-8.54866300	-1.30665100	-2.49954500
H	-6.43631900	-1.50024800	-2.19562500
C	-9.80470200	-1.15043400	-1.90382300
H	-10.87476600	-0.94096000	-0.04351200
H	-8.46704900	-1.38740600	-3.57947900
H	-10.69811900	-1.10793700	-2.51937300
C	-3.90591600	-1.43283800	1.21443200
H	-3.16976500	-2.20207000	0.96713300
H	-4.28400400	-1.58882800	2.22560300
O	-3.18240100	-0.15272600	1.31634600
H	0.56411000	3.03158500	1.81373900
Au	1.15986800	0.11709900	0.21540200
C	2.57375700	-1.34582300	-0.05299100
C	4.54176100	-2.41524400	-0.37559500
C	3.56926100	-3.36127100	-0.31014300

H	3.61516300	-4.43579100	-0.38360800
H	5.60693900	-2.49774400	-0.51965200
N	3.91570200	-1.18701700	-0.21547000
N	2.37082500	-2.69041800	-0.11075800
C	4.61508700	0.08181800	-0.22528000
C	4.79747600	0.73882900	-1.45834800
C	5.10977500	0.58635600	0.99404800
C	5.49630500	1.95219600	-1.43969100
C	5.80243800	1.80267700	0.94954800
C	5.99364300	2.47979800	-0.25165100
H	5.65609500	2.48738700	-2.37053200
H	6.20237300	2.22084400	1.86811600
H	6.53875700	3.41909800	-0.26281900
C	1.09079100	-3.35735300	0.02557400
C	0.68273500	-3.76818500	1.31041500
C	0.33090500	-3.59983900	-1.13589900
C	-0.53851500	-4.44674300	1.40781300
C	-0.87933000	-4.28575700	-0.97648400
C	-1.31036500	-4.70717000	0.27827400
H	-0.88211100	-4.78412100	2.38085100
H	-1.48943400	-4.49360700	-1.84931600
H	-2.24757900	-5.24775200	0.37555900
C	1.50721300	-3.51416100	2.56897500
C	1.94736700	-4.83424900	3.23190800
C	0.74995800	-2.61610200	3.56683200
H	2.41595500	-2.97754900	2.28156100
H	2.51568500	-5.46173400	2.53810300
H	2.58069200	-4.63072000	4.10146200
H	1.08747300	-5.41710300	3.57754000
H	0.47516700	-1.66060300	3.10832900
H	-0.16746700	-3.09609200	3.92313600
H	1.37534700	-2.40850200	4.44140300
C	0.77794100	-3.16615700	-2.52849300
C	-0.28896200	-2.30215000	-3.22854600
C	1.16141700	-4.38504500	-3.39171700
H	1.67272000	-2.54551200	-2.42158000
H	-0.59256000	-1.45849200	-2.60312400
H	0.10469000	-1.91749800	-4.17538700
H	-1.18722500	-2.88352800	-3.46185200
H	1.95817000	-4.97501900	-2.92712000
H	0.30321800	-5.04799600	-3.54377200
H	1.51095800	-4.06044500	-4.37721600
C	4.93205000	-0.13388000	2.32769800
C	4.13705100	0.72125000	3.33320900

C	6.28969700	-0.56526700	2.91689800
H	4.34933300	-1.04269600	2.15184100
H	3.15388300	0.98822700	2.93223200
H	3.98588500	0.16744300	4.26560600
H	4.66539400	1.64756300	3.58167600
H	6.84234000	-1.20639500	2.22293500
H	6.92123400	0.29985300	3.14311700
H	6.14183500	-1.12160700	3.84810300
C	4.28282900	0.18302000	-2.78269200
C	5.44338200	-0.13611800	-3.74613800
C	3.26207900	1.13389800	-3.43635800
H	3.76158900	-0.75732500	-2.58131800
H	6.15370700	-0.83988900	-3.30071500
H	5.05924700	-0.58120200	-4.66964900
H	5.99866000	0.76714200	-4.01918600
H	2.42167900	1.33561200	-2.76526300
H	3.71820500	2.09400700	-3.69899800
H	2.86847900	0.69085100	-4.35726300

Zero-point correction= 0.964268 (Hartree/Particle)
Thermal correction to Energy= 1.022516
Thermal correction to Enthalpy= 1.023460
Thermal correction to Gibbs Free Energy= 0.860159
Sum of electronic and zero-point Energies= -2522.933349
Sum of electronic and thermal Energies= -2522.875101
Sum of electronic and thermal Enthalpies= -2522.874157
Sum of electronic and thermal Free Energies= -2523.037459

10-TS2

C	2.21781800	2.88241700	-0.58108900
O	1.20398900	3.80217100	-0.54247600
C	3.55681600	3.45740800	-0.67093500
C	3.72625100	4.72280700	-1.26553800
C	4.67300800	2.79502100	-0.12910900
C	4.99007600	5.30004700	-1.33487100
H	2.86949600	5.24276400	-1.67940100
C	5.93138400	3.38488300	-0.19354000
C	6.09472100	4.63346200	-0.79882900
H	5.11313000	6.27066800	-1.80461200
H	6.78496200	2.86985800	0.23544800
C	1.67796800	1.61252700	-0.51365500
C	2.34448700	0.28798500	-0.61568800
C	0.23448400	1.72623000	-0.36273100
C	0.00410200	3.14017300	-0.42040800

C	-1.17417200	3.99344800	-0.17596400
C	-1.21047300	5.28784200	-0.72167500
C	-2.24155800	3.53491900	0.61013000
C	-2.30653900	6.11132400	-0.48347500
C	-3.33657000	4.36666500	0.84084900
H	-2.20574000	2.54394600	1.04884300
C	-3.37156500	5.65148800	0.29624600
H	-2.33091500	7.11068200	-0.90603300
H	-4.15492200	4.00734300	1.45552300
H	-4.22412800	6.29743200	0.48256300
H	7.07935300	5.08821000	-0.84851100
H	4.55900300	1.83074800	0.34885400
H	-0.38252900	5.64451100	-1.32524600
O	1.88617900	-0.72033000	-0.11085100
C	6.41054100	-1.13251500	-0.34824200
C	5.06958700	-1.20569300	-0.30153900
H	6.86737500	-0.84444900	-1.29618600
H	4.54808900	-1.48860900	0.60924800
C	7.36785500	-1.40250600	0.73203300
C	8.73832900	-1.21543300	0.47870100
C	6.98124300	-1.83877500	2.01366400
C	9.69198900	-1.44933400	1.46813200
H	9.05510700	-0.88421800	-0.50724100
C	7.93259300	-2.07244800	3.00137400
H	5.93158800	-2.00210400	2.23835300
C	9.29186400	-1.87824600	2.73396000
H	10.74510300	-1.29947500	1.24993000
H	7.61629900	-2.41076500	3.98373400
H	10.03125000	-2.06414400	3.50706400
C	4.20913300	-0.92831900	-1.49115800
H	3.47570700	-1.72085900	-1.66077600
H	4.80384600	-0.77145600	-2.39207800
O	3.46470900	0.33237300	-1.34624800
H	-0.18580500	2.37977800	-1.46195900
Au	-1.10466000	0.16254500	-0.14759500
C	-2.38753900	-1.41634000	0.04323300
C	-4.13181600	-2.73218500	0.63513300
C	-3.33106200	-3.46050500	-0.18334200
H	-3.41586600	-4.47140500	-0.54727500
H	-5.05526600	-2.97925600	1.13320300
N	-3.54198600	-1.48134200	0.76238900
N	-2.26551100	-2.64332300	-0.53466600
C	-4.11674700	-0.41190400	1.55226100
C	-3.67856000	-0.24125700	2.88144100

C	-5.13012900	0.37701600	0.97101600
C	-4.29017000	0.77117300	3.63190300
C	-5.71352000	1.36510200	1.77459700
C	-5.29952600	1.56245700	3.08979100
H	-3.98043200	0.93054500	4.65988000
H	-6.50825000	1.98075100	1.36508400
H	-5.77152300	2.32880000	3.69790000
C	-1.18390800	-3.07366400	-1.39999800
C	-1.26434300	-2.78084800	-2.77625000
C	-0.12540000	-3.81067900	-0.83085000
C	-0.22270800	-3.24290500	-3.59046400
C	0.88249700	-4.25254100	-1.69670900
C	0.83818100	-3.97103900	-3.05955600
H	-0.25119800	-3.04005500	-4.65647900
H	1.71068000	-4.82897900	-1.29749200
H	1.62871700	-4.32955500	-3.71247100
C	-2.43462700	-2.02903100	-3.40362000
C	-3.24841200	-2.94818600	-4.33683500
C	-1.97060000	-0.76017600	-4.14371300
H	-3.10430400	-1.70489100	-2.60172600
H	-3.61318100	-3.83433900	-3.80798300
H	-4.11445500	-2.41284300	-4.73949300
H	-2.64602600	-3.29192000	-5.18396800
H	-1.42221100	-0.09139700	-3.47231800
H	-1.31663000	-0.99992400	-4.98845900
H	-2.83391800	-0.21521500	-4.53954900
C	-0.06856600	-4.16874300	0.65169000
C	1.30016900	-3.85338500	1.28335600
C	-0.44447600	-5.64904800	0.87232700
H	-0.81017900	-3.55745900	1.17535100
H	1.59204600	-2.81742500	1.09788400
H	1.25500300	-4.01932800	2.36487200
H	2.08634400	-4.50728400	0.89104700
H	-1.44143000	-5.88071200	0.48384200
H	0.26780300	-6.31288200	0.37114700
H	-0.43403000	-5.89121900	1.94005100
C	-5.61670500	0.18189800	-0.46235000
C	-5.48849900	1.47408000	-1.29150300
C	-7.06227900	-0.35387800	-0.49271600
H	-4.97999800	-0.56887900	-0.93942900
H	-4.46314000	1.85569500	-1.27855100
H	-5.77084100	1.28360100	-2.33197100
H	-6.14531600	2.26468300	-0.91408400
H	-7.15386200	-1.29761700	0.05427800

H	-7.76102900	0.35868700	-0.04240500
H	-7.38313400	-0.52829600	-1.52475400
C	-2.60557000	-1.11486600	3.52460800
C	-3.18421400	-1.94296500	4.68942000
C	-1.39315900	-0.28137800	3.98207200
H	-2.24329100	-1.82135000	2.77248900
H	-4.02158100	-2.56661600	4.36076500
H	-2.41484900	-2.60092200	5.10603600
H	-3.54576900	-1.30090500	5.49918200
H	-0.95391300	0.27027100	3.14446100
H	-1.66912000	0.44126600	4.75701400
H	-0.62064400	-0.93511000	4.39946200

Zero-point correction=	0.959968 (Hartree/Particle)
Thermal correction to Energy=	1.018001
Thermal correction to Enthalpy=	1.018945
Thermal correction to Gibbs Free Energy=	0.856350
Sum of electronic and zero-point Energies=	-2522.903032
Sum of electronic and thermal Energies=	-2522.844998
Sum of electronic and thermal Enthalpies=	-2522.844054
Sum of electronic and thermal Free Energies=	-2523.006649

10-INT2

C	0.23831500	3.20798600	-0.70330600
O	-1.14898000	3.27104100	-0.68733500
C	0.89267800	4.18084200	0.16897800
C	0.26745600	5.42075900	0.40359700
C	2.11216500	3.89610700	0.80839800
C	0.85820000	6.35787900	1.24583500
H	-0.67279100	5.64982000	-0.08622300
C	2.69354100	4.83823600	1.65286200
C	2.07283600	6.07003200	1.87273100
H	0.37244600	7.31465100	1.41013300
H	3.63271800	4.60715200	2.14604400
C	0.61183600	2.19129900	-1.55158800
C	1.92216000	1.75132100	-2.08603800
C	-0.61544600	1.57056400	-2.04154300
C	-1.66596900	2.34011500	-1.52094400
C	-3.09855100	2.39229100	-1.78625500
C	-3.92349500	3.27682400	-1.06935300
C	-3.65789900	1.59032600	-2.79853600
C	-5.28254700	3.35357100	-1.36207300
C	-5.01575200	1.67571200	-3.08645100

H	-3.02920800	0.91021800	-3.36486100
C	-5.83147500	2.55679300	-2.36925300
H	-5.91316800	4.04102300	-0.80724800
H	-5.43824200	1.06124100	-3.87504200
H	-6.89016500	2.62487900	-2.59975000
H	2.53246800	6.80170700	2.53014200
H	2.59978700	2.94423900	0.64189400
H	-3.49553800	3.90096100	-0.29308600
O	2.02234200	0.78250900	-2.81711700
C	6.00631300	1.27968200	-0.82782500
C	4.93719700	1.10508700	-1.62141500
H	6.35010500	2.29889000	-0.64593700
H	4.52675400	0.11617100	-1.80799000
C	6.77949000	0.23088100	-0.14630900
C	7.58775000	0.57869400	0.94990700
C	6.75391100	-1.11654500	-0.55397000
C	8.31967900	-0.38783000	1.63836600
H	7.63517400	1.61763400	1.26634500
C	7.48729500	-2.08212100	0.13204500
H	6.18419400	-1.39911500	-1.43421300
C	8.26858800	-1.72293100	1.23487200
H	8.93502400	-0.09747900	2.48470400
H	7.46767700	-3.11455400	-0.20521300
H	8.84583500	-2.47592200	1.76279300
C	4.25065800	2.24143300	-2.30886100
H	4.09509000	2.03045700	-3.37032200
H	4.80273700	3.17533900	-2.19428500
O	2.93899000	2.54415600	-1.72374400
H	-0.65262300	0.98921800	-2.95519700
Au	-0.97701800	-0.11666700	-0.55683300
C	-1.15166500	-1.70746900	0.67530900
C	-1.89897800	-3.14167500	2.24616400
C	-0.75518300	-3.66014600	1.72951600
H	-0.22029500	-4.56920800	1.95234300
H	-2.56529600	-3.50665200	3.01092900
N	-2.13148700	-1.94210900	1.58684800
N	-0.30692300	-2.76691100	0.76614500
C	-3.27696600	-1.09117600	1.84343600
C	-3.14970900	-0.05787200	2.79299100
C	-4.47872100	-1.36596700	1.16022900
C	-4.28618300	0.72115400	3.04387900
C	-5.58022400	-0.55281500	1.45338700
C	-5.48742400	0.47857400	2.38360900
H	-4.22967500	1.52402100	3.77218400

H	-6.52400200	-0.73468100	0.94909300
H	-6.35697700	1.09220500	2.59966700
C	0.89673900	-2.96141200	-0.01920500
C	0.78836400	-3.62078300	-1.26016700
C	2.12236100	-2.51248700	0.51127900
C	1.96989600	-3.81084200	-1.98638200
C	3.26998400	-2.73161300	-0.26071800
C	3.19546700	-3.37068000	-1.49537200
H	1.92830200	-4.31412800	-2.94714400
H	4.23365300	-2.39828600	0.11062200
H	4.09842500	-3.53357300	-2.07651300
C	-0.53422400	-4.13673300	-1.81945200
C	-0.52680700	-5.67327500	-1.94653200
C	-0.87918600	-3.46985900	-3.16502200
H	-1.33060500	-3.87414200	-1.11640100
H	-0.31805500	-6.15436100	-0.98573000
H	-1.49883000	-6.03094000	-2.30104800
H	0.23174600	-6.01223000	-2.65923000
H	-0.91535600	-2.37976400	-3.06913400
H	-0.14041700	-3.71110900	-3.93567800
H	-1.85489200	-3.81638700	-3.52144900
C	2.24186400	-1.81029400	1.86102800
C	2.65147000	-0.33424700	1.68649100
C	3.21355500	-2.54596200	2.80446600
H	1.25894900	-1.81882000	2.34224400
H	1.92853800	0.20368000	1.06414300
H	2.70082000	0.16346100	2.66087300
H	3.63493200	-0.24537000	1.21426000
H	2.92493900	-3.59294000	2.94083800
H	4.23899200	-2.52860300	2.42246200
H	3.22069200	-2.06526500	3.78798200
C	-4.62104500	-2.49739400	0.14634400
C	-5.01546200	-1.96440600	-1.24415300
C	-5.61800800	-3.56715700	0.63464800
H	-3.64824800	-2.98607300	0.03734300
H	-4.29973800	-1.21706100	-1.60010600
H	-5.04753100	-2.78490500	-1.96850200
H	-6.00532900	-1.49686100	-1.23014600
H	-5.32260500	-3.97947700	1.60463300
H	-6.62639100	-3.15495100	0.74325300
H	-5.67222500	-4.39284700	-0.08208500
C	-1.85626900	0.22433800	3.55144100
C	-2.02175200	-0.05275900	5.05902800
C	-1.35266500	1.65917200	3.30283200

H	-1.08440400	-0.45523000	3.17817600
H	-2.34396000	-1.08220300	5.24493300
H	-1.07326700	0.10531800	5.58234100
H	-2.76479700	0.61372800	5.50868800
H	-1.21235500	1.85324000	2.23457900
H	-2.05402500	2.40571100	3.68929200
H	-0.39348600	1.81704200	3.80637600

Zero-point correction= 0.964285 (Hartree/Particle)
Thermal correction to Energy= 1.022649
Thermal correction to Enthalpy= 1.023593
Thermal correction to Gibbs Free Energy= 0.860879
Sum of electronic and zero-point Energies= -2522.954701
Sum of electronic and thermal Energies= -2522.896337
Sum of electronic and thermal Enthalpies= -2522.895393
Sum of electronic and thermal Free Energies= -2523.058107

3-INT1

C	-1.56087400	-2.32797300	-0.60420100
O	-2.79600900	-2.77115000	-0.40910400
C	-0.63053800	-3.43067100	-0.87968800
C	-0.92965800	-4.72293400	-0.40011700
C	0.49248600	-3.25010100	-1.70991900
C	-0.11057700	-5.79855900	-0.72340700
H	-1.80051900	-4.86849500	0.22846800
C	1.29285200	-4.33723700	-2.05096200
C	0.99792400	-5.60946600	-1.55504800
H	-0.33953100	-6.78655200	-0.33659700
H	2.14643400	-4.18755800	-2.70340700
C	-1.20083800	-0.95068300	-0.59466800
C	-2.21941500	0.00539200	-0.68898400
C	-1.98644200	1.36410400	-0.98818900
C	-1.91826700	2.51966600	-1.37945900
C	-1.83642000	3.85315100	-1.85727400
C	-2.90343500	4.75188000	-1.64109600
C	-0.69952000	4.28478400	-2.57413900
C	-2.82821700	6.05164100	-2.12945400
C	-0.63910400	5.58544900	-3.06252100
H	0.11579800	3.58955200	-2.74318500
C	-1.69936100	6.46982400	-2.84066100
H	-3.64985500	6.74002100	-1.95893600
H	0.23357900	5.91246800	-3.61909200
H	-1.64680300	7.48440500	-3.22347000
H	1.62612100	-6.45484000	-1.82006000

H	0.70872900	-2.26866200	-2.11458400
H	-3.77717800	4.42033900	-1.08972300
Au	0.71783000	-0.31337800	-0.09024700
C	2.53858300	0.31183100	0.63255000
C	4.11544600	1.27840800	1.94574400
C	4.76016800	0.67175400	0.91888100
H	5.80865100	0.59794800	0.67975900
H	4.48729300	1.83980900	2.78722400
N	2.75734100	1.05320800	1.75683700
N	3.78346400	0.07953500	0.12729000
C	1.74430300	1.52842100	2.67743300
C	1.36587400	2.88527600	2.61652700
C	1.22446800	0.63237000	3.63402100
C	0.41890600	3.33128400	3.54652800
C	0.27436000	1.13472900	4.53226400
C	-0.12622500	2.46665700	4.49123600
H	0.10740600	4.37081100	3.53280700
H	-0.14638300	0.47425800	5.28391700
H	-0.85787500	2.83473800	5.20451700
C	4.09386600	-0.75258300	-1.01584900
C	4.50951400	-2.07860900	-0.77492800
C	4.01976800	-0.19772400	-2.30862300
C	4.83941000	-2.86032600	-1.88933400
C	4.35373400	-1.02982000	-3.38473100
C	4.75900700	-2.34609700	-3.18093600
H	5.17135600	-3.88323300	-1.74052700
H	4.31032200	-0.63530000	-4.39508300
H	5.02572300	-2.96819000	-4.03043700
C	4.63254100	-2.67210300	0.62685600
C	6.09485400	-3.03728800	0.95193800
C	3.70228800	-3.88369500	0.82236100
H	4.32124100	-1.91315400	1.34987400
H	6.75838500	-2.17207100	0.85429200
H	6.17386500	-3.41108400	1.97782600
H	6.47110200	-3.81911100	0.28421900
H	2.65852000	-3.61664000	0.63574200
H	3.96306000	-4.70627700	0.14862600
H	3.78484500	-4.25928800	1.84770700
C	3.63834100	1.25614000	-2.56968500
C	2.40110500	1.36794200	-3.48038600
C	4.82992900	2.04367700	-3.15124200
H	3.37790700	1.71781200	-1.61304100
H	1.53693300	0.86139400	-3.03847200
H	2.14250800	2.42138000	-3.63539200

H	2.58262600	0.93007000	-4.46737200
H	5.70221800	1.99420000	-2.49205000
H	5.13003600	1.65341800	-4.12919600
H	4.56338200	3.09776300	-3.28160100
C	1.68136100	-0.81817200	3.76096600
C	0.50472600	-1.80670200	3.65796500
C	2.47294800	-1.03124700	5.06754600
H	2.35671500	-1.04082100	2.93044400
H	-0.03836900	-1.67457200	2.71687800
H	0.87435200	-2.83655100	3.69841200
H	-0.20628800	-1.68043800	4.48108600
H	3.33736800	-0.36222900	5.12671700
H	1.84843100	-0.84534500	5.94751500
H	2.83720500	-2.06202000	5.12921500
C	1.96664900	3.86952600	1.61667800
C	2.93881300	4.84335800	2.31365100
C	0.88422200	4.64281400	0.84297800
H	2.54061100	3.29907100	0.88016600
H	3.74895800	4.31413000	2.82523600
H	3.38894400	5.52402300	1.58351500
H	2.41820900	5.45070700	3.06146000
H	0.17898400	3.96175700	0.36006100
H	0.31415300	5.31019400	1.49703400
H	1.34467200	5.26349700	0.06765200
C	-6.82646800	-0.13198200	0.13986500
C	-5.89948400	-0.25460000	-0.82645800
H	-6.62045500	0.57209400	0.94735200
H	-6.03654500	-0.94007900	-1.65938900
C	-8.11034500	-0.83046300	0.25451600
C	-8.90267800	-0.59418200	1.39205600
C	-8.58882600	-1.72817300	-0.71913800
C	-10.12861900	-1.23535000	1.55928800
H	-8.54907100	0.09892800	2.15131000
C	-9.81266300	-2.36758400	-0.55259900
H	-8.00612000	-1.92321100	-1.61422100
C	-10.58698300	-2.12486100	0.58701300
H	-10.72490600	-1.03979300	2.44527700
H	-10.16831100	-3.05561500	-1.31364700
H	-11.54250200	-2.62508600	0.71193800
C	-4.64574200	0.54645500	-0.83236500
H	-4.64587100	1.32058300	-0.06031500
H	-4.44242100	1.00481700	-1.80433400
O	-3.52180200	-0.36828300	-0.54343700
H	-3.39584000	-2.00490600	-0.26796800

Zero-point correction=	0.957607 (Hartree/Particle)
Thermal correction to Energy=	1.015833
Thermal correction to Enthalpy=	1.016777
Thermal correction to Gibbs Free Energy=	0.854843
Sum of electronic and zero-point Energies=	-2447.643562
Sum of electronic and thermal Energies=	-2447.585336
Sum of electronic and thermal Enthalpies=	-2447.584392
Sum of electronic and thermal Free Energies=	-2447.746326

3-TS2

C	0.84904300	-1.77171800	-2.05099200
O	2.08534800	-2.11574400	-2.46011900
C	-0.16419600	-2.59061600	-2.75277600
C	-1.37158500	-2.04560200	-3.21890900
C	0.13208600	-3.93564700	-3.04151600
C	-2.26257200	-2.83206300	-3.94837900
H	-1.58685200	-0.99820100	-3.03802800
C	-0.77194600	-4.72380900	-3.74774500
C	-1.97072800	-4.17282100	-4.20752500
H	-3.18192600	-2.39452100	-4.32399100
H	-0.53730000	-5.76451100	-3.94982500
C	0.57433800	-0.80774600	-1.08094700
C	1.75194100	-0.00155900	-0.59694800
C	1.61508200	0.78555700	0.63216800
C	1.70968000	1.43852300	1.65242100
C	1.83845700	2.19919500	2.85615500
C	3.11021700	2.63695400	3.27528500
C	0.71235900	2.51750700	3.64015300
C	3.24815000	3.37449100	4.44843200
C	0.85964600	3.25641700	4.81177600
H	-0.26669500	2.17708800	3.32144700
C	2.12529100	3.68670300	5.21859900
H	4.23308200	3.70506000	4.76366800
H	-0.01394800	3.49588900	5.41048500
H	2.23605800	4.26143200	6.13292500
H	-2.66879200	-4.78243200	-4.77364400
H	1.07416600	-4.35378800	-2.70517100
H	3.98150500	2.39014900	2.67681800
Au	-1.29827900	-0.39202700	-0.30600100
C	-3.11687300	0.00441700	0.57666900
C	-5.02614400	1.02924100	1.25736500
C	-4.88422200	-0.09651100	1.99900500
H	-5.50039400	-0.51967100	2.77558400

H	-5.78814000	1.79150400	1.25972100
N	-3.94125300	1.07747700	0.38796100
N	-3.71599100	-0.71510700	1.57068100
C	-3.81749800	2.09403900	-0.63899700
C	-3.15343100	3.29850500	-0.33584800
C	-4.44850100	1.86665900	-1.88135200
C	-3.12502500	4.28783500	-1.32748800
C	-4.38496200	2.89068100	-2.83389900
C	-3.73186100	4.08924600	-2.56306400
H	-2.63141800	5.23243400	-1.12318300
H	-4.86211500	2.75078600	-3.79804900
H	-3.70319200	4.87276600	-3.31460800
C	-3.30034400	-2.01925700	2.05253200
C	-3.86842500	-3.15912600	1.44752700
C	-2.40369700	-2.10038400	3.13664800
C	-3.49145500	-4.41099900	1.94964100
C	-2.06856100	-3.37883400	3.59901800
C	-2.60109000	-4.52290800	3.01193500
H	-3.90822100	-5.30877000	1.50424700
H	-1.38579300	-3.48071800	4.43569000
H	-2.32637900	-5.50358300	3.38909400
C	-4.88085000	-3.08724000	0.30807100
C	-6.25973800	-3.61139800	0.75743000
C	-4.38476800	-3.83297100	-0.94418900
H	-5.00957700	-2.03817600	0.02723900
H	-6.63720700	-3.06086800	1.62515100
H	-6.98916300	-3.50853500	-0.05267600
H	-6.21487000	-4.67055200	1.03115200
H	-3.42716100	-3.43629000	-1.29090600
H	-4.25823300	-4.90356100	-0.75320600
H	-5.11163200	-3.72920500	-1.75707800
C	-1.84795200	-0.86686900	3.84109900
C	-0.34190300	-0.98333900	4.13390800
C	-2.63613700	-0.58062300	5.13669900
H	-1.98257000	-0.00983700	3.17294900
H	0.22692200	-1.16566500	3.21747300
H	0.02613600	-0.05674700	4.58358900
H	-0.12265900	-1.79108400	4.83905000
H	-3.70266000	-0.43469300	4.93812000
H	-2.54108000	-1.41063400	5.84475900
H	-2.25717300	0.32295300	5.62616900
C	-5.22554000	0.59073200	-2.19276800
C	-4.92152500	0.04054400	-3.59781700
C	-6.74269100	0.81666100	-2.02083400

H	-4.91837300	-0.17629500	-1.47596200
H	-3.84541300	-0.06805400	-3.76023900
H	-5.39041300	-0.94088200	-3.72245900
H	-5.31657700	0.68783800	-4.38730100
H	-6.99251200	1.14672800	-1.00808800
H	-7.10530200	1.57882900	-2.71873400
H	-7.29313700	-0.10918000	-2.21814400
C	-2.52206900	3.57722900	1.02404400
C	-3.39336100	4.55192900	1.84290900
C	-1.08209000	4.10426500	0.89389400
H	-2.47255300	2.63272400	1.57507700
H	-4.40626600	4.16260700	1.98548800
H	-2.95498600	4.72276900	2.83181600
H	-3.47890900	5.52179500	1.34166400
H	-0.45291000	3.38425700	0.36111500
H	-1.04345500	5.06042300	0.36240500
H	-0.64493600	4.26588900	1.88319800
C	5.60359000	-2.30418900	0.98510100
C	4.48558900	-2.38837700	0.24578600
H	5.60128300	-1.60608500	1.82341100
H	4.42323700	-3.06616800	-0.60352300
C	6.85768700	-3.04802300	0.81362800
C	7.93470600	-2.75746100	1.66951000
C	7.03794400	-4.03862400	-0.17045600
C	9.15251900	-3.42431800	1.54650800
H	7.81119600	-1.99929900	2.43901700
C	8.25313700	-4.70443600	-0.29386200
H	6.22246900	-4.29572900	-0.83960100
C	9.31618700	-4.40003500	0.56279800
H	9.97072300	-3.18402600	2.21876700
H	8.37335100	-5.46695000	-1.05774400
H	10.26220900	-4.92375900	0.46445000
C	3.25765900	-1.59282500	0.54147700
H	3.36012600	-1.01858500	1.46683800
H	2.36832800	-2.23120400	0.62176400
O	3.04353200	-0.66182100	-0.56667300
H	2.73105900	-1.61257000	-1.91508400
C	2.45913500	3.24236600	-1.66562400
C	3.34746100	4.30983600	-1.79806700
C	4.70186200	4.05993100	-2.03057200
C	5.13487100	2.73499400	-2.12224400
C	4.21649000	1.69228400	-1.98798100
H	5.40352000	4.87889900	-2.13985000
H	1.39612200	3.35174500	-1.48931300

H	4.47335400	0.64184800	-2.03229400
Cl	6.80332000	2.36795100	-2.40741600
Cl	2.75563800	5.93350500	-1.67502700
N	2.94104000	2.00476900	-1.76221800
O	1.78748400	0.82023000	-1.77388300

Zero-point correction= 1.031041 (Hartree/Particle)
Thermal correction to Energy= 1.097788
Thermal correction to Enthalpy= 1.098732
Thermal correction to Gibbs Free Energy= 0.913991
Sum of electronic and zero-point Energies= -3690.150102
Sum of electronic and thermal Energies= -3690.083355
Sum of electronic and thermal Enthalpies= -3690.082410
Sum of electronic and thermal Free Energies= -3690.267151

3-INT2

C	1.60003000	-1.79837400	-1.35648300
O	2.04003500	-2.01705400	-2.56293300
C	1.67819600	-2.89792400	-0.41755400
C	1.28760700	-2.73107900	0.92884100
C	2.22050700	-4.13232600	-0.83857600
C	1.45039800	-3.77340700	1.83223300
H	0.85026500	-1.79355300	1.25415200
C	2.36845800	-5.17202900	0.07056300
C	1.98733800	-4.99320700	1.40491500
H	1.14553000	-3.64069700	2.86468200
H	2.78394900	-6.11998500	-0.25507700
C	1.07713800	-0.46494200	-1.08014700
C	2.14221100	0.64032900	-1.01520400
C	1.89115100	1.87866000	-0.31898400
C	1.80882000	2.93805300	0.26887600
C	1.70852700	4.19334100	0.94205400
C	1.95486500	4.28172900	2.32609200
C	1.37853500	5.35828200	0.22214000
C	1.86720600	5.51178400	2.97289800
C	1.29347000	6.58282700	0.87963700
H	1.19839900	5.29120300	-0.84563400
C	1.53639800	6.66293000	2.25329200
H	2.06118600	5.57361200	4.03933900
H	1.04193600	7.47744100	0.31838500
H	1.47201300	7.62042900	2.76101600
H	2.10679200	-5.80788400	2.11296200
H	2.52709800	-4.25691700	-1.87068500
H	2.21658400	3.38601600	2.87999900

Au	-0.90418900	-0.31709800	-0.42546700
C	-2.86815800	-0.13596000	0.11896300
C	-5.07586900	0.35093800	0.07244700
C	-4.81288700	-0.22919300	1.27133800
H	-5.45355400	-0.45963800	2.10718400
H	-5.99260900	0.72953400	-0.34991300
N	-3.87446700	0.40080000	-0.62191700
N	-3.45492800	-0.52256700	1.28413200
C	-3.73724700	0.94731600	-1.95781100
C	-3.49672800	2.32865900	-2.09541100
C	-3.88115000	0.07893500	-3.05844000
C	-3.39068000	2.83282600	-3.39748100
C	-3.76462000	0.64105100	-4.33569500
C	-3.52096900	2.00100300	-4.50575800
H	-3.20567000	3.89236400	-3.54377900
H	-3.87008200	0.00435500	-5.20854000
H	-3.43670500	2.41487100	-5.50617400
C	-2.78110700	-1.17746200	2.38555600
C	-2.77485100	-2.58664000	2.42294500
C	-2.19153700	-0.37992300	3.38687100
C	-2.13523100	-3.19556000	3.51031300
C	-1.56249800	-1.04512000	4.44718800
C	-1.53387500	-2.43590300	4.51087800
H	-2.11902300	-4.27898700	3.57836900
H	-1.10023800	-0.46433400	5.23931400
H	-1.05355300	-2.92900600	5.35127700
C	-3.44334200	-3.44955500	1.35627200
C	-4.62294000	-4.25021000	1.94316800
C	-2.43352400	-4.37978900	0.65815900
H	-3.85241200	-2.78730100	0.58778200
H	-5.36376400	-3.59187100	2.40768700
H	-5.12421200	-4.82132000	1.15512500
H	-4.28704200	-4.96072800	2.70552300
H	-1.61374900	-3.80994100	0.21021000
H	-1.99907000	-5.10162000	1.35759800
H	-2.93006600	-4.94807700	-0.13505700
C	-2.23224800	1.14504900	3.36742400
C	-0.81712600	1.75119400	3.31082400
C	-3.02737500	1.69698200	4.56747400
H	-2.75316300	1.46191600	2.45934300
H	-0.27294400	1.40761300	2.42532000
H	-0.87357500	2.84338800	3.26819900
H	-0.23045900	1.48455300	4.19662700
H	-4.04469200	1.29399700	4.59427600

H	-2.54581900	1.44650000	5.51828800
H	-3.09636000	2.78783100	4.50754200
C	-4.16573100	-1.41287600	-2.91224300
C	-3.05207900	-2.26629100	-3.54909000
C	-5.54709300	-1.77972000	-3.49003100
H	-4.18517600	-1.65573100	-1.84558200
H	-2.07499200	-2.02216100	-3.11949900
H	-3.24596700	-3.33070300	-3.38022800
H	-2.99239700	-2.10915300	-4.63079900
H	-6.34725800	-1.20743600	-3.00998300
H	-5.59689200	-1.58145500	-4.56546900
H	-5.75352200	-2.84420200	-3.33854300
C	-3.35832500	3.27298400	-0.90523700
C	-4.48678700	4.32307200	-0.88735400
C	-1.97193600	3.94363600	-0.87588600
H	-3.44916800	2.68480700	0.01296700
H	-5.47479400	3.85185900	-0.87194200
H	-4.40092400	4.95919500	-0.00039300
H	-4.44393700	4.97323500	-1.76722400
H	-1.17115800	3.19848100	-0.84769400
H	-1.81392400	4.57466900	-1.75682800
H	-1.87629900	4.58088700	0.00910100
C	6.75747000	0.38525700	-0.14950800
C	5.60871100	-0.29643000	-0.27923000
H	6.69440900	1.42205100	0.18288200
H	5.59990600	-1.32841400	-0.62263900
C	8.12256000	-0.09302000	-0.40308900
C	9.18734600	0.81702300	-0.28269400
C	8.41996400	-1.42087300	-0.76364100
C	10.50274300	0.42188500	-0.52059100
H	8.97622400	1.84605400	-0.00266100
C	9.73242600	-1.81603300	-1.00144600
H	7.62139300	-2.15097400	-0.85445400
C	10.77984800	-0.89679200	-0.88189300
H	11.30928300	1.14239500	-0.42335100
H	9.94303600	-2.84486700	-1.27853900
H	11.80306100	-1.20943600	-1.06701700
C	4.27856400	0.29221700	0.05204300
H	4.37281900	1.32227100	0.41056400
H	3.76256800	-0.29857500	0.82401600
O	3.46287100	0.27404200	-1.15299400
H	2.03810600	-1.13186500	-3.01114400
O	1.43833400	0.40731600	-2.21883000

Zero-point correction= 0.960793 (Hartree/Particle)

Thermal correction to Energy=	1.020029
Thermal correction to Enthalpy=	1.020973
Thermal correction to Gibbs Free Energy=	0.855423
Sum of electronic and zero-point Energies=	-2522.821235
Sum of electronic and thermal Energies=	-2522.761998
Sum of electronic and thermal Enthalpies=	-2522.761054
Sum of electronic and thermal Free Energies=	-2522.926605

3-TS3

C	-1.49625600	-1.17772300	-1.06615700
O	-2.47225300	-0.87582100	-2.02408200
C	-0.72444000	-2.43209400	-1.47082700
C	-0.17905700	-3.28323000	-0.49984300
C	-0.58629000	-2.77334300	-2.82289000
C	0.43841500	-4.47797500	-0.87051400
H	-0.24515200	-2.99943600	0.54523900
C	0.03738900	-3.96724100	-3.19438600
C	0.53621600	-4.83053300	-2.21938100
H	0.84412200	-5.13350600	-0.10599200
H	0.13030700	-4.21943800	-4.24640000
C	-0.68115500	0.02473500	-0.61347300
C	-1.38966000	1.20885300	-0.43534200
C	-0.75277300	2.45582500	-0.16476100
C	-0.44383600	3.62190500	0.01966000
C	-0.10314200	4.99385600	0.21889400
C	-0.16489200	5.56747700	1.50465000
C	0.25758400	5.80182400	-0.87830400
C	0.14058400	6.91419600	1.68464000
C	0.55881600	7.14780800	-0.68645500
H	0.29302000	5.36616200	-1.87103100
C	0.50396000	7.70654400	0.59284400
H	0.09121300	7.34743100	2.67897900
H	0.83409500	7.76269000	-1.53788900
H	0.73927000	8.75646300	0.73782300
H	1.00960900	-5.76431400	-2.50695900
H	-0.95204600	-2.10074100	-3.59300500
H	-0.45337300	4.95122200	2.34946300
Au	1.33653400	-0.09057300	-0.17192800
C	3.34356700	-0.14730700	0.31001300
C	5.27630800	-0.16349000	1.50537900
C	5.60829700	-0.00671500	0.20090100
H	6.56543400	0.10162300	-0.28247500

H	5.88386100	-0.21280300	2.39409600
N	3.89051600	-0.25253100	1.55773800
N	4.41968400	-0.00541500	-0.51856000
C	3.17006800	-0.42308700	2.80287300
C	2.83366100	0.72384700	3.54716100
C	2.90597500	-1.73244600	3.25737000
C	2.18885600	0.52878800	4.77556700
C	2.25911100	-1.86541100	4.49137700
C	1.90046000	-0.74891800	5.24255000
H	1.91788500	1.39112400	5.37613600
H	2.04191500	-2.85624700	4.87570000
H	1.40351400	-0.87737300	6.19971400
C	4.39069100	0.10739900	-1.96306700
C	4.62255100	-1.05386100	-2.72830200
C	4.20987200	1.37913500	-2.54149500
C	4.64258000	-0.91227100	-4.12113000
C	4.23771800	1.45852600	-3.93935900
C	4.44749500	0.32754600	-4.72238000
H	4.82113800	-1.78405100	-4.74241700
H	4.10453200	2.42217700	-4.42019400
H	4.46938500	0.41433300	-5.80476800
C	4.89793100	-2.41776700	-2.10138900
C	6.39105200	-2.78590700	-2.22582300
C	4.01181300	-3.52519100	-2.69720700
H	4.66054900	-2.35739400	-1.03496000
H	7.03495300	-2.03504200	-1.75700000
H	6.59031800	-3.74922000	-1.74465900
H	6.68963200	-2.86740700	-3.27624900
H	2.95190400	-3.27195700	-2.61914400
H	4.24117100	-3.70709100	-3.75232700
H	4.17892300	-4.46637500	-2.16259800
C	4.05121600	2.64847000	-1.71196000
C	2.84683500	3.49406100	-2.15864000
C	5.35039900	3.48014600	-1.73828000
H	3.86614200	2.35670700	-0.67436200
H	1.92134600	2.91208500	-2.12039200
H	2.73406200	4.35828500	-1.49724300
H	2.97088900	3.87588400	-3.17748700
H	6.20517900	2.90413300	-1.36936000
H	5.58710100	3.81062700	-2.75527100
H	5.24691900	4.37174100	-1.11093500
C	3.35650100	-2.97117900	2.48775400
C	2.31537200	-4.10370000	2.51053300
C	4.71079300	-3.48420600	3.02231100

H	3.49543400	-2.68412100	1.44076400
H	1.33178800	-3.74703800	2.19158500
H	2.62817100	-4.90794900	1.83677000
H	2.20814600	-4.54442000	3.50696700
H	5.49178000	-2.72194200	2.94950800
H	4.62737800	-3.77681300	4.07439700
H	5.04177500	-4.35947500	2.45336400
C	3.18092400	2.13717300	3.09179100
C	4.31474200	2.72850700	3.95434300
C	1.95162600	3.06212600	3.08641700
H	3.54448200	2.08530800	2.06161100
H	5.21306800	2.10349700	3.92328900
H	4.58536800	3.72755600	3.59721200
H	4.00980600	2.81837000	5.00236000
H	1.15525600	2.65272100	2.45841100
H	1.55079200	3.21153000	4.09480900
H	2.22397200	4.04629900	2.69276900
C	-5.91878000	2.51252200	-0.13759900
C	-4.87493700	2.20864700	-0.92669600
H	-5.70460800	2.94907600	0.83888000
H	-5.01796000	1.75373900	-1.90453500
C	-7.34725400	2.32847200	-0.42824700
C	-8.27738100	2.51497800	0.60988100
C	-7.83277500	1.97312400	-1.70110200
C	-9.64311100	2.33656200	0.39336900
H	-7.92111600	2.80160300	1.59625400
C	-9.19604600	1.79604700	-1.91800000
H	-7.14231600	1.85179900	-2.53018800
C	-10.10725700	1.97414500	-0.87186900
H	-10.34354300	2.48636300	1.20958100
H	-9.55270600	1.52804800	-2.90821300
H	-11.17062900	1.84101700	-1.04654400
C	-3.46011100	2.50409400	-0.55042700
H	-3.39477100	2.98157500	0.43314100
H	-2.98325900	3.16387300	-1.28398600
O	-2.74253700	1.24309800	-0.52943700
H	-2.69392500	-1.69556700	-2.48707600
C	-4.55750800	-1.59897700	0.29075600
C	-5.76794800	-2.25419400	0.52855100
C	-5.77162500	-3.61759900	0.83176200
C	-4.55197500	-4.29577600	0.88521800
C	-3.36306900	-3.60730600	0.63971900
H	-6.70236400	-4.13863800	1.02452600
H	-4.45871100	-0.54233500	0.05910800

H	-2.38573900	-4.07309600	0.65279900
Cl	-4.49643600	-5.98918800	1.25898600
Cl	-7.25011700	-1.36269200	0.44867600
N	-3.43286200	-2.30797100	0.35145900
O	-2.06497500	-1.30127400	0.25353500

Zero-point correction= 1.030283 (Hartree/Particle)
Thermal correction to Energy= 1.097327
Thermal correction to Enthalpy= 1.098271
Thermal correction to Gibbs Free Energy= 0.914928
Sum of electronic and zero-point Energies= -3690.143347
Sum of electronic and thermal Energies= -3690.076304
Sum of electronic and thermal Enthalpies= -3690.075359
Sum of electronic and thermal Free Energies= -3690.258703

3-INT3

C	0.75297800	1.49781700	-3.12461100
O	0.31767300	2.72327600	-3.60339300
C	2.18897100	1.18624900	-3.41291800
C	2.58223800	-0.10979100	-3.76727700
C	3.13984200	2.21625100	-3.38233100
C	3.91473200	-0.37045700	-4.08691100
H	1.83506300	-0.89487800	-3.80904800
C	4.47293500	1.94845900	-3.69321500
C	4.86192100	0.65530100	-4.04830200
H	4.21144000	-1.37350500	-4.37794300
H	5.20451100	2.75052600	-3.66713700
C	-0.02444600	0.99854000	-1.96059000
C	-1.16613600	1.76091100	-1.48682700
C	-0.99198700	2.84619800	-0.61686700
C	-0.80823200	3.85580500	0.04768000
C	-0.58817800	5.01983200	0.81984400
C	-1.68146400	5.78764700	1.27909000
C	0.73015800	5.42394500	1.12829400
C	-1.45440300	6.93399600	2.03103700
C	0.94208600	6.57163900	1.88301800
H	1.56561600	4.83236200	0.76958100
C	-0.14614200	7.32628800	2.33355200
H	-2.29437100	7.52482100	2.38181300
H	1.95452300	6.88309500	2.11911300
H	0.02545400	8.22350700	2.92029300
H	5.89743800	0.44980200	-4.30283700
H	2.83103300	3.22363600	-3.11991800
H	-2.69221600	5.47608800	1.03754300

Au	0.63557500	-0.20249700	-0.36927900
C	1.18398200	-1.45999700	1.15875900
C	1.03419800	-2.89536000	2.90296300
C	2.35213700	-2.65918200	2.68055200
H	3.23548200	-3.02940600	3.17501900
H	0.53400100	-3.51476200	3.62978600
N	0.33130800	-2.15284000	1.96327600
N	2.42771100	-1.78103600	1.60672700
C	-1.11404600	-2.13734800	1.86472300
C	-1.83288600	-1.23745300	2.67684100
C	-1.73944800	-3.04117000	0.98234100
C	-3.22946800	-1.25541900	2.57334400
C	-3.13787900	-3.00648200	0.91574200
C	-3.87691200	-2.12564800	1.70007200
H	-3.81579300	-0.58223600	3.19163200
H	-3.65440900	-3.68356800	0.24296800
H	-4.96075400	-2.12211300	1.63050000
C	3.67861300	-1.31346600	1.04480300
C	4.35025600	-2.14661400	0.12713200
C	4.19196800	-0.07376200	1.47370900
C	5.57692800	-1.69122500	-0.37094300
C	5.41974000	0.33131800	0.93579900
C	6.10574500	-0.46595100	0.02445700
H	6.12626400	-2.30750700	-1.07551800
H	5.84772300	1.28053400	1.24284400
H	7.05976000	-0.13416600	-0.37429900
C	3.81315300	-3.50863500	-0.30408400
C	4.67055000	-4.65055100	0.27877600
C	3.70113700	-3.63215600	-1.83495100
H	2.80199200	-3.62007000	0.09860700
H	4.71775700	-4.60399400	1.37156100
H	4.25296500	-5.62328700	-0.00047900
H	5.69755600	-4.60682900	-0.09845500
H	3.09098900	-2.82735200	-2.25430500
H	4.68340100	-3.59685900	-2.31764600
H	3.24043100	-4.58875900	-2.10200600
C	3.48744800	0.80975400	2.49860700
C	3.14114500	2.19186700	1.91200300
C	4.32085800	0.94490000	3.78848500
H	2.54207900	0.33170100	2.77072600
H	2.52250900	2.09137000	1.01426400
H	2.58930000	2.78725300	2.64749500
H	4.04353700	2.75022700	1.64139300
H	4.53351800	-0.03303500	4.23160200

H	5.27955600	1.43753600	3.59698600
H	3.78159600	1.54308500	4.53038800
C	-0.96776600	-4.03976200	0.12509900
C	-1.18442200	-3.78082000	-1.37850200
C	-1.32691500	-5.49218400	0.49723700
H	0.09979600	-3.90948100	0.32545400
H	-0.89573800	-2.76141600	-1.65306000
H	-0.58450900	-4.47816800	-1.97243900
H	-2.23234700	-3.92119900	-1.66335700
H	-1.14224800	-5.69306400	1.55735700
H	-2.38077300	-5.70978700	0.29601900
H	-0.72617600	-6.19343600	-0.09079100
C	-1.15862900	-0.27558300	3.65134500
C	-1.51868800	-0.61420600	5.11170800
C	-1.49371600	1.19258100	3.32570400
H	-0.07519300	-0.38626800	3.54891300
H	-1.24584300	-1.64365800	5.36417800
H	-0.99161200	0.05443700	5.80002100
H	-2.59228000	-0.50208000	5.29513800
H	-1.20456900	1.44727400	2.30123300
H	-2.56440700	1.39468100	3.43720400
H	-0.96030600	1.86304400	4.00765500
C	-5.51401300	0.58518800	-0.77703600
C	-4.73712900	1.16985700	-1.70424400
H	-5.25139500	0.73827100	0.27039000
H	-4.94391900	1.07313200	-2.76662600
C	-6.70755600	-0.24005300	-0.99258200
C	-7.46671300	-0.63105400	0.12518500
C	-7.12800200	-0.66517500	-2.26699400
C	-8.61058000	-1.41436100	-0.02040000
H	-7.15981200	-0.30435400	1.11604800
C	-8.26859900	-1.44817400	-2.41234200
H	-6.55659200	-0.39068000	-3.14825800
C	-9.01518600	-1.82516000	-1.29099800
H	-9.18557200	-1.70081300	0.85502000
H	-8.57796400	-1.76878300	-3.40258300
H	-9.90511100	-2.43567600	-1.40973100
C	-3.56917600	2.01163500	-1.33541400
H	-3.46084600	2.11746600	-0.25290200
H	-3.59349400	3.00368000	-1.79871700
O	-2.34828100	1.35505400	-1.85785700
H	0.67551400	2.84568400	-4.49560600
O	-0.18015800	0.42162700	-3.27118000

Zero-point correction= 0.960253 (Hartree/Particle)

Thermal correction to Energy=	1.019826
Thermal correction to Enthalpy=	1.020771
Thermal correction to Gibbs Free Energy=	0.854858
Sum of electronic and zero-point Energies=	-2522.821702
Sum of electronic and thermal Energies=	-2522.762128
Sum of electronic and thermal Enthalpies=	-2522.761184
Sum of electronic and thermal Free Energies=	-2522.927097

2-INT0

C	-1.76711000	-0.79742400	3.18862200
O	-0.85413400	-1.57832400	3.43141100
C	-3.10721100	-0.90975300	3.80067800
C	-3.32849900	-1.94663100	4.72501600
C	-4.14380300	-0.01308400	3.49393400
C	-4.57194500	-2.08065500	5.33187500
H	-2.51593400	-2.62827000	4.95132600
C	-5.38811100	-0.15385400	4.10395700
C	-5.60192200	-1.18544700	5.02207600
H	-4.74262500	-2.87960100	6.04651700
H	-6.18908200	0.53931200	3.86729800
C	-1.51634700	0.32799400	2.23065500
C	-1.06956300	1.50650700	2.28727500
C	-0.62339000	2.76281400	2.30929500
C	-0.22870600	3.92712900	2.36668000
C	0.23685900	5.25244600	2.43921500
C	1.62681800	5.51868900	2.40036800
C	-0.68088500	6.32375100	2.55589200
C	2.07976400	6.82925900	2.47574800
C	-0.21213700	7.62861000	2.63035600
H	-1.74429200	6.11173800	2.58737600
C	1.16403400	7.88154000	2.59043900
H	3.14468200	7.03571300	2.44707600
H	-0.91377900	8.45138900	2.72117100
H	1.52457600	8.90396400	2.65026000
H	-6.57189300	-1.29187800	5.49860100
H	-3.97406700	0.78813600	2.78173600
H	2.32261100	4.69122900	2.31319400
Au	-1.76683300	-0.07487900	0.14578600
C	-2.14994600	-0.62560900	-1.76979200
C	-2.58916600	-0.57812500	-3.98081700
C	-2.61912700	-1.87708000	-3.58552500
H	-2.80730000	-2.78476700	-4.13533300
H	-2.73992800	-0.12343600	-4.94642400

N	-2.29924900	0.17898300	-2.85377400
N	-2.34837900	-1.88999200	-2.22415800
C	-2.15244200	1.62099100	-2.86110100
C	-3.27444400	2.41428900	-2.54851500
C	-0.89955200	2.16028700	-3.21481800
C	-3.10339300	3.80352100	-2.58440300
C	-0.79096600	3.55658900	-3.23343900
C	-1.87650200	4.36954400	-2.92070900
H	-3.94543300	4.44925500	-2.35496900
H	0.15756200	4.01004900	-3.50296900
H	-1.76875800	5.44998400	-2.94780900
C	-2.30305700	-3.09245500	-1.41505000
C	-1.06525000	-3.75012400	-1.25853200
C	-3.50592700	-3.56554500	-0.85399000
C	-1.06289700	-4.92348500	-0.49473600
C	-3.43866100	-4.74400600	-0.10016000
C	-2.23271600	-5.41513000	0.07885400
H	-0.13242700	-5.46202000	-0.35083600
H	-4.34407600	-5.14265900	0.34668900
H	-2.20410700	-6.32917500	0.66459800
C	0.21796400	-3.26320900	-1.92639900
C	0.49221100	-4.06656900	-3.21590900
C	1.43761700	-3.30646800	-0.98863300
H	0.07550700	-2.21671400	-2.21362200
H	-0.33628600	-3.99215100	-3.92778200
H	1.39607100	-3.69628900	-3.71024800
H	0.64185200	-5.12782800	-2.99084000
H	1.26551800	-2.75468700	-0.06027800
H	1.71350500	-4.33489800	-0.73082100
H	2.30072600	-2.85864000	-1.49162600
C	-4.85016300	-2.87105400	-1.05588500
C	-5.50246900	-2.47867400	0.28326500
C	-5.80259500	-3.74195100	-1.90001200
H	-4.67813200	-1.94502700	-1.61272700
H	-4.84872300	-1.82800100	0.87200000
H	-6.44197500	-1.94580500	0.10289900
H	-5.73502500	-3.35802100	0.89212400
H	-5.36571800	-3.98979000	-2.87258700
H	-6.03650600	-4.68343300	-1.39267400
H	-6.74599100	-3.21517900	-2.07666100
C	0.30089600	1.30088500	-3.60021900
C	1.52347400	1.57663600	-2.70585900
C	0.64748000	1.48446300	-5.09220000
H	0.03101000	0.25007700	-3.45750000

H	1.31346600	1.38151300	-1.65047600
H	2.35758400	0.93386900	-3.00428900
H	1.86481600	2.61322100	-2.80268100
H	-0.20539800	1.25349200	-5.73915200
H	0.95526700	2.51340100	-5.30570000
H	1.47506000	0.82529300	-5.37273900
C	-4.64219200	1.82797300	-2.20969600
C	-5.67895700	2.17099300	-3.29821900
C	-5.13000200	2.27711800	-0.81934000
H	-4.55047600	0.73823600	-2.17913000
H	-5.35807300	1.81689500	-4.28286200
H	-6.64288300	1.70565800	-3.06785800
H	-5.83931500	3.25153100	-3.37071800
H	-4.41139900	2.00010500	-0.04097800
H	-5.27645500	3.36107800	-0.77254900
H	-6.08908500	1.80403800	-0.58417200
C	4.75767000	1.78578500	-0.69194200
C	4.06254600	1.11031400	0.23584600
H	4.44073700	2.80519600	-0.92028400
H	4.32282600	0.08371100	0.49022600
C	5.91620900	1.31758100	-1.46814300
C	6.38320000	2.10739600	-2.53367100
C	6.58956700	0.11242800	-1.19291800
C	7.47135800	1.70656800	-3.30754500
H	5.88124400	3.04619800	-2.75613300
C	7.67687500	-0.28812900	-1.96440100
H	6.27429000	-0.50999800	-0.36153800
C	8.12240300	0.50467600	-3.02661100
H	7.81251700	2.33377200	-4.12626100
H	8.18376700	-1.21873000	-1.72642200
H	8.97383500	0.19107900	-3.62349600
C	2.90631200	1.69353700	0.99936200
H	2.72435100	2.72173100	0.66472900
H	3.15921500	1.73933000	2.07382300
O	1.68467100	0.98254900	0.81689200
H	1.77616600	0.10203200	1.23730100
C	5.10357500	-2.04846100	2.66819700
C	3.86215800	-2.44532800	2.34767300
H	5.21172900	-1.33021000	3.48204700
H	3.68771000	-3.14856600	1.53556700
C	6.37045900	-2.47091900	2.05148400
C	7.56460900	-1.85683100	2.46964000
C	6.45042600	-3.46626200	1.05854100
C	8.79301000	-2.21459500	1.91609300

H	7.52400900	-1.08907300	3.23825400
C	7.67642000	-3.82415100	0.50485900
H	5.54980800	-3.97214100	0.72436800
C	8.85417100	-3.20033300	0.93021400
H	9.70107200	-1.72563000	2.25609400
H	7.71679200	-4.59878200	-0.25557700
H	9.80972500	-3.48724500	0.50147400
C	2.63539700	-2.00394200	3.08221200
H	2.89551800	-1.25199300	3.84179700
H	2.19063900	-2.86178100	3.60936400
O	1.67172400	-1.48418000	2.15357000
H	0.79395500	-1.51782600	2.57944000

Zero-point correction= 1.122779 (Hartree/Particle)
Thermal correction to Energy= 1.193971
Thermal correction to Enthalpy= 1.194916
Thermal correction to Gibbs Free Energy= 0.997032
Sum of electronic and zero-point Energies= -2871.649139
Sum of electronic and thermal Energies= -2871.577947
Sum of electronic and thermal Enthalpies= -2871.577003
Sum of electronic and thermal Free Energies= -2871.774886

2-TS2

C	-0.57449000	-1.01491800	-2.04588300
O	-1.87404200	-1.27016000	-2.21408400
C	0.21559900	-1.68761900	-3.10694900
C	-0.25587200	-2.88304700	-3.67816900
C	1.36578100	-1.08627500	-3.64574200
C	0.41780900	-3.47176800	-4.74554800
H	-1.15402800	-3.33969700	-3.27851200
C	2.02848500	-1.66896200	-4.72442400
C	1.55884000	-2.86365500	-5.27577400
H	0.04821700	-4.39994100	-5.17127600
H	2.90339200	-1.18236500	-5.14503000
C	-0.01417900	-0.24990900	-1.02209100
C	-0.77914700	0.87415800	-0.41344100
C	-0.60048600	1.12958200	1.01793900
C	-0.64247800	1.36347000	2.20997700
C	-0.71858400	1.60876300	3.61641500
C	-1.08892100	0.57208200	4.49585100
C	-0.45360300	2.88923700	4.13991000
C	-1.18411800	0.81503700	5.86391500
C	-0.54938500	3.12176400	5.50956600
H	-0.17473500	3.69366900	3.46667100

C	-0.91359600	2.08704000	6.37464100
H	-1.47138200	0.00996500	6.53342600
H	-0.34259900	4.11242900	5.90297900
H	-0.98888300	2.27205700	7.44179300
H	2.07451800	-3.31474000	-6.11858400
H	1.70855600	-0.14454700	-3.23243400
H	-1.29995200	-0.41340800	4.09465200
Au	1.91132500	-0.62477500	-0.34032700
C	3.80458400	-1.05190000	0.34429200
C	5.98801500	-0.85781600	0.94700900
C	5.62257900	-2.14659100	1.15414600
H	6.17526700	-2.99050900	1.53336700
H	6.92369800	-0.34816600	1.10993500
N	4.86768600	-0.20018500	0.45064000
N	4.28890200	-2.25185100	0.77796300
C	4.85227400	1.21564400	0.15148800
C	5.12460100	1.63821100	-1.16652000
C	4.61361000	2.11685800	1.20733000
C	5.12925700	3.01696500	-1.41047200
C	4.62957100	3.48530100	0.90388400
C	4.88198100	3.93212600	-0.38981700
H	5.33944200	3.38042600	-2.41070200
H	4.45862100	4.20729400	1.69680900
H	4.90172700	4.99743600	-0.60185900
C	3.53824700	-3.48703200	0.87733500
C	2.77247300	-3.71760600	2.03696500
C	3.64805600	-4.42818600	-0.16664000
C	2.08041200	-4.93247000	2.11898600
C	2.94024200	-5.62775100	-0.02527500
C	2.16068600	-5.87734600	1.10088400
H	1.47679400	-5.14211100	2.99671700
H	3.00120700	-6.37708500	-0.80753600
H	1.61958700	-6.81506800	1.18752200
C	2.69003200	-2.72427700	3.19147600
C	3.27793700	-3.32087500	4.48567800
C	1.24876100	-2.22770600	3.41018400
H	3.29341100	-1.84936900	2.93373500
H	4.31413100	-3.64396000	4.34366400
H	3.26114200	-2.57729700	5.28944800
H	2.70347300	-4.18893900	4.82504600
H	0.85629700	-1.75319900	2.50544500
H	0.57916800	-3.05065800	3.68301000
H	1.22136900	-1.49290100	4.22165600
C	4.53001000	-4.20068700	-1.39095900

C	3.81622700	-4.55091900	-2.70799500
C	5.85283600	-4.98570400	-1.26579100
H	4.77868600	-3.13557000	-1.43414000
H	2.86579700	-4.02111600	-2.80405000
H	4.44779100	-4.27345900	-3.55817400
H	3.61816100	-5.62457500	-2.79113200
H	6.41143700	-4.70529300	-0.36717200
H	5.66454100	-6.06337700	-1.21536300
H	6.49395400	-4.79677300	-2.13319400
C	4.36847600	1.66721300	2.64437700
C	2.99156700	2.12722400	3.15390800
C	5.49846500	2.14262100	3.57915900
H	4.36668000	0.57422800	2.66607200
H	2.19066100	1.74348200	2.51538100
H	2.81702700	1.76036600	4.17028200
H	2.91818400	3.22016900	3.18478900
H	6.47604600	1.78238500	3.24338400
H	5.54724600	3.23553800	3.62726100
H	5.33196200	1.77214700	4.59581400
C	5.46787400	0.65584900	-2.28263900
C	6.99852300	0.51371800	-2.42489100
C	4.83563100	1.03113200	-3.63383600
H	5.06591900	-0.32239200	-2.00297100
H	7.46287000	0.17566300	-1.49359000
H	7.24469300	-0.21276100	-3.20630100
H	7.45555700	1.47097500	-2.69781400
H	3.75566500	1.18117000	-3.54492900
H	5.27094800	1.94314500	-4.05537400
H	5.01198200	0.22988800	-4.35854400
C	-5.56731000	1.36140700	-0.17617600
C	-4.38577000	1.72758800	-0.70524500
H	-5.56271100	0.93071600	0.82659100
H	-4.33209800	2.13421900	-1.71358500
C	-6.89531600	1.45999100	-0.79922000
C	-7.95719500	0.72493700	-0.24336700
C	-7.15080200	2.25005400	-1.93525300
C	-9.22844900	0.75878800	-0.81419600
H	-7.77933300	0.10957700	0.63424500
C	-8.42111000	2.28722500	-2.50259900
H	-6.35659000	2.85233400	-2.36633200
C	-9.46412700	1.53970800	-1.94654400
H	-10.02966700	0.17290400	-0.37436300
H	-8.60266900	2.90618800	-3.37631700
H	-10.45451700	1.57363300	-2.39049100

C	-3.09124100	1.64310000	0.04369500
H	-3.21192100	1.07228000	0.96879500
H	-2.73454400	2.64657800	0.31562900
O	-2.12612800	1.00149000	-0.82002900
H	-4.42526900	-0.74528900	-0.51155000
C	-6.80082200	-3.05810500	-0.10083500
C	-5.57064500	-2.86482000	0.40175300
H	-6.90023000	-3.11226500	-1.18584600
H	-5.40879600	-2.77908500	1.47492100
C	-8.06457500	-3.19676900	0.63748500
C	-9.27012300	-3.22447100	-0.08639900
C	-8.13020800	-3.29893200	2.04015700
C	-10.49858600	-3.33762800	0.56351500
H	-9.23817100	-3.15492600	-1.17076900
C	-9.35617600	-3.41121000	2.68945700
H	-7.21611300	-3.30456100	2.62617600
C	-10.54623400	-3.42946000	1.95524800
H	-11.41646900	-3.36019900	-0.01664800
H	-9.38569600	-3.49283700	3.77214500
H	-11.50041200	-3.52245200	2.46509500
C	-4.34906800	-2.71346200	-0.45176800
H	-4.58722300	-2.89863600	-1.50788400
H	-3.56458500	-3.41788400	-0.15594800
O	-3.75307600	-1.40845900	-0.28692700
H	-2.42718000	-1.03472600	-1.43038400
C	0.52413200	4.09834300	-0.18719400
C	0.41900900	5.48954900	-0.16123200
C	-0.51068700	6.13493800	-0.97949900
C	-1.32404200	5.36061000	-1.81129700
C	-1.19152200	3.97260900	-1.80980100
H	-0.59545400	7.21550600	-0.97468500
H	1.23092500	3.52573900	0.40149700
H	-1.77251400	3.29637600	-2.42530500
Cl	-2.49237100	6.10854500	-2.85068000
Cl	1.45392300	6.40688200	0.88747600
N	-0.29364900	3.42064500	-0.99321700
O	0.02862700	1.84320300	-1.23038200

Zero-point correction=	1.198199 (Hartree/Particle)
Thermal correction to Energy=	1.276317
Thermal correction to Enthalpy=	1.277261
Thermal correction to Gibbs Free Energy=	1.065690
Sum of electronic and zero-point Energies=	-4114.168834
Sum of electronic and thermal Energies=	-4114.090716
Sum of electronic and thermal Enthalpies=	-4114.089771

Sum of electronic and thermal Free Energies= -4114.301342