

Supporting information

Theoretical Study on the Mechanism and Chemoselectivity in Gold(I)-Catalyzed Cycloisomerization of β,β - Disubstituted Ortho-(alkynyl)styrenes

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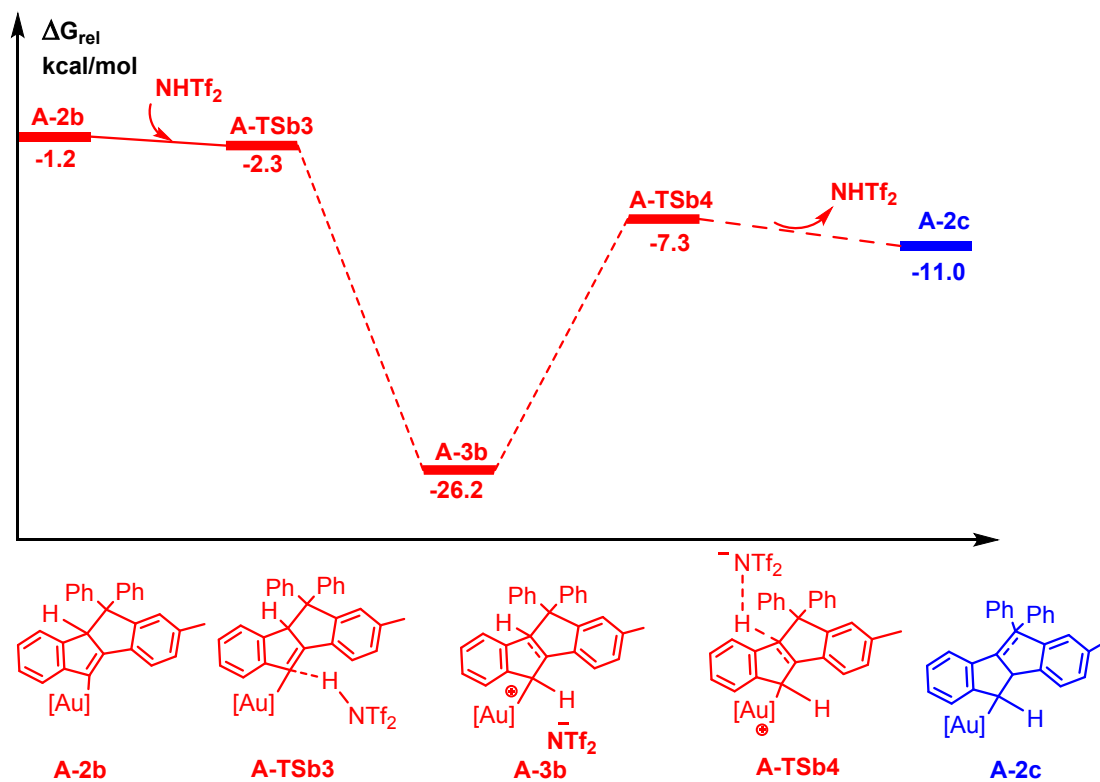


Figure S1 Energy profile calculated for the remaining pathway b of Series A. Relative energies are in kcal/mol.

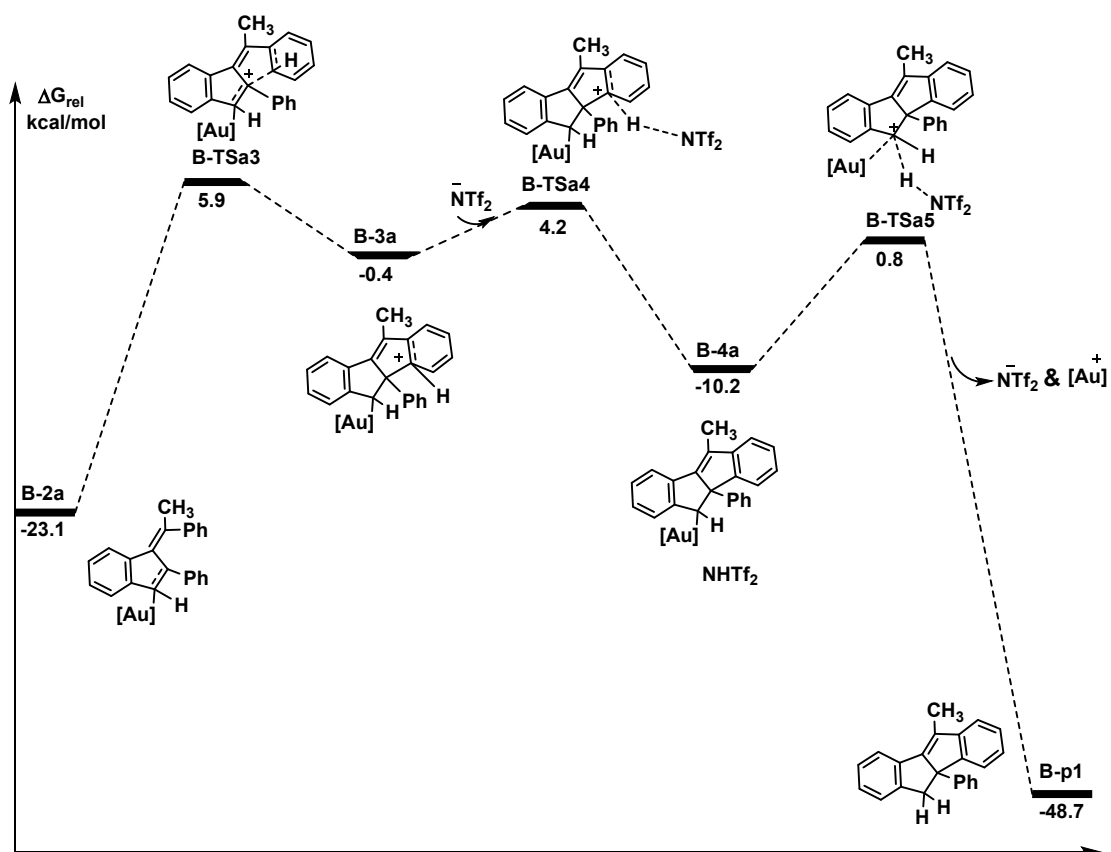


Figure S2 Energy profile calculated for the remaining pathway a of Series **B**. Relative energies are in kcal/mol.

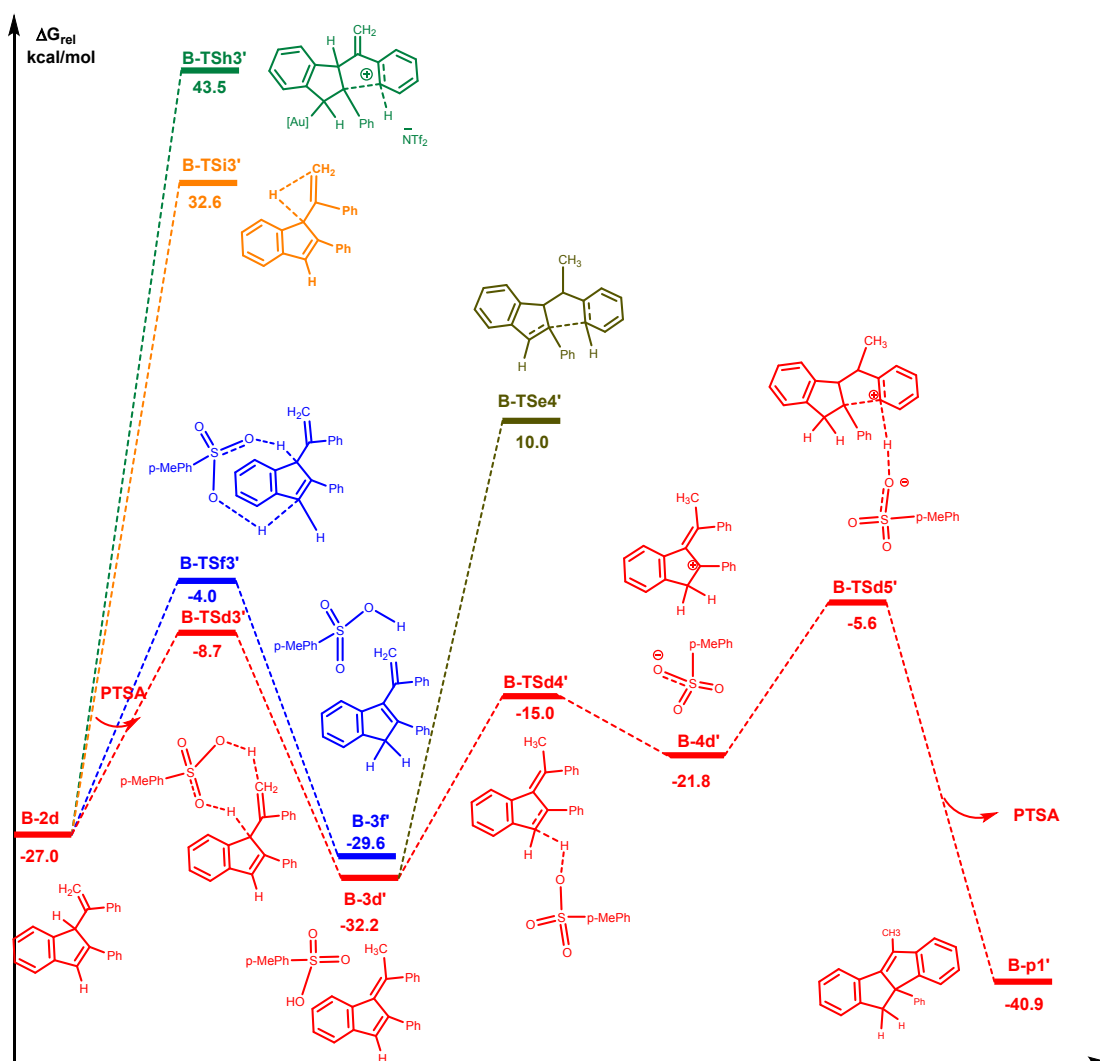


Figure S3 Second part of energy profile calculated for Series **B** catalyzed by one molecular PTSA. Relative energies are in kcal/mol.

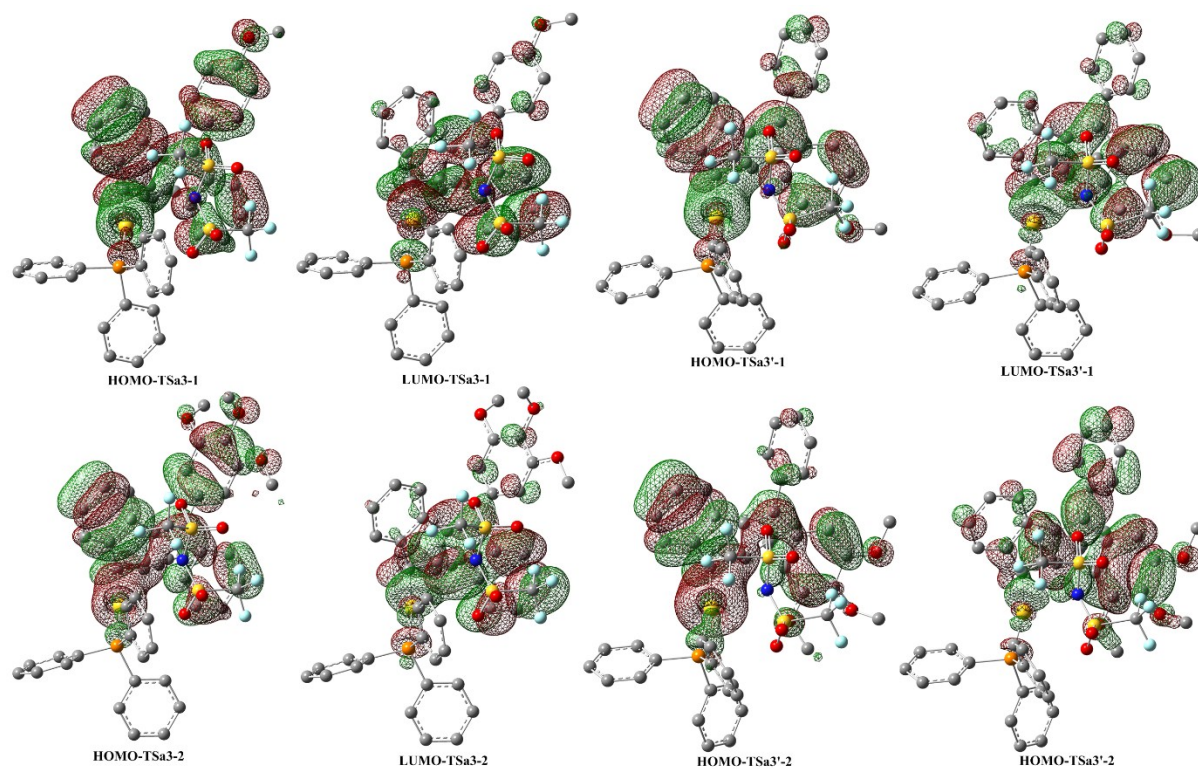


Figure S4. Comparison of the HOMOs and LUMOs of the four transition states **TSa3-1**, **TSa3'-1**, **TSa3-2**, and **TSa3'-2**.

Optimized cartesian coordinates with the self-consistent field (SCF)

energies and the imaginary frequencies of transition states

A-re

6	1.377191000	-4.584752000	-0.726580000
6	2.480353000	-3.753754000	-0.912981000
6	2.333440000	-2.376091000	-0.863367000
6	1.087347000	-1.783621000	-0.623873000
6	-0.034181000	-2.635896000	-0.453744000
6	0.129322000	-4.027397000	-0.502701000
1	1.490787000	-5.665226000	-0.764952000
1	3.460452000	-4.183266000	-1.105949000
1	3.197763000	-1.736936000	-1.026899000
1	-0.744534000	-4.659012000	-0.362728000
6	0.881372000	-0.336298000	-0.621160000
6	1.733336000	0.652558000	-0.269338000
6	-1.323951000	-2.080945000	-0.228554000
6	-2.406575000	-1.560164000	-0.047178000
6	-3.645035000	-0.893387000	0.161409000
6	-4.851959000	-1.599963000	0.246931000
6	-3.672526000	0.504843000	0.285210000
6	-6.045782000	-0.924251000	0.449391000
1	-4.838588000	-2.683308000	0.155483000
6	-4.871966000	1.166283000	0.487537000
1	-2.737361000	1.058357000	0.222878000
6	-6.078965000	0.466099000	0.570394000
1	-6.976983000	-1.485311000	0.516803000
1	-4.878469000	2.251142000	0.585937000
1	-0.115318000	-0.032041000	-0.944152000
6	3.049443000	0.400504000	0.367234000
6	4.219400000	0.924711000	-0.192438000
6	3.145137000	-0.352411000	1.541408000
6	5.456930000	0.671338000	0.386262000
1	4.150642000	1.527907000	-1.096278000
6	4.381558000	-0.597933000	2.125359000
1	2.236112000	-0.748889000	1.989421000
6	5.541501000	-0.092920000	1.546065000
1	6.359146000	1.074595000	-0.067988000
1	4.439060000	-1.185318000	3.038828000
1	6.509396000	-0.287458000	2.002122000
6	1.343680000	2.065494000	-0.468981000
6	0.527547000	2.451669000	-1.540973000
6	1.776237000	3.057446000	0.421465000

6	0.137966000	3.774476000	-1.701507000
1	0.219798000	1.705796000	-2.270891000
6	1.385477000	4.380088000	0.261358000
1	2.415230000	2.779210000	1.257081000
6	0.563476000	4.745028000	-0.799898000
1	-0.488232000	4.051849000	-2.546490000
1	1.725732000	5.130617000	0.971223000
1	0.263922000	5.782278000	-0.929696000
6	-7.374431000	1.194384000	0.762036000
1	-7.262303000	2.038979000	1.450945000
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1	-8.151672000	0.533466000	1.159472000
Zero-point correction=			0.412640 (Hartree/Particle)
Thermal correction to Energy=			0.437113
Thermal correction to Enthalpy=			0.438057
Thermal correction to Gibbs Free Energy=			0.355204
Sum of electronic and zero-point Energies=			-1117.028278
Sum of electronic and thermal Energies=			-1117.003805
Sum of electronic and thermal Enthalpies=			-1117.002861
Sum of electronic and thermal Free Energies=			-1117.085714

A-1

6	-1.185452000	4.356516000	0.155773000
6	-2.475242000	4.518168000	-0.350747000
6	-3.252607000	3.414030000	-0.671747000
6	-2.768014000	2.114674000	-0.497242000
6	-1.461434000	1.963433000	0.029824000
6	-0.678587000	3.081510000	0.345319000
1	-0.581472000	5.224645000	0.404695000
1	-2.875567000	5.517245000	-0.503114000
1	-4.252770000	3.547476000	-1.078082000
1	0.319947000	2.937247000	0.759394000
6	-3.521754000	0.917283000	-0.873218000
6	-4.809471000	0.608354000	-0.605672000
6	-1.010585000	0.624747000	0.268625000
6	-1.018491000	-0.596316000	0.500633000
6	-1.210095000	-1.990221000	0.731711000
6	-0.274687000	-2.769728000	1.426382000
6	-2.394099000	-2.586008000	0.260525000
6	-0.517225000	-4.118645000	1.632918000
1	0.635545000	-2.309022000	1.810020000
6	-2.623110000	-3.930951000	0.489427000
1	-3.133574000	-1.987001000	-0.269527000
6	-1.690886000	-4.722075000	1.171959000

1	0.212068000	-4.718199000	2.174900000
1	-3.548719000	-4.378449000	0.128568000
1	-2.934093000	0.163339000	-1.401000000
6	-5.693787000	1.451472000	0.230271000
6	-6.982216000	1.767421000	-0.216686000
6	-5.273151000	1.934295000	1.474136000
6	-7.815217000	2.576896000	0.545676000
1	-7.324236000	1.378035000	-1.174311000
6	-6.111700000	2.733524000	2.241303000
1	-4.283768000	1.667699000	1.842735000
6	-7.381219000	3.063229000	1.775546000
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1	-5.775011000	3.095858000	3.209688000
1	-8.035902000	3.690280000	2.375782000
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6	-4.971727000	-1.198001000	-2.344158000
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6	-5.384690000	-2.463730000	-2.740842000
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1	-7.198688000	-3.322733000	-0.002435000
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1	-1.932058000	-6.731162000	0.447197000
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79	1.193130000	0.136363000	0.130676000
15	3.523385000	0.173666000	-0.110481000
6	4.029992000	0.463098000	-1.826311000
6	4.242157000	-1.407214000	0.408868000
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6	5.069712000	-0.261175000	-2.413487000
6	3.382203000	1.473041000	-2.546012000
6	5.469598000	-1.468053000	1.073834000
6	3.559669000	-2.585264000	0.087271000
6	5.417381000	2.157824000	0.458598000
6	3.713640000	1.783887000	2.140304000
6	5.455826000	0.026576000	-3.719014000
1	5.574005000	-1.048550000	-1.855522000
6	3.777375000	1.758490000	-3.845859000
1	2.569082000	2.035804000	-2.084837000

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6	4.103087000	-3.817053000	0.428217000
1	2.601353000	-2.535738000	-0.432367000
6	5.998441000	3.124158000	1.272406000
1	5.850778000	1.931242000	-0.514545000
6	4.301138000	2.748613000	2.949092000
1	2.819511000	1.257606000	2.476815000
6	4.812229000	1.032758000	-4.432054000
1	6.261698000	-0.538341000	-4.180097000
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6	5.325840000	-3.875620000	1.092913000
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1	6.886740000	3.651355000	0.934521000
1	3.866426000	2.981457000	3.917551000
1	5.115484000	1.252081000	-5.452562000
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Zero-point correction=			0.688277 (Hartree/Particle)
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Thermal correction to Enthalpy=			0.733544
Thermal correction to Gibbs Free Energy=			0.602941
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Sum of electronic and thermal Energies=			-2287.711524
Sum of electronic and thermal Enthalpies=			-2287.710580
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A-TS1

6	1.408916000	-4.866002000	-1.324381000
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6	2.804591000	-2.454460000	-1.275619000
6	1.411564000	-2.478273000	-1.060239000
6	0.714648000	-3.683816000	-1.093105000
1	0.873586000	-5.811634000	-1.348223000
1	3.322876000	-5.776804000	-1.690695000
1	4.567895000	-3.628323000	-1.648128000
1	-0.361162000	-3.691651000	-0.926393000
6	3.413048000	-1.111936000	-1.288084000
6	4.350865000	-0.620639000	-0.401273000
6	0.855501000	-1.169614000	-0.756030000
6	1.620133000	-0.122705000	-0.642943000

6	1.843097000	1.240576000	-0.293908000
6	1.757193000	1.631853000	1.053991000
6	2.176830000	2.201484000	-1.264475000
6	1.972905000	2.954338000	1.409582000
1	1.511619000	0.882421000	1.805196000
6	2.408790000	3.512970000	-0.892375000
1	2.247802000	1.901510000	-2.308058000
6	2.311937000	3.911262000	0.446952000
1	1.894215000	3.253248000	2.453602000
1	2.678276000	4.249414000	-1.648079000
1	3.303942000	-0.566166000	-2.231494000
6	4.662591000	-1.280596000	0.873851000
6	5.991882000	-1.320176000	1.322483000
6	3.665901000	-1.874791000	1.662473000
6	6.317969000	-1.956934000	2.512035000
1	6.772263000	-0.863495000	0.717363000
6	3.993496000	-2.491494000	2.861124000
1	2.626757000	-1.823777000	1.344971000
6	5.319168000	-2.540656000	3.285513000
1	7.354171000	-1.994262000	2.837672000
1	3.209862000	-2.934227000	3.470576000
1	5.572547000	-3.030512000	4.222344000
6	5.004393000	0.658211000	-0.697966000
6	5.342105000	1.017639000	-2.013601000
6	5.256689000	1.576237000	0.335006000
6	5.907599000	2.254585000	-2.287167000
1	5.197625000	0.299798000	-2.818770000
6	5.799737000	2.822069000	0.055261000
1	4.991481000	1.315047000	1.357366000
6	6.130496000	3.162593000	-1.254270000
1	6.186258000	2.507998000	-3.306751000
1	5.971389000	3.529580000	0.863040000
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6	2.571518000	5.335043000	0.826227000
1	3.523338000	5.685840000	0.409424000
1	1.792238000	5.998285000	0.430894000
1	2.605193000	5.468063000	1.911565000
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15	-3.339687000	0.099664000	0.080829000
6	-4.201494000	0.793164000	-1.359878000
6	-3.302007000	1.416233000	1.335347000
6	-4.412793000	-1.207425000	0.743663000
6	-5.031877000	1.911814000	-1.251155000
6	-4.053093000	0.151765000	-2.593681000

6	-4.268753000	1.502661000	2.339820000
6	-2.290093000	2.379375000	1.257686000
6	-5.771384000	-1.278557000	0.425425000
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6	-5.707784000	2.382049000	-2.372323000
1	-5.149835000	2.414691000	-0.292401000
6	-4.735614000	0.622355000	-3.708286000
1	-3.400373000	-0.717595000	-2.677541000
6	-4.221193000	2.546673000	3.258327000
1	-5.056005000	0.753118000	2.406558000
6	-2.250187000	3.421782000	2.174897000
1	-1.533135000	2.309588000	0.474469000
6	-6.563963000	-2.268369000	0.997986000
1	-6.209064000	-0.564201000	-0.270182000
6	-4.653831000	-3.112859000	2.207752000
1	-2.795140000	-2.073546000	1.880045000
6	-5.560298000	1.739138000	-3.597400000
1	-6.350876000	3.254350000	-2.288466000
1	-4.618566000	0.122759000	-4.666496000
6	-3.214955000	3.504050000	3.176232000
1	-4.972681000	2.611713000	4.040978000
1	-1.461498000	4.167894000	2.110233000
6	-6.007194000	-3.182641000	1.886693000
1	-7.620006000	-2.325324000	0.747000000
1	-4.219521000	-3.828556000	2.901063000
1	-6.088543000	2.111127000	-4.471688000
1	-3.180314000	4.316750000	3.897478000
1	-6.630025000	-3.955613000	2.329701000
Zero-point correction=			0.688639 (Hartree/Particle)
Thermal correction to Energy=			0.731472
Thermal correction to Enthalpy=			0.732417
Thermal correction to Gibbs Free Energy=			0.607167
Sum of electronic and zero-point Energies=			-2287.749880
Sum of electronic and thermal Energies=			-2287.707047
Sum of electronic and thermal Enthalpies=			-2287.706102
Sum of electronic and thermal Free Energies=			-2287.831352

A-TS2

6	-1.471214000	5.100677000	0.201438000
6	-2.823878000	5.311855000	0.489567000
6	-3.659232000	4.228534000	0.673892000
6	-3.185292000	2.910873000	0.500816000
6	-1.801108000	2.696727000	0.236972000
6	-0.968088000	3.813032000	0.103618000

1	-0.803416000	5.950036000	0.083923000
1	-3.211637000	6.321929000	0.587797000
1	-4.711068000	4.379719000	0.909491000
1	0.093773000	3.650283000	-0.072462000
6	-4.052621000	1.814966000	0.757774000
6	-4.021592000	0.525408000	0.198213000
6	-1.276923000	1.352252000	0.251273000
6	-1.955432000	0.230043000	0.342199000
6	-1.669550000	-1.169015000	0.105353000
6	-1.931853000	-2.150854000	1.067975000
6	-1.013358000	-1.549116000	-1.085103000
6	-1.536239000	-3.466110000	0.855614000
1	-2.435407000	-1.877320000	1.990667000
6	-0.615305000	-2.856788000	-1.282096000
1	-0.825656000	-0.791368000	-1.845464000
6	-0.868700000	-3.840141000	-0.312023000
1	-1.736400000	-4.217473000	1.617584000
1	-0.092547000	-3.131916000	-2.197613000
1	-4.789533000	1.979984000	1.547938000
6	-4.817352000	-0.453524000	1.004646000
6	-5.886999000	-1.182571000	0.475040000
6	-4.565332000	-0.548179000	2.380755000
6	-6.664493000	-1.994705000	1.293489000
1	-6.132477000	-1.095223000	-0.580284000
6	-5.338667000	-1.362158000	3.197764000
1	-3.735900000	0.017785000	2.806721000
6	-6.391194000	-2.092817000	2.653521000
1	-7.497496000	-2.545492000	0.863903000
1	-5.120136000	-1.425443000	4.260878000
1	-6.999901000	-2.731236000	3.288718000
6	-3.947874000	0.327384000	-1.295382000
6	-3.958779000	1.407547000	-2.188314000
6	-3.927392000	-0.968088000	-1.831094000
6	-3.922807000	1.198259000	-3.560114000
1	-4.014329000	2.425979000	-1.812919000
6	-3.906933000	-1.176477000	-3.204062000
1	-3.914615000	-1.830140000	-1.168117000
6	-3.894507000	-0.094098000	-4.076412000
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1	-3.895169000	-2.192952000	-3.589716000
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6	-0.412004000	-5.247079000	-0.533149000
1	-0.890176000	-5.685210000	-1.417436000
1	0.670385000	-5.283014000	-0.709481000

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79	0.787730000	0.864731000	0.268416000
15	2.991734000	0.040465000	0.100356000
6	3.285032000	-0.573779000	-1.587311000
6	3.237875000	-1.397786000	1.187210000
6	4.324489000	1.208476000	0.489739000
6	4.082802000	-1.696453000	-1.827816000
6	2.707462000	0.109724000	-2.661988000
6	4.422331000	-1.599227000	1.898524000
6	2.208950000	-2.343412000	1.262675000
6	5.514199000	1.249638000	-0.240680000
6	4.153322000	2.047405000	1.596012000
6	4.301582000	-2.125175000	-3.132743000
1	4.531526000	-2.236344000	-0.994838000
6	2.931168000	-0.321312000	-3.964322000
1	2.078651000	0.980595000	-2.473580000
6	4.573820000	-2.742928000	2.677807000
1	5.224890000	-0.865217000	1.844798000
6	2.368900000	-3.484463000	2.037563000
1	1.282746000	-2.185807000	0.706746000
6	6.525342000	2.127471000	0.137411000
1	5.649651000	0.599714000	-1.103561000
6	5.170117000	2.914637000	1.973748000
1	3.221869000	2.014876000	2.162139000
6	3.726019000	-1.440131000	-4.198851000
1	4.922547000	-2.998052000	-3.317559000
1	2.480658000	0.213271000	-4.796735000
6	3.551470000	-3.683348000	2.747102000
1	5.495416000	-2.898001000	3.232983000
1	1.565928000	-4.216921000	2.096224000
6	6.354571000	2.955949000	1.241984000
1	7.449445000	2.163506000	-0.433771000
1	5.037237000	3.563766000	2.835307000
1	3.896710000	-1.780252000	-5.217239000
1	3.674375000	-4.573172000	3.359326000
1	7.147670000	3.639864000	1.533498000
Zero-point correction=			0.688303 (Hartree/Particle)
Thermal correction to Energy=			0.730974
Thermal correction to Enthalpy=			0.731919
Thermal correction to Gibbs Free Energy=			0.608524
Sum of electronic and zero-point Energies=			-2287.723035
Sum of electronic and thermal Energies=			-2287.680363
Sum of electronic and thermal Enthalpies=			-2287.679419
Sum of electronic and thermal Free Energies=			-2287.802813

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6	-0.449601000	-4.370717000	-0.685315000
6	-1.273647000	-5.155044000	0.148439000
6	-2.312483000	-4.583387000	0.849534000
6	-2.548480000	-3.201225000	0.705895000
6	-1.665475000	-2.402259000	-0.064626000
6	-0.649176000	-3.009815000	-0.817787000
1	0.372628000	-4.844405000	-1.216142000
1	-1.088923000	-6.223011000	0.226922000
1	-2.970417000	-5.186257000	1.470946000
1	-0.002854000	-2.405360000	-1.449913000
6	-3.581796000	-2.422881000	1.263153000
6	-3.865777000	-1.172727000	0.651016000
6	-1.923817000	-1.002277000	0.028397000
6	-1.365636000	0.159610000	-0.164730000
6	-1.829188000	1.529782000	-0.410679000
6	-1.796950000	2.025346000	-1.720017000
6	-2.278546000	2.363851000	0.618790000
6	-2.264072000	3.303310000	-1.996144000
1	-1.434157000	1.385359000	-2.523322000
6	-2.743566000	3.638861000	0.326230000
1	-2.289303000	2.001725000	1.644580000
6	-2.751308000	4.131127000	-0.981798000
1	-2.251736000	3.668541000	-3.022183000
1	-3.113513000	4.267978000	1.135394000
1	-4.042641000	-2.686669000	2.215379000
6	-4.377101000	-1.123642000	-0.764931000
6	-4.768924000	-2.289328000	-1.436186000
6	-4.506896000	0.102196000	-1.430729000
6	-5.243028000	-2.231310000	-2.739241000
1	-4.720949000	-3.250667000	-0.930165000
6	-4.984576000	0.157007000	-2.734348000
1	-4.231325000	1.023388000	-0.925821000
6	-5.346648000	-1.009233000	-3.398583000
1	-5.551490000	-3.147266000	-3.237126000
1	-5.067493000	1.122299000	-3.228800000
1	-5.722470000	-0.967261000	-4.417592000
6	-4.311221000	-0.130742000	1.614393000
6	-3.565936000	0.028559000	2.792363000
6	-5.460950000	0.647538000	1.438259000
6	-3.942667000	0.952772000	3.756916000
1	-2.655267000	-0.556652000	2.923578000
6	-5.833229000	1.578643000	2.400084000

1	-6.076109000	0.513509000	0.552496000
6	-5.074617000	1.739060000	3.556065000
1	-3.348783000	1.068834000	4.660015000
1	-6.729430000	2.175241000	2.250424000
1	-5.369684000	2.470856000	4.303902000
6	-3.243396000	5.515660000	-1.274376000
1	-4.206265000	5.709815000	-0.788225000
1	-2.541684000	6.273066000	-0.903525000
1	-3.368327000	5.680927000	-2.349039000
79	0.748701000	0.080114000	-0.043048000
15	3.107339000	0.154384000	0.042713000
6	3.741364000	0.459742000	1.716515000
6	3.787082000	1.449233000	-1.032694000
6	3.864899000	-1.407366000	-0.502654000
6	4.861560000	1.262302000	1.944524000
6	3.112884000	-0.181994000	2.788759000
6	5.052655000	1.318751000	-1.613608000
6	3.039009000	2.611522000	-1.243820000
6	4.860127000	-2.045739000	0.239250000
6	3.437046000	-1.959583000	-1.715437000
6	5.347736000	1.418246000	3.238726000
1	5.352698000	1.766297000	1.113832000
6	3.607704000	-0.028750000	4.077574000
1	2.237368000	-0.806352000	2.607163000
6	5.564718000	2.348918000	-2.394123000
1	5.635654000	0.412057000	-1.455854000
6	3.558307000	3.639275000	-2.022160000
1	2.046396000	2.709184000	-0.801879000
6	5.420148000	-3.231001000	-0.229989000
1	5.198480000	-1.619479000	1.182261000
6	4.003971000	-3.138247000	-2.181611000
1	2.665772000	-1.454144000	-2.298657000
6	4.723924000	0.773507000	4.301941000
1	6.216770000	2.046356000	3.416394000
1	3.119075000	-0.530098000	4.909129000
6	4.818856000	3.506873000	-2.597095000
1	6.547304000	2.245848000	-2.847416000
1	2.975018000	4.541452000	-2.186510000
6	4.994163000	-3.775776000	-1.436053000
1	6.194630000	-3.727305000	0.349121000
1	3.675422000	-3.560765000	-3.128020000
1	5.107594000	0.898398000	5.311368000
1	5.220921000	4.308563000	-3.211379000
1	5.434924000	-4.700618000	-1.799804000

Zero-point correction=	0.687958 (Hartree/Particle)
Thermal correction to Energy=	0.730923
Thermal correction to Enthalpy=	0.731867
Thermal correction to Gibbs Free Energy=	0.606774
Sum of electronic and zero-point Energies=	-2287.718745
Sum of electronic and thermal Energies=	-2287.675780
Sum of electronic and thermal Enthalpies=	-2287.674836
Sum of electronic and thermal Free Energies=	-2287.799929

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6	2.607414000	4.149153000	2.435745000
6	1.701703000	3.257141000	1.891885000
6	2.128449000	1.944687000	1.630734000
6	3.462046000	1.545453000	1.904636000
6	4.368823000	2.448386000	2.429898000
6	3.922164000	3.742015000	2.704707000
1	2.307849000	5.168710000	2.660614000
1	0.676558000	3.547442000	1.669173000
1	5.398227000	2.164244000	2.635122000
1	4.614969000	4.457870000	3.141278000
6	1.409103000	0.879350000	1.028094000
6	2.301169000	-0.271381000	0.915207000
6	3.645155000	0.150618000	1.451531000
1	4.272267000	-0.532283000	2.018581000
6	3.566745000	-0.034713000	-0.053528000
6	1.679665000	-1.624611000	0.994292000
6	1.547285000	-2.270105000	2.221268000
6	1.107968000	-2.208324000	-0.140576000
6	0.872451000	-3.485308000	2.308392000
1	1.975249000	-1.817413000	3.115633000
6	0.424414000	-3.410464000	-0.046198000
1	1.221075000	-1.714780000	-1.106941000
6	0.304715000	-4.076006000	1.179386000
1	0.784080000	-3.984983000	3.272439000
1	-0.022862000	-3.851152000	-0.936921000
6	4.154093000	-1.268237000	-0.652083000
6	4.276395000	-1.368721000	-2.046138000
6	4.570776000	-2.361041000	0.124539000
6	4.794458000	-2.512542000	-2.639276000
1	3.968685000	-0.537298000	-2.675001000
6	5.088932000	-3.502042000	-0.469071000
1	4.487148000	-2.340784000	1.208300000
6	5.203346000	-3.584092000	-1.854193000
1	4.882508000	-2.562125000	-3.721506000

1	5.408334000	-4.332593000	0.155041000
1	5.612296000	-4.478887000	-2.316459000
6	3.555299000	1.166646000	-0.949929000
6	2.459603000	1.466545000	-1.760314000
6	4.697796000	1.963281000	-1.029655000
6	2.491609000	2.565780000	-2.613336000
1	1.576017000	0.827324000	-1.727880000
6	4.730425000	3.063506000	-1.879298000
1	5.564966000	1.715616000	-0.418145000
6	3.625310000	3.369715000	-2.668563000
1	1.628813000	2.792590000	-3.234821000
1	5.621457000	3.684742000	-1.923964000
1	3.650699000	4.231907000	-3.330009000
6	-0.392756000	-5.399454000	1.257197000
1	0.232294000	-6.198351000	0.839368000
1	-0.625893000	-5.674378000	2.291277000
1	-1.328417000	-5.390640000	0.685475000
79	-0.556517000	0.721764000	0.466001000
15	-2.794707000	0.231204000	-0.189966000
6	-4.066617000	1.376888000	0.416079000
6	-3.248198000	-1.433727000	0.381279000
6	-2.969247000	0.194996000	-2.001442000
6	-5.309782000	0.936682000	0.874889000
6	-3.784796000	2.746555000	0.371910000
6	-4.204701000	-2.200729000	-0.292530000
6	-2.644247000	-1.935544000	1.537787000
6	-4.043185000	0.793895000	-2.661393000
6	-1.986548000	-0.478332000	-2.735810000
6	-6.262348000	1.863586000	1.286893000
1	-5.532859000	-0.128097000	0.914561000
6	-4.743248000	3.667443000	0.774880000
1	-2.812695000	3.088873000	0.014516000
6	-4.562919000	-3.450551000	0.199601000
1	-4.666285000	-1.818113000	-1.202654000
6	-3.011374000	-3.182597000	2.029794000
1	-1.876951000	-1.354392000	2.051323000
6	-4.129676000	0.719588000	-4.049014000
1	-4.809595000	1.319033000	-2.093503000
6	-2.081271000	-0.554478000	-4.118694000
1	-1.152455000	-0.951135000	-2.213737000
6	-5.981011000	3.224773000	1.235403000
1	-7.227249000	1.519124000	1.650012000
1	-4.523094000	4.731210000	0.737272000
6	-3.970862000	-3.938090000	1.362603000

1	-5.306747000	-4.045096000	-0.324596000
1	-2.539455000	-3.566184000	2.931727000
6	-3.151874000	0.049134000	-4.775520000
1	-4.964784000	1.189148000	-4.562587000
1	-1.318585000	-1.080542000	-4.687345000
1	-6.727613000	3.945244000	1.559752000
1	-4.255495000	-4.914993000	1.746521000
1	-3.222878000	-0.004628000	-5.858896000
Zero-point correction=			0.691228 (Hartree/Particle)
Thermal correction to Energy=			0.733498
Thermal correction to Enthalpy=			0.734442
Thermal correction to Gibbs Free Energy=			0.610587
Sum of electronic and zero-point Energies=			-2287.771130
Sum of electronic and thermal Energies=			-2287.728860
Sum of electronic and thermal Enthalpies=			-2287.727916
Sum of electronic and thermal Free Energies=			-2287.851771

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6	-2.061150000	-3.223222000	-3.244418000
6	-0.948947000	-2.537179000	-2.764730000
6	-1.132944000	-1.317599000	-2.120899000
6	-2.428555000	-0.787950000	-1.959845000
6	-3.539760000	-1.490394000	-2.411230000
6	-3.343733000	-2.704884000	-3.066481000
1	-1.931741000	-4.177661000	-3.750508000
1	0.056360000	-2.941397000	-2.877379000
1	-4.549019000	-1.118026000	-2.249080000
1	-4.206681000	-3.258854000	-3.430065000
6	-0.148512000	-0.426777000	-1.519831000
6	-0.800454000	0.619609000	-0.939092000
6	-2.302956000	0.428413000	-1.100375000
1	-2.426052000	-0.165573000	0.032443000
6	-3.272325000	1.463017000	-1.010991000
6	-0.150629000	1.758405000	-0.266924000
6	0.627607000	1.546638000	0.878387000
6	-0.226998000	3.058805000	-0.776613000
6	1.308852000	2.592280000	1.485943000
1	0.682191000	0.541011000	1.289820000
6	0.450667000	4.106002000	-0.162036000
1	-0.824521000	3.247735000	-1.668472000
6	1.234903000	3.890949000	0.974467000
1	1.922256000	2.389334000	2.365681000
1	0.378319000	5.111939000	-0.575994000
6	-3.217839000	2.492577000	0.013992000
6	-3.676743000	3.791228000	-0.285582000

6	-2.658046000	2.259189000	1.283546000
6	-3.542327000	4.817849000	0.634484000
1	-4.097174000	3.994989000	-1.267190000
6	-2.553371000	3.281732000	2.211013000
1	-2.336315000	1.260489000	1.552779000
6	-2.980054000	4.566103000	1.884412000
1	-3.875564000	5.820144000	0.377399000
1	-2.124484000	3.072277000	3.187701000
1	-2.881573000	5.371973000	2.608091000
6	-4.360211000	1.555336000	-1.985397000
6	-4.071004000	1.478357000	-3.355746000
6	-5.684532000	1.755111000	-1.569279000
6	-5.086849000	1.609606000	-4.290611000
1	-3.041859000	1.320303000	-3.672873000
6	-6.701715000	1.844060000	-2.508632000
1	-5.906105000	1.782440000	-0.505406000
6	-6.403724000	1.779470000	-3.867420000
1	-4.854469000	1.567708000	-5.351595000
1	-7.730932000	1.964300000	-2.180391000
1	-7.201568000	1.860595000	-4.602120000
6	2.015147000	5.004782000	1.605467000
1	1.681881000	5.985283000	1.248351000
1	1.925347000	4.992490000	2.697927000
1	3.085512000	4.913087000	1.373111000
79	1.887069000	-0.581952000	-1.278137000
15	4.093304000	-0.392969000	-0.395170000
6	3.925114000	-0.350806000	1.425002000
6	4.854456000	1.220179000	-0.795409000
6	5.370592000	-1.632510000	-0.782567000
6	4.816339000	0.354645000	2.240834000
6	2.824440000	-0.991593000	2.003317000
6	6.229724000	1.394193000	-0.965683000
6	4.001556000	2.326216000	-0.884333000
6	6.281360000	-2.108585000	0.162817000
6	5.432574000	-2.099378000	-2.099460000
6	4.611620000	0.406999000	3.615342000
1	5.664957000	0.875797000	1.797813000
6	2.612240000	-0.921894000	3.376240000
1	2.100270000	-1.519939000	1.382956000
6	6.745114000	2.663803000	-1.212126000
1	6.898815000	0.536422000	-0.905236000
6	4.521617000	3.591835000	-1.125759000
1	2.925662000	2.194715000	-0.762421000
6	7.247387000	-3.038340000	-0.209307000

1	6.229422000	-1.757912000	1.192455000
6	6.404354000	-3.020757000	-2.469074000
1	4.707844000	-1.740669000	-2.830947000
6	3.507611000	-0.226335000	4.182594000
1	5.308357000	0.956379000	4.244419000
1	1.734721000	-1.402270000	3.803285000
6	5.894085000	3.761781000	-1.289709000
1	7.816663000	2.794013000	-1.345390000
1	3.847023000	4.442836000	-1.198587000
6	7.310788000	-3.492017000	-1.523084000
1	7.950771000	-3.412049000	0.531111000
1	6.447581000	-3.380408000	-3.494248000
1	3.341878000	-0.168392000	5.255999000
1	6.301632000	4.751274000	-1.484137000
1	8.065052000	-4.220992000	-1.809960000
8	-4.910131000	-0.460233000	0.385157000
16	-4.274937000	-1.392912000	1.307548000
9	-3.284444000	-3.427222000	-0.092579000
9	-4.702424000	-3.989651000	1.430646000
9	-5.389248000	-3.057205000	-0.382834000
6	-4.410345000	-3.097379000	0.508865000
8	-2.073646000	-3.016370000	2.730896000
8	-0.262461000	-1.663632000	1.593973000
16	-1.581900000	-1.760798000	2.196120000
9	-2.679411000	-0.287202000	4.097419000
9	-0.808515000	-1.235855000	4.615246000
9	-0.827803000	0.491756000	3.323524000
6	-1.483740000	-0.618080000	3.656427000
7	-2.668905000	-1.024058000	1.216472000
8	-4.777295000	-1.539694000	2.657625000
Zero-point correction=			0.746508 (Hartree/Particle)
Thermal correction to Energy=			0.802742
Thermal correction to Enthalpy=			0.803686
Thermal correction to Gibbs Free Energy=			0.655092
Sum of electronic and zero-point Energies=			-4114.610382
Sum of electronic and thermal Energies=			-4114.554149
Sum of electronic and thermal Enthalpies=			-4114.553204
Sum of electronic and thermal Free Energies=			-4114.701798

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6	-2.462198000	-2.946829000	-3.226233000
6	-1.466090000	-2.195010000	-2.606011000
6	-1.830215000	-1.077780000	-1.862796000
6	-3.186240000	-0.686749000	-1.754100000

6	-4.173702000	-1.461573000	-2.355831000
6	-3.801567000	-2.586441000	-3.093420000
1	-2.193432000	-3.825722000	-3.808584000
1	-0.418154000	-2.483063000	-2.680051000
1	-5.227989000	-1.209899000	-2.262515000
1	-4.572161000	-3.186004000	-3.573430000
6	-0.999670000	-0.184695000	-1.058336000
6	-1.836500000	0.695150000	-0.414965000
6	-3.237088000	0.446511000	-0.804865000
1	-0.102924000	-1.865941000	0.098243000
6	-4.356944000	1.066680000	-0.321423000
6	-1.321708000	1.852836000	0.345272000
6	-0.435507000	1.669697000	1.416665000
6	-1.596796000	3.163111000	-0.055986000
6	0.187644000	2.751195000	2.023983000
1	-0.245717000	0.660158000	1.781114000
6	-0.981633000	4.245233000	0.565680000
1	-2.288828000	3.331727000	-0.880084000
6	-0.061888000	4.059008000	1.599222000
1	0.896486000	2.575157000	2.835850000
1	-1.202011000	5.257515000	0.225448000
6	-4.358035000	1.839901000	0.932562000
6	-5.041710000	3.060598000	1.017788000
6	-3.684355000	1.366925000	2.066326000
6	-5.001428000	3.815243000	2.181851000
1	-5.584839000	3.423932000	0.146545000
6	-3.647081000	2.121571000	3.231265000
1	-3.186612000	0.398727000	2.023333000
6	-4.295523000	3.351417000	3.289878000
1	-5.518924000	4.771094000	2.225428000
1	-3.106233000	1.745001000	4.096563000
1	-4.262257000	3.943491000	4.201797000
6	-5.646477000	0.995049000	-1.039687000
6	-5.720351000	1.343078000	-2.393665000
6	-6.819553000	0.614348000	-0.377469000
6	-6.928018000	1.277118000	-3.077030000
1	-4.811776000	1.654611000	-2.905783000
6	-8.024244000	0.533042000	-1.064946000
1	-6.772590000	0.364304000	0.681108000
6	-8.081265000	0.862052000	-2.416767000
1	-6.969398000	1.550551000	-4.128885000
1	-8.923839000	0.214612000	-0.542926000
1	-9.026145000	0.803948000	-2.952365000
6	0.662717000	5.212534000	2.225802000

1	0.431058000	5.306869000	3.294201000
1	1.750761000	5.081020000	2.146662000
1	0.403585000	6.161549000	1.743564000
79	1.038555000	0.127315000	-0.954669000
15	3.229025000	0.977281000	-0.559282000
6	4.694563000	0.033699000	-1.082548000
6	3.447207000	1.323129000	1.224555000
6	3.383355000	2.626494000	-1.324210000
6	5.957480000	0.259730000	-0.527672000
6	4.537357000	-0.932005000	-2.080317000
6	4.103805000	2.469947000	1.681170000
6	2.891780000	0.436392000	2.152263000
6	4.463946000	3.015752000	-2.115065000
6	2.339953000	3.527956000	-1.078601000
6	7.053335000	-0.468559000	-0.974955000
1	6.078835000	1.002932000	0.260099000
6	5.636886000	-1.656763000	-2.527103000
1	3.545147000	-1.124558000	-2.489837000
6	4.209035000	2.719348000	3.045843000
1	4.516986000	3.180210000	0.965499000
6	3.002137000	0.684968000	3.515418000
1	2.345715000	-0.439215000	1.803105000
6	4.501485000	4.300700000	-2.652745000
1	5.275924000	2.318417000	-2.314360000
6	2.389340000	4.810400000	-1.606374000
1	1.491522000	3.227431000	-0.461317000
6	6.892569000	-1.425123000	-1.974629000
1	8.034295000	-0.294639000	-0.539015000
1	5.509309000	-2.410866000	-3.299738000
6	3.659409000	1.827919000	3.962892000
1	4.717140000	3.616167000	3.392895000
1	2.560663000	-0.008589000	4.226987000
6	3.469896000	5.197034000	-2.397174000
1	5.343523000	4.599918000	-3.272572000
1	1.575127000	5.503466000	-1.403930000
1	7.750666000	-1.998099000	-2.318356000
1	3.736748000	2.028074000	5.028983000
1	3.505454000	6.199246000	-2.818049000
8	-1.164533000	-1.440700000	2.485743000
16	-0.955406000	-2.807505000	2.059869000
9	-2.382137000	-4.470106000	0.640321000
9	-3.361146000	-3.662736000	2.389439000
9	-3.089451000	-2.430406000	0.636058000
6	-2.570825000	-3.391121000	1.367860000

8	0.608237000	-5.218694000	0.576777000
8	1.269694000	-3.627397000	-1.300297000
16	1.022621000	-3.927868000	0.091155000
9	2.345400000	-3.352530000	2.277392000
9	3.437330000	-4.496271000	0.803888000
9	3.088191000	-2.387227000	0.498138000
6	2.586742000	-3.507548000	0.990734000
7	-0.009035000	-2.733460000	0.671349000
8	-0.452944000	-3.842006000	2.928637000
Zero-point correction=			0.750727 (Hartree/Particle)
Thermal correction to Energy=			0.807921
Thermal correction to Enthalpy=			0.808865
Thermal correction to Gibbs Free Energy=			0.657655
Sum of electronic and zero-point Energies=			-4114.645143
Sum of electronic and thermal Energies=			-4114.587948
Sum of electronic and thermal Enthalpies=			-4114.587004
Sum of electronic and thermal Free Energies=			-4114.738215

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6	-2.505283000	-2.498466000	-3.609319000
6	-1.507022000	-2.005432000	-2.773570000
6	-1.817705000	-0.968496000	-1.900732000
6	-3.116048000	-0.414418000	-1.859916000
6	-4.113243000	-0.934768000	-2.683514000
6	-3.795771000	-1.970651000	-3.558530000
1	-2.281669000	-3.310098000	-4.298292000
1	-0.502283000	-2.427833000	-2.783741000
1	-5.131180000	-0.552112000	-2.652613000
1	-4.568411000	-2.373424000	-4.209855000
6	-0.986924000	-0.361219000	-0.854505000
6	-1.797462000	0.531537000	-0.162217000
6	-3.149601000	0.532057000	-0.729724000
1	-0.458726000	-1.417704000	-0.094255000
6	-4.241950000	1.195353000	-0.221477000
6	-1.241479000	1.511437000	0.792100000
6	-0.365366000	1.118992000	1.810602000
6	-1.443158000	2.881664000	0.584332000
6	0.317914000	2.069286000	2.559563000
1	-0.220964000	0.058372000	2.016272000
6	-0.760629000	3.824348000	1.340913000
1	-2.121635000	3.204039000	-0.204755000
6	0.152508000	3.434898000	2.325892000
1	1.015918000	1.740971000	3.330418000
1	-0.917112000	4.886441000	1.147409000
6	-4.288343000	1.620027000	1.182242000

6	-4.808909000	2.870206000	1.546086000
6	-3.789822000	0.773700000	2.180702000
6	-4.762135000	3.289575000	2.867289000
1	-5.211069000	3.523823000	0.773424000
6	-3.753318000	1.191592000	3.503933000
1	-3.431708000	-0.215628000	1.904385000
6	-4.226767000	2.454074000	3.847363000
1	-5.140315000	4.272897000	3.137445000
1	-3.350224000	0.523965000	4.262027000
1	-4.191845000	2.785794000	4.882699000
6	-5.422932000	1.487381000	-1.050743000
6	-5.267092000	2.048385000	-2.325164000
6	-6.716823000	1.242861000	-0.573012000
6	-6.375006000	2.333243000	-3.111155000
1	-4.261839000	2.252359000	-2.689683000
6	-7.823584000	1.510149000	-1.368486000
1	-6.842971000	0.819004000	0.421495000
6	-7.655410000	2.055837000	-2.638224000
1	-6.240541000	2.773157000	-4.096552000
1	-8.822011000	1.295030000	-0.995008000
1	-8.523290000	2.273040000	-3.256591000
6	0.953834000	4.456722000	3.076081000
1	1.614026000	3.982634000	3.810696000
1	1.590048000	5.036696000	2.392086000
1	0.313322000	5.174108000	3.603848000
79	1.072081000	0.183110000	-0.908233000
15	3.210810000	1.101173000	-0.618033000
6	4.619622000	0.141011000	-1.247530000
6	3.530000000	1.276334000	1.174008000
6	3.316221000	2.794154000	-1.278100000
6	5.939283000	0.519246000	-0.971293000
6	4.365484000	-1.034123000	-1.958762000
6	4.048389000	2.432287000	1.758749000
6	3.219733000	0.175775000	1.977523000
6	4.258377000	3.198521000	-2.223050000
6	2.347484000	3.702330000	-0.830728000
6	6.993742000	-0.260193000	-1.426423000
1	6.138360000	1.420560000	-0.391297000
6	5.427415000	-1.814258000	-2.407771000
1	3.337390000	-1.350484000	-2.136675000
6	4.253435000	2.480413000	3.135500000
1	4.280990000	3.300345000	1.143011000
6	3.437405000	0.220440000	3.347819000
1	2.787319000	-0.713227000	1.521733000

6	4.238682000	4.504240000	-2.708420000
1	5.004129000	2.494530000	-2.587508000
6	2.341444000	5.005287000	-1.307720000
1	1.596859000	3.384411000	-0.103920000
6	6.736288000	-1.425973000	-2.146403000
1	8.018395000	0.034190000	-1.212390000
1	5.226222000	-2.731419000	-2.955421000
6	3.951638000	1.377796000	3.929417000
1	4.651123000	3.386174000	3.588323000
1	3.190180000	-0.644721000	3.958871000
6	3.287436000	5.407672000	-2.249282000
1	4.972272000	4.814025000	-3.448897000
1	1.587922000	5.704290000	-0.950096000
1	7.564063000	-2.038955000	-2.495531000
1	4.113767000	1.421331000	5.003877000
1	3.277194000	6.426377000	-2.629672000
8	-1.638529000	-1.825753000	2.409208000
16	-1.193397000	-3.030431000	1.729505000
9	-2.373686000	-4.621325000	0.020454000
9	-3.556615000	-4.075532000	1.743974000
9	-3.226189000	-2.640156000	0.161619000
6	-2.692268000	-3.643359000	0.840484000
8	0.469364000	-4.945818000	-0.255203000
8	1.438715000	-2.875642000	-1.329309000
16	0.906135000	-3.570280000	-0.166723000
9	1.923495000	-2.867009000	2.199045000
9	2.613972000	-4.765311000	1.444369000
9	3.340390000	-2.928279000	0.580326000
6	2.289786000	-3.535514000	1.114085000
7	-0.219115000	-2.560695000	0.488628000
8	-0.631174000	-4.151940000	2.453945000
Zero-point correction=			0.745540 (Hartree/Particle)
Thermal correction to Energy=			0.802326
Thermal correction to Enthalpy=			0.803270
Thermal correction to Gibbs Free Energy=			0.651138
Sum of electronic and zero-point Energies=			-4114.637312
Sum of electronic and thermal Energies=			-4114.580526
Sum of electronic and thermal Enthalpies=			-4114.579582
Sum of electronic and thermal Free Energies=			-4114.731714

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6	-0.377088000	-4.324665000	-1.925509000
6	0.074499000	-3.074114000	-2.330001000
6	-0.730239000	-1.964370000	-2.081161000

6	-1.993037000	-2.090394000	-1.464462000
6	-2.405669000	-3.345301000	-1.015007000
6	-1.596669000	-4.451182000	-1.256444000
1	0.233174000	-5.205990000	-2.109401000
1	1.047443000	-2.957277000	-2.806853000
1	-3.341049000	-3.467560000	-0.475165000
1	-1.922186000	-5.431096000	-0.914592000
6	-0.468559000	-0.539211000	-2.279247000
6	-1.538064000	0.197516000	-1.783729000
6	-2.563229000	-0.739395000	-1.303130000
1	0.258427000	-0.129045000	-2.978251000
6	-3.806245000	-0.430390000	-0.817199000
6	-1.678636000	1.651513000	-1.995574000
6	-0.789305000	2.563228000	-1.422168000
6	-2.720494000	2.155369000	-2.785140000
6	-0.942044000	3.931098000	-1.618918000
1	0.000020000	2.204276000	-0.757508000
6	-2.873501000	3.519514000	-2.969977000
1	-3.427755000	1.461420000	-3.237256000
6	-1.988943000	4.433723000	-2.388081000
1	-0.246191000	4.621003000	-1.141952000
1	-3.699757000	3.890317000	-3.576460000
6	-4.209881000	0.902967000	-0.347967000
6	-5.466851000	1.406659000	-0.714821000
6	-3.378323000	1.683337000	0.465874000
6	-5.857642000	2.680591000	-0.330794000
1	-6.123660000	0.795900000	-1.332279000
6	-3.784725000	2.948484000	0.869722000
1	-2.418237000	1.285714000	0.791153000
6	-5.014595000	3.455669000	0.461137000
1	-6.824398000	3.068104000	-0.644234000
1	-3.132104000	3.541570000	1.504308000
1	-5.323651000	4.450754000	0.773928000
6	-4.858958000	-1.465251000	-0.752960000
6	-5.227997000	-2.175862000	-1.900080000
6	-5.512997000	-1.730478000	0.455561000
6	-6.210938000	-3.155283000	-1.834951000
1	-4.726114000	-1.958090000	-2.841243000
6	-6.477731000	-2.727816000	0.522923000
1	-5.229435000	-1.170060000	1.344186000
6	-6.828156000	-3.441791000	-0.620301000
1	-6.492385000	-3.700688000	-2.732837000
1	-6.960373000	-2.947408000	1.472356000
1	-7.588681000	-4.217408000	-0.565294000

6	-2.183923000	5.907356000	-2.579336000
1	-3.143588000	6.238727000	-2.162915000
1	-1.392242000	6.484070000	-2.090167000
1	-2.188154000	6.177474000	-3.642508000
79	0.842076000	-0.190042000	-0.325724000
15	3.209988000	-0.124536000	-0.582809000
6	3.776345000	1.468223000	-1.275702000
6	3.859781000	-1.379369000	-1.737420000
6	4.145751000	-0.347141000	0.958736000
6	4.762118000	1.542914000	-2.263682000
6	3.218814000	2.644986000	-0.762269000
6	4.867843000	-2.275248000	-1.379442000
6	3.316581000	-1.435796000	-3.026529000
6	5.412392000	0.212008000	1.142414000
6	3.559105000	-1.093517000	1.980797000
6	5.179639000	2.782607000	-2.738557000
1	5.204598000	0.632336000	-2.664827000
6	3.644022000	3.878945000	-1.239312000
1	2.468971000	2.588287000	0.025813000
6	5.323958000	-3.216070000	-2.299934000
1	5.297190000	-2.236680000	-0.379980000
6	3.780937000	-2.367041000	-3.945326000
1	2.528316000	-0.737327000	-3.310505000
6	6.080474000	0.021035000	2.346850000
1	5.870157000	0.802644000	0.349640000
6	4.224891000	-1.275447000	3.186191000
1	2.567016000	-1.518216000	1.836911000
6	4.620099000	3.949598000	-2.229587000
1	5.945168000	2.834818000	-3.509216000
1	3.208937000	4.790009000	-0.835083000
6	4.784822000	-3.262441000	-3.579941000
1	6.107299000	-3.913138000	-2.012141000
1	3.355578000	-2.399720000	-4.945664000
6	5.485422000	-0.715070000	3.368454000
1	7.064113000	0.461013000	2.494016000
1	3.743143000	-1.832555000	3.986033000
1	4.946739000	4.916854000	-2.604491000
1	5.145269000	-3.996706000	-4.296404000
1	6.003711000	-0.842947000	4.315917000
8	-2.353760000	-1.284452000	1.611799000
16	-1.246016000	-1.054272000	2.522671000
9	0.883455000	-2.455201000	3.098486000
9	-0.914975000	-3.612888000	2.793238000
9	0.128256000	-2.780127000	1.098152000

6	-0.217727000	-2.576567000	2.366482000
8	1.019106000	0.559771000	4.084220000
8	1.676764000	1.646576000	1.909604000
16	0.652945000	1.073770000	2.779088000
9	-0.757054000	3.069105000	1.877430000
9	-1.593086000	2.164991000	3.647559000
9	0.168526000	3.403524000	3.800511000
6	-0.468537000	2.517117000	3.054762000
7	-0.256684000	0.076800000	1.852862000
8	-1.482114000	-0.895358000	3.944289000
Zero-point correction=			0.751438 (Hartree/Particle)
Thermal correction to Energy=			0.807613
Thermal correction to Enthalpy=			0.808557
Thermal correction to Gibbs Free Energy=			0.660647
Sum of electronic and zero-point Energies=			-4114.671228
Sum of electronic and thermal Energies=			-4114.615053
Sum of electronic and thermal Enthalpies=			-4114.614109
Sum of electronic and thermal Free Energies=			-4114.762019

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6	1.537033000	-4.368770000	-1.541318000
6	0.743826000	-3.286531000	-1.188522000
6	1.352334000	-2.049840000	-0.952836000
6	2.758121000	-1.922847000	-1.091652000
6	3.546865000	-3.005413000	-1.440860000
6	2.924843000	-4.232522000	-1.661275000
1	1.080061000	-5.338628000	-1.721200000
1	-0.334677000	-3.392606000	-1.079922000
1	4.628282000	-2.906004000	-1.528048000
1	3.524456000	-5.098229000	-1.931498000
6	0.751380000	-0.786060000	-0.552502000
6	1.798589000	0.086960000	-0.387699000
6	3.112470000	-0.488426000	-0.873107000
1	3.270668000	-0.016971000	-1.856895000
6	4.254109000	-0.080204000	0.026049000
6	1.959802000	1.422898000	0.084762000
6	1.116409000	2.506705000	-0.193521000
6	3.240847000	1.665432000	0.693527000
6	1.609145000	3.789070000	-0.065641000
1	0.130549000	2.324350000	-0.619248000
6	3.722564000	3.005767000	0.758999000
1	3.437155000	1.095148000	1.602747000
6	2.935134000	4.063085000	0.367172000
1	0.979735000	4.630564000	-0.354665000

1	4.702759000	3.200150000	1.193054000
6	5.485913000	0.458856000	-0.584241000
6	6.442464000	1.104654000	0.219029000
6	5.756406000	0.316013000	-1.951318000
6	7.614193000	1.600341000	-0.326823000
1	6.251478000	1.214478000	1.286169000
6	6.942898000	0.796952000	-2.495185000
1	5.058870000	-0.206250000	-2.602166000
6	7.869368000	1.446816000	-1.689852000
1	8.336077000	2.105311000	0.309777000
1	7.140707000	0.659877000	-3.555030000
1	8.791555000	1.830962000	-2.118016000
6	4.419344000	-0.942043000	1.233975000
6	3.333805000	-1.243117000	2.072653000
6	5.639911000	-1.588175000	1.474733000
6	3.471070000	-2.142330000	3.118755000
1	2.363250000	-0.779103000	1.898565000
6	5.771668000	-2.495883000	2.520066000
1	6.487237000	-1.400375000	0.820582000
6	4.692127000	-2.772697000	3.348426000
1	2.618776000	-2.354253000	3.759150000
1	6.727116000	-2.988131000	2.682430000
1	4.797953000	-3.476920000	4.169439000
6	3.411940000	5.480536000	0.431726000
1	3.420161000	5.938373000	-0.564872000
1	2.756276000	6.094857000	1.059896000
1	4.425438000	5.545594000	0.837708000
79	-1.247324000	-0.396019000	-0.273563000
15	-3.565079000	0.086361000	0.031579000
6	-3.897338000	1.877558000	0.017538000
6	-4.221396000	-0.528950000	1.611637000
6	-4.625970000	-0.614307000	-1.268252000
6	-4.712736000	2.493306000	0.968612000
6	-3.327858000	2.640172000	-1.008454000
6	-5.512106000	-1.049349000	1.729596000
6	-3.403182000	-0.437799000	2.742768000
6	-5.774866000	0.044651000	-1.714651000
6	-4.292106000	-1.865343000	-1.796146000
6	-4.953386000	3.862434000	0.893007000
1	-5.159882000	1.905533000	1.768622000
6	-3.578094000	4.004026000	-1.084317000
1	-2.696839000	2.155718000	-1.755398000
6	-5.976146000	-1.475817000	2.969897000
1	-6.152906000	-1.126269000	0.852704000

6	-3.874812000	-0.856123000	3.980552000
1	-2.392892000	-0.038171000	2.647391000
6	-6.581627000	-0.547273000	-2.680429000
1	-6.037028000	1.020855000	-1.308926000
6	-5.104256000	-2.454560000	-2.757572000
1	-3.391154000	-2.374368000	-1.451322000
6	-4.388907000	4.615942000	-0.130265000
1	-5.587576000	4.339821000	1.635703000
1	-3.141756000	4.591889000	-1.888182000
6	-5.160249000	-1.379312000	4.092957000
1	-6.978681000	-1.886682000	3.058454000
1	-3.236225000	-0.783939000	4.857242000
6	-6.246691000	-1.794005000	-3.200663000
1	-7.473294000	-0.032317000	-3.028861000
1	-4.842106000	-3.426567000	-3.167414000
1	-4.581761000	5.684343000	-0.187229000
1	-5.526394000	-1.716935000	5.059299000
1	-6.877689000	-2.251912000	-3.958250000
Zero-point correction=			0.689767 (Hartree/Particle)
Thermal correction to Energy=			0.731869
Thermal correction to Enthalpy=			0.732814
Thermal correction to Gibbs Free Energy=			0.609571
Sum of electronic and zero-point Energies=			-2287.724209
Sum of electronic and thermal Energies=			-2287.682106
Sum of electronic and thermal Enthalpies=			-2287.681162
Sum of electronic and thermal Free Energies=			-2287.804405

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6	1.706389000	-4.426537000	-1.377128000
6	0.866810000	-3.355997000	-1.124825000
6	1.425693000	-2.077818000	-0.976164000
6	2.834659000	-1.895121000	-1.079917000
6	3.663842000	-2.971483000	-1.347748000
6	3.090984000	-4.234005000	-1.484181000
1	1.295896000	-5.425966000	-1.493513000
1	-0.210578000	-3.489973000	-1.040771000
1	4.741123000	-2.841527000	-1.432791000
1	3.731032000	-5.091972000	-1.675623000
6	0.753680000	-0.831193000	-0.697591000
6	1.770486000	0.118140000	-0.622086000
6	3.126754000	-0.437412000	-0.959423000
1	3.389600000	-0.054346000	-1.961001000
6	4.085335000	0.219408000	0.072593000
6	1.912956000	1.404909000	-0.124863000

6	1.030746000	2.502820000	-0.065943000
6	3.314785000	1.581825000	0.359757000
6	1.586749000	3.753646000	0.001767000
1	-0.035881000	2.367612000	-0.243528000
6	3.858847000	2.945265000	0.131187000
1	3.173559000	1.600419000	1.467306000
6	3.009673000	3.998526000	0.020747000
1	0.930889000	4.623236000	-0.049073000
1	4.934489000	3.104446000	0.180799000
6	5.495029000	0.469974000	-0.435245000
6	6.412979000	1.098387000	0.418402000
6	5.937060000	0.076514000	-1.697062000
6	7.714922000	1.353578000	0.012418000
1	6.101726000	1.372327000	1.427310000
6	7.247096000	0.324795000	-2.106379000
1	5.272055000	-0.448339000	-2.380459000
6	8.136641000	0.969511000	-1.258940000
1	8.406846000	1.842991000	0.693439000
1	7.568795000	0.004868000	-3.094439000
1	9.156927000	1.163457000	-1.579359000
6	4.105131000	-0.679141000	1.319980000
6	3.053930000	-0.693953000	2.244237000
6	5.140086000	-1.603524000	1.500548000
6	3.051172000	-1.579030000	3.318776000
1	2.201165000	-0.025014000	2.137366000
6	5.136978000	-2.490576000	2.569972000
1	5.969425000	-1.630320000	0.797261000
6	4.094018000	-2.479743000	3.489447000
1	2.224053000	-1.559393000	4.024409000
1	5.960087000	-3.191400000	2.685962000
1	4.094227000	-3.167597000	4.330973000
6	3.488858000	5.412763000	-0.092105000
1	3.111691000	5.887570000	-1.005762000
1	3.138330000	6.018771000	0.752190000
1	4.580909000	5.464063000	-0.111856000
79	-1.235710000	-0.477737000	-0.345156000
15	-3.529285000	0.066678000	0.027063000
6	-3.812116000	1.846979000	-0.240330000
6	-4.124417000	-0.280516000	1.708261000
6	-4.663293000	-0.788965000	-1.106165000
6	-4.506543000	2.637540000	0.676641000
6	-3.321882000	2.418863000	-1.420802000
6	-5.461347000	-0.601788000	1.958498000
6	-3.227939000	-0.153138000	2.773535000

6	-5.818736000	-0.174174000	-1.597360000
6	-4.382262000	-2.115589000	-1.447175000
6	-4.708471000	3.989596000	0.412855000
1	-4.889374000	2.199018000	1.596953000
6	-3.534862000	3.765804000	-1.683178000
1	-2.781844000	1.800485000	-2.139516000
6	-5.895234000	-0.787414000	3.266267000
1	-6.162522000	-0.708067000	1.132008000
6	-3.667991000	-0.334632000	4.079307000
1	-2.183386000	0.088925000	2.574331000
6	-6.686595000	-0.887344000	-2.417159000
1	-6.039421000	0.861254000	-1.340608000
6	-5.254809000	-2.824627000	-2.263705000
1	-3.475908000	-2.590474000	-1.069293000
6	-4.226744000	4.552306000	-0.763991000
1	-5.249508000	4.602990000	1.128882000
1	-3.162208000	4.203272000	-2.606144000
6	-5.001017000	-0.652089000	4.324413000
1	-6.934707000	-1.039470000	3.459969000
1	-2.969249000	-0.234594000	4.905880000
6	-6.405937000	-2.209755000	-2.748348000
1	-7.584432000	-0.408493000	-2.799551000
1	-5.034228000	-3.855901000	-2.526908000
1	-4.391871000	5.607278000	-0.968405000
1	-5.344327000	-0.799159000	5.345346000
1	-7.085529000	-2.763447000	-3.391196000
Zero-point correction=			0.690996 (Hartree/Particle)
Thermal correction to Energy=			0.733114
Thermal correction to Enthalpy=			0.734058
Thermal correction to Gibbs Free Energy=			0.610552
Sum of electronic and zero-point Energies=			-2287.747132
Sum of electronic and thermal Energies=			-2287.705014
Sum of electronic and thermal Enthalpies=			-2287.704069
Sum of electronic and thermal Free Energies=			-2287.827575

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6	0.187041000	5.779509000	-1.125276000
6	-0.459289000	4.707641000	-0.520531000
6	0.302421000	3.736624000	0.130329000
6	1.714611000	3.853143000	0.165843000
6	2.352784000	4.923665000	-0.439045000
6	1.579131000	5.884070000	-1.090385000
1	-0.393887000	6.542089000	-1.639440000
1	-1.543934000	4.612366000	-0.554125000

1	3.439440000	5.001186000	-0.431187000
1	2.066752000	6.720416000	-1.586567000
6	-0.137756000	2.501325000	0.782077000
6	1.003124000	1.922937000	1.261339000
6	2.248917000	2.718106000	0.975570000
1	2.618779000	3.106507000	1.939316000
6	3.287321000	1.660005000	0.470033000
6	1.413875000	0.641498000	1.724146000
6	0.774894000	-0.306437000	2.526849000
6	2.752946000	0.382075000	1.240290000
6	1.515916000	-1.362413000	3.018663000
1	-0.270561000	-0.174217000	2.799255000
6	3.522045000	-0.620795000	1.927618000
1	2.366212000	-0.546839000	0.407262000
6	2.898397000	-1.523888000	2.760534000
1	1.027110000	-2.097681000	3.658738000
1	4.569841000	-0.760282000	1.673801000
6	4.723627000	1.982705000	0.867763000
6	5.746485000	1.079370000	0.539278000
6	5.088541000	3.166997000	1.508975000
6	7.068715000	1.336261000	0.874590000
1	5.500674000	0.179643000	-0.022748000
6	6.416632000	3.430252000	1.841768000
1	4.340482000	3.919274000	1.749075000
6	7.411698000	2.513119000	1.535568000
1	7.838012000	0.615680000	0.605891000
1	6.666636000	4.363872000	2.341039000
1	8.447751000	2.717274000	1.795808000
6	3.147841000	1.523633000	-1.057155000
6	1.956872000	1.044293000	-1.616490000
6	4.155767000	1.926773000	-1.936091000
6	1.805595000	0.907180000	-2.990483000
1	1.122870000	0.757208000	-0.984192000
6	4.004524000	1.794243000	-3.313718000
1	5.084653000	2.338431000	-1.550638000
6	2.836704000	1.268391000	-3.849426000
1	0.877036000	0.494330000	-3.382570000
1	4.817731000	2.099303000	-3.968805000
1	2.729281000	1.144486000	-4.924202000
6	3.635986000	-2.673132000	3.376512000
1	3.656477000	-2.600490000	4.470859000
1	3.153516000	-3.625015000	3.122364000
1	4.668875000	-2.719838000	3.018711000
79	-1.924947000	1.525892000	0.529648000

15	-3.832113000	0.189250000	0.023373000
6	-3.800464000	-1.428591000	0.873304000
6	-3.962424000	-0.215463000	-1.749549000
6	-5.449378000	0.899257000	0.478376000
6	-3.807383000	-2.641133000	0.183414000
6	-3.781868000	-1.429551000	2.272744000
6	-5.191343000	-0.320839000	-2.405678000
6	-2.778486000	-0.489448000	-2.443130000
6	-6.550891000	0.099749000	0.799283000
6	-5.588349000	2.289636000	0.461253000
6	-3.817984000	-3.842371000	0.889006000
1	-3.805922000	-2.650742000	-0.905380000
6	-3.804980000	-2.629200000	2.971605000
1	-3.763433000	-0.482382000	2.813854000
6	-5.232473000	-0.698040000	-3.744022000
1	-6.116341000	-0.104707000	-1.873742000
6	-2.828129000	-0.886296000	-3.774203000
1	-1.820849000	-0.412828000	-1.929629000
6	-7.775488000	0.687582000	1.094729000
1	-6.447729000	-0.984691000	0.819243000
6	-6.815947000	2.874102000	0.752378000
1	-4.723940000	2.910040000	0.223359000
6	-3.825836000	-3.838241000	2.278710000
1	-3.819065000	-4.783814000	0.344872000
1	-3.803814000	-2.622280000	4.059071000
6	-4.054038000	-0.985736000	-4.426132000
1	-6.190515000	-0.771892000	-4.253544000
1	-1.903608000	-1.120386000	-4.296732000
6	-7.908345000	2.073428000	1.070689000
1	-8.628831000	0.062329000	1.346628000
1	-6.916936000	3.956522000	0.739032000
1	-3.841353000	-4.778084000	2.825750000
1	-4.091152000	-1.288556000	-5.470037000
1	-8.866819000	2.530734000	1.305175000
8	4.374275000	-1.625503000	-0.839975000
16	3.183768000	-2.284650000	-1.353077000
9	2.280958000	-4.731991000	-1.086585000
9	4.380140000	-4.574139000	-1.569504000
9	3.700646000	-4.132169000	0.428981000
6	3.396592000	-4.052951000	-0.858526000
8	-0.387337000	-0.912234000	-0.294469000
8	0.106032000	-2.735525000	-1.955920000
16	0.380751000	-2.090245000	-0.686053000
9	-0.773549000	-2.777690000	1.587890000

9	-0.743238000	-4.333360000	0.095690000
9	1.042135000	-3.863667000	1.209601000
6	-0.045677000	-3.356986000	0.646660000
7	1.953371000	-1.774717000	-0.392022000
8	2.885096000	-2.305373000	-2.767523000
Zero-point correction=			0.749019 (Hartree/Particle)
Thermal correction to Energy=			0.803754
Thermal correction to Enthalpy=			0.804698
Thermal correction to Gibbs Free Energy=			0.660656
Sum of electronic and zero-point Energies=			-4114.606207
Sum of electronic and thermal Energies=			-4114.551471
Sum of electronic and thermal Enthalpies=			-4114.550527
Sum of electronic and thermal Free Energies=			-4114.694569

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6	0.432774000	-5.980710000	1.133943000
6	-0.224648000	-4.906541000	0.539012000
6	0.518507000	-3.954703000	-0.154894000
6	1.925005000	-4.086839000	-0.237674000
6	2.572284000	-5.163220000	0.345301000
6	1.817780000	-6.110439000	1.040415000
1	-0.139602000	-6.729019000	1.678834000
1	-1.307472000	-4.803339000	0.610014000
1	3.655931000	-5.262822000	0.279405000
1	2.314706000	-6.952737000	1.517188000
6	0.074331000	-2.727965000	-0.834198000
6	1.187505000	-2.185536000	-1.386371000
6	2.442131000	-2.961925000	-1.076499000
1	2.872887000	-3.344226000	-2.016357000
6	3.394212000	-1.834971000	-0.545169000
6	1.597790000	-0.880919000	-1.863422000
6	0.916375000	0.118160000	-2.555844000
6	2.925002000	-0.668366000	-1.437398000
6	1.578315000	1.305304000	-2.858547000
1	-0.125611000	-0.027224000	-2.842287000
6	3.574686000	0.517803000	-1.746711000
1	2.029188000	1.834206000	-0.443705000
6	2.911093000	1.517421000	-2.477119000
1	1.058029000	2.089623000	-3.408727000
1	4.599558000	0.694974000	-1.422981000
6	4.882406000	-2.105896000	-0.698939000
6	5.797471000	-1.182487000	-0.172283000
6	5.390704000	-3.233281000	-1.343739000
6	7.165870000	-1.366876000	-0.314071000

1	5.422576000	-0.320366000	0.379840000
6	6.764415000	-3.425059000	-1.480788000
1	4.715225000	-3.989380000	-1.738032000
6	7.657324000	-2.490714000	-0.974138000
1	7.853400000	-0.634118000	0.102969000
1	7.132674000	-4.316362000	-1.984290000
1	8.729324000	-2.639940000	-1.081032000
6	3.047978000	-1.553722000	0.927037000
6	2.024339000	-0.675450000	1.286510000
6	3.720133000	-2.225235000	1.953118000
6	1.714456000	-0.430024000	2.620738000
1	1.444281000	-0.179522000	0.515753000
6	3.401312000	-1.998681000	3.287075000
1	4.517105000	-2.924518000	1.705373000
6	2.406631000	-1.088198000	3.630243000
1	0.937635000	0.297190000	2.863257000
1	3.944515000	-2.530823000	4.065002000
1	2.175416000	-0.893954000	4.675057000
6	3.614857000	2.793838000	-2.835138000
1	4.055628000	2.738459000	-3.838894000
1	2.926207000	3.647377000	-2.829814000
1	4.428607000	3.013788000	-2.134376000
79	-1.685471000	-1.727182000	-0.542873000
15	-3.584966000	-0.390630000	0.007135000
6	-3.770513000	1.123440000	-0.999727000
6	-3.592004000	0.161784000	1.746617000
6	-5.190671000	-1.240870000	-0.201703000
6	-3.979117000	2.390972000	-0.452940000
6	-3.749159000	0.969321000	-2.390316000
6	-4.762011000	0.631099000	2.354154000
6	-2.405474000	0.110580000	2.483898000
6	-6.351539000	-0.590044000	-0.628145000
6	-5.240172000	-2.603297000	0.108441000
6	-4.201236000	3.483437000	-1.289202000
1	-3.981264000	2.523230000	0.628482000
6	-3.981984000	2.058569000	-3.220400000
1	-3.568716000	-0.016814000	-2.820629000
6	-4.739609000	1.059137000	3.675537000
1	-5.694394000	0.654120000	1.790506000
6	-2.387973000	0.540366000	3.807357000
1	-1.495470000	-0.272361000	2.020670000
6	-7.546740000	-1.294437000	-0.733152000
1	-6.319459000	0.468489000	-0.884895000
6	-6.437045000	-3.302427000	0.007819000

1	-4.329608000	-3.115051000	0.422732000
6	-4.216061000	3.316667000	-2.669925000
1	-4.361470000	4.467939000	-0.855053000
1	-3.979404000	1.926027000	-4.299751000
6	-3.551731000	1.015776000	4.401293000
1	-5.652379000	1.422419000	4.142079000
1	-1.462302000	0.498896000	4.376041000
6	-7.590841000	-2.648063000	-0.414052000
1	-8.446470000	-0.783526000	-1.068342000
1	-6.466352000	-4.361973000	0.250004000
1	-4.400786000	4.169046000	-3.319596000
1	-3.536435000	1.348638000	5.436479000
1	-8.526160000	-3.196158000	-0.500575000
8	4.039811000	2.371262000	0.973577000
16	2.800434000	2.976754000	1.402888000
9	1.592591000	5.221307000	0.880377000
9	3.568394000	5.427186000	1.736911000
9	3.341523000	4.849549000	-0.331584000
6	2.831213000	4.751971000	0.881383000
8	-0.581979000	1.226777000	0.086971000
8	-0.363849000	3.221824000	1.645210000
16	-0.026866000	2.514134000	0.435036000
9	-1.029839000	2.962718000	-1.947143000
9	-1.176551000	4.629944000	-0.583009000
9	0.704253000	4.166128000	-1.523732000
6	-0.406610000	3.656474000	-1.019955000
7	1.642963000	2.396577000	0.330645000
8	2.312951000	2.959330000	2.756407000
Zero-point correction=			0.754661 (Hartree/Particle)
Thermal correction to Energy=			0.810012
Thermal correction to Enthalpy=			0.810956
Thermal correction to Gibbs Free Energy=			0.664650
Sum of electronic and zero-point Energies=			-4114.643046
Sum of electronic and thermal Energies=			-4114.587694
Sum of electronic and thermal Enthalpies=			-4114.586750
Sum of electronic and thermal Free Energies=			-4114.733056

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6	0.968205000	-0.593220000	4.671414000
6	0.398937000	0.329186000	3.810485000
6	1.094032000	0.694945000	2.653134000
6	2.363009000	0.127410000	2.389532000
6	2.899905000	-0.855761000	3.235473000
6	2.203705000	-1.196904000	4.378173000

1	0.442485000	-0.872512000	5.582178000
1	-0.579508000	0.762444000	4.018189000
1	3.847762000	-1.331575000	2.995840000
1	2.609616000	-1.943149000	5.056572000
6	0.692832000	1.625362000	1.579462000
6	1.866308000	1.686954000	0.673580000
6	2.818456000	0.659611000	1.137797000
1	0.370356000	2.611970000	1.932028000
6	3.758951000	0.246654000	0.195147000
6	2.322361000	3.071355000	0.321873000
6	1.389068000	3.998565000	-0.157349000
6	3.644502000	3.489781000	0.477883000
6	1.767630000	5.293257000	-0.472956000
1	0.351875000	3.688465000	-0.290131000
6	4.017653000	4.791893000	0.158649000
1	4.390787000	2.799346000	0.865459000
6	3.093029000	5.714043000	-0.325518000
1	1.022827000	5.996363000	-0.844997000
1	5.053892000	5.098701000	0.297420000
6	3.299335000	0.641020000	-1.088217000
6	4.094875000	0.981110000	-2.198848000
6	1.871465000	0.891759000	-1.102431000
6	3.517586000	1.662661000	-3.243053000
1	5.164993000	0.787762000	-2.175216000
6	1.320829000	1.602730000	-2.218051000
1	1.256989000	0.058411000	-0.744168000
6	2.132453000	1.983431000	-3.249034000
1	4.135715000	1.990755000	-4.075812000
1	0.244689000	1.762231000	-2.256392000
1	1.716301000	2.497712000	-4.112121000
6	5.009575000	-0.463628000	0.443291000
6	5.797452000	-0.153085000	1.558993000
6	5.451342000	-1.448805000	-0.449349000
6	7.002420000	-0.808900000	1.774509000
1	5.456026000	0.614467000	2.253606000
6	6.656876000	-2.100993000	-0.232466000
1	4.812763000	-1.724578000	-1.286790000
6	7.435741000	-1.781058000	0.876767000
1	7.608400000	-0.556922000	2.641638000
1	6.983822000	-2.873998000	-0.923577000
1	8.379459000	-2.294656000	1.045440000
6	3.503991000	7.106600000	-0.698041000
1	2.725783000	7.836543000	-0.448353000
1	4.424748000	7.404664000	-0.185497000

1	3.689537000	7.192250000	-1.776646000
79	-1.155708000	0.900912000	0.748748000
15	-3.371611000	0.362297000	0.119074000
6	-4.023172000	1.479116000	-1.170744000
6	-4.489510000	0.611826000	1.543436000
6	-3.719504000	-1.328940000	-0.439091000
6	-5.139169000	2.290056000	-0.954915000
6	-3.351778000	1.530409000	-2.399587000
6	-5.682942000	-0.104739000	1.668794000
6	-4.170278000	1.585925000	2.494258000
6	-4.630722000	-1.593289000	-1.463853000
6	-3.103178000	-2.383339000	0.239779000
6	-5.580232000	3.148832000	-1.958164000
1	-5.667040000	2.254655000	-0.003577000
6	-3.806151000	2.382718000	-3.398009000
1	-2.489185000	0.886649000	-2.570503000
6	-6.545105000	0.155881000	2.728191000
1	-5.934580000	-0.869535000	0.935410000
6	-5.037032000	1.848065000	3.549223000
1	-3.234266000	2.138540000	2.401394000
6	-4.932693000	-2.908869000	-1.796142000
1	-5.103462000	-0.771158000	-1.998835000
6	-3.420691000	-3.694650000	-0.089456000
1	-2.357581000	-2.178583000	1.010377000
6	-4.915852000	3.195660000	-3.178153000
1	-6.448473000	3.779819000	-1.782980000
1	-3.288900000	2.412961000	-4.354232000
6	-6.224976000	1.132554000	3.666687000
1	-7.470486000	-0.407612000	2.821455000
1	-4.781430000	2.607807000	4.284038000
6	-4.332421000	-3.956584000	-1.105775000
1	-5.636031000	-3.114799000	-2.599513000
1	-2.929378000	-4.512374000	0.428893000
1	-5.263535000	3.865751000	-3.961218000
1	-6.900814000	1.333014000	4.494801000
1	-4.564779000	-4.984983000	-1.371739000
8	2.592815000	-2.390274000	0.436801000
16	1.386567000	-2.995636000	-0.115160000
9	-0.623827000	-4.229123000	1.012867000
9	1.249902000	-4.394426000	2.071199000
9	0.134071000	-2.547661000	2.134617000
6	0.475646000	-3.578838000	1.373043000
8	-1.211921000	-3.095947000	-2.255465000
8	-0.968812000	-0.591454000	-2.240654000

16	-0.386171000	-1.921258000	-2.039090000
9	2.099475000	-1.519504000	-2.876818000
9	1.154113000	-3.261405000	-3.725746000
9	0.583754000	-1.296090000	-4.394759000
6	0.955180000	-2.018205000	-3.346867000
7	0.397780000	-1.831502000	-0.635312000
8	1.507909000	-4.142823000	-1.002901000
Zero-point correction=			0.748620 (Hartree/Particle)
Thermal correction to Energy=			0.804348
Thermal correction to Enthalpy=			0.805293
Thermal correction to Gibbs Free Energy=			0.657004
Sum of electronic and zero-point Energies=			-4114.626003
Sum of electronic and thermal Energies=			-4114.570274
Sum of electronic and thermal Enthalpies=			-4114.569330
Sum of electronic and thermal Free Energies=			-4114.717619

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6	-1.188070000	-0.008555000	-4.600016000
6	-0.585549000	0.721218000	-3.593815000
6	-1.276314000	0.922934000	-2.390823000
6	-2.586513000	0.394218000	-2.251581000
6	-3.168186000	-0.391543000	-3.266053000
6	-2.467653000	-0.579021000	-4.435661000
1	-0.657086000	-0.166944000	-5.536646000
1	0.422236000	1.118606000	-3.714184000
1	-4.147298000	-0.841057000	-3.115970000
1	-2.894099000	-1.176260000	-5.237324000
6	-0.824303000	1.622564000	-1.178159000
6	-2.030600000	1.575879000	-0.242124000
6	-3.021177000	0.688800000	-0.935419000
1	-0.534576000	2.656603000	-1.409201000
6	-3.961037000	0.151158000	-0.052211000
6	-2.526680000	2.992552000	0.044315000
6	-1.622912000	3.920153000	0.578340000
6	-3.834468000	3.414494000	-0.185575000
6	-2.016399000	5.215880000	0.872638000
1	-0.590500000	3.620068000	0.759402000
6	-4.223913000	4.719466000	0.109865000
1	-4.568210000	2.723758000	-0.593723000
6	-3.327826000	5.642041000	0.640406000
1	-1.292919000	5.916376000	1.289585000
1	-5.252703000	5.024332000	-0.079953000
6	-3.455802000	0.367325000	1.242164000
6	-4.122345000	0.294927000	2.481246000

6	-2.035847000	0.795705000	1.170650000
6	-3.486469000	0.779453000	3.595201000
1	-5.150844000	-0.055882000	2.526779000
6	-1.466869000	1.370708000	2.391179000
1	-1.433177000	-0.108753000	0.932233000
6	-2.161465000	1.321286000	3.554633000
1	-4.016152000	0.785134000	4.545975000
1	-0.439675000	1.732328000	2.362442000
1	-1.715117000	1.677570000	4.479391000
6	-5.198384000	-0.554466000	-0.392478000
6	-6.048661000	-0.047303000	-1.382810000
6	-5.555778000	-1.737331000	0.265897000
6	-7.230833000	-0.702141000	-1.704093000
1	-5.775607000	0.872707000	-1.899861000
6	-6.739721000	-2.389042000	-0.055481000
1	-4.870708000	-2.164906000	0.996209000
6	-7.581037000	-1.872572000	-1.037030000
1	-7.883809000	-0.295035000	-2.472657000
1	-6.999438000	-3.314352000	0.453213000
1	-8.505763000	-2.387007000	-1.287874000
6	-3.739075000	7.052270000	0.939119000
1	-4.828012000	7.165405000	0.920775000
1	-3.382857000	7.374833000	1.924559000
1	-3.323215000	7.753865000	0.204673000
79	1.078251000	0.889696000	-0.528903000
15	3.386272000	0.476564000	-0.141572000
6	4.087236000	1.466535000	1.222599000
6	4.344531000	0.992326000	-1.612465000
6	3.926414000	-1.233193000	0.152581000
6	5.218743000	2.268995000	1.060029000
6	3.458679000	1.394670000	2.471865000
6	5.556742000	0.385471000	-1.952637000
6	3.868035000	2.054460000	-2.387042000
6	4.901981000	-1.556798000	1.097540000
6	3.385701000	-2.230656000	-0.662958000
6	5.718390000	2.993688000	2.138532000
1	5.711742000	2.330643000	0.091303000
6	3.970478000	2.113314000	3.545383000
1	2.582834000	0.758785000	2.596069000
6	6.280364000	0.838391000	-3.050759000
1	5.931724000	-0.445619000	-1.356840000
6	4.596109000	2.508551000	-3.480995000
1	2.916579000	2.520663000	-2.127064000
6	5.341013000	-2.871098000	1.214095000

1	5.318472000	-0.782851000	1.740163000
6	3.843167000	-3.537221000	-0.554985000
1	2.589239000	-1.988172000	-1.369007000
6	5.097179000	2.915206000	3.380047000
1	6.598331000	3.618914000	2.006049000
1	3.486121000	2.046014000	4.516828000
6	5.802010000	1.899132000	-3.814402000
1	7.220555000	0.358325000	-3.312181000
1	4.217661000	3.334924000	-4.078062000
6	4.818236000	-3.857117000	0.383768000
1	6.093985000	-3.124451000	1.956658000
1	3.416140000	-4.311823000	-1.185681000
1	5.491496000	3.480048000	4.221849000
1	6.368524000	2.247843000	-4.674828000
1	5.163358000	-4.884075000	0.477735000
8	-2.414435000	-2.332521000	-0.762761000
16	-1.227643000	-2.936991000	-0.173318000
9	0.944853000	-3.935103000	-1.211641000
9	-0.852209000	-4.298393000	-2.350896000
9	0.067675000	-2.346520000	-2.380998000
6	-0.197457000	-3.405738000	-1.624652000
8	1.497343000	-3.122247000	1.759554000
8	1.027105000	-0.689234000	2.224757000
16	0.555978000	-2.018390000	1.827680000
9	-1.853846000	-2.005623000	2.930838000
9	-0.703398000	-3.779239000	3.361387000
9	-0.212484000	-1.920429000	4.325875000
6	-0.637671000	-2.476824000	3.199597000
7	-0.355951000	-1.764674000	0.517853000
8	-1.347025000	-4.150671000	0.621625000
Zero-point correction=			0.748964 (Hartree/Particle)
Thermal correction to Energy=			0.806108
Thermal correction to Enthalpy=			0.807052
Thermal correction to Gibbs Free Energy=			0.654061
Sum of electronic and zero-point Energies=			-4114.630223
Sum of electronic and thermal Energies=			-4114.573079
Sum of electronic and thermal Enthalpies=			-4114.572135
Sum of electronic and thermal Free Energies=			-4114.725126

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6	1.199351000	3.986951000	2.814046000
6	0.726865000	3.554239000	1.584297000
6	1.392173000	2.521407000	0.918515000
6	2.555206000	1.962842000	1.497742000

6	3.005498000	2.383244000	2.756499000
6	2.325074000	3.397781000	3.407545000
1	0.683292000	4.792793000	3.332572000
1	-0.167711000	3.996919000	1.145793000
1	3.883283000	1.928550000	3.209347000
1	2.668178000	3.745583000	4.378839000
6	1.026030000	1.869294000	-0.366586000
6	2.318857000	1.085465000	-0.727844000
6	3.022336000	0.942070000	0.600238000
1	0.807264000	2.635263000	-1.121319000
6	3.787522000	-0.193809000	0.675393000
6	3.140960000	1.967427000	-1.692750000
6	2.554718000	2.385210000	-2.894078000
6	4.462645000	2.338139000	-1.453967000
6	3.262763000	3.143582000	-3.813685000
1	1.522717000	2.110225000	-3.114115000
6	5.168780000	3.104534000	-2.378102000
1	4.959536000	2.021995000	-0.540221000
6	4.585309000	3.524380000	-3.569727000
1	2.781102000	3.450649000	-4.741934000
1	6.200656000	3.381598000	-2.163085000
6	3.532535000	-0.953482000	-0.520465000
6	4.156547000	-2.114785000	-0.988030000
6	2.458065000	-0.351664000	-1.286360000
6	3.821496000	-2.587259000	-2.242448000
1	4.911860000	-2.612524000	-0.384812000
6	2.292559000	-0.768881000	-2.647882000
1	1.500398000	-1.142350000	-0.873623000
6	2.910087000	-1.913634000	-3.084341000
1	4.299729000	-3.493446000	-2.609395000
1	1.565743000	-0.256972000	-3.272657000
1	2.699325000	-2.309846000	-4.073690000
6	4.708407000	-0.579660000	1.754676000
6	5.658826000	0.338504000	2.219794000
6	4.674062000	-1.857438000	2.324662000
6	6.542687000	-0.003898000	3.235570000
1	5.707381000	1.329041000	1.767945000
6	5.561880000	-2.198642000	3.339118000
1	3.926397000	-2.568369000	1.982024000
6	6.496535000	-1.276146000	3.798607000
1	7.275244000	0.721427000	3.582755000
1	5.515561000	-3.192392000	3.779027000
1	7.188567000	-1.547460000	4.592566000
6	5.335544000	4.377151000	-4.548149000

1	6.418718000	4.264489000	-4.431093000
1	5.078950000	4.124141000	-5.583161000
1	5.102807000	5.441088000	-4.410560000
79	-0.917953000	1.041387000	-0.112063000
15	-3.268591000	0.717955000	0.239252000
6	-4.268700000	0.253328000	-1.215676000
6	-3.993760000	2.335057000	0.719224000
6	-3.736038000	-0.411356000	1.588003000
6	-5.662002000	0.155835000	-1.132774000
6	-3.633092000	0.044152000	-2.439894000
6	-5.085801000	2.455107000	1.583735000
6	-3.458699000	3.488078000	0.136217000
6	-4.254274000	-1.682098000	1.335870000
6	-3.441751000	-0.033506000	2.903263000
6	-6.406515000	-0.161876000	-2.260829000
1	-6.166123000	0.326786000	-0.182229000
6	-4.383726000	-0.269146000	-3.569361000
1	-2.547859000	0.106058000	-2.503487000
6	-5.627840000	3.705854000	1.859529000
1	-5.505883000	1.569345000	2.057794000
6	-4.005212000	4.736943000	0.408781000
1	-2.604563000	3.400530000	-0.536770000
6	-4.492317000	-2.556889000	2.391115000
1	-4.450997000	-1.996382000	0.313848000
6	-3.690122000	-0.906495000	3.953432000
1	-3.007918000	0.946213000	3.104397000
6	-5.766649000	-0.374599000	-3.480263000
1	-7.488834000	-0.241110000	-2.190137000
1	-3.880932000	-0.437639000	-4.518589000
6	-5.089630000	4.847246000	1.273616000
1	-6.473810000	3.788077000	2.538143000
1	-3.578849000	5.625827000	-0.050382000
6	-4.215398000	-2.171083000	3.697529000
1	-4.888275000	-3.548634000	2.187061000
1	-3.462461000	-0.604812000	4.973157000
1	-6.351816000	-0.623431000	-4.362794000
1	-5.514378000	5.824070000	1.493238000
1	-4.400253000	-2.859592000	4.518776000
8	2.114902000	-3.296050000	0.997670000
16	0.691145000	-3.078866000	0.813730000
9	-1.056648000	-1.625288000	2.095539000
9	0.472943000	-2.522505000	3.327408000
9	0.950280000	-0.819933000	2.087199000
6	0.224711000	-1.925529000	2.173893000

8	-2.086579000	-2.281277000	-0.778476000
8	-0.603265000	-1.220199000	-2.524454000
16	-0.818253000	-2.218922000	-1.484418000
9	0.607805000	-4.062744000	-2.687133000
9	-1.150060000	-4.835658000	-1.700501000
9	-1.354124000	-3.711982000	-3.522065000
6	-0.664921000	-3.834344000	-2.397876000
7	0.499656000	-2.138607000	-0.518619000
8	-0.243066000	-4.185269000	0.866430000
Zero-point correction=			0.745058 (Hartree/Particle)
Thermal correction to Energy=			0.801602
Thermal correction to Enthalpy=			0.802546
Thermal correction to Gibbs Free Energy=			0.651498
Sum of electronic and zero-point Energies=			-4114.624630
Sum of electronic and thermal Energies=			-4114.568087
Sum of electronic and thermal Enthalpies=			-4114.567143
Sum of electronic and thermal Free Energies=			-4114.718190

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6	-2.422334000	0.359965000	-3.696015000
6	-1.182675000	0.835165000	-3.275137000
6	-1.064606000	1.455063000	-2.033584000
6	-2.215808000	1.604289000	-1.222366000
6	-3.461155000	1.136821000	-1.653024000
6	-3.556299000	0.506305000	-2.894471000
1	-2.509614000	-0.131475000	-4.662911000
1	-0.298254000	0.699382000	-3.897174000
1	-4.345078000	1.246062000	-1.026895000
1	-4.521436000	0.139501000	-3.237510000
6	0.161901000	1.994025000	-1.376077000
6	-0.415013000	2.828438000	-0.192332000
6	-1.764030000	2.179009000	0.032066000
1	0.723121000	2.622922000	-2.079306000
6	-2.026280000	1.974478000	1.348475000
6	-0.544158000	4.300085000	-0.600872000
6	0.594533000	4.994032000	-1.027837000
6	-1.743142000	5.005211000	-0.523738000
6	0.532894000	6.337440000	-1.362846000
1	1.548770000	4.469919000	-1.093796000
6	-1.803356000	6.353922000	-0.866609000
1	-2.644762000	4.498749000	-0.183527000
6	-0.671705000	7.043903000	-1.290966000
1	1.435824000	6.855897000	-1.686385000
1	-2.754790000	6.881443000	-0.799865000

6	-0.826184000	2.363651000	2.104460000
6	-0.570044000	2.314948000	3.471110000
6	0.172322000	2.789947000	1.204578000
6	0.697075000	2.675801000	3.931344000
1	-1.346470000	2.004843000	4.168650000
6	1.422056000	3.157899000	1.670413000
1	-2.818103000	-0.697715000	-0.749992000
6	1.687967000	3.082028000	3.040714000
1	0.911496000	2.643818000	4.998270000
1	2.197709000	3.483559000	0.977656000
1	2.676264000	3.343552000	3.413475000
6	-3.225358000	1.353025000	1.920797000
6	-4.496919000	1.807089000	1.550256000
6	-3.135964000	0.295195000	2.836178000
6	-5.644162000	1.215722000	2.065180000
1	-4.571782000	2.650522000	0.864049000
6	-4.283157000	-0.304817000	3.341166000
1	-2.155575000	-0.070346000	3.133641000
6	-5.540894000	0.152892000	2.956503000
1	-6.622835000	1.581804000	1.763674000
1	-4.194058000	-1.142533000	4.029493000
1	-6.437602000	-0.318940000	3.350968000
6	-0.734722000	8.492559000	-1.673223000
1	-1.686540000	8.944493000	-1.374541000
1	0.072381000	9.067134000	-1.202939000
1	-0.632151000	8.627402000	-2.757684000
79	1.550447000	0.517183000	-0.772601000
15	3.289086000	-0.980844000	-0.102832000
6	4.787263000	-0.770796000	-1.127594000
6	2.914932000	-2.763075000	-0.194515000
6	3.859676000	-0.694318000	1.605775000
6	5.573264000	-1.845881000	-1.547570000
6	5.156364000	0.532076000	-1.478855000
6	3.304133000	-3.671354000	0.791836000
6	2.185502000	-3.210982000	-1.300642000
6	5.171747000	-0.974965000	2.002722000
6	2.943665000	-0.206889000	2.542610000
6	6.716954000	-1.617264000	-2.307452000
1	5.289305000	-2.863367000	-1.282489000
6	6.302179000	0.756695000	-2.231478000
1	4.532511000	1.369109000	-1.163159000
6	2.955672000	-5.013640000	0.676483000
1	3.866044000	-3.326433000	1.658341000
6	1.841035000	-4.552234000	-1.412534000

1	1.857782000	-2.497242000	-2.055892000
6	5.556746000	-0.782326000	3.323928000
1	5.892031000	-1.345161000	1.273699000
6	3.332716000	-0.021666000	3.865728000
1	1.927421000	0.045420000	2.235333000
6	7.082257000	-0.318979000	-2.647868000
1	7.323409000	-2.458453000	-2.635115000
1	6.581617000	1.772186000	-2.501769000
6	2.221477000	-5.452643000	-0.420752000
1	3.252203000	-5.716717000	1.451329000
1	1.251662000	-4.888615000	-2.262035000
6	4.636234000	-0.308977000	4.255928000
1	6.578512000	-0.999453000	3.626615000
1	2.614494000	0.362917000	4.586131000
1	7.974672000	-0.143895000	-3.244199000
1	1.937073000	-6.499171000	-0.500205000
1	4.940301000	-0.156470000	5.289006000
8	-5.270401000	-1.102638000	-0.214789000
16	-4.390350000	-2.232042000	-0.028516000
9	-4.300512000	-4.547625000	-1.290362000
9	-5.904029000	-3.236573000	-1.873219000
9	-3.890592000	-2.831968000	-2.538481000
6	-4.627763000	-3.304901000	-1.547456000
8	-1.725444000	-3.889882000	-0.364162000
8	-0.550521000	-1.805978000	-1.239948000
16	-1.415896000	-2.479946000	-0.300028000
9	-0.493860000	-0.870099000	1.526963000
9	-1.588913000	-2.562662000	2.299934000
9	0.400980000	-2.831293000	1.493485000
6	-0.730866000	-2.160592000	1.386248000
7	-2.837308000	-1.598171000	-0.236918000
8	-4.410828000	-3.104840000	1.118044000
Zero-point correction=			0.753416 (Hartree/Particle)
Thermal correction to Energy=			0.809446
Thermal correction to Enthalpy=			0.810390
Thermal correction to Gibbs Free Energy=			0.662387
Sum of electronic and zero-point Energies=			-4114.657803
Sum of electronic and thermal Energies=			-4114.601773
Sum of electronic and thermal Enthalpies=			-4114.600829
Sum of electronic and thermal Free Energies=			-4114.748832

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6	-0.347710000	1.362678000	4.344903000
6	-1.095165000	1.090718000	3.200710000

6	-0.669759000	1.596469000	1.978687000
6	0.502864000	2.382936000	1.903861000
6	1.248856000	2.641981000	3.053552000
6	0.816233000	2.127231000	4.273028000
1	-0.676463000	0.969244000	5.304136000
1	-1.982570000	0.464872000	3.254812000
1	2.157702000	3.236761000	3.002671000
1	1.386171000	2.331525000	5.176810000
6	-1.260429000	1.357156000	0.608061000
6	-0.571570000	2.460944000	-0.259458000
6	0.729315000	2.672507000	0.497496000
1	-2.347791000	1.528877000	0.637065000
6	1.798513000	2.731645000	-0.337845000
6	-1.442523000	3.723221000	-0.265829000
6	-2.744502000	3.655047000	-0.774241000
6	-0.975671000	4.956519000	0.184408000
6	-3.546726000	4.785516000	-0.823326000
1	-3.138621000	2.706801000	-1.141807000
6	-1.787068000	6.086637000	0.135320000
1	0.036749000	5.041393000	0.576475000
6	-3.084822000	6.022440000	-0.365676000
1	-4.555674000	4.708908000	-1.228328000
1	-1.401076000	7.039787000	0.496500000
6	1.313939000	2.487761000	-1.705206000
6	2.011304000	2.456743000	-2.909534000
6	-0.070753000	2.220022000	-1.671031000
6	1.321581000	2.123889000	-4.076084000
1	3.074268000	2.690772000	-2.939609000
6	-0.749896000	1.898772000	-2.833781000
1	-1.896639000	0.067067000	0.236806000
6	-0.038761000	1.829605000	-4.035892000
1	1.851695000	2.100966000	-5.026911000
1	-1.817191000	1.689567000	-2.815946000
1	-0.560802000	1.559424000	-4.950984000
6	3.210163000	2.869211000	0.030337000
6	3.619796000	3.854765000	0.936007000
6	4.180492000	2.011966000	-0.507765000
6	4.953511000	3.968249000	1.312410000
1	2.877679000	4.553374000	1.321781000
6	5.513769000	2.131110000	-0.138019000
1	3.876556000	1.228072000	-1.201391000
6	5.905199000	3.106946000	0.775421000
1	5.252809000	4.743657000	2.014237000
1	6.250757000	1.450756000	-0.559389000

1	6.950389000	3.199601000	1.062206000
6	-3.970130000	7.232171000	-0.392163000
1	-4.594496000	7.253205000	-1.292682000
1	-4.649974000	7.248660000	0.469577000
1	-3.385994000	8.158350000	-0.363657000
79	0.100836000	-0.423293000	0.157668000
15	1.874946000	-1.906179000	-0.008994000
6	1.445538000	-3.547558000	0.640426000
6	3.299527000	-1.278285000	0.933630000
6	2.456697000	-2.154140000	-1.713689000
6	2.318507000	-4.307372000	1.421693000
6	0.171116000	-4.040039000	0.341245000
6	4.602438000	-1.718563000	0.676014000
6	3.078576000	-0.311965000	1.920104000
6	3.049264000	-3.350687000	-2.126677000
6	2.319499000	-1.095534000	-2.617463000
6	1.915365000	-5.552679000	1.893928000
1	3.305547000	-3.921832000	1.673095000
6	-0.227908000	-5.281140000	0.817221000
1	-0.519437000	-3.441435000	-0.254259000
6	5.665871000	-1.211409000	1.413695000
1	4.783557000	-2.451353000	-0.110235000
6	4.147681000	0.206881000	2.640838000
1	2.069179000	0.054511000	2.117114000
6	3.518638000	-3.476712000	-3.429695000
1	3.132480000	-4.185608000	-1.431119000
6	2.797014000	-1.225405000	-3.915876000
1	1.830427000	-0.167955000	-2.312082000
6	0.645876000	-6.037283000	1.594277000
1	2.592880000	-6.141522000	2.507704000
1	-1.230560000	-5.638828000	0.598830000
6	5.438666000	-0.246706000	2.392643000
1	6.676892000	-1.558551000	1.213259000
1	3.964876000	0.985787000	3.378533000
6	3.396026000	-2.414494000	-4.321729000
1	3.974893000	-4.409694000	-3.751961000
1	2.680556000	-0.394715000	-4.609089000
1	0.330446000	-7.004545000	1.978230000
1	6.275786000	0.166697000	2.950735000
1	3.760562000	-2.519286000	-5.340984000
8	-1.878402000	-1.862166000	2.103021000
16	-3.004259000	-2.055401000	1.203436000
9	-5.565468000	-1.535900000	1.437262000
9	-4.600260000	-2.280321000	3.219833000

9	-4.268354000	-0.243280000	2.578798000
6	-4.474819000	-1.488526000	2.169671000
8	-4.936775000	-1.576232000	-1.341925000
8	-3.573005000	0.496094000	-1.865117000
16	-3.676124000	-0.868032000	-1.375545000
9	-1.365076000	-1.304408000	-2.523806000
9	-2.475304000	-3.094322000	-2.057086000
9	-3.094811000	-1.837049000	-3.701100000
6	-2.573520000	-1.850320000	-2.488060000
7	-2.863130000	-0.885687000	0.053296000
8	-3.328686000	-3.364664000	0.672938000
Zero-point correction=			0.747090 (Hartree/Particle)
Thermal correction to Energy=			0.803239
Thermal correction to Enthalpy=			0.804183
Thermal correction to Gibbs Free Energy=			0.655310
Sum of electronic and zero-point Energies=			-4114.644709
Sum of electronic and thermal Energies=			-4114.588561
Sum of electronic and thermal Enthalpies=			-4114.587616
Sum of electronic and thermal Free Energies=			-4114.736489

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6	0.927841000	-1.906085000	-3.050006000
6	0.795130000	-0.645875000	-2.460528000
6	1.811742000	-0.183508000	-1.640083000
6	2.960280000	-0.969129000	-1.402527000
6	3.106625000	-2.202396000	-2.034016000
6	2.078534000	-2.665466000	-2.853100000
1	0.130602000	-2.292290000	-3.683484000
1	-0.072622000	-0.018263000	-2.660118000
1	3.998097000	-2.806260000	-1.874626000
1	2.167495000	-3.642280000	-3.324599000
6	1.935977000	1.147385000	-0.938194000
6	2.912934000	0.808668000	0.215773000
6	3.797552000	-0.210097000	-0.484065000
1	2.418653000	1.875007000	-1.606879000
6	5.114721000	0.081693000	-0.331797000
6	2.187279000	0.192486000	1.414690000
6	0.950051000	0.671662000	1.849872000
6	2.773116000	-0.841847000	2.151406000
6	0.287644000	0.093895000	2.931195000
1	0.481701000	1.517617000	1.352211000
6	2.116409000	-1.412607000	3.234910000
1	3.755805000	-1.212111000	1.858384000
6	0.850075000	-0.973631000	3.630669000

1	-0.685889000	0.491648000	3.219909000
1	2.591564000	-2.229177000	3.779326000
6	5.214340000	1.339353000	0.427962000
6	6.329508000	2.050985000	0.861641000
6	3.918585000	1.816234000	0.708854000
6	6.134841000	3.241000000	1.560825000
1	7.335021000	1.681685000	0.667541000
6	3.730536000	2.980149000	1.430829000
1	0.976796000	1.579354000	-0.639574000
6	4.851483000	3.704998000	1.841354000
1	6.997551000	3.810496000	1.899838000
1	2.726845000	3.325106000	1.674579000
1	4.722108000	4.634657000	2.390664000
6	6.246562000	-0.664311000	-0.886682000
6	6.290737000	-2.058842000	-0.768246000
6	7.300183000	-0.016066000	-1.543449000
6	7.344481000	-2.787952000	-1.305428000
1	5.490387000	-2.561024000	-0.223565000
6	8.353389000	-0.745169000	-2.081358000
1	7.272006000	1.066515000	-1.653226000
6	8.379304000	-2.132297000	-1.965499000
1	7.363716000	-3.870504000	-1.200506000
1	9.157572000	-0.227593000	-2.599668000
1	9.206150000	-2.700015000	-2.385785000
6	0.112553000	-1.651656000	4.745181000
1	0.797543000	-2.017345000	5.518475000
1	-0.611454000	-0.978394000	5.216951000
1	-0.450968000	-2.519543000	4.372036000
79	-1.704543000	0.186541000	-0.100366000
15	-2.038904000	-2.078881000	0.207463000
6	-3.384662000	-2.624218000	-0.892757000
6	-2.587778000	-2.412357000	1.912428000
6	-0.672095000	-3.237349000	-0.087632000
6	-4.410268000	-3.469252000	-0.465318000
6	-3.351282000	-2.189496000	-2.222572000
6	-2.436356000	-3.678981000	2.486316000
6	-3.198691000	-1.389185000	2.643982000
6	-0.871885000	-4.459186000	-0.736071000
6	0.580321000	-2.923521000	0.445101000
6	-5.394326000	-3.874284000	-1.362510000
1	-4.445828000	-3.806577000	0.569330000
6	-4.331254000	-2.603044000	-3.115267000
1	-2.558232000	-1.516858000	-2.553263000
6	-2.908143000	-3.920423000	3.772334000

1	-1.946844000	-4.476087000	1.927826000
6	-3.667749000	-1.635946000	3.929728000
1	-3.296182000	-0.392511000	2.211861000
6	0.177317000	-5.367387000	-0.834900000
1	-1.846374000	-4.702721000	-1.156746000
6	1.619231000	-3.839383000	0.349370000
1	0.755072000	-1.960984000	0.924121000
6	-5.354778000	-3.443571000	-2.684296000
1	-6.196445000	-4.525855000	-1.024497000
1	-4.302913000	-2.259009000	-4.146045000
6	-3.524650000	-2.900474000	4.492486000
1	-2.788997000	-4.906632000	4.214700000
1	-4.138518000	-0.834395000	4.493171000
6	1.419154000	-5.061532000	-0.286053000
1	0.021697000	-6.318381000	-1.338996000
1	2.592465000	-3.582093000	0.764627000
1	-6.127650000	-3.758606000	-3.381247000
1	-3.887661000	-3.090793000	5.499728000
1	2.236578000	-5.774877000	-0.364039000
8	-1.137854000	2.032029000	-2.770455000
16	-1.865903000	2.935049000	-1.896215000
9	-4.443524000	3.294071000	-1.522760000
9	-3.804366000	3.179555000	-3.581814000
9	-3.916088000	1.387359000	-2.382507000
6	-3.639052000	2.685973000	-2.367333000
8	-3.109592000	4.209292000	0.822569000
8	-1.985490000	2.336736000	2.094978000
16	-2.027766000	3.259408000	0.969757000
9	0.498433000	3.785704000	0.313971000
9	-0.693337000	5.525741000	0.770872000
9	-0.024650000	4.226595000	2.353945000
6	-0.447910000	4.281118000	1.102268000
7	-1.777968000	2.313695000	-0.370322000
8	-1.637746000	4.366030000	-1.910606000
Zero-point correction=			0.753577 (Hartree/Particle)
Thermal correction to Energy=			0.809700
Thermal correction to Enthalpy=			0.810644
Thermal correction to Gibbs Free Energy=			0.661532
Sum of electronic and zero-point Energies=			-4114.705040
Sum of electronic and thermal Energies=			-4114.648917
Sum of electronic and thermal Enthalpies=			-4114.647973
Sum of electronic and thermal Free Energies=			-4114.797084

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6	1.765570000	5.207788000	-1.461106000
6	1.845052000	4.658610000	-0.191613000
6	0.866475000	3.746471000	0.217533000
6	-0.200553000	3.419147000	-0.672309000
6	-0.257028000	3.969902000	-1.960966000
6	0.729137000	4.858886000	-2.346135000
1	2.523301000	5.917973000	-1.785510000
1	2.664755000	4.916982000	0.477393000
1	-1.063960000	3.694081000	-2.638466000
1	0.704128000	5.298335000	-3.340517000
6	0.735687000	2.972026000	1.466449000
6	-0.543067000	2.295115000	1.310891000
6	-1.090954000	2.564724000	0.051467000
6	-2.422044000	2.037579000	-0.232211000
6	-1.331254000	1.346067000	2.018110000
6	-2.143879000	0.547126000	1.135829000
6	-1.532191000	1.267810000	3.404295000
6	-3.216546000	-0.208632000	1.683724000
1	-1.617677000	0.027898000	0.334854000
6	-2.583603000	0.518364000	3.885111000
1	-0.913517000	1.858694000	4.076769000
6	-3.453038000	-0.222851000	3.035295000
1	-3.787756000	-0.854137000	1.020760000
1	-2.773038000	0.493872000	4.958427000
6	-2.633735000	1.508480000	-1.598401000
6	-3.736008000	1.881795000	-2.384148000
6	-1.690992000	0.619666000	-2.139253000
6	-3.907776000	1.348440000	-3.654140000
1	-4.454101000	2.602533000	-2.001920000
6	-1.885499000	0.062247000	-3.392528000
1	-0.824634000	0.314750000	-1.548742000
6	-2.999292000	0.418201000	-4.148803000
1	-4.765081000	1.648274000	-4.252218000
1	-1.190466000	-0.690514000	-3.754540000
1	-3.158990000	-0.036265000	-5.123767000
6	-3.577251000	2.720818000	0.426489000
6	-4.845040000	2.121136000	0.453249000
6	-3.421029000	3.984781000	1.001582000
6	-5.918934000	2.764428000	1.047309000
1	-4.973320000	1.134102000	0.008125000
6	-4.500966000	4.628397000	1.599982000
1	-2.450171000	4.474548000	0.960816000
6	-5.749737000	4.021897000	1.627014000
1	-6.893446000	2.282079000	1.063910000

1	-4.361620000	5.613514000	2.039091000
1	-6.592811000	4.524980000	2.094740000
6	-4.530226000	-1.071744000	3.633811000
1	-5.289566000	-0.459848000	4.136790000
1	-5.027894000	-1.673208000	2.866470000
1	-4.120314000	-1.759522000	4.383355000
79	2.091318000	1.345876000	0.988414000
15	3.404794000	-0.333216000	0.001218000
6	3.524923000	-1.932939000	0.854229000
6	5.134181000	0.170109000	-0.296756000
6	2.695152000	-0.602640000	-1.652643000
6	4.470551000	-2.882910000	0.456569000
6	2.662978000	-2.211872000	1.917917000
6	5.800317000	-0.122444000	-1.489331000
6	5.811635000	0.841754000	0.724904000
6	2.274299000	-1.855109000	-2.094771000
6	2.485596000	0.529523000	-2.451455000
6	4.542224000	-4.106880000	1.109597000
1	5.152320000	-2.662632000	-0.364319000
6	2.748011000	-3.433565000	2.575782000
1	1.906645000	-1.483487000	2.206826000
6	7.130724000	0.250308000	-1.652975000
1	5.274052000	-0.636148000	-2.292785000
6	7.141758000	1.207986000	0.560200000
1	5.286413000	1.080482000	1.650274000
6	1.650622000	-1.976512000	-3.334091000
1	2.379565000	-2.731258000	-1.459147000
6	1.886315000	0.399506000	-3.696706000
1	2.780853000	1.516859000	-2.088820000
6	3.682517000	-4.380264000	2.169526000
1	5.272537000	-4.847400000	0.792728000
1	2.076999000	-3.647053000	3.403712000
6	7.801178000	0.913301000	-0.630220000
1	7.643929000	0.023372000	-2.584553000
1	7.662657000	1.731098000	1.358620000
6	1.471694000	-0.856394000	-4.138836000
1	1.286821000	-2.949691000	-3.654902000
1	1.721423000	1.281633000	-4.311029000
1	3.742382000	-5.337769000	2.681555000
1	8.840041000	1.206483000	-0.762635000
1	0.989052000	-0.957812000	-5.108898000
1	1.049384000	3.390537000	2.424178000
8	0.253642000	-1.209642000	0.325697000
16	-0.438117000	-2.481595000	0.083292000

9	-2.309692000	-3.215427000	1.843161000
9	-0.383013000	-4.116064000	2.168537000
9	-0.703496000	-2.046623000	2.682030000
6	-1.001550000	-3.006091000	1.805196000
8	-2.357805000	-3.048457000	-2.998665000
8	-2.603624000	-4.579587000	-1.012918000
16	-2.581762000	-3.235692000	-1.571203000
9	-4.361838000	-1.279874000	-1.562838000
9	-5.126864000	-3.240927000	-2.039603000
9	-4.630103000	-2.743643000	-0.000464000
6	-4.278317000	-2.574716000	-1.274170000
7	-1.786074000	-2.135778000	-0.687114000
8	0.337058000	-3.607717000	-0.419313000
Zero-point correction=			0.752324 (Hartree/Particle)
Thermal correction to Energy=			0.807535
Thermal correction to Enthalpy=			0.808479
Thermal correction to Gibbs Free Energy=			0.663721
Sum of electronic and zero-point Energies=			-4114.616821
Sum of electronic and thermal Energies=			-4114.561610
Sum of electronic and thermal Enthalpies=			-4114.560666
Sum of electronic and thermal Free Energies=			-4114.705424

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6	-2.359368000	-5.119137000	-0.209051000
6	-2.304298000	-4.272053000	0.883432000
6	-1.190320000	-3.436091000	1.039304000
6	-0.129129000	-3.505517000	0.080098000
6	-0.213989000	-4.355413000	-1.037412000
6	-1.329876000	-5.154397000	-1.173613000
1	-3.222015000	-5.770068000	-0.335200000
1	-3.120227000	-4.235744000	1.603833000
1	0.590903000	-4.369938000	-1.770623000
1	-1.420284000	-5.824594000	-2.024912000
6	-0.900513000	-2.400744000	2.047039000
6	0.462930000	-1.998058000	1.697475000
6	0.882745000	-2.619243000	0.523080000
6	2.218883000	-2.146192000	0.023462000
6	1.462972000	-1.114874000	2.124297000
6	2.459194000	-0.956255000	1.040966000
6	1.624794000	-0.412899000	3.327615000
6	3.772512000	-0.434720000	1.442595000
1	2.068272000	-0.037286000	0.537078000
6	2.815735000	0.233902000	3.545357000
1	0.839363000	-0.423322000	4.079479000

6	3.919886000	0.212486000	2.628668000
1	4.577847000	-0.408991000	0.712243000
1	2.953368000	0.784329000	4.476855000
6	2.040894000	-1.669348000	-1.424472000
6	2.595783000	-2.335279000	-2.518132000
6	1.218626000	-0.563429000	-1.668881000
6	2.383500000	-1.867590000	-3.813824000
1	3.211029000	-3.219076000	-2.364602000
6	1.033054000	-0.077543000	-2.954745000
1	0.720782000	-0.047073000	-0.846590000
6	1.620890000	-0.727825000	-4.035622000
1	2.837119000	-2.393897000	-4.651081000
1	0.443961000	0.825760000	-3.101142000
1	1.487137000	-0.342431000	-5.043925000
6	3.326968000	-3.178420000	0.211122000
6	4.611326000	-2.915168000	-0.283001000
6	3.120174000	-4.361304000	0.920423000
6	5.653307000	-3.807680000	-0.071675000
1	4.786142000	-2.009515000	-0.862241000
6	4.165901000	-5.256664000	1.134134000
1	2.131502000	-4.592427000	1.311571000
6	5.434796000	-4.984251000	0.640941000
1	6.640549000	-3.584976000	-0.470102000
1	3.979972000	-6.173340000	1.689344000
1	6.249862000	-5.685069000	0.805321000
6	5.163527000	0.971577000	2.972331000
1	5.473454000	0.798048000	4.009438000
1	5.993120000	0.697213000	2.314673000
1	4.992165000	2.049116000	2.852700000
79	-2.140583000	-0.814488000	1.241156000
15	-3.561551000	0.525333000	-0.088757000
6	-3.697722000	2.315032000	0.176520000
6	-5.270952000	-0.106393000	-0.066624000
6	-2.999315000	0.308109000	-1.811876000
6	-4.921727000	2.989166000	0.184176000
6	-2.502647000	3.025751000	0.315706000
6	-6.069560000	-0.090733000	-1.212889000
6	-5.800490000	-0.572232000	1.139646000
6	-2.941318000	1.364533000	-2.722439000
6	-2.631961000	-0.980646000	-2.219138000
6	-4.940240000	4.372823000	0.328292000
1	-5.855184000	2.438890000	0.076923000
6	-2.528179000	4.408752000	0.439268000
1	-1.550263000	2.498280000	0.306921000

6	-7.385009000	-0.536919000	-1.149481000
1	-5.658286000	0.270411000	-2.154966000
6	-7.117635000	-1.012990000	1.200450000
1	-5.171743000	-0.590587000	2.030219000
6	-2.528976000	1.129126000	-4.031898000
1	-3.210195000	2.371534000	-2.408258000
6	-2.221596000	-1.209259000	-3.525225000
1	-2.664006000	-1.807556000	-1.506685000
6	-3.747717000	5.080644000	0.450113000
1	-5.891351000	4.900275000	0.338893000
1	-1.587928000	4.947985000	0.520438000
6	-7.908440000	-0.997524000	0.055390000
1	-8.002798000	-0.526946000	-2.044278000
1	-7.524709000	-1.375529000	2.141327000
6	-2.170994000	-0.153472000	-4.432753000
1	-2.478055000	1.955991000	-4.735926000
1	-1.916976000	-2.208603000	-3.827015000
1	-3.769616000	6.163219000	0.552331000
1	-8.936642000	-1.348718000	0.101126000
1	-1.835057000	-0.330302000	-5.452130000
1	-1.184008000	-2.570330000	3.087713000
8	0.473053000	1.584495000	0.933213000
16	1.226259000	2.684775000	0.315007000
9	2.435959000	4.748264000	1.377551000
9	0.559311000	4.209383000	2.303425000
9	2.327252000	3.028485000	2.675998000
6	1.677093000	3.740457000	1.757260000
8	2.758654000	2.664853000	-2.745730000
8	3.911101000	4.161253000	-1.081214000
16	3.381353000	2.855690000	-1.444912000
9	4.467658000	0.485019000	-1.780500000
9	5.693139000	2.166187000	-2.351748000
9	5.429605000	1.686779000	-0.265382000
6	4.830867000	1.721120000	-1.453021000
7	2.604637000	2.107544000	-0.221361000
8	0.516592000	3.597297000	-0.575658000
Zero-point correction=			0.751426 (Hartree/Particle)
Thermal correction to Energy=			0.807640
Thermal correction to Enthalpy=			0.808584
Thermal correction to Gibbs Free Energy=			0.658766
Sum of electronic and zero-point Energies=			-4114.631462
Sum of electronic and thermal Energies=			-4114.575248
Sum of electronic and thermal Enthalpies=			-4114.574304
Sum of electronic and thermal Free Energies=			-4114.724122

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6	-1.960470000	-5.091357000	0.287288000
6	-1.923017000	-4.106928000	1.263702000
6	-0.854454000	-3.203613000	1.281421000
6	0.188130000	-3.341213000	0.317919000
6	0.124309000	-4.323974000	-0.680443000
6	-0.953142000	-5.191936000	-0.689143000
1	-2.790325000	-5.794928000	0.269170000
1	-2.724843000	-4.018793000	1.996473000
1	0.913053000	-4.392853000	-1.428599000
1	-1.022454000	-5.965098000	-1.451071000
6	-0.600731000	-2.019205000	2.136096000
6	0.733425000	-1.600603000	1.698727000
6	1.170524000	-2.356161000	0.633974000
6	2.464599000	-1.875021000	0.033783000
6	1.735859000	-0.646166000	2.019441000
6	2.778535000	-0.672757000	1.013997000
6	1.875947000	0.149499000	3.164027000
6	4.080935000	-0.241654000	1.451462000
1	2.586354000	0.516630000	0.368958000
6	3.103475000	0.714217000	3.424939000
1	1.046114000	0.250684000	3.860179000
6	4.236035000	0.501878000	2.596813000
1	4.943428000	-0.410275000	0.812440000
1	3.232245000	1.317455000	4.324195000
6	2.092805000	-1.454697000	-1.405011000
6	2.729627000	-1.932080000	-2.549709000
6	0.958207000	-0.645165000	-1.576066000
6	2.268664000	-1.585905000	-3.820110000
1	3.582546000	-2.599730000	-2.465451000
6	0.504372000	-0.296106000	-2.837530000
1	0.400993000	-0.294347000	-0.706663000
6	1.158818000	-0.768191000	-3.971833000
1	2.787241000	-1.971855000	-4.695326000
1	-0.369928000	0.346598000	-2.929710000
1	0.802946000	-0.497181000	-4.963394000
6	3.584093000	-2.909902000	0.131292000
6	4.848211000	-2.662854000	-0.421223000
6	3.401074000	-4.110709000	0.820830000
6	5.881173000	-3.583396000	-0.299037000
1	5.028392000	-1.740526000	-0.966960000
6	4.435733000	-5.034004000	0.946957000
1	2.434752000	-4.333990000	1.266200000

6	5.679683000	-4.777925000	0.386123000
1	6.849246000	-3.365029000	-0.744746000
1	4.259906000	-5.960954000	1.488385000
1	6.486647000	-5.500667000	0.481395000
6	5.557602000	1.088033000	2.991189000
1	5.824306000	0.819396000	4.020502000
1	6.361441000	0.742974000	2.333344000
1	5.534262000	2.184034000	2.939665000
79	-2.031296000	-0.687796000	1.227132000
15	-3.684039000	0.324976000	-0.127257000
6	-3.783030000	2.138797000	-0.148330000
6	-5.371241000	-0.257567000	0.236228000
6	-3.347525000	-0.177029000	-1.849790000
6	-4.949366000	2.850813000	0.135253000
6	-2.594819000	2.823827000	-0.418297000
6	-6.357689000	-0.308626000	-0.752838000
6	-5.690062000	-0.612139000	1.549406000
6	-3.594046000	0.668800000	-2.935024000
6	-2.813201000	-1.451559000	-2.072317000
6	-4.918226000	4.242989000	0.148712000
1	-5.878064000	2.324652000	0.349939000
6	-2.568915000	4.210912000	-0.406458000
1	-1.682617000	2.271142000	-0.638029000
6	-7.648889000	-0.707060000	-0.427225000
1	-6.113343000	-0.039739000	-1.779961000
6	-6.984206000	-1.006061000	1.872686000
1	-4.914828000	-0.581541000	2.315436000
6	-3.312682000	0.239443000	-4.228262000
1	-3.994019000	1.667826000	-2.765763000
6	-2.535020000	-1.875857000	-3.365866000
1	-2.600753000	-2.108463000	-1.226446000
6	-3.733239000	4.920820000	-0.118969000
1	-5.825968000	4.798738000	0.372666000
1	-1.629851000	4.719654000	-0.612424000
6	-7.962218000	-1.054372000	0.884418000
1	-8.412625000	-0.750319000	-1.200055000
1	-7.226900000	-1.281330000	2.896190000
6	-2.783496000	-1.030225000	-4.443175000
1	-3.499177000	0.903103000	-5.069175000
1	-2.096250000	-2.858026000	-3.525219000
1	-3.715477000	6.008110000	-0.101088000
1	-8.972891000	-1.367856000	1.135428000
1	-2.551827000	-1.356928000	-5.454469000
1	-0.825762000	-2.084161000	3.203852000

8	0.222204000	1.595744000	0.957136000
16	1.021697000	2.560954000	0.216210000
9	2.124734000	4.836921000	0.948449000
9	0.253332000	4.341687000	1.899458000
9	2.071559000	3.333670000	2.493202000
6	1.413846000	3.863061000	1.471762000
8	2.730064000	1.896422000	-2.756139000
8	3.380180000	3.931103000	-1.403269000
16	3.198836000	2.496693000	-1.524351000
9	4.830904000	0.467300000	-1.356013000
9	5.646327000	2.260663000	-2.234139000
9	5.377826000	2.142958000	-0.098622000
6	4.876449000	1.793145000	-1.270428000
7	2.451881000	1.861531000	-0.158082000
8	0.444860000	3.288944000	-0.903578000
Zero-point correction=			0.751426 (Hartree/Particle)
Thermal correction to Energy=			0.807640
Thermal correction to Enthalpy=			0.808584
Thermal correction to Gibbs Free Energy=			0.658766
Sum of electronic and zero-point Energies=			-4114.631462
Sum of electronic and thermal Energies=			-4114.575248
Sum of electronic and thermal Enthalpies=			-4114.574304
Sum of electronic and thermal Free Energies=			-4114.724122

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6	0.508322000	3.428273000	3.185296000
6	0.063597000	3.268125000	1.876481000
6	0.810040000	2.497946000	0.989872000
6	2.031178000	1.899647000	1.412677000
6	2.461769000	2.064226000	2.732195000
6	1.692875000	2.819204000	3.609384000
1	-0.067548000	4.032726000	3.883543000
1	-0.863394000	3.736118000	1.540316000
1	3.385410000	1.606722000	3.076928000
1	2.024887000	2.947279000	4.637577000
6	0.539603000	2.160658000	-0.436821000
6	1.737022000	1.397196000	-0.802932000
6	2.593857000	1.242282000	0.252889000
6	3.935189000	0.675087000	-0.195156000
6	2.345528000	0.890916000	-2.014383000
6	3.637625000	0.432573000	-1.684552000
6	1.886380000	0.817232000	-3.324302000
6	4.458655000	-0.093203000	-2.663259000
1	1.900586000	-1.522362000	0.507851000

6	2.721989000	0.275363000	-4.299096000
1	0.888363000	1.173661000	-3.577851000
6	4.004505000	-0.182381000	-3.989053000
1	5.466618000	-0.435451000	-2.420700000
1	2.376510000	0.209397000	-5.330493000
6	4.313993000	-0.583311000	0.583422000
6	4.832436000	-0.467388000	1.879738000
6	4.126043000	-1.867815000	0.067385000
6	5.133032000	-1.590864000	2.634723000
1	5.016387000	0.523934000	2.290143000
6	4.418422000	-3.001708000	0.829652000
1	3.770358000	-1.987869000	-0.954220000
6	4.919792000	-2.866913000	2.115880000
1	5.530598000	-1.470946000	3.639958000
1	4.245078000	-3.986922000	0.403693000
1	5.150043000	-3.747185000	2.710924000
6	5.051451000	1.728711000	-0.133484000
6	6.392648000	1.335503000	-0.182746000
6	4.761569000	3.094300000	-0.118102000
6	7.413640000	2.277824000	-0.208279000
1	6.642742000	0.275538000	-0.187716000
6	5.783688000	4.038338000	-0.142846000
1	3.724722000	3.423168000	-0.083547000
6	7.113444000	3.636187000	-0.186305000
1	8.449645000	1.947166000	-0.241393000
1	5.533662000	5.096948000	-0.123253000
1	7.911108000	4.375496000	-0.200278000
6	4.904512000	-0.740274000	-5.051276000
1	5.764545000	-0.082484000	-5.231243000
1	5.308514000	-1.718851000	-4.764407000
1	4.377080000	-0.861140000	-6.003299000
79	-1.338699000	1.171426000	-0.510407000
15	-3.615994000	0.474353000	-0.387775000
6	-4.120133000	-1.051719000	-1.242297000
6	-4.736078000	1.766340000	-1.020740000
6	-4.094171000	0.231529000	1.356005000
6	-5.331981000	-1.178059000	-1.925396000
6	-3.249294000	-2.142117000	-1.165115000
6	-5.979262000	2.026291000	-0.438325000
6	-4.342267000	2.479082000	-2.157105000
6	-4.909449000	-0.822236000	1.771211000
6	-3.552083000	1.104760000	2.305805000
6	-5.664571000	-2.390158000	-2.522926000
1	-6.013505000	-0.331502000	-1.993234000

6	-3.589762000	-3.352973000	-1.753741000
1	-2.304373000	-2.048458000	-0.633454000
6	-6.818591000	2.988267000	-0.990826000
1	-6.289182000	1.474002000	0.447947000
6	-5.185947000	3.435301000	-2.709594000
1	-3.365913000	2.284002000	-2.601516000
6	-5.169935000	-1.006568000	3.126132000
1	-5.323808000	-1.511929000	1.037279000
6	-3.815483000	0.917639000	3.656623000
1	-2.897839000	1.917336000	1.985992000
6	-4.797419000	-3.475316000	-2.436215000
1	-6.606384000	-2.486324000	-3.058231000
1	-2.905637000	-4.194161000	-1.674890000
6	-6.423271000	3.690870000	-2.125345000
1	-7.784074000	3.189668000	-0.532694000
1	-4.874005000	3.988274000	-3.592227000
6	-4.620068000	-0.142788000	4.067465000
1	-5.795212000	-1.836538000	3.446391000
1	-3.377578000	1.591109000	4.389543000
1	-5.063446000	-4.420115000	-2.904664000
1	-7.080967000	4.443878000	-2.553121000
1	-4.812284000	-0.300138000	5.126145000
1	0.357309000	3.029806000	-1.085383000
8	1.854096000	-1.258832000	3.016211000
16	0.792083000	-2.038759000	2.431254000
9	-1.667986000	-1.525011000	1.768445000
9	-1.206612000	-1.247021000	3.859075000
9	-0.528863000	0.202014000	2.411352000
6	-0.774144000	-1.070372000	2.625423000
8	1.677473000	-4.264794000	-0.234788000
8	-0.767046000	-3.678333000	0.104517000
16	0.595915000	-3.306291000	-0.203157000
9	1.810083000	-2.318442000	-2.293813000
9	-0.040097000	-3.364626000	-2.680362000
9	-0.081195000	-1.369353000	-1.860954000
6	0.574221000	-2.508440000	-1.884249000
7	0.978132000	-1.934684000	0.735953000
8	0.487553000	-3.401374000	2.799648000
Zero-point correction=			0.752145 (Hartree/Particle)
Thermal correction to Energy=			0.808600
Thermal correction to Enthalpy=			0.809545
Thermal correction to Gibbs Free Energy=			0.660471
Sum of electronic and zero-point Energies=			-4114.657986
Sum of electronic and thermal Energies=			-4114.601531

Sum of electronic and thermal Enthalpies=	-4114.600586
Sum of electronic and thermal Free Energies=	-4114.749660

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6	-1.092614000	2.959456000	-4.072157000
6	-0.981414000	3.458414000	-2.780115000
6	-1.286528000	2.628697000	-1.703979000
6	-1.706070000	1.285836000	-1.929680000
6	-1.781648000	0.791429000	-3.232217000
6	-1.481679000	1.635090000	-4.295467000
1	-0.868259000	3.603794000	-4.919469000
1	-0.659708000	4.484575000	-2.606051000
1	-2.078167000	-0.240617000	-3.416941000
1	-1.559025000	1.262442000	-5.314614000
6	-1.232686000	2.891945000	-0.261771000
6	-1.780511000	1.740897000	0.341473000
6	-1.966310000	0.674235000	-0.611204000
6	-3.155999000	-0.199124000	-0.109851000
6	-2.461175000	1.413447000	1.576980000
6	-3.253747000	0.274290000	1.344495000
6	-2.498904000	2.063512000	2.809219000
6	-4.087190000	-0.206682000	2.341038000
1	0.224148000	2.895112000	-0.010118000
6	-3.323513000	1.554984000	3.804290000
1	-1.884559000	2.942728000	2.982078000
6	-4.125706000	0.428362000	3.587661000
1	-4.731680000	-1.067470000	2.155908000
1	-3.360477000	2.046250000	4.775702000
6	-2.891253000	-1.694655000	-0.276775000
6	-2.950632000	-2.259670000	-1.556553000
6	-2.518557000	-2.519186000	0.786345000
6	-2.624496000	-3.592366000	-1.768254000
1	-3.271013000	-1.639111000	-2.392412000
6	-2.185930000	-3.856687000	0.575904000
1	-2.473280000	-2.108314000	1.793193000
6	-2.235695000	-4.398898000	-0.701192000
1	-2.671799000	-4.006314000	-2.773786000
1	-1.882098000	-4.472610000	1.421023000
1	-1.965448000	-5.439534000	-0.868315000
6	-4.493470000	0.205439000	-0.755642000
6	-5.566876000	-0.691543000	-0.774082000
6	-4.711281000	1.501598000	-1.227429000
6	-6.810989000	-0.310665000	-1.264282000
1	-5.427607000	-1.706759000	-0.406519000

6	-5.953851000	1.882323000	-1.721890000
1	-3.904631000	2.230528000	-1.215076000
6	-7.009771000	0.978324000	-1.745416000
1	-7.627434000	-1.029730000	-1.271180000
1	-6.092643000	2.895477000	-2.092371000
1	-7.980511000	1.277032000	-2.134325000
6	-5.047304000	-0.073400000	4.658308000
1	-5.031089000	-1.167441000	4.723796000
1	-4.781412000	0.330496000	5.640568000
1	-6.085544000	0.217966000	4.453504000
79	-0.096483000	-0.460391000	-0.294158000
15	1.666559000	-2.007747000	-0.040650000
6	3.326600000	-1.600992000	-0.665325000
6	1.238968000	-3.546069000	-0.926284000
6	1.919294000	-2.491267000	1.699250000
6	4.165613000	-2.582434000	-1.205285000
6	3.792323000	-0.293483000	-0.521966000
6	1.363852000	-4.808489000	-0.345639000
6	0.832318000	-3.433423000	-2.259717000
6	3.148390000	-2.976291000	2.154740000
6	0.842890000	-2.393059000	2.585734000
6	5.462870000	-2.252589000	-1.579495000
1	3.803975000	-3.602150000	-1.330048000
6	5.092503000	0.030955000	-0.892263000
1	3.137922000	0.480505000	-0.124990000
6	1.096885000	-5.949559000	-1.097566000
1	1.676560000	-4.900638000	0.693506000
6	0.578524000	-4.574608000	-3.009709000
1	0.705604000	-2.445815000	-2.707030000
6	3.292302000	-3.368703000	3.480950000
1	3.994958000	-3.039593000	1.472195000
6	0.990452000	-2.788608000	3.909950000
1	-0.107291000	-1.992769000	2.230663000
6	5.926961000	-0.949379000	-1.418349000
1	6.113547000	-3.015713000	-2.000223000
1	5.432116000	1.056443000	-0.775067000
6	0.712115000	-5.833929000	-2.429545000
1	1.197659000	-6.931779000	-0.641503000
1	0.267868000	-4.481150000	-4.047767000
6	2.214745000	-3.276791000	4.357091000
1	4.251555000	-3.740432000	3.833001000
1	0.151632000	-2.703420000	4.596352000
1	6.942980000	-0.696114000	-1.712199000
1	0.510641000	-6.726824000	-3.016891000

1	2.332466000	-3.577952000	5.395347000
1	-1.363556000	3.882148000	0.176079000
8	0.166739000	3.705695000	2.404614000
16	1.491706000	3.305483000	1.971129000
9	2.811356000	1.053951000	2.213824000
9	1.875263000	1.780658000	4.018830000
9	0.672665000	0.876355000	2.471847000
6	1.734517000	1.631909000	2.714285000
8	2.619254000	4.865442000	-0.913602000
8	3.943541000	2.882605000	-0.063451000
16	2.717399000	3.458045000	-0.586284000
9	1.848833000	3.372155000	-3.065637000
9	3.577269000	2.169292000	-2.659198000
9	1.632408000	1.481836000	-2.037860000
6	2.397063000	2.548071000	-2.202146000
7	1.414866000	2.947880000	0.351592000
8	2.670113000	4.073014000	2.305997000
Zero-point correction=			0.748170 (Hartree/Particle)
Thermal correction to Energy=			0.803823
Thermal correction to Enthalpy=			0.804767
Thermal correction to Gibbs Free Energy=			0.657979
Sum of electronic and zero-point Energies=			-4114.648651
Sum of electronic and thermal Energies=			-4114.592998
Sum of electronic and thermal Enthalpies=			-4114.592054
Sum of electronic and thermal Free Energies=			-4114.738841

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6	-1.310313000	-2.716042000	-4.547154000
6	-0.454902000	-2.715286000	-3.440736000
6	-0.946279000	-2.306658000	-2.214505000
6	-2.292224000	-1.884224000	-2.078186000
6	-3.140110000	-1.890728000	-3.183284000
6	-2.637503000	-2.311476000	-4.413880000
1	-0.938545000	-3.039676000	-5.516572000
1	0.581860000	-3.032397000	-3.538538000
1	-4.174557000	-1.565929000	-3.091684000
1	-3.291065000	-2.322306000	-5.283545000
6	-0.237187000	-2.204926000	-0.886370000
6	-1.303852000	-1.624555000	-0.022215000
6	-2.467276000	-1.464547000	-0.697975000
6	-3.584905000	-0.988631000	0.213257000
6	-1.457889000	-1.208816000	1.352389000
6	-2.793082000	-0.779990000	1.515805000
6	-0.568716000	-1.193332000	2.419322000

6	-3.222037000	-0.327708000	2.747780000
1	0.670463000	-1.581650000	-0.936796000
6	-1.022050000	-0.743204000	3.657734000
1	0.456544000	-1.535737000	2.299289000
6	-2.337850000	-0.314578000	3.839958000
1	-4.248547000	0.012106000	2.894650000
1	-0.333396000	-0.726681000	4.502493000
6	-4.585813000	-2.149831000	0.334181000
6	-5.617352000	-2.280597000	-0.600435000
6	-4.438607000	-3.144741000	1.302826000
6	-6.481063000	-3.369038000	-0.564346000
1	-5.756859000	-1.511342000	-1.359042000
6	-5.303519000	-4.233630000	1.340139000
1	-3.639855000	-3.067598000	2.037886000
6	-6.328737000	-4.351140000	0.408408000
1	-7.277814000	-3.447676000	-1.300838000
1	-5.172521000	-4.994653000	2.106426000
1	-7.004905000	-5.202290000	0.440205000
6	-4.273059000	0.294999000	-0.230426000
6	-5.403033000	0.756311000	0.455691000
6	-3.803621000	1.043903000	-1.308155000
6	-6.027019000	1.941501000	0.089289000
1	-5.812661000	0.161794000	1.271013000
6	-4.434213000	2.228915000	-1.686147000
1	-2.935736000	0.699418000	-1.866098000
6	-5.543086000	2.687248000	-0.985115000
1	-6.905712000	2.278149000	0.635641000
1	-4.046785000	2.789110000	-2.536787000
1	-6.040324000	3.608379000	-1.281112000
6	-2.822135000	0.134600000	5.186031000
1	-3.385304000	1.074450000	5.116931000
1	-3.495146000	-0.605305000	5.638230000
1	-1.990004000	0.288569000	5.881917000
79	1.831792000	0.557681000	0.338128000
15	0.482054000	2.383185000	-0.046238000
6	-0.252336000	2.362024000	-1.710987000
6	1.516477000	3.884379000	-0.016277000
6	-0.849219000	2.670698000	1.152537000
6	-0.691795000	3.547413000	-2.311268000
6	-0.377506000	1.153721000	-2.399189000
6	1.054031000	5.092256000	0.511257000
6	2.793845000	3.812846000	-0.584193000
6	-2.117566000	3.104825000	0.765711000
6	-0.552474000	2.505478000	2.509812000

6	-1.271639000	3.512163000	-3.573607000
1	-0.572439000	4.498105000	-1.792389000
6	-0.954751000	1.119702000	-3.665457000
1	-0.032199000	0.227931000	-1.942331000
6	1.863376000	6.223211000	0.464401000
1	0.064068000	5.147868000	0.962703000
6	3.594184000	4.947499000	-0.630233000
1	3.169118000	2.867790000	-0.981744000
6	-3.083064000	3.377405000	1.729894000
1	-2.365620000	3.220138000	-0.286980000
6	-1.513672000	2.798470000	3.467823000
1	0.427072000	2.135355000	2.815241000
6	-1.405903000	2.299403000	-4.248479000
1	-1.611445000	4.435383000	-4.037202000
1	-1.052551000	0.167089000	-4.184591000
6	3.129778000	6.151167000	-0.106823000
1	1.503100000	7.161821000	0.878700000
1	4.587532000	4.886247000	-1.067311000
6	-2.777547000	3.235820000	3.078368000
1	-4.077789000	3.683800000	1.412388000
1	-1.279770000	2.668522000	4.522428000
1	-1.855022000	2.277775000	-5.238638000
1	3.761790000	7.035579000	-0.136922000
1	-3.531252000	3.454826000	3.832226000
1	0.104963000	-3.185584000	-0.525034000
8	2.674768000	-1.083798000	2.799367000
16	3.677072000	-1.623719000	1.892109000
9	4.009707000	-4.004346000	0.841540000
9	3.344186000	-3.980325000	2.894574000
9	1.961721000	-3.505646000	1.305247000
6	3.221556000	-3.406622000	1.711677000
8	4.530330000	0.422894000	-1.314616000
8	5.565432000	-1.787387000	-0.621919000
16	4.409755000	-0.947044000	-0.843859000
9	2.409617000	-1.043599000	-2.561584000
9	4.246274000	-1.970951000	-3.205684000
9	2.979842000	-2.964677000	-1.765690000
6	3.437795000	-1.793132000	-2.177770000
7	3.315241000	-0.996281000	0.403321000
8	5.084978000	-1.592842000	2.217153000
Zero-point correction=			0.753262 (Hartree/Particle)
Thermal correction to Energy=			0.809265
Thermal correction to Enthalpy=			0.810210
Thermal correction to Gibbs Free Energy=			0.663254

Sum of electronic and zero-point Energies=	-4114.702947
Sum of electronic and thermal Energies=	-4114.646944
Sum of electronic and thermal Enthalpies=	-4114.646000
Sum of electronic and thermal Free Energies=	-4114.792956

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6	-1.932753000	-2.349210000	-4.111773000
6	-1.071772000	-1.810070000	-3.158274000
6	-1.606115000	-1.346925000	-1.958977000
6	-2.995741000	-1.424886000	-1.726974000
6	-3.842792000	-1.983935000	-2.670508000
6	-3.303110000	-2.439105000	-3.873555000
1	-1.527778000	-2.712922000	-5.053793000
1	-0.000203000	-1.749970000	-3.341290000
1	-4.913260000	-2.062493000	-2.479610000
1	-3.956339000	-2.869208000	-4.629489000
6	-0.914482000	-0.754208000	-0.786865000
6	-1.910624000	-0.468056000	0.117230000
6	-3.259344000	-0.925528000	-0.343311000
1	-3.520718000	-1.774361000	0.312732000
6	-4.177349000	0.276501000	0.056763000
6	-2.105001000	0.334288000	1.304765000
6	-1.219544000	0.817663000	2.268114000
6	-3.464186000	0.706095000	1.343026000
6	-1.715973000	1.606457000	3.296987000
1	-0.158319000	0.578970000	2.222990000
6	-3.946987000	1.486387000	2.379206000
1	0.070760000	-1.631391000	-0.357903000
6	-3.075987000	1.932641000	3.380129000
1	-1.034723000	1.978322000	4.062195000
1	-4.999714000	1.766637000	2.417226000
6	-5.642311000	-0.062132000	0.281540000
6	-6.562111000	0.982771000	0.440342000
6	-6.118361000	-1.370898000	0.365890000
6	-7.902225000	0.729116000	0.698793000
1	-6.218077000	2.011390000	0.337581000
6	-7.464759000	-1.628737000	0.614857000
1	-5.443746000	-2.213014000	0.228693000
6	-8.360979000	-0.582338000	0.788299000
1	-8.594427000	1.559472000	0.820002000
1	-7.809863000	-2.658777000	0.669127000
1	-9.411533000	-0.785206000	0.982759000
6	-4.029443000	1.369787000	-1.014079000
6	-3.191057000	2.476848000	-0.863361000

6	-4.730275000	1.233430000	-2.217570000
6	-3.056357000	3.413398000	-1.886784000
1	-2.635240000	2.622787000	0.061490000
6	-4.593134000	2.162644000	-3.239058000
1	-5.395724000	0.382712000	-2.351632000
6	-3.752398000	3.260656000	-3.078421000
1	-2.406312000	4.274449000	-1.740464000
1	-5.146430000	2.028433000	-4.165747000
1	-3.646064000	3.992896000	-3.875535000
6	-3.597151000	2.743781000	4.527213000
1	-4.053576000	2.098456000	5.288988000
1	-2.798336000	3.310899000	5.016531000
1	-4.369572000	3.450138000	4.202988000
79	0.732012000	0.573430000	-0.756248000
15	2.571156000	1.909251000	-0.184074000
6	2.563407000	1.932835000	1.644145000
6	2.591862000	3.652454000	-0.697611000
6	4.169360000	1.174907000	-0.642881000
6	2.492273000	3.116939000	2.376864000
6	2.535526000	0.700366000	2.312887000
6	3.775881000	4.393227000	-0.742665000
6	1.374159000	4.268841000	-1.000245000
6	5.297414000	1.282924000	0.176944000
6	4.236339000	0.429133000	-1.822818000
6	2.394005000	3.072097000	3.765922000
1	2.507426000	4.077571000	1.864201000
6	2.441242000	0.662196000	3.697544000
1	2.577318000	-0.233852000	1.750174000
6	3.739333000	5.740090000	-1.083474000
1	4.727428000	3.913543000	-0.516953000
6	1.342234000	5.618124000	-1.335196000
1	0.453925000	3.683303000	-0.976941000
6	6.482559000	0.656046000	-0.189485000
1	5.242158000	1.841049000	1.111311000
6	5.423785000	-0.196161000	-2.184500000
1	3.344520000	0.300398000	-2.433921000
6	2.367862000	1.848799000	4.425992000
1	2.337962000	3.999154000	4.331642000
1	2.418184000	-0.298397000	4.206747000
6	2.523500000	6.352284000	-1.377319000
1	4.662261000	6.313668000	-1.121938000
1	0.393808000	6.094589000	-1.571820000
6	6.544488000	-0.084390000	-1.367293000
1	7.356860000	0.734479000	0.452217000

1	5.462053000	-0.794035000	-3.091620000
1	2.288817000	1.816125000	5.510039000
1	2.498426000	7.405583000	-1.646458000
1	7.468721000	-0.586946000	-1.642714000
8	2.052108000	-1.951314000	-2.082369000
16	1.956630000	-3.091433000	-1.181671000
9	3.598026000	-4.051217000	0.625104000
9	4.535801000	-3.194189000	-1.120541000
9	3.688467000	-1.907378000	0.390037000
6	3.551125000	-3.063811000	-0.247008000
8	-1.292224000	-3.480660000	1.015888000
8	0.695312000	-5.058744000	0.961087000
16	0.136787000	-3.725995000	1.011809000
9	0.329809000	-1.731142000	2.695918000
9	0.236061000	-3.693178000	3.595856000
9	2.057989000	-3.014209000	2.656969000
6	0.734639000	-2.990736000	2.595226000
7	0.841875000	-2.669366000	-0.045109000
8	1.819534000	-4.438475000	-1.686567000
Zero-point correction=			0.748083 (Hartree/Particle)
Thermal correction to Energy=			0.803759
Thermal correction to Enthalpy=			0.804703
Thermal correction to Gibbs Free Energy=			0.657086
Sum of electronic and zero-point Energies=			-4114.639934
Sum of electronic and thermal Energies=			-4114.584257
Sum of electronic and thermal Enthalpies=			-4114.583313
Sum of electronic and thermal Free Energies=			-4114.730930

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6	-1.036108000	0.377319000	-4.668030000
6	-0.393284000	-0.313278000	-3.643649000
6	-1.154340000	-0.743137000	-2.560599000
6	-2.542255000	-0.483336000	-2.499632000
6	-3.174227000	0.178533000	-3.540641000
6	-2.408178000	0.621348000	-4.620182000
1	-0.457594000	0.725946000	-5.520772000
1	0.678003000	-0.499794000	-3.670289000
1	-4.249787000	0.353254000	-3.521553000
1	-2.890342000	1.154314000	-5.436623000
6	-0.727101000	-1.459811000	-1.336832000
6	-1.856251000	-1.659517000	-0.567348000
6	-3.078699000	-1.181697000	-1.285365000
1	-3.513369000	-2.132368000	-1.648038000
6	-4.021371000	-0.710284000	-0.140683000

6	-2.289856000	-2.195852000	0.701045000
6	-1.641704000	-3.020423000	1.618980000
6	-3.605608000	-1.741810000	0.922411000
6	-2.348313000	-3.420624000	2.744215000
1	-0.619987000	-3.352257000	1.432265000
6	-4.300663000	-2.172121000	2.040007000
1	0.231646000	-1.962145000	-1.197991000
6	-3.676230000	-3.023643000	2.960067000
1	-1.872286000	-4.074958000	3.473257000
1	-5.327240000	-1.849915000	2.215229000
6	-5.505489000	-0.755446000	-0.471691000
6	-6.422929000	-0.207003000	0.433268000
6	-6.002246000	-1.332010000	-1.641769000
6	-7.789112000	-0.261993000	0.191728000
1	-6.053407000	0.285393000	1.332358000
6	-7.371706000	-1.379248000	-1.891303000
1	-5.323548000	-1.740458000	-2.388120000
6	-8.270637000	-0.851863000	-0.973650000
1	-8.481234000	0.167536000	0.912597000
1	-7.732676000	-1.829005000	-2.813436000
1	-9.339697000	-0.889523000	-1.168488000
6	-3.630709000	0.701841000	0.313834000
6	-3.152378000	0.975709000	1.598100000
6	-3.795521000	1.771784000	-0.572726000
6	-2.858688000	2.281259000	1.983432000
1	-3.022207000	0.167764000	2.315674000
6	-3.465615000	3.068754000	-0.200311000
1	-4.200541000	1.587497000	-1.564815000
6	-3.000555000	3.330734000	1.085500000
1	-2.509746000	2.475101000	2.995121000
1	-3.595806000	3.881262000	-0.911851000
1	-2.750271000	4.346272000	1.387842000
6	-4.422520000	-3.523181000	4.159681000
1	-4.786258000	-4.545997000	3.997522000
1	-3.782680000	-3.549123000	5.048830000
1	-5.293700000	-2.898753000	4.382971000
79	-0.169596000	0.328273000	-0.017238000
15	1.189837000	2.147622000	0.625575000
6	2.530747000	1.713871000	1.772080000
6	0.447357000	3.626799000	1.402430000
6	1.945603000	2.722003000	-0.924377000
6	3.277502000	2.731808000	2.382061000
6	2.828542000	0.376540000	2.036333000
6	0.300450000	4.832077000	0.715621000

6	0.040566000	3.541257000	2.738057000
6	3.328500000	2.798431000	-1.082592000
6	1.102557000	2.966741000	-2.014239000
6	4.310679000	2.409921000	3.250040000
1	3.044257000	3.776369000	2.177668000
6	3.862088000	0.062164000	2.915454000
1	2.274648000	-0.421575000	1.539430000
6	-0.248056000	5.939211000	1.358553000
1	0.624582000	4.912615000	-0.319859000
6	-0.495327000	4.649645000	3.379475000
1	0.153605000	2.601484000	3.279570000
6	3.864169000	3.124174000	-2.324099000
1	3.987760000	2.565313000	-0.248925000
6	1.642728000	3.311479000	-3.245407000
1	0.019954000	2.864417000	-1.902747000
6	4.598090000	1.073324000	3.520166000
1	4.889045000	3.201345000	3.720625000
1	4.095494000	-0.978945000	3.116003000
6	-0.643926000	5.851433000	2.688349000
1	-0.354538000	6.876581000	0.817758000
1	-0.799737000	4.577124000	4.421180000
6	3.025074000	3.384793000	-3.401252000
1	4.943336000	3.159980000	-2.451135000
1	0.984850000	3.499424000	-4.090380000
1	5.404452000	0.820789000	4.204836000
1	-1.063733000	6.719697000	3.190782000
1	3.448807000	3.630523000	-4.372091000
8	2.334140000	-0.037380000	-1.889412000
16	2.979277000	-1.342710000	-1.748166000
9	5.397629000	-2.005530000	-0.982814000
9	5.281637000	-0.253359000	-2.246520000
9	4.686226000	-0.137798000	-0.177340000
6	4.702776000	-0.916081000	-1.254981000
8	1.093567000	-4.126224000	0.119792000
8	3.392949000	-4.381471000	-0.883146000
16	2.437647000	-3.604002000	-0.114559000
9	2.336020000	-2.799743000	2.376538000
9	3.363946000	-4.672433000	2.071108000
9	4.320125000	-2.814825000	1.515351000
6	3.162682000	-3.465890000	1.569214000
7	2.347136000	-2.025806000	-0.443044000
8	3.101398000	-2.194936000	-2.918577000
Zero-point correction=			0.752628 (Hartree/Particle)
Thermal correction to Energy=			0.809107

Thermal correction to Enthalpy=	0.810051
Thermal correction to Gibbs Free Energy=	0.660182
Sum of electronic and zero-point Energies=	-4114.673367
Sum of electronic and thermal Energies=	-4114.616888
Sum of electronic and thermal Enthalpies=	-4114.615944
Sum of electronic and thermal Free Energies=	-4114.765812

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6	0.689443000	-4.279955000	0.855449000
6	0.396617000	-3.578496000	-0.306320000
6	0.643080000	-2.205798000	-0.341224000
6	1.218831000	-1.546964000	0.774754000
6	1.504839000	-2.264105000	1.935247000
6	1.225288000	-3.623961000	1.970320000
1	0.497191000	-5.349708000	0.902857000
1	-0.039902000	-4.080524000	-1.169239000
1	1.950337000	-1.762644000	2.790132000
1	1.439566000	-4.190460000	2.873747000
6	0.284572000	-1.205202000	-1.371219000
6	0.739963000	0.040091000	-0.840343000
6	1.412468000	-0.131154000	0.404612000
6	1.336376000	1.208488000	1.185346000
6	0.559952000	1.445790000	-1.109726000
6	0.970178000	2.156298000	0.030953000
6	0.049044000	2.104173000	-2.227792000
6	0.923996000	3.542875000	0.021858000
1	2.708247000	-0.192670000	-0.142262000
6	-0.012622000	3.488739000	-2.210167000
1	-0.282033000	1.536424000	-3.097006000
6	0.439567000	4.221563000	-1.101283000
1	1.265623000	4.114436000	0.884943000
1	-0.402404000	4.027011000	-3.072950000
6	2.634495000	1.552249000	1.908240000
6	2.850377000	1.095633000	3.211112000
6	3.665980000	2.230745000	1.261547000
6	4.062055000	1.318588000	3.851071000
1	2.059141000	0.554229000	3.728777000
6	4.886208000	2.445690000	1.896099000
1	3.537766000	2.575100000	0.237292000
6	5.086112000	1.994178000	3.194708000
1	4.212241000	0.947171000	4.862298000
1	5.684208000	2.946364000	1.353936000
1	6.041645000	2.154783000	3.688333000
6	0.140529000	1.288979000	2.154289000

6	0.005802000	2.432625000	2.954638000
6	-0.851492000	0.314259000	2.243833000
6	-1.087541000	2.604145000	3.790425000
1	0.784615000	3.192498000	2.933374000
6	-1.949195000	0.480675000	3.089938000
1	-0.764154000	-0.605610000	1.669166000
6	-2.078411000	1.627077000	3.859534000
1	-1.162334000	3.503935000	4.397866000
1	-2.709496000	-0.298624000	3.140528000
1	-2.941604000	1.760876000	4.507889000
6	0.415714000	5.720095000	-1.126925000
1	-0.379034000	6.100001000	-1.778016000
1	0.267974000	6.138776000	-0.125141000
1	1.364466000	6.121311000	-1.505949000
79	-1.817656000	-0.822748000	-0.916484000
15	-4.024447000	-0.320060000	-0.284012000
6	-4.691088000	-1.545044000	0.889963000
6	-5.242643000	-0.256345000	-1.635962000
6	-4.067970000	1.302026000	0.541802000
6	-6.067374000	-1.711984000	1.075001000
6	-3.795701000	-2.331245000	1.623320000
6	-6.186991000	0.765568000	-1.748222000
6	-5.230991000	-1.297256000	-2.570866000
6	-5.066652000	1.636403000	1.461739000
6	-3.053817000	2.222022000	0.255876000
6	-6.538658000	-2.633031000	2.003707000
1	-6.770975000	-1.128449000	0.481657000
6	-4.271661000	-3.249256000	2.553205000
1	-2.720680000	-2.234084000	1.457468000
6	-7.116240000	0.740194000	-2.784360000
1	-6.194059000	1.582650000	-1.028705000
6	-6.163727000	-1.320641000	-3.599124000
1	-4.486254000	-2.089666000	-2.488449000
6	-5.052578000	2.881625000	2.079769000
1	-5.847406000	0.917226000	1.706895000
6	-3.039700000	3.462656000	0.882168000
1	-2.253625000	1.963680000	-0.440099000
6	-5.641734000	-3.396828000	2.745591000
1	-7.609453000	-2.759644000	2.143570000
1	-3.569317000	-3.855886000	3.119001000
6	-7.106486000	-0.300738000	-3.706272000
1	-7.848797000	1.538944000	-2.871256000
1	-6.151269000	-2.131904000	-4.322650000
6	-4.038661000	3.791720000	1.792820000

1	-5.829019000	3.137334000	2.796876000
1	-2.230353000	4.158621000	0.668534000
1	-6.013703000	-4.118433000	3.468960000
1	-7.832451000	-0.316284000	-4.515536000
1	-4.022031000	4.758426000	2.290914000
1	0.278221000	-1.431587000	-2.439597000
8	4.166949000	-1.325256000	1.785340000
16	4.933749000	-1.226944000	0.559335000
9	5.628880000	-3.019983000	-1.236210000
9	5.585039000	-3.707630000	0.807213000
9	3.740626000	-3.405542000	-0.272356000
6	4.971856000	-2.956405000	-0.097189000
8	5.515710000	1.632186000	-1.227063000
8	5.697401000	-0.527480000	-2.519595000
16	4.924063000	0.397561000	-1.712759000
9	3.016332000	2.076115000	-2.335833000
9	4.120301000	1.259437000	-3.991571000
9	2.634625000	0.050479000	-3.002331000
6	3.567944000	0.976771000	-2.826001000
7	4.018303000	-0.409085000	-0.554395000
8	6.316083000	-0.788576000	0.560559000
Zero-point correction=			0.744600 (Hartree/Particle)
Thermal correction to Energy=			0.800772
Thermal correction to Enthalpy=			0.801716
Thermal correction to Gibbs Free Energy=			0.651847
Sum of electronic and zero-point Energies=			-4114.641800
Sum of electronic and thermal Energies=			-4114.585628
Sum of electronic and thermal Enthalpies=			-4114.584683
Sum of electronic and thermal Free Energies=			-4114.734553

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6	-1.029694000	-0.464217000	-4.642571000
6	-0.278570000	0.383469000	-3.843645000
6	-0.854153000	0.903930000	-2.682729000
6	-2.184285000	0.564914000	-2.344985000
6	-2.911070000	-0.347702000	-3.122364000
6	-2.330865000	-0.843244000	-4.276080000
1	-0.598856000	-0.859567000	-5.560277000
1	0.747191000	0.640928000	-4.106518000
1	-3.915206000	-0.645572000	-2.828931000
1	-2.886003000	-1.534403000	-4.905503000
6	-0.271611000	1.808301000	-1.668049000
6	-1.380725000	2.104197000	-0.740021000
6	-2.496011000	1.223690000	-1.100640000

1	0.184767000	2.717040000	-2.082782000
6	-3.448567000	0.956001000	-0.117274000
6	-2.904465000	1.261879000	1.158486000
6	-3.630190000	1.589758000	2.324268000
6	-1.466235000	1.362389000	1.152792000
6	-2.962332000	2.114854000	3.404592000
1	-4.713746000	1.492787000	2.326393000
6	-0.822451000	1.975400000	2.268155000
1	-0.935233000	0.500619000	0.738249000
6	-1.560869000	2.336568000	3.365782000
1	-3.518944000	2.405137000	4.292810000
1	0.264046000	2.046575000	2.274181000
1	-1.067059000	2.748033000	4.243288000
6	-4.794547000	0.444513000	-0.342435000
6	-5.568262000	0.933648000	-1.407530000
6	-5.356022000	-0.521560000	0.498212000
6	-6.853082000	0.476127000	-1.622304000
1	-5.144850000	1.693073000	-2.064412000
6	-6.647389000	-0.990035000	0.293879000
1	-4.746041000	-0.947624000	1.292270000
6	-7.402391000	-0.489640000	-0.769804000
1	-7.465402000	0.850127000	-2.438567000
1	-7.045968000	-1.755598000	0.952247000
79	1.505932000	0.945612000	-0.824382000
15	3.671798000	0.217408000	-0.190164000
6	4.464107000	1.228051000	1.109139000
6	4.802837000	0.369694000	-1.618269000
6	3.829013000	-1.511585000	0.334447000
6	5.730866000	1.791553000	0.936976000
6	3.775524000	1.425256000	2.312873000
6	5.811320000	-0.563178000	-1.869924000
6	4.677014000	1.487581000	-2.449282000
6	4.711511000	-1.905359000	1.341956000
6	3.084026000	-2.469662000	-0.356522000
6	6.302290000	2.547853000	1.956424000
1	6.275108000	1.641159000	0.005986000
6	4.357614000	2.174530000	3.327801000
1	2.799306000	0.964777000	2.457682000
6	6.681694000	-0.377011000	-2.939857000
1	5.912892000	-1.437395000	-1.228837000
6	5.553837000	1.675799000	-3.510483000
1	3.885507000	2.212840000	-2.256256000
6	4.849939000	-3.254825000	1.647009000
1	5.287221000	-1.159544000	1.887856000

6	3.235849000	-3.816424000	-0.054863000
1	2.366823000	-2.151033000	-1.114747000
6	5.617661000	2.740265000	3.151023000
1	7.288151000	2.984755000	1.814361000
1	3.823356000	2.315704000	4.264541000
6	6.555962000	0.740996000	-3.757788000
1	7.461241000	-1.110148000	-3.133355000
1	5.451025000	2.549007000	-4.150320000
6	4.117925000	-4.207928000	0.946733000
1	5.528987000	-3.561684000	2.439047000
1	2.638549000	-4.555382000	-0.581033000
1	6.067341000	3.329480000	3.947040000
1	7.238090000	0.883096000	-4.592778000
1	4.222384000	-5.261490000	1.194366000
8	-2.725220000	-1.873012000	-0.237481000
16	-1.567396000	-2.585074000	0.289972000
9	0.255380000	-4.069481000	-0.840758000
9	-1.680966000	-4.126972000	-1.796139000
9	-0.408053000	-2.400125000	-2.040383000
6	-0.797673000	-3.344405000	-1.195602000
8	1.133762000	-2.959978000	2.194682000
8	1.266740000	-0.449478000	2.099518000
16	0.473611000	-1.678726000	2.015759000
9	-1.915772000	-1.099316000	3.055136000
9	-0.863156000	-2.679803000	4.075957000
9	-0.243867000	-0.632497000	4.324431000
6	-0.721997000	-1.523031000	3.464843000
7	-0.432128000	-1.511360000	0.697523000
8	-1.767203000	-3.667290000	1.243508000
8	-8.665139000	-0.874105000	-1.058835000
6	-9.262691000	-1.853390000	-0.242080000
1	-10.266745000	-2.015443000	-0.638751000
1	-8.707405000	-2.801086000	-0.272910000
1	-9.338860000	-1.518634000	0.801975000
6	-1.546679000	3.596758000	-0.479760000
6	-2.740020000	4.152327000	0.275006000
1	-1.560237000	4.044799000	-1.488191000
1	-0.611129000	3.953189000	-0.019019000
6	-2.783886000	5.672935000	0.181240000
1	-3.676871000	3.737764000	-0.130708000
1	-2.708222000	3.867933000	1.333818000
6	-3.955534000	6.263281000	0.946705000
1	-1.838553000	6.087248000	0.564057000
1	-2.836871000	5.973502000	-0.876198000

1	-3.984330000	7.355496000	0.873329000
1	-4.909105000	5.878506000	0.563716000
1	-3.902470000	6.001627000	2.010961000
Zero-point correction=			0.787507 (Hartree/Particle)
Thermal correction to Energy=			0.845209
Thermal correction to Enthalpy=			0.846154
Thermal correction to Gibbs Free Energy=			0.694377
Sum of electronic and zero-point Energies=			-4116.020405
Sum of electronic and thermal Energies=			-4115.962703
Sum of electronic and thermal Enthalpies=			-4115.961759
Sum of electronic and thermal Free Energies=			-4116.113535

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6	-0.840937000	-3.711260000	-3.170359000
6	-0.255249000	-2.456137000	-3.145100000
6	-0.996630000	-1.372404000	-2.668829000
6	-2.327235000	-1.568417000	-2.232227000
6	-2.893306000	-2.850733000	-2.214243000
6	-2.146712000	-3.910984000	-2.693492000
1	-0.275191000	-4.561632000	-3.545281000
1	0.774419000	-2.309690000	-3.472633000
1	-3.899543000	-3.007019000	-1.832029000
1	-2.571455000	-4.911816000	-2.697634000
6	-0.588251000	0.038152000	-2.496847000
6	-1.792542000	0.725088000	-1.986067000
6	-2.803062000	-0.306617000	-1.723983000
1	-0.190140000	0.507280000	-3.406720000
6	-3.782211000	-0.004384000	-0.777766000
6	-3.338390000	1.075602000	0.021833000
6	-4.134387000	1.966819000	0.769786000
6	-1.915564000	1.306173000	-0.076697000
6	-3.571737000	3.101168000	1.302657000
1	-5.203211000	1.785197000	0.861897000
6	-1.379558000	2.526679000	0.412291000
1	-1.285935000	0.437757000	0.140619000
6	-2.190139000	3.396876000	1.108296000
1	-4.200503000	3.802415000	1.844076000
1	-0.306223000	2.705592000	0.386758000
6	-5.039185000	-0.721134000	-0.572975000
6	-5.828047000	-1.091256000	-1.669322000
6	-5.471618000	-1.042281000	0.720164000
6	-7.026848000	-1.765293000	-1.477619000
1	-5.490266000	-0.835618000	-2.673463000
6	-6.670287000	-1.717106000	0.907820000

1	-4.829419000	-0.800984000	1.564930000
6	-7.450028000	-2.077567000	-0.187949000
1	-7.634645000	-2.045079000	-2.334882000
1	-6.989665000	-1.977927000	1.913857000
79	1.197054000	0.142040000	-1.301989000
15	3.386332000	0.234171000	-0.395745000
6	4.008277000	1.941254000	-0.208067000
6	4.549197000	-0.547126000	-1.571164000
6	3.715923000	-0.617289000	1.173337000
6	5.165850000	2.380155000	-0.854519000
6	3.278619000	2.831628000	0.591231000
6	5.734738000	-1.147104000	-1.137180000
6	4.268432000	-0.493215000	-2.939439000
6	4.512737000	-0.055135000	2.171601000
6	3.200797000	-1.906610000	1.330284000
6	5.589991000	3.697895000	-0.707143000
1	5.740223000	1.695647000	-1.476344000
6	3.715701000	4.142112000	0.740011000
1	2.386868000	2.485815000	1.113351000
6	6.625010000	-1.683335000	-2.061330000
1	5.958727000	-1.194635000	-0.072258000
6	5.162978000	-1.024875000	-3.861494000
1	3.339564000	-0.031381000	-3.277194000
6	4.792606000	-0.784493000	3.322194000
1	4.908958000	0.951673000	2.051183000
6	3.493391000	-2.632160000	2.477408000
1	2.561840000	-2.336068000	0.557207000
6	4.866587000	4.578784000	0.088460000
1	6.490783000	4.033210000	-1.216083000
1	3.149863000	4.826619000	1.367576000
6	6.340837000	-1.621967000	-3.422410000
1	7.543560000	-2.152021000	-1.715976000
1	4.935934000	-0.979935000	-4.924022000
6	4.285328000	-2.070046000	3.473316000
1	5.404290000	-0.342629000	4.105218000
1	3.080722000	-3.628692000	2.604739000
1	5.199994000	5.607834000	0.202532000
1	7.037836000	-2.044296000	-4.142653000
1	4.498174000	-2.634174000	4.378145000
8	-2.464030000	-2.026571000	0.871416000
16	-1.358983000	-2.100906000	1.820974000
9	0.624528000	-3.783784000	2.066570000
9	-1.179665000	-4.621578000	1.229635000
9	0.083199000	-3.356444000	0.021345000

6	-0.391241000	-3.558107000	1.245203000
8	1.097146000	-0.823305000	3.694103000
8	1.071374000	1.051809000	2.018207000
16	0.385241000	-0.052146000	2.690064000
9	-2.182500000	0.605617000	3.019476000
9	-1.096146000	0.314910000	4.854774000
9	-0.785638000	2.097930000	3.686077000
6	-1.015565000	0.789995000	3.629823000
7	-0.341292000	-0.887949000	1.521788000
8	-1.640447000	-2.343470000	3.229286000
1	-8.387600000	-2.607818000	-0.037317000
8	-1.601296000	4.494511000	1.627662000
6	-2.284592000	5.219445000	2.624880000
1	-1.575481000	5.954383000	3.010462000
1	-3.158017000	5.750936000	2.221692000
1	-2.604283000	4.564810000	3.447133000
6	-2.100274000	2.018248000	-2.729242000
6	-3.381320000	2.792369000	-2.480854000
1	-2.087834000	1.731276000	-3.794606000
1	-1.230701000	2.682086000	-2.597372000
6	-3.556160000	3.901577000	-3.510851000
1	-4.252096000	2.118937000	-2.523660000
1	-3.381614000	3.237644000	-1.477416000
6	-4.810354000	4.723349000	-3.267727000
1	-2.670501000	4.554927000	-3.495779000
1	-3.586850000	3.460770000	-4.518855000
1	-4.937563000	5.509212000	-4.019761000
1	-5.706350000	4.090328000	-3.292857000
1	-4.779453000	5.206187000	-2.282884000
Zero-point correction=			0.787255 (Hartree/Particle)
Thermal correction to Energy=			0.845126
Thermal correction to Enthalpy=			0.846070
Thermal correction to Gibbs Free Energy=			0.693563
Sum of electronic and zero-point Energies=			-4116.019140
Sum of electronic and thermal Energies=			-4115.961269
Sum of electronic and thermal Enthalpies=			-4115.960325
Sum of electronic and thermal Free Energies=			-4116.112832

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6	-0.576423000	-0.110668000	-4.507354000
6	0.219766000	0.699949000	-3.712440000
6	-0.334483000	1.275815000	-2.568174000
6	-1.681003000	1.009079000	-2.228878000
6	-2.467947000	0.164714000	-3.021801000

6	-1.909768000	-0.379469000	-4.164037000
1	-0.159611000	-0.552340000	-5.410339000
1	1.262780000	0.886942000	-3.966724000
1	-3.491443000	-0.063965000	-2.736236000
1	-2.507078000	-1.029436000	-4.798380000
6	0.299589000	2.154453000	-1.558158000
6	-0.772954000	2.456770000	-0.594712000
6	-1.928580000	1.618807000	-0.944590000
1	0.768048000	3.057127000	-1.971617000
6	-2.828404000	1.313894000	0.076371000
6	-2.215701000	1.558290000	1.335424000
6	-2.876662000	1.867096000	2.543771000
6	-0.779208000	1.611067000	1.265553000
6	-2.144569000	2.348626000	3.602056000
1	-3.960461000	1.788749000	2.595097000
6	-0.064441000	2.165927000	2.366185000
1	-0.296136000	0.765638000	0.772420000
6	-0.739766000	2.531019000	3.502063000
1	-2.650220000	2.633130000	4.521993000
1	1.022905000	2.208955000	2.318394000
1	-0.194758000	2.913989000	4.361883000
6	-4.172560000	0.764595000	-0.069501000
6	-5.052652000	1.268847000	-1.026432000
6	-4.570149000	-0.281951000	0.772969000
6	-6.324357000	0.716102000	-1.153061000
1	-4.765513000	2.087487000	-1.683991000
6	-5.828206000	-0.855987000	0.629392000
1	-3.846539000	-0.698871000	1.469126000
6	-6.723837000	-0.338785000	-0.326400000
79	2.042373000	1.193610000	-0.756228000
15	4.066400000	0.107277000	-0.182198000
6	4.900122000	0.628121000	1.357073000
6	5.311157000	0.404119000	-1.485880000
6	3.895443000	-1.696818000	-0.094926000
6	6.240179000	1.023155000	1.368830000
6	4.167013000	0.618969000	2.550359000
6	6.208240000	-0.585080000	-1.895574000
6	5.392997000	1.682687000	-2.046566000
6	4.679151000	-2.468042000	0.765496000
6	2.989810000	-2.316880000	-0.961413000
6	6.841194000	1.412299000	2.562440000
1	6.818629000	1.026198000	0.446894000
6	4.777863000	1.002754000	3.737933000
1	3.129430000	0.287799000	2.543454000

6	7.175098000	-0.295619000	-2.853501000
1	6.147333000	-1.583628000	-1.465311000
6	6.365493000	1.970923000	-2.996271000
1	4.687392000	2.452473000	-1.731983000
6	4.561013000	-3.853336000	0.751868000
1	5.378540000	-1.985773000	1.447177000
6	2.891970000	-3.701864000	-0.982925000
1	2.341235000	-1.713696000	-1.600399000
6	6.111704000	1.403583000	3.745583000
1	7.884211000	1.720127000	2.564900000
1	4.207678000	0.986653000	4.663894000
6	7.255958000	0.980318000	-3.402086000
1	7.867342000	-1.071303000	-3.172339000
1	6.424432000	2.967980000	-3.426312000
6	3.672729000	-4.468248000	-0.123432000
1	5.162354000	-4.453380000	1.430679000
1	2.180729000	-4.180878000	-1.648659000
1	6.583327000	1.707322000	4.677517000
1	8.012075000	1.202597000	-4.151436000
1	3.577128000	-5.551225000	-0.127176000
8	-2.595391000	-1.787577000	-0.898745000
16	-1.652147000	-2.498685000	-0.051523000
9	-0.038493000	-4.509121000	-0.576446000
9	-1.776360000	-4.367560000	-1.842439000
9	-0.129450000	-2.998620000	-2.119250000
6	-0.835730000	-3.673631000	-1.218113000
8	1.013062000	-3.161588000	1.704112000
8	1.401362000	-0.672183000	1.731809000
16	0.482021000	-1.810273000	1.634990000
9	-1.624126000	-0.844051000	2.951642000
9	-0.995833000	-2.802596000	3.602343000
9	0.166239000	-1.070815000	4.127060000
6	-0.573320000	-1.632091000	3.178457000
7	-0.480613000	-1.474481000	0.383656000
8	-2.160045000	-3.325805000	1.041517000
8	-7.969202000	-0.877093000	-0.455164000
6	-8.006956000	-1.988698000	-1.335713000
1	-9.042461000	-2.336435000	-1.365302000
1	-7.692381000	-1.697918000	-2.347649000
1	-7.363769000	-2.800455000	-0.972381000
8	-7.153693000	1.188446000	-2.127877000
8	-6.269566000	-1.912786000	1.339380000
6	-5.335231000	-2.553460000	2.189243000
1	-5.851244000	-3.417447000	2.611711000

1	-4.445358000	-2.886161000	1.637488000
1	-5.019861000	-1.890717000	3.007956000
6	-8.300715000	1.870558000	-1.650583000
1	-8.934613000	1.215487000	-1.041274000
1	-8.010934000	2.750532000	-1.057550000
1	-8.858209000	2.202616000	-2.530014000
6	-0.888267000	3.938228000	-0.267853000
6	-2.040540000	4.491108000	0.550201000
1	-0.926437000	4.424651000	-1.257825000
1	0.072378000	4.254446000	0.170012000
6	-2.061933000	6.014386000	0.502983000
1	-2.999425000	4.103854000	0.170461000
1	-1.970751000	4.175124000	1.598008000
6	-3.192875000	6.599202000	1.331489000
1	-1.095660000	6.402661000	0.860060000
1	-2.151984000	6.347268000	-0.542128000
1	-3.206165000	7.693403000	1.292167000
1	-4.166649000	6.241141000	0.974504000
1	-3.102959000	6.304177000	2.384507000
Zero-point correction=			0.853488 (Hartree/Particle)
Thermal correction to Energy=			0.916422
Thermal correction to Enthalpy=			0.917366
Thermal correction to Gibbs Free Energy=			0.754257
Sum of electronic and zero-point Energies=			-4344.870585
Sum of electronic and thermal Energies=			-4344.807651
Sum of electronic and thermal Enthalpies=			-4344.806707
Sum of electronic and thermal Free Energies=			-4344.969816

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6	-0.001828000	-4.922980000	-1.305706000
6	0.344389000	-3.694839000	-1.848400000
6	-0.577084000	-2.647177000	-1.792871000
6	-1.844972000	-2.858058000	-1.210209000
6	-2.166200000	-4.084711000	-0.616945000
6	-1.242047000	-5.113539000	-0.679106000
1	0.705936000	-5.748243000	-1.350014000
1	1.328714000	-3.535394000	-2.289313000
1	-3.125975000	-4.228630000	-0.125009000
1	-1.477503000	-6.078677000	-0.237206000
6	-0.431018000	-1.238805000	-2.230843000
6	-1.753007000	-0.634551000	-2.018317000
6	-2.545474000	-1.593580000	-1.238488000
1	-0.050675000	-1.099788000	-3.250598000
6	-3.580357000	-1.119057000	-0.453003000

6	-3.467467000	0.286127000	-0.253333000
6	-4.535610000	1.142007000	0.050395000
6	-2.162386000	0.806257000	-0.535687000
6	-4.340334000	2.508090000	-0.044473000
1	-5.516099000	0.716522000	0.241809000
6	-2.003551000	2.219932000	-0.677705000
1	-1.309077000	0.339308000	-0.040832000
6	-3.080318000	3.061852000	-0.437904000
6	-4.649712000	-1.938104000	0.123851000
6	-5.368237000	-2.822472000	-0.690419000
6	-4.977510000	-1.839704000	1.481643000
6	-6.396842000	-3.590915000	-0.160854000
1	-5.108754000	-2.895175000	-1.746424000
6	-6.002986000	-2.614145000	2.008918000
1	-4.384410000	-1.188675000	2.120052000
6	-6.716256000	-3.486359000	1.190624000
1	-6.952172000	-4.270783000	-0.802757000
1	-6.238857000	-2.546221000	3.068289000
79	1.268407000	-0.460866000	-1.146287000
15	3.480303000	0.163374000	-0.543569000
6	3.903162000	1.788559000	-1.257988000
6	4.667407000	-0.974516000	-1.357773000
6	4.029821000	0.180290000	1.189831000
6	5.228172000	2.220581000	-1.373661000
6	2.871305000	2.602691000	-1.727081000
6	5.929522000	-1.247257000	-0.821858000
6	4.304772000	-1.551314000	-2.578739000
6	4.566604000	1.313315000	1.802058000
6	3.902396000	-1.007544000	1.916139000
6	5.511984000	3.459998000	-1.934113000
1	6.040986000	1.582157000	-1.029271000
6	3.158006000	3.841987000	-2.291642000
1	1.842183000	2.250376000	-1.648299000
6	6.813088000	-2.079882000	-1.501235000
1	6.216707000	-0.817286000	0.136794000
6	5.190257000	-2.380963000	-3.256818000
1	3.315709000	-1.348841000	-2.992768000
6	4.992290000	1.248890000	3.123825000
1	4.635311000	2.249889000	1.252629000
6	4.338698000	-1.067536000	3.233022000
1	3.444620000	-1.883876000	1.454980000
6	4.476470000	4.271983000	-2.391398000
1	6.544116000	3.791652000	-2.019367000
1	2.346965000	4.469928000	-2.655109000

6	6.445390000	-2.646580000	-2.717443000
1	7.791359000	-2.289657000	-1.074747000
1	4.896463000	-2.826640000	-4.204352000
6	4.886729000	0.059737000	3.836067000
1	5.399948000	2.136930000	3.600892000
1	4.230438000	-1.991417000	3.795448000
1	4.700973000	5.240163000	-2.833287000
1	7.136296000	-3.301418000	-3.243442000
1	5.215286000	0.015553000	4.871612000
8	-1.837875000	-1.660130000	1.764861000
16	-0.720411000	-1.149258000	2.550661000
9	0.877491000	-2.797436000	1.277255000
9	1.558077000	-2.241201000	3.248719000
9	-0.087609000	-3.619748000	3.024363000
6	0.491305000	-2.539221000	2.523326000
8	1.606660000	0.923417000	3.535564000
8	1.384747000	2.006708000	1.274318000
16	0.801441000	1.228476000	2.365809000
9	-1.654707000	2.229083000	2.252080000
9	-0.876681000	2.036335000	4.253347000
9	-0.152762000	3.600016000	2.962232000
6	-0.561891000	2.332384000	3.012558000
7	0.026819000	-0.011020000	1.681382000
8	-0.926040000	-0.829985000	3.955273000
1	-7.518666000	-4.090427000	1.608025000
8	-2.946637000	4.410025000	-0.554776000
6	-3.034199000	5.160566000	0.650858000
1	-2.536893000	6.116182000	0.460799000
1	-4.076216000	5.340038000	0.933647000
1	-2.517407000	4.645808000	1.473198000
8	-0.755127000	2.611680000	-0.972750000
8	-5.307551000	3.423754000	0.145034000
6	-6.592053000	2.961130000	0.503894000
1	-7.210450000	3.848956000	0.644245000
1	-7.025380000	2.339014000	-0.290795000
1	-6.563919000	2.383636000	1.437205000
6	-0.246524000	3.853794000	-0.489667000
1	0.839991000	3.749854000	-0.492173000
1	-0.567712000	4.688350000	-1.119842000
1	-0.551817000	4.024243000	0.547933000
6	-2.286029000	0.125976000	-3.220556000
6	-3.732204000	0.583215000	-3.275241000
1	-2.122688000	-0.557834000	-4.071567000
1	-1.608617000	0.975683000	-3.401075000

6	-4.103415000	1.099652000	-4.659035000
1	-4.401394000	-0.249415000	-3.003613000
1	-3.923571000	1.378436000	-2.544391000
6	-5.541416000	1.586115000	-4.718954000
1	-3.419591000	1.916088000	-4.936607000
1	-3.943440000	0.306127000	-5.404777000
1	-5.806399000	1.964567000	-5.711813000
1	-6.240211000	0.776229000	-4.473585000
1	-5.711748000	2.395074000	-3.996963000
Zero-point correction=			0.854707 (Hartree/Particle)
Thermal correction to Energy=			0.916805
Thermal correction to Enthalpy=			0.917749
Thermal correction to Gibbs Free Energy=			0.758216
Sum of electronic and zero-point Energies=			-4344.878438
Sum of electronic and thermal Energies=			-4344.816340
Sum of electronic and thermal Enthalpies=			-4344.815396
Sum of electronic and thermal Free Energies=			-4344.974930

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6	4.556566000	-2.183245000	-0.040179000
6	4.979286000	-0.861395000	-0.158420000
6	4.042674000	0.158987000	-0.248559000
6	2.669742000	-0.100095000	-0.205666000
6	2.246999000	-1.446927000	-0.113754000
6	3.202291000	-2.471301000	-0.024792000
1	5.284030000	-2.987981000	0.030312000
1	6.040593000	-0.625925000	-0.179248000
1	4.371683000	1.193086000	-0.338689000
1	2.854546000	-3.499156000	0.045959000
6	1.722831000	1.020850000	-0.326405000
6	0.742047000	1.361746000	0.529765000
6	0.865332000	-1.779865000	-0.150779000
6	-0.320585000	-2.037797000	-0.176547000
6	-1.726629000	-2.251244000	-0.190229000
6	-2.269186000	-3.530744000	-0.007002000
6	-2.591125000	-1.160554000	-0.377032000
6	-3.644375000	-3.712875000	-0.008919000
1	-1.596902000	-4.372920000	0.137188000
6	-3.964954000	-1.352418000	-0.377619000
1	-2.162301000	-0.170083000	-0.525477000
6	-4.495309000	-2.626654000	-0.193389000
1	-4.056909000	-4.708816000	0.133819000
1	-4.627272000	-0.502666000	-0.524866000
1	1.859306000	1.634658000	-1.218873000

6	-0.140474000	2.514057000	0.235217000
6	0.302573000	3.619171000	-0.503588000
6	-1.461481000	2.529488000	0.702877000
6	-0.545107000	4.680434000	-0.786584000
1	1.337856000	3.656641000	-0.836156000
6	-2.313400000	3.589089000	0.415413000
1	-1.833575000	1.691620000	1.289716000
6	-1.860727000	4.669569000	-0.332481000
1	-0.172278000	5.529121000	-1.355583000
1	-3.337309000	3.569824000	0.781920000
1	-2.523807000	5.502781000	-0.551964000
6	0.485642000	0.630255000	1.813205000
1	-0.405451000	-0.009190000	1.747020000
1	1.323803000	-0.019182000	2.080185000
1	0.320869000	1.340147000	2.632596000
1	-5.572668000	-2.773154000	-0.195036000
Zero-point correction=			0.333756 (Hartree/Particle)
Thermal correction to Energy=			0.352752
Thermal correction to Enthalpy=			0.353696
Thermal correction to Gibbs Free Energy=			0.284549
Sum of electronic and zero-point Energies=			-886.223041
Sum of electronic and thermal Energies=			-886.204044
Sum of electronic and thermal Enthalpies=			-886.203100
Sum of electronic and thermal Free Energies=			-886.272247

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6	1.081263000	4.865051000	-0.117880000
6	2.418156000	5.228913000	0.011435000
6	3.397203000	4.257152000	0.197372000
6	3.067397000	2.904246000	0.252534000
6	1.706149000	2.543735000	0.108528000
6	0.726405000	3.524715000	-0.068147000
1	0.317226000	5.624870000	-0.257581000
1	2.702172000	6.277410000	-0.028674000
1	4.441176000	4.544574000	0.302275000
1	-0.316762000	3.226868000	-0.174430000
6	4.087142000	1.861516000	0.487197000
6	4.747651000	1.186426000	-0.472831000
6	1.395971000	1.133012000	0.128969000
6	1.890828000	-0.018187000	0.104460000
6	2.406276000	-1.334786000	0.038882000
6	2.214646000	-2.114417000	-1.117168000
6	3.173897000	-1.835250000	1.106045000
6	2.770700000	-3.381312000	-1.191069000

1	1.624467000	-1.710066000	-1.937987000
6	3.743742000	-3.094660000	1.009248000
1	3.330798000	-1.215524000	1.985712000
6	3.537507000	-3.867254000	-0.131876000
1	2.618381000	-3.989687000	-2.078422000
1	4.354222000	-3.475053000	1.823458000
1	4.246566000	1.585303000	1.532392000
6	5.681232000	0.095662000	-0.119589000
6	6.352310000	0.073772000	1.111696000
6	5.894509000	-0.969444000	-1.003817000
6	7.181034000	-0.984779000	1.456034000
1	6.248111000	0.914461000	1.794813000
6	6.723538000	-2.030974000	-0.659373000
1	5.386980000	-0.983977000	-1.966247000
6	7.368398000	-2.045367000	0.572510000
1	7.701312000	-0.972600000	2.410881000
1	6.867522000	-2.849390000	-1.361341000
1	8.026065000	-2.869423000	0.838090000
79	-0.604883000	0.279423000	0.123682000
15	-2.883377000	-0.285438000	0.030827000
6	-3.581824000	-0.729326000	1.643727000
6	-3.191283000	-1.682007000	-1.084221000
6	-3.841351000	1.124941000	-0.589973000
6	-4.515385000	-1.760423000	1.774706000
6	-3.212324000	0.028271000	2.759954000
6	-4.313120000	-1.718108000	-1.915740000
6	-2.305951000	-2.764505000	-1.053718000
6	-5.107830000	1.426705000	-0.083122000
6	-3.299450000	1.896918000	-1.623760000
6	-5.074918000	-2.028117000	3.019922000
1	-4.803643000	-2.353199000	0.908033000
6	-3.779432000	-0.240839000	3.998547000
1	-2.481968000	0.831391000	2.654557000
6	-4.544870000	-2.835592000	-2.711540000
1	-5.002832000	-0.875863000	-1.942441000
6	-2.546945000	-3.879354000	-1.845966000
1	-1.430418000	-2.733560000	-0.403352000
6	-5.823457000	2.497176000	-0.609880000
1	-5.532233000	0.830531000	0.723129000
6	-4.021485000	2.961207000	-2.148189000
1	-2.311311000	1.657788000	-2.020324000
6	-4.709156000	-1.270200000	4.127657000
1	-5.799349000	-2.831595000	3.124087000
1	-3.492925000	0.348587000	4.865545000

6	-3.665015000	-3.912815000	-2.676015000
1	-5.415813000	-2.863362000	-3.361064000
1	-1.861076000	-4.722104000	-1.819678000
6	-5.281965000	3.262748000	-1.637760000
1	-6.807041000	2.734688000	-0.213121000
1	-3.599680000	3.558850000	-2.951988000
1	-5.148414000	-1.483345000	5.098846000
1	-3.850550000	-4.783266000	-3.300014000
1	-5.843849000	4.100422000	-2.042810000
6	4.508614000	1.456678000	-1.928649000
1	3.932388000	0.642919000	-2.391808000
1	3.947747000	2.383045000	-2.080074000
1	5.453726000	1.527592000	-2.478869000
1	3.982582000	-4.856882000	-0.199711000
Zero-point correction=			0.609712 (Hartree/Particle)
Thermal correction to Energy=			0.648392
Thermal correction to Enthalpy=			0.649336
Thermal correction to Gibbs Free Energy=			0.533208
Sum of electronic and zero-point Energies=			-2056.956681
Sum of electronic and thermal Energies=			-2056.918002
Sum of electronic and thermal Enthalpies=			-2056.917058
Sum of electronic and thermal Free Energies=			-2057.033185

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6	1.426833000	5.025494000	-0.040172000
6	2.798793000	5.213470000	0.111615000
6	3.649406000	4.122131000	0.280470000
6	3.120885000	2.836279000	0.298945000
6	1.734388000	2.648450000	0.137830000
6	0.889194000	3.743915000	-0.026002000
1	0.774261000	5.884935000	-0.168606000
1	3.211576000	6.218926000	0.100838000
1	4.720234000	4.273125000	0.400860000
1	-0.181723000	3.585035000	-0.146158000
6	3.912739000	1.604953000	0.489636000
6	4.644397000	0.996059000	-0.505823000
6	1.331634000	1.253572000	0.155111000
6	2.204676000	0.291429000	0.224937000
6	2.517910000	-1.100041000	0.128751000
6	2.135108000	-1.804539000	-1.028327000
6	3.200939000	-1.775614000	1.152532000
6	2.411915000	-3.159405000	-1.141011000
1	1.602665000	-1.273742000	-1.816378000
6	3.497390000	-3.123852000	1.019374000

1	3.489514000	-1.230972000	2.048716000
6	3.099685000	-3.816646000	-0.122473000
1	2.100117000	-3.703362000	-2.029284000
1	4.033712000	-3.639389000	1.811841000
1	4.088471000	1.295361000	1.523748000
6	5.546510000	-0.110292000	-0.188598000
6	6.193923000	-0.180421000	1.057072000
6	5.774050000	-1.138461000	-1.117346000
6	7.019894000	-1.249076000	1.369887000
1	6.078286000	0.631968000	1.771360000
6	6.586970000	-2.215734000	-0.796292000
1	5.281800000	-1.114496000	-2.086766000
6	7.211665000	-2.274461000	0.446801000
1	7.527134000	-1.277456000	2.330688000
1	6.738699000	-3.011109000	-1.521375000
1	7.858612000	-3.113069000	0.691770000
79	-0.642094000	0.540984000	0.140401000
15	-2.863464000	-0.251535000	0.029843000
6	-3.504709000	-0.822715000	1.629630000
6	-2.972067000	-1.670668000	-1.102119000
6	-4.031495000	0.997306000	-0.580946000
6	-4.352912000	-1.928772000	1.728996000
6	-3.166076000	-0.096500000	2.775625000
6	-4.013645000	-1.811003000	-2.021003000
6	-1.977932000	-2.652430000	-1.018886000
6	-5.365070000	1.013384000	-0.162566000
6	-3.585287000	1.928898000	-1.523929000
6	-4.858629000	-2.301215000	2.970017000
1	-4.615710000	-2.498328000	0.838551000
6	-3.677285000	-0.471397000	4.011790000
1	-2.499190000	0.762439000	2.695480000
6	-4.058845000	-2.928708000	-2.849351000
1	-4.785882000	-1.046855000	-2.094203000
6	-2.032795000	-3.768832000	-1.842634000
1	-1.161436000	-2.539077000	-0.303535000
6	-6.243987000	1.952887000	-0.690191000
1	-5.714387000	0.294679000	0.577685000
6	-4.469012000	2.863061000	-2.050153000
1	-2.542623000	1.918828000	-1.844196000
6	-4.521636000	-1.574239000	4.107982000
1	-5.516457000	-3.162979000	3.047962000
1	-3.412496000	0.093734000	4.901685000
6	-3.072448000	-3.905252000	-2.760102000
1	-4.867782000	-3.035306000	-3.567492000

1	-1.261394000	-4.531976000	-1.771431000
6	-5.796929000	2.874932000	-1.632203000
1	-7.280208000	1.966838000	-0.362473000
1	-4.120161000	3.586476000	-2.782608000
1	-4.916257000	-1.871526000	5.076319000
1	-3.111490000	-4.776107000	-3.409616000
1	-6.486595000	3.609843000	-2.039730000
1	3.326275000	-4.875642000	-0.218445000
6	4.467283000	1.382722000	-1.936719000
1	5.438063000	1.518722000	-2.426089000
1	3.947952000	0.585256000	-2.486815000
1	3.881213000	2.298460000	-2.042573000
Zero-point correction=			0.609002 (Hartree/Particle)
Thermal correction to Energy=			0.646848
Thermal correction to Enthalpy=			0.647792
Thermal correction to Gibbs Free Energy=			0.533372
Sum of electronic and zero-point Energies=			-2056.950514
Sum of electronic and thermal Energies=			-2056.912668
Sum of electronic and thermal Enthalpies=			-2056.911724
Sum of electronic and thermal Free Energies=			-2057.026145

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6	-2.228958000	5.114311000	-0.354612000
6	-1.475796000	3.955780000	-0.287414000
6	-2.136553000	2.721176000	-0.391721000
6	-3.545207000	2.660866000	-0.557976000
6	-4.296318000	3.821955000	-0.585108000
6	-3.621172000	5.042151000	-0.501811000
1	-1.748601000	6.086481000	-0.290763000
1	-0.394625000	3.983758000	-0.163856000
1	-5.378154000	3.795791000	-0.687139000
1	-4.192793000	5.965925000	-0.554100000
6	-1.595739000	1.409799000	-0.281021000
6	-2.678025000	0.458843000	-0.430927000
6	-3.962660000	1.241550000	-0.575140000
1	-4.746619000	0.922646000	-1.257813000
6	-3.824080000	0.517761000	0.742591000
6	-2.357230000	-0.874938000	-1.014720000
6	-2.577490000	-1.126140000	-2.367060000
6	-1.757724000	-1.859473000	-0.222538000
6	-2.219369000	-2.354047000	-2.920241000
1	-3.036984000	-0.358245000	-2.988583000
6	-1.384484000	-3.076458000	-0.776483000
1	-1.598682000	-1.663054000	0.839068000

6	-1.623329000	-3.327988000	-2.126685000
1	-2.406735000	-2.546580000	-3.973855000
1	-0.914384000	-3.835071000	-0.155213000
6	-4.525643000	-0.785091000	0.911343000
6	-4.423919000	-1.479958000	2.126364000
6	-5.246220000	-1.393434000	-0.127862000
6	-5.000714000	-2.732274000	2.289042000
1	-3.880124000	-1.048398000	2.961774000
6	-5.824200000	-2.643365000	0.034169000
1	-5.359518000	-0.900741000	-1.089705000
6	-5.699659000	-3.322444000	1.242361000
1	-4.903397000	-3.247336000	3.241271000
1	-6.377364000	-3.088729000	-0.788463000
1	-6.151103000	-4.303123000	1.368378000
79	0.344561000	0.781416000	-0.065365000
15	2.540848000	-0.132995000	0.094079000
6	3.849470000	0.991413000	-0.473906000
6	2.686657000	-1.672859000	-0.858261000
6	2.973611000	-0.574202000	1.806679000
6	4.927696000	0.557509000	-1.247396000
6	3.780986000	2.327286000	-0.061918000
6	3.672865000	-2.617263000	-0.548521000
6	1.819581000	-1.899858000	-1.930628000
6	4.191887000	-0.216071000	2.386260000
6	2.041879000	-1.312414000	2.545244000
6	5.931227000	1.454541000	-1.600569000
1	4.982459000	-0.478518000	-1.576822000
6	4.790572000	3.215219000	-0.408329000
1	2.937540000	2.665203000	0.542005000
6	3.796928000	-3.767767000	-1.316987000
1	4.341435000	-2.450409000	0.295578000
6	1.952530000	-3.050962000	-2.700102000
1	1.033440000	-1.178336000	-2.160183000
6	4.471541000	-0.590407000	3.697850000
1	4.922470000	0.356606000	1.817145000
6	2.329213000	-1.688832000	3.850271000
1	1.090988000	-1.596023000	2.090325000
6	5.865512000	2.778486000	-1.179359000
1	6.767927000	1.116244000	-2.206314000
1	4.738659000	4.250570000	-0.081376000
6	2.940035000	-3.981759000	-2.394436000
1	4.563236000	-4.499924000	-1.075794000
1	1.283091000	-3.219148000	-3.539950000
6	3.543014000	-1.323086000	4.428591000

1	5.419629000	-0.307402000	4.147960000
1	1.604745000	-2.264000000	4.421302000
1	6.652840000	3.475225000	-1.455501000
1	3.041006000	-4.882207000	-2.995207000
1	3.764092000	-1.611159000	5.453193000
1	-1.343965000	-4.286571000	-2.557563000
6	-3.514108000	1.252738000	2.025242000
1	-4.428165000	1.344969000	2.621813000
1	-2.775390000	0.706334000	2.621727000
1	-3.119620000	2.256501000	1.863595000
Zero-point correction=			0.611047 (Hartree/Particle)
Thermal correction to Energy=			0.648426
Thermal correction to Enthalpy=			0.649370
Thermal correction to Gibbs Free Energy=			0.537358
Sum of electronic and zero-point Energies=			-2056.970945
Sum of electronic and thermal Energies=			-2056.933566
Sum of electronic and thermal Enthalpies=			-2056.932621
Sum of electronic and thermal Free Energies=			-2057.044633

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6	-1.222751000	-2.090770000	-4.188965000
6	-0.279001000	-1.438365000	-3.415831000
6	-0.722609000	-0.487077000	-2.485542000
6	-2.102079000	-0.208319000	-2.338935000
6	-3.041006000	-0.837653000	-3.134049000
6	-2.585177000	-1.795171000	-4.040266000
1	-0.915909000	-2.849759000	-4.903535000
1	0.783163000	-1.663525000	-3.499164000
1	-4.102050000	-0.636860000	-3.018790000
1	-3.310196000	-2.342956000	-4.637999000
6	0.027195000	0.275440000	-1.544808000
6	-0.871879000	1.108056000	-0.790542000
6	-2.278834000	0.807094000	-1.280982000
1	-3.042486000	0.629479000	-0.524820000
6	-1.852445000	2.184304000	-1.614280000
6	-0.497766000	1.498692000	0.598348000
6	-1.176750000	0.971688000	1.696104000
6	0.587748000	2.356042000	0.810391000
6	-0.760935000	1.289843000	2.987192000
1	-2.031268000	0.315421000	1.539789000
6	1.007399000	2.662836000	2.099091000
1	1.092767000	2.792971000	-0.053824000
6	0.331759000	2.125732000	3.192644000
1	-1.299675000	0.872858000	3.835449000

1	1.854207000	3.329414000	2.252060000
6	-2.341638000	3.288294000	-0.741837000
6	-1.677287000	4.523036000	-0.728530000
6	-3.458340000	3.124020000	0.086512000
6	-2.111501000	5.555437000	0.090352000
1	-0.794518000	4.672804000	-1.347564000
6	-3.895939000	4.160414000	0.901400000
1	-4.019916000	2.193864000	0.103900000
6	-3.224961000	5.377882000	0.907966000
1	-1.576898000	6.502597000	0.092782000
1	-4.768370000	3.997655000	1.529693000
1	-3.566115000	6.188325000	1.547968000
79	1.969162000	0.001352000	-0.948911000
15	4.095433000	-0.315570000	0.078613000
6	4.935077000	-1.874630000	-0.338837000
6	3.922668000	-0.260203000	1.889219000
6	5.293262000	1.001482000	-0.317285000
6	5.680719000	-2.602145000	0.591215000
6	4.848993000	-2.321208000	-1.661322000
6	4.996720000	0.092390000	2.714825000
6	2.685763000	-0.577998000	2.457366000
6	6.624711000	0.741860000	-0.645067000
6	4.836618000	2.322853000	-0.262944000
6	6.337787000	-3.763016000	0.196619000
1	5.740281000	-2.266163000	1.625118000
6	5.513352000	-3.476677000	-2.052569000
1	4.254207000	-1.758315000	-2.381676000
6	4.835090000	0.108050000	4.094578000
1	5.956808000	0.361837000	2.274681000
6	2.530825000	-0.564398000	3.839674000
1	1.834910000	-0.823285000	1.820064000
6	7.490813000	1.798051000	-0.915356000
1	6.984952000	-0.284907000	-0.689422000
6	5.705697000	3.372674000	-0.526888000
1	3.794781000	2.522837000	-0.008317000
6	6.256736000	-4.198364000	-1.122381000
1	6.911995000	-4.331349000	0.924142000
1	5.443225000	-3.820601000	-3.081443000
6	3.603448000	-0.222874000	4.655838000
1	5.670351000	0.383975000	4.733749000
1	1.563955000	-0.808083000	4.272933000
6	7.033509000	3.109831000	-0.856186000
1	8.527044000	1.592443000	-1.172865000
1	5.346528000	4.397885000	-0.482526000

1	6.769562000	-5.107935000	-1.425619000
1	3.479194000	-0.206020000	5.736020000
1	7.712527000	3.931701000	-1.070048000
8	-5.652880000	0.928806000	1.430489000
16	-5.566742000	-0.449772000	0.962654000
9	-6.071947000	-1.485945000	-1.411095000
9	-7.482634000	0.004468000	-0.745114000
9	-5.528960000	0.600819000	-1.442983000
6	-6.205367000	-0.338600000	-0.767153000
8	-4.241745000	-3.234995000	-0.077132000
8	-2.025117000	-2.037702000	-0.012977000
16	-3.369969000	-2.238326000	0.523543000
9	-4.199115000	-2.914770000	2.919986000
9	-2.483544000	-4.011867000	2.198838000
9	-2.256957000	-1.976712000	2.878958000
6	-3.067844000	-2.821949000	2.247746000
7	-4.002259000	-0.770115000	0.741915000
8	-6.357772000	-1.492925000	1.590743000
6	-1.450525000	2.599923000	-3.005330000
1	-2.319605000	3.047207000	-3.502753000
1	-0.660589000	3.357124000	-2.984295000
1	-1.102223000	1.766198000	-3.618383000
1	0.658283000	2.361816000	4.203430000
Zero-point correction=			0.670131 (Hartree/Particle)
Thermal correction to Energy=			0.722643
Thermal correction to Enthalpy=			0.723587
Thermal correction to Gibbs Free Energy=			0.579048
Sum of electronic and zero-point Energies=			-3883.817153
Sum of electronic and thermal Energies=			-3883.764641
Sum of electronic and thermal Enthalpies=			-3883.763697
Sum of electronic and thermal Free Energies=			-3883.908236

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6	1.110451000	-3.851363000	-1.229582000
6	0.082217000	-2.988488000	-0.867525000
6	0.341652000	-1.619221000	-0.825872000
6	1.618672000	-1.132348000	-1.163226000
6	2.647245000	-1.991459000	-1.514839000
6	2.378190000	-3.359307000	-1.548488000
1	0.929912000	-4.923545000	-1.260929000
1	-0.906588000	-3.365123000	-0.608243000
1	3.632836000	-1.603265000	-1.759062000
1	3.172603000	-4.050099000	-1.820320000
6	-0.534197000	-0.514931000	-0.461995000

6	0.168649000	0.653150000	-0.541433000
6	1.627890000	0.358705000	-1.005700000
1	1.876443000	0.898611000	-1.926698000
6	2.351149000	0.872844000	0.169070000
6	-0.340680000	2.000400000	-0.250657000
6	-0.208764000	3.053153000	-1.163683000
6	-0.973066000	2.256287000	0.974602000
6	-0.699123000	4.319603000	-0.864687000
1	0.269622000	2.871091000	-2.124992000
6	-1.464708000	3.521336000	1.274024000
1	-1.060528000	1.444324000	1.696010000
6	-1.324201000	4.559120000	0.356307000
1	-0.588239000	5.123988000	-1.588525000
1	-1.953785000	3.698865000	2.229729000
6	2.699144000	2.275951000	0.238462000
6	2.640534000	2.963334000	1.465000000
6	3.062615000	2.992303000	-0.918941000
6	2.920125000	4.318348000	1.529059000
1	2.322886000	2.442528000	2.363883000
6	3.378099000	4.336939000	-0.842560000
1	3.181911000	2.465552000	-1.860394000
6	3.298339000	5.004312000	0.378071000
1	2.848385000	4.840275000	2.479308000
1	3.696149000	4.867958000	-1.735632000
1	3.538057000	6.063566000	0.433258000
79	-2.568854000	-0.550059000	-0.158242000
15	-4.934024000	-0.384566000	0.077476000
6	-5.830405000	-0.754623000	-1.465579000
6	-5.441559000	1.299930000	0.557751000
6	-5.664423000	-1.483406000	1.335116000
6	-6.982773000	-0.067616000	-1.854785000
6	-5.339784000	-1.792085000	-2.264760000
6	-6.594198000	1.540911000	1.312373000
6	-4.652799000	2.376352000	0.139410000
6	-6.918775000	-2.078896000	1.181338000
6	-4.931389000	-1.705872000	2.505104000
6	-7.639068000	-0.421869000	-3.029279000
1	-7.363821000	0.748212000	-1.242293000
6	-6.001361000	-2.146068000	-3.434109000
1	-4.431079000	-2.316663000	-1.968167000
6	-6.956686000	2.843985000	1.634467000
1	-7.205768000	0.706358000	1.653628000
6	-5.020678000	3.677830000	0.463027000
1	-3.739210000	2.198174000	-0.431002000

6	-7.434627000	-2.882623000	2.193107000
1	-7.490325000	-1.917536000	0.268204000
6	-5.452767000	-2.504725000	3.515143000
1	-3.944995000	-1.254477000	2.616244000
6	-7.150294000	-1.459647000	-3.816945000
1	-8.532860000	0.118593000	-3.331648000
1	-5.613926000	-2.951689000	-4.052676000
6	-6.171142000	3.911981000	1.209576000
1	-7.852327000	3.025839000	2.223640000
1	-4.394682000	4.506150000	0.138759000
6	-6.704196000	-3.094136000	3.358391000
1	-8.409558000	-3.347816000	2.068179000
1	-4.877400000	-2.676518000	4.421384000
1	-7.663684000	-1.730666000	-4.736410000
1	-6.453822000	4.929908000	1.467679000
1	-7.108517000	-3.726905000	4.144780000
8	6.243359000	-1.719214000	2.678373000
16	6.490636000	-1.753071000	1.247599000
9	5.568662000	-3.310531000	-0.655325000
9	6.152545000	-4.335426000	1.153461000
9	4.317697000	-3.198553000	1.102013000
6	5.574299000	-3.246491000	0.671832000
8	6.772666000	-0.600699000	-1.768813000
8	4.571666000	0.536422000	-1.369536000
16	5.873661000	0.080242000	-0.856006000
9	7.895479000	1.398050000	0.134615000
9	6.883199000	2.384017000	-1.500670000
9	5.980349000	2.342213000	0.457622000
6	6.718475000	1.652548000	-0.405073000
7	5.595947000	-0.583068000	0.569854000
8	7.836791000	-1.891375000	0.724120000
6	2.624612000	-0.012897000	1.293488000
1	3.680213000	-0.342744000	1.120262000
1	2.636279000	0.483472000	2.266179000
1	2.010011000	-0.916835000	1.298046000
1	-1.696149000	5.553826000	0.593717000
Zero-point correction=			0.669350 (Hartree/Particle)
Thermal correction to Energy=			0.721787
Thermal correction to Enthalpy=			0.722732
Thermal correction to Gibbs Free Energy=			0.577882
Sum of electronic and zero-point Energies=			-3883.815557
Sum of electronic and thermal Energies=			-3883.763120
Sum of electronic and thermal Enthalpies=			-3883.762176
Sum of electronic and thermal Free Energies=			-3883.907026

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6	-1.956831000	-3.539091000	-3.173886000
6	-0.912074000	-2.787543000	-2.640768000
6	-1.158150000	-1.483117000	-2.229455000
6	-2.448404000	-0.928539000	-2.344638000
6	-3.496514000	-1.696030000	-2.841464000
6	-3.236091000	-2.998016000	-3.272916000
1	-1.776284000	-4.559724000	-3.504377000
1	0.089001000	-3.204842000	-2.539184000
1	-4.515343000	-1.319800000	-2.876588000
1	-4.049816000	-3.599277000	-3.672347000
6	-0.240416000	-0.508910000	-1.652490000
6	-0.925814000	0.629513000	-1.369377000
6	-2.406633000	0.425711000	-1.714496000
1	-2.759664000	0.109991000	-0.532655000
6	-3.303713000	1.476659000	-2.033151000
6	-0.314365000	1.861070000	-0.828111000
6	0.215063000	1.877075000	0.469343000
6	-0.167450000	3.005779000	-1.620469000
6	0.865340000	3.004561000	0.960884000
1	0.105647000	0.990506000	1.091066000
6	0.482416000	4.134081000	-1.131404000
1	-0.562039000	3.001858000	-2.636097000
6	0.998729000	4.138222000	0.163293000
1	1.273725000	2.991311000	1.970415000
1	0.587466000	5.013158000	-1.764301000
6	-3.289614000	2.735450000	-1.305421000
6	-3.568747000	3.949678000	-1.960728000
6	-2.969938000	2.774903000	0.063451000
6	-3.489713000	5.153451000	-1.279906000
1	-3.790299000	3.958271000	-3.025099000
6	-2.931428000	3.977396000	0.749905000
1	-2.790616000	1.850005000	0.599342000
6	-3.176072000	5.170654000	0.077940000
1	-3.676425000	6.084849000	-1.808391000
1	-2.690443000	3.973265000	1.810041000
1	-3.127744000	6.117021000	0.611387000
79	1.725041000	-0.688108000	-1.085127000
15	3.800190000	-0.446864000	0.052921000
6	3.391858000	-0.009607000	1.779143000
6	4.721079000	1.007384000	-0.561736000
6	5.028459000	-1.789595000	0.108786000
6	4.228190000	0.798639000	2.556601000

6	2.164129000	-0.430264000	2.300475000
6	6.108475000	1.024073000	-0.712300000
6	3.975395000	2.149585000	-0.877553000
6	5.786804000	-2.074795000	1.245905000
6	5.238223000	-2.520546000	-1.064974000
6	3.842019000	1.171822000	3.839115000
1	5.175425000	1.151718000	2.148575000
6	1.771799000	-0.040378000	3.576274000
1	1.483318000	-1.036272000	1.702645000
6	6.743850000	2.173861000	-1.174353000
1	6.694225000	0.138172000	-0.470226000
6	4.615481000	3.295961000	-1.329039000
1	2.889702000	2.142922000	-0.764923000
6	6.750769000	-3.077109000	1.204605000
1	5.619106000	-1.515840000	2.165209000
6	6.208177000	-3.514570000	-1.104722000
1	4.634576000	-2.304210000	-1.946939000
6	2.611788000	0.757891000	4.346702000
1	4.496072000	1.800308000	4.439296000
1	0.796308000	-0.350648000	3.944776000
6	5.999918000	3.308083000	-1.481950000
1	7.824730000	2.181071000	-1.294587000
1	4.024689000	4.177395000	-1.569367000
6	6.964288000	-3.793156000	0.030839000
1	7.335951000	-3.300673000	2.093481000
1	6.368738000	-4.078450000	-2.020397000
1	2.305026000	1.068271000	5.343063000
1	6.499683000	4.203452000	-1.844735000
1	7.718364000	-4.576169000	0.001870000
8	-5.272494000	-0.137727000	-0.532117000
16	-4.824933000	-0.827457000	0.671607000
9	-3.649239000	-3.079542000	-0.086422000
9	-5.284714000	-3.352523000	1.291715000
9	-5.687129000	-2.838386000	-0.757136000
6	-4.853113000	-2.665689000	0.258095000
8	-2.929429000	-2.245524000	2.583628000
8	-0.918341000	-1.079151000	1.577967000
16	-2.313778000	-1.076075000	1.985318000
9	-3.619495000	0.491061000	3.654289000
9	-1.675904000	-0.161823000	4.324756000
9	-1.840573000	1.366614000	2.805703000
6	-2.384276000	0.246224000	3.278466000
7	-3.222050000	-0.453206000	0.775259000
8	-5.553561000	-0.676489000	1.913520000

6	-4.334362000	1.299039000	-3.082812000
1	-3.983147000	0.666643000	-3.903183000
1	-5.187281000	0.791511000	-2.608719000
1	-4.715587000	2.249866000	-3.461211000
1	1.508463000	5.020463000	0.545422000
Zero-point correction=			0.665088 (Hartree/Particle)
Thermal correction to Energy=			0.716716
Thermal correction to Enthalpy=			0.717660
Thermal correction to Gibbs Free Energy=			0.578794
Sum of electronic and zero-point Energies=			-3883.813079
Sum of electronic and thermal Energies=			-3883.761452
Sum of electronic and thermal Enthalpies=			-3883.760507
Sum of electronic and thermal Free Energies=			-3883.899373

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6	-2.519749000	-2.553512000	-3.805038000
6	-1.589530000	-1.868176000	-3.025011000
6	-2.001984000	-0.754642000	-2.303908000
6	-3.342236000	-0.298190000	-2.364266000
6	-4.263043000	-1.003839000	-3.134837000
6	-3.842342000	-2.124938000	-3.854736000
1	-2.211465000	-3.427807000	-4.374292000
1	-0.554110000	-2.200147000	-2.966967000
1	-5.305162000	-0.708964000	-3.200935000
1	-4.563197000	-2.664997000	-4.464943000
6	-1.232902000	0.102502000	-1.405149000
6	-2.091222000	1.044431000	-0.893168000
6	-3.456147000	0.840150000	-1.430280000
1	-0.715171000	-1.525123000	-0.003449000
6	-4.600046000	1.488309000	-1.070022000
6	-1.609527000	2.203474000	-0.112297000
6	-0.853064000	2.024398000	1.053559000
6	-1.792913000	3.508700000	-0.584311000
6	-0.280366000	3.107182000	1.712923000
1	-0.731831000	1.019754000	1.456270000
6	-1.225082000	4.593538000	0.075099000
1	-2.377044000	3.664983000	-1.490102000
6	-0.463092000	4.398488000	1.225600000
1	0.316021000	2.931979000	2.608403000
1	-1.376520000	5.598361000	-0.314709000
6	-4.679940000	2.355901000	0.121794000
6	-5.275700000	3.622070000	0.054264000
6	-4.195816000	1.910936000	1.357830000
6	-5.348092000	4.434910000	1.177419000

1	-5.653872000	3.986915000	-0.900200000
6	-4.276736000	2.720624000	2.484008000
1	-3.754404000	0.917841000	1.429244000
6	-4.847665000	3.986171000	2.396823000
1	-5.794605000	5.423962000	1.100971000
1	-3.889915000	2.357174000	3.433378000
1	-4.906514000	4.620864000	3.278101000
79	0.790320000	0.223181000	-1.013725000
15	2.976779000	0.772888000	-0.244081000
6	4.356509000	-0.358083000	-0.605683000
6	2.929046000	0.995527000	1.570926000
6	3.489050000	2.414686000	-0.852995000
6	5.520558000	-0.402179000	0.166685000
6	4.228611000	-1.199257000	-1.714615000
6	3.737874000	1.925040000	2.231600000
6	2.007739000	0.246383000	2.308665000
6	4.779607000	2.707462000	-1.295626000
6	2.516053000	3.421097000	-0.832134000
6	6.551821000	-1.267874000	-0.179485000
1	5.616080000	0.237023000	1.043766000
6	5.263964000	-2.060573000	-2.059968000
1	3.307802000	-1.183480000	-2.298602000
6	3.637643000	2.082831000	3.610029000
1	4.434356000	2.541056000	1.663198000
6	1.907508000	0.404107000	3.685695000
1	1.349126000	-0.449228000	1.791081000
6	5.094092000	4.000327000	-1.707291000
1	5.538961000	1.927242000	-1.320553000
6	2.838296000	4.710149000	-1.233499000
1	1.504523000	3.194721000	-0.491540000
6	6.424659000	-2.093757000	-1.293570000
1	7.455410000	-1.301392000	0.424631000
1	5.159056000	-2.713592000	-2.922680000
6	2.725499000	1.322877000	4.337633000
1	4.268062000	2.809655000	4.116876000
1	1.181439000	-0.183945000	4.242494000
6	4.128063000	5.000417000	-1.673194000
1	6.099754000	4.225163000	-2.054980000
1	2.074322000	5.483970000	-1.205457000
1	7.232100000	-2.771779000	-1.559957000
1	2.645030000	1.454716000	5.414061000
1	4.379500000	6.008850000	-1.993699000
8	-1.908774000	-0.950933000	2.311550000
16	-1.878020000	-2.324963000	1.857764000

9	-3.358475000	-3.652982000	0.164716000
9	-4.392421000	-2.883952000	1.899937000
9	-3.816818000	-1.548983000	0.303849000
6	-3.483385000	-2.628415000	0.978621000
8	-0.516317000	-4.936164000	0.472847000
8	0.638996000	-3.411143000	-1.209063000
16	0.143338000	-3.707145000	0.114763000
9	1.185447000	-3.280423000	2.483708000
9	2.286178000	-4.641619000	1.214988000
9	2.341172000	-2.517704000	0.831184000
6	1.594255000	-3.521846000	1.253352000
7	-0.780554000	-2.382563000	0.588607000
8	-1.650917000	-3.446122000	2.734612000
1	-0.016164000	5.247695000	1.738383000
6	-5.889663000	1.298179000	-1.816301000
1	-5.748992000	1.321149000	-2.901966000
1	-6.345309000	0.330040000	-1.562819000
1	-6.618717000	2.066745000	-1.544003000
Zero-point correction=			0.670115 (Hartree/Particle)
Thermal correction to Energy=			0.722485
Thermal correction to Enthalpy=			0.723430
Thermal correction to Gibbs Free Energy=			0.582326
Sum of electronic and zero-point Energies=			-3883.846708
Sum of electronic and thermal Energies=			-3883.794338
Sum of electronic and thermal Enthalpies=			-3883.793394
Sum of electronic and thermal Free Energies=			-3883.934498

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6	-2.601480000	-1.696829000	-4.109449000
6	-1.717151000	-1.431594000	-3.066758000
6	-1.960063000	-0.336799000	-2.249392000
6	-3.074779000	0.505656000	-2.447671000
6	-3.964987000	0.212969000	-3.481469000
6	-3.715031000	-0.883223000	-4.307498000
1	-2.431693000	-2.548905000	-4.763934000
1	-0.859133000	-2.073932000	-2.866649000
1	-4.855358000	0.806809000	-3.661567000
1	-4.406958000	-1.104926000	-5.117113000
6	-1.222028000	0.090377000	-1.054749000
6	-1.883418000	1.201068000	-0.549269000
6	-3.067879000	1.508577000	-1.363193000
1	-1.261562000	-0.990799000	-0.224813000
6	-3.985679000	2.502599000	-1.148354000
6	-1.304602000	1.984744000	0.558611000

6	-0.995131000	1.368033000	1.775508000
6	-0.941005000	3.321129000	0.365698000
6	-0.338190000	2.074934000	2.774760000
1	-1.293933000	0.335145000	1.939063000
6	-0.292341000	4.028031000	1.370809000
1	-1.174734000	3.803450000	-0.582596000
6	0.016928000	3.406355000	2.577771000
1	-0.110698000	1.581415000	3.718144000
1	-0.021601000	5.069132000	1.207851000
6	-4.059176000	3.261298000	0.111335000
6	-4.127257000	4.661297000	0.099760000
6	-4.061663000	2.594815000	1.343428000
6	-4.130584000	5.379005000	1.287433000
1	-4.124406000	5.192826000	-0.851235000
6	-4.081616000	3.316052000	2.530179000
1	-4.046185000	1.506653000	1.362784000
6	-4.102287000	4.706509000	2.506922000
1	-4.153108000	6.466060000	1.262819000
1	-4.070070000	2.783834000	3.478484000
1	-4.107104000	5.268121000	3.438346000
79	0.878657000	0.066694000	-0.751241000
15	3.183316000	0.342165000	-0.365727000
6	4.176498000	-1.176408000	-0.254433000
6	3.479868000	1.198543000	1.220017000
6	3.963407000	1.406108000	-1.623390000
6	5.427209000	-1.175767000	0.375148000
6	3.671279000	-2.358507000	-0.799950000
6	4.210320000	2.383190000	1.317750000
6	2.933575000	0.622865000	2.372168000
6	5.231262000	1.154110000	-2.149537000
6	3.249861000	2.533941000	-2.045826000
6	6.170419000	-2.346943000	0.441512000
1	5.810951000	-0.256468000	0.817664000
6	4.417975000	-3.530306000	-0.723989000
1	2.680940000	-2.371231000	-1.252664000
6	4.393366000	2.985878000	2.559661000
1	4.636474000	2.836485000	0.424144000
6	3.131317000	1.220830000	3.609351000
1	2.349846000	-0.294442000	2.294512000
6	5.780371000	2.024322000	-3.086872000
1	5.787710000	0.273547000	-1.833414000
6	3.807082000	3.405631000	-2.972372000
1	2.255301000	2.724385000	-1.638607000
6	5.664494000	-3.523569000	-0.107836000

1	7.141456000	-2.345898000	0.930999000
1	4.014365000	-4.451506000	-1.136419000
6	3.858913000	2.404933000	3.704072000
1	4.961291000	3.910613000	2.630502000
1	2.708908000	0.765924000	4.502510000
6	5.072340000	3.149145000	-3.495554000
1	6.765545000	1.820417000	-3.499571000
1	3.248744000	4.281215000	-3.294495000
1	6.243869000	-4.441925000	-0.045673000
1	4.006633000	2.875834000	4.673319000
1	5.503901000	3.826786000	-4.228462000
8	-3.489417000	-0.795482000	1.222693000
16	-2.995343000	-2.161524000	1.212480000
9	-3.656628000	-4.284820000	-0.154062000
9	-5.312216000	-3.142607000	0.637283000
9	-4.215911000	-2.412690000	-1.074601000
6	-4.120797000	-3.071038000	0.065004000
8	-0.927550000	-4.619095000	0.739889000
8	0.511297000	-3.018132000	-0.585822000
16	-0.421173000	-3.286502000	0.498572000
9	0.288145000	-1.490824000	2.307979000
9	0.101363000	-3.497825000	3.078357000
9	1.793955000	-2.959651000	1.853587000
6	0.496703000	-2.780689000	2.051099000
7	-1.585259000	-2.139926000	0.371894000
8	-2.908168000	-2.942317000	2.430291000
6	-5.020508000	2.843321000	-2.176006000
1	-4.614946000	2.835589000	-3.192849000
1	-5.840187000	2.111223000	-2.142470000
1	-5.468049000	3.821047000	-1.976344000
1	0.530343000	3.958524000	3.361696000
Zero-point correction=			0.665154 (Hartree/Particle)
Thermal correction to Energy=			0.716940
Thermal correction to Enthalpy=			0.717885
Thermal correction to Gibbs Free Energy=			0.578849
Sum of electronic and zero-point Energies=			-3883.841149
Sum of electronic and thermal Energies=			-3883.789362
Sum of electronic and thermal Enthalpies=			-3883.788418
Sum of electronic and thermal Free Energies=			-3883.927453

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6	-1.567426000	-4.336553000	-1.943897000
6	-1.004090000	-3.482207000	-1.002907000
6	-1.085069000	-2.112665000	-1.212725000

6	-1.739665000	-1.567528000	-2.336173000
6	-2.309520000	-2.438767000	-3.265709000
6	-2.205773000	-3.814118000	-3.066923000
1	-1.514140000	-5.413422000	-1.802554000
1	-0.507460000	-3.869871000	-0.114451000
1	-2.823301000	-2.083460000	-4.151359000
1	-2.639806000	-4.488612000	-3.801368000
6	-0.522202000	-1.022366000	-0.415835000
6	-0.858266000	0.196091000	-1.054983000
6	-1.702747000	-0.095274000	-2.201453000
1	-0.495733000	-1.063881000	0.683529000
6	-2.550126000	0.798663000	-2.821951000
6	-0.280833000	1.490801000	-0.653392000
6	-0.041982000	1.779180000	0.696526000
6	0.154456000	2.400364000	-1.627642000
6	0.587865000	2.963385000	1.058885000
1	-0.375738000	1.081366000	1.462744000
6	0.766375000	3.591169000	-1.259341000
1	0.004913000	2.165062000	-2.679331000
6	0.987469000	3.876906000	0.087079000
1	0.765046000	3.168989000	2.112891000
1	1.077753000	4.296120000	-2.027918000
6	-2.760331000	2.178318000	-2.357092000
6	-2.703545000	3.237138000	-3.274737000
6	-3.034767000	2.455979000	-1.012142000
6	-2.834799000	4.549037000	-2.842622000
1	-2.504023000	3.028909000	-4.325523000
6	-3.197580000	3.769068000	-0.590335000
1	-3.133019000	1.635710000	-0.303597000
6	-3.080540000	4.816907000	-1.497587000
1	-2.754149000	5.364639000	-3.557597000
1	-3.417057000	3.967170000	0.455543000
1	-3.197523000	5.844551000	-1.161016000
79	1.672385000	-0.889546000	-0.491361000
15	3.853115000	-0.346907000	0.187291000
6	5.012174000	-1.703079000	0.520473000
6	3.630415000	0.588580000	1.737383000
6	4.705323000	0.801062000	-0.935806000
6	6.006714000	-1.595060000	1.496795000
6	4.926244000	-2.856600000	-0.263341000
6	4.446568000	1.677002000	2.059381000
6	2.577296000	0.238953000	2.589649000
6	6.044859000	0.651805000	-1.295947000
6	3.962836000	1.879503000	-1.429514000

6	6.911712000	-2.634431000	1.678708000
1	6.067544000	-0.700399000	2.115214000
6	5.836457000	-3.891044000	-0.080257000
1	4.140008000	-2.941973000	-1.013466000
6	4.208171000	2.403060000	3.221536000
1	5.257749000	1.967361000	1.392389000
6	2.338519000	0.969803000	3.747245000
1	1.922963000	-0.596348000	2.337854000
6	6.637157000	1.579518000	-2.149365000
1	6.624077000	-0.187063000	-0.913088000
6	4.562503000	2.804847000	-2.271871000
1	2.914287000	2.000244000	-1.148259000
6	6.827620000	-3.779080000	0.890221000
1	7.682609000	-2.551925000	2.440880000
1	5.767111000	-4.788226000	-0.689972000
6	3.154084000	2.053656000	4.061458000
1	4.841932000	3.251961000	3.466695000
1	1.501301000	0.699611000	4.386306000
6	5.899459000	2.653207000	-2.635511000
1	7.679789000	1.460526000	-2.433830000
1	3.980111000	3.642789000	-2.648532000
1	7.535930000	-4.590643000	1.038154000
1	2.962108000	2.633492000	4.961144000
1	6.365844000	3.373933000	-3.302923000
8	-4.768207000	-0.397434000	-1.086224000
16	-4.812299000	-0.730247000	0.334925000
9	-4.901912000	-3.036421000	1.587187000
9	-6.068815000	-2.921334000	-0.225325000
9	-3.922799000	-3.105934000	-0.331335000
6	-4.925817000	-2.572414000	0.351361000
8	-3.842943000	-1.100830000	3.402714000
8	-1.547769000	-0.406747000	2.643235000
16	-3.007234000	-0.327808000	2.500409000
9	-2.541263000	2.243127000	2.237346000
9	-4.606287000	1.763464000	2.609992000
9	-3.161480000	1.629749000	4.210155000
6	-3.364775000	1.438195000	2.914693000
7	-3.337108000	-0.419504000	0.931556000
8	-5.932580000	-0.280527000	1.145420000
6	-3.426173000	0.365080000	-3.948040000
1	-2.874938000	-0.153916000	-4.738931000
1	-4.172276000	-0.329917000	-3.532951000
1	-3.970929000	1.207371000	-4.380045000
1	1.471615000	4.806909000	0.376200000

Zero-point correction=	0.669800 (Hartree/Particle)
Thermal correction to Energy=	0.722246
Thermal correction to Enthalpy=	0.723190
Thermal correction to Gibbs Free Energy=	0.579139
Sum of electronic and zero-point Energies=	-3883.848693
Sum of electronic and thermal Energies=	-3883.796247
Sum of electronic and thermal Enthalpies=	-3883.795303
Sum of electronic and thermal Free Energies=	-3883.939354

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6	1.426833000	5.025494000	-0.040172000
6	2.798793000	5.213470000	0.111615000
6	3.649406000	4.122131000	0.280470000
6	3.120885000	2.836279000	0.298945000
6	1.734388000	2.648450000	0.137830000
6	0.889194000	3.743915000	-0.026002000
1	0.774261000	5.884935000	-0.168606000
1	3.211576000	6.218926000	0.100838000
1	4.720234000	4.273125000	0.400860000
1	-0.181723000	3.585035000	-0.146158000
6	3.912739000	1.604953000	0.489636000
6	4.644397000	0.996059000	-0.505823000
6	1.331634000	1.253572000	0.155111000
6	2.204676000	0.291429000	0.224937000
6	2.517910000	-1.100041000	0.128751000
6	2.135108000	-1.804539000	-1.028327000
6	3.200939000	-1.775614000	1.152532000
6	2.411915000	-3.159405000	-1.141011000
1	1.602665000	-1.273742000	-1.816378000
6	3.497390000	-3.123852000	1.019374000
1	3.489514000	-1.230972000	2.048716000
6	3.099685000	-3.816646000	-0.122473000
1	2.100117000	-3.703362000	-2.029284000
1	4.033712000	-3.639389000	1.811841000
1	4.088471000	1.295361000	1.523748000
6	5.546510000	-0.110292000	-0.188598000
6	6.193923000	-0.180421000	1.057072000
6	5.774050000	-1.138461000	-1.117346000
6	7.019894000	-1.249076000	1.369887000
1	6.078286000	0.631968000	1.771360000
6	6.586970000	-2.215734000	-0.796292000
1	5.281800000	-1.114496000	-2.086766000
6	7.211665000	-2.274461000	0.446801000
1	7.527134000	-1.277456000	2.330688000

1	6.738699000	-3.011109000	-1.521375000
1	7.858612000	-3.113069000	0.691770000
79	-0.642094000	0.540984000	0.140401000
15	-2.863464000	-0.251535000	0.029843000
6	-3.504709000	-0.822715000	1.629630000
6	-2.972067000	-1.670668000	-1.102119000
6	-4.031495000	0.997306000	-0.580946000
6	-4.352912000	-1.928772000	1.728996000
6	-3.166076000	-0.096500000	2.775625000
6	-4.013645000	-1.811003000	-2.021003000
6	-1.977932000	-2.652430000	-1.018886000
6	-5.365070000	1.013384000	-0.162566000
6	-3.585287000	1.928898000	-1.523929000
6	-4.858629000	-2.301215000	2.970017000
1	-4.615710000	-2.498328000	0.838551000
6	-3.677285000	-0.471397000	4.011790000
1	-2.499190000	0.762439000	2.695480000
6	-4.058845000	-2.928708000	-2.849351000
1	-4.785882000	-1.046855000	-2.094203000
6	-2.032795000	-3.768832000	-1.842634000
1	-1.161436000	-2.539077000	-0.303535000
6	-6.243987000	1.952887000	-0.690191000
1	-5.714387000	0.294679000	0.577685000
6	-4.469012000	2.863061000	-2.050153000
1	-2.542623000	1.918828000	-1.844196000
6	-4.521636000	-1.574239000	4.107982000
1	-5.516457000	-3.162979000	3.047962000
1	-3.412496000	0.093734000	4.901685000
6	-3.072448000	-3.905252000	-2.760102000
1	-4.867782000	-3.035306000	-3.567492000
1	-1.261394000	-4.531976000	-1.771431000
6	-5.796929000	2.874932000	-1.632203000
1	-7.280208000	1.966838000	-0.362473000
1	-4.120161000	3.586476000	-2.782608000
1	-4.916257000	-1.871526000	5.076319000
1	-3.111490000	-4.776107000	-3.409616000
1	-6.486595000	3.609843000	-2.039730000
1	3.326275000	-4.875642000	-0.218445000
6	4.467283000	1.382722000	-1.936719000
1	5.438063000	1.518722000	-2.426089000
1	3.947952000	0.585256000	-2.486815000
1	3.881213000	2.298460000	-2.042573000
Zero-point correction=			0.664454 (Hartree/Particle)
Thermal correction to Energy=			0.716331

Thermal correction to Enthalpy=	0.717275
Thermal correction to Gibbs Free Energy=	0.572935
Sum of electronic and zero-point Energies=	-3883.813803
Sum of electronic and thermal Energies=	-3883.761926
Sum of electronic and thermal Enthalpies=	-3883.760981
Sum of electronic and thermal Free Energies=	-3883.905322

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6	-0.881539000	-4.288108000	0.825123000
6	0.147264000	-3.368222000	0.632709000
6	-0.167390000	-2.018811000	0.498163000
6	-1.507587000	-1.601528000	0.563629000
6	-2.527820000	-2.513821000	0.776062000
6	-2.208843000	-3.867307000	0.897010000
1	-0.648023000	-5.346443000	0.923311000
1	1.186850000	-3.691340000	0.584313000
1	-3.567259000	-2.191746000	0.843481000
1	-3.004016000	-4.594749000	1.047595000
6	0.702246000	-0.854434000	0.301370000
6	-0.084885000	0.245880000	0.228410000
6	-1.563792000	-0.107262000	0.411917000
1	-1.907703000	0.321271000	1.367260000
6	-2.441455000	0.432908000	-0.698670000
6	0.369423000	1.643514000	0.082055000
6	0.872314000	2.334792000	1.190215000
6	0.289089000	2.315251000	-1.143157000
6	1.257849000	3.668162000	1.085228000
1	0.947273000	1.810720000	2.142408000
6	0.669173000	3.647959000	-1.250185000
1	-0.090087000	1.780430000	-2.013171000
6	1.144856000	4.331857000	-0.133658000
1	1.637813000	4.192532000	1.959678000
1	0.590851000	4.156783000	-2.208895000
6	-2.802269000	1.874489000	-0.671509000
6	-3.132352000	2.546604000	-1.857936000
6	-2.831283000	2.608565000	0.521882000
6	-3.501083000	3.883944000	-1.849403000
1	-3.065883000	2.019854000	-2.807650000
6	-3.197068000	3.949303000	0.531831000
1	-2.575183000	2.132847000	1.463682000
6	-3.538698000	4.592829000	-0.651895000
1	-3.747079000	4.379547000	-2.785942000
1	-3.211453000	4.491921000	1.474152000
1	-3.822006000	5.642775000	-0.644846000

79	2.744892000	-0.728024000	0.184859000
15	5.082182000	-0.287279000	-0.004210000
6	5.967173000	-0.094197000	1.578532000
6	5.344486000	1.282689000	-0.898326000
6	6.043464000	-1.517239000	-0.949576000
6	7.097636000	0.718355000	1.707104000
6	5.501384000	-0.809604000	2.685057000
6	6.435788000	1.486639000	-1.748200000
6	4.413679000	2.309973000	-0.709087000
6	7.280651000	-2.008773000	-0.530612000
6	5.493719000	-1.965987000	-2.155692000
6	7.756555000	0.806005000	2.927964000
1	7.457290000	1.288126000	0.850922000
6	6.164984000	-0.722014000	3.904005000
1	4.608401000	-1.427182000	2.587118000
6	6.597002000	2.707779000	-2.393800000
1	7.156986000	0.685714000	-1.909336000
6	4.581095000	3.528982000	-1.355590000
1	3.550995000	2.157727000	-0.057051000
6	7.961538000	-2.937121000	-1.313801000
1	7.711853000	-1.668585000	0.409400000
6	6.181265000	-2.883431000	-2.938804000
1	4.521103000	-1.591261000	-2.476633000
6	7.291546000	0.085551000	4.025120000
1	8.633132000	1.442256000	3.024486000
1	5.796269000	-1.278341000	4.762251000
6	5.670329000	3.728027000	-2.198566000
1	7.445734000	2.860650000	-3.056420000
1	3.843142000	4.313567000	-1.204171000
6	7.415615000	-3.371963000	-2.516299000
1	8.922777000	-3.321021000	-0.979989000
1	5.749561000	-3.226290000	-3.875989000
1	7.805702000	0.160539000	4.980561000
1	5.795336000	4.679749000	-2.710107000
1	7.949997000	-4.097715000	-3.124807000
8	-6.058316000	-1.071216000	-2.489980000
16	-6.610887000	-1.200963000	-1.160823000
9	-5.157256000	-3.336275000	-0.964382000
9	-6.617935000	-3.113032000	0.609442000
9	-7.251384000	-3.696095000	-1.373396000
6	-6.395116000	-2.973221000	-0.679227000
8	-6.836609000	-0.586647000	2.079220000
8	-4.521293000	0.461266000	1.946413000
16	-5.827305000	0.179709000	1.393257000

9	-7.878856000	1.672640000	0.766060000
9	-6.346331000	2.652491000	1.934244000
9	-6.033489000	2.277896000	-0.168964000
6	-6.585441000	1.822071000	0.937851000
7	-5.516051000	-0.486311000	-0.117492000
8	-7.946905000	-0.796154000	-0.797744000
6	-2.858650000	-0.369790000	-1.696984000
1	-2.585671000	-1.422293000	-1.720554000
1	-4.566092000	-0.318357000	-0.507875000
1	-3.481689000	-0.006553000	-2.512300000
1	1.428483000	5.379786000	-0.213963000
Zero-point correction=			0.670317 (Hartree/Particle)
Thermal correction to Energy=			0.722828
Thermal correction to Enthalpy=			0.723772
Thermal correction to Gibbs Free Energy=			0.577817
Sum of electronic and zero-point Energies=			-3883.822283
Sum of electronic and thermal Energies=			-3883.769772
Sum of electronic and thermal Enthalpies=			-3883.768828
Sum of electronic and thermal Free Energies=			-3883.914783

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6	2.207005000	-1.345924000	-4.140163000
6	1.364949000	-0.942318000	-3.106624000
6	1.872376000	-0.099756000	-2.123100000
6	3.199550000	0.343208000	-2.185275000
6	4.046247000	-0.083147000	-3.195327000
6	3.535975000	-0.928456000	-4.181225000
1	1.827278000	-2.008219000	-4.914931000
1	0.340392000	-1.305300000	-3.047426000
1	5.092515000	0.220050000	-3.218670000
1	4.183175000	-1.266984000	-4.987305000
6	1.219452000	0.455877000	-0.918695000
6	2.129732000	1.301130000	-0.306416000
6	3.484063000	1.217709000	-0.989900000
1	3.777227000	2.236582000	-1.286322000
6	4.586286000	0.626439000	-0.109374000
6	1.875087000	2.208821000	0.808717000
6	0.660152000	2.910292000	0.879171000
6	2.825265000	2.445147000	1.816430000
6	0.372283000	3.749519000	1.947080000
1	-0.045382000	2.828330000	0.053297000
6	2.535115000	3.281441000	2.883704000
1	3.780479000	1.929452000	1.790233000
6	1.304238000	3.926567000	2.963593000

1	-0.574899000	4.286405000	1.971003000
1	3.276515000	3.424708000	3.666060000
6	5.904920000	1.294190000	-0.107573000
6	6.729627000	1.227968000	1.024226000
6	6.371548000	2.010617000	-1.217545000
6	7.980321000	1.829625000	1.036603000
1	6.368908000	0.715656000	1.914565000
6	7.625925000	2.610268000	-1.207556000
1	5.756302000	2.089126000	-2.113029000
6	8.436734000	2.521668000	-0.081741000
1	8.597279000	1.769782000	1.930378000
1	7.968818000	3.151759000	-2.086360000
1	9.414440000	2.997441000	-0.071254000
79	-0.914597000	0.569434000	-0.764499000
15	-3.247975000	0.651948000	-0.494002000
6	-4.043696000	2.081657000	-1.296790000
6	-3.661374000	0.796591000	1.273556000
6	-4.106462000	-0.816666000	-1.132803000
6	-5.095771000	2.783925000	-0.704136000
6	-3.584952000	2.458225000	-2.562834000
6	-4.699647000	0.078258000	1.868812000
6	-2.879683000	1.658825000	2.049143000
6	-5.464995000	-0.786973000	-1.466323000
6	-3.379112000	-2.002354000	-1.271717000
6	-5.685625000	3.848911000	-1.378102000
1	-5.449598000	2.500042000	0.286256000
6	-4.180348000	3.518934000	-3.234071000
1	-2.753554000	1.918327000	-3.017072000
6	-4.953280000	0.229256000	3.228860000
1	-5.300409000	-0.608167000	1.274228000
6	-3.145795000	1.817054000	3.402493000
1	-2.042519000	2.190396000	1.596034000
6	-6.090449000	-1.941762000	-1.920007000
1	-6.029218000	0.141240000	-1.377642000
6	-4.011749000	-3.154988000	-1.724505000
1	-2.315483000	-2.027567000	-1.033594000
6	-5.229839000	4.215261000	-2.640503000
1	-6.502066000	4.395724000	-0.912394000
1	-3.818698000	3.808877000	-4.217483000
6	-4.180455000	1.097264000	3.993931000
1	-5.755066000	-0.339448000	3.693707000
1	-2.521869000	2.478275000	3.999486000
6	-5.364590000	-3.124425000	-2.046348000
1	-7.145671000	-1.918485000	-2.181529000

1	-3.437722000	-4.072122000	-1.828801000
1	-5.691122000	5.050650000	-3.161942000
1	-4.377897000	1.204654000	5.057834000
1	-5.857291000	-4.025086000	-2.405366000
8	0.004118000	-2.993919000	-1.216873000
16	0.647637000	-3.163308000	0.078098000
9	2.904230000	-2.776123000	-1.181078000
9	3.116646000	-3.632808000	0.787300000
9	2.381109000	-4.844735000	-0.844904000
6	2.389860000	-3.632697000	-0.315711000
8	1.539653000	-2.261748000	3.179839000
8	0.767192000	0.046013000	2.486169000
16	0.707450000	-1.401328000	2.363730000
9	-1.155822000	-3.054660000	3.268471000
9	-1.484286000	-0.974240000	3.696074000
9	-1.832250000	-1.730325000	1.703758000
6	-1.063791000	-1.837410000	2.785852000
7	0.826268000	-1.685554000	0.749362000
8	0.162403000	-4.153016000	1.022680000
6	4.349468000	-0.485998000	0.596062000
1	3.365763000	-0.950600000	0.612343000
1	0.902824000	-0.500300000	-0.068726000
1	5.130158000	-0.981270000	1.167432000
1	1.082998000	4.581362000	3.803306000
Zero-point correction=			0.664012 (Hartree/Particle)
Thermal correction to Energy=			0.715908
Thermal correction to Enthalpy=			0.716853
Thermal correction to Gibbs Free Energy=			0.574624
Sum of electronic and zero-point Energies=			-3883.821234
Sum of electronic and thermal Energies=			-3883.769337
Sum of electronic and thermal Enthalpies=			-3883.768393
Sum of electronic and thermal Free Energies=			-3883.910621

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6	-2.083000000	0.358711000	-4.714574000
6	-0.998344000	0.846862000	-3.987683000
6	-1.229836000	1.344356000	-2.708029000
6	-2.515682000	1.306639000	-2.143844000
6	-3.594108000	0.850597000	-2.880299000
6	-3.370262000	0.378497000	-4.176974000
1	-1.927514000	-0.025232000	-5.720452000
1	0.005048000	0.851149000	-4.409579000
1	-4.600237000	0.863298000	-2.460370000
1	-4.208671000	0.024051000	-4.773698000

6	-0.325934000	1.951292000	-1.745124000
6	-0.994465000	2.262756000	-0.601962000
6	-2.441200000	1.809933000	-0.723512000
1	-2.565134000	0.940957000	-0.050390000
6	-3.480444000	2.856440000	-0.363133000
6	-0.450405000	2.888198000	0.599563000
6	0.754942000	3.603730000	0.550680000
6	-1.106723000	2.775059000	1.832731000
6	1.290950000	4.176736000	1.693801000
1	1.272661000	3.712980000	-0.399224000
6	-0.567076000	3.347344000	2.977805000
1	-2.048333000	2.229814000	1.898295000
6	0.631074000	4.050280000	2.913823000
1	2.233783000	4.715354000	1.632288000
1	-1.088206000	3.243556000	3.927025000
6	-4.582658000	2.460752000	0.537076000
6	-5.127617000	3.382052000	1.440947000
6	-5.101438000	1.159153000	0.526722000
6	-6.174987000	3.025608000	2.279998000
1	-4.696420000	4.379569000	1.502075000
6	-6.152748000	0.804061000	1.364195000
1	-4.695164000	0.412878000	-0.157408000
6	-6.696467000	1.735176000	2.242321000
1	-6.577257000	3.755398000	2.979229000
1	-6.544992000	-0.211098000	1.327118000
1	-7.514447000	1.455299000	2.902054000
79	0.693502000	-0.362876000	-0.329058000
15	-0.590009000	-2.237124000	0.088393000
6	-2.399534000	-2.233137000	-0.131610000
6	-0.309532000	-2.634385000	1.844099000
6	-0.008753000	-3.668321000	-0.875750000
6	-3.266954000	-2.482479000	0.935130000
6	-2.915194000	-2.020054000	-1.414442000
6	-0.232738000	-3.950746000	2.306998000
6	-0.171069000	-1.571382000	2.742665000
6	-0.810934000	-4.801382000	-1.050770000
6	1.278189000	-3.639050000	-1.421394000
6	-4.640259000	-2.532825000	0.715576000
1	-2.868809000	-2.644122000	1.935213000
6	-4.286159000	-2.092704000	-1.629479000
1	-2.244749000	-1.799752000	-2.246998000
6	-0.011828000	-4.197106000	3.657579000
1	-0.331448000	-4.782056000	1.610471000
6	0.052581000	-1.824406000	4.090560000

1	-0.207011000	-0.540802000	2.387862000
6	-0.323443000	-5.895621000	-1.755491000
1	-1.820065000	-4.824047000	-0.640131000
6	1.760930000	-4.737385000	-2.124524000
1	1.899427000	-2.749926000	-1.306223000
6	-5.149303000	-2.347617000	-0.565889000
1	-5.312323000	-2.724282000	1.549156000
1	-4.680903000	-1.940336000	-2.631182000
6	0.133954000	-3.136247000	4.547425000
1	0.056660000	-5.221946000	4.014501000
1	0.182444000	-0.990885000	4.776062000
6	0.961540000	-5.863306000	-2.291249000
1	-0.950275000	-6.773460000	-1.892063000
1	2.760225000	-4.705324000	-2.550761000
1	-6.222577000	-2.396656000	-0.737185000
1	0.321342000	-3.334370000	5.600187000
1	1.337655000	-6.718397000	-2.847909000
8	2.860138000	0.298079000	-2.467433000
16	3.580860000	0.825649000	-1.317593000
9	2.785207000	3.123348000	-2.297263000
9	4.174175000	3.307752000	-0.660170000
9	4.869698000	2.662250000	-2.599716000
6	3.874264000	2.607870000	-1.733527000
8	4.063607000	1.859142000	1.751383000
8	1.776366000	0.917814000	2.298110000
16	2.996383000	0.910531000	1.508454000
9	5.033306000	-0.776831000	1.704873000
9	3.405175000	-1.140738000	3.063874000
9	3.212779000	-1.690295000	0.988456000
6	3.726395000	-0.794359000	1.828045000
7	2.501195000	0.879434000	-0.079133000
8	4.877019000	0.300394000	-0.928142000
6	-3.389685000	4.086583000	-0.877955000
1	-2.555346000	4.362369000	-1.520659000
1	0.725547000	2.134641000	-1.941757000
1	-4.145130000	4.845764000	-0.692507000
1	1.053156000	4.494886000	3.811834000
Zero-point correction=			0.670696 (Hartree/Particle)
Thermal correction to Energy=			0.722546
Thermal correction to Enthalpy=			0.723491
Thermal correction to Gibbs Free Energy=			0.583573
Sum of electronic and zero-point Energies=			-3883.872460
Sum of electronic and thermal Energies=			-3883.820609
Sum of electronic and thermal Enthalpies=			-3883.819665

Sum of electronic and thermal Free Energies= -3883.959582

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6	-0.191821000	-2.909526000	-4.168466000
6	-1.454166000	-2.325536000	-4.221569000
6	-1.889043000	-1.586594000	-3.124521000
6	-1.067408000	-1.434080000	-1.995348000
6	0.182229000	-2.022716000	-1.943455000
6	0.618083000	-2.760538000	-3.042939000
1	0.167314000	-3.489768000	-5.015415000
1	-2.085397000	-2.441332000	-5.100135000
1	0.801102000	-1.912068000	-1.060661000
1	1.602840000	-3.221760000	-3.017448000
6	-3.121420000	-0.859353000	-2.888398000
6	-3.104051000	-0.256432000	-1.678649000
6	-1.788661000	-0.618821000	-0.959111000
1	-1.233195000	0.288263000	-0.673939000
6	-2.222951000	-1.385725000	0.255358000
6	-4.144223000	0.607844000	-1.121096000
6	-3.815253000	1.791309000	-0.447480000
6	-5.493234000	0.258008000	-1.253326000
6	-4.815028000	2.592788000	0.087014000
1	-2.770709000	2.089101000	-0.359046000
6	-6.490199000	1.066254000	-0.723521000
1	-5.749202000	-0.672430000	-1.757985000
6	-6.153161000	2.233884000	-0.046060000
1	-4.545016000	3.506265000	0.612064000
1	-7.533504000	0.777720000	-0.829207000
6	-2.739999000	-0.653721000	1.407725000
6	-2.095511000	0.481065000	1.919897000
6	-3.960897000	-1.060084000	1.969368000
6	-2.649636000	1.172481000	2.985487000
1	-1.149743000	0.804273000	1.500301000
6	-4.536518000	-0.330679000	2.997364000
1	-4.487170000	-1.912985000	1.546262000
6	-3.874704000	0.778792000	3.515102000
1	-2.126891000	2.033395000	3.392948000
1	-5.500775000	-0.630637000	3.398788000
1	-4.318541000	1.340221000	4.333758000
6	-2.199081000	-2.782426000	0.272699000
1	-2.123109000	-3.296773000	-0.687505000
1	-3.921059000	-0.745258000	-3.616488000
1	-2.797571000	-3.276545000	1.040117000
1	-6.931989000	2.863091000	0.378253000

16	1.047269000	-2.307158000	1.810216000
8	1.183667000	-2.378053000	3.256489000
8	0.555817000	-1.002374000	1.267241000
8	0.191321000	-3.410154000	1.224760000
1	-1.032273000	-2.973058000	0.736852000
6	2.660663000	-2.570545000	1.109445000
6	3.395932000	-3.653567000	1.586242000
6	4.648925000	-3.912013000	1.055164000
6	5.188488000	-3.096002000	0.055544000
6	4.434600000	-2.016321000	-0.401761000
6	3.172004000	-1.742244000	0.116241000
1	2.980508000	-4.279411000	2.372580000
1	5.227011000	-4.759870000	1.420297000
1	4.841573000	-1.373793000	-1.181633000
1	2.601691000	-0.893157000	-0.260459000
6	6.558054000	-3.367046000	-0.488773000
1	6.717986000	-2.861143000	-1.446332000
1	7.334304000	-3.015333000	0.202615000
1	6.725601000	-4.439508000	-0.638357000
16	1.134872000	1.926936000	-0.095779000
8	-0.249490000	2.390392000	-0.056109000
8	1.496381000	0.942239000	-1.107438000
8	1.567651000	1.389142000	1.331723000
1	1.254770000	0.434673000	1.430467000
6	2.206875000	3.323375000	-0.205480000
6	1.683431000	4.606627000	-0.145536000
6	2.551612000	5.687565000	-0.244122000
6	3.924743000	5.495796000	-0.397381000
6	4.421003000	4.188623000	-0.460565000
6	3.571734000	3.099221000	-0.366572000
1	0.611863000	4.743502000	-0.028624000
1	2.156889000	6.701177000	-0.202512000
1	5.490883000	4.031294000	-0.587566000
1	3.951967000	2.081292000	-0.418984000
6	4.859667000	6.663581000	-0.473105000
1	5.632278000	6.510606000	-1.234529000
1	4.327657000	7.590551000	-0.708326000
1	5.376393000	6.813972000	0.483021000
Zero-point correction=			0.619127 (Hartree/Particle)
Thermal correction to Energy=			0.659684
Thermal correction to Enthalpy=			0.660628
Thermal correction to Gibbs Free Energy=			0.543361
Sum of electronic and zero-point Energies=			-2676.087164
Sum of electronic and thermal Energies=			-2676.046606

Sum of electronic and thermal Enthalpies= -2676.045662
 Sum of electronic and thermal Free Energies= -2676.162929

B-3d

6	1.385094000	-3.687469000	1.687740000
6	0.342398000	-2.922530000	2.206188000
6	0.087209000	-1.673203000	1.642415000
6	0.854530000	-1.198235000	0.560710000
6	1.880859000	-1.973066000	0.044005000
6	2.146190000	-3.216949000	0.619564000
1	1.598176000	-4.664854000	2.114144000
1	-0.264260000	-3.293244000	3.029944000
1	2.468273000	-1.623491000	-0.799736000
1	2.949314000	-3.828940000	0.213938000
6	-0.949311000	-0.694131000	1.923919000
6	-0.853254000	0.351306000	1.070209000
6	0.348655000	0.167338000	0.158857000
1	0.031912000	0.162397000	-0.894536000
6	1.433395000	1.282991000	0.303181000
6	-1.820249000	1.448305000	0.986076000
6	-2.260486000	1.926617000	-0.255071000
6	-2.376626000	1.988823000	2.152025000
6	-3.210921000	2.935165000	-0.322123000
1	-1.875690000	1.477831000	-1.168796000
6	-3.333480000	2.993756000	2.081520000
1	-2.023911000	1.632624000	3.119287000
6	-3.748998000	3.474268000	0.843204000
1	-3.537687000	3.299651000	-1.293149000
1	-3.745831000	3.412198000	2.997047000
6	0.901436000	2.635724000	-0.132133000
6	0.757134000	2.916073000	-1.493114000
6	0.484419000	3.588176000	0.796915000
6	0.196337000	4.115819000	-1.911752000
1	1.101203000	2.191216000	-2.228034000
6	-0.091004000	4.781970000	0.378393000
1	0.583102000	3.394440000	1.862384000
6	-0.239257000	5.049211000	-0.977087000
1	0.100718000	4.320885000	-2.975328000
1	-0.428452000	5.503219000	1.119076000
1	-0.684632000	5.985548000	-1.305025000
6	2.029393000	1.272926000	1.701813000
1	2.547860000	0.325016000	1.878233000
1	-1.741617000	-0.833013000	2.656626000
1	1.227957000	1.349990000	2.444574000

1	-4.490658000	4.267499000	0.785928000
16	3.879191000	1.462831000	-0.928573000
8	3.992235000	1.649378000	-2.359681000
8	2.404576000	0.827634000	-0.693369000
8	4.118088000	2.552743000	-0.001821000
1	2.728461000	2.099992000	1.843170000
6	4.856337000	0.062277000	-0.459687000
6	5.326342000	-0.041586000	0.843881000
6	5.988466000	-1.199334000	1.227740000
6	6.180531000	-2.251782000	0.329550000
6	5.716091000	-2.109518000	-0.981107000
6	5.055149000	-0.957855000	-1.384391000
1	5.177685000	0.780382000	1.539842000
1	6.365806000	-1.292499000	2.244692000
1	5.880087000	-2.914452000	-1.695722000
1	4.693406000	-0.839477000	-2.403191000
6	6.846467000	-3.519019000	0.769902000
1	7.352131000	-4.019593000	-0.062084000
1	7.584067000	-3.335401000	1.557851000
1	6.109439000	-4.224953000	1.174497000
16	-2.666572000	-2.422178000	-1.401417000
8	-2.884497000	-3.345746000	-2.493084000
8	-1.796794000	-1.265376000	-1.563891000
8	-2.089964000	-3.253794000	-0.142190000
1	-1.232161000	-2.863054000	0.114399000
6	-4.235607000	-1.894272000	-0.783354000
6	-5.397947000	-2.431709000	-1.318804000
6	-6.623567000	-1.970047000	-0.852917000
6	-6.696480000	-0.983167000	0.130875000
6	-5.506977000	-0.458517000	0.648863000
6	-4.277184000	-0.910215000	0.200989000
1	-5.332032000	-3.190726000	-2.093499000
1	-7.544360000	-2.378495000	-1.265755000
1	-5.543438000	0.323732000	1.406761000
1	-3.355593000	-0.491768000	0.597394000
6	-8.019268000	-0.497368000	0.638545000
1	-8.039955000	0.595367000	0.715223000
1	-8.841508000	-0.809408000	-0.012698000
1	-8.223747000	-0.892422000	1.641454000
Zero-point correction=			0.627667 (Hartree/Particle)
Thermal correction to Energy=			0.667879
Thermal correction to Enthalpy=			0.668823
Thermal correction to Gibbs Free Energy=			0.554762
Sum of electronic and zero-point Energies=			-2676.114575

Sum of electronic and thermal Energies=	-2676.074363
Sum of electronic and thermal Enthalpies=	-2676.073419
Sum of electronic and thermal Free Energies=	-2676.187480

B-TSd4

6	4.442677000	2.507852000	3.370984000
6	5.085283000	1.709829000	2.430452000
6	4.340905000	0.759115000	1.741309000
6	2.965868000	0.589278000	1.991477000
6	2.322701000	1.421127000	2.902238000
6	3.074647000	2.369385000	3.596271000
1	5.007183000	3.256283000	3.922383000
1	6.147547000	1.830683000	2.227451000
1	1.248902000	1.371142000	3.050480000
1	2.579452000	3.014779000	4.317786000
6	4.734927000	-0.157805000	0.692484000
6	3.685931000	-0.890419000	0.266328000
6	2.447580000	-0.444689000	1.037857000
1	1.896713000	0.275686000	0.187932000
6	1.359893000	-1.328260000	1.337237000
6	3.776423000	-1.892596000	-0.811250000
6	3.901539000	-1.462234000	-2.135659000
6	3.779427000	-3.264163000	-0.541433000
6	4.000688000	-2.384195000	-3.170795000
1	3.891531000	-0.392940000	-2.341214000
6	3.876225000	-4.185114000	-1.576308000
1	3.696045000	-3.605118000	0.489447000
6	3.981541000	-3.747413000	-2.893633000
1	4.089131000	-2.036742000	-4.197477000
1	3.870740000	-5.249730000	-1.353946000
6	0.878435000	-2.286661000	0.368300000
6	0.875153000	-2.000100000	-1.012845000
6	0.395098000	-3.538399000	0.800825000
6	0.423408000	-2.942484000	-1.918422000
1	1.159959000	-1.011778000	-1.362303000
6	-0.010194000	-4.489216000	-0.117414000
1	0.384855000	-3.782689000	1.859315000
6	-0.002117000	-4.190384000	-1.477210000
1	0.394889000	-2.694851000	-2.975415000
1	-0.362923000	-5.455918000	0.230132000
1	-0.354634000	-4.927394000	-2.194270000
6	0.603010000	-1.178572000	2.592549000
1	1.235486000	-0.922487000	3.447011000
1	5.742689000	-0.252174000	0.297217000

1	-0.050075000	-2.028514000	2.800786000
1	4.053960000	-4.470085000	-3.703005000
16	-2.877403000	-1.965130000	0.235602000
8	-2.584921000	-2.220626000	-1.164755000
8	-1.921503000	-0.803325000	0.756373000
8	-2.795311000	-3.024897000	1.223656000
1	-0.083188000	-0.331709000	2.407522000
6	-4.473596000	-1.206630000	0.343042000
6	-5.396350000	-1.660116000	1.273475000
6	-6.640820000	-1.043016000	1.340049000
6	-6.962414000	0.019248000	0.496434000
6	-6.010291000	0.453904000	-0.433151000
6	-4.768088000	-0.152241000	-0.518449000
1	-5.132689000	-2.486572000	1.928071000
1	-7.377336000	-1.391678000	2.062147000
1	-6.254986000	1.281478000	-1.097423000
1	-4.025997000	0.184021000	-1.240676000
6	-8.293209000	0.701741000	0.587160000
1	-8.193348000	1.702324000	1.026014000
1	-8.745010000	0.830997000	-0.402938000
1	-8.994040000	0.136395000	1.209165000
16	0.002030000	1.646577000	-0.391165000
8	1.381741000	1.176634000	-0.810580000
8	-0.151619000	1.604663000	1.069318000
8	-1.070179000	0.929105000	-1.124477000
1	-1.676789000	-0.176758000	0.016065000
6	-0.044546000	3.339150000	-0.902901000
6	0.725345000	4.257576000	-0.192309000
6	0.727664000	5.583178000	-0.592399000
6	-0.026104000	6.005341000	-1.693909000
6	-0.787438000	5.064143000	-2.384905000
6	-0.801641000	3.728276000	-1.997287000
1	1.306692000	3.925560000	0.666419000
1	1.321911000	6.312878000	-0.043821000
1	-1.379825000	5.383275000	-3.241054000
1	-1.393591000	2.987202000	-2.527674000
6	-0.002626000	7.443340000	-2.114974000
1	-0.263144000	8.106568000	-1.281743000
1	0.996271000	7.739867000	-2.457688000
1	-0.705687000	7.635738000	-2.931286000
Zero-point correction=			0.620484 (Hartree/Particle)
Thermal correction to Energy=			0.660771
Thermal correction to Enthalpy=			0.661715
Thermal correction to Gibbs Free Energy=			0.546240

Sum of electronic and zero-point Energies=	-2676.078962
Sum of electronic and thermal Energies=	-2676.038675
Sum of electronic and thermal Enthalpies=	-2676.037731
Sum of electronic and thermal Free Energies=	-2676.153206

B-4d

6	-0.722833000	-2.032104000	3.847383000
6	-0.050285000	-0.815912000	3.890877000
6	0.928080000	-0.560884000	2.937797000
6	1.257872000	-1.511641000	1.943780000
6	0.536038000	-2.701523000	1.878846000
6	-0.435398000	-2.957238000	2.844929000
1	-1.486433000	-2.257510000	4.588681000
1	-0.290424000	-0.071279000	4.647728000
1	0.696715000	-3.424607000	1.084460000
1	-0.979742000	-3.899757000	2.813332000
6	1.736589000	0.618882000	2.712306000
6	2.534059000	0.438881000	1.614401000
6	2.278024000	-0.915187000	1.065817000
1	0.581525000	1.564488000	1.235243000
6	2.880441000	-1.510990000	-0.010552000
6	3.586833000	-0.726472000	-1.036555000
6	3.016609000	0.455231000	-1.526761000
6	4.828662000	-1.129342000	-1.545530000
6	3.688353000	1.234870000	-2.457126000
1	2.033536000	0.756697000	-1.168164000
6	5.503035000	-0.345983000	-2.471002000
1	5.294119000	-2.041028000	-1.175289000
6	4.937590000	0.841808000	-2.925232000
1	3.232798000	2.154491000	-2.816051000
1	6.477102000	-0.661822000	-2.837141000
1	5.466636000	1.454565000	-3.651202000
6	2.825119000	-2.990479000	-0.227397000
1	2.781469000	-3.543818000	0.714644000
1	1.792781000	1.477283000	3.378246000
1	3.696198000	-3.331877000	-0.794712000
16	-1.073101000	-2.833552000	-1.931630000
8	-1.263360000	-2.499237000	-3.331008000
8	0.088643000	-1.908072000	-1.322731000
8	-0.715683000	-4.173638000	-1.511084000
1	1.942318000	-3.256812000	-0.824511000
6	-2.496640000	-2.286075000	-1.035531000
6	-3.271966000	-1.257874000	-1.560920000
6	-4.308055000	-0.742157000	-0.794689000

6	-4.581310000	-1.248705000	0.478540000
6	-3.797094000	-2.294567000	0.970529000
6	-2.751098000	-2.814462000	0.223665000
1	-3.046252000	-0.863455000	-2.549300000
1	-4.910315000	0.079541000	-1.183445000
1	-3.997146000	-2.691505000	1.965022000
1	-2.123391000	-3.614193000	0.607620000
6	-5.707118000	-0.689932000	1.293964000
1	-5.486939000	-0.737910000	2.365961000
1	-5.908404000	0.355099000	1.031003000
1	-6.635441000	-1.251304000	1.128236000
16	-1.075993000	1.094558000	-0.025630000
8	-0.039820000	2.097932000	0.670957000
8	-1.397936000	0.042493000	0.914495000
8	-0.551241000	0.744145000	-1.349993000
1	-0.085055000	-0.958233000	-1.520572000
6	-2.466297000	2.146809000	-0.264767000
6	-3.363469000	2.308109000	0.787533000
6	-4.500066000	3.073734000	0.581786000
6	-4.753126000	3.670374000	-0.658925000
6	-3.838665000	3.479530000	-1.696399000
6	-2.691367000	2.718739000	-1.510249000
1	-3.181719000	1.810500000	1.737738000
1	-5.215901000	3.205827000	1.391926000
1	-4.033616000	3.929153000	-2.668202000
1	-1.984772000	2.548081000	-2.318080000
6	-5.978478000	4.507584000	-0.858970000
1	-6.199358000	4.652143000	-1.920790000
1	-6.855726000	4.053838000	-0.385274000
1	-5.850074000	5.500775000	-0.411011000
6	3.595854000	1.395014000	1.246586000
6	3.294716000	2.744552000	1.038441000
6	4.931298000	0.988377000	1.149675000
6	4.293418000	3.654341000	0.710590000
1	2.260811000	3.081082000	1.098514000
6	5.926677000	1.895150000	0.816022000
1	5.184378000	-0.053502000	1.335176000
6	5.611611000	3.232013000	0.588719000
1	4.035683000	4.697252000	0.540202000
1	6.957460000	1.556874000	0.738235000
1	6.392168000	3.941017000	0.323371000
Zero-point correction=			0.625147 (Hartree/Particle)
Thermal correction to Energy=			0.666208
Thermal correction to Enthalpy=			0.667153

Thermal correction to Gibbs Free Energy=	0.551172
Sum of electronic and zero-point Energies=	-2676.114492
Sum of electronic and thermal Energies=	-2676.073430
Sum of electronic and thermal Enthalpies=	-2676.072486
Sum of electronic and thermal Free Energies=	-2676.188467

B-TSd5

6	-0.478986000	-1.141260000	4.338645000
6	0.110820000	0.074380000	4.015137000
6	1.040771000	0.108840000	2.987660000
6	1.397101000	-1.054264000	2.276095000
6	0.754985000	-2.258642000	2.571141000
6	-0.165922000	-2.291264000	3.613850000
1	-1.202976000	-1.194202000	5.148350000
1	-0.164471000	0.986328000	4.540670000
1	0.930643000	-3.163319000	1.997735000
1	-0.653456000	-3.232266000	3.859071000
6	1.722281000	1.257909000	2.375011000
6	2.605539000	0.742479000	1.391684000
6	2.350946000	-0.664700000	1.223781000
1	0.861839000	1.741762000	1.516513000
6	2.889316000	-1.484021000	0.238237000
6	3.639110000	1.582956000	0.786247000
6	4.968293000	1.149678000	0.710769000
6	3.313249000	2.868365000	0.335694000
6	5.946844000	1.978917000	0.182765000
1	5.230767000	0.161690000	1.083613000
6	4.294408000	3.686141000	-0.208036000
1	2.275970000	3.197100000	0.366973000
6	5.611621000	3.245407000	-0.286645000
1	6.976995000	1.634347000	0.137212000
1	4.026541000	4.673303000	-0.576553000
6	3.402855000	-0.946866000	-1.019331000
6	2.730891000	0.105909000	-1.662141000
6	4.559259000	-1.474687000	-1.616479000
6	3.223833000	0.633515000	-2.845307000
1	1.801406000	0.490540000	-1.244634000
6	5.058015000	-0.930755000	-2.789022000
1	5.102369000	-2.281134000	-1.128167000
6	4.390529000	0.124470000	-3.406296000
1	2.685475000	1.440270000	-3.335274000
1	5.970085000	-1.330374000	-3.224973000
1	4.776024000	0.541214000	-4.333741000
6	2.895445000	-2.959858000	0.405191000

1	3.021096000	-3.258640000	1.449694000
1	1.997918000	2.147180000	2.944569000
1	3.662951000	-3.433879000	-0.211634000
1	6.378023000	3.890528000	-0.709139000
16	-0.739180000	-3.068310000	-1.219000000
8	-0.698172000	-3.239340000	-2.660094000
8	0.158671000	-1.830385000	-0.774914000
8	-0.301071000	-4.146472000	-0.345399000
1	1.930032000	-3.361343000	0.054333000
6	-2.365838000	-2.531864000	-0.771847000
6	-3.334875000	-2.380327000	-1.757386000
6	-4.595826000	-1.923226000	-1.391704000
6	-4.888017000	-1.608769000	-0.062375000
6	-3.895013000	-1.780496000	0.906068000
6	-2.634940000	-2.241517000	0.562135000
1	-3.091375000	-2.616520000	-2.789722000
1	-5.366404000	-1.798511000	-2.151424000
1	-4.105962000	-1.522249000	1.942503000
1	-1.852718000	-2.342849000	1.310838000
6	-6.221014000	-1.043432000	0.320600000
1	-6.602965000	-1.498619000	1.241102000
1	-6.138443000	0.036099000	0.506690000
1	-6.966190000	-1.189449000	-0.468215000
16	-1.017959000	1.271307000	0.128364000
8	0.015333000	2.282369000	0.610866000
8	-1.374081000	0.318185000	1.175035000
8	-0.593917000	0.653728000	-1.156301000
1	-0.212703000	-0.939479000	-1.045253000
6	-2.453386000	2.230648000	-0.265175000
6	-2.565778000	3.568863000	0.076704000
6	-3.747978000	4.242596000	-0.217679000
6	-4.812411000	3.593555000	-0.840544000
6	-4.671739000	2.240017000	-1.170771000
6	-3.501615000	1.555638000	-0.889253000
1	-1.733238000	4.070891000	0.561515000
1	-3.845840000	5.295735000	0.041183000
1	-5.492926000	1.721148000	-1.666768000
1	-3.393815000	0.504443000	-1.155319000
6	-6.084060000	4.318698000	-1.160524000
1	-6.945784000	3.842593000	-0.677372000
1	-6.048357000	5.361364000	-0.830125000
1	-6.282667000	4.315467000	-2.239046000
Zero-point correction=			0.620362 (Hartree/Particle)
Thermal correction to Energy=			0.660592

Thermal correction to Enthalpy=	0.661536
Thermal correction to Gibbs Free Energy=	0.547160
Sum of electronic and zero-point Energies=	-2676.096644
Sum of electronic and thermal Energies=	-2676.056414
Sum of electronic and thermal Enthalpies=	-2676.055470
Sum of electronic and thermal Free Energies=	-2676.169846

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6	-0.290024000	4.164971000	2.762825000
6	-0.370780000	2.840720000	3.184193000
6	-1.106646000	1.945033000	2.428376000
6	-1.756020000	2.332220000	1.244588000
6	-1.645625000	3.656363000	0.815094000
6	-0.921374000	4.561072000	1.587004000
1	0.269252000	4.889823000	3.349525000
1	0.129747000	2.512782000	4.092973000
1	-2.077572000	4.006237000	-0.112925000
1	-0.844341000	5.592822000	1.253276000
6	-1.340918000	0.496512000	2.676881000
6	-2.287770000	0.091828000	1.610464000
6	-2.445704000	1.140747000	0.689316000
1	-0.418600000	-0.086956000	2.479121000
6	-3.097861000	1.047454000	-0.562816000
6	-3.329356000	-0.217953000	-1.226818000
6	-2.387677000	-1.254712000	-1.121982000
6	-4.491733000	-0.434812000	-1.992515000
6	-2.598702000	-2.475777000	-1.733757000
1	-1.464908000	-1.081795000	-0.583582000
6	-4.717124000	-1.667633000	-2.578841000
1	-5.245617000	0.344681000	-2.074933000
6	-3.770835000	-2.686657000	-2.454675000
1	-1.832600000	-3.241327000	-1.635965000
1	-5.631528000	-1.839610000	-3.140427000
1	-3.947624000	-3.646222000	-2.934904000
6	-3.472657000	2.281476000	-1.283905000
1	-3.891901000	3.046015000	-0.622830000
1	-1.693708000	0.232650000	3.681467000
1	-4.141701000	2.089808000	-2.124303000
16	0.432934000	2.176474000	-2.329349000
8	0.906220000	1.899074000	-3.673019000
8	-0.490301000	0.984757000	-1.825405000
8	-0.346676000	3.379949000	-2.062846000
1	-2.536002000	2.688513000	-1.712651000
6	1.811274000	2.098423000	-1.223547000

6	2.836652000	1.196515000	-1.496695000
6	3.862883000	1.054127000	-0.577122000
6	3.881855000	1.803201000	0.603198000
6	2.846287000	2.705428000	0.844264000
6	1.804030000	2.856130000	-0.061428000
1	2.808987000	0.596028000	-2.402561000
1	4.657706000	0.331765000	-0.762425000
1	2.853503000	3.295339000	1.759945000
1	0.987203000	3.549092000	0.125965000
6	5.003793000	1.631141000	1.580212000
1	4.790162000	2.125252000	2.533571000
1	5.188609000	0.567193000	1.775599000
1	5.939478000	2.051303000	1.190323000
16	0.983997000	-1.665319000	-0.180019000
8	0.240177000	-2.899948000	0.126268000
8	0.714793000	-0.557292000	0.765784000
8	0.811431000	-1.232778000	-1.605844000
1	0.030065000	0.109483000	-1.783724000
6	2.719981000	-2.041650000	-0.044009000
6	3.369523000	-1.868153000	1.171616000
6	4.716484000	-2.194512000	1.278976000
6	5.427785000	-2.689155000	0.183421000
6	4.754178000	-2.846985000	-1.031269000
6	3.407206000	-2.532365000	-1.149113000
1	2.820567000	-1.450102000	2.012450000
1	5.231589000	-2.059360000	2.230280000
1	5.299813000	-3.219153000	-1.897715000
1	2.885381000	-2.636601000	-2.097176000
6	6.874119000	-3.062774000	0.307914000
1	7.434390000	-2.811344000	-0.599424000
1	7.350873000	-2.554580000	1.152728000
1	6.991907000	-4.142048000	0.468527000
6	-2.968831000	-1.189443000	1.718284000
6	-2.227208000	-2.332686000	2.048105000
6	-4.356571000	-1.290788000	1.545648000
6	-2.863366000	-3.561422000	2.151426000
1	-1.142112000	-2.273471000	2.111660000
6	-4.986836000	-2.516834000	1.681888000
1	-4.935595000	-0.397849000	1.318137000
6	-4.240434000	-3.655821000	1.977029000
1	-2.273714000	-4.450111000	2.359118000
1	-6.064561000	-2.586585000	1.558605000
1	-4.735181000	-4.619639000	2.069272000
Zero-point correction=			0.625716 (Hartree/Particle)

Thermal correction to Energy=	0.665986
Thermal correction to Enthalpy=	0.666930
Thermal correction to Gibbs Free Energy=	0.554369
Sum of electronic and zero-point Energies=	-2676.106835
Sum of electronic and thermal Energies=	-2676.066565
Sum of electronic and thermal Enthalpies=	-2676.065621
Sum of electronic and thermal Free Energies=	-2676.178182

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6	0.466317000	-4.104778000	1.946161000
6	-0.472703000	-4.109886000	0.918864000
6	-1.263912000	-2.987051000	0.735458000
6	-1.088273000	-1.853275000	1.542177000
6	-0.126613000	-1.837758000	2.552156000
6	0.636121000	-2.978826000	2.756313000
1	1.078809000	-4.986549000	2.119007000
1	-0.585725000	-4.979750000	0.275609000
1	0.034609000	-0.950993000	3.159119000
1	1.382091000	-2.993087000	3.547129000
6	-2.851072000	-1.375823000	0.042745000
6	-1.939245000	-0.803904000	1.011473000
6	-1.828910000	0.577797000	1.065165000
6	-2.407940000	1.149430000	-0.103653000
6	-3.033832000	2.412049000	-0.144923000
6	-2.499989000	0.264671000	-1.234984000
6	-3.898706000	2.690318000	-1.173314000
1	-2.887671000	3.115886000	0.670488000
6	-3.394434000	0.597917000	-2.284503000
1	-1.613329000	-0.331685000	-1.508039000
6	-4.103749000	1.768567000	-2.231359000
1	-4.447094000	3.628784000	-1.175589000
1	-3.469728000	-0.057562000	-3.148620000
1	-4.780185000	2.035697000	-3.039418000
6	-1.126507000	1.339906000	2.124537000
1	-1.475495000	1.068905000	3.127727000
1	-0.058465000	1.084322000	2.050029000
1	-1.199781000	2.422864000	1.986409000
16	0.952598000	3.799370000	0.027612000
8	1.568113000	4.621110000	-0.998198000
8	-0.040645000	2.754624000	-0.646944000
8	0.174565000	4.404950000	1.097822000
6	2.208209000	2.767672000	0.735446000
6	3.154561000	2.188987000	-0.103425000
6	4.070363000	1.296336000	0.430830000

6	4.058615000	0.980111000	1.791090000
6	3.126215000	1.608484000	2.618593000
6	2.196587000	2.499866000	2.098383000
1	3.151291000	2.413067000	-1.167545000
1	4.799916000	0.818058000	-0.222386000
1	3.128398000	1.390644000	3.686007000
1	1.467613000	2.995022000	2.735429000
6	5.001463000	-0.048348000	2.335115000
1	5.207251000	0.107286000	3.399531000
1	4.572317000	-1.053388000	2.221820000
1	5.954387000	-0.047994000	1.794379000
16	1.020838000	-0.398759000	-1.210106000
8	0.043115000	-1.398807000	-1.710271000
8	0.866854000	-0.096510000	0.222249000
8	1.054408000	0.828541000	-2.062313000
1	0.420761000	2.096285000	-1.256090000
6	2.628695000	-1.140840000	-1.371615000
6	3.042678000	-2.037210000	-0.388872000
6	4.299418000	-2.614730000	-0.484449000
6	5.154596000	-2.309814000	-1.549738000
6	4.714003000	-1.413538000	-2.523135000
6	3.454205000	-0.826959000	-2.441055000
1	2.381558000	-2.253506000	0.450331000
1	4.636279000	-3.313073000	0.282274000
1	5.371261000	-1.167376000	-3.356080000
1	3.110109000	-0.111795000	-3.184522000
6	6.513046000	-2.938927000	-1.630912000
1	7.068348000	-2.587119000	-2.506023000
1	7.112312000	-2.712013000	-0.740517000
1	6.443251000	-4.031564000	-1.696815000
6	-2.294726000	-2.735130000	-0.328872000
1	-1.776257000	-2.676201000	-1.298832000
1	-3.067217000	-3.509296000	-0.386940000
6	-4.324824000	-1.219259000	0.089157000
6	-5.112356000	-1.819072000	-0.902147000
6	-4.961889000	-0.504134000	1.108228000
6	-6.492650000	-1.695295000	-0.884211000
1	-4.629062000	-2.366252000	-1.710795000
6	-6.346113000	-0.383936000	1.126115000
1	-4.370011000	-0.056416000	1.902900000
6	-7.116163000	-0.975693000	0.132138000
1	-7.085693000	-2.162932000	-1.666124000
1	-6.825036000	0.166751000	1.931868000
1	-8.198996000	-0.883608000	0.151583000

Zero-point correction=	0.624713 (Hartree/Particle)
Thermal correction to Energy=	0.664410
Thermal correction to Enthalpy=	0.665355
Thermal correction to Gibbs Free Energy=	0.553461
Sum of electronic and zero-point Energies=	-2676.076160
Sum of electronic and thermal Energies=	-2676.036462
Sum of electronic and thermal Enthalpies=	-2676.035518
Sum of electronic and thermal Free Energies=	-2676.147411

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6	-0.673648000	-4.233780000	2.015577000
6	-1.380132000	-4.042375000	0.831359000
6	-1.844982000	-2.771479000	0.528688000
6	-1.592930000	-1.705211000	1.414552000
6	-0.853730000	-1.893329000	2.586546000
6	-0.407344000	-3.169892000	2.884719000
1	-0.312201000	-5.228342000	2.267019000
1	-1.555251000	-4.873302000	0.151547000
1	-0.633834000	-1.054215000	3.241665000
1	0.158895000	-3.349184000	3.794831000
6	-2.969023000	-0.859274000	-0.363099000
6	-2.086464000	-0.512269000	0.798916000
6	-1.810858000	0.836854000	0.892321000
6	-2.273467000	1.414048000	-0.311686000
6	-2.409253000	2.774148000	-0.645820000
6	-2.639643000	0.362330000	-1.295150000
6	-3.107464000	3.096100000	-1.780963000
1	-2.017637000	3.544942000	0.011519000
6	-3.488320000	0.792108000	-2.411880000
1	-1.663084000	0.055362000	-1.769342000
6	-3.675661000	2.111339000	-2.651985000
1	-3.261392000	4.145792000	-2.021956000
1	-3.865154000	0.042316000	-3.104202000
1	-4.235166000	2.441981000	-3.522483000
6	-1.062688000	1.513465000	1.984421000
1	-1.548868000	1.365059000	2.956843000
1	-0.053035000	1.082205000	2.026350000
1	-0.941694000	2.587456000	1.812936000
16	1.594548000	3.786546000	0.302645000
8	2.368335000	4.569556000	-0.643639000
8	0.484481000	2.953473000	-0.474886000
8	0.877156000	4.434816000	1.389531000
6	2.647046000	2.524778000	0.965272000
6	3.543447000	1.881055000	0.115255000

6	4.293357000	0.825075000	0.605959000
6	4.172847000	0.412977000	1.936538000
6	3.290274000	1.095226000	2.773555000
6	2.519944000	2.148744000	2.295145000
1	3.625402000	2.189004000	-0.924222000
1	4.972700000	0.291466000	-0.059196000
1	3.202587000	0.790889000	3.815684000
1	1.828137000	2.686015000	2.939336000
6	4.988760000	-0.739163000	2.436724000
1	4.692516000	-1.038256000	3.447310000
1	4.878735000	-1.606723000	1.773248000
1	6.056831000	-0.489649000	2.462035000
16	1.056396000	-0.310180000	-1.231484000
8	-0.022091000	-1.054184000	-1.934834000
8	0.831702000	-0.175236000	0.215100000
8	1.357845000	0.984116000	-1.916164000
1	0.876599000	2.246373000	-1.083582000
6	2.536773000	-1.281587000	-1.393936000
6	2.794036000	-2.259417000	-0.439718000
6	3.947440000	-3.026760000	-0.546788000
6	4.852011000	-2.825386000	-1.592166000
6	4.574409000	-1.829480000	-2.532622000
6	3.421671000	-1.059852000	-2.442493000
1	2.099666000	-2.385829000	0.390258000
1	4.158183000	-3.794277000	0.197947000
1	5.279107000	-1.654845000	-3.344994000
1	3.210556000	-0.271592000	-3.160637000
6	6.085534000	-3.667852000	-1.717649000
1	6.954229000	-3.068249000	-2.011921000
1	6.325427000	-4.173553000	-0.776615000
1	5.958823000	-4.443835000	-2.483288000
6	-2.528717000	-2.297114000	-0.725186000
1	-1.785540000	-2.272725000	-1.533556000
1	-3.358471000	-2.946508000	-1.023441000
6	-4.457236000	-0.816715000	0.000496000
6	-5.393928000	-1.296133000	-0.921137000
6	-4.925707000	-0.302701000	1.209897000
6	-6.754398000	-1.251833000	-0.649686000
1	-5.054780000	-1.718420000	-1.866515000
6	-6.289407000	-0.262711000	1.486157000
1	-4.224265000	0.070792000	1.951851000
6	-7.208676000	-0.733616000	0.559030000
1	-7.462363000	-1.629732000	-1.383489000
1	-6.630200000	0.138275000	2.437748000

1	-8.273209000	-0.702779000	0.776885000
Zero-point correction=			0.625403 (Hartree/Particle)
Thermal correction to Energy=			0.665841
Thermal correction to Enthalpy=			0.666785
Thermal correction to Gibbs Free Energy=			0.550228
Sum of electronic and zero-point Energies=			-2676.094026
Sum of electronic and thermal Energies=			-2676.053589
Sum of electronic and thermal Enthalpies=			-2676.052644
Sum of electronic and thermal Free Energies=			-2676.169202

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6	-1.706635000	-3.697476000	2.939115000
6	-2.005748000	-3.603239000	1.580323000
6	-2.196687000	-2.349877000	1.023136000
6	-2.084929000	-1.196528000	1.823181000
6	-1.762335000	-1.291216000	3.176061000
6	-1.583337000	-2.553697000	3.728442000
1	-1.565398000	-4.676688000	3.390951000
1	-2.086541000	-4.500057000	0.969061000
1	-1.671923000	-0.399432000	3.791569000
1	-1.347679000	-2.652620000	4.785052000
6	-2.964892000	-0.520377000	-0.310129000
6	-2.298266000	-0.058847000	0.960734000
6	-1.810606000	1.212589000	0.899399000
6	-2.007090000	1.661304000	-0.449763000
6	-1.735549000	2.906977000	-1.025598000
6	-2.482987000	0.571345000	-1.288471000
6	-2.102759000	3.117865000	-2.340866000
1	-1.261281000	3.694369000	-0.446884000
6	-3.013356000	0.900726000	-2.584699000
1	-1.410905000	0.144827000	-1.705151000
6	-2.764432000	2.136917000	-3.116258000
1	-1.897276000	4.085857000	-2.792895000
1	-3.486629000	0.123203000	-3.180868000
1	-3.059196000	2.369638000	-4.135103000
6	-1.032739000	1.919456000	1.954061000
1	-1.613497000	2.047361000	2.874561000
1	-0.136815000	1.325955000	2.185666000
1	-0.678049000	2.900528000	1.626754000
16	2.489190000	3.525962000	0.706764000
8	3.445695000	4.085615000	-0.230815000
8	1.146456000	3.145272000	-0.074664000
8	2.044330000	4.275059000	1.866718000
6	3.098210000	1.949359000	1.234692000

6	3.908563000	1.209642000	0.378979000
6	4.311162000	-0.059382000	0.766297000
6	3.922549000	-0.593311000	1.998261000
6	3.124121000	0.178321000	2.843693000
6	2.705217000	1.447731000	2.468450000
1	4.203028000	1.625849000	-0.581347000
1	4.924578000	-0.658578000	0.092816000
1	2.823645000	-0.227287000	3.808637000
1	2.089145000	2.061297000	3.121781000
6	4.373419000	-1.964075000	2.400122000
1	5.429024000	-1.964033000	2.700141000
1	3.790597000	-2.348987000	3.243082000
1	4.276576000	-2.668256000	1.564631000
16	1.016292000	-0.055820000	-1.347378000
8	-0.154409000	-0.485256000	-2.207156000
8	0.677192000	-0.084990000	0.078392000
8	1.594368000	1.223389000	-1.832330000
1	1.333649000	2.477321000	-0.797887000
6	2.261493000	-1.288803000	-1.622839000
6	2.225886000	-2.449999000	-0.860041000
6	3.203967000	-3.417268000	-1.052227000
6	4.220619000	-3.235070000	-1.993465000
6	4.237191000	-2.053881000	-2.740131000
6	3.262356000	-1.080544000	-2.564335000
1	1.454331000	-2.568513000	-0.101037000
1	3.187798000	-4.329150000	-0.456032000
1	5.031247000	-1.896205000	-3.468927000
1	3.280132000	-0.152366000	-3.129842000
6	5.263396000	-4.288681000	-2.214243000
1	6.251523000	-3.846582000	-2.382526000
1	5.335967000	-4.969582000	-1.360098000
1	5.029067000	-4.896021000	-3.097646000
6	-2.452928000	-1.983100000	-0.416256000
1	-1.509329000	-2.005484000	-0.980288000
1	-3.156709000	-2.662052000	-0.909605000
6	-4.492157000	-0.482762000	-0.230746000
6	-5.247906000	-1.100346000	-1.231592000
6	-5.165778000	0.192393000	0.786604000
6	-6.635285000	-1.043497000	-1.218448000
1	-4.745476000	-1.638082000	-2.035580000
6	-6.556283000	0.246010000	0.804419000
1	-4.600228000	0.681867000	1.575912000
6	-7.296276000	-0.369596000	-0.196333000
1	-7.201648000	-1.531663000	-2.008104000

1	-7.061238000	0.772187000	1.611124000
1	-8.382402000	-0.327979000	-0.180418000
Zero-point correction=			0.622909 (Hartree/Particle)
Thermal correction to Energy=			0.662358
Thermal correction to Enthalpy=			0.663302
Thermal correction to Gibbs Free Energy=			0.551556
Sum of electronic and zero-point Energies=			-2676.096031
Sum of electronic and thermal Energies=			-2676.056582
Sum of electronic and thermal Enthalpies=			-2676.055638
Sum of electronic and thermal Free Energies=			-2676.167384

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6	-0.948650000	-3.580535000	2.235753000
6	-1.491037000	-3.301404000	0.979561000
6	-1.873436000	-2.002688000	0.682652000
6	-1.732131000	-0.977306000	1.639366000
6	-1.183890000	-1.258874000	2.888943000
6	-0.794374000	-2.564709000	3.177980000
1	-0.651428000	-4.597198000	2.484495000
1	-1.603267000	-4.090973000	0.237089000
1	-1.082405000	-0.478083000	3.640254000
1	-0.371426000	-2.795761000	4.153885000
6	-2.975243000	-0.078708000	-0.223573000
6	-2.151721000	0.261862000	1.006220000
6	-1.673814000	1.524660000	0.975702000
6	-2.039861000	2.100849000	-0.321465000
6	-1.669133000	3.317997000	-0.884816000
6	-2.736965000	1.141881000	-1.087304000
6	-2.012547000	3.576771000	-2.212411000
1	-1.099141000	4.046307000	-0.311016000
6	-3.090783000	1.412870000	-2.399214000
1	-0.766292000	0.808055000	-2.337153000
6	-2.714288000	2.638278000	-2.964202000
1	-1.717953000	4.518537000	-2.668808000
1	-3.632437000	0.679188000	-2.994985000
1	-2.961758000	2.851369000	-4.001030000
6	-0.748890000	2.190394000	1.925858000
1	-1.240550000	3.014367000	2.459323000
1	-0.370388000	1.482470000	2.671354000
1	0.114750000	2.612235000	1.392872000
16	3.403260000	3.157608000	0.770992000
8	4.577080000	3.312954000	-0.067395000
8	2.091438000	3.319426000	-0.150486000
8	3.155281000	4.008241000	1.914691000

6	3.320015000	1.463495000	1.287120000
6	4.000562000	0.492851000	0.561911000
6	3.871635000	-0.839399000	0.936748000
6	3.062202000	-1.209745000	2.012037000
6	2.397991000	-0.209594000	2.729290000
6	2.530214000	1.125301000	2.381189000
1	4.621101000	0.787453000	-0.281229000
1	4.397050000	-1.611237000	0.374859000
1	1.766900000	-0.491072000	3.572753000
1	2.034980000	1.910612000	2.947013000
6	2.882420000	-2.648944000	2.384175000
1	1.882718000	-3.001160000	2.091635000
1	3.620399000	-3.290009000	1.890229000
1	2.966691000	-2.797014000	3.467130000
16	1.194614000	0.344228000	-1.588928000
8	0.002007000	0.294280000	-2.671440000
8	0.610869000	0.527345000	-0.276298000
8	2.198797000	1.295021000	-2.064317000
1	2.203014000	2.782855000	-0.968111000
6	1.838633000	-1.286582000	-1.739478000
6	1.368078000	-2.264123000	-0.866208000
6	1.888337000	-3.545315000	-0.966658000
6	2.872836000	-3.854399000	-1.911011000
6	3.334832000	-2.843728000	-2.758360000
6	2.823415000	-1.555070000	-2.681660000
1	0.628911000	-2.020819000	-0.101391000
1	1.532239000	-4.320115000	-0.287947000
1	4.111873000	-3.071684000	-3.485515000
1	3.190389000	-0.760827000	-3.326591000
6	3.410656000	-5.247940000	-2.017956000
1	2.738716000	-5.881649000	-2.610132000
1	4.390092000	-5.265874000	-2.505815000
1	3.509719000	-5.716420000	-1.032951000
6	-2.373004000	-1.449837000	-0.630836000
1	-1.529233000	-1.309427000	-1.323607000
1	-3.088783000	-2.114056000	-1.128079000
6	-4.470727000	-0.215533000	0.070452000
6	-5.321510000	-0.771440000	-0.889163000
6	-5.030629000	0.244142000	1.261932000
6	-6.687982000	-0.873113000	-0.663097000
1	-4.913037000	-1.134963000	-1.831968000
6	-6.398627000	0.139855000	1.493280000
1	-4.385871000	0.687324000	2.017512000
6	-7.232926000	-0.419823000	0.533958000

1	-7.329814000	-1.309785000	-1.424901000
1	-6.811869000	0.498700000	2.433267000
1	-8.301583000	-0.503254000	0.716197000
Zero-point correction=			0.627521 (Hartree/Particle)
Thermal correction to Energy=			0.667763
Thermal correction to Enthalpy=			0.668708
Thermal correction to Gibbs Free Energy=			0.555254
Sum of electronic and zero-point Energies=			-2676.131302
Sum of electronic and thermal Energies=			-2676.091060
Sum of electronic and thermal Enthalpies=			-2676.090115
Sum of electronic and thermal Free Energies=			-2676.203569

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6	-0.644194000	-2.372037000	3.737904000
6	0.024633000	-1.177566000	3.876435000
6	0.921957000	-0.797883000	2.862798000
6	1.153662000	-1.617226000	1.722067000
6	0.425770000	-2.804654000	1.578616000
6	-0.445293000	-3.166530000	2.591867000
1	-1.345457000	-2.700588000	4.500522000
1	-0.140871000	-0.530401000	4.734699000
1	0.495999000	-3.418857000	0.685156000
1	-1.002258000	-4.096670000	2.493908000
6	1.659744000	0.386786000	2.704948000
6	2.266386000	0.446064000	1.425412000
6	2.073751000	-0.929235000	0.837393000
1	1.317978000	1.156681000	0.903145000
6	2.718008000	-1.436148000	-0.251731000
6	3.434723000	-0.561357000	-1.199661000
6	2.731118000	0.400649000	-1.930454000
6	4.810046000	-0.712486000	-1.410526000
6	3.397174000	1.192440000	-2.858796000
1	1.657828000	0.514724000	-1.785333000
6	5.476057000	0.107099000	-2.309902000
1	5.362385000	-1.454182000	-0.834694000
6	4.767664000	1.054923000	-3.044402000
1	2.837308000	1.924669000	-3.435398000
1	6.549448000	0.000084000	-2.446570000
1	5.286987000	1.683979000	-3.763556000
6	2.745109000	-2.895254000	-0.569748000
1	2.647937000	-3.525725000	0.318319000
1	1.722166000	1.194398000	3.431004000
1	3.671519000	-3.152547000	-1.094037000
16	-1.371791000	-2.867505000	-1.867073000

8	-1.651062000	-2.761308000	-3.286998000
8	-0.141761000	-1.919533000	-1.495115000
8	-1.034098000	-4.146628000	-1.265633000
1	1.915148000	-3.134319000	-1.250898000
6	-2.725689000	-2.140871000	-0.985668000
6	-3.372949000	-1.031097000	-1.525113000
6	-4.377827000	-0.419654000	-0.792252000
6	-4.757000000	-0.912564000	0.460998000
6	-4.110466000	-2.040845000	0.963520000
6	-3.090524000	-2.656671000	0.249215000
1	-3.077934000	-0.648548000	-2.499443000
1	-4.871811000	0.469065000	-1.186127000
1	-4.409151000	-2.438089000	1.932549000
1	-2.579764000	-3.535638000	0.632579000
6	-5.842462000	-0.229643000	1.235057000
1	-5.971271000	-0.670817000	2.228551000
1	-5.617189000	0.837836000	1.360465000
1	-6.805250000	-0.292553000	0.713238000
16	-0.804093000	1.121713000	-0.166573000
8	0.394608000	1.957901000	0.255237000
8	-1.089789000	0.067515000	0.805541000
8	-0.647133000	0.669784000	-1.575149000
1	-0.353010000	-0.952345000	-1.635236000
6	-2.179653000	2.237823000	-0.183644000
6	-2.983195000	2.333840000	0.947364000
6	-4.081415000	3.182027000	0.924553000
6	-4.392678000	3.929452000	-0.215489000
6	-3.574437000	3.804835000	-1.339905000
6	-2.468271000	2.964531000	-1.331999000
1	-2.754876000	1.723445000	1.818165000
1	-4.718526000	3.264075000	1.805119000
1	-3.814782000	4.372440000	-2.237524000
1	-1.842797000	2.848085000	-2.213034000
6	-5.571677000	4.854227000	-0.218283000
1	-5.878476000	5.112756000	-1.236656000
1	-6.431887000	4.409550000	0.294195000
1	-5.337828000	5.791729000	0.301745000
6	3.546303000	1.212375000	1.271278000
6	3.642327000	2.360392000	0.486820000
6	4.682557000	0.746479000	1.939314000
6	4.860412000	3.019166000	0.359136000
1	2.760573000	2.723850000	-0.037582000
6	5.898660000	1.404302000	1.811367000
1	4.604888000	-0.155357000	2.547303000

6	5.989473000	2.543239000	1.016658000
1	4.926309000	3.909460000	-0.261991000
1	6.776737000	1.028219000	2.331551000
1	6.941121000	3.058835000	0.910235000
Zero-point correction=			0.619186 (Hartree/Particle)
Thermal correction to Energy=			0.658914
Thermal correction to Enthalpy=			0.659858
Thermal correction to Gibbs Free Energy=			0.547492
Sum of electronic and zero-point Energies=			-2676.092430
Sum of electronic and thermal Energies=			-2676.052702
Sum of electronic and thermal Enthalpies=			-2676.051758
Sum of electronic and thermal Free Energies=			-2676.164124

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6	-1.604380000	2.024553000	3.128300000
6	-0.730901000	2.683681000	2.309891000
6	0.289244000	1.926788000	1.674022000
6	0.436802000	0.511846000	1.899221000
6	-0.529409000	-0.145519000	2.682273000
6	-1.510781000	0.616187000	3.281813000
1	-2.405036000	2.562152000	3.629565000
1	-0.814389000	3.750567000	2.114642000
1	-0.545399000	-1.227347000	2.773529000
1	-2.258119000	0.112770000	3.891957000
6	1.220218000	2.320625000	0.738958000
6	2.016668000	1.182427000	0.266110000
6	1.554355000	0.030621000	1.143221000
1	1.629510000	0.991625000	-0.768690000
6	2.146098000	-1.202633000	1.190884000
6	3.144140000	-1.587532000	0.181790000
6	2.825848000	-1.544836000	-1.181274000
6	4.420538000	-2.011266000	0.575941000
6	3.770950000	-1.921511000	-2.127453000
1	1.833676000	-1.228292000	-1.494599000
6	5.371539000	-2.346424000	-0.375504000
1	4.678986000	-2.030078000	1.633575000
6	5.044890000	-2.310294000	-1.729531000
1	3.504920000	-1.900393000	-3.181108000
1	6.369506000	-2.642535000	-0.062005000
1	5.786379000	-2.590964000	-2.473827000
6	1.846368000	-2.210224000	2.244624000
1	1.530962000	-1.761476000	3.190929000
1	1.353569000	3.333147000	0.364239000
1	2.713649000	-2.854303000	2.420574000

16	-1.692139000	-3.472230000	0.489228000
8	-2.093447000	-4.842815000	0.251007000
8	-0.609063000	-3.117818000	-0.599719000
8	-1.202373000	-3.109173000	1.820805000
1	1.029897000	-2.865397000	1.901470000
6	-3.016542000	-2.355739000	0.106696000
6	-3.359187000	-2.108952000	-1.219583000
6	-4.405705000	-1.242574000	-1.492698000
6	-5.126063000	-0.631130000	-0.462065000
6	-4.771900000	-0.907320000	0.859962000
6	-3.717425000	-1.765340000	1.151289000
1	-2.781549000	-2.547100000	-2.029023000
1	-4.648367000	-1.011903000	-2.528524000
1	-5.325983000	-0.435482000	1.670846000
1	-3.424251000	-1.975314000	2.177049000
6	-6.220041000	0.339622000	-0.785148000
1	-6.930927000	-0.081998000	-1.504752000
1	-6.777549000	0.635063000	0.109710000
1	-5.807217000	1.249505000	-1.240583000
16	-0.581330000	0.240617000	-2.067599000
8	0.742584000	0.679798000	-2.563564000
8	-0.438249000	-0.578243000	-0.810725000
8	-1.471412000	-0.364055000	-3.057326000
1	-0.502618000	-2.111768000	-0.715386000
6	-1.361261000	1.723855000	-1.442569000
6	-2.423899000	1.604090000	-0.550528000
6	-3.019900000	2.747111000	-0.041999000
6	-2.570894000	4.022381000	-0.406868000
6	-1.503379000	4.119409000	-1.298502000
6	-0.898706000	2.977446000	-1.821107000
1	-2.751999000	0.617272000	-0.232556000
1	-3.837331000	2.654519000	0.675581000
1	-1.141183000	5.104677000	-1.590359000
1	-0.060193000	3.045022000	-2.510428000
6	-3.224202000	5.244064000	0.165483000
1	-3.324442000	5.169272000	1.256220000
1	-2.655564000	6.151545000	-0.061518000
1	-4.236286000	5.380588000	-0.235149000
6	3.497215000	1.469190000	0.187679000
6	4.171124000	1.436137000	-1.030709000
6	4.203291000	1.751913000	1.358382000
6	5.543406000	1.655791000	-1.073381000
1	3.615625000	1.212673000	-1.940387000
6	5.572611000	1.977659000	1.314404000

1	3.672365000	1.769220000	2.311291000
6	6.245576000	1.924630000	0.096640000
1	6.065880000	1.612424000	-2.026001000
1	6.117594000	2.191335000	2.230935000
1	7.319230000	2.092845000	0.060912000
Zero-point correction=			0.625716 (Hartree/Particle)
Thermal correction to Energy=			0.665986
Thermal correction to Enthalpy=			0.666930
Thermal correction to Gibbs Free Energy=			0.554369
Sum of electronic and zero-point Energies=			-2676.106835
Sum of electronic and thermal Energies=			-2676.066565
Sum of electronic and thermal Enthalpies=			-2676.065621
Sum of electronic and thermal Free Energies=			-2676.178182

B-TSf3

6	-1.859084000	-3.783005000	3.427356000
6	-1.873245000	-4.020682000	2.056219000
6	-2.097657000	-2.946901000	1.206711000
6	-2.283312000	-1.659337000	1.713605000
6	-2.265691000	-1.420496000	3.077525000
6	-2.050160000	-2.497834000	3.933335000
1	-1.683440000	-4.607908000	4.113413000
1	-1.696570000	-5.018442000	1.660777000
1	-2.410251000	-0.414093000	3.466696000
1	-2.022764000	-2.334750000	5.007750000
6	-2.032606000	-2.863289000	-0.274117000
6	-2.310325000	-1.525037000	-0.642680000
6	-2.504428000	-0.687029000	0.591473000
1	-1.793820000	0.149110000	0.613359000
6	-3.937397000	-0.131107000	0.516059000
6	-4.101992000	1.290723000	0.157637000
6	-5.042453000	1.673235000	-0.805584000
6	-3.321115000	2.278841000	0.766642000
6	-5.200365000	3.010022000	-1.147111000
1	-5.624729000	0.902052000	-1.307737000
6	-3.479592000	3.615245000	0.426069000
1	-2.580527000	2.007637000	1.519133000
6	-4.418742000	3.983522000	-0.532221000
1	-5.926812000	3.291533000	-1.906011000
1	-2.850847000	4.361591000	0.904770000
1	-4.533832000	5.029070000	-0.807941000
6	-4.981213000	-0.940820000	0.719055000
1	-4.851520000	-1.990748000	0.973052000
1	-2.297957000	-3.703213000	-0.921197000

1	-5.998705000	-0.560556000	0.677837000
16	1.257946000	-1.951656000	0.294262000
8	1.415403000	-2.243306000	1.713094000
8	0.531527000	-0.675843000	-0.000544000
8	0.620004000	-3.052740000	-0.521201000
1	-0.803280000	-2.849764000	-0.486408000
6	2.881896000	-1.768668000	-0.401921000
6	3.982458000	-1.802117000	0.441809000
6	5.250943000	-1.589189000	-0.087709000
6	5.428904000	-1.340478000	-1.447385000
6	4.303075000	-1.329879000	-2.281185000
6	3.032553000	-1.539530000	-1.768084000
1	3.831848000	-1.988434000	1.501752000
1	6.120308000	-1.610305000	0.568121000
1	4.433307000	-1.147229000	-3.347448000
1	2.157001000	-1.526500000	-2.413856000
6	6.786269000	-1.047255000	-2.010402000
1	7.011693000	-1.679595000	-2.876916000
1	6.850710000	-0.005021000	-2.352107000
1	7.573207000	-1.198967000	-1.264713000
16	0.287588000	2.492860000	0.990787000
8	-0.107969000	3.576864000	1.868666000
8	-0.312113000	2.364300000	-0.330712000
8	0.017454000	1.153364000	1.815665000
1	0.259361000	0.364602000	1.241331000
6	2.045558000	2.493495000	0.793822000
6	2.838443000	3.171100000	1.711844000
6	4.219374000	3.121458000	1.569930000
6	4.808990000	2.401409000	0.528750000
6	3.983835000	1.743026000	-0.386186000
6	2.604165000	1.778696000	-0.262011000
1	2.368347000	3.731306000	2.515977000
1	4.853477000	3.649585000	2.280224000
1	4.433261000	1.180459000	-1.204467000
1	1.960645000	1.249759000	-0.961285000
6	6.298079000	2.301224000	0.400738000
1	6.611720000	2.319392000	-0.649503000
1	6.809106000	3.115079000	0.925141000
1	6.661927000	1.356484000	0.826742000
6	-2.356193000	-1.003417000	-1.982567000
6	-2.084532000	0.355919000	-2.220036000
6	-2.633187000	-1.849514000	-3.072405000
6	-2.100145000	0.850097000	-3.515629000
1	-1.807985000	1.011946000	-1.398230000

6	-2.654554000	-1.347281000	-4.360106000
1	-2.858470000	-2.898646000	-2.895576000
6	-2.388540000	0.004839000	-4.581843000
1	-1.878366000	1.899618000	-3.687615000
1	-2.882980000	-2.002891000	-5.196096000
1	-2.404146000	0.397556000	-5.595882000
Zero-point correction=			0.621315 (Hartree/Particle)
Thermal correction to Energy=			0.661113
Thermal correction to Enthalpy=			0.662057
Thermal correction to Gibbs Free Energy=			0.548617
Sum of electronic and zero-point Energies=			-2676.079935
Sum of electronic and thermal Energies=			-2676.040137
Sum of electronic and thermal Enthalpies=			-2676.039193
Sum of electronic and thermal Free Energies=			-2676.152632

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6	-6.733669000	3.608508000	0.269497000
6	-6.615662000	2.510475000	1.117366000
6	-5.579478000	1.613892000	0.898373000
6	-4.680864000	1.803238000	-0.150865000
6	-4.798507000	2.894163000	-0.999380000
6	-5.831789000	3.800110000	-0.776584000
1	-7.533238000	4.327759000	0.428213000
1	-7.317774000	2.366555000	1.936269000
1	-4.091193000	3.038552000	-1.812913000
1	-5.935036000	4.667833000	-1.423042000
6	-5.225148000	0.371434000	1.666924000
6	-3.924185000	-0.058682000	1.057399000
6	-3.690610000	0.678610000	-0.210015000
1	-2.647336000	0.988583000	-0.387907000
6	-4.086974000	-0.454751000	-1.212898000
6	-3.049872000	-1.434602000	-1.577840000
6	-3.288330000	-2.803050000	-1.387990000
6	-1.808612000	-1.023599000	-2.074400000
6	-2.300328000	-3.735224000	-1.673937000
1	-4.247064000	-3.122376000	-0.979562000
6	-0.823591000	-1.959331000	-2.364311000
1	-1.585079000	0.032969000	-2.212600000
6	-1.062920000	-3.313481000	-2.154559000
1	-2.489123000	-4.792628000	-1.503609000
1	0.142119000	-1.608223000	-2.720072000
1	-0.273054000	-4.035389000	-2.346120000
6	-5.357182000	-0.573618000	-1.620123000
1	-6.139379000	0.115058000	-1.309488000

1	-5.986669000	-0.420052000	1.582572000
1	-5.627703000	-1.348620000	-2.332904000
16	2.938981000	-2.868972000	0.210956000
8	2.206053000	-2.871831000	1.473105000
8	1.977699000	-2.348774000	-0.941554000
8	3.541528000	-4.091115000	-0.281134000
1	-5.090380000	0.539223000	2.745124000
6	4.177484000	-1.604623000	0.300088000
6	3.919138000	-0.436268000	1.014224000
6	4.871306000	0.570067000	1.013220000
6	6.071550000	0.429508000	0.309830000
6	6.310150000	-0.757674000	-0.382541000
6	5.367320000	-1.778457000	-0.394975000
1	2.972712000	-0.313860000	1.534862000
1	4.674500000	1.498047000	1.551469000
1	7.246120000	-0.880118000	-0.925401000
1	5.540707000	-2.706493000	-0.933567000
6	7.060328000	1.554569000	0.291711000
1	7.972897000	1.287170000	-0.250237000
1	6.624912000	2.440224000	-0.191540000
1	7.344092000	1.854978000	1.307921000
16	0.661759000	1.043150000	-0.809605000
8	-0.640026000	1.625750000	-0.408790000
8	0.813936000	0.767407000	-2.243028000
8	0.988068000	-0.147329000	0.049790000
1	1.554986000	-1.477169000	-0.654291000
6	1.903219000	2.246906000	-0.381168000
6	1.863779000	2.856288000	0.870520000
6	2.874982000	3.733139000	1.233058000
6	3.932587000	4.013404000	0.359810000
6	3.942338000	3.401637000	-0.892995000
6	2.936479000	2.515329000	-1.266773000
1	1.035895000	2.642681000	1.542974000
1	2.850262000	4.216586000	2.209441000
1	4.751091000	3.624423000	-1.588858000
1	2.939269000	2.031059000	-2.239809000
6	5.039489000	4.931145000	0.783982000
1	5.687178000	5.198186000	-0.057858000
1	4.650326000	5.859299000	1.218515000
1	5.670819000	4.461441000	1.550805000
6	-3.074233000	-1.043858000	1.580520000
6	-1.719358000	-1.100176000	1.163417000
6	-3.560648000	-2.015779000	2.498353000
6	-0.888664000	-2.107629000	1.622355000

1	-1.299839000	-0.313904000	0.540733000
6	-2.735513000	-3.030013000	2.920389000
1	-4.597456000	-1.980741000	2.825687000
6	-1.401944000	-3.076323000	2.476033000
1	0.155506000	-2.133034000	1.319984000
1	-3.109534000	-3.794985000	3.595115000
1	-0.745829000	-3.874453000	2.817094000
Zero-point correction=			0.625325 (Hartree/Particle)
Thermal correction to Energy=			0.665788
Thermal correction to Enthalpy=			0.666732
Thermal correction to Gibbs Free Energy=			0.551931
Sum of electronic and zero-point Energies=			-2676.075339
Sum of electronic and thermal Energies=			-2676.034876
Sum of electronic and thermal Enthalpies=			-2676.033932
Sum of electronic and thermal Free Energies=			-2676.148733

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6	-2.958019000	0.027704000	-4.674647000
6	-2.231467000	1.012425000	-4.010489000
6	-2.335762000	1.094380000	-2.631442000
6	-3.143320000	0.201862000	-1.923482000
6	-3.881979000	-0.770651000	-2.583138000
6	-3.780581000	-0.848583000	-3.968513000
1	-2.886890000	-0.055956000	-5.756260000
1	-1.597344000	1.702430000	-4.562935000
1	-4.527627000	-1.451443000	-2.032023000
1	-4.346540000	-1.605313000	-4.506025000
6	-1.709641000	2.062384000	-1.681624000
6	-2.224522000	1.658647000	-0.338785000
6	-3.018791000	0.481634000	-0.460568000
1	-2.029423000	-0.222818000	-0.084993000
6	-4.181318000	0.172601000	0.450080000
6	-4.271533000	-1.132113000	1.140004000
6	-4.949782000	-1.231286000	2.362514000
6	-3.708325000	-2.293285000	0.596719000
6	-5.093331000	-2.454032000	3.002585000
1	-5.347543000	-0.329494000	2.825040000
6	-3.856014000	-3.516879000	1.236989000
1	-3.137591000	-2.246258000	-0.327561000
6	-4.552405000	-3.604424000	2.436818000
1	-5.619061000	-2.507022000	3.953118000
1	-3.413492000	-4.405738000	0.794623000
1	-4.660371000	-4.563499000	2.937756000
6	-5.150853000	1.092062000	0.542150000

1	-5.070092000	2.050867000	0.035325000
1	-2.018118000	3.102133000	-1.880512000
1	-6.063522000	0.907601000	1.102666000
16	2.271105000	2.556918000	0.017013000
8	1.686873000	2.990188000	-1.245949000
8	1.214812000	1.596918000	0.731714000
8	2.680461000	3.528620000	1.011588000
1	-0.608537000	2.066190000	-1.705011000
6	3.614684000	1.447661000	-0.304736000
6	3.492942000	0.511138000	-1.330831000
6	4.499560000	-0.424932000	-1.498962000
6	5.623199000	-0.438455000	-0.666358000
6	5.725274000	0.521637000	0.340474000
6	4.722461000	1.465410000	0.532276000
1	2.605725000	0.498250000	-1.959968000
1	4.409389000	-1.173744000	-2.284981000
1	6.601156000	0.524385000	0.987902000
1	4.787376000	2.210729000	1.320371000
6	6.685520000	-1.474766000	-0.868045000
1	7.169306000	-1.364768000	-1.846178000
1	7.464300000	-1.414994000	-0.100661000
1	6.252230000	-2.483377000	-0.838422000
16	-0.008214000	-1.345104000	-0.718123000
8	-0.454173000	-2.287032000	-1.735667000
8	-1.003232000	-1.114739000	0.402809000
8	0.412189000	-0.007323000	-1.239655000
1	0.826878000	1.002065000	0.023914000
6	1.424035000	-2.021007000	0.084386000
6	2.145799000	-3.014443000	-0.562907000
6	3.342162000	-3.455143000	-0.005462000
6	3.821800000	-2.911346000	1.185858000
6	3.065770000	-1.922282000	1.824713000
6	1.873285000	-1.471499000	1.283973000
1	1.762145000	-3.429048000	-1.492200000
1	3.913914000	-4.237480000	-0.504048000
1	3.433149000	-1.491837000	2.755640000
1	1.296606000	-0.694711000	1.779645000
6	5.117799000	-3.365376000	1.784761000
1	5.831567000	-2.533029000	1.850497000
1	4.976425000	-3.744153000	2.804002000
1	5.582112000	-4.161084000	1.192773000
6	-1.810249000	2.309446000	0.872991000
6	-2.004100000	1.708741000	2.133081000
6	-1.103385000	3.525119000	0.803543000

6	-1.505837000	2.309805000	3.274152000
1	-2.507288000	0.748251000	2.209098000
6	-0.622674000	4.129787000	1.950528000
1	-0.901616000	3.981778000	-0.162747000
6	-0.820523000	3.520578000	3.186105000
1	-1.639443000	1.828018000	4.238879000
1	-0.055167000	5.052630000	1.877710000
1	-0.423579000	3.983238000	4.086329000
Zero-point correction=			0.621619 (Hartree/Particle)
Thermal correction to Energy=			0.661056
Thermal correction to Enthalpy=			0.662000
Thermal correction to Gibbs Free Energy=			0.550766
Sum of electronic and zero-point Energies=			-2676.079468
Sum of electronic and thermal Energies=			-2676.040032
Sum of electronic and thermal Enthalpies=			-2676.039088
Sum of electronic and thermal Free Energies=			-2676.150322

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6	3.541038000	0.016603000	4.691289000
6	2.668585000	0.895844000	4.047509000
6	2.728283000	1.009002000	2.669472000
6	3.653170000	0.250300000	1.933642000
6	4.536692000	-0.613733000	2.575707000
6	4.467577000	-0.726422000	3.961597000
1	3.502619000	-0.084722000	5.773471000
1	1.956188000	1.485175000	4.622443000
1	5.270263000	-1.181949000	2.005024000
1	5.146621000	-1.398488000	4.481667000
6	1.964304000	1.879256000	1.724582000
6	2.531132000	1.521414000	0.374786000
6	3.501024000	0.577408000	0.516427000
1	1.401205000	-2.088499000	-1.265869000
6	4.367635000	0.000111000	-0.539648000
6	4.036687000	-1.342747000	-1.069775000
6	4.324653000	-1.685282000	-2.397438000
6	3.387662000	-2.293848000	-0.268941000
6	4.011261000	-2.942638000	-2.897628000
1	4.768443000	-0.938472000	-3.053036000
6	3.079951000	-3.558344000	-0.769418000
1	3.120254000	-2.044407000	0.756514000
6	3.393038000	-3.889000000	-2.085481000
1	4.235685000	-3.179153000	-3.935099000
1	2.574145000	-4.273113000	-0.124520000
1	3.141967000	-4.870619000	-2.479081000

6	5.432870000	0.685280000	-0.971146000
1	5.648507000	1.676255000	-0.580845000
1	2.099965000	2.946138000	1.957592000
1	6.122937000	0.279892000	-1.708008000
16	-1.999380000	2.737703000	-0.188038000
8	-1.077949000	2.991397000	0.906744000
8	-1.266200000	1.777811000	-1.250152000
8	-2.578640000	3.813293000	-0.962537000
1	0.878577000	1.705885000	1.749127000
6	-3.308715000	1.713023000	0.426819000
6	-3.029476000	0.790807000	1.433341000
6	-4.044865000	-0.036801000	1.883001000
6	-5.336394000	0.052442000	1.353509000
6	-5.589233000	0.991191000	0.352638000
6	-4.580362000	1.824436000	-0.119469000
1	-2.024226000	0.724066000	1.843903000
1	-3.837727000	-0.773260000	2.658863000
1	-6.593962000	1.072862000	-0.060498000
1	-4.767735000	2.565153000	-0.892876000
6	-6.415160000	-0.852019000	1.865291000
1	-6.635431000	-0.650035000	2.920471000
1	-7.347062000	-0.734237000	1.302494000
1	-6.105879000	-1.903892000	1.800414000
16	-0.186143000	-1.582933000	0.055724000
8	0.391013000	-2.541787000	0.978993000
8	0.477806000	-1.775352000	-1.394768000
8	-0.124512000	-0.160224000	0.386060000
1	-0.575807000	1.252549000	-0.783862000
6	-1.856425000	-2.015061000	-0.305424000
6	-2.426917000	-3.082879000	0.374160000
6	-3.765412000	-3.382288000	0.143543000
6	-4.522614000	-2.635306000	-0.758595000
6	-3.913923000	-1.568799000	-1.430226000
6	-2.587970000	-1.242688000	-1.206263000
1	-1.827929000	-3.659388000	1.073724000
1	-4.231692000	-4.211092000	0.674011000
1	-4.503718000	-0.969854000	-2.122475000
1	-2.134517000	-0.392122000	-1.711700000
6	-5.961859000	-2.954898000	-1.020204000
1	-6.580163000	-2.049979000	-0.964915000
1	-6.096837000	-3.373076000	-2.025159000
1	-6.354934000	-3.681793000	-0.302089000
6	2.038822000	2.134629000	-0.859939000
6	2.021115000	1.431214000	-2.074308000

6	1.537489000	3.444065000	-0.850120000
6	1.541773000	2.023428000	-3.234321000
1	2.360918000	0.397673000	-2.097328000
6	1.067798000	4.038805000	-2.013583000
1	1.505917000	4.000754000	0.083439000
6	1.070924000	3.332486000	-3.211184000
1	1.526601000	1.453883000	-4.160923000
1	0.677530000	5.052942000	-1.978411000
1	0.690543000	3.793570000	-4.119379000
Zero-point correction=			0.625869 (Hartree/Particle)
Thermal correction to Energy=			0.666471
Thermal correction to Enthalpy=			0.667415
Thermal correction to Gibbs Free Energy=			0.553570
Sum of electronic and zero-point Energies=			-2676.113080
Sum of electronic and thermal Energies=			-2676.072477
Sum of electronic and thermal Enthalpies=			-2676.071533
Sum of electronic and thermal Free Energies=			-2676.185378

B-TSf5

6	0.662447000	1.123422000	4.087029000
6	1.554571000	0.061435000	3.975021000
6	2.228390000	-0.117794000	2.777126000
6	2.035807000	0.753648000	1.696632000
6	1.117701000	1.797130000	1.801923000
6	0.440602000	1.973416000	3.003177000
1	0.124042000	1.282568000	5.018571000
1	1.710805000	-0.624586000	4.805741000
1	0.886309000	2.449943000	0.964347000
1	-0.284644000	2.779984000	3.080931000
6	3.157830000	-1.212342000	2.369806000
6	3.520747000	-0.871990000	0.960042000
6	2.846270000	0.255656000	0.559804000
1	1.621974000	-0.535239000	-2.022344000
6	2.775417000	0.753890000	-0.797044000
6	2.478010000	2.168442000	-1.009082000
6	1.521004000	2.556788000	-1.955189000
6	3.129873000	3.145866000	-0.243919000
6	1.193699000	3.896941000	-2.103386000
1	0.982843000	1.799231000	-2.521306000
6	2.837044000	4.486427000	-0.434435000
1	3.863331000	2.839385000	0.499864000
6	1.855865000	4.861302000	-1.350586000
1	0.401392000	4.182633000	-2.790311000
1	3.354205000	5.242249000	0.150617000

1	1.597192000	5.910552000	-1.467294000
6	2.825078000	-0.106399000	-1.909293000
1	3.271976000	-1.088866000	-1.758259000
1	2.649732000	-2.190922000	2.372088000
1	3.043131000	0.356807000	-2.872018000
16	-2.323941000	2.650827000	-0.505976000
8	-1.446372000	3.192935000	0.519230000
8	-1.456921000	1.742647000	-1.497016000
8	-3.102235000	3.527359000	-1.356774000
1	4.047839000	-1.325827000	3.005022000
6	-3.399270000	1.460259000	0.247953000
6	-2.911768000	0.657624000	1.278504000
6	-3.738509000	-0.322244000	1.804424000
6	-5.037961000	-0.510286000	1.321289000
6	-5.505562000	0.325237000	0.306386000
6	-4.690435000	1.310025000	-0.240255000
1	-1.896246000	0.792787000	1.647807000
1	-3.366439000	-0.970643000	2.596716000
1	-6.521672000	0.196911000	-0.065509000
1	-5.039998000	1.964781000	-1.034805000
6	-5.894522000	-1.600734000	1.887134000
1	-6.005138000	-1.501060000	2.973404000
1	-6.896252000	-1.601870000	1.444978000
1	-5.440932000	-2.584106000	1.701586000
16	-0.041957000	-1.434452000	-0.695804000
8	0.774665000	-2.370755000	0.076128000
8	0.446629000	-1.222160000	-2.122598000
8	-0.213618000	-0.099948000	-0.059757000
1	-0.910042000	1.098315000	-0.958019000
6	-1.660701000	-2.120124000	-0.899261000
6	-2.020423000	-3.261642000	-0.198100000
6	-3.327251000	-3.729245000	-0.296010000
6	-4.269350000	-3.068226000	-1.083460000
6	-3.876196000	-1.921748000	-1.782426000
6	-2.581746000	-1.439632000	-1.694644000
1	-1.278757000	-3.766763000	0.414933000
1	-3.623227000	-4.623867000	0.250770000
1	-4.608026000	-1.392903000	-2.391800000
1	-2.289703000	-0.537094000	-2.227827000
6	-5.678018000	-3.566064000	-1.194402000
1	-6.396027000	-2.748066000	-1.054771000
1	-5.871485000	-3.995556000	-2.185211000
1	-5.894241000	-4.339336000	-0.449664000
6	4.525418000	-1.661803000	0.247788000

6	4.389255000	-3.052877000	0.170544000
6	5.647803000	-1.052718000	-0.326790000
6	5.348632000	-3.813532000	-0.485184000
1	3.498737000	-3.522818000	0.583250000
6	6.609926000	-1.819105000	-0.969151000
1	5.758665000	0.028100000	-0.254643000
6	6.461845000	-3.200780000	-1.051756000
1	5.223313000	-4.890929000	-0.558355000
1	7.480837000	-1.336558000	-1.406050000
1	7.214535000	-3.799207000	-1.558904000
Zero-point correction=			0.620664 (Hartree/Particle)
Thermal correction to Energy=			0.660426
Thermal correction to Enthalpy=			0.661370
Thermal correction to Gibbs Free Energy=			0.548251
Sum of electronic and zero-point Energies=			-2676.095298
Sum of electronic and thermal Energies=			-2676.055537
Sum of electronic and thermal Enthalpies=			-2676.054592
Sum of electronic and thermal Free Energies=			-2676.167711

B-TSg3

6	-3.645732000	4.985126000	-1.301514000
6	-3.718008000	4.421873000	-0.044288000
6	-3.387772000	3.062561000	0.084915000
6	-2.997778000	2.286043000	-1.029467000
6	-2.896507000	2.873016000	-2.280188000
6	-3.231078000	4.216611000	-2.402511000
1	-3.892665000	6.033147000	-1.446117000
1	-4.011005000	5.007619000	0.823583000
1	-2.565798000	2.295040000	-3.138839000
1	-3.166458000	4.691898000	-3.378461000
6	-3.273509000	2.253887000	1.238292000
6	-2.690939000	1.003006000	0.934807000
6	-2.743202000	0.875218000	-0.617899000
1	-1.780884000	0.516796000	-1.012538000
6	-3.846433000	-0.100363000	-1.021246000
6	-3.533779000	-1.545019000	-0.934991000
6	-4.476896000	-2.426731000	-0.393418000
6	-2.310949000	-2.062816000	-1.373335000
6	-4.208526000	-3.785135000	-0.302948000
1	-5.411540000	-2.026714000	-0.004174000
6	-2.042461000	-3.423169000	-1.286444000
1	-1.546316000	-1.408213000	-1.788135000
6	-2.990323000	-4.287412000	-0.750251000
1	-4.948333000	-4.453075000	0.132713000

1	-1.084022000	-3.805489000	-1.632205000
1	-2.773516000	-5.349843000	-0.670931000
6	-5.061798000	0.325884000	-1.382087000
1	-5.323228000	1.379729000	-1.431460000
1	-3.482970000	2.588142000	2.254109000
1	-5.832605000	-0.386220000	-1.665230000
16	0.627614000	1.734672000	-0.254144000
8	0.422963000	2.336155000	-1.569818000
8	0.562013000	0.244962000	-0.243644000
8	-0.279564000	2.264390000	0.825399000
1	-1.578776000	1.499605000	1.053176000
6	2.257229000	2.175550000	0.298487000
6	3.200768000	2.594394000	-0.628969000
6	4.494242000	2.877600000	-0.201430000
6	4.850254000	2.752948000	1.140693000
6	3.875882000	2.341918000	2.058490000
6	2.585562000	2.047100000	1.646065000
1	2.909919000	2.700300000	-1.671043000
1	5.240940000	3.207593000	-0.922507000
1	4.141839000	2.251410000	3.111260000
1	1.825961000	1.731015000	2.357197000
6	6.251232000	3.018734000	1.601483000
1	6.270587000	3.694085000	2.464546000
1	6.744413000	2.088201000	1.915154000
1	6.860161000	3.464044000	0.808214000
16	1.518427000	-2.921643000	-0.636585000
8	1.540109000	-4.213484000	-1.293745000
8	0.848109000	-2.750092000	0.643519000
8	0.894888000	-1.911186000	-1.703593000
1	0.775230000	-1.019281000	-1.269560000
6	3.172502000	-2.310788000	-0.482781000
6	4.157805000	-2.786030000	-1.338721000
6	5.429115000	-2.228535000	-1.273552000
6	5.717157000	-1.203941000	-0.371286000
6	4.708808000	-0.758027000	0.487717000
6	3.435313000	-1.301356000	0.438475000
1	3.920671000	-3.580715000	-2.041229000
1	6.211247000	-2.588232000	-1.940168000
1	4.919740000	0.046707000	1.192343000
1	2.640927000	-0.947386000	1.091748000
6	7.072789000	-0.567819000	-0.319508000
1	7.519021000	-0.658074000	0.678653000
1	7.763141000	-1.019134000	-1.038850000
1	7.006298000	0.505125000	-0.543778000

6	-2.785200000	-0.187488000	1.816077000
6	-1.772438000	-1.149850000	1.777690000
6	-3.900193000	-0.390550000	2.632962000
6	-1.875156000	-2.300993000	2.546477000
1	-0.905121000	-1.008147000	1.134533000
6	-3.994993000	-1.537879000	3.411295000
1	-4.711942000	0.337241000	2.627193000
6	-2.984315000	-2.494224000	3.365783000
1	-1.087277000	-3.047258000	2.476980000
1	-4.868705000	-1.695606000	4.039442000
1	-3.067777000	-3.398780000	3.963880000
Zero-point correction=			0.621652 (Hartree/Particle)
Thermal correction to Energy=			0.661365
Thermal correction to Enthalpy=			0.662309
Thermal correction to Gibbs Free Energy=			0.549381
Sum of electronic and zero-point Energies=			-2676.071095
Sum of electronic and thermal Energies=			-2676.031382
Sum of electronic and thermal Enthalpies=			-2676.030438
Sum of electronic and thermal Free Energies=			-2676.143366

B-3g

6	-0.426055000	4.572615000	-0.889149000
6	-0.969166000	4.120688000	0.283565000
6	-1.577871000	2.840189000	0.276524000
6	-1.654456000	2.053792000	-0.909473000
6	-1.073063000	2.516468000	-2.075652000
6	-0.459231000	3.762832000	-2.046646000
1	0.091734000	5.525917000	-0.926516000
1	-0.895562000	4.692745000	1.204353000
1	-1.074136000	1.910400000	-2.976993000
1	0.031697000	4.129946000	-2.944098000
6	-2.015667000	2.060406000	1.331503000
6	-2.331957000	0.699770000	0.920482000
6	-2.360785000	0.770113000	-0.648726000
1	-1.783902000	-0.061350000	-1.079519000
6	-3.780621000	0.724650000	-1.195242000
6	-4.440045000	-0.601383000	-1.237605000
6	-5.802672000	-0.705235000	-0.929416000
6	-3.738140000	-1.767773000	-1.563746000
6	-6.447886000	-1.933034000	-0.952134000
1	-6.344718000	0.185114000	-0.615051000
6	-4.389670000	-2.995718000	-1.591449000
1	-2.672087000	-1.740154000	-1.780279000
6	-5.742654000	-3.085075000	-1.286268000

1	-7.502033000	-1.992439000	-0.690699000
1	-3.824570000	-3.889211000	-1.845325000
1	-6.244239000	-4.050071000	-1.296926000
6	-4.419676000	1.834305000	-1.585128000
1	-3.962765000	2.819793000	-1.542141000
1	-2.033424000	2.379611000	2.373567000
1	-5.425920000	1.783207000	-1.992403000
16	0.432343000	-1.347440000	-0.218113000
8	0.085718000	-1.120914000	1.205302000
8	0.777961000	-0.051408000	-0.902741000
8	-0.561685000	-2.108059000	-0.987783000
1	-1.368047000	0.163245000	1.163022000
6	1.933833000	-2.300896000	-0.217150000
6	2.679198000	-2.436347000	0.944877000
6	3.872019000	-3.152589000	0.906913000
6	4.330695000	-3.723798000	-0.279180000
6	3.560495000	-3.571670000	-1.438582000
6	2.367060000	-2.867128000	-1.413987000
1	2.315592000	-1.985791000	1.864629000
1	4.458158000	-3.271436000	1.817975000
1	3.905201000	-4.022170000	-2.368962000
1	1.757470000	-2.761820000	-2.308556000
6	5.627203000	-4.474682000	-0.331123000
1	5.500795000	-5.463480000	-0.787552000
1	6.372278000	-3.939754000	-0.935496000
1	6.051978000	-4.617455000	0.668203000
16	2.460621000	2.774615000	0.058705000
8	2.625300000	3.923937000	0.930010000
8	2.227182000	2.971812000	-1.366963000
8	1.265573000	1.926571000	0.670226000
1	1.073092000	1.125036000	0.071534000
6	3.848784000	1.692723000	0.236042000
6	4.751593000	1.903839000	1.269275000
6	5.821352000	1.028939000	1.414880000
6	5.989433000	-0.049114000	0.546002000
6	5.069004000	-0.230178000	-0.491128000
6	3.997581000	0.632421000	-0.655971000
1	4.611887000	2.748057000	1.938745000
1	6.540284000	1.183300000	2.217929000
1	5.187307000	-1.076608000	-1.167872000
1	3.273589000	0.486722000	-1.455239000
6	7.114332000	-1.021316000	0.725556000
1	7.619891000	-1.229506000	-0.224729000
1	7.861403000	-0.653719000	1.436092000

1	6.738198000	-1.981985000	1.103774000
6	-3.418069000	-0.027406000	1.649055000
6	-3.301760000	-1.405904000	1.838203000
6	-4.559896000	0.638592000	2.095575000
6	-4.326809000	-2.108119000	2.457351000
1	-2.404767000	-1.912650000	1.480884000
6	-5.576924000	-0.063967000	2.731322000
1	-4.664484000	1.709186000	1.911989000
6	-5.461562000	-1.438938000	2.908763000
1	-4.239251000	-3.183602000	2.589270000
1	-6.465143000	0.459752000	3.076998000
1	-6.261019000	-1.991590000	3.396686000
Zero-point correction=			0.624199 (Hartree/Particle)
Thermal correction to Energy=			0.664479
Thermal correction to Enthalpy=			0.665423
Thermal correction to Gibbs Free Energy=			0.551116
Sum of electronic and zero-point Energies=			-2676.076385
Sum of electronic and thermal Energies=			-2676.036105
Sum of electronic and thermal Enthalpies=			-2676.035161
Sum of electronic and thermal Free Energies=			-2676.149468

B-TSd3'

6	0.551927000	4.779865000	-0.413490000
6	-0.829340000	4.628818000	-0.492025000
6	-1.372269000	3.372865000	-0.242652000
6	-0.546434000	2.285049000	0.084633000
6	0.828150000	2.436737000	0.159773000
6	1.369596000	3.697470000	-0.092227000
1	0.999084000	5.752743000	-0.604428000
1	-1.469458000	5.472197000	-0.742554000
1	1.457209000	1.584913000	0.406235000
1	2.446851000	3.834242000	-0.037067000
6	-2.751633000	2.914711000	-0.240800000
6	-2.822355000	1.609798000	0.081534000
6	-1.400691000	1.061224000	0.314000000
1	-1.277337000	0.698254000	1.344003000
6	-1.180512000	-0.067036000	-0.654564000
6	-4.048426000	0.803097000	0.230503000
6	-4.639021000	0.654135000	1.489136000
6	-4.616940000	0.147745000	-0.864218000
6	-5.761528000	-0.148995000	1.652672000
1	-4.200044000	1.169171000	2.342983000
6	-5.740830000	-0.653819000	-0.701254000
1	-4.162307000	0.264897000	-1.847197000

6	-6.311308000	-0.808593000	0.557783000
1	-6.209918000	-0.258532000	2.637385000
1	-6.171585000	-1.161607000	-1.560853000
6	-1.506565000	-1.431023000	-0.283532000
6	-2.207727000	-1.725441000	0.899141000
6	-1.097360000	-2.504838000	-1.097962000
6	-2.548712000	-3.027902000	1.218025000
1	-2.518622000	-0.928489000	1.565385000
6	-1.402947000	-3.809292000	-0.755118000
1	-0.479933000	-2.322250000	-1.973000000
6	-2.145269000	-4.073467000	0.392535000
1	-3.116368000	-3.229720000	2.122436000
1	-1.047855000	-4.625024000	-1.377921000
1	-2.393902000	-5.099262000	0.653792000
6	-0.660835000	0.232784000	-1.927830000
1	-0.619076000	1.289246000	-2.193784000
1	-3.614817000	3.544195000	-0.441500000
1	-0.953816000	-0.426270000	-2.745682000
1	-7.187320000	-1.439762000	0.685163000
16	2.060487000	-1.303055000	-0.300462000
8	2.059608000	-2.763392000	-0.323882000
8	1.179042000	-0.662679000	0.699372000
8	1.801961000	-0.714313000	-1.683595000
1	0.530258000	-0.122828000	-1.767138000
6	3.719884000	-0.778098000	0.064576000
6	4.755530000	-1.165347000	-0.783156000
6	6.052771000	-0.778792000	-0.489884000
6	6.338696000	-0.012499000	0.646150000
6	5.286605000	0.360196000	1.479838000
6	3.977745000	-0.019330000	1.196518000
1	4.535207000	-1.763281000	-1.664687000
1	6.867990000	-1.075107000	-1.149329000
1	5.496705000	0.954431000	2.368215000
1	3.152179000	0.258783000	1.847196000
6	7.751725000	0.380208000	0.955271000
1	7.801765000	1.065746000	1.807167000
1	8.363183000	-0.497500000	1.198902000
1	8.227670000	0.871372000	0.098242000
Zero-point correction=			0.475273 (Hartree/Particle)
Thermal correction to Energy=			0.504223
Thermal correction to Enthalpy=			0.505168
Thermal correction to Gibbs Free Energy=			0.413295
Sum of electronic and zero-point Energies=			-1781.146447
Sum of electronic and thermal Energies=			-1781.117496

Sum of electronic and thermal Enthalpies= -1781.116552
 Sum of electronic and thermal Free Energies= -1781.208424

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6	2.372094000	3.573492000	2.457052000
6	1.725570000	2.442769000	2.949132000
6	0.686197000	1.886055000	2.215280000
6	0.268999000	2.444644000	0.978961000
6	0.924357000	3.583993000	0.505852000
6	1.973544000	4.136168000	1.248456000
1	3.195746000	4.014265000	3.012970000
1	2.034624000	1.992119000	3.890251000
1	0.661086000	4.045760000	-0.438676000
1	2.490399000	5.011327000	0.862835000
6	-0.098580000	0.696549000	2.457945000
6	-0.966628000	0.494391000	1.430689000
6	-0.837709000	1.612303000	0.465947000
1	2.320712000	1.985860000	-0.255838000
6	-1.592194000	1.858074000	-0.642077000
6	-2.787133000	1.067011000	-0.992609000
6	-3.829132000	0.866786000	-0.083334000
6	-2.893399000	0.516621000	-2.275959000
6	-4.937394000	0.108336000	-0.436576000
1	-3.759701000	1.309388000	0.908570000
6	-3.995275000	-0.251570000	-2.623910000
1	-2.074808000	0.659263000	-2.981218000
6	-5.020724000	-0.457368000	-1.704531000
1	-5.736537000	-0.045022000	0.284814000
1	-4.055019000	-0.693671000	-3.615669000
1	-5.886768000	-1.055043000	-1.978862000
6	-1.259037000	2.957478000	-1.607667000
1	-0.269216000	2.795968000	-2.054689000
1	0.056124000	0.006473000	3.283499000
1	-1.996313000	3.007503000	-2.412407000
16	2.487229000	0.453321000	-1.741777000
8	3.064185000	1.480028000	-0.644329000
8	3.390824000	0.474588000	-2.870565000
8	1.070153000	0.756075000	-1.905572000
1	-1.257672000	3.934170000	-1.108915000
6	2.647139000	-1.099318000	-0.914514000
6	1.846156000	-1.348096000	0.195704000
6	1.941060000	-2.573563000	0.832343000
6	2.829681000	-3.553046000	0.374625000
6	3.627184000	-3.270919000	-0.735106000

6	3.543039000	-2.046873000	-1.389122000
1	1.153519000	-0.590377000	0.558333000
1	1.309039000	-2.777844000	1.696510000
1	4.324526000	-4.025469000	-1.095063000
1	4.156233000	-1.818250000	-2.256740000
6	2.901757000	-4.884177000	1.057556000
1	3.785207000	-5.450385000	0.746866000
1	2.933356000	-4.772998000	2.147085000
1	2.018936000	-5.492299000	0.824264000
6	-1.726657000	-0.759402000	1.291607000
6	-1.606100000	-1.548576000	0.141061000
6	-2.519413000	-1.222755000	2.344898000
6	-2.284537000	-2.754932000	0.040154000
1	-0.976240000	-1.202039000	-0.678210000
6	-3.202198000	-2.429231000	2.240439000
1	-2.614479000	-0.611044000	3.241042000
6	-3.092168000	-3.195843000	1.085703000
1	-2.183876000	-3.354234000	-0.861811000
1	-3.826651000	-2.768878000	3.063896000
1	-3.630182000	-4.137193000	1.001317000
Zero-point correction=			0.479406 (Hartree/Particle)
Thermal correction to Energy=			0.509495
Thermal correction to Enthalpy=			0.510440
Thermal correction to Gibbs Free Energy=			0.417420
Sum of electronic and zero-point Energies=			-1781.192305
Sum of electronic and thermal Energies=			-1781.162216
Sum of electronic and thermal Enthalpies=			-1781.161272
Sum of electronic and thermal Free Energies=			-1781.254292

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6	-4.061157000	3.739830000	0.793520000
6	-3.172717000	3.061688000	1.622303000
6	-2.639552000	1.862449000	1.179721000
6	-2.953408000	1.339443000	-0.085870000
6	-3.849492000	2.025365000	-0.906156000
6	-4.397544000	3.221691000	-0.455608000
1	-4.495500000	4.680831000	1.121868000
1	-2.900374000	3.462691000	2.595805000
1	-4.140391000	1.644430000	-1.880276000
1	-5.095874000	3.760678000	-1.091008000
6	-1.651956000	0.965127000	1.810153000
6	-1.569104000	-0.204130000	0.991640000
6	-2.271180000	0.042696000	-0.234560000
1	-0.581352000	1.464833000	1.505470000

6	-2.090756000	-0.671758000	-1.407510000
6	-1.664223000	-2.068423000	-1.426628000
6	-2.251947000	-3.002428000	-0.562334000
6	-0.665393000	-2.496958000	-2.313473000
6	-1.841811000	-4.326947000	-0.573426000
1	-3.043519000	-2.675287000	0.108682000
6	-0.239775000	-3.816004000	-2.303231000
1	-0.172534000	-1.770075000	-2.956210000
6	-0.829375000	-4.733914000	-1.437706000
1	-2.310001000	-5.043589000	0.096323000
1	0.558861000	-4.130313000	-2.970104000
1	-0.501246000	-5.770372000	-1.439658000
6	-2.331515000	-0.016670000	-2.722005000
1	-2.046978000	1.039470000	-2.694154000
1	-1.547818000	0.867787000	2.893917000
1	-1.783979000	-0.524291000	-3.519974000
16	1.051496000	2.130183000	-0.288630000
8	0.632616000	2.264904000	1.158125000
8	1.058698000	3.389900000	-1.024920000
8	0.308266000	1.019270000	-0.933460000
1	-3.395671000	-0.089271000	-2.989230000
6	2.747073000	1.582562000	-0.187178000
6	3.122205000	0.638636000	0.762846000
6	4.424242000	0.156103000	0.772999000
6	5.366736000	0.609900000	-0.152279000
6	4.973001000	1.570552000	-1.086089000
6	3.671851000	2.055888000	-1.110547000
1	2.396907000	0.298009000	1.499009000
1	4.722080000	-0.579507000	1.520058000
1	5.703275000	1.946616000	-1.802194000
1	3.359826000	2.811971000	-1.826694000
6	6.766530000	0.072806000	-0.153727000
1	7.500473000	0.863980000	-0.343759000
1	7.017356000	-0.398229000	0.802562000
1	6.902676000	-0.684279000	-0.936886000
6	-0.708741000	-1.317902000	1.416484000
6	0.484182000	-1.635023000	0.757517000
6	-1.071764000	-2.026449000	2.566486000
6	1.279106000	-2.668532000	1.234716000
1	0.779942000	-1.041549000	-0.105982000
6	-0.283811000	-3.076424000	3.021073000
1	-1.990371000	-1.764389000	3.089753000
6	0.892888000	-3.400239000	2.354485000
1	2.214567000	-2.896014000	0.727514000

1	-0.583715000	-3.633564000	3.905294000
1	1.517225000	-4.213705000	2.716288000
Zero-point correction=			0.475717 (Hartree/Particle)
Thermal correction to Energy=			0.504736
Thermal correction to Enthalpy=			0.505680
Thermal correction to Gibbs Free Energy=			0.414683
Sum of electronic and zero-point Energies=			-1781.152745
Sum of electronic and thermal Energies=			-1781.123726
Sum of electronic and thermal Enthalpies=			-1781.122782
Sum of electronic and thermal Free Energies=			-1781.213779

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6	0.275077000	5.050983000	-0.541725000
6	0.238576000	3.959327000	-1.404214000
6	-0.523138000	2.857164000	-1.057330000
6	-1.247364000	2.817814000	0.146068000
6	-1.188478000	3.909047000	1.014687000
6	-0.431683000	5.020096000	0.657336000
1	0.863580000	5.927692000	-0.800628000
1	0.804105000	3.964668000	-2.333476000
1	-1.710898000	3.920375000	1.965624000
1	-0.390842000	5.873480000	1.329740000
6	-0.696573000	1.577203000	-1.795659000
6	-1.611521000	0.787381000	-0.947422000
6	-1.886812000	1.488359000	0.253207000
1	-1.083964000	1.678377000	-2.818756000
6	-2.608556000	0.983677000	1.345976000
6	-2.662651000	-0.432819000	1.645938000
6	-1.537591000	-1.232911000	1.372335000
6	-3.809296000	-1.032665000	2.205209000
6	-1.576327000	-2.600138000	1.595143000
1	-0.615009000	-0.772116000	1.019279000
6	-3.843554000	-2.398449000	2.414934000
1	-4.699461000	-0.439586000	2.406243000
6	-2.729498000	-3.185069000	2.105832000
1	-0.689396000	-3.179814000	1.350288000
1	-4.743467000	-2.861719000	2.811537000
1	-2.768144000	-4.258922000	2.273949000
6	-3.243183000	1.923894000	2.308469000
1	-3.601850000	2.839125000	1.829473000
1	0.257123000	1.001272000	-1.892919000
1	-4.057239000	1.448782000	2.861032000
16	1.658278000	-0.793781000	-0.426875000
8	1.608270000	-0.446189000	-1.875862000

8	1.159230000	-2.148996000	-0.127055000
8	1.033465000	0.271525000	0.400539000
1	-2.494576000	2.210282000	3.062674000
6	3.389220000	-0.780022000	0.000504000
6	4.071396000	0.434565000	0.009145000
6	5.425019000	0.455888000	0.303098000
6	6.117180000	-0.725000000	0.593902000
6	5.414179000	-1.927948000	0.582727000
6	4.054546000	-1.962239000	0.287126000
1	3.529276000	1.352559000	-0.208022000
1	5.964402000	1.403076000	0.311286000
1	5.942177000	-2.853800000	0.809130000
1	3.497011000	-2.894993000	0.277127000
6	7.580324000	-0.682367000	0.918625000
1	8.000629000	-1.688670000	1.016416000
1	8.147108000	-0.155647000	0.141362000
1	7.765846000	-0.152579000	1.861552000
6	-2.235358000	-0.415455000	-1.467084000
6	-3.604812000	-0.664424000	-1.276869000
6	-1.461980000	-1.331522000	-2.199241000
6	-4.180675000	-1.820885000	-1.771436000
1	-4.214848000	0.070824000	-0.756230000
6	-2.044681000	-2.503584000	-2.661714000
1	-0.392884000	-1.158294000	-2.333136000
6	-3.396487000	-2.751544000	-2.452130000
1	-5.243898000	-1.998528000	-1.630691000
1	-1.430569000	-3.228524000	-3.188756000
1	-3.846187000	-3.667684000	-2.827678000
Zero-point correction=			0.478715 (Hartree/Particle)
Thermal correction to Energy=			0.508458
Thermal correction to Enthalpy=			0.509402
Thermal correction to Gibbs Free Energy=			0.417034
Sum of electronic and zero-point Energies=			-1781.163988
Sum of electronic and thermal Energies=			-1781.134245
Sum of electronic and thermal Enthalpies=			-1781.133300
Sum of electronic and thermal Free Energies=			-1781.225668

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6	-0.478986000	-1.141260000	4.338645000
6	0.110820000	0.074380000	4.015137000
6	1.040771000	0.108840000	2.987660000
6	1.397101000	-1.054264000	2.276095000
6	0.754985000	-2.258642000	2.571141000
6	-0.165922000	-2.291264000	3.613850000

1	-1.202976000	-1.194202000	5.148350000
1	-0.164471000	0.986328000	4.540670000
1	0.930643000	-3.163319000	1.997735000
1	-0.653456000	-3.232266000	3.859071000
6	1.722281000	1.257909000	2.375011000
6	2.605539000	0.742479000	1.391684000
6	2.350946000	-0.664700000	1.223781000
1	0.861839000	1.741762000	1.516513000
6	2.889316000	-1.484021000	0.238237000
6	3.639110000	1.582956000	0.786247000
6	4.968293000	1.149678000	0.710769000
6	3.313249000	2.868365000	0.335694000
6	5.946844000	1.978917000	0.182765000
1	5.230767000	0.161690000	1.083613000
6	4.294408000	3.686141000	-0.208036000
1	2.275970000	3.197100000	0.366973000
6	5.611621000	3.245407000	-0.286645000
1	6.976995000	1.634347000	0.137212000
1	4.026541000	4.673303000	-0.576553000
6	3.402855000	-0.946866000	-1.019331000
6	2.730891000	0.105909000	-1.662141000
6	4.559259000	-1.474687000	-1.616479000
6	3.223833000	0.633515000	-2.845307000
1	1.801406000	0.490540000	-1.244634000
6	5.058015000	-0.930755000	-2.789022000
1	5.102369000	-2.281134000	-1.128167000
6	4.390529000	0.124470000	-3.406296000
1	2.685475000	1.440270000	-3.335274000
1	5.970085000	-1.330374000	-3.224973000
1	4.776024000	0.541214000	-4.333741000
6	2.895445000	-2.959858000	0.405191000
1	3.021096000	-3.258640000	1.449694000
1	1.997918000	2.147180000	2.944569000
1	3.662951000	-3.433879000	-0.211634000
1	6.378023000	3.890528000	-0.709139000
16	-0.739180000	-3.068310000	-1.219000000
8	-0.698172000	-3.239340000	-2.660094000
8	0.158671000	-1.830385000	-0.774914000
8	-0.301071000	-4.146472000	-0.345399000
1	1.930032000	-3.361343000	0.054333000
6	-2.365838000	-2.531864000	-0.771847000
6	-3.334875000	-2.380327000	-1.757386000
6	-4.595826000	-1.923226000	-1.391704000
6	-4.888017000	-1.608769000	-0.062375000

6	-3.895013000	-1.780496000	0.906068000
6	-2.634940000	-2.241517000	0.562135000
1	-3.091375000	-2.616520000	-2.789722000
1	-5.366404000	-1.798511000	-2.151424000
1	-4.105962000	-1.522249000	1.942503000
1	-1.852718000	-2.342849000	1.310838000
6	-6.221014000	-1.043432000	0.320600000
1	-6.602965000	-1.498619000	1.241102000
1	-6.138443000	0.036099000	0.506690000
1	-6.966190000	-1.189449000	-0.468215000
16	-1.017959000	1.271307000	0.128364000
8	0.015333000	2.282369000	0.610866000
8	-1.374081000	0.318185000	1.175035000
8	-0.593917000	0.653728000	-1.156301000
1	-0.212703000	-0.939479000	-1.045253000
6	-2.453386000	2.230648000	-0.265175000
6	-2.565778000	3.568863000	0.076704000
6	-3.747978000	4.242596000	-0.217679000
6	-4.812411000	3.593555000	-0.840544000
6	-4.671739000	2.240017000	-1.170771000
6	-3.501615000	1.555638000	-0.889253000
1	-1.733238000	4.070891000	0.561515000
1	-3.845840000	5.295735000	0.041183000
1	-5.492926000	1.721148000	-1.666768000
1	-3.393815000	0.504443000	-1.155319000
6	-6.084060000	4.318698000	-1.160524000
1	-6.945784000	3.842593000	-0.677372000
1	-6.048357000	5.361364000	-0.830125000
1	-6.282667000	4.315467000	-2.239046000
Zero-point correction=			0.477299 (Hartree/Particle)
Thermal correction to Energy=			0.506441
Thermal correction to Enthalpy=			0.507385
Thermal correction to Gibbs Free Energy=			0.417358
Sum of electronic and zero-point Energies=			-1781.135771
Sum of electronic and thermal Energies=			-1781.106629
Sum of electronic and thermal Enthalpies=			-1781.105684
Sum of electronic and thermal Free Energies=			-1781.195712

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6	0.494980000	-4.300494000	0.417634000
6	0.575472000	-3.358211000	-0.610605000
6	0.751279000	-2.024776000	-0.286587000
6	0.866569000	-1.629544000	1.062074000
6	0.773631000	-2.566249000	2.085358000

6	0.584331000	-3.906856000	1.751125000
1	0.363145000	-5.352804000	0.174711000
1	0.501957000	-3.669293000	-1.652009000
1	0.878231000	-2.267082000	3.126458000
1	0.525681000	-4.655247000	2.537956000
6	1.578824000	0.205248000	-0.312015000
6	1.048864000	-0.186731000	1.055194000
6	0.562779000	0.871056000	1.741948000
6	3.087194000	0.008137000	-0.458686000
6	3.670352000	-0.048584000	-1.726562000
6	3.921632000	-0.054862000	0.657633000
6	5.046151000	-0.177739000	-1.875724000
1	3.044890000	0.009716000	-2.616592000
6	5.298213000	-0.185798000	0.511594000
1	3.483024000	-0.004401000	1.652581000
6	5.866215000	-0.250650000	-0.755372000
1	5.478097000	-0.223417000	-2.872927000
1	5.929445000	-0.239246000	1.395694000
6	0.719131000	2.057062000	0.890500000
6	0.360613000	3.383521000	1.127197000
6	1.259775000	1.678312000	-0.356702000
6	0.570417000	4.325683000	0.117452000
1	-0.089342000	3.676310000	2.073909000
6	1.481143000	2.620372000	-1.344327000
1	-1.205623000	2.580209000	-0.354181000
6	1.124931000	3.950078000	-1.103993000
1	0.288906000	5.362255000	0.284910000
1	1.916109000	2.331186000	-2.299668000
1	1.270816000	4.696820000	-1.880183000
1	6.942243000	-0.356835000	-0.869819000
6	-0.135547000	0.886163000	3.053959000
1	-0.284841000	-0.128776000	3.438677000
1	-1.115651000	1.374300000	2.962345000
1	0.436429000	1.446346000	3.805446000
16	-3.156663000	1.816438000	0.019378000
8	-1.968598000	2.357304000	-0.925819000
8	-2.764433000	2.068108000	1.397808000
8	-4.385880000	2.343922000	-0.528662000
6	-3.101720000	0.076422000	-0.285716000
6	-3.585103000	-0.407530000	-1.499260000
6	-3.517254000	-1.768458000	-1.749798000
6	-2.978037000	-2.650584000	-0.806601000
6	-2.504145000	-2.137157000	0.400870000
6	-2.560328000	-0.774830000	0.668740000

1	-4.016341000	0.279298000	-2.223476000
1	-3.897422000	-2.162932000	-2.691116000
1	-2.075073000	-2.814767000	1.138270000
1	-2.200874000	-0.370366000	1.612337000
6	-2.905365000	-4.117227000	-1.102172000
1	-2.105444000	-4.334004000	-1.822252000
1	-3.840453000	-4.482975000	-1.541205000
1	-2.698465000	-4.699839000	-0.199068000
6	0.796962000	-0.811539000	-1.186694000
1	-0.224545000	-0.430439000	-1.351859000
1	1.241248000	-1.007113000	-2.168377000
Zero-point correction=			0.481748 (Hartree/Particle)
Thermal correction to Energy=			0.510694
Thermal correction to Enthalpy=			0.511638
Thermal correction to Gibbs Free Energy=			0.422901
Sum of electronic and zero-point Energies=			-1781.210953
Sum of electronic and thermal Energies=			-1781.182006
Sum of electronic and thermal Enthalpies=			-1781.181062
Sum of electronic and thermal Free Energies=			-1781.269799

B-TSe4'

6	0.582878000	4.622987000	-0.411412000
6	0.694358000	3.554663000	-1.263085000
6	1.199563000	2.329157000	-0.764513000
6	1.607601000	2.250825000	0.613037000
6	1.454769000	3.361802000	1.470134000
6	0.958743000	4.532361000	0.954808000
1	0.183781000	5.564269000	-0.782766000
1	0.374442000	3.630120000	-2.300243000
1	1.739479000	3.291938000	2.518255000
1	0.842285000	5.403370000	1.594582000
6	1.337370000	1.070592000	-1.389367000
6	1.875039000	0.138194000	-0.420218000
6	1.958339000	0.912543000	0.866114000
1	1.418562000	0.935571000	-2.465641000
6	2.036062000	0.115454000	2.013944000
6	3.071298000	-0.626253000	-0.916242000
6	2.965471000	-1.374977000	-2.093097000
6	4.299146000	-0.601882000	-0.253107000
6	4.052590000	-2.075654000	-2.594505000
1	2.012736000	-1.405057000	-2.621388000
6	5.390195000	-1.304983000	-0.756643000
1	4.406651000	-0.018310000	0.657655000
6	5.273862000	-2.043306000	-1.926488000

1	3.946848000	-2.649205000	-3.512601000
1	6.339681000	-1.268025000	-0.227040000
6	1.620882000	-1.176775000	1.664875000
6	1.971184000	-2.409964000	2.259073000
6	0.861583000	-1.144864000	0.403351000
6	1.730349000	-3.575558000	1.582704000
1	2.508733000	-2.421191000	3.205806000
6	0.652316000	-2.414992000	-0.264160000
1	-0.041308000	-0.530475000	0.476662000
6	1.088079000	-3.570289000	0.305043000
1	2.055554000	-4.523806000	2.003600000
1	0.093953000	-2.427408000	-1.199490000
1	0.909980000	-4.521812000	-0.191669000
1	6.128076000	-2.589971000	-2.318644000
6	2.435058000	0.588179000	3.367648000
1	3.327879000	1.223310000	3.331921000
1	1.628431000	1.186990000	3.813682000
1	2.630868000	-0.246365000	4.048497000
16	-2.276304000	1.157196000	-0.335636000
8	-2.730366000	2.439145000	-0.839865000
8	-1.488677000	1.098139000	0.890124000
8	-1.462745000	0.372713000	-1.475376000
1	-0.509408000	0.683126000	-1.464339000
6	-3.654143000	0.059533000	-0.206878000
6	-4.893951000	0.464186000	-0.679653000
6	-5.970886000	-0.407490000	-0.567702000
6	-5.818542000	-1.668120000	0.008775000
6	-4.554514000	-2.048099000	0.475111000
6	-3.470652000	-1.191840000	0.375826000
1	-5.000241000	1.449368000	-1.126054000
1	-6.949902000	-0.104093000	-0.934510000
1	-4.426754000	-3.031835000	0.924546000
1	-2.488645000	-1.482980000	0.744207000
6	-6.983950000	-2.598701000	0.149036000
1	-7.331905000	-2.638994000	1.188743000
1	-7.829625000	-2.282411000	-0.469299000
1	-6.715553000	-3.621604000	-0.137798000
Zero-point correction=			0.476348 (Hartree/Particle)
Thermal correction to Energy=			0.505818
Thermal correction to Enthalpy=			0.506762
Thermal correction to Gibbs Free Energy=			0.414666
Sum of electronic and zero-point Energies=			-1781.122399
Sum of electronic and thermal Energies=			-1781.092929
Sum of electronic and thermal Enthalpies=			-1781.091985

Sum of electronic and thermal Free Energies= -1781.184081

B-TSf3'

6	-0.577987000	5.168586000	0.229699000
6	-0.582211000	4.250832000	1.275455000
6	-0.907389000	2.933014000	0.990005000
6	-1.207313000	2.529656000	-0.312166000
6	-1.191030000	3.441575000	-1.354745000
6	-0.876869000	4.767542000	-1.072000000
1	-0.332777000	6.208976000	0.428603000
1	-0.331609000	4.558654000	2.288144000
1	-1.425118000	3.127390000	-2.369705000
1	-0.860337000	5.499353000	-1.875754000
6	-0.907982000	1.729193000	1.858812000
6	-1.409228000	0.641156000	1.086502000
6	-1.503183000	1.056583000	-0.351425000
1	-0.722774000	0.508425000	-0.918739000
6	-2.896544000	0.661314000	-0.849250000
6	-1.688093000	-0.675856000	1.590592000
6	-1.278576000	-1.821079000	0.883930000
6	-2.406789000	-0.810994000	2.790179000
6	-1.617615000	-3.075214000	1.364920000
1	-0.641149000	-1.707222000	0.008748000
6	-2.766743000	-2.069233000	3.243001000
1	-2.722129000	0.080351000	3.328688000
6	-2.374837000	-3.199209000	2.526877000
1	-1.299763000	-3.959665000	0.818984000
1	-3.351654000	-2.173466000	4.152745000
6	-3.078168000	-0.712053000	-1.360617000
6	-4.191138000	-1.461409000	-0.962008000
6	-2.141222000	-1.301545000	-2.217764000
6	-4.370267000	-2.761720000	-1.413499000
1	-4.896145000	-1.023093000	-0.257298000
6	-2.325522000	-2.600549000	-2.673656000
1	-1.245161000	-0.756196000	-2.510825000
6	-3.437452000	-3.334856000	-2.272117000
1	-5.233405000	-3.334915000	-1.083177000
1	-1.589106000	-3.043110000	-3.339637000
1	-3.571898000	-4.355684000	-2.622030000
6	-3.916430000	1.518779000	-0.739959000
1	-3.782005000	2.517860000	-0.333197000
1	-1.046295000	1.764368000	2.941612000
1	-4.907692000	1.252379000	-1.098331000
1	-2.656690000	-4.186504000	2.885448000

16	1.845764000	0.311125000	-0.208415000
8	1.863668000	1.674611000	-0.748775000
8	1.063130000	-0.661821000	-1.014200000
8	1.433198000	0.261663000	1.239032000
1	0.170817000	1.234192000	1.706118000
6	3.519382000	-0.291463000	-0.212243000
6	4.569147000	0.582452000	-0.455480000
6	5.874866000	0.105111000	-0.417216000
6	6.143424000	-1.234551000	-0.139580000
6	5.068476000	-2.095576000	0.103413000
6	3.762310000	-1.632985000	0.067083000
1	4.347974000	1.623758000	-0.674952000
1	6.704441000	0.785253000	-0.607133000
1	5.267017000	-3.144317000	0.323055000
1	2.924387000	-2.302036000	0.248765000
6	7.550433000	-1.752023000	-0.127569000
1	7.699534000	-2.494237000	0.664759000
1	7.801766000	-2.242195000	-1.077038000
1	8.274865000	-0.944823000	0.023285000
Zero-point correction=			0.475687 (Hartree/Particle)
Thermal correction to Energy=			0.504792
Thermal correction to Enthalpy=			0.505736
Thermal correction to Gibbs Free Energy=			0.413930
Sum of electronic and zero-point Energies=			-1781.135181
Sum of electronic and thermal Energies=			-1781.106076
Sum of electronic and thermal Enthalpies=			-1781.105131
Sum of electronic and thermal Free Energies=			-1781.196937

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6	1.372744000	4.277301000	0.178946000
6	0.888814000	3.517661000	1.244399000
6	-0.216716000	2.705089000	1.040315000
6	-0.839887000	2.635441000	-0.221415000
6	-0.347197000	3.391679000	-1.285779000
6	0.757120000	4.211473000	-1.071099000
1	2.241250000	4.916112000	0.319871000
1	1.378591000	3.546670000	2.216183000
1	-0.803044000	3.318386000	-2.270701000
1	1.155308000	4.797883000	-1.895901000
6	-0.894302000	1.746020000	1.962860000
6	-1.889149000	1.050727000	1.073814000
6	-1.886861000	1.603880000	-0.173005000
1	0.959772000	1.243134000	-0.243337000
6	-2.708400000	1.225414000	-1.341360000

6	-2.677292000	-0.083796000	1.558451000
6	-4.043614000	-0.208849000	1.286187000
6	-2.031438000	-1.109434000	2.261757000
6	-4.740534000	-1.342184000	1.681505000
1	-4.554172000	0.591444000	0.752994000
6	-2.730613000	-2.243039000	2.653141000
1	-0.960328000	-1.038430000	2.450941000
6	-4.085435000	-2.364251000	2.361395000
1	-5.800689000	-1.429676000	1.454931000
1	-2.211571000	-3.041814000	3.177666000
6	-2.904134000	-0.213766000	-1.635575000
6	-4.122772000	-0.686608000	-2.132034000
6	-1.883708000	-1.133487000	-1.383366000
6	-4.315976000	-2.042665000	-2.361791000
1	-4.939056000	0.015874000	-2.294628000
6	-2.077034000	-2.489521000	-1.602633000
1	-0.926795000	-0.788079000	-1.001493000
6	-3.295764000	-2.950054000	-2.090873000
1	-5.275106000	-2.396067000	-2.734300000
1	-1.264117000	-3.177630000	-1.381564000
1	-3.454551000	-4.013766000	-2.253580000
6	-3.257223000	2.176153000	-2.114240000
1	-3.158224000	3.232454000	-1.876491000
1	-1.416962000	2.260554000	2.783917000
1	-3.828784000	1.920102000	-3.002924000
1	-4.631606000	-3.254943000	2.663320000
16	1.772612000	-0.659821000	0.350771000
8	1.060184000	-1.857563000	-0.047930000
8	1.590258000	-0.117996000	1.691455000
8	1.442647000	0.517630000	-0.695136000
1	-0.185551000	1.052299000	2.434824000
6	3.494713000	-0.882124000	0.036194000
6	4.370293000	0.167857000	0.306146000
6	5.725276000	-0.025108000	0.101760000
6	6.217179000	-1.251509000	-0.362684000
6	5.315996000	-2.283196000	-0.620653000
6	3.950576000	-2.108047000	-0.425162000
1	3.986436000	1.119167000	0.669433000
1	6.424057000	0.784600000	0.306119000
1	5.690065000	-3.239909000	-0.980395000
1	3.239817000	-2.905282000	-0.623772000
6	7.687284000	-1.434969000	-0.582606000
1	7.932691000	-2.473358000	-0.824622000
1	8.043436000	-0.806676000	-1.408024000

1	8.260958000	-1.149008000	0.306494000
Zero-point correction=			0.479386 (Hartree/Particle)
Thermal correction to Energy=			0.509289
Thermal correction to Enthalpy=			0.510233
Thermal correction to Gibbs Free Energy=			0.417726
Sum of electronic and zero-point Energies=			-1781.187997
Sum of electronic and thermal Energies=			-1781.158094
Sum of electronic and thermal Enthalpies=			-1781.157150
Sum of electronic and thermal Free Energies=			-1781.249657

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6	-0.144766000	-3.369171000	-1.790637000
6	-0.245179000	-2.545054000	-0.668944000
6	-0.618129000	-1.213975000	-0.834101000
6	-0.940123000	-0.738133000	-2.127520000
6	-0.872660000	-1.565211000	-3.233397000
6	-0.437134000	-2.883825000	-3.062763000
1	0.159541000	-4.406258000	-1.666600000
1	-0.012434000	-2.927766000	0.324368000
1	-1.168938000	-1.209756000	-4.218072000
1	-0.358742000	-3.541274000	-3.925641000
6	-0.617209000	-0.107450000	0.170950000
6	-1.048802000	1.109279000	-0.571428000
6	-1.618590000	0.573270000	-1.884283000
1	-1.013889000	-0.280136000	1.178097000
6	-0.088028000	2.270177000	-0.547810000
6	0.132026000	2.998028000	0.626987000
6	0.649394000	2.594960000	-1.690214000
6	1.030590000	4.055450000	0.647167000
1	-0.408812000	2.718298000	1.530916000
6	1.545206000	3.662591000	-1.669773000
1	0.519762000	2.013343000	-2.600623000
6	1.729190000	4.404022000	-0.508363000
1	1.180347000	4.616088000	1.566982000
1	2.096471000	3.914739000	-2.573132000
6	-2.653208000	2.639966000	-1.659622000
6	-2.802433000	4.007022000	-1.860209000
6	-2.699638000	2.110083000	-0.313223000
6	-3.008918000	4.851728000	-0.776128000
1	-2.697799000	4.421246000	-2.860734000
6	-2.907178000	3.013995000	0.768037000
1	-3.169515000	1.130759000	-0.120914000
6	-3.049436000	4.364287000	0.539638000
1	-3.115720000	5.920485000	-0.950288000

1	-3.006084000	2.590004000	1.767470000
1	-3.217836000	5.051686000	1.364292000
79	1.539941000	-0.037978000	0.466715000
15	3.865742000	-0.407995000	0.413786000
6	4.436987000	-1.712765000	1.547312000
6	4.918418000	1.037674000	0.749618000
6	4.309976000	-0.958683000	-1.267623000
6	5.460284000	-2.603077000	1.211522000
6	3.840303000	-1.786231000	2.809864000
6	4.469468000	2.278414000	0.287482000
6	6.141491000	0.946026000	1.418194000
6	5.569795000	-0.710101000	-1.820581000
6	3.352361000	-1.655501000	-2.013509000
6	5.885636000	-3.551853000	2.135599000
1	5.920961000	-2.557300000	0.225564000
6	4.271601000	-2.733106000	3.730990000
1	3.029709000	-1.102837000	3.063674000
6	5.243947000	3.414674000	0.483032000
1	3.506924000	2.356886000	-0.221669000
6	6.910918000	2.088786000	1.614426000
1	6.490960000	-0.016651000	1.788989000
6	5.869955000	-1.162193000	-3.101132000
1	6.314961000	-0.154816000	-1.251569000
6	3.658722000	-2.106198000	-3.292280000
1	2.359916000	-1.844526000	-1.598614000
6	5.293692000	-3.615704000	3.393518000
1	6.679215000	-4.246102000	1.870003000
1	3.801575000	-2.789244000	4.709605000
6	6.464330000	3.320838000	1.146739000
1	4.885608000	4.376646000	0.122882000
1	7.861163000	2.015851000	2.138075000
6	4.915539000	-1.859654000	-3.836475000
1	6.850286000	-0.964040000	-3.528043000
1	2.903966000	-2.641906000	-3.863287000
1	5.625933000	-4.361463000	4.111740000
1	7.066546000	4.212084000	1.306721000
1	5.150997000	-2.205869000	-4.840164000
8	-4.590994000	-0.716745000	-1.906274000
16	-4.911513000	-1.257591000	-0.587515000
9	-3.187450000	-3.152945000	-1.107796000
9	-4.574211000	-3.622306000	0.478352000
9	-5.241150000	-3.627873000	-1.574235000
6	-4.441266000	-3.037757000	-0.696539000
8	-4.356069000	-1.776284000	2.706225000

8	-2.873877000	0.258590000	2.503418000
16	-4.013053000	-0.534989000	2.035241000
9	-5.577664000	1.476817000	1.334755000
9	-6.589030000	-0.072135000	2.451923000
9	-5.240697000	1.274839000	3.452997000
6	-5.468263000	0.601118000	2.331037000
7	-3.830127000	-0.624219000	0.433171000
8	-6.283051000	-1.255173000	-0.102667000
1	2.413124000	5.250365000	-0.500008000
6	-2.135890000	1.714248000	-2.685484000
6	-2.167901000	1.893802000	-4.008483000
1	-1.710355000	1.179516000	-4.686922000
1	-2.681103000	2.739558000	-4.459741000
1	-2.580964000	0.133944000	-1.555609000
Zero-point correction=			0.666378 (Hartree/Particle)
Thermal correction to Energy=			0.718373
Thermal correction to Enthalpy=			0.719317
Thermal correction to Gibbs Free Energy=			0.575008
Sum of electronic and zero-point Energies=			-3883.745370
Sum of electronic and thermal Energies=			-3883.693375
Sum of electronic and thermal Enthalpies=			-3883.692431
Sum of electronic and thermal Free Energies=			-3883.836740

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6	4.771072000	-0.574451000	0.674216000
6	3.767375000	-1.493548000	0.941559000
6	2.490035000	-1.272135000	0.422177000
6	2.234385000	-0.142035000	-0.386746000
6	3.243466000	0.779356000	-0.641658000
6	4.507006000	0.555836000	-0.106869000
1	5.769093000	-0.727931000	1.078110000
1	3.963338000	-2.368620000	1.558804000
1	3.051990000	1.654778000	-1.260750000
1	5.303337000	1.270248000	-0.303388000
6	1.262294000	-2.010686000	0.570483000
6	0.246351000	-1.368150000	-0.080823000
6	0.792199000	-0.197781000	-0.781589000
1	1.251861000	0.134399000	-2.132010000
6	0.094516000	1.026222000	-1.108345000
6	-1.157560000	-1.774526000	-0.120149000
6	-1.979956000	-1.471945000	-1.213601000
6	-1.719906000	-2.479651000	0.952719000
6	-3.311156000	-1.867129000	-1.235813000
1	-1.560490000	-0.936185000	-2.062929000

6	-3.048090000	-2.879207000	0.927698000
1	-1.103126000	-2.694100000	1.823736000
6	-3.851857000	-2.574328000	-0.167282000
1	-3.928847000	-1.625332000	-2.097908000
1	-3.463375000	-3.422654000	1.773517000
6	-0.679447000	1.845382000	-0.202076000
6	-1.465740000	2.901722000	-0.687237000
6	-0.636040000	1.609857000	1.181691000
6	-2.179710000	3.706862000	0.186637000
1	-1.523625000	3.066593000	-1.761459000
6	-1.369121000	2.402732000	2.050414000
1	-0.004236000	0.808704000	1.562221000
6	-2.136905000	3.454769000	1.555868000
1	-2.785387000	4.523762000	-0.197841000
1	-1.332379000	2.211701000	3.119905000
1	-2.706531000	4.079322000	2.239936000
6	0.473443000	1.309174000	-2.436750000
1	0.585952000	2.332275000	-2.818055000
1	1.173429000	-2.956085000	1.100066000
1	0.123413000	0.613784000	-3.204034000
1	-4.894350000	-2.882692000	-0.185065000
Zero-point correction=			0.328813 (Hartree/Particle)
Thermal correction to Energy=			0.346641
Thermal correction to Enthalpy=			0.347585
Thermal correction to Gibbs Free Energy=			0.281719
Sum of electronic and zero-point Energies=			-886.167740
Sum of electronic and thermal Energies=			-886.149912
Sum of electronic and thermal Enthalpies=			-886.148968
Sum of electronic and thermal Free Energies=			-886.214834

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6	-0.856978000	-3.410094000	-1.512766000
6	-0.792517000	-2.529122000	-0.444101000
6	-0.749711000	-1.157994000	-0.703370000
6	-0.817340000	-0.692231000	-2.039715000
6	-0.879405000	-1.590043000	-3.109988000
6	-0.879340000	-2.948426000	-2.837361000
1	-0.898050000	-4.480041000	-1.320959000
1	-0.786345000	-2.889009000	0.583256000
1	-0.926896000	-1.234614000	-4.136879000
1	-0.925318000	-3.664479000	-3.654207000
6	-0.579572000	-0.029547000	0.224252000
6	-0.788492000	1.188143000	-0.573829000
6	-0.999108000	0.735298000	-1.966411000

1	-0.988902000	-0.081007000	1.238653000
6	-1.715668000	1.577371000	-2.792563000
6	0.001315000	2.410975000	-0.201364000
6	0.058231000	2.796984000	1.145368000
6	0.704148000	3.160622000	-1.145533000
6	0.793210000	3.906496000	1.532205000
1	-0.497503000	2.221503000	1.885701000
6	1.435776000	4.282186000	-0.754142000
1	0.682373000	2.864735000	-2.192247000
6	1.483371000	4.659782000	0.581734000
1	0.820437000	4.192752000	2.580878000
1	1.972743000	4.858275000	-1.505614000
6	-2.365593000	2.565377000	-1.993344000
6	-2.657398000	3.888633000	-2.366022000
6	-2.560010000	2.134700000	-0.632914000
6	-2.992429000	4.798367000	-1.387108000
1	-2.521962000	4.207594000	-3.397730000
6	-2.910848000	3.106693000	0.345464000
1	-2.965307000	1.129006000	-0.461838000
6	-3.098515000	4.413064000	-0.028939000
1	-3.156924000	5.839636000	-1.655151000
1	-3.070572000	2.773622000	1.369505000
1	-3.384024000	5.157929000	0.709963000
79	1.577799000	-0.158706000	0.441885000
15	3.905305000	-0.479941000	0.326675000
6	4.584680000	-1.712805000	1.479974000
6	4.874014000	1.039477000	0.586459000
6	4.319933000	-1.063734000	-1.350496000
6	5.635976000	-2.565962000	1.134364000
6	4.034402000	-1.774571000	2.764052000
6	4.290182000	2.256154000	0.219221000
6	6.164178000	1.022820000	1.124208000
6	5.551020000	-0.785233000	-1.951620000
6	3.365196000	-1.814436000	-2.045592000
6	6.134348000	-3.466480000	2.070064000
1	6.059760000	-2.530103000	0.131600000
6	4.538508000	-2.672859000	3.696370000
1	3.201752000	-1.121831000	3.026622000
6	4.999928000	3.441062000	0.370449000
1	3.272039000	2.281829000	-0.175292000
6	6.867465000	2.212924000	1.277361000
1	6.614598000	0.079615000	1.431493000
6	5.826494000	-1.263497000	-3.228144000
1	6.291965000	-0.184728000	-1.424829000

6	3.645161000	-2.289226000	-3.321618000
1	2.394388000	-2.019707000	-1.590580000
6	5.587881000	-3.518989000	3.348791000
1	6.949632000	-4.132177000	1.797280000
1	4.104002000	-2.720515000	4.691660000
6	6.287449000	3.420337000	0.898401000
1	4.534225000	4.382478000	0.086605000
1	7.869608000	2.197348000	1.699017000
6	4.874853000	-2.014357000	-3.912490000
1	6.784639000	-1.042740000	-3.692578000
1	2.893280000	-2.864956000	-3.855604000
1	5.976707000	-4.228170000	4.075616000
1	6.838267000	4.349539000	1.024395000
1	5.090281000	-2.380413000	-4.913579000
8	-3.977422000	-1.245239000	-1.957932000
16	-4.690350000	-1.280879000	-0.686931000
9	-3.548721000	-3.486612000	0.203665000
9	-5.618776000	-3.258023000	0.763970000
9	-5.104874000	-3.778804000	-1.262340000
6	-4.739390000	-3.070450000	-0.200903000
8	-4.296266000	-1.590218000	2.674391000
8	-2.930940000	0.520400000	2.433040000
16	-3.995736000	-0.364548000	1.949298000
9	-5.519308000	1.650394000	1.229991000
9	-6.612308000	-0.044966000	2.010437000
9	-5.501914000	1.226810000	3.345942000
6	-5.520207000	0.678495000	2.136429000
7	-3.728183000	-0.552062000	0.381311000
8	-6.083089000	-0.859698000	-0.627998000
1	2.051581000	5.536497000	0.885395000
6	-1.961963000	1.367881000	-4.243523000
1	-1.042426000	1.167897000	-4.803971000
1	-2.621462000	0.494734000	-4.361306000
1	-2.472168000	2.223814000	-4.696175000
Zero-point correction=			0.666936 (Hartree/Particle)
Thermal correction to Energy=			0.717523
Thermal correction to Enthalpy=			0.718467
Thermal correction to Gibbs Free Energy=			0.579525
Sum of electronic and zero-point Energies=			-3883.807670
Sum of electronic and thermal Energies=			-3883.757083
Sum of electronic and thermal Enthalpies=			-3883.756139
Sum of electronic and thermal Free Energies=			-3883.895081

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6	-1.275884000	2.543125000	-3.896359000
6	-0.693347000	1.596027000	-3.065062000
6	-0.983367000	1.612844000	-1.701416000
6	-1.867749000	2.606824000	-1.205192000
6	-2.467220000	3.548642000	-2.053863000
6	-2.156784000	3.516619000	-3.400564000
1	-1.045338000	2.532401000	-4.959757000
1	-0.014847000	0.844896000	-3.466304000
1	-3.156691000	4.290709000	-1.657093000
1	-2.596205000	4.241760000	-4.080514000
6	-0.557545000	0.653452000	-0.644735000
6	-1.022559000	1.363376000	0.657867000
6	-2.049196000	2.355375000	0.185689000
1	-1.141945000	-0.270788000	-0.773003000
6	-2.997843000	2.646208000	1.147753000
6	0.146061000	2.098206000	1.341847000
6	1.041007000	1.409915000	2.169047000
6	0.398721000	3.450412000	1.098861000
6	2.135890000	2.045664000	2.742270000
1	0.909316000	0.347022000	2.357042000
6	1.499916000	4.090966000	1.665424000
1	-0.265111000	4.021453000	0.454039000
6	2.372094000	3.395299000	2.492922000
1	2.810933000	1.473675000	3.377089000
1	1.664953000	5.146771000	1.460487000
6	-2.829974000	1.684074000	2.169328000
6	-3.443251000	1.593521000	3.431754000
6	-1.885429000	0.628866000	1.736966000
6	-2.999337000	0.634747000	4.311586000
1	-4.207455000	2.306583000	3.731501000
6	-1.398231000	-0.294761000	2.760103000
1	-2.532938000	-0.027578000	1.088517000
6	-1.967687000	-0.299364000	3.993703000
1	-3.448769000	0.584525000	5.301908000
1	-0.696336000	-1.069965000	2.456677000
1	-1.684207000	-1.042749000	4.733418000
79	1.449739000	0.029071000	-0.677760000
15	3.724791000	-0.606756000	-0.371957000
6	4.401689000	-1.997516000	-1.330950000
6	3.906095000	-1.095737000	1.379713000
6	4.892481000	0.777626000	-0.579169000
6	5.396723000	-2.836431000	-0.819825000
6	3.907741000	-2.214053000	-2.620191000
6	4.913572000	-0.594763000	2.206113000

6	2.944850000	-1.964145000	1.911039000
6	6.201024000	0.607894000	-1.035687000
6	4.448394000	2.050654000	-0.203715000
6	5.896145000	-3.875371000	-1.596565000
1	5.775208000	-2.678656000	0.189777000
6	4.413059000	-3.251677000	-3.395375000
1	3.116847000	-1.571458000	-3.006626000
6	4.956085000	-0.955188000	3.550782000
1	5.659295000	0.088529000	1.801522000
6	2.992182000	-2.322849000	3.252395000
1	2.148993000	-2.348443000	1.270453000
6	7.057693000	1.702294000	-1.110902000
1	6.551506000	-0.378974000	-1.334364000
6	5.311992000	3.137035000	-0.267795000
1	3.423732000	2.187663000	0.146425000
6	5.405051000	-4.082112000	-2.882999000
1	6.666019000	-4.529946000	-1.195075000
1	4.021783000	-3.419467000	-4.395675000
6	3.995586000	-1.813770000	4.074947000
1	5.741631000	-0.559844000	4.190645000
1	2.241266000	-2.997368000	3.657230000
6	6.616174000	2.963774000	-0.723953000
1	8.074101000	1.567838000	-1.473508000
1	4.959965000	4.122217000	0.030865000
1	5.792215000	-4.900005000	-3.486022000
1	4.027010000	-2.088343000	5.126685000
1	7.289501000	3.815811000	-0.782464000
8	-5.020796000	1.013713000	-0.484643000
16	-4.904325000	-0.397134000	-0.833796000
9	-4.503203000	-1.597995000	-3.127782000
9	-5.880463000	0.062932000	-3.183045000
9	-3.758128000	0.424981000	-3.034495000
6	-4.742813000	-0.383976000	-2.669016000
8	-3.589395000	-3.482577000	-0.795039000
8	-1.774624000	-2.422086000	0.599506000
16	-3.153117000	-2.437335000	0.111615000
9	-4.447130000	-1.481087000	2.217583000
9	-5.301234000	-3.293642000	1.412492000
9	-3.468386000	-3.374802000	2.539604000
6	-4.175914000	-2.666377000	1.667603000
7	-3.449527000	-0.910630000	-0.342580000
8	-5.996312000	-1.314210000	-0.544002000
6	-4.099993000	3.641197000	1.042419000
1	-4.830682000	3.290918000	0.301827000

1	-4.627010000	3.768449000	1.993307000
1	-3.731931000	4.625583000	0.731203000
1	3.228978000	3.895950000	2.938541000
Zero-point correction=			0.669045 (Hartree/Particle)
Thermal correction to Energy=			0.721000
Thermal correction to Enthalpy=			0.721944
Thermal correction to Gibbs Free Energy=			0.578564
Sum of electronic and zero-point Energies=			-3883.818524
Sum of electronic and thermal Energies=			-3883.766568
Sum of electronic and thermal Enthalpies=			-3883.765624
Sum of electronic and thermal Free Energies=			-3883.909005

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6	1.309937000	-4.046803000	-3.393793000
6	0.711924000	-2.997072000	-2.694878000
6	1.281660000	-2.563341000	-1.507058000
6	2.452823000	-3.195205000	-1.034704000
6	3.055080000	-4.237211000	-1.733190000
6	2.467127000	-4.665440000	-2.920128000
1	0.863025000	-4.393732000	-4.323304000
1	-0.190161000	-2.516754000	-3.072656000
1	3.951386000	-4.722487000	-1.349696000
1	2.907544000	-5.488624000	-3.477544000
6	0.912439000	-1.397950000	-0.630122000
6	1.605735000	-1.796758000	0.729645000
6	2.826406000	-2.488190000	0.173079000
1	1.496217000	-0.544194000	-1.010276000
6	4.000288000	-2.042190000	0.701811000
6	0.738781000	-2.719468000	1.585250000
6	-0.464272000	-2.250907000	2.124490000
6	1.119336000	-4.028833000	1.881575000
6	-1.270064000	-3.060992000	2.912422000
1	-0.791679000	-1.233685000	1.914476000
6	0.314957000	-4.847130000	2.672746000
1	2.053077000	-4.424521000	1.486881000
6	-0.883300000	-4.370253000	3.188309000
1	-2.202559000	-2.659002000	3.307721000
1	0.631911000	-5.866664000	2.881818000
6	3.669397000	-1.046867000	1.683529000
6	4.502507000	-0.363266000	2.573895000
6	2.258704000	-0.719385000	1.615237000
6	3.922665000	0.482980000	3.499874000
1	5.578258000	-0.519561000	2.556726000
6	1.689713000	0.022659000	2.707542000

1	2.401346000	0.305131000	0.900446000
6	2.524440000	0.658138000	3.591773000
1	4.561893000	1.017058000	4.200158000
1	0.617135000	0.194153000	2.738557000
1	2.115909000	1.311804000	4.357076000
79	-1.049595000	-0.661457000	-0.634605000
15	-3.210158000	0.297642000	-0.339005000
6	-3.316571000	2.096612000	-0.585346000
6	-3.608711000	0.088017000	1.436678000
6	-4.598995000	-0.470875000	-1.235875000
6	-4.361877000	2.851383000	-0.037558000
6	-2.289262000	2.738057000	-1.278812000
6	-4.702335000	-0.641018000	1.900601000
6	-2.710775000	0.653174000	2.353192000
6	-5.656397000	0.256645000	-1.784872000
6	-4.578715000	-1.864408000	-1.368995000
6	-4.387192000	4.228930000	-0.209329000
1	-5.147954000	2.357814000	0.534517000
6	-2.310105000	4.120799000	-1.435771000
1	-1.447549000	2.164500000	-1.665515000
6	-4.896519000	-0.810557000	3.270387000
1	-5.404840000	-1.079664000	1.193727000
6	-2.909062000	0.479335000	3.716524000
1	-1.854445000	1.226703000	1.989597000
6	-6.685062000	-0.403513000	-2.450273000
1	-5.671814000	1.341679000	-1.702069000
6	-5.614521000	-2.520564000	-2.022052000
1	-3.742473000	-2.430689000	-0.956429000
6	-3.360682000	4.862621000	-0.908592000
1	-5.200323000	4.813076000	0.215407000
1	-1.489238000	4.608889000	-1.955062000
6	-4.001448000	-0.255143000	4.177617000
1	-5.752659000	-1.379294000	3.626049000
1	-2.208395000	0.917642000	4.424021000
6	-6.668029000	-1.789260000	-2.565119000
1	-7.501974000	0.169614000	-2.882442000
1	-5.593014000	-3.603387000	-2.118248000
1	-3.375810000	5.943632000	-1.027821000
1	-4.153274000	-0.391786000	5.245825000
1	-7.473558000	-2.301660000	-3.086019000
8	4.979266000	1.084822000	-0.216111000
16	3.902536000	1.832406000	-0.844194000
9	2.348700000	1.193462000	-2.871571000
9	4.463272000	1.271406000	-3.306660000

9	3.650247000	-0.392720000	-2.203896000
6	3.555119000	0.912409000	-2.416423000
8	0.891727000	3.041034000	-1.285432000
8	0.226125000	1.825779000	0.828861000
16	1.229693000	2.521108000	0.027284000
9	2.063446000	3.612214000	2.251596000
9	2.528520000	4.775400000	0.497192000
9	0.498376000	4.681692000	1.214550000
6	1.627732000	4.003696000	1.063254000
7	2.563500000	1.581508000	0.074291000
8	4.072736000	3.214977000	-1.242359000
1	-1.511350000	-5.011948000	3.802247000
6	5.386422000	-2.365347000	0.266080000
1	5.926693000	-2.967818000	1.007578000
1	5.375451000	-2.921707000	-0.677176000
1	5.955777000	-1.441837000	0.104500000
Zero-point correction=			0.665831 (Hartree/Particle)
Thermal correction to Energy=			0.717102
Thermal correction to Enthalpy=			0.718046
Thermal correction to Gibbs Free Energy=			0.578886
Sum of electronic and zero-point Energies=			-3883.826556
Sum of electronic and thermal Energies=			-3883.775285
Sum of electronic and thermal Enthalpies=			-3883.774341
Sum of electronic and thermal Free Energies=			-3883.913502

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6	2.023135000	-2.728389000	1.925928000
6	1.168220000	-2.094306000	1.022524000
6	1.129288000	-0.705366000	0.967139000
6	1.974490000	0.041376000	1.825177000
6	2.814181000	-0.593220000	2.740944000
6	2.831000000	-1.986559000	2.787461000
1	2.054044000	-3.815221000	1.963299000
1	0.536001000	-2.678283000	0.354403000
1	3.453211000	-0.012090000	3.402512000
1	3.488432000	-2.493042000	3.490423000
6	0.352363000	0.189988000	0.037146000
6	0.492034000	1.595829000	0.725067000
6	1.812836000	1.441267000	1.459044000
1	0.874304000	0.221022000	-0.931532000
6	2.658145000	2.467951000	1.220126000
6	-0.670487000	1.853958000	1.696638000
6	-1.865949000	2.427717000	1.243854000
6	-0.607480000	1.476858000	3.041202000

6	-2.955086000	2.607909000	2.087792000
1	-1.955697000	2.742981000	0.207426000
6	-1.697433000	1.654003000	3.892874000
1	0.303767000	1.037698000	3.439131000
6	-2.877076000	2.219208000	3.423073000
1	-3.869194000	3.049275000	1.691862000
1	-1.613525000	1.351822000	4.935225000
6	2.006251000	3.361786000	0.258066000
6	2.515026000	4.490335000	-0.374429000
6	0.770478000	2.806965000	-0.136139000
6	1.792587000	5.055464000	-1.425382000
1	3.473414000	4.912455000	-0.074869000
6	0.071609000	3.363417000	-1.193902000
1	3.658352000	-0.661796000	0.449987000
6	0.591836000	4.489278000	-1.841137000
1	2.180981000	5.933167000	-1.937691000
1	-0.851368000	2.911787000	-1.557347000
1	0.056789000	4.919433000	-2.685061000
79	-1.638546000	-0.395133000	-0.304164000
15	-3.998561000	-0.754190000	-0.422308000
6	-4.708102000	-1.817018000	-1.720578000
6	-4.812593000	0.868476000	-0.633831000
6	-4.656860000	-1.389825000	1.155293000
6	-5.988896000	-1.605576000	-2.239696000
6	-3.945672000	-2.895576000	-2.177678000
6	-5.925861000	1.265620000	0.109219000
6	-4.252621000	1.753332000	-1.561668000
6	-5.729350000	-2.280080000	1.236643000
6	-4.058080000	-0.916685000	2.328627000
6	-6.502701000	-2.471004000	-3.198597000
1	-6.582441000	-0.760265000	-1.892784000
6	-4.465352000	-3.762394000	-3.132524000
1	-2.939752000	-3.044586000	-1.784792000
6	-6.471724000	2.532962000	-0.076590000
1	-6.359720000	0.587070000	0.842456000
6	-4.797810000	3.018061000	-1.743667000
1	-3.372118000	1.447948000	-2.129075000
6	-6.198578000	-2.689710000	2.481646000
1	-6.195652000	-2.657159000	0.327407000
6	-4.540227000	-1.316951000	3.568023000
1	-3.214669000	-0.226470000	2.275660000
6	-5.742616000	-3.549769000	-3.642584000
1	-7.498077000	-2.302256000	-3.602836000
1	-3.868284000	-4.599774000	-3.485209000

6	-5.907673000	3.409688000	-0.998063000
1	-7.337913000	2.837481000	0.506384000
1	-4.351604000	3.703030000	-2.460864000
6	-5.608345000	-2.206935000	3.645672000
1	-7.029534000	-3.388827000	2.541134000
1	-4.069356000	-0.933820000	4.471038000
1	-6.145640000	-4.224455000	-4.394311000
1	-6.330903000	4.402274000	-1.133371000
1	-5.979347000	-2.530043000	4.615694000
8	5.819634000	-0.250581000	1.849422000
16	5.992495000	-0.689712000	0.483505000
9	6.502846000	-3.021297000	-0.609032000
9	7.545054000	-2.588065000	1.231488000
9	5.450842000	-3.118917000	1.269601000
6	6.394547000	-2.497390000	0.589754000
8	5.196080000	-1.436766000	-2.532398000
8	2.726959000	-1.317500000	-1.912207000
16	4.084009000	-0.828794000	-1.846097000
9	3.009770000	1.534909000	-1.797208000
9	5.157743000	1.545446000	-2.011593000
9	3.907916000	0.968520000	-3.678516000
6	4.039840000	0.946801000	-2.366565000
7	4.455284000	-0.684534000	-0.205454000
8	6.929158000	-0.101218000	-0.439953000
6	4.089669000	2.598106000	1.601087000
1	4.415882000	1.796538000	2.269486000
1	4.727046000	2.562216000	0.702693000
1	4.294122000	3.557047000	2.094756000
1	-3.727055000	2.356561000	4.088489000
Zero-point correction=			0.671713 (Hartree/Particle)
Thermal correction to Energy=			0.723679
Thermal correction to Enthalpy=			0.724623
Thermal correction to Gibbs Free Energy=			0.581568
Sum of electronic and zero-point Energies=			-3883.849286
Sum of electronic and thermal Energies=			-3883.797320
Sum of electronic and thermal Enthalpies=			-3883.796376
Sum of electronic and thermal Free Energies=			-3883.939431

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6	0.630415000	-2.088278000	-4.336689000
6	0.664976000	-1.185142000	-3.272504000
6	1.452553000	-1.472072000	-2.164675000
6	2.236586000	-2.645947000	-2.144527000
6	2.201195000	-3.540674000	-3.210943000

6	1.381970000	-3.260436000	-4.301829000
1	0.014124000	-1.868023000	-5.205479000
1	0.105485000	-0.251745000	-3.323102000
1	2.802677000	-4.447826000	-3.194821000
1	1.338508000	-3.955450000	-5.137380000
6	1.726523000	-0.626986000	-0.925762000
6	2.423732000	-1.641729000	0.047946000
6	3.061752000	-2.589363000	-0.950515000
1	2.514509000	0.080377000	-1.242761000
6	4.364127000	-2.824413000	-0.674972000
6	1.422392000	-2.375007000	0.951721000
6	0.829054000	-1.702685000	2.030136000
6	1.048481000	-3.702449000	0.723807000
6	-0.123776000	-2.323880000	2.830250000
1	1.096341000	-0.668898000	2.237083000
6	0.099733000	-4.329519000	1.531356000
1	1.502514000	-4.257199000	-0.093918000
6	-0.498051000	-3.641677000	2.581111000
1	-0.578720000	-1.768011000	3.648582000
1	-0.172121000	-5.364541000	1.330556000
6	4.736700000	-1.976768000	0.462334000
6	5.974921000	-1.794969000	1.068223000
6	3.627716000	-1.196394000	0.852909000
6	6.108076000	-0.813731000	2.050932000
1	6.835842000	-2.390976000	0.768607000
6	3.765372000	-0.232887000	1.835530000
1	1.270289000	0.723790000	-0.521143000
6	5.018733000	-0.032723000	2.422007000
1	7.075644000	-0.650375000	2.520792000
1	2.924787000	0.386548000	2.139311000
1	5.136527000	0.750307000	3.168598000
79	-0.477850000	-0.386637000	-0.315598000
15	-2.711601000	-0.377087000	0.338368000
6	-3.669936000	0.972846000	-0.415457000
6	-2.835806000	-0.167034000	2.140826000
6	-3.600202000	-1.911718000	-0.050173000
6	-4.393326000	1.895630000	0.340366000
6	-3.638393000	1.085827000	-1.808925000
6	-3.568827000	-1.041143000	2.945341000
6	-2.114650000	0.880093000	2.725383000
6	-4.989794000	-1.928468000	-0.201717000
6	-2.874726000	-3.104060000	-0.112510000
6	-5.072484000	2.930837000	-0.296363000
1	-4.418089000	1.813185000	1.425243000

6	-4.324173000	2.114715000	-2.439610000
1	-3.057000000	0.373264000	-2.394951000
6	-3.577792000	-0.866561000	4.326396000
1	-4.121833000	-1.864299000	2.495830000
6	-2.127396000	1.049447000	4.103232000
1	-1.525654000	1.556849000	2.107211000
6	-5.647274000	-3.134822000	-0.412719000
1	-5.553879000	-0.997546000	-0.152820000
6	-3.539424000	-4.308620000	-0.313394000
1	-1.790064000	-3.089065000	0.005531000
6	-5.037063000	3.041489000	-1.681530000
1	-5.626893000	3.654961000	0.295381000
1	-4.291603000	2.202652000	-3.522875000
6	-2.857538000	0.174106000	4.904799000
1	-4.147524000	-1.549664000	4.951879000
1	-1.554241000	1.859442000	4.547338000
6	-4.922669000	-4.323189000	-0.465543000
1	-6.727512000	-3.148381000	-0.535410000
1	-2.971532000	-5.235156000	-0.357546000
1	-5.561871000	3.856008000	-2.175021000
1	-2.860887000	0.301593000	5.984760000
1	-5.440029000	-5.265573000	-0.630186000
8	1.853157000	2.140860000	-2.758341000
16	1.258411000	2.971728000	-1.729195000
9	-1.290884000	3.366728000	-1.146171000
9	-0.695721000	3.933604000	-3.142340000
9	-0.918602000	1.848721000	-2.632224000
6	-0.541522000	3.043109000	-2.180083000
8	0.180619000	3.826570000	1.238436000
8	0.976683000	1.585151000	2.049314000
16	1.115674000	2.722779000	1.148862000
9	3.727673000	2.806135000	0.772222000
9	2.833812000	4.712729000	1.237725000
9	3.074501000	3.226254000	2.782423000
6	2.817227000	3.425668000	1.498233000
7	1.255237000	2.072835000	-0.353167000
8	1.673960000	4.338941000	-1.491978000
1	-1.249334000	-4.125134000	3.202687000
6	5.335238000	-3.623195000	-1.476561000
1	5.628106000	-3.087381000	-2.389854000
1	6.250517000	-3.831741000	-0.912179000
1	4.916773000	-4.586458000	-1.784937000
Zero-point correction=			0.665455 (Hartree/Particle)
Thermal correction to Energy=			0.716267

Thermal correction to Enthalpy=	0.717211
Thermal correction to Gibbs Free Energy=	0.579635
Sum of electronic and zero-point Energies=	-3883.833125
Sum of electronic and thermal Energies=	-3883.782314
Sum of electronic and thermal Enthalpies=	-3883.781370
Sum of electronic and thermal Free Energies=	-3883.918945