

Electronic Supplementary Information (ESI)

Insight into the Reaction Mechanism and Chemoselectivity in the Cycloaddition of Ynamides and Isoxazoles with H₂O

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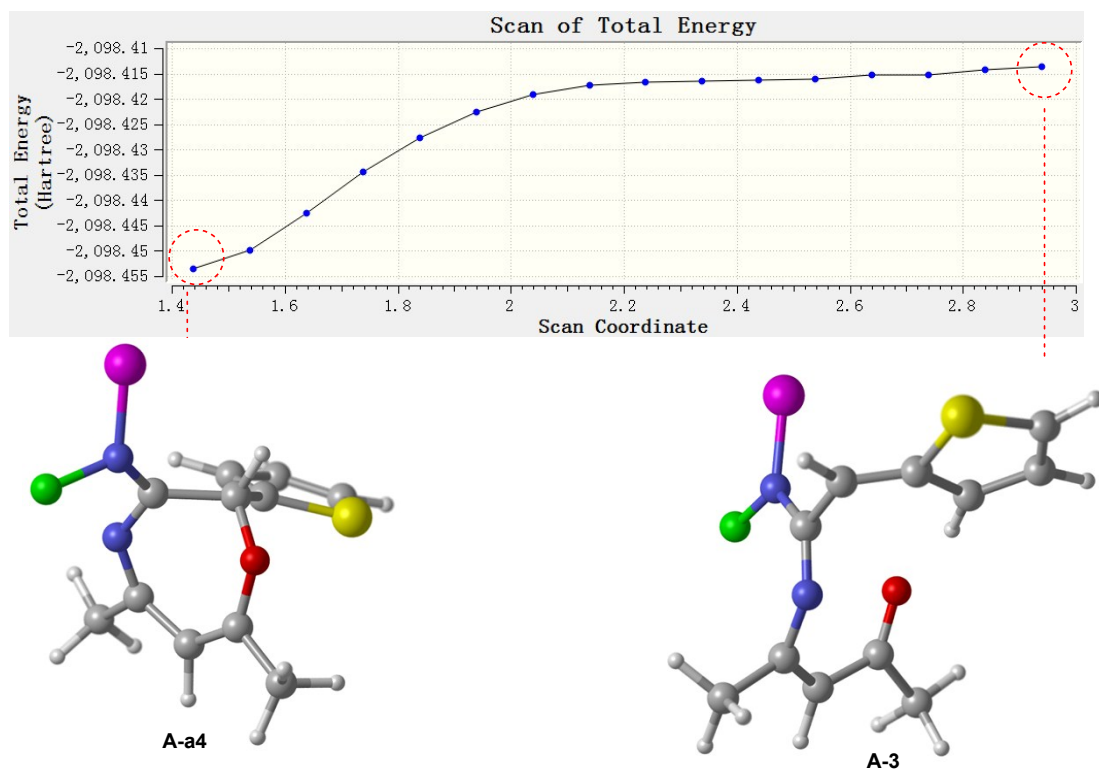


Fig. S1. PES scan results for A-a4.

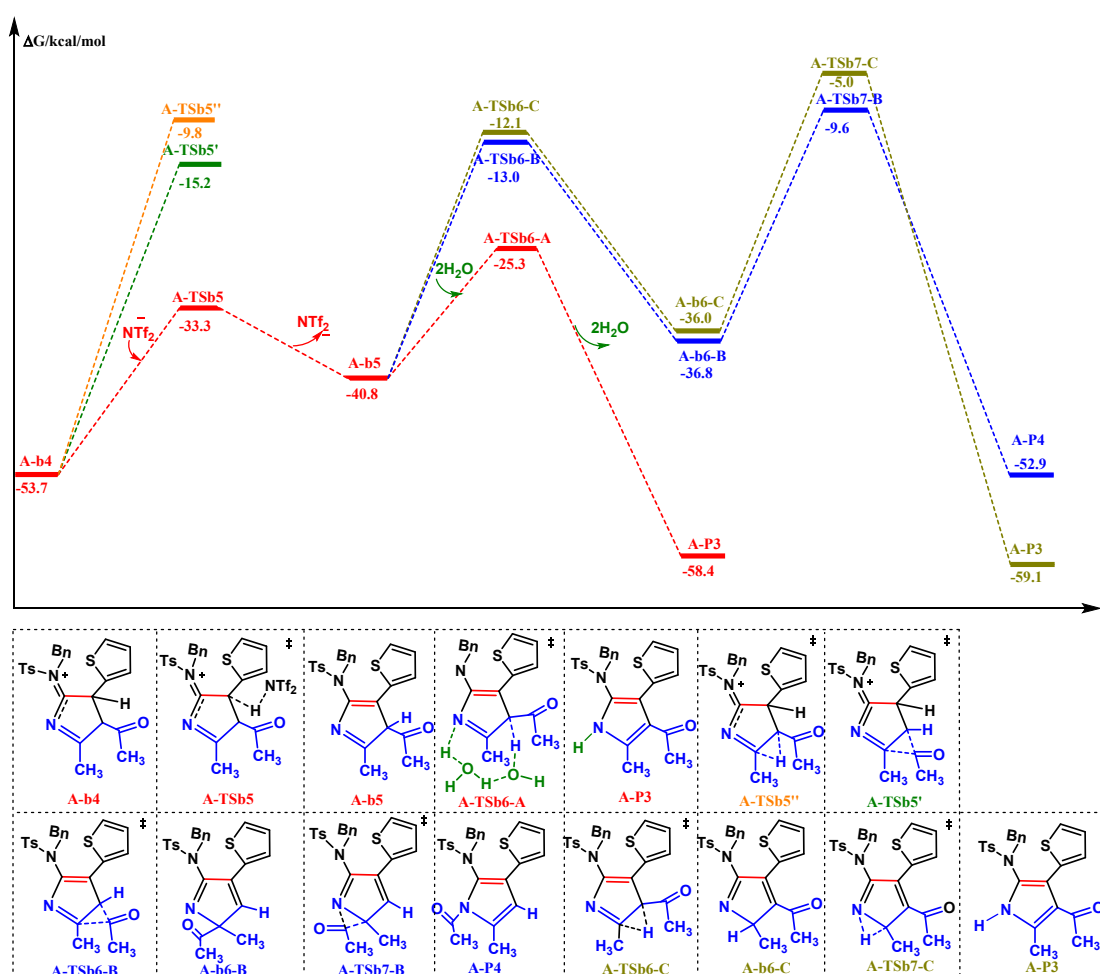


Fig. S2. Free energy profiles for the competition pathways of 1,3-H-shift or 1,3-acyl-shift for the series A. The values are given in kcal/mol.

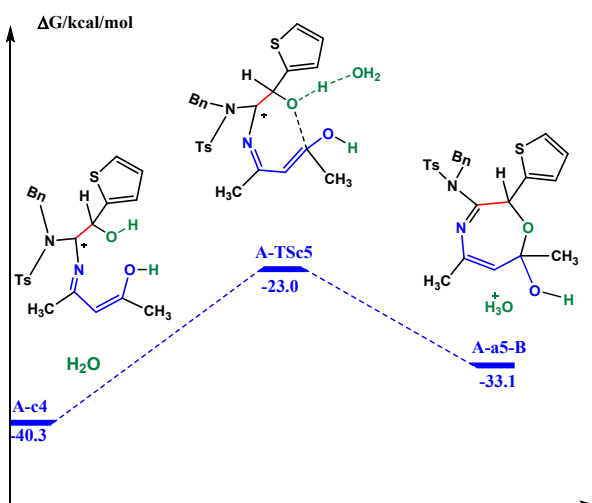


Fig. S3. Free energy profiles of nucleophilic attack for path **c** of the series **A**. The values are given in kcal/mol.

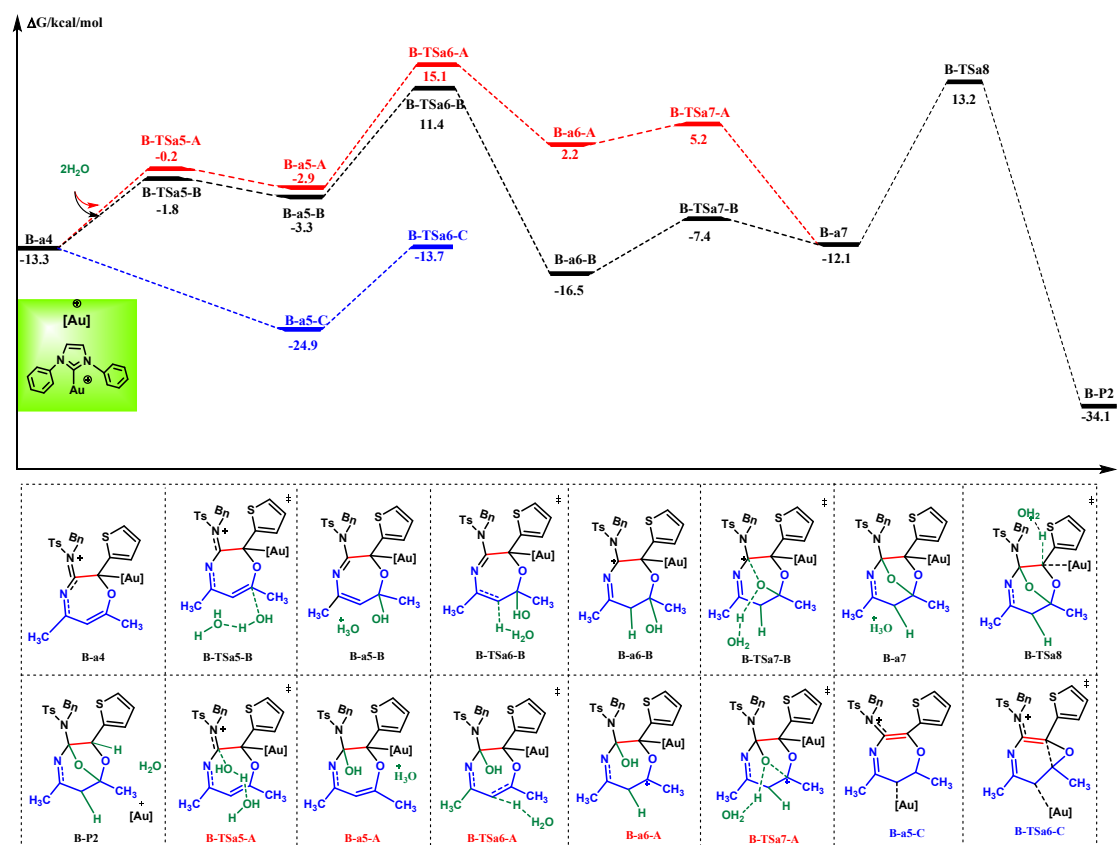


Fig. S4. Free energy profiles for the competition pathways to O-bridged tetrahydro-1,4-oxazepines of the series **B**. The values are given in kcal/mol.

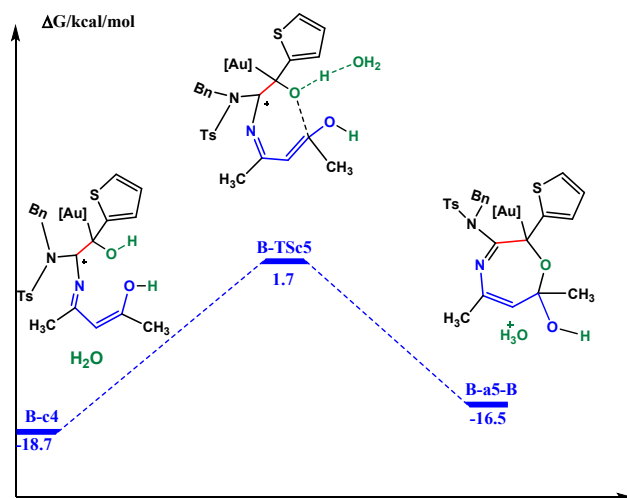


Fig. S5. Free energy profiles of nucleophilic attack for path **c** of the series **B**. The values are given in kcal/mol.

Optimized cartesian coordinates with the self-consistent field (SCF) energies and the imaginary frequencies of transition states

Re1

6	-2.427550000	-0.837794000	0.533674000
6	-2.734180000	0.521916000	0.568909000
6	-3.690130000	1.009171000	-0.314666000
6	-4.333603000	0.161325000	-1.223193000
6	-3.999508000	-1.197720000	-1.234441000
6	-3.046041000	-1.708007000	-0.361765000
16	-1.151237000	-1.455951000	1.588059000
8	-1.274123000	-2.900741000	1.693967000
8	-1.057644000	-0.619490000	2.770637000
7	0.293992000	-1.190181000	0.716143000
6	0.678333000	0.103130000	0.629245000
6	1.036457000	1.258086000	0.547951000
6	1.421434000	2.615628000	0.440127000
6	2.479156000	3.254775000	1.040336000
6	2.557262000	4.633294000	0.700396000
6	1.561093000	5.023009000	-0.149317000
16	0.510883000	3.723984000	-0.553088000
6	-5.389776000	0.694465000	-2.151666000
6	0.535592000	-2.048338000	-0.475649000
6	2.015097000	-2.141125000	-0.746852000
6	2.843173000	-2.835368000	0.139450000
6	4.210657000	-2.917028000	-0.098406000
6	4.761415000	-2.303930000	-1.224752000
6	3.941314000	-1.606494000	-2.106944000
6	2.570573000	-1.521746000	-1.865078000
1	-2.242847000	1.178633000	1.279902000
1	-3.943302000	2.065280000	-0.298774000
1	-4.494188000	-1.864202000	-1.935119000
1	-2.792835000	-2.763473000	-0.364648000
1	3.168827000	2.741714000	1.699819000
1	3.319518000	5.307049000	1.072061000
1	1.385872000	6.008065000	-0.561855000
1	-5.229689000	1.753765000	-2.364560000
1	-6.381409000	0.591914000	-1.697798000

1	-5.401123000	0.143043000	-3.094789000
1	0.125070000	-3.031097000	-0.235170000
1	0.004764000	-1.634776000	-1.340566000
1	2.407185000	-3.307195000	1.016765000
1	4.848479000	-3.461019000	0.591405000
1	5.828795000	-2.370101000	-1.411617000
1	4.367015000	-1.125047000	-2.981839000
1	1.927127000	-0.971474000	-2.546752000

Zero-point correction= 0.325218 (Hartree/Particle)

Thermal correction to Energy= 0.348003

Thermal correction to Enthalpy= 0.348947

Thermal correction to Gibbs Free Energy= 0.267514

Sum of electronic and zero-point Energies= -1773.052571

Sum of electronic and thermal Energies= -1773.029786

Sum of electronic and thermal Enthalpies= -1773.028842

Sum of electronic and thermal Free Energies= -1773.110275

A-TS1

6	-2.046608000	0.771315000	2.047217000
6	-3.032757000	-0.211644000	2.031652000
6	-2.699844000	-1.483380000	2.482142000
6	-1.410240000	-1.770307000	2.940614000
6	-0.452573000	-0.748008000	2.965555000
6	-0.753483000	0.528523000	2.515227000
16	-2.422412000	2.369133000	1.425877000
8	-1.586463000	3.360356000	2.073023000
8	-3.854017000	2.549571000	1.280240000
7	-1.826853000	2.300868000	-0.247214000
6	-0.556290000	2.211338000	-0.402179000
6	0.684504000	1.982167000	-0.485688000
6	1.874807000	2.793669000	-0.541753000
6	2.008601000	4.127547000	-0.236483000
6	3.342524000	4.591774000	-0.376128000
6	4.199096000	3.607868000	-0.787381000
16	3.401160000	2.104041000	-1.002480000
6	-1.038528000	-3.149826000	3.404202000
6	-2.798455000	2.379711000	-1.385309000
6	-3.240285000	1.015651000	-1.837680000

6	-4.351078000	0.402711000	-1.253897000
6	-4.731739000	-0.876753000	-1.651044000
6	-4.006398000	-1.544642000	-2.635927000
6	-2.901423000	-0.932519000	-3.225511000
6	-2.518454000	0.344669000	-2.826460000
1	-4.032326000	0.011698000	1.673712000
1	-3.450762000	-2.267907000	2.468537000
1	0.543919000	-0.960196000	3.339561000
1	-0.006851000	1.316611000	2.535382000
1	1.171217000	4.735693000	0.086880000
1	3.654919000	5.610503000	-0.181810000
1	5.260351000	3.687061000	-0.983028000
1	-1.038398000	-3.198192000	4.498411000
1	-0.032907000	-3.406085000	3.059830000
1	-1.743483000	-3.896211000	3.032133000
1	-3.634416000	2.986299000	-1.036308000
1	-2.273185000	2.917447000	-2.175685000
1	-4.918075000	0.934461000	-0.493959000
1	-5.596477000	-1.349348000	-1.195574000
1	-4.301791000	-2.542791000	-2.944671000
1	-2.331534000	-1.452864000	-3.988798000
1	-1.650981000	0.819804000	-3.276778000
1	0.909226000	0.581525000	-0.416073000
9	-1.564650000	-1.221793000	-0.389915000
9	-0.596464000	-2.995425000	0.388302000
9	-1.465347000	-3.029193000	-1.589448000
6	-0.831657000	-2.280467000	-0.699147000
8	1.641073000	-2.856759000	-1.489548000
8	0.395059000	-0.965374000	-2.626735000
16	0.758450000	-1.706979000	-1.437578000
9	4.856751000	-0.728055000	0.670967000
9	4.165817000	-2.696473000	0.102650000
9	3.864636000	-1.021479000	-1.226788000
6	3.909938000	-1.404300000	0.040455000
8	1.904505000	-2.307592000	1.527891000
8	2.472521000	0.150970000	1.688994000
16	2.281303000	-1.054510000	0.905207000
7	1.276778000	-0.624103000	-0.322199000

Zero-point correction= 0.390037 (Hartree/Particle)

Thermal correction to Energy= 0.427390

Thermal correction to Enthalpy= 0.428334

Thermal correction to Gibbs Free Energy= 0.318834

Sum of electronic and zero-point Energies= -3600.297039

Sum of electronic and thermal Energies= -3600.259687

Sum of electronic and thermal Enthalpies= -3600.258743

Sum of electronic and thermal Free Energies= -3600.368243

A-1

6	-1.185008000	-1.831538000	1.583238000
6	-1.473523000	-0.505357000	1.904878000
6	-2.806592000	-0.128487000	1.969908000
6	-3.831274000	-1.052284000	1.720103000
6	-3.498691000	-2.378276000	1.412152000
6	-2.173414000	-2.781612000	1.327717000
16	0.487974000	-2.273598000	1.351308000
8	0.696188000	-3.702202000	1.474086000
8	1.384803000	-1.310054000	1.940331000
7	0.632913000	-2.053896000	-0.497386000
6	-0.178854000	-1.302311000	-1.070329000
6	-1.189407000	-0.584914000	-1.491338000
6	-2.485945000	-1.185141000	-1.765415000
6	-2.789053000	-2.508532000	-1.976666000
6	-4.184104000	-2.731928000	-2.112660000
6	-4.910988000	-1.577872000	-2.002839000
16	-3.916118000	-0.204962000	-1.744873000
6	-5.269831000	-0.625362000	1.785973000
6	1.687397000	-2.884000000	-1.180625000
6	3.079967000	-2.456394000	-0.798416000
6	3.704549000	-3.009158000	0.322493000
6	4.991751000	-2.611217000	0.671867000
6	5.665073000	-1.671518000	-0.105617000
6	5.051662000	-1.131081000	-1.234254000
6	3.760469000	-1.519874000	-1.579370000
1	-0.680594000	0.214553000	2.077098000
1	-3.048137000	0.905162000	2.198792000
1	-4.289030000	-3.097895000	1.221283000

1	-1.912606000	-3.803661000	1.070557000
1	-2.033315000	-3.284982000	-2.041898000
1	-4.630484000	-3.702751000	-2.289243000
1	-5.983872000	-1.455196000	-2.075235000
1	-5.387350000	0.403013000	1.435132000
1	-5.629651000	-0.665539000	2.820008000
1	-5.902856000	-1.281101000	1.183622000
1	1.480843000	-3.915129000	-0.886086000
1	1.499393000	-2.760238000	-2.247814000
1	3.184199000	-3.754151000	0.918371000
1	5.470552000	-3.042187000	1.545271000
1	6.671261000	-1.365833000	0.164169000
1	5.576925000	-0.402915000	-1.843888000
1	3.274021000	-1.091814000	-2.450214000
1	-1.020422000	0.484161000	-1.597304000
9	3.147591000	0.430953000	0.759809000
9	3.134612000	2.560508000	1.133510000
9	4.196981000	1.769279000	-0.579484000
6	3.123247000	1.624049000	0.190698000
8	1.761409000	3.110688000	-1.494347000
8	1.564654000	0.620656000	-1.676265000
16	1.612750000	1.819259000	-0.840533000
9	-2.380184000	4.294272000	0.111251000
9	-1.248591000	3.371520000	-1.488814000
9	-2.494724000	2.156165000	-0.207471000
6	-1.689281000	3.219431000	-0.244333000
8	0.470138000	4.213035000	0.885281000
8	-0.907981000	2.544544000	2.152452000
16	-0.277163000	2.965901000	0.907799000
7	0.438274000	1.690111000	0.246480000

Zero-point correction= 0.394092 (Hartree/Particle)

Thermal correction to Energy= 0.432485

Thermal correction to Enthalpy= 0.433429

Thermal correction to Gibbs Free Energy= 0.320628

Sum of electronic and zero-point Energies= -3600.307490

Sum of electronic and thermal Energies= -3600.269098

Sum of electronic and thermal Enthalpies= -3600.268153

Sum of electronic and thermal Free Energies= -3600.380954

A-TS2

6	-1.838154000	-1.398010000	-1.185594000
6	-2.647602000	-2.280722000	-0.474407000
6	-3.983768000	-1.943545000	-0.299244000
6	-4.499035000	-0.747791000	-0.813294000
6	-3.655058000	0.105574000	-1.537000000
6	-2.317608000	-0.204104000	-1.726906000
16	-0.124074000	-1.725629000	-1.287893000
8	0.490576000	-0.948628000	-2.342156000
8	0.168979000	-3.128233000	-1.080584000
7	0.494341000	-0.944467000	0.227854000
6	0.506884000	0.318026000	0.262233000
6	0.921592000	1.556866000	0.119506000
6	2.225493000	1.862034000	-0.451151000
6	3.163616000	1.015692000	-0.993306000
6	4.329062000	1.700204000	-1.423725000
6	4.260168000	3.048456000	-1.202586000
16	2.780151000	3.507716000	-0.468458000
6	-5.937862000	-0.374582000	-0.597015000
6	1.065754000	-1.793028000	1.331884000
6	2.566225000	-1.717871000	1.250556000
6	3.251490000	-0.759439000	1.998390000
6	4.625008000	-0.597573000	1.833044000
6	5.314359000	-1.391487000	0.918660000
6	4.633089000	-2.357232000	0.177983000
6	3.260554000	-2.521713000	0.342801000
1	-2.243690000	-3.203149000	-0.068834000
1	-4.634745000	-2.612802000	0.255436000
1	-4.052068000	1.031459000	-1.943439000
1	-1.657605000	0.462242000	-2.272923000
1	3.024310000	-0.057660000	-1.078666000
1	5.182628000	1.213176000	-1.878730000
1	5.002143000	3.802359000	-1.430240000
1	-6.040872000	0.704623000	-0.452492000
1	-6.355229000	-0.889402000	0.271121000
1	-6.536966000	-0.649459000	-1.471822000
1	0.676129000	-1.381738000	2.264712000

1	0.681957000	-2.803120000	1.183165000
1	2.706308000	-0.136091000	2.702848000
1	5.154824000	0.151582000	2.412775000
1	6.383765000	-1.260918000	0.785123000
1	5.171062000	-2.981324000	-0.528533000
1	2.722824000	-3.267308000	-0.237899000
1	0.269256000	2.360772000	0.447269000
6	-3.323771000	2.279115000	0.967713000
6	-3.704747000	1.270949000	1.794832000
6	-2.576493000	0.401824000	1.840168000
8	-2.064706000	2.053186000	0.544508000
1	-4.652253000	1.147575000	2.296920000
7	-1.607032000	0.879174000	1.098580000
6	-3.990797000	3.500501000	0.453108000
1	-4.049992000	3.470317000	-0.638665000
1	-4.998651000	3.568541000	0.863220000
1	-3.428501000	4.393833000	0.738428000
6	-2.420358000	-0.866513000	2.611307000
1	-2.129569000	-0.647479000	3.642976000
1	-3.368259000	-1.407905000	2.633426000
1	-1.662224000	-1.508832000	2.159507000

Zero-point correction= 0.453523 (Hartree/Particle)

Thermal correction to Energy= 0.483598

Thermal correction to Enthalpy= 0.484542

Thermal correction to Gibbs Free Energy= 0.390131

Sum of electronic and zero-point Energies= -2097.920943

Sum of electronic and thermal Energies= -2097.890867

Sum of electronic and thermal Enthalpies= -2097.889923

Sum of electronic and thermal Free Energies= -2097.984334

A-2

6	-1.863990000	1.212869000	-1.154338000
6	-2.544363000	0.093344000	-1.625668000
6	-3.919851000	0.024792000	-1.439686000
6	-4.613716000	1.058659000	-0.800411000
6	-3.903915000	2.187051000	-0.372667000
6	-2.527247000	2.271221000	-0.537644000
16	-0.099451000	1.244625000	-1.216156000

8	0.358866000	2.618696000	-1.085951000
8	0.339640000	0.408507000	-2.329306000
7	0.389716000	0.466869000	0.197512000
6	0.348552000	-0.937955000	0.209726000
6	-0.638230000	-1.716312000	0.690980000
6	-1.870083000	-1.280172000	1.308776000
6	-2.219981000	-0.062887000	1.849507000
6	-3.544682000	-0.047491000	2.356196000
6	-4.185054000	-1.246518000	2.194068000
16	-3.183151000	-2.413318000	1.440016000
6	-6.089253000	0.939500000	-0.541147000
6	1.109177000	1.224237000	1.232796000
6	2.593233000	1.435888000	0.990960000
6	3.381216000	1.826924000	2.075674000
6	4.743660000	2.064920000	1.916384000
6	5.338547000	1.908513000	0.665428000
6	4.560140000	1.508995000	-0.419095000
6	3.195154000	1.276795000	-0.258435000
1	-2.008443000	-0.706616000	-2.127396000
1	-4.465412000	-0.845733000	-1.793173000
1	-4.436496000	3.004366000	0.104898000
1	-1.974838000	3.141330000	-0.197203000
1	-1.548824000	0.787085000	1.882659000
1	-4.006670000	0.815800000	2.819594000
1	-5.193852000	-1.508628000	2.485530000
1	-6.585937000	0.360860000	-1.323404000
1	-6.561849000	1.921867000	-0.473156000
1	-6.256180000	0.422641000	0.411437000
1	0.612657000	2.194465000	1.336753000
1	0.954209000	0.683852000	2.172227000
1	2.922406000	1.946367000	3.054408000
1	5.340786000	2.369301000	2.770427000
1	6.400652000	2.092546000	0.537497000
1	5.013713000	1.376988000	-1.396850000
1	2.611739000	0.949290000	-1.115691000
1	-0.485592000	-2.789987000	0.595950000
6	3.641254000	-2.048169000	-0.192021000
6	3.205448000	-2.479542000	-1.414071000

6	1.829650000	-2.181004000	-1.462341000
8	2.614793000	-1.528483000	0.498200000
1	3.786962000	-2.955034000	-2.188359000
7	1.512559000	-1.606218000	-0.308150000
6	4.950267000	-2.049448000	0.494969000
1	5.185716000	-1.037648000	0.838162000
1	4.915935000	-2.714239000	1.362712000
1	5.720036000	-2.394203000	-0.194619000
6	0.844098000	-2.457241000	-2.534890000
1	1.114469000	-1.884424000	-3.424385000
1	0.889046000	-3.521302000	-2.779394000
1	-0.165104000	-2.185986000	-2.227753000

Zero-point correction= 0.456865 (Hartree/Particle)

Thermal correction to Energy= 0.485642

Thermal correction to Enthalpy= 0.486587

Thermal correction to Gibbs Free Energy= 0.395836

Sum of electronic and zero-point Energies= -2097.971731

Sum of electronic and thermal Energies= -2097.942954

Sum of electronic and thermal Enthalpies= -2097.942009

Sum of electronic and thermal Free Energies= -2098.032760

A-TS3

6	-2.256226000	-1.472918000	0.414995000
6	-3.098350000	-0.705194000	1.220798000
6	-4.419040000	-0.534417000	0.831939000
6	-4.907602000	-1.119743000	-0.344450000
6	-4.045141000	-1.902705000	-1.117196000
6	-2.716143000	-2.086646000	-0.746018000
16	-0.549512000	-1.629351000	0.867051000
8	-0.073519000	-2.905795000	0.352725000
8	-0.443923000	-1.291589000	2.279319000
7	0.333728000	-0.456261000	0.051199000
6	0.513499000	0.811387000	0.670774000
6	-0.482926000	1.808256000	0.690940000
6	-1.662209000	1.871536000	-0.055334000
6	-2.073232000	1.147635000	-1.187001000
6	-3.314963000	1.555203000	-1.673684000
6	-3.868673000	2.572480000	-0.912966000

16	-2.872582000	3.067093000	0.364242000
6	-6.330809000	-0.882595000	-0.765810000
6	0.908556000	-0.724077000	-1.284435000
6	2.397469000	-0.996128000	-1.269942000
6	3.249403000	-0.219931000	-2.055214000
6	4.625063000	-0.450207000	-2.048114000
6	5.157239000	-1.463936000	-1.254835000
6	4.308094000	-2.253583000	-0.479050000
6	2.935514000	-2.024182000	-0.489433000
1	-2.721239000	-0.254675000	2.133345000
1	-5.085218000	0.062913000	1.448762000
1	-4.417911000	-2.376227000	-2.020645000
1	-2.053224000	-2.705341000	-1.343080000
1	-1.476738000	0.367842000	-1.641831000
1	-3.805175000	1.127474000	-2.538955000
1	-4.831870000	3.046971000	-1.061840000
1	-6.587392000	-1.464796000	-1.652892000
1	-6.487202000	0.177718000	-0.993339000
1	-7.024895000	-1.147196000	0.037101000
1	0.368131000	-1.578640000	-1.702753000
1	0.701966000	0.143752000	-1.918811000
1	2.835825000	0.581266000	-2.662849000
1	5.277748000	0.162584000	-2.662790000
1	6.227840000	-1.643987000	-1.245806000
1	4.716302000	-3.051904000	0.133393000
1	2.273500000	-2.643542000	0.109728000
1	-0.273167000	2.627393000	1.376483000
6	3.830501000	1.885963000	0.141058000
6	3.970996000	0.875247000	1.138134000
6	2.755105000	0.505978000	1.624451000
8	2.654284000	2.188788000	-0.163380000
1	4.913748000	0.490236000	1.497789000
7	1.668535000	1.206419000	1.172056000
6	4.985438000	2.621495000	-0.462774000
1	5.890108000	2.013682000	-0.416688000
1	4.759713000	2.896197000	-1.494043000
1	5.148170000	3.538905000	0.113209000
6	2.522344000	-0.520935000	2.689348000

1	3.472569000	-0.751293000	3.171892000
1	1.801260000	-0.162424000	3.425512000
1	2.116630000	-1.431011000	2.239231000

Zero-point correction= 0.453300 (Hartree/Particle)

Thermal correction to Energy= 0.482865

Thermal correction to Enthalpy= 0.483809

Thermal correction to Gibbs Free Energy= 0.392068

Sum of electronic and zero-point Energies= -2097.938292

Sum of electronic and thermal Energies= -2097.908728

Sum of electronic and thermal Enthalpies= -2097.907784

Sum of electronic and thermal Free Energies= -2097.999524

A-3

6	2.517465000	-0.734935000	-1.069742000
6	3.637978000	-0.043073000	-1.522532000
6	4.881491000	-0.382978000	-1.001435000
6	5.010035000	-1.395403000	-0.045724000
6	3.859526000	-2.067855000	0.387902000
6	2.606370000	-1.747917000	-0.115097000
16	0.956254000	-0.326139000	-1.793882000
8	0.611676000	-1.259121000	-2.851492000
8	0.927793000	1.109152000	-2.059771000
7	-0.162798000	-0.606534000	-0.537511000
6	-0.417414000	0.397937000	0.384647000
6	0.541236000	1.539516000	0.438093000
6	0.146654000	2.833346000	0.557585000
6	-1.164179000	3.390891000	0.452613000
6	-1.170414000	4.760521000	0.597802000
6	0.117665000	5.273314000	0.804924000
16	1.332713000	4.111778000	0.820618000
6	6.355747000	-1.768711000	0.510925000
6	-1.050860000	-1.771840000	-0.648204000
6	-2.444295000	-1.411424000	-1.117225000
6	-3.504752000	-2.248378000	-0.762535000
6	-4.799480000	-1.961896000	-1.183862000
6	-5.047634000	-0.827205000	-1.955152000
6	-3.993291000	0.011845000	-2.309075000
6	-2.694688000	-0.279227000	-1.892467000

1	3.540167000	0.749729000	-2.257322000
1	5.764921000	0.151690000	-1.337147000
1	3.948296000	-2.845295000	1.141385000
1	1.716967000	-2.247896000	0.256572000
1	-2.037416000	2.777815000	0.263615000
1	-2.049380000	5.389639000	0.552422000
1	0.370323000	6.319755000	0.944833000
1	7.132346000	-1.085686000	0.161505000
1	6.628007000	-2.783495000	0.203568000
1	6.342829000	-1.752716000	1.604543000
1	-0.585082000	-2.462176000	-1.353471000
1	-1.081321000	-2.265346000	0.323624000
1	-3.311266000	-3.122353000	-0.145022000
1	-5.617174000	-2.617604000	-0.901192000
1	-6.058498000	-0.597391000	-2.276723000
1	-4.180491000	0.897036000	-2.909120000
1	-1.881665000	0.391288000	-2.162956000
1	1.601176000	1.292642000	0.488634000
6	-0.656564000	-1.978528000	2.824397000
6	-2.007665000	-1.481167000	2.530530000
6	-2.286415000	-0.394309000	1.768908000
8	0.338233000	-1.602875000	2.211626000
1	-2.840939000	-1.965995000	3.028861000
7	-1.336060000	0.468450000	1.259993000
6	-0.554220000	-2.994068000	3.934964000
1	0.479874000	-3.318989000	4.050664000
1	-0.914580000	-2.559454000	4.872830000
1	-1.192283000	-3.855575000	3.712869000
6	-3.687159000	0.132392000	1.616028000
1	-3.907646000	0.323873000	0.561217000
1	-4.411535000	-0.579577000	2.013380000
1	-3.779537000	1.080108000	2.156795000

Zero-point correction= 0.454474 (Hartree/Particle)

Thermal correction to Energy= 0.483935

Thermal correction to Enthalpy= 0.484879

Thermal correction to Gibbs Free Energy= 0.393143

Sum of electronic and zero-point Energies= -2097.955575

Sum of electronic and thermal Energies= -2097.926114

Sum of electronic and thermal Enthalpies= -2097.925170

Sum of electronic and thermal Free Energies= -2098.016905

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6	-1.967851000	2.096427000	0.075318000
6	-2.317605000	2.258320000	-1.267091000
6	-3.447773000	1.603693000	-1.731517000
6	-4.217964000	0.796693000	-0.879237000
6	-3.848272000	0.677604000	0.464685000
6	-2.725026000	1.330737000	0.959543000
16	-0.476828000	2.821100000	0.639172000
8	-0.577016000	3.152237000	2.049674000
8	-0.006377000	3.811793000	-0.309943000
7	0.713337000	1.540479000	0.563259000
6	0.489078000	0.207303000	0.662088000
6	-0.436923000	-0.540510000	-0.307472000
6	-1.187587000	-1.678039000	0.309010000
6	-1.460302000	-1.923474000	1.626660000
6	-2.333901000	-3.038268000	1.806040000
6	-2.699024000	-3.611176000	0.625284000
16	-2.003893000	-2.801418000	-0.727468000
6	-5.428632000	0.084489000	-1.411487000
6	2.064723000	2.009300000	0.977448000
6	3.112759000	1.303062000	0.147344000
6	4.164553000	0.627951000	0.766201000
6	5.105989000	-0.056973000	0.000570000
6	4.998449000	-0.072559000	-1.388517000
6	3.950189000	0.604802000	-2.011241000
6	3.008397000	1.288068000	-1.245821000
1	-1.707813000	2.869749000	-1.923637000
1	-3.738892000	1.710935000	-2.772304000
1	-4.442946000	0.058821000	1.129947000
1	-2.441102000	1.239440000	2.003649000
1	-1.062221000	-1.332379000	2.444190000
1	-2.663527000	-3.398479000	2.772574000
1	-3.330280000	-4.475070000	0.463126000
1	-5.186160000	-0.456942000	-2.330204000
1	-6.217017000	0.804046000	-1.654565000
1	-5.824328000	-0.623910000	-0.681386000

1	2.092768000	3.087599000	0.801078000
1	2.207159000	1.818851000	2.044944000
1	4.233771000	0.626146000	1.851085000
1	5.919830000	-0.582110000	0.490696000
1	5.730126000	-0.608580000	-1.984976000
1	3.867849000	0.604000000	-3.093782000
1	2.184732000	1.809481000	-1.728298000
6	1.682102000	-1.757152000	1.232557000
6	1.917229000	-2.314195000	-0.043376000
6	1.424797000	-1.834046000	-1.233467000
8	0.444724000	-0.944549000	-1.368916000
1	2.589467000	-3.163124000	-0.101193000
7	1.272013000	-0.508332000	1.401495000
6	1.905912000	-2.312969000	-2.557012000
1	2.861871000	-2.825626000	-2.460715000
1	1.163069000	-2.997304000	-2.982089000
1	2.001786000	-1.462837000	-3.236978000
6	2.098237000	-2.498244000	2.456498000
1	3.185013000	-2.397628000	2.568803000
1	1.620365000	-2.078533000	3.342268000
1	1.866697000	-3.560051000	2.356572000
1	-1.116108000	0.132635000	-0.823926000

Zero-point correction= 0.456444 (Hartree/Particle)

Thermal correction to Energy= 0.486125

Thermal correction to Enthalpy= 0.487069

Thermal correction to Gibbs Free Energy= 0.393926

Sum of electronic and zero-point Energies= -2097.990134

Sum of electronic and thermal Energies= -2097.960453

Sum of electronic and thermal Enthalpies= -2097.959509

Sum of electronic and thermal Free Energies= -2098.052651

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6	2.936496000	-0.073161000	-0.636526000
6	3.189105000	-1.386547000	-0.242733000
6	4.105346000	-1.602397000	0.777392000
6	4.779845000	-0.532354000	1.381617000
6	4.516229000	0.768879000	0.942554000
6	3.591373000	1.011264000	-0.067361000

16	1.838734000	0.197554000	-1.990350000
8	1.852071000	1.602179000	-2.391563000
8	2.101321000	-0.827230000	-2.986734000
7	0.232126000	-0.154641000	-1.418728000
6	-0.370390000	0.809845000	-0.630470000
6	-1.756190000	0.430211000	-0.078200000
6	-1.639541000	-0.310119000	1.225835000
6	-0.541854000	-0.664218000	1.961718000
6	-0.871800000	-1.488535000	3.078630000
6	-2.207746000	-1.744094000	3.165560000
16	-3.088466000	-0.992179000	1.892586000
6	5.782545000	-0.793027000	2.471334000
6	-0.584900000	-1.038892000	-2.283416000
6	-1.186625000	-2.222419000	-1.555940000
6	-2.430963000	-2.697961000	-1.974726000
6	-3.007257000	-3.805435000	-1.357451000
6	-2.349952000	-4.436025000	-0.303122000
6	-1.112088000	-3.958735000	0.124526000
6	-0.528116000	-2.861416000	-0.504649000
1	2.689918000	-2.219207000	-0.729036000
1	4.312623000	-2.617907000	1.102422000
1	5.040127000	1.603766000	1.398349000
1	3.374917000	2.018399000	-0.407728000
1	0.472690000	-0.375555000	1.709783000
1	-0.143599000	-1.867655000	3.785086000
1	-2.733679000	-2.314093000	3.920160000
1	6.603377000	-1.412796000	2.097664000
1	6.202376000	0.138761000	2.854959000
1	5.319943000	-1.333148000	3.302782000
1	0.071228000	-1.396800000	-3.077014000
1	-1.361941000	-0.433591000	-2.761222000
1	-2.950802000	-2.195712000	-2.787002000
1	-3.973811000	-4.167210000	-1.693784000
1	-2.803218000	-5.291955000	0.186915000
1	-0.598138000	-4.442263000	0.949675000
1	0.431092000	-2.484062000	-0.160419000
1	-2.267743000	-0.202156000	-0.802480000
6	-2.389088000	2.596190000	0.790875000

6	-1.170838000	2.969250000	1.268370000
6	0.130841000	2.419818000	1.009641000
8	-2.639556000	1.545190000	0.003254000
1	-1.184880000	3.814280000	1.947547000
7	0.501830000	1.519363000	0.135829000
6	-3.642695000	3.338458000	1.099483000
1	-4.282708000	2.713578000	1.731110000
1	-4.176935000	3.536496000	0.167245000
1	-3.429791000	4.277109000	1.609683000
6	1.232820000	2.997508000	1.848315000
1	2.155782000	2.434707000	1.714514000
1	0.941941000	2.995536000	2.902296000
1	1.400630000	4.041527000	1.559845000
8	-2.272948000	4.146935000	-1.571501000
1	-1.772821000	4.897973000	-1.219213000
1	-2.686487000	4.462477000	-2.389076000
8	-0.930416000	1.977625000	-1.971239000
1	-0.071233000	2.252182000	-2.345763000
1	-1.451956000	2.814123000	-1.748079000

Zero-point correction= 0.508823 (Hartree/Particle)

Thermal correction to Energy= 0.542118

Thermal correction to Enthalpy= 0.543062

Thermal correction to Gibbs Free Energy= 0.444349

Sum of electronic and zero-point Energies= -2250.745122

Sum of electronic and thermal Energies= -2250.711827

Sum of electronic and thermal Enthalpies= -2250.710883

Sum of electronic and thermal Free Energies= -2250.809595

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6	2.857161000	-0.608331000	-0.605432000
6	2.797320000	-1.755856000	0.179546000
6	3.733963000	-1.910377000	1.194833000
6	4.733607000	-0.952999000	1.407724000
6	4.774039000	0.175952000	0.581841000
6	3.836217000	0.361446000	-0.427422000
16	1.742932000	-0.450410000	-1.966702000
8	1.967524000	0.840785000	-2.642190000
8	1.841219000	-1.667516000	-2.757756000

7	0.145132000	-0.422615000	-1.347022000
6	-0.262348000	0.866702000	-0.818881000
6	-1.654667000	0.759324000	-0.157932000
6	-1.620121000	0.076172000	1.178974000
6	-0.585644000	-0.482726000	1.877028000
6	-1.018710000	-1.156321000	3.058213000
6	-2.369162000	-1.095001000	3.231651000
16	-3.138021000	-0.221564000	1.963767000
6	5.765816000	-1.152964000	2.483154000
6	-0.842314000	-1.166771000	-2.175817000
6	-1.743188000	-2.085638000	-1.378286000
6	-3.076695000	-2.225685000	-1.768184000
6	-3.926875000	-3.089479000	-1.080632000
6	-3.451507000	-3.810521000	0.011809000
6	-2.122034000	-3.669664000	0.408364000
6	-1.269857000	-2.817705000	-0.289135000
1	2.041675000	-2.514554000	0.000984000
1	3.696516000	-2.793555000	1.825699000
1	5.546096000	0.924369000	0.735190000
1	3.852037000	1.245191000	-1.056123000
1	0.448273000	-0.443911000	1.552131000
1	-0.348906000	-1.656952000	3.746839000
1	-2.961121000	-1.495475000	4.044095000
1	5.352632000	-1.706657000	3.329556000
1	6.613506000	-1.727075000	2.093731000
1	6.150968000	-0.196464000	2.843543000
1	-0.277608000	-1.761772000	-2.894421000
1	-1.439793000	-0.453969000	-2.754495000
1	-3.450844000	-1.651691000	-2.612864000
1	-4.961618000	-3.189386000	-1.393276000
1	-4.114459000	-4.475464000	0.556648000
1	-1.747193000	-4.225592000	1.262569000
1	-0.238465000	-2.696433000	0.028343000
1	-2.305939000	0.198644000	-0.830881000
6	-1.834555000	3.013136000	0.679000000
6	-0.558636000	3.146299000	1.110594000
6	0.628993000	2.360800000	0.800629000
8	-2.297800000	2.029306000	-0.117462000

1	-0.384979000	3.981091000	1.780688000
7	0.791011000	1.390006000	-0.036459000
6	-2.916408000	3.991440000	0.989209000
1	-3.715740000	3.491157000	1.544573000
1	-3.346535000	4.360126000	0.052631000
1	-2.536398000	4.830683000	1.570770000
6	1.846241000	2.763869000	1.586512000
1	2.706410000	2.159788000	1.300482000
1	1.644718000	2.631625000	2.654804000
1	2.066733000	3.823968000	1.427343000
8	-1.134616000	4.085640000	-1.865854000
1	-0.647501000	4.635169000	-1.228200000
1	-1.096105000	4.530395000	-2.730516000
8	-0.466520000	1.761356000	-2.016743000
1	0.399840000	1.726513000	-2.502829000
1	-0.780058000	2.822896000	-1.879802000

Zero-point correction= 0.507657 (Hartree/Particle)

Thermal correction to Energy= 0.540771

Thermal correction to Enthalpy= 0.541715

Thermal correction to Gibbs Free Energy= 0.443632

Sum of electronic and zero-point Energies= -2250.750536

Sum of electronic and thermal Energies= -2250.717422

Sum of electronic and thermal Enthalpies= -2250.716478

Sum of electronic and thermal Free Energies= -2250.814561

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6	2.830516000	-0.267504000	-0.668420000
6	3.030284000	-1.579569000	-0.245659000
6	3.947337000	-1.817458000	0.770369000
6	4.676265000	-0.768929000	1.345017000
6	4.465206000	0.533546000	0.880485000
6	3.542506000	0.794867000	-0.126836000
16	1.704845000	0.020729000	-2.004543000
8	1.812808000	1.419394000	-2.438054000
8	1.935402000	-1.031928000	-2.986039000
7	0.135746000	-0.236075000	-1.395191000
6	-0.474212000	0.963583000	-0.784486000
6	-1.755537000	0.515030000	-0.035493000

6	-1.535288000	-0.230064000	1.245504000
6	-0.383541000	-0.600250000	1.886013000
6	-0.624957000	-1.456978000	3.000552000
6	-1.949680000	-1.722793000	3.183047000
16	-2.926773000	-0.941562000	2.004179000
6	5.692358000	-1.049996000	2.417750000
6	-0.748221000	-1.053653000	-2.257155000
6	-1.401968000	-2.205731000	-1.520817000
6	-2.676141000	-2.625214000	-1.909575000
6	-3.287365000	-3.708068000	-1.280395000
6	-2.633247000	-4.373463000	-0.245937000
6	-1.364530000	-3.953727000	0.151766000
6	-0.749943000	-2.879033000	-0.486319000
1	2.489036000	-2.398947000	-0.708991000
1	4.109250000	-2.834208000	1.116678000
1	5.029520000	1.354003000	1.314750000
1	3.366207000	1.803106000	-0.486356000
1	0.605159000	-0.298403000	1.560936000
1	0.157099000	-1.851060000	3.638007000
1	-2.414587000	-2.315672000	3.959746000
1	5.951646000	-0.142323000	2.966737000
1	5.319966000	-1.793888000	3.126830000
1	6.611492000	-1.449882000	1.976574000
1	-0.146404000	-1.451615000	-3.075004000
1	-1.505540000	-0.406174000	-2.713414000
1	-3.192010000	-2.100107000	-2.710177000
1	-4.277361000	-4.025071000	-1.593442000
1	-3.111531000	-5.211543000	0.251272000
1	-0.851178000	-4.464006000	0.961299000
1	0.230848000	-2.541798000	-0.164523000
1	-2.347539000	-0.101138000	-0.713039000
6	-2.351648000	2.761407000	0.711235000
6	-1.062833000	3.277404000	0.893284000
6	0.231174000	2.542679000	0.818216000
8	-2.670321000	1.624608000	0.169778000
1	-1.057873000	4.121593000	1.582003000
7	0.518417000	1.537993000	0.087472000
6	-3.550577000	3.586787000	1.021667000

1	-4.059074000	3.131266000	1.878544000
1	-4.240980000	3.562372000	0.174754000
1	-3.277533000	4.612628000	1.264678000
6	1.298323000	3.106895000	1.709525000
1	2.227807000	2.550612000	1.590342000
1	0.969683000	3.052715000	2.752534000
1	1.466319000	4.163764000	1.477068000
8	-1.288494000	4.680333000	-1.337987000
1	-1.150980000	3.983116000	-0.279735000
1	-0.511135000	5.227472000	-1.555117000
8	-0.898652000	1.877438000	-1.771035000
1	-0.093829000	2.079453000	-2.286078000
1	-1.436397000	4.066267000	-2.080337000

Zero-point correction= 0.506263 (Hartree/Particle)

Thermal correction to Energy= 0.538675

Thermal correction to Enthalpy= 0.539619

Thermal correction to Gibbs Free Energy= 0.443700

Sum of electronic and zero-point Energies= -2250.732763

Sum of electronic and thermal Energies= -2250.700352

Sum of electronic and thermal Enthalpies= -2250.699408

Sum of electronic and thermal Free Energies= -2250.795327

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6	0.646179000	1.994096000	-1.236312000
6	1.703189000	2.216742000	-0.358784000
6	1.692560000	3.370579000	0.416912000
6	0.652859000	4.301383000	0.310624000
6	-0.379790000	4.059293000	-0.603883000
6	-0.389869000	2.909196000	-1.384401000
16	0.652903000	0.513750000	-2.204322000
8	-0.399315000	0.615910000	-3.221447000
8	2.014761000	0.278791000	-2.666049000
7	0.364064000	-0.755408000	-1.126104000
6	-0.990502000	-1.015690000	-0.597551000
6	-0.790618000	-1.439572000	0.884249000
6	-0.503253000	-0.392702000	1.910522000
6	-0.537115000	0.976849000	1.860526000
6	-0.107712000	1.582339000	3.078569000

6	0.235729000	0.669449000	4.030674000
16	0.062448000	-0.942917000	3.462871000
6	0.661867000	5.555773000	1.140926000
6	1.209090000	-1.946003000	-1.360227000
6	2.530693000	-1.921877000	-0.623412000
6	3.559968000	-2.753890000	-1.070984000
6	4.774330000	-2.805975000	-0.393207000
6	4.977178000	-2.022276000	0.742106000
6	3.957515000	-1.187592000	1.190979000
6	2.740201000	-1.138804000	0.511859000
1	2.514962000	1.500136000	-0.277177000
1	2.502998000	3.550793000	1.117292000
1	-1.185235000	4.781542000	-0.704062000
1	-1.190599000	2.707723000	-2.087635000
1	-0.837601000	1.545106000	0.989218000
1	-0.062844000	2.653847000	3.232616000
1	0.577928000	0.848862000	5.041623000
1	1.196970000	6.354737000	0.616446000
1	-0.353742000	5.909653000	1.333321000
1	1.165781000	5.393329000	2.096774000
1	1.387173000	-2.087861000	-2.429459000
1	0.617186000	-2.809831000	-1.045205000
1	3.408387000	-3.359921000	-1.961137000
1	5.566111000	-3.454394000	-0.755805000
1	5.925554000	-2.059058000	1.268869000
1	4.105704000	-0.569468000	2.071720000
1	1.952714000	-0.474148000	0.857976000
1	-0.012842000	-2.207203000	0.909757000
6	-3.155694000	-2.096735000	0.967646000
6	-3.747663000	-0.947107000	0.244856000
6	-2.955934000	0.215505000	-0.318256000
8	-1.954435000	-2.251093000	1.325245000
1	-4.494557000	-0.561000000	0.955314000
7	-1.748829000	0.208528000	-0.713244000
6	-4.056308000	-3.198673000	1.364438000
1	-5.075902000	-2.844619000	1.514607000
1	-3.670199000	-3.723170000	2.238305000
1	-4.059060000	-3.894267000	0.512457000

6	-3.754124000	1.478505000	-0.420112000
1	-3.190212000	2.246222000	-0.948338000
1	-3.998613000	1.832024000	0.588005000
1	-4.700173000	1.289105000	-0.937749000
8	-2.644690000	-1.015495000	-3.341359000
1	-4.357870000	-1.377429000	-0.564286000
1	-2.009893000	-0.281141000	-3.429966000
8	-1.607944000	-2.091742000	-1.212357000
1	-1.986315000	-1.779786000	-2.087604000
1	-2.591749000	-1.502798000	-4.176026000

Zero-point correction= 0.509622 (Hartree/Particle)

Thermal correction to Energy= 0.542905

Thermal correction to Enthalpy= 0.543849

Thermal correction to Gibbs Free Energy= 0.443958

Sum of electronic and zero-point Energies= -2250.750560

Sum of electronic and thermal Energies= -2250.717278

Sum of electronic and thermal Enthalpies= -2250.716334

Sum of electronic and thermal Free Energies= -2250.816225

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6	-1.402866000	-1.629809000	-1.281278000
6	-2.434181000	-1.631160000	-0.344822000
6	-2.698842000	-2.805618000	0.349253000
6	-1.960149000	-3.970314000	0.105069000
6	-0.947784000	-3.938490000	-0.860561000
6	-0.661712000	-2.772012000	-1.560797000
16	-1.049949000	-0.121008000	-2.134707000
8	-0.123608000	-0.406447000	-3.234589000
8	-2.312569000	0.527430000	-2.459537000
7	-0.349121000	0.902771000	-0.981012000
6	1.051671000	0.742427000	-0.602000000
6	1.174803000	1.129455000	0.921163000
6	1.043873000	0.028991000	1.929431000
6	0.419797000	-1.184584000	1.834864000
6	0.384283000	-1.883955000	3.078662000
6	0.980381000	-1.190983000	4.088401000
16	1.581923000	0.332022000	3.553847000
6	-2.271775000	-5.240593000	0.847634000

6	-0.865437000	2.286795000	-0.993505000
6	-2.070531000	2.504121000	-0.105715000
6	-2.907608000	3.586875000	-0.385704000
6	-3.997834000	3.870600000	0.430302000
6	-4.268789000	3.067958000	1.537711000
6	-3.442483000	1.983479000	1.819740000
6	-2.346151000	1.702308000	1.003483000
1	-3.010123000	-0.730161000	-0.154172000
1	-3.492951000	-2.821879000	1.090497000
1	-0.375655000	-4.838797000	-1.065700000
1	0.131164000	-2.735689000	-2.299838000
1	0.008028000	-1.575971000	0.912372000
1	-0.055771000	-2.866217000	3.202812000
1	1.121658000	-1.489615000	5.118892000
1	-3.117978000	-5.755495000	0.380324000
1	-1.418787000	-5.922700000	0.837462000
1	-2.545281000	-5.033660000	1.885336000
1	-1.099072000	2.598864000	-2.014237000
1	-0.037598000	2.926006000	-0.673555000
1	-2.702045000	4.207680000	-1.254389000
1	-4.640901000	4.713589000	0.196870000
1	-5.122480000	3.284260000	2.172305000
1	-3.650407000	1.349800000	2.676688000
1	-1.717792000	0.841271000	1.221592000
1	0.460093000	1.926729000	1.142836000
6	3.402161000	1.459586000	0.266556000
6	3.710555000	0.032176000	-0.063545000
6	2.650934000	-0.921404000	-0.581818000
8	2.450161000	1.822687000	1.054981000
1	4.104940000	-0.377188000	0.881323000
7	1.444654000	-0.621765000	-0.846901000
6	4.449114000	2.472218000	0.038863000
1	5.339033000	2.169354000	0.604678000
1	4.116269000	3.460196000	0.351567000
1	4.723584000	2.460841000	-1.019475000
6	3.134042000	-2.320064000	-0.797031000
1	2.308250000	-2.954320000	-1.119575000
1	3.562990000	-2.714426000	0.129516000

1	3.923099000	-2.328570000	-1.556465000
8	2.496104000	0.460839000	-3.443968000
1	4.547633000	0.022000000	-0.768636000
1	1.673258000	-0.049122000	-3.563448000
8	1.902193000	1.642231000	-1.271760000
1	2.138651000	1.254140000	-2.186911000
1	2.596798000	0.993887000	-4.246665000

Zero-point correction= 0.508235 (Hartree/Particle)

Thermal correction to Energy= 0.540038

Thermal correction to Enthalpy= 0.540982

Thermal correction to Gibbs Free Energy= 0.443513

Sum of electronic and zero-point Energies= -2250.747551

Sum of electronic and thermal Energies= -2250.715748

Sum of electronic and thermal Enthalpies= -2250.714804

Sum of electronic and thermal Free Energies= -2250.812273

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6	-1.339533000	-1.383342000	-1.517014000
6	-2.566590000	-0.895982000	-1.074160000
6	-3.435814000	-1.776360000	-0.441335000
6	-3.098857000	-3.123515000	-0.270837000
6	-1.866696000	-3.582327000	-0.757271000
6	-0.976408000	-2.720395000	-1.382653000
16	-0.245443000	-0.229980000	-2.271746000
8	0.826391000	-1.019954000	-2.947922000
8	-1.005651000	0.692831000	-3.093559000
7	0.455703000	0.728346000	-1.089765000
6	1.400534000	0.206700000	-0.133012000
6	1.241865000	0.756291000	1.305827000
6	0.238416000	0.089517000	2.197821000
6	-0.570328000	-0.998621000	2.008571000
6	-1.448639000	-1.233571000	3.110433000
6	-1.289602000	-0.326131000	4.113924000
16	-0.078182000	0.836215000	3.733903000
6	-4.053161000	-4.074491000	0.395809000
6	0.364710000	2.193287000	-1.285585000
6	-0.913844000	2.819257000	-0.772857000
6	-1.284942000	4.073237000	-1.265075000

6	-2.421974000	4.712763000	-0.781089000
6	-3.206470000	4.102916000	0.197479000
6	-2.845568000	2.850724000	0.685804000
6	-1.703084000	2.212321000	0.203772000
1	-2.835562000	0.146222000	-1.216689000
1	-4.391998000	-1.412285000	-0.078032000
1	-1.602617000	-4.629416000	-0.639604000
1	-0.015999000	-3.064463000	-1.748464000
1	-0.550276000	-1.611848000	1.115659000
1	-2.161664000	-2.048821000	3.148631000
1	-1.806832000	-0.275622000	5.062877000
1	-3.516850000	-4.811234000	0.998969000
1	-4.760643000	-3.541666000	1.034702000
1	-4.628355000	-4.622152000	-0.358559000
1	0.495396000	2.424984000	-2.344298000
1	1.233918000	2.615554000	-0.773411000
1	-0.680164000	4.547835000	-2.034001000
1	-2.701080000	5.685687000	-1.173717000
1	-4.095867000	4.600001000	0.571752000
1	-3.449570000	2.363508000	1.445509000
1	-1.438057000	1.230241000	0.586138000
1	1.001224000	1.825096000	1.235715000
6	3.472314000	0.391033000	0.743123000
6	3.738755000	-1.103172000	0.643019000
6	2.480952000	-1.824226000	0.210320000
8	2.571228000	0.625076000	1.816889000
1	4.063913000	-1.484040000	1.615935000
7	1.414943000	-1.225936000	-0.167756000
6	4.686377000	1.267385000	0.856567000
1	5.227456000	1.008762000	1.769648000
1	4.378703000	2.313809000	0.901581000
1	5.346277000	1.111100000	-0.000066000
6	2.514836000	-3.317385000	0.236546000
1	1.578624000	-3.735829000	-0.133909000
1	2.683150000	-3.653900000	1.265068000
1	3.353961000	-3.684504000	-0.363195000
8	3.037094000	0.020640000	-2.829451000
1	4.539079000	-1.315897000	-0.076829000

1	3.796525000	-0.536732000	-3.083404000
8	2.711193000	0.755461000	-0.430110000
1	3.098373000	0.328855000	-1.856396000
1	2.096897000	-0.477773000	-2.959005000

Zero-point correction= 0.509252 (Hartree/Particle)

Thermal correction to Energy= 0.540291

Thermal correction to Enthalpy= 0.541235

Thermal correction to Gibbs Free Energy= 0.446303

Sum of electronic and zero-point Energies= -2250.775045

Sum of electronic and thermal Energies= -2250.744007

Sum of electronic and thermal Enthalpies= -2250.743063

Sum of electronic and thermal Free Energies= -2250.837995

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6	-2.986381000	-0.316701000	-0.377040000
6	-3.707244000	0.852531000	-0.613735000
6	-4.518612000	1.352125000	0.398501000
6	-4.626541000	0.691421000	1.626200000
6	-3.908933000	-0.495975000	1.821308000
6	-3.085769000	-1.009554000	0.828856000
16	-1.957691000	-0.924513000	-1.680772000
8	-1.745272000	-2.356399000	-1.512647000
8	-2.482377000	-0.435350000	-2.943227000
7	-0.426393000	-0.161088000	-1.533453000
6	0.411916000	-0.543132000	-0.503462000
6	1.891016000	-0.167874000	-0.617956000
6	2.384512000	0.657578000	0.534715000
6	1.667805000	1.347870000	1.468552000
6	2.497418000	2.130295000	2.329804000
6	3.820295000	2.011696000	2.030424000
16	4.085271000	0.956388000	0.692043000
6	-5.518047000	1.223456000	2.713633000
6	-0.099296000	0.976500000	-2.429796000
6	0.262643000	2.231845000	-1.665067000
6	1.457402000	2.900668000	-1.935111000
6	1.800224000	4.048842000	-1.222202000
6	0.945737000	4.539906000	-0.238391000
6	-0.254811000	3.882305000	0.027609000

6	-0.591379000	2.733186000	-0.680069000
1	-3.638231000	1.358855000	-1.571473000
1	-5.080166000	2.265801000	0.228533000
1	-3.997222000	-1.023400000	2.767013000
1	-2.530895000	-1.927461000	0.984875000
1	0.586371000	1.311655000	1.538580000
1	2.119891000	2.746303000	3.136906000
1	4.665185000	2.473524000	2.523653000
1	-5.780736000	2.267931000	2.534635000
1	-6.446600000	0.644942000	2.762163000
1	-5.033595000	1.144481000	3.690234000
1	-0.982174000	1.142727000	-3.047651000
1	0.706803000	0.677605000	-3.106141000
1	2.128671000	2.514541000	-2.698834000
1	2.737318000	4.554561000	-1.432779000
1	1.214008000	5.430204000	0.321489000
1	-0.927024000	4.260851000	0.791384000
1	-1.518508000	2.213341000	-0.452822000
1	2.079460000	0.362653000	-1.549301000
6	2.607695000	-2.405566000	0.000276000
6	1.940380000	-2.336162000	1.283523000
6	0.739789000	-1.741320000	1.489281000
8	2.675213000	-1.364357000	-0.813623000
1	2.409219000	-2.887749000	2.090549000
7	-0.050962000	-1.212568000	0.484072000
6	3.801610000	-3.292997000	-0.140964000
1	4.621178000	-2.820448000	0.411131000
1	4.093874000	-3.376122000	-1.188820000
1	3.608810000	-4.275828000	0.289008000
6	0.082525000	-1.733893000	2.831638000
1	-0.826721000	-2.342551000	2.791759000
1	-0.214854000	-0.712145000	3.089191000
1	0.747063000	-2.125000000	3.602518000
8	1.344891000	-3.440977000	-1.031764000
1	1.786643000	-4.189248000	-1.464319000
1	0.602162000	-3.804820000	-0.457972000
8	-0.729924000	-4.093473000	0.383846000
1	-1.301167000	-3.499263000	-0.135258000

1	-1.112538000	-4.978193000	0.293252000
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Zero-point correction= 0.509246 (Hartree/Particle)

Thermal correction to Energy= 0.542180

Thermal correction to Enthalpy= 0.543124

Thermal correction to Gibbs Free Energy= 0.446203

Sum of electronic and zero-point Energies= -2250.750062

Sum of electronic and thermal Energies= -2250.717128

Sum of electronic and thermal Enthalpies= -2250.716184

Sum of electronic and thermal Free Energies= -2250.813104

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6	-2.975328000	-0.458279000	-0.317031000
6	-3.767575000	0.669846000	-0.532327000
6	-4.591136000	1.108842000	0.496354000
6	-4.643170000	0.429671000	1.719077000
6	-3.853967000	-0.713471000	1.891534000
6	-3.018679000	-1.168925000	0.880322000
16	-1.953432000	-1.000785000	-1.652290000
8	-1.742742000	-2.452389000	-1.532543000
8	-2.530555000	-0.525737000	-2.895053000
7	-0.431290000	-0.243410000	-1.545072000
6	0.432354000	-0.604474000	-0.508796000
6	1.884029000	-0.113856000	-0.592436000
6	2.250553000	0.763363000	0.577140000
6	1.446915000	1.448239000	1.440492000
6	2.184992000	2.282147000	2.337853000
6	3.528919000	2.207574000	2.133637000
16	3.923722000	1.127064000	0.846686000
6	-5.562330000	0.896024000	2.812703000
6	-0.134268000	0.880827000	-2.470862000
6	0.150082000	2.181142000	-1.750987000
6	1.326359000	2.882912000	-2.018158000
6	1.605494000	4.074105000	-1.351176000
6	0.703383000	4.576848000	-0.416735000
6	-0.480331000	3.887836000	-0.155979000
6	-0.752962000	2.694949000	-0.818213000
1	-3.746009000	1.187686000	-1.486070000
1	-5.210044000	1.988213000	0.344598000

1	-3.896424000	-1.255987000	2.831490000
1	-2.410800000	-2.055190000	1.013598000
1	0.365539000	1.366568000	1.438263000
1	1.728646000	2.900473000	3.101624000
1	4.320046000	2.713561000	2.670894000
1	-5.704481000	1.978311000	2.774271000
1	-6.546814000	0.428701000	2.702194000
1	-5.174862000	0.623823000	3.797051000
1	-1.003648000	0.983404000	-3.120013000
1	0.704571000	0.593104000	-3.110298000
1	2.034179000	2.485824000	-2.742397000
1	2.529611000	4.604379000	-1.558520000
1	0.922068000	5.501151000	0.108660000
1	-1.188506000	4.275892000	0.569559000
1	-1.666612000	2.151116000	-0.592987000
1	2.022106000	0.467126000	-1.503336000
6	2.739485000	-2.363282000	-0.018107000
6	2.061981000	-2.239398000	1.319147000
6	0.824994000	-1.752161000	1.492672000
8	2.803965000	-1.184385000	-0.784407000
1	2.623412000	-2.580676000	2.182102000
7	-0.011874000	-1.336402000	0.438719000
6	4.156499000	-2.886518000	0.089341000
1	4.756693000	-2.201709000	0.692214000
1	4.598910000	-2.960834000	-0.907529000
1	4.151490000	-3.872136000	0.558604000
6	0.162607000	-1.658165000	2.833182000
1	-0.757360000	-2.252474000	2.842474000
1	-0.120095000	-0.618838000	3.033200000
1	0.824584000	-2.007372000	3.626666000
8	1.967931000	-3.323645000	-0.791812000
1	2.298441000	-3.361442000	-1.706433000
1	0.723419000	-3.770728000	-0.501143000
8	-0.285946000	-4.111234000	-0.340278000
1	-0.459593000	-4.245077000	0.609271000
1	-0.915564000	-3.404315000	-0.717010000

Zero-point correction= 0.509461 (Hartree/Particle)

Thermal correction to Energy= 0.541701

Thermal correction to Enthalpy= 0.542645
 Thermal correction to Gibbs Free Energy= 0.447007
 Sum of electronic and zero-point Energies= -2250.759691
 Sum of electronic and thermal Energies= -2250.727451
 Sum of electronic and thermal Enthalpies= -2250.726506
 Sum of electronic and thermal Free Energies= -2250.822145

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6	-2.813976000	-0.820007000	-0.284749000
6	-3.689604000	0.263174000	-0.323230000
6	-4.567427000	0.442361000	0.739112000
6	-4.585452000	-0.449957000	1.815906000
6	-3.700591000	-1.536926000	1.812976000
6	-2.807556000	-1.732451000	0.769237000
16	-1.738798000	-1.051807000	-1.662546000
8	-1.217375000	-2.412604000	-1.661732000
8	-2.386581000	-0.549444000	-2.859710000
7	-0.402534000	0.030889000	-1.420752000
6	0.497010000	-0.266718000	-0.448510000
6	1.866731000	0.443640000	-0.425553000
6	2.220939000	0.876293000	0.975468000
6	1.412827000	1.343233000	1.972992000
6	2.146314000	1.750031000	3.130032000
6	3.490216000	1.581217000	2.979349000
16	3.890393000	0.929740000	1.434607000
6	-5.555652000	-0.272735000	2.950284000
6	-0.244757000	1.189443000	-2.320675000
6	-0.292091000	2.515420000	-1.590759000
6	0.340875000	3.617190000	-2.172577000
6	0.293733000	4.862809000	-1.554823000
6	-0.379628000	5.018476000	-0.343856000
6	-1.005001000	3.922136000	0.242622000
6	-0.963139000	2.674098000	-0.378274000
1	-3.691584000	0.946118000	-1.167293000
1	-5.255040000	1.282409000	0.726712000
1	-3.716726000	-2.239689000	2.641205000
1	-2.122314000	-2.572999000	0.762016000
1	0.331592000	1.379265000	1.895068000

1	1.689003000	2.140379000	4.031186000
1	4.275840000	1.789350000	3.693483000
1	-6.330413000	-1.045644000	2.910775000
1	-5.049902000	-0.368686000	3.914916000
1	-6.045200000	0.701734000	2.905632000
1	-1.051442000	1.129118000	-3.052069000
1	0.692551000	1.077954000	-2.873619000
1	0.872608000	3.495238000	-3.112797000
1	0.789703000	5.710986000	-2.016051000
1	-0.411593000	5.988498000	0.141918000
1	-1.527011000	4.033286000	1.188048000
1	-1.456815000	1.826190000	0.090138000
1	1.845632000	1.328194000	-1.064042000
6	2.743442000	-1.802956000	-0.877047000
6	2.293101000	-2.300452000	0.500393000
6	1.181296000	-1.769025000	1.153989000
8	2.883091000	-0.386226000	-0.973019000
1	3.064809000	-2.733802000	1.132279000
7	0.203922000	-1.147286000	0.451625000
6	4.107468000	-2.359380000	-1.234316000
1	4.855420000	-2.029785000	-0.510085000
1	4.396216000	-2.004687000	-2.227677000
1	4.065832000	-3.450863000	-1.240495000
6	0.898326000	-2.080693000	2.584115000
1	1.196013000	-1.207714000	3.177937000
1	1.471396000	-2.943885000	2.924808000
1	-0.170575000	-2.243711000	2.735839000
8	1.764724000	-2.209183000	-1.809124000
1	2.066909000	-1.941271000	-2.691417000
1	1.429249000	-3.351225000	0.155874000
8	0.519764000	-4.102614000	-0.308508000
1	0.010842000	-3.502251000	-0.901630000
1	0.906334000	-4.793399000	-0.875652000

Zero-point correction= 0.505568 (Hartree/Particle)

Thermal correction to Energy= 0.537170

Thermal correction to Enthalpy= 0.538114

Thermal correction to Gibbs Free Energy= 0.443236

Sum of electronic and zero-point Energies= -2250.739559

Sum of electronic and thermal Energies= -2250.707958
Sum of electronic and thermal Enthalpies= -2250.707014
Sum of electronic and thermal Free Energies= -2250.801892

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6	-2.854171000	-0.122088000	-0.364508000
6	-3.446379000	1.090988000	-0.014493000
6	-4.270566000	1.118573000	1.102573000
6	-4.521412000	-0.043233000	1.844081000
6	-3.915363000	-1.244334000	1.455116000
6	-3.075071000	-1.297308000	0.351888000
16	-1.888829000	-0.196913000	-1.830904000
8	-1.682767000	-1.573787000	-2.230628000
8	-2.363550000	0.792800000	-2.776581000
7	-0.277241000	0.426050000	-1.387218000
6	0.438359000	-0.227133000	-0.483989000
6	1.913506000	0.124334000	-0.236298000
6	2.257009000	0.153702000	1.230562000
6	1.471367000	0.394241000	2.323041000
6	2.220714000	0.445436000	3.538274000
6	3.552875000	0.244047000	3.337801000
16	3.925002000	-0.008534000	1.673517000
6	-5.454495000	-0.005006000	3.021162000
6	0.261543000	1.572390000	-2.147056000
6	0.487533000	2.801714000	-1.292034000
6	1.343444000	3.788276000	-1.789464000
6	1.576669000	4.948241000	-1.059308000
6	0.962773000	5.130549000	0.179846000
6	0.114512000	4.147893000	0.680124000
6	-0.125268000	2.985325000	-0.052605000
1	-3.273166000	1.986040000	-0.604276000
1	-4.739528000	2.052604000	1.397055000
1	-4.105803000	-2.149205000	2.024577000
1	-2.587012000	-2.219994000	0.052385000
1	0.395717000	0.524471000	2.272238000
1	1.779084000	0.611994000	4.513194000
1	4.344582000	0.210244000	4.074833000
1	-5.371572000	0.942762000	3.558110000

1	-6.490880000	-0.101580000	2.679704000
1	-5.252457000	-0.824787000	3.713529000
1	-0.457177000	1.786917000	-2.938392000
1	1.187504000	1.250151000	-2.632454000
1	1.829196000	3.642402000	-2.750916000
1	2.245590000	5.706381000	-1.453965000
1	1.150997000	6.032936000	0.752606000
1	-0.364985000	4.280842000	1.644838000
1	-0.794521000	2.229397000	0.350294000
1	2.145476000	1.098518000	-0.670476000
6	2.297883000	-2.157619000	-1.101073000
6	1.745628000	-2.787783000	0.179730000
6	0.468402000	-2.223128000	0.727146000
8	2.721870000	-0.801597000	-0.949094000
1	2.494344000	-2.719303000	0.979372000
7	-0.114388000	-1.173595000	0.251967000
6	3.527886000	-2.894908000	-1.590527000
1	4.308636000	-2.879703000	-0.827250000
1	3.909015000	-2.406186000	-2.491603000
1	3.267290000	-3.929090000	-1.823533000
6	-0.150940000	-2.925911000	1.878959000
1	-1.004209000	-2.368076000	2.264741000
1	0.600216000	-3.065779000	2.662909000
1	-0.470676000	-3.916539000	1.539493000
8	1.252639000	-2.204692000	-2.044062000
1	1.611325000	-1.994130000	-2.920874000
1	1.579174000	-3.855642000	-0.001323000
8	-0.769730000	-3.988718000	-1.033538000
1	-0.311069000	-3.364342000	-1.617367000
1	-1.688803000	-3.936926000	-1.324966000

Zero-point correction= 0.510499 (Hartree/Particle)

Thermal correction to Energy= 0.543866

Thermal correction to Enthalpy= 0.544810

Thermal correction to Gibbs Free Energy= 0.446202

Sum of electronic and zero-point Energies= -2250.765585

Sum of electronic and thermal Energies= -2250.732218

Sum of electronic and thermal Enthalpies= -2250.731274

Sum of electronic and thermal Free Energies= -2250.829882

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6	-2.634814000	-1.373289000	-0.180283000
6	-2.682502000	-1.627896000	-1.550899000
6	-3.646523000	-0.976977000	-2.303248000
6	-4.547214000	-0.083927000	-1.704038000
6	-4.481599000	0.127695000	-0.322452000
6	-3.526744000	-0.516563000	0.456231000
16	-1.367294000	-2.130774000	0.758947000
8	-1.698254000	-2.049433000	2.181097000
8	-1.012842000	-3.419038000	0.189346000
7	0.057624000	-1.155910000	0.563670000
6	-0.024664000	0.199471000	0.360078000
6	1.194291000	1.091130000	0.678481000
6	2.120312000	1.324468000	-0.478352000
6	2.133427000	0.782007000	-1.730485000
6	3.253097000	1.215872000	-2.504734000
6	4.058254000	2.079000000	-1.824862000
16	3.473467000	2.379693000	-0.231795000
6	-5.560594000	0.634640000	-2.548685000
6	1.209826000	-1.781729000	1.284171000
6	2.427176000	-1.864799000	0.398619000
6	3.629086000	-1.275162000	0.783572000
6	4.737160000	-1.324974000	-0.061363000
6	4.647055000	-1.977076000	-1.288164000
6	3.450527000	-2.588639000	-1.666501000
6	2.344352000	-2.532176000	-0.826055000
1	-1.974077000	-2.309803000	-2.010286000
1	-3.701406000	-1.153137000	-3.373587000
1	-5.186582000	0.807228000	0.147394000
1	-3.461492000	-0.345393000	1.525304000
1	1.382060000	0.087145000	-2.086966000
1	3.441682000	0.898282000	-3.523179000
1	4.956339000	2.573895000	-2.169944000
1	-6.106438000	1.381533000	-1.969032000
1	-5.072299000	1.132624000	-3.392026000
1	-6.283546000	-0.074319000	-2.964668000
1	0.890411000	-2.791752000	1.551948000

1	1.412565000	-1.253793000	2.219004000
1	3.696697000	-0.761666000	1.740202000
1	5.665598000	-0.848340000	0.237716000
1	5.506961000	-2.009478000	-1.949990000
1	3.380656000	-3.104825000	-2.618973000
1	1.404060000	-2.994684000	-1.118928000
1	1.748168000	0.651117000	1.514209000
6	-0.678413000	2.231935000	1.600898000
6	-1.624370000	2.637588000	0.483107000
6	-1.410903000	1.761901000	-0.728151000
8	0.653521000	2.339079000	1.098128000
1	-1.431610000	3.677229000	0.200096000
7	-0.762624000	0.656565000	-0.712708000
6	-0.806702000	3.017261000	2.880119000
1	-0.606203000	4.070841000	2.674580000
1	-0.077788000	2.659137000	3.611950000
1	-1.817442000	2.917814000	3.281438000
6	-1.990864000	2.240704000	-2.017643000
1	-1.935905000	1.466408000	-2.783048000
1	-1.423433000	3.120036000	-2.344436000
1	-3.027124000	2.560550000	-1.869764000
8	-0.924689000	0.844779000	1.802159000
1	-0.584412000	0.445419000	2.705051000
1	-2.671112000	2.566599000	0.801496000
8	-0.189792000	-0.365690000	3.844730000
1	-0.317975000	-0.001170000	4.734194000
1	-0.725631000	-1.175138000	3.779214000

Zero-point correction= 0.509315 (Hartree/Particle)

Thermal correction to Energy= 0.540334

Thermal correction to Enthalpy= 0.541278

Thermal correction to Gibbs Free Energy= 0.449267

Sum of electronic and zero-point Energies= -2250.760042

Sum of electronic and thermal Energies= -2250.729024

Sum of electronic and thermal Enthalpies= -2250.728079

Sum of electronic and thermal Free Energies= -2250.820090

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6	-3.179900000	1.612336000	0.071446000
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6	-3.009072000	2.490715000	-0.992021000
6	-2.902304000	3.849478000	-0.714095000
6	-2.955001000	4.324685000	0.599614000
6	-3.130993000	3.410029000	1.646788000
6	-3.253189000	2.051143000	1.393255000
16	-3.348598000	-0.118992000	-0.249874000
8	-4.419867000	-0.642561000	0.587603000
8	-3.385913000	-0.362541000	-1.679875000
7	-1.904518000	-0.822024000	0.434786000
6	-0.947745000	0.028939000	0.951989000
6	-0.242541000	0.943941000	0.114842000
6	-0.257130000	0.976311000	-1.356436000
6	-0.494922000	-0.023647000	-2.264568000
6	-0.246673000	0.380189000	-3.609225000
6	0.201761000	1.663958000	-3.702075000
16	0.318587000	2.412816000	-2.154617000
6	-2.839661000	5.798214000	0.880645000
6	-2.154053000	-2.132170000	1.091617000
6	-2.727247000	-3.145001000	0.125442000
6	-3.956432000	-3.750347000	0.388261000
6	-4.468750000	-4.714442000	-0.478223000
6	-3.759798000	-5.070687000	-1.622914000
6	-2.533900000	-4.464907000	-1.894270000
6	-2.018497000	-3.510702000	-1.022442000
1	-2.948852000	2.113829000	-2.008569000
1	-2.762275000	4.551241000	-1.531323000
1	-3.176385000	3.770127000	2.670390000
1	-3.394832000	1.343011000	2.205356000
1	-0.862585000	-1.001139000	-1.983787000
1	-0.400646000	-0.264324000	-4.466643000
1	0.464614000	2.222703000	-4.590349000
1	-3.802988000	6.294601000	0.720942000
1	-2.538639000	5.982886000	1.914437000
1	-2.113778000	6.268806000	0.212716000
1	-2.813945000	-2.003150000	1.952701000
1	-1.174929000	-2.455253000	1.448588000
1	-4.516548000	-3.456087000	1.271478000
1	-5.425319000	-5.180745000	-0.263080000

1	-4.160918000	-5.816182000	-2.302596000
1	-1.974891000	-4.739617000	-2.783484000
1	-1.054448000	-3.053247000	-1.221244000
1	1.081076000	0.273696000	0.259560000
6	0.659055000	2.547901000	1.635490000
6	0.973251000	1.660031000	2.625128000
6	0.309884000	0.430469000	2.921154000
8	-0.161765000	2.279348000	0.621036000
1	1.683682000	2.009334000	3.365385000
7	-0.619375000	-0.214820000	2.237910000
6	1.122472000	3.958771000	1.612560000
1	0.245709000	4.615686000	1.580185000
1	1.699535000	4.127872000	0.698608000
1	1.727108000	4.195736000	2.486641000
6	0.676597000	-0.181328000	4.241726000
1	1.751810000	-0.389201000	4.259529000
1	0.118172000	-1.100409000	4.411510000
1	0.473513000	0.528747000	5.050085000
9	2.582719000	0.011360000	-2.462198000
9	4.701236000	-0.335988000	-2.189974000
9	3.959012000	1.678659000	-2.420548000
6	3.699137000	0.478830000	-1.927586000
8	4.709745000	0.138047000	0.518983000
8	3.071578000	2.030714000	0.142160000
16	3.499444000	0.662302000	-0.074557000
9	2.924143000	-3.786772000	1.677674000
9	3.521932000	-1.807909000	2.326246000
9	1.461510000	-2.438194000	2.528566000
6	2.552285000	-2.522170000	1.782483000
8	3.258473000	-2.328949000	-0.767136000
8	0.792924000	-2.263271000	-0.164112000
16	2.172607000	-1.890262000	0.086747000
7	2.185029000	-0.267823000	0.287459000

Zero-point correction= 0.507963 (Hartree/Particle)

Thermal correction to Energy= 0.552538

Thermal correction to Enthalpy= 0.553483

Thermal correction to Gibbs Free Energy= 0.428727

Sum of electronic and zero-point Energies= -3924.787885

Sum of electronic and thermal Energies= -3924.743310
Sum of electronic and thermal Enthalpies= -3924.742365
Sum of electronic and thermal Free Energies= -3924.867120

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6	4.266148000	-0.591757000	0.197334000
6	4.147737000	-0.389127000	1.572104000
6	4.506526000	0.845247000	2.094018000
6	4.997179000	1.865273000	1.265132000
6	5.136992000	1.616415000	-0.102285000
6	4.769569000	0.389674000	-0.648426000
16	3.747798000	-2.132697000	-0.499532000
8	4.266861000	-2.230523000	-1.862870000
8	4.037023000	-3.223287000	0.428771000
7	2.050795000	-1.985483000	-0.511811000
6	1.552651000	-0.686982000	-0.852447000
6	1.002694000	0.059412000	0.139188000
6	0.773397000	-0.296861000	1.534389000
6	1.021314000	-1.450364000	2.246851000
6	0.598988000	-1.364562000	3.601465000
6	0.045228000	-0.153900000	3.906333000
16	0.019305000	0.901012000	2.553310000
6	5.358944000	3.202528000	1.851324000
6	1.442723000	-3.100798000	-1.284456000
6	-0.032882000	-3.174461000	-0.991670000
6	-0.957251000	-2.631704000	-1.887424000
6	-2.324018000	-2.705836000	-1.617146000
6	-2.770436000	-3.310483000	-0.442421000
6	-1.849610000	-3.839226000	0.462078000
6	-0.487689000	-3.773110000	0.186052000
1	3.776813000	-1.179990000	2.216071000
1	4.407594000	1.025693000	3.161096000
1	5.527942000	2.394707000	-0.751452000
1	4.860593000	0.197578000	-1.712974000
1	1.501635000	-2.316259000	1.813053000
1	0.707704000	-2.169873000	4.317957000
1	-0.352642000	0.179583000	4.855768000
1	4.501439000	3.641657000	2.371250000

1	6.164231000	3.100264000	2.585532000
1	5.686951000	3.900247000	1.077820000
1	1.938009000	-4.019207000	-0.956151000
1	1.619785000	-2.961509000	-2.355117000
1	-0.601064000	-2.153766000	-2.796433000
1	-3.035755000	-2.291420000	-2.325060000
1	-3.832924000	-3.374142000	-0.229558000
1	-2.195986000	-4.304005000	1.379850000
1	0.233411000	-4.193605000	0.882385000
1	-1.634323000	-0.584958000	-0.209682000
6	1.525568000	2.174832000	-0.595648000
6	2.079530000	1.995406000	-1.798371000
6	1.781488000	0.833904000	-2.640919000
8	0.496579000	1.308726000	-0.202551000
1	2.799710000	2.721193000	-2.164642000
7	1.583022000	-0.363257000	-2.198560000
6	1.824982000	3.245966000	0.391798000
1	2.172313000	2.794014000	1.328453000
1	0.918851000	3.817562000	0.616935000
1	2.595999000	3.919608000	0.012743000
6	1.789704000	1.049583000	-4.124610000
1	1.689984000	0.097899000	-4.647713000
1	2.715436000	1.545920000	-4.433934000
1	0.960627000	1.707858000	-4.405998000
9	-1.552421000	2.821043000	0.645976000
9	-2.929259000	3.759964000	-0.718315000
9	-0.902137000	3.367856000	-1.346847000
6	-1.909572000	2.928208000	-0.614540000
8	-3.883542000	1.440689000	-1.573044000
8	-1.531622000	0.877677000	-2.358431000
16	-2.465594000	1.277591000	-1.334406000
9	-5.460216000	-1.513615000	1.140327000
9	-5.836056000	0.412288000	0.235699000
9	-4.716074000	-1.088529000	-0.843179000
6	-4.973709000	-0.575227000	0.345688000
8	-3.729311000	1.409328000	1.599560000
8	-2.928794000	-0.971568000	2.036758000
16	-3.407896000	0.071095000	1.162371000

7	-2.287157000	0.197490000	-0.070618000
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Zero-point correction= 0.514025 (Hartree/Particle)

Thermal correction to Energy= 0.558680

Thermal correction to Enthalpy= 0.559624

Thermal correction to Gibbs Free Energy= 0.435907

Sum of electronic and zero-point Energies= -3924.819756

Sum of electronic and thermal Energies= -3924.775102

Sum of electronic and thermal Enthalpies= -3924.774158

Sum of electronic and thermal Free Energies= -3924.897875

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6	-2.185860000	0.245178000	1.339218000
6	-3.146556000	1.167177000	1.738790000
6	-4.485425000	0.906688000	1.457489000
6	-4.864134000	-0.252327000	0.776908000
6	-3.871396000	-1.165622000	0.395553000
6	-2.532524000	-0.930356000	0.673166000
16	-0.477792000	0.613280000	1.668552000
8	0.096756000	-0.386756000	2.557304000
8	-0.420116000	2.022527000	2.040893000
7	0.346663000	0.480994000	0.215490000
6	1.099727000	-0.683792000	-0.079397000
6	2.456506000	-0.485379000	-0.449113000
6	3.191088000	0.779646000	-0.393853000
6	4.224775000	1.128116000	-1.227876000
6	4.821947000	2.374219000	-0.883052000
6	4.239681000	2.943483000	0.211462000
16	2.949624000	1.986194000	0.833609000
6	-6.302348000	-0.506647000	0.417119000
6	0.017362000	1.435806000	-0.866164000
6	-1.189949000	1.012474000	-1.673714000
6	-1.138038000	-0.132234000	-2.474916000
6	-2.272293000	-0.567325000	-3.154788000
6	-3.467860000	0.142691000	-3.047703000
6	-3.521403000	1.295234000	-2.266636000
6	-2.385541000	1.726995000	-1.584621000
1	-2.848583000	2.077904000	2.246935000
1	-5.244644000	1.620892000	1.763502000

1	-4.155281000	-2.067733000	-0.140014000
1	-1.756890000	-1.621610000	0.353702000
1	4.541775000	0.498735000	-2.050970000
1	5.642098000	2.826416000	-1.427358000
1	4.477166000	3.889094000	0.681304000
1	-6.461339000	-0.328611000	-0.652395000
1	-6.974353000	0.150732000	0.972980000
1	-6.581008000	-1.544347000	0.619989000
1	-0.137184000	2.416671000	-0.410646000
1	0.907795000	1.501765000	-1.498811000
1	-0.208259000	-0.689593000	-2.559377000
1	-2.224347000	-1.460145000	-3.770711000
1	-4.352884000	-0.198313000	-3.576522000
1	-4.448659000	1.854418000	-2.181639000
1	-2.428539000	2.617747000	-0.962321000
6	1.196893000	-2.993277000	0.263517000
6	2.576795000	-3.030960000	0.391089000
6	3.397797000	-2.025058000	-0.138559000
8	2.979087000	-1.431179000	-1.330325000
1	3.039724000	-3.818508000	0.977901000
7	0.510388000	-1.855320000	0.032758000
6	4.852657000	-1.894977000	0.178606000
1	5.136064000	-0.846671000	0.308881000
1	5.091003000	-2.443113000	1.091108000
1	5.443345000	-2.297399000	-0.650909000
6	0.350393000	-4.197324000	0.569814000
1	-0.366795000	-3.967891000	1.363471000
1	-0.221370000	-4.484083000	-0.318838000
1	0.962910000	-5.048971000	0.871414000

Zero-point correction= 0.441776 (Hartree/Particle)

Thermal correction to Energy= 0.469965

Thermal correction to Enthalpy= 0.470909

Thermal correction to Gibbs Free Energy= 0.382036

Sum of electronic and zero-point Energies= -2097.559979

Sum of electronic and thermal Energies= -2097.531790

Sum of electronic and thermal Enthalpies= -2097.530846

Sum of electronic and thermal Free Energies= -2097.619719

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6	-2.261945000	-0.615295000	-1.259022000
6	-3.237933000	-1.605253000	-1.284650000
6	-4.550992000	-1.261280000	-0.972840000
6	-4.887881000	0.048542000	-0.626273000
6	-3.881940000	1.025149000	-0.621474000
6	-2.569696000	0.707555000	-0.939579000
16	-0.580293000	-1.090547000	-1.589422000
8	-0.064472000	-0.398815000	-2.759624000
8	-0.538912000	-2.547269000	-1.542319000
7	0.345767000	-0.583691000	-0.274760000
6	1.036580000	0.643557000	-0.295034000
6	2.420931000	0.628826000	0.279932000
6	3.154767000	-0.651615000	0.447061000
6	3.822492000	-1.061671000	1.567407000
6	4.481318000	-2.315466000	1.389097000
6	4.305474000	-2.823657000	0.136923000
16	3.330311000	-1.792190000	-0.844467000
6	-6.292308000	0.412520000	-0.229291000
6	0.099219000	-1.240089000	1.030942000
6	-1.018847000	-0.575188000	1.802368000
6	-0.851777000	0.718926000	2.304966000
6	-1.904771000	1.364629000	2.947950000
6	-3.131190000	0.719199000	3.102295000
6	-3.297812000	-0.577867000	2.620924000
6	-2.244417000	-1.220715000	1.973880000
1	-2.970776000	-2.628389000	-1.525889000
1	-5.321178000	-2.027261000	-0.986997000
1	-4.133952000	2.047617000	-0.352776000
1	-1.784047000	1.457388000	-0.917161000
1	3.838830000	-0.475702000	2.478937000
1	5.054810000	-2.814574000	2.160824000
1	4.679060000	-3.753757000	-0.270140000
1	-6.335728000	0.638975000	0.841794000
1	-6.988716000	-0.403477000	-0.432866000
1	-6.632413000	1.303765000	-0.764237000
1	-0.118580000	-2.291473000	0.834452000
1	1.038290000	-1.196517000	1.589688000

1	0.106109000	1.224160000	2.191596000
1	-1.767236000	2.370294000	3.333114000
1	-3.952139000	1.224242000	3.602141000
1	-4.249741000	-1.086752000	2.741423000
1	-2.375739000	-2.227185000	1.584238000
6	1.203884000	2.859635000	-1.011533000
6	2.500032000	2.986335000	-0.671570000
6	3.194777000	1.930957000	0.074910000
8	2.604662000	1.564328000	1.328461000
1	3.066458000	3.865370000	-0.963805000
7	0.478076000	1.684648000	-0.789594000
6	4.697955000	1.944265000	0.048443000
1	5.114842000	1.107063000	0.608380000
1	5.050082000	1.895237000	-0.985451000
1	5.057350000	2.878153000	0.490600000
6	0.418975000	3.924359000	-1.715415000
1	0.016106000	3.533468000	-2.655042000
1	-0.432861000	4.231475000	-1.099388000
1	1.034389000	4.800860000	-1.925386000

Zero-point correction= 0.444512 (Hartree/Particle)

Thermal correction to Energy= 0.473310

Thermal correction to Enthalpy= 0.474254

Thermal correction to Gibbs Free Energy= 0.384907

Sum of electronic and zero-point Energies= -2097.566559

Sum of electronic and thermal Energies= -2097.537761

Sum of electronic and thermal Enthalpies= -2097.536816

Sum of electronic and thermal Free Energies= -2097.626164

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6	2.319581000	0.513370000	1.032420000
6	3.199725000	-0.408910000	0.474271000
6	4.356676000	0.064321000	-0.137938000
6	4.643867000	1.430945000	-0.180223000
6	3.745229000	2.329985000	0.411815000
6	2.580296000	1.882924000	1.016679000
16	0.866338000	-0.079061000	1.853860000
8	0.344789000	0.943656000	2.740052000
8	1.136732000	-1.411051000	2.370383000

7	-0.337823000	-0.376686000	0.627699000
6	-0.909031000	0.667374000	-0.019497000
6	-2.136711000	0.387391000	-0.899504000
6	-3.250021000	-0.314727000	-0.142279000
6	-4.017361000	-1.334872000	-0.622500000
6	-5.036948000	-1.741641000	0.293604000
6	-5.024150000	-1.017181000	1.446933000
16	-3.769590000	0.171510000	1.439229000
6	5.892904000	1.941750000	-0.843869000
6	-0.577263000	-1.796723000	0.270127000
6	0.614249000	-2.407028000	-0.432812000
6	1.040616000	-1.891049000	-1.659789000
6	2.156847000	-2.434589000	-2.291310000
6	2.842655000	-3.501419000	-1.709783000
6	2.403664000	-4.031669000	-0.497634000
6	1.293572000	-3.481628000	0.140272000
1	2.993080000	-1.474298000	0.518685000
1	5.049206000	-0.644326000	-0.582686000
1	3.965552000	3.393951000	0.396487000
1	1.874395000	2.572152000	1.465808000
1	-3.837484000	-1.775033000	-1.596742000
1	-5.744073000	-2.540019000	0.101436000
1	-5.670552000	-1.111355000	2.309310000
1	6.530592000	1.119740000	-1.175171000
1	6.467673000	2.571761000	-0.158551000
1	5.642775000	2.554340000	-1.715906000
1	-0.827235000	-2.347221000	1.177312000
1	-1.428390000	-1.801194000	-0.407015000
1	0.482137000	-1.068585000	-2.103759000
1	2.493307000	-2.027702000	-3.240254000
1	3.713790000	-3.922465000	-2.202715000
1	2.929550000	-4.865851000	-0.043371000
1	0.962365000	-3.870351000	1.098912000
6	-0.800270000	2.881602000	-0.617243000
6	-1.852775000	2.793018000	-1.527658000
6	-2.595332000	1.629399000	-1.596667000
8	-1.723414000	-0.218246000	-2.054463000
1	-2.118936000	3.657213000	-2.126414000

7	-0.328343000	1.838825000	0.103074000
6	-3.855083000	1.553967000	-2.385659000
1	-3.984983000	0.554858000	-2.801271000
1	-4.701903000	1.760542000	-1.718713000
1	-3.861012000	2.297495000	-3.185449000
6	-0.076049000	4.167731000	-0.400270000
1	-0.514775000	4.984756000	-0.972991000
1	-0.092932000	4.413253000	0.666573000
1	0.974882000	4.045258000	-0.685048000

Zero-point correction= 0.441991 (Hartree/Particle)

Thermal correction to Energy= 0.470936

Thermal correction to Enthalpy= 0.471880

Thermal correction to Gibbs Free Energy= 0.381788

Sum of electronic and zero-point Energies= -2097.530804

Sum of electronic and thermal Energies= -2097.501859

Sum of electronic and thermal Enthalpies= -2097.500915

Sum of electronic and thermal Free Energies= -2097.591007

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6	1.786061000	-0.988963000	1.120173000
6	2.605247000	-2.109842000	1.153714000
6	3.976717000	-1.933438000	1.326496000
6	4.525377000	-0.656440000	1.456022000
6	3.668846000	0.454617000	1.426747000
6	2.300950000	0.300526000	1.261545000
16	0.044939000	-1.199205000	0.835319000
8	-0.713623000	-0.633938000	1.945851000
8	-0.153442000	-2.593435000	0.453875000
7	-0.298675000	-0.243182000	-0.472049000
6	-1.102031000	0.926273000	-0.275903000
6	-2.623330000	0.761157000	-0.282750000
6	-3.207868000	-0.582109000	-0.517599000
6	-3.393500000	-1.184394000	-1.731061000
6	-3.956900000	-2.490033000	-1.619186000
6	-4.181400000	-2.850686000	-0.323466000
16	-3.699957000	-1.618396000	0.778903000
6	6.009878000	-0.456327000	1.594249000
6	0.301225000	-0.548548000	-1.779718000

6	1.661335000	0.084293000	-1.977248000
6	1.787290000	1.475494000	-2.029691000
6	3.043958000	2.065015000	-2.132269000
6	4.187880000	1.268450000	-2.192599000
6	4.067919000	-0.118931000	-2.158786000
6	2.808181000	-0.706273000	-2.053372000
1	2.177728000	-3.099046000	1.030083000
1	4.628841000	-2.801761000	1.348022000
1	4.088618000	1.452760000	1.520764000
1	1.637768000	1.160571000	1.204015000
1	-3.135219000	-0.701158000	-2.666225000
1	-4.185069000	-3.127664000	-2.464775000
1	-4.593937000	-3.776480000	0.054965000
1	6.406426000	0.063279000	0.715238000
1	6.532876000	-1.409862000	1.692770000
1	6.242813000	0.159344000	2.468025000
1	0.359879000	-1.636623000	-1.871426000
1	-0.410518000	-0.193880000	-2.529775000
1	0.897263000	2.098527000	-1.973804000
1	3.132508000	3.146648000	-2.166861000
1	5.168180000	1.728995000	-2.270216000
1	4.954333000	-0.744989000	-2.203481000
1	2.713479000	-1.788695000	-2.009160000
6	-1.228651000	2.926652000	0.871461000
6	-2.684266000	2.880841000	0.887141000
6	-3.375157000	1.807604000	0.450422000
8	-1.867662000	1.247577000	-1.399736000
1	-3.203107000	3.693088000	1.388512000
7	-0.477493000	1.984836000	0.403776000
6	-4.849652000	1.651588000	0.670878000
1	-5.349583000	1.326254000	-0.246877000
1	-5.057902000	0.897875000	1.436953000
1	-5.282980000	2.596934000	1.003252000
6	-0.573315000	4.101912000	1.535518000
1	0.511654000	3.995884000	1.517422000
1	-0.855877000	5.024435000	1.017670000
1	-0.915654000	4.193337000	2.571045000

Zero-point correction= 0.444093 (Hartree/Particle)

Thermal correction to Energy= 0.473162
 Thermal correction to Enthalpy= 0.474106
 Thermal correction to Gibbs Free Energy= 0.382887
 Sum of electronic and zero-point Energies= -2097.571028
 Sum of electronic and thermal Energies= -2097.541959
 Sum of electronic and thermal Enthalpies= -2097.541014
 Sum of electronic and thermal Free Energies= -2097.632233

A-TSa8-C

6	-1.745134000	-0.869310000	-1.199918000
6	-2.552730000	-1.989788000	-1.342966000
6	-3.918762000	-1.807853000	-1.547993000
6	-4.472418000	-0.527411000	-1.600146000
6	-3.626244000	0.583211000	-1.462548000
6	-2.263267000	0.424583000	-1.263887000
16	-0.014588000	-1.089376000	-0.874750000
8	0.775673000	-0.499265000	-1.945704000
8	0.179900000	-2.488406000	-0.511871000
7	0.277858000	-0.166464000	0.483842000
6	1.037900000	1.013997000	0.373750000
6	2.786245000	0.750274000	0.382127000
6	3.225264000	-0.637768000	0.567534000
6	3.082272000	-1.371540000	1.718024000
6	3.511714000	-2.720513000	1.575330000
6	3.961503000	-2.992741000	0.315950000
16	3.865458000	-1.617419000	-0.712054000
6	-5.954234000	-0.325904000	-1.762975000
6	-0.300825000	-0.572891000	1.777978000
6	-1.698897000	-0.031753000	1.980197000
6	-1.900511000	1.342666000	2.138865000
6	-3.189060000	1.858119000	2.245638000
6	-4.289989000	1.002746000	2.199168000
6	-4.095806000	-0.369017000	2.052119000
6	-2.804324000	-0.882413000	1.944836000
1	-2.122937000	-2.983460000	-1.274443000
1	-4.564351000	-2.675015000	-1.653809000
1	-4.050298000	1.583302000	-1.497132000
1	-1.607645000	1.281649000	-1.125555000

1	2.678575000	-0.948172000	2.630127000
1	3.488382000	-3.453140000	2.373056000
1	4.353100000	-3.924341000	-0.070487000
1	-6.388276000	0.056434000	-0.832466000
1	-6.459084000	-1.260877000	-2.014833000
1	-6.166454000	0.407432000	-2.546198000
1	-0.285548000	-1.664930000	1.824666000
1	0.382171000	-0.198501000	2.545007000
1	-1.044390000	2.013060000	2.167544000
1	-3.335639000	2.927152000	2.366629000
1	-5.295148000	1.405252000	2.280794000
1	-4.949084000	-1.039888000	2.013967000
1	-2.650326000	-1.950948000	1.813690000
6	1.360401000	3.062081000	-0.608371000
6	2.769229000	2.933249000	-0.656553000
6	3.430413000	1.747112000	-0.401276000
8	1.933890000	1.208433000	1.405453000
1	3.316020000	3.731376000	-1.150305000
7	0.547781000	2.066849000	-0.294277000
6	4.782670000	1.495150000	-1.012285000
1	5.438186000	0.936827000	-0.339525000
1	4.695108000	0.928743000	-1.945732000
1	5.254065000	2.449600000	-1.257166000
6	0.721054000	4.328263000	-1.107312000
1	-0.283790000	4.120458000	-1.479786000
1	0.634610000	5.047073000	-0.285047000
1	1.314878000	4.795553000	-1.895815000

Zero-point correction= 0.442595 (Hartree/Particle)

Thermal correction to Energy= 0.470507

Thermal correction to Enthalpy= 0.471451

Thermal correction to Gibbs Free Energy= 0.383652

Sum of electronic and zero-point Energies= -2097.566847

Sum of electronic and thermal Energies= -2097.538935

Sum of electronic and thermal Enthalpies= -2097.537991

Sum of electronic and thermal Free Energies= -2097.625791

A-P1

6	-1.931098000	-0.396571000	-1.370042000
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6	-2.757832000	-1.397562000	-1.866001000
6	-4.122998000	-1.145025000	-1.971450000
6	-4.659243000	0.081286000	-1.573505000
6	-3.794442000	1.072322000	-1.087385000
6	-2.429513000	0.847753000	-0.986057000
16	-0.204347000	-0.752883000	-1.172365000
8	0.596376000	0.032877000	-2.096392000
8	-0.063555000	-2.202856000	-1.144112000
7	0.194214000	-0.222853000	0.375015000
6	0.873878000	0.975123000	0.564622000
6	3.049630000	0.669203000	0.529456000
6	3.492005000	-0.718087000	0.479950000
6	3.211329000	-1.680513000	1.421802000
6	3.695641000	-2.969422000	1.069282000
6	4.325279000	-2.977458000	-0.141888000
16	4.338184000	-1.420182000	-0.869683000
6	-6.140183000	0.337332000	-1.625066000
6	-0.229164000	-1.023436000	1.544712000
6	-1.661029000	-0.719508000	1.920833000
6	-1.978915000	0.503389000	2.518219000
6	-3.305223000	0.841339000	2.770402000
6	-4.327296000	-0.042303000	2.424307000
6	-4.016542000	-1.266413000	1.836321000
6	-2.687025000	-1.604944000	1.589910000
1	-2.343792000	-2.361950000	-2.140749000
1	-4.782334000	-1.919773000	-2.351785000
1	-4.203656000	2.028061000	-0.770777000
1	-1.758839000	1.608926000	-0.594970000
1	2.680884000	-1.458731000	2.339751000
1	3.584275000	-3.850358000	1.689832000
1	4.796792000	-3.809591000	-0.647757000
1	-6.544050000	0.425719000	-0.610666000
1	-6.667914000	-0.472443000	-2.132837000
1	-6.358797000	1.274716000	-2.144654000
1	-0.085323000	-2.079053000	1.306775000
1	0.454983000	-0.756615000	2.353089000
1	-1.181650000	1.196735000	2.777627000
1	-3.541870000	1.793338000	3.235669000

1	-5.363045000	0.221808000	2.615551000
1	-4.809334000	-1.956670000	1.563440000
1	-2.443865000	-2.554136000	1.117889000
6	1.418026000	3.146085000	0.006294000
6	2.769079000	3.006001000	-0.103466000
6	3.508528000	1.763509000	-0.134722000
8	1.966205000	0.867711000	1.406330000
1	3.336431000	3.909189000	-0.314733000
7	0.531153000	2.079081000	0.031472000
6	4.780122000	1.743696000	-0.943486000
1	5.521174000	1.052438000	-0.536840000
1	4.585396000	1.468780000	-1.986019000
1	5.218714000	2.745240000	-0.952862000
6	0.749488000	4.488513000	-0.057214000
1	0.042817000	4.521202000	-0.892401000
1	0.176476000	4.670595000	0.858298000
1	1.480325000	5.290321000	-0.175103000

Zero-point correction= 0.444512 (Hartree/Particle)

Thermal correction to Energy= 0.473310

Thermal correction to Enthalpy= 0.474254

Thermal correction to Gibbs Free Energy= 0.384907

Sum of electronic and zero-point Energies= -2097.566559

Sum of electronic and thermal Energies= -2097.537761

Sum of electronic and thermal Enthalpies= -2097.536816

Sum of electronic and thermal Free Energies= -2097.626164

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6	2.343459000	-1.212821000	-0.662483000
6	3.210922000	-0.236271000	-1.146305000
6	4.388933000	0.005605000	-0.451344000
6	4.704209000	-0.716411000	0.706174000
6	3.811836000	-1.697276000	1.160181000
6	2.630793000	-1.960755000	0.479456000
16	0.863017000	-1.547899000	-1.564399000
8	0.792645000	-2.958023000	-1.907906000
8	0.699485000	-0.556011000	-2.613607000
7	-0.380220000	-1.326205000	-0.378870000
6	-0.214879000	-0.501892000	0.708272000

6	0.572170000	0.765129000	0.594282000
6	0.450132000	1.642874000	-0.464131000
6	-0.588615000	1.702555000	-1.423310000
6	-0.483752000	2.808860000	-2.258631000
6	0.627534000	3.585898000	-1.959552000
16	1.552304000	2.993191000	-0.667869000
6	5.996581000	-0.461100000	1.428907000
6	-1.426153000	-2.379431000	-0.284914000
6	-2.802883000	-1.765979000	-0.327411000
6	-3.661138000	-1.861275000	0.764945000
6	-4.936920000	-1.302433000	0.704998000
6	-5.354139000	-0.638018000	-0.444699000
6	-4.496172000	-0.537809000	-1.540353000
6	-3.227791000	-1.104246000	-1.482191000
1	2.959662000	0.322580000	-2.042371000
1	5.075630000	0.765577000	-0.812405000
1	4.050455000	-2.263067000	2.055511000
1	1.943763000	-2.724655000	0.834219000
1	-1.376089000	0.957855000	-1.469344000
1	-1.172408000	3.048278000	-3.057977000
1	0.936660000	4.490518000	-2.471820000
1	6.242624000	0.603549000	1.429605000
1	6.815879000	-0.986902000	0.927086000
1	5.952286000	-0.816088000	2.460382000
1	-1.276686000	-3.046599000	-1.133331000
1	-1.267851000	-2.949120000	0.634101000
1	-3.328257000	-2.373482000	1.663997000
1	-5.602894000	-1.382583000	1.558702000
1	-6.346921000	-0.200955000	-0.491117000
1	-4.821011000	-0.027113000	-2.441797000
1	-2.559068000	-1.039954000	-2.339199000
1	1.399380000	0.867268000	1.294689000
6	-1.813267000	1.967560000	1.452462000
6	-0.894718000	1.448649000	2.508504000
6	-0.661887000	0.121765000	2.806615000
8	-2.501810000	1.249687000	0.751405000
1	-0.628017000	2.174909000	3.273482000
7	-0.723748000	-0.847773000	1.848585000

6	-1.834610000	3.468563000	1.329183000
1	-2.456923000	3.765127000	0.485140000
1	-2.227465000	3.908365000	2.252046000
1	-0.814452000	3.850479000	1.204392000
6	-0.291620000	-0.351406000	4.174310000
1	-1.054550000	-1.061049000	4.512367000
1	0.659543000	-0.891371000	4.142852000
1	-0.231370000	0.474392000	4.882155000

Zero-point correction= 0.452919 (Hartree/Particle)

Thermal correction to Energy= 0.482779

Thermal correction to Enthalpy= 0.483724

Thermal correction to Gibbs Free Energy= 0.390810

Sum of electronic and zero-point Energies= -2097.953630

Sum of electronic and thermal Energies= -2097.923769

Sum of electronic and thermal Enthalpies= -2097.922825

Sum of electronic and thermal Free Energies= -2098.015738

A-b4

6	-1.802110000	-1.984648000	-0.446351000
6	-2.840502000	-1.077513000	-0.244220000
6	-3.922218000	-1.475255000	0.529495000
6	-3.976861000	-2.756653000	1.088405000
6	-2.924180000	-3.650512000	0.845987000
6	-1.831146000	-3.279937000	0.077215000
16	-0.424475000	-1.480511000	-1.406662000
8	0.280333000	-2.637023000	-1.915479000
8	-0.756260000	-0.357680000	-2.254586000
7	0.696492000	-0.834384000	-0.176948000
6	0.928838000	0.439689000	0.034478000
6	0.369750000	1.658640000	-0.687302000
6	-1.063688000	1.890517000	-0.268531000
6	-1.590080000	1.788819000	0.990557000
6	-2.971319000	2.142024000	1.041910000
6	-3.460617000	2.511354000	-0.176714000
16	-2.253602000	2.433610000	-1.402302000
6	-5.157829000	-3.188201000	1.910181000
6	1.395456000	-1.860649000	0.660097000
6	2.876478000	-1.933811000	0.364647000

6	3.793736000	-1.715397000	1.393181000
6	5.160721000	-1.822836000	1.149141000
6	5.618257000	-2.136373000	-0.128669000
6	4.704804000	-2.346692000	-1.160233000
6	3.337750000	-2.250812000	-0.915100000
1	-2.816059000	-0.093086000	-0.698007000
1	-4.737544000	-0.777637000	0.695926000
1	-2.967999000	-4.652823000	1.261424000
1	-1.030832000	-3.983784000	-0.127034000
1	-1.012653000	1.477724000	1.855489000
1	-3.569596000	2.118543000	1.944420000
1	-4.464385000	2.825551000	-0.431091000
1	-5.796204000	-3.861284000	1.328317000
1	-4.835574000	-3.732767000	2.801385000
1	-5.761030000	-2.332013000	2.217699000
1	0.914466000	-2.815446000	0.446302000
1	1.211411000	-1.603676000	1.703605000
1	3.433461000	-1.453763000	2.384353000
1	5.867843000	-1.655387000	1.955356000
1	6.683585000	-2.216017000	-0.321283000
1	5.055797000	-2.593939000	-2.157197000
1	2.627118000	-2.426789000	-1.717611000
1	0.444793000	1.535781000	-1.766810000
6	0.689521000	4.078989000	0.187637000
6	1.355437000	2.745626000	-0.164458000
6	2.021870000	2.047776000	0.985923000
8	0.471850000	4.380479000	1.339306000
1	2.125365000	2.934364000	-0.925580000
7	1.782347000	0.766166000	1.053800000
6	0.358742000	4.969671000	-0.974964000
1	-0.456548000	5.643803000	-0.710655000
1	0.111183000	4.396199000	-1.871214000
1	1.252951000	5.562818000	-1.202318000
6	2.913422000	2.723138000	1.946039000
1	3.486639000	1.997787000	2.522364000
1	2.285920000	3.325654000	2.613723000
1	3.572474000	3.420195000	1.419861000

Zero-point correction= 0.456432 (Hartree/Particle)

Thermal correction to Energy= 0.486080
 Thermal correction to Enthalpy= 0.487024
 Thermal correction to Gibbs Free Energy= 0.394590
 Sum of electronic and zero-point Energies= -2098.016699
 Sum of electronic and thermal Energies= -2097.987051
 Sum of electronic and thermal Enthalpies= -2097.986107
 Sum of electronic and thermal Free Energies= -2098.078541

A-TSb5

6	-3.691438000	0.528305000	0.548569000
6	-4.085489000	-0.800926000	0.635465000
6	-5.439577000	-1.103651000	0.535930000
6	-6.390822000	-0.097061000	0.355867000
6	-5.961704000	1.236870000	0.294124000
6	-4.618290000	1.563535000	0.398319000
16	-1.980816000	0.917722000	0.736436000
8	-1.883359000	2.186946000	1.432593000
8	-1.258443000	-0.251209000	1.203130000
7	-1.374494000	1.262462000	-0.846561000
6	-0.559382000	0.432576000	-1.555267000
6	-0.275786000	-0.952786000	-1.391786000
6	-1.404752000	-1.909276000	-1.188126000
6	-2.531112000	-1.934840000	-1.972530000
6	-3.407162000	-3.021492000	-1.684085000
6	-2.928263000	-3.812825000	-0.681658000
16	-1.423508000	-3.239709000	-0.070455000
6	-7.853241000	-0.423351000	0.232734000
6	-1.512454000	2.670744000	-1.280160000
6	-0.352378000	3.563438000	-0.889904000
6	-0.349456000	4.878597000	-1.360090000
6	0.687955000	5.744343000	-1.026487000
6	1.736660000	5.302159000	-0.220981000
6	1.738590000	3.991619000	0.248341000
6	0.696439000	3.128748000	-0.084139000
1	-3.348328000	-1.579807000	0.796560000
1	-5.757612000	-2.139956000	0.604391000
1	-6.696047000	2.028828000	0.178768000
1	-4.302849000	2.601564000	0.393622000

1	-2.713520000	-1.196118000	-2.747062000
1	-4.347914000	-3.197203000	-2.192294000
1	-3.379845000	-4.697342000	-0.251269000
1	-8.449089000	0.201992000	0.903458000
1	-8.202020000	-0.230937000	-0.787215000
1	-8.047565000	-1.471572000	0.467698000
1	-2.440208000	3.054441000	-0.852201000
1	-1.633228000	2.659897000	-2.363630000
1	-1.164384000	5.224420000	-1.991767000
1	0.678821000	6.764377000	-1.398191000
1	2.547897000	5.975447000	0.037654000
1	2.548789000	3.628733000	0.873371000
1	0.705161000	2.111779000	0.295377000
1	0.728665000	-0.796748000	-0.251418000
6	1.912459000	-2.088193000	-2.325516000
6	0.660743000	-1.233239000	-2.582251000
6	0.886944000	0.137481000	-3.138979000
8	3.004867000	-1.748818000	-2.722504000
1	0.092276000	-1.792202000	-3.345235000
7	0.150244000	1.047147000	-2.574990000
6	1.689721000	-3.389827000	-1.604587000
1	2.606372000	-3.979040000	-1.632931000
1	0.865426000	-3.940472000	-2.067379000
1	1.413800000	-3.200227000	-0.561243000
6	1.843348000	0.469403000	-4.218130000
1	1.637552000	1.465556000	-4.610872000
1	1.810038000	-0.278444000	-5.014456000
1	2.850388000	0.437993000	-3.789338000
9	-0.150237000	-0.334315000	3.748941000
9	0.722761000	1.159174000	2.443722000
9	1.880698000	0.323517000	4.056891000
6	0.954518000	0.065784000	3.148406000
8	2.930848000	-1.609256000	2.539654000
8	0.572805000	-2.362300000	2.031846000
16	1.588445000	-1.333527000	2.060121000
9	5.070358000	-0.610923000	-1.087560000
9	5.197612000	-0.797381000	1.057789000
9	3.974322000	-2.177135000	-0.072642000

6	4.407182000	-0.930018000	0.010639000
8	3.301453000	1.150253000	1.263732000
8	2.715181000	0.772648000	-1.167681000
16	2.966805000	0.263453000	0.165128000
7	1.672345000	-0.688359000	0.543436000

Zero-point correction= 0.508188 (Hartree/Particle)

Thermal correction to Energy= 0.551579

Thermal correction to Enthalpy= 0.552523

Thermal correction to Gibbs Free Energy= 0.432211

Sum of electronic and zero-point Energies= -3924.828807

Sum of electronic and thermal Energies= -3924.785416

Sum of electronic and thermal Enthalpies= -3924.784472

Sum of electronic and thermal Free Energies= -3924.904784

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6	-3.457782000	0.536465000	0.580982000
6	-3.829784000	-0.467501000	1.467992000
6	-5.173059000	-0.826965000	1.540109000
6	-6.131060000	-0.200763000	0.739941000
6	-5.720548000	0.808138000	-0.142214000
6	-4.388694000	1.188935000	-0.224522000
16	-1.786883000	1.114386000	0.654590000
8	-1.769623000	2.314518000	1.477998000
8	-0.926379000	-0.010298000	1.018460000
7	-1.372202000	1.607545000	-0.903577000
6	-0.626224000	0.758704000	-1.743787000
6	-0.726105000	-0.584110000	-1.943033000
6	-1.911158000	-1.404071000	-1.643416000
6	-3.131533000	-1.225085000	-2.246920000
6	-4.133336000	-2.129411000	-1.792226000
6	-3.657897000	-2.987734000	-0.843653000
16	-2.000781000	-2.704254000	-0.490171000
6	-7.574113000	-0.621821000	0.793197000
6	-1.274473000	3.064645000	-1.122369000
6	-0.018819000	3.726790000	-0.588422000
6	0.144939000	5.096770000	-0.803595000
6	1.276357000	5.757744000	-0.332996000
6	2.259360000	5.054833000	0.361855000

6	2.101877000	3.688570000	0.580700000
6	0.969053000	3.032160000	0.106347000
1	-3.082670000	-0.957555000	2.084892000
1	-5.478756000	-1.611155000	2.226796000
1	-6.457727000	1.300760000	-0.770005000
1	-4.076027000	1.968184000	-0.913521000
1	-3.296704000	-0.457501000	-2.995466000
1	-5.156137000	-2.137014000	-2.150421000
1	-4.190918000	-3.773925000	-0.324617000
1	-8.240204000	0.235739000	0.668736000
1	-7.793258000	-1.329071000	-0.014501000
1	-7.808398000	-1.113564000	1.739895000
1	-2.154040000	3.526328000	-0.667448000
1	-1.346747000	3.216629000	-2.201317000
1	-0.620489000	5.648503000	-1.344706000
1	1.390626000	6.822979000	-0.509793000
1	3.142237000	5.568798000	0.729028000
1	2.859817000	3.125942000	1.118565000
1	0.860656000	1.965258000	0.279505000
1	0.892150000	-0.509286000	0.027948000
6	1.439271000	-1.944551000	-2.568838000
6	0.365746000	-0.905678000	-2.952495000
6	0.936595000	0.466261000	-3.223096000
8	2.612984000	-1.736495000	-2.785955000
1	-0.093933000	-1.300193000	-3.873861000
7	0.362475000	1.387443000	-2.528885000
6	0.975001000	-3.228370000	-1.942601000
1	1.771325000	-3.969984000	-2.014139000
1	0.061767000	-3.595073000	-2.416512000
1	0.754771000	-3.047896000	-0.883189000
6	2.059473000	0.756640000	-4.153640000
1	2.084340000	1.824620000	-4.375904000
1	1.964390000	0.182091000	-5.078856000
1	2.997872000	0.459347000	-3.677498000
9	-0.213101000	-0.424234000	3.634507000
9	1.098787000	0.959918000	2.601369000
9	1.863906000	-0.268721000	4.202633000
6	1.010134000	-0.214382000	3.196284000

8	2.771321000	-2.080032000	2.421998000
8	0.329799000	-2.460441000	1.847407000
16	1.473325000	-1.596672000	2.003089000
9	4.971252000	-1.242885000	-1.260955000
9	5.137773000	-1.673205000	0.848127000
9	3.592287000	-2.626040000	-0.322821000
6	4.302385000	-1.526880000	-0.160250000
8	3.705661000	0.577456000	1.388904000
8	2.964357000	0.662312000	-1.030823000
16	3.183518000	-0.058861000	0.199863000
7	1.728649000	-0.822440000	0.545718000

Zero-point correction= 0.513197 (Hartree/Particle)

Thermal correction to Energy= 0.557203

Thermal correction to Enthalpy= 0.558147

Thermal correction to Gibbs Free Energy= 0.435529

Sum of electronic and zero-point Energies= -3924.839051

Sum of electronic and thermal Energies= -3924.795046

Sum of electronic and thermal Enthalpies= -3924.794102

Sum of electronic and thermal Free Energies= -3924.916720

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6	-2.728824000	-1.370329000	-0.850870000
6	-3.371358000	-0.401584000	-1.614213000
6	-4.561332000	0.147382000	-1.139075000
6	-5.102308000	-0.252763000	0.085457000
6	-4.433625000	-1.235433000	0.829270000
6	-3.253859000	-1.801994000	0.368126000
16	-1.169510000	-2.023542000	-1.393324000
8	-1.132056000	-3.436395000	-1.030639000
8	-0.970914000	-1.609147000	-2.773187000
7	0.010953000	-1.285769000	-0.478466000
6	0.512490000	-0.018291000	-0.870260000
6	0.335592000	1.192129000	-0.243882000
6	-0.448365000	1.475680000	0.957948000
6	-1.790778000	1.320482000	1.172715000
6	-2.194930000	1.674647000	2.496759000
6	-1.155647000	2.098331000	3.268922000
16	0.336661000	2.060960000	2.402281000

6	-6.380654000	0.346576000	0.605022000
6	0.217923000	-1.733255000	0.909168000
6	1.671398000	-2.063185000	1.155908000
6	2.451040000	-1.277326000	2.002794000
6	3.785839000	-1.607160000	2.242247000
6	4.345349000	-2.730528000	1.637195000
6	3.570451000	-3.516451000	0.776900000
6	2.242023000	-3.177868000	0.533097000
1	-2.947025000	-0.086254000	-2.561820000
1	-5.075126000	0.901293000	-1.728505000
1	-4.850456000	-1.564226000	1.777501000
1	-2.754111000	-2.577777000	0.939819000
1	-2.471189000	0.990024000	0.397048000
1	-3.219130000	1.623444000	2.848156000
1	-1.174657000	2.431547000	4.298062000
1	-6.779939000	1.090475000	-0.087236000
1	-7.139926000	-0.427377000	0.753125000
1	-6.217070000	0.830249000	1.573203000
1	-0.383235000	-2.632580000	1.057415000
1	-0.133544000	-0.970569000	1.612159000
1	2.011000000	-0.402530000	2.474978000
1	4.386868000	-0.985912000	2.899015000
1	5.381143000	-2.993527000	1.828106000
1	4.004445000	-4.390169000	0.300767000
1	1.632325000	-3.779559000	-0.137229000
6	1.186014000	3.586604000	-1.024773000
6	1.268254000	2.103397000	-0.913678000
6	1.812017000	1.303869000	-2.003207000
8	2.095534000	4.206381000	-1.552957000
1	2.383964000	1.836331000	-0.179087000
7	1.412608000	0.052117000	-1.923201000
6	-0.038180000	4.296586000	-0.502273000
1	-0.034652000	5.323338000	-0.870305000
1	-0.026529000	4.312011000	0.592199000
1	-0.950931000	3.779848000	-0.810864000
6	2.829960000	1.745473000	-3.001285000
1	3.018932000	0.937507000	-3.710575000
1	3.769458000	2.011103000	-2.505285000

1	2.494015000	2.637682000	-3.535968000
8	3.402358000	1.407877000	0.476248000
1	3.676901000	0.543260000	0.001723000
1	4.134598000	2.038888000	0.379092000
8	3.953877000	-0.667387000	-0.914229000
1	3.128424000	-0.789693000	-1.424575000
1	4.094748000	-1.490512000	-0.422518000

Zero-point correction= 0.489790 (Hartree/Particle)

Thermal correction to Energy= 0.523612

Thermal correction to Enthalpy= 0.524556

Thermal correction to Gibbs Free Energy= 0.423701

Sum of electronic and zero-point Energies= -2250.344747

Sum of electronic and thermal Energies= -2250.310926

Sum of electronic and thermal Enthalpies= -2250.309982

Sum of electronic and thermal Free Energies= -2250.410836

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6	-1.401454000	-1.798548000	-1.067701000
6	-1.671694000	-0.935465000	-2.123343000
6	-3.000444000	-0.681078000	-2.450661000
6	-4.043805000	-1.276843000	-1.736580000
6	-3.736020000	-2.149499000	-0.684277000
6	-2.417974000	-2.412162000	-0.337496000
16	0.277712000	-2.088719000	-0.591676000
8	0.401035000	-3.410259000	0.018751000
8	1.147183000	-1.750071000	-1.717577000
7	0.462195000	-0.980555000	0.659329000
6	0.301748000	0.368882000	0.293096000
6	-0.774474000	1.198797000	0.547597000
6	-2.024554000	0.768020000	1.172794000
6	-3.304897000	1.027406000	0.757584000
6	-4.298488000	0.416464000	1.579035000
6	-3.760298000	-0.305977000	2.603256000
16	-2.038318000	-0.248359000	2.583678000
6	-5.478419000	-0.960157000	-2.058228000
6	1.426925000	-1.334924000	1.727412000
6	2.878277000	-1.193913000	1.328676000
6	3.580631000	-0.020159000	1.612338000

6	4.909731000	0.121661000	1.218608000
6	5.549343000	-0.910541000	0.534480000
6	4.857712000	-2.089041000	0.253149000
6	3.528088000	-2.229305000	0.647795000
1	-0.858108000	-0.472318000	-2.673336000
1	-3.230242000	-0.007982000	-3.271602000
1	-4.541719000	-2.621179000	-0.128536000
1	-2.175776000	-3.085550000	0.478736000
1	-3.522666000	1.621309000	-0.123355000
1	-5.365302000	0.505811000	1.408706000
1	-4.274716000	-0.870720000	3.369288000
1	-5.575856000	-0.515017000	-3.050709000
1	-6.100882000	-1.857727000	-2.013734000
1	-5.879165000	-0.247029000	-1.328821000
1	1.202996000	-2.360017000	2.029388000
1	1.192569000	-0.671641000	2.563963000
1	3.080884000	0.783795000	2.147466000
1	5.449303000	1.036236000	1.444564000
1	6.583467000	-0.798086000	0.223921000
1	5.353989000	-2.900150000	-0.270679000
1	2.988344000	-3.147812000	0.431081000
6	-1.137456000	3.762345000	-0.003841000
6	-0.462089000	2.458708000	-0.071941000
6	0.781323000	2.308042000	-0.698556000
8	-0.834052000	4.658157000	-0.783153000
1	4.869579000	2.697278000	-0.416563000
7	1.222583000	1.055505000	-0.461681000
6	-2.165792000	4.033481000	1.073641000
1	-2.097505000	5.089615000	1.342553000
1	-2.028899000	3.407307000	1.956689000
1	-3.170145000	3.851082000	0.679835000
6	1.615186000	3.274233000	-1.473926000
1	2.623227000	2.872717000	-1.609963000
1	1.673621000	4.235240000	-0.957923000
1	1.179528000	3.468262000	-2.457759000
8	5.253725000	2.165238000	-1.126488000
1	4.202132000	0.721880000	-1.499156000
1	5.345327000	2.773115000	-1.873269000

8	3.439060000	0.184265000	-1.785984000
1	2.091991000	0.658063000	-0.878946000
1	3.598002000	-0.719094000	-1.479269000

Zero-point correction= 0.494612 (Hartree/Particle)

Thermal correction to Energy= 0.530056

Thermal correction to Enthalpy= 0.531000

Thermal correction to Gibbs Free Energy= 0.427140

Sum of electronic and zero-point Energies= -2250.393397

Sum of electronic and thermal Energies= -2250.357953

Sum of electronic and thermal Enthalpies= -2250.357009

Sum of electronic and thermal Free Energies= -2250.460869

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6	-1.953499000	-1.433842000	-0.245714000
6	-2.930493000	-1.102350000	-1.175983000
6	-4.267194000	-1.285067000	-0.833826000
6	-4.629194000	-1.788997000	0.417428000
6	-3.618439000	-2.113704000	1.332311000
6	-2.279139000	-1.948733000	1.006838000
16	-0.254445000	-1.325088000	-0.741148000
8	0.212056000	-2.684645000	-0.993252000
8	-0.139325000	-0.318599000	-1.785410000
7	0.576571000	-0.811592000	0.631030000
6	0.831914000	0.561971000	0.844674000
6	-0.036125000	1.662204000	0.680357000
6	-1.448423000	1.754010000	0.291183000
6	-2.549644000	1.507388000	1.067335000
6	-3.779714000	1.825929000	0.420051000
6	-3.594919000	2.322344000	-0.837603000
16	-1.925803000	2.388203000	-1.255158000
6	-6.076113000	-1.996666000	0.775381000
6	1.525233000	-1.772448000	1.218366000
6	2.802699000	-2.011149000	0.437321000
6	3.661297000	-3.021341000	0.876195000
6	4.849871000	-3.287377000	0.201450000
6	5.191967000	-2.544705000	-0.927150000
6	4.338073000	-1.537227000	-1.370055000
6	3.150646000	-1.269123000	-0.691720000

1	-2.648998000	-0.692943000	-2.140848000
1	-5.042124000	-1.016172000	-1.546399000
1	-3.889089000	-2.497956000	2.311966000
1	-1.499488000	-2.189993000	1.723703000
1	-2.473131000	1.119090000	2.076921000
1	-4.755851000	1.691662000	0.871935000
1	-4.345416000	2.644109000	-1.547669000
1	-6.368390000	-3.037640000	0.598912000
1	-6.256618000	-1.779748000	1.831272000
1	-6.727668000	-1.361431000	0.170920000
1	1.001411000	-2.721280000	1.352287000
1	1.765609000	-1.383237000	2.210566000
1	3.393600000	-3.607565000	1.752607000
1	5.505843000	-4.077659000	0.554107000
1	6.116015000	-2.751713000	-1.458132000
1	4.595500000	-0.953451000	-2.248805000
1	2.496568000	-0.473986000	-1.041863000
6	2.084510000	2.886696000	-0.519570000
6	0.775885000	2.776626000	0.961352000
6	2.062210000	2.257069000	1.364019000
8	2.034108000	2.033851000	-1.335176000
1	0.444981000	3.805907000	1.042692000
7	2.055651000	0.910437000	1.282952000
6	2.647538000	4.266499000	-0.665699000
1	2.460840000	4.598214000	-1.689277000
1	3.729195000	4.208145000	-0.507453000
1	2.219324000	4.966254000	0.049999000
6	3.166305000	2.977566000	2.080299000
1	4.143897000	2.624158000	1.742939000
1	3.082741000	2.768867000	3.151322000
1	3.103449000	4.058303000	1.948585000

Zero-point correction= 0.441753 (Hartree/Particle)

Thermal correction to Energy= 0.471046

Thermal correction to Enthalpy= 0.471990

Thermal correction to Gibbs Free Energy= 0.380257

Sum of electronic and zero-point Energies= -2097.553935

Sum of electronic and thermal Energies= -2097.524642

Sum of electronic and thermal Enthalpies= -2097.523698

Sum of electronic and thermal Free Energies= -2097.615431

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6	-1.066613000	-1.837079000	-1.138747000
6	-2.080720000	-0.971746000	-1.539522000
6	-3.394613000	-1.280511000	-1.210132000
6	-3.701529000	-2.439288000	-0.486931000
6	-2.663531000	-3.306012000	-0.127562000
6	-1.341339000	-3.011042000	-0.443436000
16	0.620798000	-1.361330000	-1.397689000
8	1.431103000	-2.570579000	-1.461623000
8	0.647858000	-0.383152000	-2.478499000
7	1.070736000	-0.567943000	-0.002906000
6	0.805680000	0.814725000	0.081541000
6	-0.298436000	1.403933000	0.607862000
6	-1.441076000	0.797716000	1.266901000
6	-1.556339000	-0.443715000	1.843127000
6	-2.851305000	-0.692308000	2.380157000
6	-3.704898000	0.359706000	2.213308000
16	-2.940302000	1.674997000	1.405991000
6	-5.119664000	-2.720481000	-0.074327000
6	1.900707000	-1.235489000	1.001706000
6	3.397043000	-1.057244000	0.829727000
6	4.225739000	-1.340844000	1.918814000
6	5.608963000	-1.242738000	1.802332000
6	6.180253000	-0.852740000	0.591956000
6	5.358519000	-0.562569000	-0.494079000
6	3.973050000	-0.665679000	-0.377867000
1	-1.837529000	-0.077369000	-2.103144000
1	-4.195477000	-0.611107000	-1.513228000
1	-2.894038000	-4.219265000	0.413658000
1	-0.536086000	-3.681116000	-0.158179000
1	-0.741518000	-1.157053000	1.878117000
1	-3.134126000	-1.615706000	2.872422000
1	-4.736043000	0.446405000	2.528982000
1	-5.259413000	-3.772187000	0.185005000
1	-5.377770000	-2.118179000	0.804757000
1	-5.822745000	-2.458161000	-0.869091000

1	1.654800000	-2.302161000	0.982846000
1	1.589725000	-0.854205000	1.980043000
1	3.781132000	-1.641612000	2.864923000
1	6.239816000	-1.466982000	2.657180000
1	7.258762000	-0.770899000	0.498111000
1	5.794504000	-0.251029000	-1.438490000
1	3.341510000	-0.416362000	-1.224675000
6	-1.104914000	3.526591000	-0.588706000
6	-0.113657000	2.880981000	0.400464000
6	1.261153000	2.916175000	-0.244507000
8	-1.542748000	4.632687000	-0.370380000
1	-0.143694000	3.463540000	1.327078000
7	1.749653000	1.739730000	-0.428783000
6	-1.451099000	2.735316000	-1.822261000
1	-1.751898000	3.416878000	-2.618795000
1	-2.300651000	2.084082000	-1.584018000
1	-0.619316000	2.100868000	-2.144470000
6	1.928199000	4.179460000	-0.664336000
1	2.928150000	3.965868000	-1.043633000
1	1.995069000	4.876665000	0.176281000
1	1.349028000	4.675545000	-1.451541000

Zero-point correction= 0.443300 (Hartree/Particle)

Thermal correction to Energy= 0.472925

Thermal correction to Enthalpy= 0.473870

Thermal correction to Gibbs Free Energy= 0.381389

Sum of electronic and zero-point Energies= -2097.596617

Sum of electronic and thermal Energies= -2097.566992

Sum of electronic and thermal Enthalpies= -2097.566048

Sum of electronic and thermal Free Energies= -2097.65852

A-TSb7-B

6	-2.098680000	-1.367619000	-0.276384000
6	-3.162788000	-1.045707000	-1.112548000
6	-4.457627000	-1.271737000	-0.660312000
6	-4.696375000	-1.804337000	0.610712000
6	-3.602951000	-2.120912000	1.425055000
6	-2.299975000	-1.913991000	0.987387000
16	-0.455066000	-1.175158000	-0.914144000

8	0.046414000	-2.506402000	-1.242016000
8	-0.474415000	-0.140694000	-1.934214000
7	0.476928000	-0.651538000	0.385977000
6	0.726546000	0.712097000	0.610560000
6	-0.114831000	1.835448000	0.412631000
6	-1.569238000	1.882613000	0.204656000
6	-2.546282000	1.532668000	1.097957000
6	-3.861776000	1.822752000	0.629703000
6	-3.860778000	2.393879000	-0.609435000
16	-2.262455000	2.575871000	-1.224827000
6	-6.106650000	-2.005147000	1.095861000
6	1.368727000	-1.623830000	1.044008000
6	2.780442000	-1.722876000	0.495435000
6	3.826890000	-1.925504000	1.399001000
6	5.135782000	-2.090116000	0.951747000
6	5.415654000	-2.046407000	-0.412653000
6	4.378171000	-1.834589000	-1.318609000
6	3.068556000	-1.672679000	-0.869928000
1	-2.977956000	-0.608856000	-2.088713000
1	-5.299216000	-1.015792000	-1.298483000
1	-3.775125000	-2.536681000	2.413678000
1	-1.457653000	-2.155823000	1.629457000
1	-2.324716000	1.092759000	2.064084000
1	-4.765321000	1.612783000	1.190407000
1	-4.709331000	2.706094000	-1.203827000
1	-6.713284000	-2.508154000	0.337636000
1	-6.130570000	-2.599809000	2.011460000
1	-6.581225000	-1.040417000	1.305390000
1	0.886148000	-2.601528000	0.979766000
1	1.409725000	-1.340717000	2.099008000
1	3.612359000	-1.951413000	2.464849000
1	5.935163000	-2.246443000	1.669810000
1	6.433951000	-2.171759000	-0.767575000
1	4.586961000	-1.791994000	-2.383597000
1	2.275151000	-1.504168000	-1.590481000
6	2.846390000	1.599052000	-0.519193000
6	0.705387000	2.949280000	0.568511000
6	2.000254000	2.502145000	0.889147000

8	2.271196000	1.450936000	-1.552757000
1	0.383540000	3.982963000	0.525915000
7	1.972352000	1.076275000	0.952123000
6	4.332693000	1.543128000	-0.306621000
1	4.761599000	1.022341000	-1.163871000
1	4.577713000	1.013616000	0.613888000
1	4.740530000	2.556802000	-0.267434000
6	2.973376000	3.297612000	1.718170000
1	3.168819000	4.266193000	1.250391000
1	3.918709000	2.774619000	1.857680000
1	2.548345000	3.478770000	2.710126000

Zero-point correction= 0.442275 (Hartree/Particle)

Thermal correction to Energy= 0.471356

Thermal correction to Enthalpy= 0.472300

Thermal correction to Gibbs Free Energy= 0.381388

Sum of electronic and zero-point Energies= -2097.550297

Sum of electronic and thermal Energies= -2097.521216

Sum of electronic and thermal Enthalpies= -2097.520272

Sum of electronic and thermal Free Energies= -2097.611183

A-P4

6	-1.503710000	-1.360387000	-1.264146000
6	-2.295109000	-0.277641000	-1.642726000
6	-3.663607000	-0.337849000	-1.410951000
6	-4.245178000	-1.460998000	-0.810740000
6	-3.427986000	-2.544844000	-0.471515000
6	-2.055093000	-2.501562000	-0.687784000
16	0.258008000	-1.222569000	-1.381631000
8	0.827255000	-2.564800000	-1.346529000
8	0.561125000	-0.310924000	-2.480114000
7	0.743326000	-0.461606000	0.021442000
6	0.541006000	0.919877000	0.106298000
6	-0.507210000	1.628422000	0.665471000
6	-1.692354000	1.102930000	1.338436000
6	-1.967838000	-0.142573000	1.842509000
6	-3.291837000	-0.261419000	2.361229000
6	-4.011823000	0.889984000	2.243961000
16	-3.085719000	2.137953000	1.498551000

6	-5.716288000	-1.477656000	-0.500471000
6	1.210748000	-1.247123000	1.184038000
6	2.712998000	-1.341486000	1.302019000
6	3.400025000	-0.483846000	2.160507000
6	4.788240000	-0.549754000	2.263573000
6	5.497922000	-1.481070000	1.509193000
6	4.814573000	-2.347662000	0.656461000
6	3.428908000	-2.277994000	0.553566000
1	-1.845283000	0.594718000	-2.106028000
1	-4.291374000	0.502766000	-1.693367000
1	-3.872140000	-3.429994000	-0.024975000
1	-1.420111000	-3.339516000	-0.418034000
1	-1.264577000	-0.964927000	1.831015000
1	-3.686801000	-1.170996000	2.799204000
1	-5.027391000	1.085817000	2.561242000
1	-6.090470000	-2.497511000	-0.386659000
1	-5.902549000	-0.943745000	0.438898000
1	-6.292237000	-0.977157000	-1.282913000
1	0.767802000	-2.244391000	1.109779000
1	0.801269000	-0.762171000	2.074116000
1	2.844174000	0.240981000	2.750936000
1	5.314651000	0.123072000	2.934023000
1	6.579448000	-1.536193000	1.589115000
1	5.364200000	-3.079451000	0.071892000
1	2.891248000	-2.940727000	-0.118424000
6	2.498907000	1.432772000	-1.352408000
6	-0.258205000	3.007400000	0.384504000
6	0.879916000	3.106788000	-0.371182000
8	3.228244000	0.553540000	-0.975930000
1	-0.843963000	3.851329000	0.725478000
7	1.382186000	1.828525000	-0.540800000
6	2.655200000	2.139155000	-2.670013000
1	3.279212000	3.029174000	-2.549833000
1	1.690713000	2.431471000	-3.086419000
1	3.165783000	1.452686000	-3.346036000
6	1.557284000	4.348756000	-0.854005000
1	1.442029000	4.495869000	-1.931508000
1	2.626270000	4.343902000	-0.621733000

1	1.104956000	5.204576000	-0.349331000
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Zero-point correction= 0.444278 (Hartree/Particle)

Thermal correction to Energy= 0.473706

Thermal correction to Enthalpy= 0.474650

Thermal correction to Gibbs Free Energy= 0.383202

Sum of electronic and zero-point Energies= -2097.619470

Sum of electronic and thermal Energies= -2097.590042

Sum of electronic and thermal Enthalpies= -2097.589098

Sum of electronic and thermal Free Energies= -2097.680546

A-TSb6-C

6	1.411703000	-1.965012000	-0.108983000
6	2.529142000	-2.108077000	0.709213000
6	3.775448000	-2.255186000	0.114179000
6	3.914584000	-2.262908000	-1.278702000
6	2.769365000	-2.136900000	-2.071493000
6	1.511649000	-1.991730000	-1.495842000
16	-0.181675000	-1.843652000	0.659845000
8	-0.824331000	-3.152060000	0.591841000
8	-0.035787000	-1.203502000	1.958546000
7	-1.069095000	-0.845880000	-0.340831000
6	-0.912969000	0.556909000	-0.354732000
6	0.182937000	1.375524000	0.001519000
6	1.567086000	1.124581000	0.447344000
6	2.682928000	1.242144000	-0.341915000
6	3.904534000	1.196126000	0.390642000
6	3.695988000	1.065409000	1.734100000
16	2.023230000	0.975125000	2.117540000
6	5.279480000	-2.374173000	-1.901504000
6	-2.203246000	-1.422293000	-1.095359000
6	-3.551128000	-1.274286000	-0.419699000
6	-4.603291000	-0.659024000	-1.099827000
6	-5.862374000	-0.552588000	-0.513725000
6	-6.079153000	-1.053366000	0.768099000
6	-5.032144000	-1.664726000	1.455358000
6	-3.776382000	-1.778709000	0.863327000
1	2.422811000	-2.078763000	1.788633000
1	4.658614000	-2.350488000	0.740217000

1	2.864626000	-2.147893000	-3.153361000
1	0.627511000	-1.882233000	-2.117605000
1	2.619006000	1.369098000	-1.417460000
1	4.888170000	1.250807000	-0.061267000
1	4.436127000	0.976667000	2.518844000
1	5.870206000	-3.154925000	-1.414767000
1	5.212756000	-2.600243000	-2.967792000
1	5.826208000	-1.431577000	-1.788518000
1	-1.977268000	-2.477857000	-1.250041000
1	-2.220284000	-0.927710000	-2.067842000
1	-4.427308000	-0.248325000	-2.090783000
1	-6.670615000	-0.068444000	-1.053514000
1	-7.057698000	-0.964831000	1.230056000
1	-5.193170000	-2.059613000	2.453937000
1	-2.970619000	-2.272650000	1.399115000
6	0.450782000	4.011327000	-0.211151000
6	-0.215857000	2.680847000	-0.404524000
6	-1.561673000	2.537550000	-0.977749000
8	0.319074000	4.874353000	-1.057937000
1	-0.475524000	2.642752000	-1.699076000
7	-1.921682000	1.239920000	-0.921283000
6	1.229643000	4.239409000	1.052732000
1	1.384207000	5.311542000	1.179462000
1	2.203194000	3.742451000	0.971146000
1	0.712094000	3.817655000	1.917406000
6	-2.535316000	3.618617000	-1.331986000
1	-3.142442000	3.856325000	-0.453725000
1	-3.198915000	3.266200000	-2.123994000
1	-2.023184000	4.523074000	-1.657968000

Zero-point correction= 0.439959 (Hartree/Particle)

Thermal correction to Energy= 0.469323

Thermal correction to Enthalpy= 0.470267

Thermal correction to Gibbs Free Energy= 0.378298

Sum of electronic and zero-point Energies= -2097.552609

Sum of electronic and thermal Energies= -2097.523245

Sum of electronic and thermal Enthalpies= -2097.522301

Sum of electronic and thermal Free Energies= -2097.614271

A-b6-C

6	-1.610153000	-1.980655000	-0.964366000
6	-2.427402000	-1.000445000	-1.520426000
6	-3.774252000	-0.980031000	-1.178511000
6	-4.308421000	-1.927995000	-0.297258000
6	-3.469152000	-2.925330000	0.211181000
6	-2.116299000	-2.954550000	-0.108649000
16	0.138000000	-1.899988000	-1.233777000
8	0.711264000	-3.215084000	-0.974264000
8	0.362222000	-1.233840000	-2.511574000
7	0.702117000	-0.907601000	-0.022091000
6	0.573616000	0.486581000	-0.176427000
6	-0.410254000	1.276086000	0.319570000
6	-1.567377000	0.913612000	1.116458000
6	-1.799990000	-0.229476000	1.841437000
6	-3.070181000	-0.234504000	2.484491000
6	-3.786922000	0.903114000	2.250449000
16	-2.921273000	2.003281000	1.248286000
6	-5.749369000	-1.844346000	0.123802000
6	1.568628000	-1.416314000	1.046144000
6	3.052686000	-1.390621000	0.739453000
6	3.947305000	-1.249513000	1.803221000
6	5.322690000	-1.281651000	1.585245000
6	5.820325000	-1.447216000	0.291707000
6	4.932093000	-1.571988000	-0.776100000
6	3.555934000	-1.544337000	-0.553958000
1	-2.012713000	-0.269924000	-2.207530000
1	-4.423413000	-0.215677000	-1.597738000
1	-3.878397000	-3.678910000	0.878137000
1	-1.460528000	-3.717347000	0.299442000
1	-1.085124000	-1.041152000	1.904469000
1	-3.433515000	-1.051208000	3.097523000
1	-4.768524000	1.168846000	2.619506000
1	-6.107534000	-2.799142000	0.514881000
1	-5.860929000	-1.092736000	0.914425000
1	-6.389580000	-1.542891000	-0.709161000
1	1.253850000	-2.439312000	1.274548000
1	1.374060000	-0.790666000	1.922213000

1	3.558957000	-1.104916000	2.808057000
1	6.006542000	-1.169625000	2.421085000
1	6.891366000	-1.468794000	0.116617000
1	5.310915000	-1.686238000	-1.786990000
1	2.878378000	-1.614677000	-1.399835000
6	-0.990896000	3.421705000	-0.990711000
6	-0.031650000	2.684890000	-0.040126000
6	1.289237000	2.462360000	-0.750009000
8	-1.213653000	4.600694000	-0.835001000
1	0.121703000	3.308912000	0.847322000
7	1.600135000	1.214767000	-0.826733000
6	-1.576885000	2.615300000	-2.119045000
1	-1.959837000	3.285095000	-2.889349000
1	-2.403285000	2.007479000	-1.731660000
1	-0.830138000	1.931631000	-2.535959000
6	2.126714000	3.571175000	-1.282378000
1	3.015589000	3.173865000	-1.773548000
1	2.433957000	4.228775000	-0.462474000
1	1.558117000	4.179845000	-1.993682000
8	2.288570000	1.620285000	2.091336000
1	3.028752000	1.620348000	1.455493000
1	2.703946000	1.802319000	2.942818000
8	4.277299000	1.598817000	0.065377000
1	3.587397000	1.189031000	-0.486133000
1	4.900807000	0.882133000	0.248987000

Zero-point correction= 0.492712 (Hartree/Particle)

Thermal correction to Energy= 0.528480

Thermal correction to Enthalpy= 0.529424

Thermal correction to Gibbs Free Energy= 0.423766

Sum of electronic and zero-point Energies= -2250.360060

Sum of electronic and thermal Energies= -2250.324293

Sum of electronic and thermal Enthalpies= -2250.323349

Sum of electronic and thermal Free Energies= -2250.429007

A-TSb7-C

6	1.593350000	-1.796199000	0.297954000
6	2.628125000	-1.804230000	1.225784000
6	3.899124000	-2.197846000	0.812625000

6	4.141993000	-2.576437000	-0.508655000
6	3.077653000	-2.559520000	-1.420385000
6	1.802701000	-2.178394000	-1.026342000
16	-0.052126000	-1.479719000	0.893123000
8	-0.716116000	-2.775330000	0.989646000
8	0.037210000	-0.616677000	2.063146000
7	-0.840791000	-0.634283000	-0.322826000
6	-1.023080000	0.768540000	-0.202157000
6	-0.044588000	1.776761000	-0.164313000
6	1.407439000	1.538291000	-0.162301000
6	2.184972000	1.190924000	-1.233106000
6	3.567035000	1.065105000	-0.901824000
6	3.809611000	1.317384000	0.417062000
16	2.366859000	1.701181000	1.272523000
6	5.524548000	-2.959370000	-0.961982000
6	-1.783053000	-1.384103000	-1.168005000
6	-3.149259000	-1.696462000	-0.582226000
6	-4.074316000	-2.328940000	-1.416119000
6	-5.338656000	-2.672701000	-0.946194000
6	-5.693683000	-2.385866000	0.370439000
6	-4.776265000	-1.752827000	1.205843000
6	-3.511226000	-1.410854000	0.733253000
1	2.441932000	-1.504872000	2.252105000
1	4.714872000	-2.205366000	1.530187000
1	3.253988000	-2.850555000	-2.452300000
1	0.988076000	-2.165363000	-1.744221000
1	1.775170000	1.036950000	-2.225383000
1	4.340511000	0.793113000	-1.610615000
1	4.755279000	1.282621000	0.941954000
1	6.149351000	-3.258736000	-0.117653000
1	5.489971000	-3.781486000	-1.681568000
1	6.012195000	-2.111225000	-1.455373000
1	-1.302903000	-2.324688000	-1.451001000
1	-1.899606000	-0.798916000	-2.085209000
1	-3.799531000	-2.556528000	-2.443928000
1	-6.045339000	-3.164004000	-1.608236000
1	-6.678192000	-2.652832000	0.741891000
1	-5.043692000	-1.522194000	2.232616000

1	-2.810561000	-0.906847000	1.393100000
6	-0.231598000	4.400407000	-0.282643000
6	-0.734284000	3.003059000	-0.228699000
6	-2.117390000	2.697617000	-0.302269000
8	-1.031278000	5.318226000	-0.370325000
1	-2.375163000	1.980530000	-1.325254000
7	-2.269876000	1.271507000	-0.244102000
6	1.247580000	4.677370000	-0.228670000
1	1.410874000	5.729476000	-0.464058000
1	1.804279000	4.039857000	-0.920362000
1	1.622412000	4.472396000	0.778917000
6	-3.324499000	3.558758000	-0.066862000
1	-3.303721000	3.952949000	0.952938000
1	-4.225919000	2.954468000	-0.189264000
1	-3.347263000	4.404745000	-0.752108000

Zero-point correction= 0.439248 (Hartree/Particle)

Thermal correction to Energy= 0.468800

Thermal correction to Enthalpy= 0.469744

Thermal correction to Gibbs Free Energy= 0.376420

Sum of electronic and zero-point Energies= -2097.540848

Sum of electronic and thermal Energies= -2097.511296

Sum of electronic and thermal Enthalpies= -2097.510352

Sum of electronic and thermal Free Energies= -2097.603675

A-P3

6	-1.239860000	-1.983560000	-0.671795000
6	-1.797288000	-1.673635000	-1.905052000
6	-3.185550000	-1.634904000	-2.018169000
6	-4.004203000	-1.902821000	-0.919848000
6	-3.408521000	-2.216482000	0.310563000
6	-2.029799000	-2.256101000	0.445609000
16	0.518708000	-2.111271000	-0.509502000
8	0.854144000	-3.352331000	0.183859000
8	1.121244000	-1.844459000	-1.813471000
7	0.870583000	-0.870621000	0.570747000
6	0.762326000	0.428460000	0.045409000
6	-0.206588000	1.385201000	0.272127000
6	-1.391299000	1.139034000	1.098008000

6	-1.440724000	0.642674000	2.374385000
6	-2.772350000	0.442577000	2.847472000
6	-3.713929000	0.781783000	1.919961000
16	-2.993985000	1.340608000	0.459339000
6	-5.501637000	-1.814076000	-1.028395000
6	1.900424000	-1.122438000	1.609757000
6	3.315944000	-0.942695000	1.111733000
6	3.999415000	0.252512000	1.346001000
6	5.279342000	0.448455000	0.830312000
6	5.884588000	-0.552280000	0.073253000
6	5.209703000	-1.749793000	-0.162367000
6	3.931883000	-1.944633000	0.354805000
1	-1.156771000	-1.469454000	-2.756637000
1	-3.637256000	-1.391796000	-2.975604000
1	-4.037621000	-2.427069000	1.171082000
1	-1.568940000	-2.494486000	1.399984000
1	-0.547741000	0.436233000	2.954294000
1	-3.015574000	0.070368000	3.835728000
1	-4.791443000	0.743694000	2.012781000
1	-5.825587000	-1.794389000	-2.071014000
1	-5.986187000	-2.656586000	-0.527370000
1	-5.860266000	-0.897826000	-0.545388000
1	1.736529000	-2.134010000	1.984525000
1	1.684091000	-0.414761000	2.414387000
1	3.518706000	1.035194000	1.928352000
1	5.801565000	1.381533000	1.018290000
1	6.880912000	-0.402184000	-0.331052000
1	5.681095000	-2.533998000	-0.746686000
1	3.403866000	-2.877512000	0.172639000
6	-0.397980000	3.891214000	-0.562421000
6	0.165391000	2.532351000	-0.513759000
6	1.342868000	2.206555000	-1.193853000
8	-0.055692000	4.670523000	-1.442748000
1	2.485483000	0.439757000	-1.191055000
7	1.682974000	0.949287000	-0.837732000
6	-1.361619000	4.351913000	0.508550000
1	-1.192321000	5.417163000	0.677842000
1	-1.254478000	3.799824000	1.443850000

1	-2.388914000	4.227536000	0.152475000
6	2.195216000	3.005167000	-2.120993000
1	1.701488000	3.143464000	-3.086231000
1	3.151819000	2.501627000	-2.281880000
1	2.375008000	4.000899000	-1.710675000

Zero-point correction= 0.445582 (Hartree/Particle)

Thermal correction to Energy= 0.474959

Thermal correction to Enthalpy= 0.475903

Thermal correction to Gibbs Free Energy= 0.384330

Sum of electronic and zero-point Energies= -2097.628314

Sum of electronic and thermal Energies= -2097.598937

Sum of electronic and thermal Enthalpies= -2097.597993

Sum of electronic and thermal Free Energies= -2097.689566

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6	1.609529000	-1.937728000	0.281602000
6	2.779132000	-1.642192000	0.972884000
6	3.998610000	-1.882212000	0.346956000
6	4.055591000	-2.409009000	-0.945668000
6	2.856213000	-2.705481000	-1.608078000
6	1.628182000	-2.479597000	-1.002878000
16	0.065635000	-1.680123000	1.107962000
8	-0.557371000	-2.961216000	1.392686000
8	0.257754000	-0.710849000	2.175820000
7	-0.946862000	-0.956041000	-0.051794000
6	-0.968655000	0.395202000	-0.291329000
6	-0.143236000	1.433910000	0.474010000
6	1.352705000	1.415622000	0.250004000
6	1.989244000	1.206056000	-0.945240000
6	3.402325000	1.344516000	-0.833773000
6	3.794101000	1.683515000	0.429826000
16	2.461202000	1.824420000	1.507741000
6	5.375583000	-2.630149000	-1.631303000
6	-1.864703000	-1.806107000	-0.851054000
6	-3.308784000	-1.651443000	-0.429183000
6	-4.259705000	-1.185506000	-1.337057000
6	-5.595452000	-1.065876000	-0.959182000
6	-5.986680000	-1.403981000	0.334140000

6	-5.038942000	-1.866731000	1.246502000
6	-3.706130000	-1.993779000	0.866013000
1	2.736038000	-1.232723000	1.976561000
1	4.920058000	-1.650978000	0.873612000
1	2.888532000	-3.121773000	-2.610792000
1	0.708704000	-2.718991000	-1.529186000
1	1.466484000	0.946073000	-1.861067000
1	4.094962000	1.191705000	-1.652234000
1	4.798883000	1.840855000	0.800052000
1	6.192085000	-2.687388000	-0.908472000
1	5.364090000	-3.550976000	-2.219720000
1	5.591795000	-1.804049000	-2.317681000
1	-1.539055000	-2.838241000	-0.718572000
1	-1.735709000	-1.528776000	-1.899969000
1	-3.947988000	-0.907050000	-2.340179000
1	-6.327764000	-0.701294000	-1.672890000
1	-7.026439000	-1.308127000	0.631286000
1	-5.339367000	-2.135892000	2.254400000
1	-2.969202000	-2.367074000	1.572942000
1	-0.386873000	1.441304000	1.547450000
6	-0.273054000	4.052780000	0.338109000
6	-0.651323000	2.674064000	-0.137103000
6	-1.512901000	2.323339000	-1.230150000
8	-0.640449000	4.281223000	1.467085000
1	-0.634493000	2.548003000	-1.935474000
7	-1.723392000	0.894668000	-1.205463000
6	0.456618000	4.958153000	-0.589276000
1	0.615800000	5.924306000	-0.110383000
1	-0.117777000	5.074876000	-1.515685000
1	1.416381000	4.496033000	-0.851046000
6	-2.673982000	3.196442000	-1.670529000
1	-2.992944000	2.893292000	-2.667192000
1	-2.381483000	4.248185000	-1.681905000
1	-3.497529000	3.053443000	-0.968499000

Zero-point correction= 0.453097 (Hartree/Particle)

Thermal correction to Energy= 0.482414

Thermal correction to Enthalpy= 0.483358

Thermal correction to Gibbs Free Energy= 0.392318

Sum of electronic and zero-point Energies= -2097.944889
Sum of electronic and thermal Energies= -2097.915572
Sum of electronic and thermal Enthalpies= -2097.914628
Sum of electronic and thermal Free Energies= -2098.005668

A-TSb5''

6	-2.298825000	-1.529058000	-0.388391000
6	-3.196955000	-0.465759000	-0.371467000
6	-4.358068000	-0.584194000	0.383842000
6	-4.628760000	-1.747126000	1.111143000
6	-3.710745000	-2.804482000	1.062292000
6	-2.545329000	-2.709472000	0.314396000
16	-0.817377000	-1.374883000	-1.341601000
8	-0.425689000	-2.692372000	-1.809438000
8	-0.966953000	-0.264885000	-2.268280000
7	0.402158000	-0.921043000	-0.243218000
6	0.758812000	0.378452000	0.017655000
6	0.403352000	1.582308000	-0.839416000
6	-0.942754000	2.169189000	-0.431832000
6	-1.520285000	2.148979000	0.821145000
6	-2.766466000	2.827292000	0.853571000
6	-3.101653000	3.359873000	-0.360331000
16	-1.910211000	3.056632000	-1.563370000
6	-5.899097000	-1.884963000	1.902846000
6	0.937695000	-1.962819000	0.664305000
6	2.413793000	-2.186837000	0.427928000
6	3.335880000	-1.995536000	1.455545000
6	4.693093000	-2.221178000	1.231882000
6	5.133648000	-2.631597000	-0.023964000
6	4.214133000	-2.819487000	-1.055720000
6	2.858821000	-2.600005000	-0.830085000
1	-3.002330000	0.427959000	-0.955921000
1	-5.068054000	0.237726000	0.400702000
1	-3.919120000	-3.717900000	1.611888000
1	-1.854320000	-3.544365000	0.259480000
1	-1.076319000	1.643919000	1.673009000
1	-3.391630000	2.903469000	1.734126000
1	-3.997888000	3.907386000	-0.623792000

1	-5.703256000	-2.319363000	2.886728000
1	-6.389672000	-0.918822000	2.036677000
1	-6.597530000	-2.551112000	1.385441000
1	0.386283000	-2.881978000	0.461909000
1	0.742755000	-1.656911000	1.694628000
1	2.988221000	-1.659421000	2.428779000
1	5.406483000	-2.070616000	2.036213000
1	6.190798000	-2.804528000	-0.200398000
1	4.553681000	-3.141691000	-2.035211000
1	2.135988000	-2.746076000	-1.629367000
1	0.523073000	1.492424000	-1.916854000
6	3.282831000	2.182064000	0.084564000
6	1.101017000	2.653705000	-0.119350000
6	1.754788000	2.077294000	1.006387000
8	3.518157000	1.263723000	-0.621170000
1	1.149203000	3.691005000	-0.437594000
7	1.442753000	0.682109000	1.068225000
6	4.118400000	3.371960000	0.411441000
1	4.495710000	3.275491000	1.433381000
1	3.521245000	4.284657000	0.349085000
1	4.953740000	3.403514000	-0.288738000
6	1.931530000	2.769913000	2.335599000
1	2.728039000	2.293956000	2.910041000
1	0.992481000	2.660584000	2.885644000
1	2.142186000	3.832417000	2.211835000

Zero-point correction= 0.454803 (Hartree/Particle)

Thermal correction to Energy= 0.483904

Thermal correction to Enthalpy= 0.484848

Thermal correction to Gibbs Free Energy= 0.394277

Sum of electronic and zero-point Energies= -2097.955809

Sum of electronic and thermal Energies= -2097.926708

Sum of electronic and thermal Enthalpies= -2097.925764

Sum of electronic and thermal Free Energies= -2098.016335

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6	2.361471000	0.269509000	1.442041000
6	3.276637000	-0.776772000	1.417431000
6	4.583738000	-0.506875000	1.012736000

6	4.970649000	0.784621000	0.641499000
6	4.018936000	1.816294000	0.681799000
6	2.714582000	1.571899000	1.082509000
16	0.722688000	-0.039951000	2.031374000
8	0.442522000	0.808493000	3.173622000
8	0.516702000	-1.480467000	2.118609000
7	-0.288508000	0.518243000	0.779377000
6	-0.583084000	-0.279135000	-0.318524000
6	0.069911000	-1.628457000	-0.397522000
6	-0.686871000	-2.778980000	-0.476932000
6	-2.090961000	-2.910767000	-0.475018000
6	-2.504204000	-4.237614000	-0.512844000
6	-1.430889000	-5.118419000	-0.547300000
16	0.078342000	-4.353427000	-0.525292000
6	6.367894000	1.068333000	0.168094000
6	-0.948344000	1.821673000	0.941444000
6	-2.446604000	1.702661000	1.124311000
6	-3.249771000	2.781183000	0.748621000
6	-4.630214000	2.724595000	0.918211000
6	-5.221369000	1.581018000	1.453045000
6	-4.423627000	0.500435000	1.824638000
6	-3.039909000	0.561684000	1.664895000
1	2.978140000	-1.777952000	1.712133000
1	5.311997000	-1.311973000	0.989992000
1	4.310009000	2.821262000	0.390546000
1	1.985533000	2.377047000	1.106659000
1	-2.754502000	-2.054437000	-0.437542000
1	-3.535412000	-4.564743000	-0.511215000
1	-1.484345000	-6.200930000	-0.578808000
1	7.037485000	0.234286000	0.385542000
1	6.763586000	1.971261000	0.640372000
1	6.369278000	1.235957000	-0.914267000
1	-0.506726000	2.296160000	1.819150000
1	-0.713162000	2.440024000	0.074502000
1	-2.788740000	3.663340000	0.310623000
1	-5.244928000	3.569224000	0.622876000
1	-6.298384000	1.531607000	1.578443000
1	-4.877007000	-0.392524000	2.243840000

1	-2.426135000	-0.288484000	1.954244000
1	1.142213000	-1.686553000	-0.251344000
6	0.189149000	2.268747000	-2.337647000
6	-1.263982000	2.131746000	-2.357558000
6	-1.955401000	1.085809000	-1.822968000
8	0.903703000	1.639711000	-1.551181000
1	-1.824979000	2.843101000	-2.954581000
7	-1.373492000	-0.024219000	-1.274646000
6	0.790152000	3.219724000	-3.338929000
1	1.862530000	3.320079000	-3.167980000
1	0.613207000	2.842517000	-4.351555000
1	0.306372000	4.198457000	-3.268277000
6	-3.435940000	0.931373000	-2.033449000
1	-3.924093000	0.638460000	-1.098981000
1	-3.877285000	1.859968000	-2.397162000
1	-3.612653000	0.136993000	-2.766177000
8	0.862833000	-1.326769000	-2.528214000
1	1.717196000	-0.842312000	-2.419500000
1	1.094048000	-2.176601000	-2.929169000
8	3.089033000	0.103450000	-2.019160000
1	2.558990000	0.883562000	-1.768655000
1	3.525269000	-0.191988000	-1.209068000

Zero-point correction= 0.504887 (Hartree/Particle)

Thermal correction to Energy= 0.539813

Thermal correction to Enthalpy= 0.540757

Thermal correction to Gibbs Free Energy= 0.437403

Sum of electronic and zero-point Energies= -2250.716811

Sum of electronic and thermal Energies= -2250.681886

Sum of electronic and thermal Enthalpies= -2250.680942

Sum of electronic and thermal Free Energies= -2250.784295

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6	-1.616801000	-2.365156000	-0.056847000
6	-2.189972000	-2.166037000	1.200872000
6	-3.572512000	-2.157890000	1.302099000
6	-4.381857000	-2.344431000	0.171552000
6	-3.773533000	-2.561737000	-1.067610000
6	-2.388088000	-2.578184000	-1.194599000
16	0.139345000	-2.303472000	-0.187325000

8	0.565397000	-2.952508000	-1.413827000
8	0.712517000	-2.678397000	1.092442000
7	0.425465000	-0.602230000	-0.415128000
6	1.305409000	0.128680000	0.337914000
6	1.331723000	1.653987000	0.151009000
6	0.318637000	2.286385000	1.066786000
6	-0.237188000	1.791511000	2.214988000
6	-1.164658000	2.697481000	2.810159000
6	-1.285272000	3.859603000	2.105501000
16	-0.276632000	3.870579000	0.711694000
6	-5.878531000	-2.312123000	0.305596000
6	-0.114217000	-0.060578000	-1.690114000
6	-1.196170000	0.989066000	-1.550824000
6	-2.136583000	0.953532000	-0.520260000
6	-3.151848000	1.903288000	-0.460407000
6	-3.242059000	2.894861000	-1.435714000
6	-2.303340000	2.939021000	-2.463182000
6	-1.280435000	1.993810000	-2.516649000
1	-1.563639000	-2.016895000	2.075141000
1	-4.037525000	-2.005157000	2.271820000
1	-4.390285000	-2.724651000	-1.946065000
1	-1.920132000	-2.762338000	-2.156762000
1	-0.006702000	0.810296000	2.616444000
1	-1.714128000	2.491403000	3.720606000
1	-1.904225000	4.718077000	2.330922000
1	-6.208271000	-1.334414000	0.670589000
1	-6.217837000	-3.060423000	1.028018000
1	-6.367559000	-2.505536000	-0.650944000
1	0.725589000	0.313957000	-2.282287000
1	-0.501976000	-0.915915000	-2.248181000
1	-2.065843000	0.195777000	0.252711000
1	-3.872215000	1.865556000	0.351356000
1	-4.035708000	3.634176000	-1.389825000
1	-2.361766000	3.712932000	-3.222331000
1	-0.545221000	2.032866000	-3.317321000
1	1.097151000	1.897854000	-0.887462000
6	4.168346000	-1.198422000	-0.595133000
6	3.892014000	-1.755236000	0.633676000

6	2.888166000	-1.300723000	1.528364000
8	3.307190000	-0.387320000	-1.168019000
1	4.596120000	-2.477164000	1.028460000
7	2.064526000	-0.319038000	1.259990000
6	5.438159000	-1.467879000	-1.328864000
1	5.209165000	-1.909811000	-2.303667000
1	5.954110000	-0.518073000	-1.510425000
1	6.093023000	-2.131794000	-0.766364000
6	2.884084000	-1.845556000	2.922261000
1	2.920768000	-2.936456000	2.876692000
1	3.780111000	-1.502695000	3.449927000
1	1.995976000	-1.523239000	3.464354000
8	2.638045000	2.145128000	0.354752000
1	3.740399000	0.338941000	-1.726813000
1	2.895971000	1.966109000	1.274016000
8	4.250583000	1.792374000	-1.944472000
1	3.980604000	2.298316000	-2.723700000
1	3.820002000	2.205609000	-1.173311000

Zero-point correction= 0.507628 (Hartree/Particle)

Thermal correction to Energy= 0.541567

Thermal correction to Enthalpy= 0.542511

Thermal correction to Gibbs Free Energy= 0.441040

Sum of electronic and zero-point Energies= -2250.761325

Sum of electronic and thermal Energies= -2250.727385

Sum of electronic and thermal Enthalpies= -2250.726441

Sum of electronic and thermal Free Energies= -2250.827913

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6	-2.349376000	1.274519000	-0.857590000
6	-3.453638000	0.436569000	-0.761454000
6	-4.366176000	0.645711000	0.267195000
6	-4.185362000	1.680671000	1.189613000
6	-3.071137000	2.520142000	1.054023000
6	-2.153279000	2.333937000	0.028632000
16	-1.223846000	1.050762000	-2.204676000
8	-0.738007000	2.363251000	-2.614145000
8	-1.819428000	0.176291000	-3.202256000
7	0.165702000	0.322758000	-1.503074000
6	0.042495000	-0.862736000	-0.774685000

6	1.264815000	-1.131520000	0.118352000
6	1.220836000	-0.185560000	1.288890000
6	0.121238000	0.420055000	1.836023000
6	0.447958000	1.233623000	2.960633000
6	1.783448000	1.214697000	3.245125000
16	2.661000000	0.217185000	2.154343000
6	-5.180224000	1.921273000	2.291393000
6	1.455430000	0.677231000	-2.149579000
6	2.392196000	1.494914000	-1.289385000
6	1.920686000	2.545261000	-0.500543000
6	2.806394000	3.314030000	0.247428000
6	4.175042000	3.046026000	0.205595000
6	4.651134000	2.000574000	-0.580172000
6	3.760668000	1.224441000	-1.320928000
1	-3.587695000	-0.362391000	-1.481859000
1	-5.232075000	-0.004649000	0.352432000
1	-2.930063000	3.337229000	1.755953000
1	-1.309885000	3.006686000	-0.084940000
1	-0.883527000	0.300887000	1.441498000
1	-0.276805000	1.808541000	3.524388000
1	2.305451000	1.734309000	4.037701000
1	-4.674882000	2.073764000	3.249036000
1	-5.875082000	1.084931000	2.390250000
1	-5.763525000	2.824412000	2.083802000
1	1.938613000	-0.244976000	-2.483394000
1	1.211625000	1.242930000	-3.051109000
1	0.855641000	2.752400000	-0.473588000
1	2.429798000	4.125817000	0.862377000
1	4.865148000	3.648685000	0.787877000
1	5.714201000	1.782949000	-0.614539000
1	4.131635000	0.404534000	-1.932145000
1	2.170195000	-0.955540000	-0.468993000
6	0.732500000	-3.849927000	-0.623124000
6	-0.665387000	-3.820480000	-0.218198000
6	-1.419545000	-2.696763000	-0.224496000
8	1.039684000	-3.291992000	-1.774946000
1	-1.048171000	-4.724239000	0.242227000
7	-1.059864000	-1.498216000	-0.817261000

6	1.599062000	-4.953743000	-0.123030000
1	1.329038000	-5.855372000	-0.684566000
1	2.654349000	-4.727236000	-0.287552000
1	1.416367000	-5.133650000	0.936945000
6	-2.804007000	-2.699482000	0.350310000
1	-3.533088000	-2.501982000	-0.441295000
1	-3.035387000	-3.656783000	0.819245000
1	-2.901114000	-1.896861000	1.089217000
8	1.361370000	-2.473365000	0.589815000
1	1.972124000	-3.462834000	-2.005964000
1	0.818572000	-2.580509000	1.440001000
8	0.036536000	-2.748570000	2.769019000
1	-0.873042000	-3.070794000	2.683099000
1	-0.019595000	-1.914902000	3.261520000

Zero-point correction= 0.508763 (Hartree/Particle)

Thermal correction to Energy= 0.541936

Thermal correction to Enthalpy= 0.542881

Thermal correction to Gibbs Free Energy= 0.444441

Sum of electronic and zero-point Energies= -2250.737551

Sum of electronic and thermal Energies= -2250.704377

Sum of electronic and thermal Enthalpies= -2250.703433

Sum of electronic and thermal Free Energies= -2250.801873

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6	4.662788000	0.533335000	-0.313421000
6	5.260842000	-0.510485000	0.392846000
6	6.558655000	-0.869627000	0.060137000
6	7.256263000	-0.202734000	-0.956899000
6	6.624189000	0.839905000	-1.642597000
6	5.324034000	1.219005000	-1.329586000
16	3.008741000	0.979557000	0.082626000
8	2.653086000	2.201703000	-0.618759000
8	2.748817000	0.816922000	1.498287000
7	2.086336000	-0.292785000	-0.681666000
6	1.331570000	-1.043315000	0.063445000
6	0.493974000	-1.694292000	0.736084000
6	0.257644000	-2.907149000	1.461075000
6	-0.893130000	-3.281892000	2.112909000
6	-0.786959000	-4.555608000	2.733337000

6	0.440295000	-5.127526000	2.546147000
16	1.485305000	-4.132309000	1.614559000
6	8.672793000	-0.584431000	-1.282899000
6	1.958953000	-0.293219000	-2.172669000
6	0.569109000	0.119892000	-2.578942000
6	0.225874000	1.472806000	-2.654360000
6	-1.084330000	1.846877000	-2.943092000
6	-2.058226000	0.871192000	-3.157302000
6	-1.720340000	-0.479106000	-3.089919000
6	-0.407942000	-0.853534000	-2.803353000
1	4.725467000	-1.024828000	1.185420000
1	7.043256000	-1.679698000	0.596725000
1	7.156173000	1.362110000	-2.432049000
1	4.833684000	2.031717000	-1.855069000
1	-1.774498000	-2.649647000	2.138890000
1	-1.583769000	-5.027334000	3.294738000
1	0.791178000	-6.084713000	2.909403000
1	8.851250000	-1.644220000	-1.087775000
1	9.368639000	-0.010591000	-0.661153000
1	8.908740000	-0.371720000	-2.327853000
1	2.717259000	0.394837000	-2.554194000
1	2.199159000	-1.303565000	-2.508364000
1	0.986187000	2.228965000	-2.478308000
1	-1.344797000	2.899415000	-3.002453000
1	-3.079878000	1.164077000	-3.380307000
1	-2.478810000	-1.239766000	-3.253317000
1	-0.139584000	-1.905831000	-2.747841000
7	-3.911080000	0.835652000	-0.192256000
6	-4.700151000	1.974146000	-0.139501000
6	-3.960400000	2.931044000	0.465343000
7	-2.734922000	2.355997000	0.760609000
6	-4.336326000	-0.400739000	-0.775482000
6	-5.025355000	-0.372853000	-1.986343000
6	-5.420353000	-1.572527000	-2.571634000
6	-5.121114000	-2.787052000	-1.956808000
6	-4.447199000	-2.800149000	-0.737231000
6	-4.063739000	-1.606245000	-0.132548000
6	-1.670573000	3.048752000	1.426021000

6	-1.951579000	3.711127000	2.617889000
6	-0.927765000	4.392269000	3.270971000
6	0.359734000	4.400242000	2.738450000
6	0.626294000	3.733189000	1.544028000
6	-0.391312000	3.058302000	0.874561000
1	-5.711182000	1.986852000	-0.514539000
1	-4.180049000	3.960065000	0.703122000
1	-5.954402000	-1.554811000	-3.515929000
1	-4.231538000	-3.741041000	-0.241099000
1	-1.137771000	4.908221000	4.202067000
1	1.624810000	3.737061000	1.119750000
6	-2.696001000	1.065763000	0.360425000
79	-1.118032000	-0.208725000	0.503552000
1	-5.423263000	-3.720006000	-2.421289000
1	1.156232000	4.927158000	3.253593000
1	-5.233644000	0.574864000	-2.473500000
1	-3.571828000	-1.607679000	0.834883000
1	-0.201117000	2.551936000	-0.067897000
1	-2.954988000	3.678219000	3.031286000

Zero-point correction= 0.564049 (Hartree/Particle)

Thermal correction to Energy= 0.601997

Thermal correction to Enthalpy= 0.602941

Thermal correction to Gibbs Free Energy= 0.488575

Sum of electronic and zero-point Energies= -2596.101173

Sum of electronic and thermal Energies= -2596.063225

Sum of electronic and thermal Enthalpies= -2596.062281

Sum of electronic and thermal Free Energies= -2596.176647

B-TS2

6	3.906034000	-1.752759000	0.267630000
6	4.665771000	-1.278018000	-0.799341000
6	6.029901000	-1.100719000	-0.611683000
6	6.633802000	-1.387952000	0.618789000
6	5.842293000	-1.877780000	1.664148000
6	4.475209000	-2.067372000	1.499932000
16	2.164568000	-1.916658000	0.056687000
8	1.677580000	-2.996156000	0.902777000
8	1.832153000	-1.849322000	-1.353223000
7	1.493702000	-0.488331000	0.748135000

6	1.165208000	0.507509000	-0.044123000
6	0.256256000	1.229233000	-0.612713000
6	0.277790000	2.565714000	-1.175273000
6	-0.434621000	3.009939000	-2.262793000
6	-0.234848000	4.391767000	-2.537856000
6	0.592334000	4.989718000	-1.630138000
16	1.171788000	3.876210000	-0.454489000
6	8.111486000	-1.179803000	0.801176000
6	1.309198000	-0.390447000	2.227125000
6	-0.151685000	-0.462849000	2.586900000
6	-0.802300000	-1.699072000	2.626410000
6	-2.170761000	-1.764142000	2.875509000
6	-2.896256000	-0.592901000	3.095205000
6	-2.250667000	0.641874000	3.069743000
6	-0.880716000	0.705971000	2.815444000
1	4.195100000	-1.058332000	-1.752192000
1	6.637795000	-0.728704000	-1.431657000
1	6.304175000	-2.114209000	2.618202000
1	3.869010000	-2.464143000	2.308203000
1	-1.074251000	2.353018000	-2.842512000
1	-0.698615000	4.919078000	-3.362555000
1	0.892542000	6.028405000	-1.582699000
1	8.384220000	-1.171492000	1.858598000
1	8.430962000	-0.237149000	0.348336000
1	8.673603000	-1.983348000	0.313624000
1	1.869578000	-1.212202000	2.677140000
1	1.759041000	0.553494000	2.541919000
1	-0.232840000	-2.607452000	2.445943000
1	-2.671100000	-2.727987000	2.899599000
1	-3.964066000	-0.644352000	3.288085000
1	-2.812778000	1.556066000	3.237503000
1	-0.374650000	1.668099000	2.784123000
7	-4.530349000	-0.258597000	0.113714000
6	-5.522246000	-1.221281000	0.219805000
6	-4.983880000	-2.378954000	-0.224025000
7	-3.673644000	-2.096838000	-0.581802000
6	-4.710210000	1.111392000	0.486707000
6	-5.376924000	1.406717000	1.673627000

6	-5.547453000	2.737554000	2.045948000
6	-5.046298000	3.761045000	1.244406000
6	-4.392078000	3.453005000	0.052969000
6	-4.233052000	2.127025000	-0.339568000
6	-2.786471000	-3.077000000	-1.136710000
6	-3.258407000	-3.889947000	-2.165328000
6	-2.420874000	-4.864765000	-2.700010000
6	-1.123522000	-5.017805000	-2.215377000
6	-0.662935000	-4.196214000	-1.188787000
6	-1.493539000	-3.223449000	-0.638975000
1	-6.513834000	-0.986380000	0.573569000
1	-5.399782000	-3.370083000	-0.313785000
1	-6.065509000	2.970406000	2.970503000
1	-4.014005000	4.245253000	-0.585207000
1	-2.783125000	-5.498850000	-3.502531000
1	0.342754000	-4.310201000	-0.798798000
6	-3.383111000	-0.791359000	-0.373230000
79	-1.581971000	0.162077000	-0.540713000
1	-5.173005000	4.796559000	1.542840000
1	-0.472060000	-5.776935000	-2.635931000
1	-5.746508000	0.604506000	2.304635000
1	-3.752279000	1.878652000	-1.280360000
1	-1.149377000	-2.592702000	0.175300000
1	-4.264753000	-3.750961000	-2.548491000
6	3.787333000	1.868015000	-1.304470000
6	5.075698000	2.227863000	-0.824285000
6	5.047863000	1.914547000	0.500053000
8	3.838867000	1.412019000	0.814333000
1	5.898395000	2.639879000	-1.388123000
7	3.066602000	1.393526000	-0.317552000
6	6.038685000	2.004469000	1.600152000
1	6.994443000	2.350951000	1.206360000
1	5.695381000	2.704956000	2.366724000
1	6.173084000	1.024589000	2.067883000
6	3.228593000	1.964535000	-2.682774000
1	2.364489000	1.305757000	-2.790142000
1	2.915046000	2.992692000	-2.892883000
1	3.990311000	1.685771000	-3.413965000

Zero-point correction= 0.680044 (Hartree/Particle)
 Thermal correction to Energy= 0.725826
 Thermal correction to Enthalpy= 0.726771
 Thermal correction to Gibbs Free Energy= 0.596099
 Sum of electronic and zero-point Energies= -2920.541233
 Sum of electronic and thermal Energies= -2920.495451
 Sum of electronic and thermal Enthalpies= -2920.494506
 Sum of electronic and thermal Free Energies= -2920.625178

B-2

6	3.974450000	-1.661176000	0.328183000
6	4.814355000	-1.179760000	-0.670996000
6	6.159439000	-0.972177000	-0.377211000
6	6.669365000	-1.246781000	0.894538000
6	5.804465000	-1.756759000	1.872784000
6	4.460156000	-1.970888000	1.599691000
16	2.237111000	-1.814649000	-0.005683000
8	1.743276000	-2.972561000	0.731229000
8	2.045155000	-1.696653000	-1.445045000
7	1.497809000	-0.480650000	0.665642000
6	1.417024000	0.704194000	-0.098038000
6	0.277052000	1.244721000	-0.576707000
6	0.226040000	2.601905000	-1.122509000
6	-0.590663000	3.041795000	-2.137427000
6	-0.433028000	4.424423000	-2.441924000
6	0.474193000	5.039117000	-1.629170000
16	1.171770000	3.937778000	-0.502549000
6	8.122903000	-1.020609000	1.208135000
6	1.298819000	-0.421012000	2.136080000
6	-0.155417000	-0.531674000	2.524598000
6	-0.782662000	-1.780139000	2.524323000
6	-2.139252000	-1.887356000	2.820025000
6	-2.876917000	-0.744819000	3.130637000
6	-2.253284000	0.501422000	3.151457000
6	-0.895514000	0.606029000	2.850614000
1	4.420217000	-0.979498000	-1.662970000
1	6.823106000	-0.590269000	-1.148071000
1	6.194101000	-1.990915000	2.859557000
1	3.803835000	-2.387790000	2.356606000
1	-1.278743000	2.375921000	-2.647699000

1	-0.982949000	4.941772000	-3.218807000
1	0.759419000	6.082845000	-1.610881000
1	8.580302000	-0.338220000	0.488265000
1	8.673737000	-1.966469000	1.171972000
1	8.248136000	-0.607254000	2.212375000
1	1.864067000	-1.240711000	2.585277000
1	1.726091000	0.518507000	2.496665000
1	-0.201388000	-2.664630000	2.274820000
1	-2.620761000	-2.861212000	2.808687000
1	-3.935765000	-0.827483000	3.359552000
1	-2.824560000	1.392775000	3.393808000
1	-0.408722000	1.578532000	2.856235000
7	-4.439069000	-0.330689000	0.157824000
6	-5.413895000	-1.310029000	0.269154000
6	-4.862052000	-2.454556000	-0.190902000
7	-3.560914000	-2.147288000	-0.562595000
6	-4.642571000	1.034531000	0.535674000
6	-5.310585000	1.315828000	1.725301000
6	-5.506007000	2.642452000	2.100708000
6	-5.027541000	3.677322000	1.299968000
6	-4.370859000	3.383747000	0.106300000
6	-4.187617000	2.061911000	-0.289024000
6	-2.674232000	-3.104021000	-1.156910000
6	-3.174498000	-3.935050000	-2.158016000
6	-2.338526000	-4.885988000	-2.736059000
6	-1.012561000	-4.997280000	-2.323468000
6	-0.522766000	-4.157701000	-1.325260000
6	-1.352175000	-3.210263000	-0.730610000
1	-6.404919000	-1.095899000	0.637429000
1	-5.264041000	-3.451241000	-0.281647000
1	-6.024450000	2.863613000	3.027982000
1	-4.008402000	4.184016000	-0.531108000
1	-2.725630000	-5.533762000	-3.515790000
1	0.505717000	-4.236000000	-0.989568000
6	-3.285510000	-0.838605000	-0.344959000
79	-1.489443000	0.175348000	-0.502054000
1	-5.173453000	4.709614000	1.600991000
1	-0.361898000	-5.737514000	-2.777844000

1	-5.660301000	0.505429000	2.357209000
1	-3.701890000	1.826012000	-1.230213000
1	-0.979646000	-2.567605000	0.060923000
1	-4.203059000	-3.827406000	-2.488834000
6	3.323229000	1.641944000	-1.481082000
6	4.584829000	2.156069000	-1.125330000
6	4.665268000	2.041946000	0.234246000
8	3.520190000	1.528217000	0.717397000
1	5.344814000	2.519641000	-1.799161000
7	2.707023000	1.290995000	-0.358119000
6	5.726562000	2.322053000	1.224811000
1	6.635902000	2.621336000	0.703900000
1	5.412665000	3.123641000	1.899338000
1	5.921506000	1.423378000	1.817543000
6	2.709700000	1.453169000	-2.816795000
1	2.053044000	0.579391000	-2.814338000
1	2.115899000	2.336535000	-3.077579000
1	3.500698000	1.332160000	-3.557525000

Zero-point correction= 0.683343 (Hartree/Particle)

Thermal correction to Energy= 0.728570

Thermal correction to Enthalpy= 0.729514

Thermal correction to Gibbs Free Energy= 0.601153

Sum of electronic and zero-point Energies= -2920.570918

Sum of electronic and thermal Energies= -2920.525691

Sum of electronic and thermal Enthalpies= -2920.524747

Sum of electronic and thermal Free Energies= -2920.653108

B-TS3

6	3.971522000	-1.683379000	0.534351000
6	4.845623000	-1.237277000	-0.452318000
6	6.166647000	-0.969350000	-0.108529000
6	6.619170000	-1.145999000	1.202664000
6	5.722841000	-1.622694000	2.167843000
6	4.401167000	-1.899759000	1.843521000
16	2.261184000	-1.930518000	0.129232000
8	1.762616000	-3.025391000	0.955250000
8	2.138623000	-1.979376000	-1.322099000
7	1.406599000	-0.578894000	0.620089000
6	1.457253000	0.580481000	-0.206146000

6	0.262105000	1.264820000	-0.539871000
6	0.274316000	2.642926000	-0.871503000
6	-0.790143000	3.336062000	-1.453264000
6	-0.549563000	4.706368000	-1.631786000
6	0.692700000	5.074448000	-1.162251000
16	1.585793000	3.770183000	-0.531250000
6	8.046779000	-0.851720000	1.574096000
6	1.207645000	-0.366868000	2.078418000
6	-0.244349000	-0.466396000	2.478558000
6	-0.864101000	-1.717939000	2.523646000
6	-2.218455000	-1.822514000	2.828973000
6	-2.959651000	-0.674411000	3.110017000
6	-2.342583000	0.575014000	3.089222000
6	-0.987499000	0.677663000	2.773283000
1	4.496281000	-1.105156000	-1.471466000
1	6.856301000	-0.613448000	-0.869338000
1	6.069219000	-1.783302000	3.185047000
1	3.720665000	-2.294548000	2.590938000
1	-1.706243000	2.825393000	-1.729460000
1	-1.252418000	5.404262000	-2.068521000
1	1.117188000	6.071312000	-1.153030000
1	8.096342000	-0.222596000	2.467564000
1	8.571518000	-0.344980000	0.761378000
1	8.584871000	-1.778218000	1.799663000
1	1.786389000	-1.123262000	2.613308000
1	1.622274000	0.611398000	2.338318000
1	-0.278129000	-2.606491000	2.300572000
1	-2.695221000	-2.798372000	2.852198000
1	-4.015930000	-0.756623000	3.349950000
1	-2.916046000	1.470252000	3.311215000
1	-0.505081000	1.652172000	2.743467000
7	-4.461126000	-0.330827000	0.091677000
6	-5.417596000	-1.326061000	0.210306000
6	-4.838135000	-2.468109000	-0.221805000
7	-3.539435000	-2.142885000	-0.584463000
6	-4.703465000	1.037160000	0.433291000
6	-5.379260000	1.330533000	1.615478000
6	-5.622061000	2.660332000	1.949383000

6	-5.184805000	3.685856000	1.113710000
6	-4.520079000	3.379294000	-0.072261000
6	-4.287682000	2.052918000	-0.425366000
6	-2.631379000	-3.097452000	-1.151022000
6	-3.107676000	-3.946647000	-2.148626000
6	-2.255086000	-4.901397000	-2.695047000
6	-0.937083000	-4.998714000	-2.254101000
6	-0.471286000	-4.140369000	-1.260537000
6	-1.317104000	-3.187037000	-0.698803000
1	-6.416709000	-1.123610000	0.562870000
1	-5.219782000	-3.473923000	-0.298691000
1	-6.147461000	2.891852000	2.870115000
1	-4.194349000	4.173810000	-0.736375000
1	-2.623080000	-5.563757000	-3.471703000
1	0.551573000	-4.206384000	-0.906076000
6	-3.292774000	-0.825181000	-0.389137000
79	-1.504177000	0.212137000	-0.525490000
1	-5.370641000	4.721025000	1.380735000
1	-0.273492000	-5.742760000	-2.682647000
1	-5.700779000	0.527720000	2.271502000
1	-3.797557000	1.800904000	-1.360536000
1	-0.964600000	-2.529239000	0.089450000
1	-4.130582000	-3.851292000	-2.499921000
6	3.231450000	1.307581000	-1.792588000
6	4.419521000	1.994194000	-1.647991000
6	4.721320000	2.136260000	-0.278943000
8	3.830252000	1.734590000	0.527739000
1	5.061674000	2.280324000	-2.466847000
7	2.641467000	0.938618000	-0.654646000
6	6.016460000	2.655349000	0.262742000
1	5.826197000	3.530294000	0.889967000
1	6.470537000	1.882264000	0.890114000
1	6.696595000	2.923480000	-0.545874000
6	2.606204000	0.861533000	-3.077011000
1	2.370419000	-0.204645000	-3.017100000
1	1.672027000	1.409815000	-3.238127000
1	3.286468000	1.055047000	-3.905928000

Zero-point correction= 0.680121 (Hartree/Particle)

Thermal correction to Energy= 0.725352
 Thermal correction to Enthalpy= 0.726297
 Thermal correction to Gibbs Free Energy= 0.598766
 Sum of electronic and zero-point Energies= -2920.543120
 Sum of electronic and thermal Energies= -2920.497888
 Sum of electronic and thermal Enthalpies= -2920.496944
 Sum of electronic and thermal Free Energies= -2920.624474

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6	-4.532513000	-0.022189000	1.172555000
6	-4.824391000	-1.074680000	0.305307000
6	-6.072433000	-1.678630000	0.383829000
6	-7.029318000	-1.242699000	1.309339000
6	-6.703175000	-0.191120000	2.170461000
6	-5.456833000	0.423187000	2.113786000
16	-2.987941000	0.845677000	1.074797000
8	-2.579703000	1.172204000	2.434502000
8	-3.048154000	1.905898000	0.084892000
7	-1.913068000	-0.312826000	0.498949000
6	-1.426901000	-0.366337000	-0.823605000
6	-0.130794000	-1.092056000	-0.992465000
6	-0.117471000	-2.304077000	-1.655512000
6	1.026267000	-3.073410000	-1.954443000
6	0.735286000	-4.279048000	-2.584615000
6	-0.630041000	-4.442161000	-2.780182000
16	-1.564307000	-3.151666000	-2.207802000
6	-8.381277000	-1.898194000	1.361325000
6	-1.701416000	-1.490611000	1.385245000
6	-0.322571000	-1.598772000	1.994786000
6	0.174341000	-0.590022000	2.825027000
6	1.448312000	-0.703191000	3.376072000
6	2.233412000	-1.825020000	3.104467000
6	1.735478000	-2.839962000	2.290242000
6	0.457238000	-2.728199000	1.744433000
1	-4.088717000	-1.426256000	-0.413969000
1	-6.309656000	-2.505521000	-0.279589000
1	-7.431486000	0.148820000	2.900612000
1	-5.205209000	1.229973000	2.794763000
1	2.019028000	-2.725031000	-1.684514000

1	1.467646000	-5.011107000	-2.898866000
1	-1.114280000	-5.285866000	-3.259196000
1	-8.938081000	-1.590322000	2.248501000
1	-8.286678000	-2.987529000	1.369157000
1	-8.970869000	-1.628129000	0.479069000
1	-2.450535000	-1.423630000	2.179577000
1	-1.935989000	-2.393320000	0.812461000
1	-0.441102000	0.281770000	3.033379000
1	1.828328000	0.083707000	4.020939000
1	3.227744000	-1.911075000	3.532061000
1	2.340598000	-3.716192000	2.077378000
1	0.068913000	-3.512044000	1.097358000
7	4.375741000	0.685801000	0.479964000
6	5.169737000	1.731137000	0.922415000
6	4.370274000	2.821688000	0.980934000
7	3.109126000	2.409213000	0.582610000
6	4.833481000	-0.661551000	0.321950000
6	5.477845000	-1.279234000	1.390250000
6	5.908503000	-2.596577000	1.253138000
6	5.689002000	-3.285299000	0.061958000
6	5.048585000	-2.651900000	-1.002399000
6	4.621695000	-1.331840000	-0.880844000
6	1.958953000	3.264361000	0.548187000
6	2.044376000	4.484881000	-0.113995000
6	0.927263000	5.315886000	-0.143820000
6	-0.258131000	4.922212000	0.474555000
6	-0.325874000	3.699444000	1.139876000
6	0.787273000	2.865782000	1.186005000
1	6.218403000	1.600833000	1.139179000
1	4.571233000	3.839619000	1.276294000
1	6.408687000	-3.085373000	2.082661000
1	4.891612000	-3.179549000	-1.937878000
1	0.983127000	6.268276000	-0.661482000
1	-1.242255000	3.389921000	1.631920000
6	3.102923000	1.094215000	0.267644000
79	1.496870000	-0.039489000	-0.365829000
1	6.023869000	-4.312473000	-0.039716000
1	-1.127625000	5.571198000	0.444029000

1	5.623403000	-0.736393000	2.319312000
1	4.137559000	-0.820224000	-1.707010000
1	0.755626000	1.917988000	1.715367000
1	2.967372000	4.769494000	-0.610326000
6	-2.662541000	1.062843000	-2.464515000
6	-2.266972000	2.301150000	-2.844368000
6	-0.927154000	2.848154000	-2.618017000
8	-0.037696000	2.240836000	-2.033357000
1	-2.991949000	2.925913000	-3.355049000
7	-1.797756000	0.159315000	-1.903526000
6	-0.680548000	4.229485000	-3.185993000
1	0.347027000	4.535112000	-2.985911000
1	-0.867514000	4.232893000	-4.264917000
1	-1.372913000	4.948589000	-2.735374000
6	-4.041056000	0.541529000	-2.758637000
1	-3.990115000	-0.469645000	-3.172819000
1	-4.622318000	0.498895000	-1.831667000
1	-4.556491000	1.195075000	-3.463736000

Zero-point correction= 0.679974 (Hartree/Particle)

Thermal correction to Energy= 0.726524

Thermal correction to Enthalpy= 0.727469

Thermal correction to Gibbs Free Energy= 0.596284

Sum of electronic and zero-point Energies= -2920.558236

Sum of electronic and thermal Energies= -2920.511686

Sum of electronic and thermal Enthalpies= -2920.510742

Sum of electronic and thermal Free Energies= -2920.641926

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6	-0.300390000	-2.791149000	1.547762000
6	0.870732000	-3.025378000	0.834689000
6	2.083967000	-2.661940000	1.411783000
6	2.128191000	-2.037554000	2.662020000
6	0.929099000	-1.819102000	3.355039000
6	-0.289630000	-2.201383000	2.811569000
16	-1.857662000	-3.192982000	0.811829000
8	-2.663925000	-3.974968000	1.738593000
8	-1.615562000	-3.711890000	-0.523219000
7	-2.653640000	-1.666550000	0.704842000
6	-1.827333000	-0.521198000	0.545126000
6	-0.987080000	-0.367430000	-0.689042000

6	-1.354612000	-1.069206000	-1.861339000
6	-2.599088000	-1.531246000	-2.289501000
6	-2.564323000	-2.130167000	-3.556593000
6	-1.294909000	-2.131389000	-4.097731000
16	-0.151704000	-1.374827000	-3.093914000
6	3.438343000	-1.574924000	3.236832000
6	-3.813269000	-1.479948000	1.619508000
6	-4.752395000	-0.451995000	1.035293000
6	-5.533444000	-0.781047000	-0.076666000
6	-6.386069000	0.160644000	-0.645423000
6	-6.474899000	1.440451000	-0.097946000
6	-5.711908000	1.770549000	1.020547000
6	-4.849360000	0.828854000	1.580962000
1	0.831057000	-3.486672000	-0.147280000
1	3.008552000	-2.861938000	0.878681000
1	0.955914000	-1.348171000	4.333704000
1	-1.216596000	-2.034232000	3.353668000
1	-3.493700000	-1.411674000	-1.691040000
1	-3.423830000	-2.556471000	-4.058271000
1	-0.989542000	-2.555707000	-5.046642000
1	3.388021000	-1.496136000	4.325306000
1	3.693496000	-0.584097000	2.840840000
1	4.250085000	-2.255639000	2.968386000
1	-4.310858000	-2.445669000	1.691725000
1	-3.473689000	-1.178838000	2.615206000
1	-5.472535000	-1.785070000	-0.491563000
1	-6.987143000	-0.105447000	-1.509235000
1	-7.144671000	2.174052000	-0.535906000
1	-5.787902000	2.761565000	1.458043000
1	-4.248952000	1.084246000	2.449662000
7	4.032173000	0.650334000	-0.255313000
6	5.024227000	1.585549000	0.001644000
6	4.402407000	2.775786000	0.156034000
7	3.048642000	2.535176000	-0.013966000
6	4.308140000	-0.729892000	-0.510921000
6	3.629389000	-1.397994000	-1.528329000
6	3.915731000	-2.738620000	-1.770400000
6	4.888930000	-3.397281000	-1.020184000

6	5.574668000	-2.712111000	-0.018176000
6	5.282357000	-1.376117000	0.246930000
6	2.058482000	3.571778000	0.005058000
6	1.308535000	3.821677000	-1.142342000
6	0.396537000	4.873741000	-1.136134000
6	0.245858000	5.665767000	0.002046000
6	0.997094000	5.397620000	1.145604000
6	1.909257000	4.344077000	1.152689000
1	6.069583000	1.320462000	0.015695000
1	4.788298000	3.766959000	0.336262000
1	3.386779000	-3.261828000	-2.560534000
1	6.334102000	-3.218736000	0.568381000
1	-0.184810000	5.084136000	-2.028371000
1	0.877534000	6.008355000	2.034620000
6	2.805614000	1.226716000	-0.254874000
79	0.916407000	0.394370000	-0.464340000
1	5.116134000	-4.439322000	-1.219591000
1	-0.457500000	6.492696000	-0.002326000
1	2.897156000	-0.866601000	-2.127115000
1	5.795840000	-0.845153000	1.042791000
1	2.504373000	4.120392000	2.033225000
1	1.458091000	3.210842000	-2.027623000
6	-1.219934000	1.546356000	1.584048000
6	-1.435876000	2.561643000	0.705972000
6	-2.136217000	2.401924000	-0.553057000
8	-2.138723000	1.334428000	-1.186406000
1	-1.153848000	3.567035000	1.000091000
7	-1.814030000	0.307286000	1.515443000
6	-2.913962000	3.568009000	-1.095984000
1	-2.933899000	3.539118000	-2.186415000
1	-3.942774000	3.479837000	-0.727069000
1	-2.505547000	4.515999000	-0.740580000
6	-0.439520000	1.754287000	2.846851000
1	-1.015961000	1.419873000	3.714030000
1	0.472514000	1.145480000	2.800541000
1	-0.156405000	2.801575000	2.965935000

Zero-point correction= 0.680593 (Hartree/Particle)

Thermal correction to Energy= 0.725533

Thermal correction to Enthalpy= 0.726477

Thermal correction to Gibbs Free Energy= 0.601193
Sum of electronic and zero-point Energies= -2920.567143
Sum of electronic and thermal Energies= -2920.522203
Sum of electronic and thermal Enthalpies= -2920.521259
Sum of electronic and thermal Free Energies= -2920.646543

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6	4.474635000	0.078925000	-0.570847000
6	5.112770000	0.987218000	0.270820000
6	6.285346000	0.596796000	0.905656000
6	6.828247000	-0.676075000	0.700717000
6	6.174045000	-1.558169000	-0.168250000
6	5.000561000	-1.190061000	-0.812521000
16	3.004596000	0.582611000	-1.418395000
8	2.842607000	-0.245144000	-2.601691000
8	2.988540000	2.032528000	-1.509111000
7	1.635052000	0.236887000	-0.428183000
6	1.189559000	-1.054014000	-0.378279000
6	-0.313396000	-1.407894000	-0.402067000
6	-0.617559000	-2.548751000	0.514321000
6	0.053417000	-2.977891000	1.629648000
6	-0.617391000	-4.040028000	2.313823000
6	-1.773711000	-4.411000000	1.699697000
16	-2.087822000	-3.450770000	0.298175000
6	8.111439000	-1.077810000	1.373224000
6	1.111824000	1.331089000	0.418767000
6	2.114518000	1.777298000	1.456641000
6	2.532083000	3.107301000	1.493950000
6	3.456385000	3.526085000	2.449783000
6	3.970598000	2.613055000	3.368705000
6	3.553270000	1.281988000	3.335497000
6	2.627394000	0.866609000	2.383707000
1	4.698909000	1.977735000	0.431234000
1	6.786259000	1.293333000	1.571933000
1	6.594513000	-2.544358000	-0.343116000
1	4.499295000	-1.866259000	-1.495919000
1	0.999011000	-2.558867000	1.955671000
1	-0.237618000	-4.511589000	3.212290000
1	-2.461452000	-5.198848000	1.977152000

1	8.967932000	-0.828010000	0.737738000
1	8.140323000	-2.154197000	1.558107000
1	8.240766000	-0.554197000	2.323090000
1	0.806016000	2.165189000	-0.215542000
1	0.228202000	0.927918000	0.919115000
1	2.142033000	3.806156000	0.758609000
1	3.780005000	4.562088000	2.471267000
1	4.694650000	2.937892000	4.109518000
1	3.954128000	0.568187000	4.048417000
1	2.313442000	-0.174588000	2.343670000
7	-4.473005000	1.535626000	0.427446000
6	-5.059128000	2.792759000	0.411749000
6	-4.125998000	3.647997000	-0.064624000
7	-2.999869000	2.887956000	-0.336432000
6	-5.159339000	0.347471000	0.838671000
6	-4.565633000	-0.529692000	1.743163000
6	-5.255202000	-1.680129000	2.118676000
6	-6.526552000	-1.937528000	1.609743000
6	-7.113276000	-1.043616000	0.715903000
6	-6.429189000	0.102449000	0.321778000
6	-1.781135000	3.417848000	-0.871793000
6	-1.166565000	4.485622000	-0.225225000
6	0.020942000	4.998422000	-0.745203000
6	0.590696000	4.434090000	-1.884966000
6	-0.038224000	3.365538000	-2.523883000
6	-1.235413000	2.858701000	-2.026791000
1	-6.069880000	2.956307000	0.751314000
1	-4.156963000	4.710087000	-0.250208000
1	-4.796842000	-2.371445000	2.818640000
1	-8.101868000	-1.240298000	0.314355000
1	0.506239000	5.831843000	-0.247601000
1	0.400484000	2.927897000	-3.414491000
6	-3.201883000	1.584633000	-0.032685000
79	-1.790849000	0.097535000	-0.201114000
1	-7.061217000	-2.832807000	1.909819000
1	1.524942000	4.823672000	-2.275407000
1	-3.582492000	-0.309762000	2.147620000
1	-6.865340000	0.795844000	-0.390583000

1	-1.748273000	2.042493000	-2.525605000
1	-1.608333000	4.900560000	0.675627000
6	1.895692000	-3.280716000	-0.813791000
6	1.016939000	-3.698072000	-1.825032000
6	0.011874000	-2.916636000	-2.356321000
8	-0.462291000	-1.808867000	-1.818045000
1	1.182583000	-4.670138000	-2.275823000
7	2.060016000	-2.007253000	-0.462804000
6	-0.691452000	-3.266614000	-3.621718000
1	-1.736360000	-3.506816000	-3.398726000
1	-0.687618000	-2.398132000	-4.287190000
1	-0.215020000	-4.111721000	-4.116776000
6	2.852186000	-4.256674000	-0.207458000
1	3.631236000	-4.500763000	-0.939556000
1	3.327146000	-3.829441000	0.676517000
1	2.333392000	-5.183451000	0.047872000

Zero-point correction= 0.682031 (Hartree/Particle)

Thermal correction to Energy= 0.727608

Thermal correction to Enthalpy= 0.728552

Thermal correction to Gibbs Free Energy= 0.598228

Sum of electronic and zero-point Energies= -2920.582497

Sum of electronic and thermal Energies= -2920.536921

Sum of electronic and thermal Enthalpies= -2920.535977

Sum of electronic and thermal Free Energies= -2920.666301

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6	3.852563000	-1.099880000	-1.520017000
6	3.373646000	-0.663957000	-2.752418000
6	4.054603000	0.358973000	-3.405259000
6	5.206613000	0.925993000	-2.851671000
6	5.687803000	0.426482000	-1.632982000
6	5.018429000	-0.586026000	-0.960394000
16	2.946859000	-2.364296000	-0.684016000
8	3.767006000	-2.980846000	0.357971000
8	2.369202000	-3.236660000	-1.694171000
7	1.556794000	-1.578300000	-0.009885000
6	1.696258000	-0.713840000	1.078010000
6	0.629607000	0.403443000	1.264527000
6	1.148925000	1.677844000	0.649999000

6	2.040330000	1.876294000	-0.370730000
6	2.160288000	3.249301000	-0.755698000
6	1.371936000	4.074533000	-0.014093000
16	0.449336000	3.194489000	1.149296000
6	5.929498000	2.047675000	-3.544831000
6	0.302798000	-2.317392000	-0.250857000
6	-0.397620000	-1.956531000	-1.538245000
6	-1.432646000	-2.783645000	-1.976417000
6	-2.167121000	-2.453631000	-3.112669000
6	-1.864315000	-1.296842000	-3.830484000
6	-0.827430000	-0.471136000	-3.400583000
6	-0.103488000	-0.793231000	-2.252251000
1	2.487359000	-1.110216000	-3.191630000
1	3.686976000	0.717531000	-4.361851000
1	6.597211000	0.840986000	-1.206442000
1	5.379306000	-0.972346000	-0.015045000
1	2.608563000	1.075232000	-0.830086000
1	2.825190000	3.596347000	-1.538537000
1	1.286357000	5.152032000	-0.063952000
1	5.459009000	2.293637000	-4.498842000
1	6.973624000	1.780241000	-3.732557000
1	5.932085000	2.946884000	-2.920562000
1	0.514415000	-3.389356000	-0.231732000
1	-0.345021000	-2.120861000	0.605634000
1	-1.672974000	-3.684097000	-1.414464000
1	-2.972977000	-3.104020000	-3.440022000
1	-2.430122000	-1.043803000	-4.721586000
1	-0.584187000	0.431425000	-3.953771000
1	0.684090000	-0.130431000	-1.900507000
7	-4.035324000	1.380681000	-0.447442000
6	-5.365198000	1.085919000	-0.701795000
6	-5.521360000	-0.231958000	-0.443343000
7	-4.284123000	-0.704543000	-0.029347000
6	-3.450337000	2.672202000	-0.653894000
6	-2.343311000	2.797593000	-1.490531000
6	-1.789946000	4.058424000	-1.694370000
6	-2.345205000	5.177385000	-1.075609000
6	-3.458044000	5.037582000	-0.248831000

6	-4.017869000	3.780496000	-0.032402000
6	-4.025283000	-2.078878000	0.274936000
6	-4.560106000	-3.059254000	-0.558434000
6	-4.304601000	-4.400133000	-0.285665000
6	-3.506963000	-4.756228000	0.800744000
6	-2.982261000	-3.766435000	1.629982000
6	-3.250236000	-2.422157000	1.380840000
1	-6.059474000	1.832919000	-1.053363000
1	-6.388856000	-0.870546000	-0.497084000
1	-0.924193000	4.163158000	-2.340396000
1	-3.892564000	5.906484000	0.234412000
1	-4.717580000	-5.164706000	-0.935542000
1	-2.375300000	-4.038039000	2.487769000
6	-3.360164000	0.287237000	-0.025448000
79	-1.383519000	0.247228000	0.547794000
1	-1.910929000	6.158722000	-1.238345000
1	-3.301176000	-5.801875000	1.005071000
1	-1.929548000	1.916569000	-1.972484000
1	-4.878138000	3.653856000	0.617953000
1	-2.872907000	-1.646457000	2.039756000
1	-5.149722000	-2.773188000	-1.423991000
6	3.447837000	0.351385000	2.260656000
6	2.718517000	0.970805000	3.328954000
6	1.373538000	1.042581000	3.527884000
8	0.417526000	0.614618000	2.697075000
1	3.320686000	1.434000000	4.100931000
7	3.012452000	-0.436366000	1.313825000
6	0.779466000	1.625513000	4.766285000
1	0.214044000	2.526725000	4.506829000
1	0.072817000	0.912009000	5.201620000
1	1.547053000	1.872819000	5.498490000
6	4.931970000	0.599756000	2.244956000
1	5.186197000	1.150705000	1.332855000
1	5.260639000	1.177689000	3.108195000
1	5.469110000	-0.352229000	2.221958000
8	1.196665000	-1.859704000	2.439965000
1	0.700807000	-1.393319000	3.132812000
1	2.079881000	-2.213945000	2.823194000

8	3.499524000	-2.659391000	3.123840000
1	3.568507000	-3.559979000	3.474065000
1	3.855905000	-2.696662000	2.216437000

Zero-point correction= 0.734088 (Hartree/Particle)

Thermal correction to Energy= 0.782785

Thermal correction to Enthalpy= 0.783729

Thermal correction to Gibbs Free Energy= 0.650062

Sum of electronic and zero-point Energies= -3073.330501

Sum of electronic and thermal Energies= -3073.281805

Sum of electronic and thermal Enthalpies= -3073.280861

Sum of electronic and thermal Free Energies= -3073.414528

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6	3.847889000	-1.123458000	-1.430638000
6	3.426558000	-0.729840000	-2.698344000
6	4.173356000	0.225796000	-3.378929000
6	5.334688000	0.766371000	-2.818017000
6	5.749528000	0.315672000	-1.557345000
6	5.013273000	-0.628385000	-0.855257000
16	2.864153000	-2.332279000	-0.600246000
8	3.721620000	-2.994557000	0.425668000
8	2.334241000	-3.229752000	-1.615031000
7	1.502145000	-1.584359000	0.057650000
6	1.595599000	-0.776150000	1.293563000
6	0.614373000	0.450926000	1.303517000
6	1.185571000	1.662612000	0.626907000
6	2.070344000	1.774462000	-0.411251000
6	2.241723000	3.119846000	-0.867847000
6	1.494890000	4.014166000	-0.164035000
16	0.554307000	3.231910000	1.053931000
6	6.130415000	1.813943000	-3.545951000
6	0.264708000	-2.356884000	-0.181030000
6	-0.428646000	-2.019709000	-1.480241000
6	-1.473637000	-2.842446000	-1.902833000
6	-2.195695000	-2.534723000	-3.053545000
6	-1.871193000	-1.403734000	-3.801978000
6	-0.824355000	-0.582251000	-3.387869000
6	-0.112206000	-0.882497000	-2.226580000
1	2.535257000	-1.159887000	-3.143947000

1	3.853799000	0.547850000	-4.365399000
1	6.663749000	0.710455000	-1.122841000
1	5.326848000	-0.979889000	0.119301000
1	2.594369000	0.927949000	-0.835923000
1	2.907984000	3.399208000	-1.676293000
1	1.450753000	5.089687000	-0.272966000
1	5.827101000	1.887024000	-4.592266000
1	7.199819000	1.589385000	-3.507064000
1	5.986112000	2.794938000	-3.080795000
1	0.464741000	-3.430871000	-0.137712000
1	-0.396870000	-2.139336000	0.660508000
1	-1.732608000	-3.722830000	-1.317465000
1	-3.009543000	-3.181912000	-3.367390000
1	-2.427287000	-1.167523000	-4.703806000
1	-0.563645000	0.300589000	-3.964502000
1	0.683363000	-0.222490000	-1.888751000
7	-3.997730000	1.428777000	-0.515865000
6	-5.330329000	1.158507000	-0.781957000
6	-5.520169000	-0.148904000	-0.495013000
7	-4.299374000	-0.639195000	-0.053329000
6	-3.382969000	2.702345000	-0.746263000
6	-2.268211000	2.784336000	-1.578050000
6	-1.685368000	4.027367000	-1.806652000
6	-2.220005000	5.171974000	-1.217311000
6	-3.341001000	5.075508000	-0.395191000
6	-3.930301000	3.836457000	-0.154087000
6	-4.077251000	-2.012130000	0.283249000
6	-4.623665000	-2.997386000	-0.536754000
6	-4.406690000	-4.337734000	-0.230645000
6	-3.636265000	-4.689385000	0.876710000
6	-3.099605000	-3.694691000	1.692195000
6	-3.328206000	-2.350008000	1.408412000
1	-6.003266000	1.912710000	-1.158680000
1	-6.401419000	-0.768745000	-0.545084000
1	-0.812316000	4.097452000	-2.447388000
1	-3.758851000	5.964936000	0.064892000
1	-4.828908000	-5.106138000	-0.870024000
1	-2.514489000	-3.962357000	2.566246000

6	-3.352446000	0.331117000	-0.058287000
79	-1.381939000	0.278423000	0.556765000
1	-1.763010000	6.139660000	-1.398617000
1	-3.461125000	-5.735119000	1.107529000
1	-1.871733000	1.883434000	-2.036869000
1	-4.797890000	3.743480000	0.492244000
1	-2.940742000	-1.568948000	2.054812000
1	-5.193204000	-2.716215000	-1.417221000
6	3.421791000	0.324616000	2.348189000
6	2.681120000	1.059850000	3.359157000
6	1.346847000	1.213762000	3.528733000
8	0.369827000	0.763242000	2.714295000
1	3.291696000	1.544250000	4.112189000
7	2.984336000	-0.474656000	1.434723000
6	0.758842000	1.923348000	4.704756000
1	0.240663000	2.826271000	4.364990000
1	0.014611000	1.280818000	5.185553000
1	1.524890000	2.195106000	5.430386000
6	4.918882000	0.521335000	2.386052000
1	5.205319000	1.225404000	1.596509000
1	5.249446000	0.931274000	3.341258000
1	5.432738000	-0.424823000	2.205992000
8	1.185366000	-1.646314000	2.371766000
1	0.576952000	-1.170223000	2.964803000
1	2.336645000	-2.443321000	2.830190000
8	3.226266000	-2.979525000	2.827109000
1	3.087575000	-3.885854000	3.158807000
1	3.502974000	-2.997625000	1.801484000

Zero-point correction= 0.733943 (Hartree/Particle)

Thermal correction to Energy= 0.782137

Thermal correction to Enthalpy= 0.783081

Thermal correction to Gibbs Free Energy= 0.650745

Sum of electronic and zero-point Energies= -3073.339456

Sum of electronic and thermal Energies= -3073.291263

Sum of electronic and thermal Enthalpies= -3073.290319

Sum of electronic and thermal Free Energies= -3073.422655

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6	4.407074000	0.164509000	-0.391872000
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6	5.245930000	1.251643000	-0.184098000
6	6.385958000	1.070160000	0.593646000
6	6.684987000	-0.174111000	1.156552000
6	5.823273000	-1.251823000	0.912252000
6	4.682030000	-1.093780000	0.137762000
16	2.946596000	0.368468000	-1.378130000
8	3.054159000	-0.565721000	-2.505372000
8	2.780568000	1.786546000	-1.680685000
7	1.694432000	-0.122253000	-0.349302000
6	0.846205000	-1.205659000	-0.905721000
6	-0.453360000	-1.480395000	-0.093584000
6	-0.224071000	-2.117535000	1.236330000
6	0.943607000	-2.354983000	1.912711000
6	0.739521000	-2.897482000	3.218879000
6	-0.578361000	-3.078363000	3.511915000
16	-1.594167000	-2.561573000	2.218391000
6	7.890163000	-0.343185000	2.040744000
6	1.169472000	0.959091000	0.513031000
6	2.234173000	1.595173000	1.381596000
6	2.574393000	2.935531000	1.207484000
6	3.537132000	3.532469000	2.020820000
6	4.173322000	2.786069000	3.009088000
6	3.836329000	1.443158000	3.189793000
6	2.867039000	0.854547000	2.384777000
1	4.998551000	2.220972000	-0.604132000
1	7.048693000	1.911647000	0.775840000
1	6.051074000	-2.224114000	1.340445000
1	3.995121000	-1.916700000	-0.045943000
1	1.917686000	-2.155899000	1.481900000
1	1.544351000	-3.153672000	3.897720000
1	-1.014527000	-3.496467000	4.409413000
1	8.704985000	0.315174000	1.730047000
1	8.248924000	-1.375007000	2.028874000
1	7.638310000	-0.091076000	3.076937000
1	0.657467000	1.731734000	-0.075352000
1	0.441232000	0.483827000	1.172306000
1	2.090707000	3.502414000	0.416216000
1	3.793918000	4.577529000	1.876157000

1	4.929055000	3.246091000	3.638626000
1	4.328550000	0.858092000	3.961104000
1	2.600344000	-0.189904000	2.525860000
7	-4.556520000	1.633821000	0.266687000
6	-5.160996000	2.853168000	0.001080000
6	-4.217246000	3.633467000	-0.574693000
7	-3.067696000	2.864199000	-0.653749000
6	-5.217950000	0.535050000	0.902792000
6	-4.628500000	-0.074230000	2.007753000
6	-5.279557000	-1.142670000	2.618005000
6	-6.510852000	-1.583093000	2.136157000
6	-7.095062000	-0.954715000	1.038084000
6	-6.449173000	0.108817000	0.412424000
6	-1.813553000	3.325575000	-1.170398000
6	-1.225196000	4.448051000	-0.598670000
6	0.014554000	4.876567000	-1.070750000
6	0.657632000	4.176028000	-2.088433000
6	0.051566000	3.056686000	-2.659142000
6	-1.195336000	2.631982000	-2.210755000
1	-6.189898000	3.048915000	0.259800000
1	-4.252451000	4.647792000	-0.939975000
1	-4.826388000	-1.621803000	3.479745000
1	-8.053235000	-1.295635000	0.660175000
1	0.483481000	5.748492000	-0.626245000
1	0.553392000	2.512742000	-3.452151000
6	-3.264989000	1.630230000	-0.135110000
79	-1.867324000	0.117971000	-0.058474000
1	-7.016716000	-2.412640000	2.619128000
1	1.634263000	4.496173000	-2.435928000
1	-3.679570000	0.293424000	2.385201000
1	-6.886311000	0.597809000	-0.452838000
1	-1.691739000	1.775230000	-2.657441000
1	-1.725603000	4.965213000	0.214250000
6	1.449387000	-3.429258000	-1.568481000
6	0.238073000	-3.651757000	-2.384636000
6	-1.015706000	-3.260985000	-1.886070000
8	-1.280190000	-2.452399000	-0.913434000
1	0.191434000	-4.600827000	-2.918233000

7	1.728763000	-2.359506000	-0.936644000
6	-2.265351000	-3.831101000	-2.475524000
1	-2.994774000	-3.033408000	-2.632789000
1	-2.059953000	-4.350997000	-3.410479000
1	-2.693084000	-4.538685000	-1.757283000
6	2.444713000	-4.553020000	-1.564624000
1	3.334392000	-4.277531000	-0.997725000
1	1.993238000	-5.452199000	-1.133595000
1	2.729297000	-4.796429000	-2.594479000
8	0.406167000	-0.849579000	-2.203519000
1	-0.253730000	-0.141317000	-2.102011000
1	1.736998000	-1.416568000	-3.636106000
8	1.343688000	-2.122166000	-4.203486000
1	0.667056000	-2.807636000	-3.432102000
1	2.069566000	-2.640980000	-4.593326000

Zero-point correction= 0.729254 (Hartree/Particle)

Thermal correction to Energy= 0.778144

Thermal correction to Enthalpy= 0.779089

Thermal correction to Gibbs Free Energy= 0.644025

Sum of electronic and zero-point Energies= -3073.308463

Sum of electronic and thermal Energies= -3073.259573

Sum of electronic and thermal Enthalpies= -3073.258629

Sum of electronic and thermal Free Energies= -3073.393692

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6	3.805860000	0.655911000	-1.584022000
6	4.770521000	0.829258000	-0.591974000
6	5.924228000	0.060725000	-0.644561000
6	6.121659000	-0.875377000	-1.668957000
6	5.142284000	-1.011155000	-2.657651000
6	3.976803000	-0.250023000	-2.623496000
16	2.292647000	1.561767000	-1.433269000
8	1.652750000	1.574447000	-2.753472000
8	2.584465000	2.853603000	-0.824364000
7	1.302953000	0.751186000	-0.331902000
6	1.206516000	-0.724224000	-0.477525000
6	-0.080071000	-1.283913000	0.259489000
6	0.073601000	-1.733221000	1.689754000
6	0.733444000	-2.825400000	2.197826000

6	0.641715000	-2.945075000	3.615038000
6	-0.101121000	-1.947355000	4.174234000
16	-0.728246000	-0.883704000	2.981214000
6	7.363950000	-1.723554000	-1.685771000
6	1.172342000	1.406161000	0.991652000
6	2.377728000	1.441953000	1.911657000
6	3.035919000	2.657136000	2.124610000
6	4.136743000	2.734925000	2.975732000
6	4.589903000	1.593419000	3.633239000
6	3.923723000	0.382634000	3.449647000
6	2.821077000	0.308329000	2.601953000
1	4.616108000	1.549355000	0.206496000
1	6.683568000	0.182384000	0.123151000
1	5.292934000	-1.725342000	-3.462232000
1	3.205324000	-0.365056000	-3.376598000
1	1.270050000	-3.549463000	1.595087000
1	1.114326000	-3.735662000	4.185410000
1	-0.322826000	-1.778951000	5.219859000
1	7.385414000	-2.379988000	-2.558251000
1	7.417063000	-2.345183000	-0.785895000
1	8.262925000	-1.099969000	-1.701222000
1	0.834189000	2.426317000	0.799839000
1	0.342000000	0.897731000	1.479401000
1	2.686997000	3.542912000	1.601824000
1	4.638551000	3.686310000	3.123891000
1	5.449857000	1.648090000	4.293868000
1	4.258494000	-0.507759000	3.973691000
1	2.313829000	-0.641117000	2.464535000
7	-4.802430000	0.665197000	-0.206750000
6	-5.660623000	1.753712000	-0.243816000
6	-4.880375000	2.858553000	-0.262234000
7	-3.568409000	2.412435000	-0.246496000
6	-5.247706000	-0.695722000	-0.170414000
6	-4.769593000	-1.554988000	0.816503000
6	-5.211382000	-2.874902000	0.835944000
6	-6.132668000	-3.321306000	-0.109851000
6	-6.614934000	-2.446043000	-1.081240000
6	-6.171131000	-1.126705000	-1.118772000

6	-2.426220000	3.276735000	-0.278656000
6	-2.300838000	4.271772000	0.685522000
6	-1.190413000	5.113155000	0.647042000
6	-0.222746000	4.952940000	-0.342840000
6	-0.366749000	3.954333000	-1.306305000
6	-1.471633000	3.108422000	-1.279619000
1	-6.732636000	1.634761000	-0.239229000
1	-5.125843000	3.908466000	-0.297328000
1	-4.843287000	-3.550144000	1.601514000
1	-7.332940000	-2.791037000	-1.817884000
1	-1.080622000	5.888308000	1.398266000
1	0.385485000	3.828836000	-2.077313000
6	-3.507849000	1.062201000	-0.211303000
79	-1.807290000	-0.090875000	-0.055275000
1	-6.478693000	-4.349503000	-0.086644000
1	0.644765000	5.604592000	-0.366030000
1	-4.070257000	-1.186170000	1.559965000
1	-6.526502000	-0.437475000	-1.878838000
1	-1.604090000	2.327465000	-2.022653000
1	-3.056280000	4.375978000	1.458402000
6	2.673300000	-2.545249000	-0.255158000
6	1.818977000	-3.483179000	-1.083246000
6	0.334156000	-3.377864000	-1.106154000
8	-0.407814000	-2.578641000	-0.478706000
1	2.005328000	-4.518506000	-0.763585000
7	2.417072000	-1.336917000	0.027797000
6	-0.398575000	-4.360432000	-1.943776000
1	-0.427774000	-3.935390000	-2.956448000
1	0.130906000	-5.312117000	-1.995061000
1	-1.421826000	-4.486069000	-1.590176000
6	3.938505000	-3.165582000	0.262549000
1	4.554096000	-2.406507000	0.746866000
1	3.699104000	-3.958867000	0.980544000
1	4.498150000	-3.630661000	-0.556487000
8	1.099103000	-1.000044000	-1.838220000
1	0.307755000	-0.545522000	-2.223603000
1	-0.077335000	1.074144000	-3.215460000
8	-0.783425000	0.403785000	-3.179635000

1	2.151299000	-3.458514000	-2.131034000
1	-0.877037000	0.074896000	-4.084700000

Zero-point correction= 0.735574 (Hartree/Particle)

Thermal correction to Energy= 0.783752

Thermal correction to Enthalpy= 0.784696

Thermal correction to Gibbs Free Energy= 0.652825

Sum of electronic and zero-point Energies= -3073.330347

Sum of electronic and thermal Energies= -3073.282170

Sum of electronic and thermal Enthalpies= -3073.281225

Sum of electronic and thermal Free Energies= -3073.413097

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6	3.734390000	0.535954000	-1.697129000
6	4.704740000	0.744520000	-0.717128000
6	5.847257000	-0.041879000	-0.735959000
6	6.029687000	-1.027939000	-1.715674000
6	5.046258000	-1.197494000	-2.694948000
6	3.891414000	-0.419929000	-2.693290000
16	2.221944000	1.448067000	-1.576225000
8	1.518549000	1.334875000	-2.857437000
8	2.521108000	2.788500000	-1.088571000
7	1.281988000	0.723792000	-0.373553000
6	1.229607000	-0.750123000	-0.356785000
6	-0.075929000	-1.285834000	0.388497000
6	0.066172000	-1.659739000	1.837269000
6	0.689091000	-2.742820000	2.404154000
6	0.592122000	-2.781780000	3.826167000
6	-0.116878000	-1.731477000	4.329454000
16	-0.706825000	-0.712519000	3.078585000
6	7.267982000	-1.881920000	-1.702945000
6	1.162145000	1.489270000	0.892775000
6	2.373109000	1.611685000	1.798858000
6	3.066933000	2.824607000	1.857590000
6	4.166952000	2.978309000	2.700083000
6	4.581459000	1.919979000	3.505094000
6	3.877544000	0.716750000	3.477919000
6	2.777022000	0.567270000	2.638747000
1	4.559119000	1.496903000	0.052678000
1	6.608820000	0.102781000	0.025416000

1	5.184362000	-1.950229000	-3.465803000
1	3.116064000	-0.559865000	-3.438066000
1	1.194587000	-3.513938000	1.835553000
1	1.034561000	-3.556303000	4.441256000
1	-0.336932000	-1.502286000	5.363779000
1	7.415296000	-2.337902000	-0.719229000
1	8.155904000	-1.277988000	-1.916053000
1	7.210424000	-2.676647000	-2.449715000
1	0.816048000	2.486584000	0.615718000
1	0.339636000	1.016875000	1.429997000
1	2.747208000	3.646758000	1.224332000
1	4.697428000	3.925244000	2.728381000
1	5.439433000	2.035144000	4.160581000
1	4.180586000	-0.107083000	4.117130000
1	2.236585000	-0.373873000	2.628031000
7	-4.795223000	0.615458000	-0.271676000
6	-5.657405000	1.697278000	-0.362493000
6	-4.882602000	2.805873000	-0.400006000
7	-3.569533000	2.367863000	-0.341716000
6	-5.234246000	-0.746867000	-0.209741000
6	-4.768677000	-1.580270000	0.804682000
6	-5.203886000	-2.901936000	0.846639000
6	-6.105557000	-3.375246000	-0.104996000
6	-6.575192000	-2.525410000	-1.104622000
6	-6.138296000	-1.204719000	-1.164533000
6	-2.430061000	3.236160000	-0.380562000
6	-2.283481000	4.210635000	0.601085000
6	-1.176723000	5.056543000	0.552799000
6	-0.232950000	4.920713000	-0.463372000
6	-0.395654000	3.941576000	-1.443826000
6	-1.498790000	3.095090000	-1.406749000
1	-6.728684000	1.572630000	-0.375963000
1	-5.132624000	3.852824000	-0.472920000
1	-4.846287000	-3.557141000	1.634223000
1	-7.278288000	-2.890960000	-1.845661000
1	-1.051531000	5.817125000	1.316294000
1	0.339816000	3.830225000	-2.232329000
6	-3.503289000	1.019898000	-0.258522000

79	-1.799305000	-0.109382000	0.005328000
1	-6.446393000	-4.404603000	-0.064339000
1	0.631806000	5.575723000	-0.493407000
1	-4.084510000	-1.190822000	1.551972000
1	-6.484239000	-0.535572000	-1.946610000
1	-1.651160000	2.337779000	-2.168717000
1	-3.021783000	4.296254000	1.392546000
6	2.735801000	-2.493160000	0.049517000
6	1.920342000	-3.476418000	-0.758170000
6	0.507234000	-3.139174000	-1.118496000
8	-0.353107000	-2.570731000	-0.358263000
1	1.842126000	-4.424330000	-0.202328000
7	2.435875000	-1.275483000	0.238975000
6	-0.065629000	-3.842831000	-2.293264000
1	0.113719000	-4.918110000	-2.190187000
1	-1.130009000	-3.635366000	-2.393119000
1	0.474901000	-3.510557000	-3.185455000
6	3.987448000	-3.051378000	0.657759000
1	4.541241000	-2.258402000	1.162045000
1	3.736368000	-3.839809000	1.376267000
1	4.615235000	-3.505402000	-0.116857000
8	1.160937000	-1.187538000	-1.693049000
1	0.363888000	-0.795972000	-2.182148000
1	-0.289636000	0.650746000	-3.245600000
8	-0.727307000	-0.212823000	-3.144772000
1	2.458665000	-3.721265000	-1.680532000
1	-1.558553000	-0.049016000	-2.672541000

Zero-point correction= 0.735797 (Hartree/Particle)

Thermal correction to Energy= 0.783566

Thermal correction to Enthalpy= 0.784510

Thermal correction to Gibbs Free Energy= 0.654147

Sum of electronic and zero-point Energies= -3073.327929

Sum of electronic and thermal Energies= -3073.280160

Sum of electronic and thermal Enthalpies= -3073.279216

Sum of electronic and thermal Free Energies= -3073.409579

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6	3.471310000	1.176162000	1.635800000
6	2.838989000	0.964736000	2.859016000

6	3.352792000	-0.007133000	3.709784000
6	4.485907000	-0.746852000	3.355328000
6	5.115915000	-0.479286000	2.132937000
6	4.618571000	0.481924000	1.264365000
16	2.735912000	2.366825000	0.565720000
8	3.757733000	2.788165000	-0.439268000
8	2.159705000	3.435261000	1.362426000
7	1.429054000	1.630520000	-0.190187000
6	1.616875000	0.638282000	-1.238977000
6	0.715309000	-0.629500000	-1.180100000
6	1.389320000	-1.733050000	-0.419144000
6	1.642527000	-1.817054000	0.924586000
6	2.358831000	-2.999006000	1.289456000
6	2.620136000	-3.804871000	0.221346000
16	2.022347000	-3.120936000	-1.248618000
6	5.038011000	-1.800923000	4.274232000
6	0.185751000	2.441541000	-0.201594000
6	-0.537845000	2.506443000	1.122698000
6	-1.265844000	3.652262000	1.442055000
6	-1.997888000	3.718218000	2.626212000
6	-2.004519000	2.639409000	3.507382000
6	-1.270289000	1.495070000	3.199082000
6	-0.539851000	1.431555000	2.014215000
1	1.961486000	1.540475000	3.137269000
1	2.866488000	-0.192738000	4.662794000
1	6.004723000	-1.039439000	1.857423000
1	5.094316000	0.687947000	0.313677000
1	1.336946000	-1.056354000	1.634199000
1	2.647811000	-3.238669000	2.307279000
1	3.116027000	-4.766222000	0.209291000
1	5.925170000	-1.426641000	4.796010000
1	5.340632000	-2.688417000	3.711997000
1	4.303878000	-2.095230000	5.027113000
1	0.396790000	3.454181000	-0.561498000
1	-0.457225000	1.964988000	-0.947367000
1	-1.258427000	4.499994000	0.761394000
1	-2.560345000	4.616735000	2.861753000
1	-2.570148000	2.692003000	4.432443000

1	-1.259067000	0.651838000	3.883564000
1	0.038934000	0.544242000	1.776353000
7	-3.824928000	-1.857597000	0.519394000
6	-5.150528000	-1.660090000	0.873639000
6	-5.406674000	-0.347018000	0.680528000
7	-4.232621000	0.219906000	0.203892000
6	-3.164814000	-3.128394000	0.560401000
6	-1.927782000	-3.251706000	1.190533000
6	-1.281735000	-4.484596000	1.178570000
6	-1.882089000	-5.586136000	0.570307000
6	-3.132054000	-5.455304000	-0.031553000
6	-3.777145000	-4.221447000	-0.046234000
6	-4.106113000	1.607471000	-0.123897000
6	-4.680049000	2.552800000	0.722397000
6	-4.606644000	3.902049000	0.386494000
6	-3.948413000	4.302831000	-0.773369000
6	-3.365558000	3.347916000	-1.605536000
6	-3.453069000	1.993855000	-1.293852000
1	-5.773666000	-2.463088000	1.235180000
1	-6.308467000	0.228467000	0.818676000
1	-0.307792000	-4.581301000	1.648412000
1	-3.602888000	-6.310227000	-0.505510000
1	-5.054323000	4.639820000	1.044579000
1	-2.859062000	3.652580000	-2.516068000
6	-3.249550000	-0.705296000	0.098586000
79	-1.280585000	-0.534234000	-0.529871000
1	-1.375989000	-6.546057000	0.566831000
1	-3.889875000	5.355925000	-1.029303000
1	-1.480734000	-2.390918000	1.678555000
1	-4.737361000	-4.098280000	-0.537763000
1	-3.037707000	1.240659000	-1.955925000
1	-5.166223000	2.236638000	1.640290000
6	3.479524000	-0.112456000	-2.434691000
6	2.664924000	-0.175631000	-3.709908000
6	1.199955000	0.074161000	-3.383185000
8	0.717928000	-0.988861000	-2.598170000
1	2.772276000	-1.166253000	-4.162209000
7	3.009932000	0.282353000	-1.313078000

6	0.297863000	0.336202000	-4.556981000
1	0.298115000	-0.539343000	-5.210372000
1	-0.717698000	0.515508000	-4.195303000
1	0.647513000	1.200763000	-5.126507000
6	4.912671000	-0.525869000	-2.543403000
1	5.423651000	0.106058000	-3.277907000
1	5.418730000	-0.453720000	-1.581125000
1	4.971746000	-1.556186000	-2.908452000
8	1.174101000	1.221875000	-2.494618000
1	2.585374000	3.917744000	-2.942627000
1	2.109214000	2.329024000	-2.758206000
8	2.891228000	3.017622000	-2.724583000
1	3.054753000	0.557242000	-4.427856000
1	3.320485000	2.980102000	-1.746508000

Zero-point correction= 0.734307 (Hartree/Particle)

Thermal correction to Energy= 0.781755

Thermal correction to Enthalpy= 0.782699

Thermal correction to Gibbs Free Energy= 0.652087

Sum of electronic and zero-point Energies= -3073.358186

Sum of electronic and thermal Energies= -3073.310739

Sum of electronic and thermal Enthalpies= -3073.309795

Sum of electronic and thermal Free Energies= -3073.440407

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6	4.051602000	0.375226000	1.411384000
6	3.484994000	-0.170617000	2.557945000
6	4.017563000	-1.350099000	3.070178000
6	5.111532000	-1.970683000	2.459238000
6	5.673044000	-1.379843000	1.320062000
6	5.148519000	-0.208935000	0.787794000
16	3.391836000	1.899137000	0.792144000
8	4.262672000	2.426253000	-0.249063000
8	3.097934000	2.741754000	1.946302000
7	1.845346000	1.504476000	0.168617000
6	1.788296000	1.019899000	-1.193585000
6	0.531046000	0.152699000	-1.596419000
6	0.768747000	-1.314413000	-1.350700000
6	1.368024000	-1.930811000	-0.280825000
6	1.431004000	-3.349192000	-0.422866000

6	0.870984000	-3.788277000	-1.585665000
16	0.272092000	-2.480933000	-2.537020000
6	5.677449000	-3.253261000	3.005333000
6	0.783345000	2.380636000	0.693689000
6	0.295986000	1.994804000	2.070360000
6	-0.052846000	2.990412000	2.983306000
6	-0.645947000	2.659017000	4.200103000
6	-0.880961000	1.323433000	4.522343000
6	-0.503940000	0.321336000	3.629183000
6	0.083569000	0.656211000	2.409752000
1	2.649276000	0.320883000	3.047196000
1	3.584543000	-1.787307000	3.965207000
1	6.532296000	-1.845554000	0.845138000
1	5.572278000	0.249624000	-0.099277000
1	1.802795000	-1.383428000	0.549446000
1	1.886405000	-4.007577000	0.307985000
1	0.783965000	-4.803192000	-1.949994000
1	6.769966000	-3.219335000	3.032236000
1	5.393612000	-4.100177000	2.371605000
1	5.310344000	-3.450064000	4.014901000
1	1.083626000	3.432155000	0.677439000
1	-0.063865000	2.282255000	0.020227000
1	0.144688000	4.031562000	2.739893000
1	-0.916373000	3.444013000	4.899529000
1	-1.341742000	1.063987000	5.470334000
1	-0.664245000	-0.722436000	3.883539000
1	0.387159000	-0.124434000	1.715575000
7	-3.901593000	-1.673739000	0.673911000
6	-5.207553000	-1.450829000	1.083675000
6	-5.402565000	-0.111615000	1.049646000
7	-4.210094000	0.446689000	0.623035000
6	-3.315975000	-2.973165000	0.532594000
6	-2.058897000	-3.227352000	1.075500000
6	-1.510339000	-4.499862000	0.938618000
6	-2.213760000	-5.501311000	0.272165000
6	-3.472061000	-5.232186000	-0.261646000
6	-4.031071000	-3.963091000	-0.136317000
6	-3.988604000	1.841481000	0.385155000

6	-2.947115000	2.484564000	1.051124000
6	-2.679313000	3.819815000	0.753687000
6	-3.458517000	4.499146000	-0.185628000
6	-4.512767000	3.845664000	-0.824082000
6	-4.781439000	2.507271000	-0.544064000
1	-5.856529000	-2.259225000	1.382070000
1	-6.258116000	0.492849000	1.307346000
1	-0.534473000	-4.707574000	1.363885000
1	-4.020784000	-6.008957000	-0.783734000
1	-1.870274000	4.329139000	1.268379000
1	-5.120161000	4.373437000	-1.551683000
6	-3.284972000	-0.509259000	0.380131000
79	-1.460853000	-0.172547000	-0.444890000
1	-1.782121000	-6.491734000	0.171325000
1	-3.248027000	5.539004000	-0.413204000
1	-1.530718000	-2.444272000	1.610871000
1	-5.004372000	-3.737255000	-0.561018000
1	-5.580854000	1.975876000	-1.051512000
1	-2.363559000	1.944050000	1.791386000
6	3.427265000	0.122508000	-2.603038000
6	2.751179000	0.749065000	-3.791646000
6	1.444349000	1.402138000	-3.364789000
8	0.492678000	0.386867000	-3.022923000
1	2.541212000	-0.017317000	-4.544887000
7	2.991976000	0.247262000	-1.413505000
6	0.889749000	2.318366000	-4.427465000
1	0.813293000	1.763599000	-5.365933000
1	-0.102910000	2.688311000	-4.169624000
1	1.571496000	3.158572000	-4.576061000
6	4.672111000	-0.670296000	-2.856396000
1	5.478109000	0.000519000	-3.175045000
1	4.978448000	-1.203207000	-1.955458000
1	4.506778000	-1.386590000	-3.666885000
8	1.660889000	2.096691000	-2.137221000
1	-0.315245000	2.945920000	-2.072286000
1	-1.749199000	2.705911000	-1.422095000
8	-1.072298000	2.325447000	-2.019332000
1	3.423759000	1.485052000	-4.248220000

1	-0.650646000	1.272380000	-1.577785000
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Zero-point correction= 0.732648 (Hartree/Particle)

Thermal correction to Energy= 0.779695

Thermal correction to Enthalpy= 0.780640

Thermal correction to Gibbs Free Energy= 0.652111

Sum of electronic and zero-point Energies= -3073.319640

Sum of electronic and thermal Energies= -3073.272592

Sum of electronic and thermal Enthalpies= -3073.271648

Sum of electronic and thermal Free Energies= -3073.400176

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6	4.044858000	-1.961584000	-0.945061000
6	3.286602000	-2.060015000	-2.108344000
6	3.822030000	-1.574759000	-3.297521000
6	5.099072000	-1.004998000	-3.330809000
6	5.843619000	-0.944448000	-2.145728000
6	5.324732000	-1.418093000	-0.947184000
16	3.312445000	-2.519790000	0.568670000
8	4.336714000	-2.666563000	1.590578000
8	2.466275000	-3.667015000	0.255682000
7	2.206237000	-1.290508000	0.943448000
6	2.638896000	-0.120875000	1.672124000
6	1.867628000	1.180669000	1.285546000
6	2.476700000	1.964941000	0.161959000
6	2.843088000	1.533895000	-1.081275000
6	3.359056000	2.586852000	-1.898292000
6	3.373359000	3.788940000	-1.255308000
16	2.764288000	3.657647000	0.352828000
6	5.674149000	-0.461882000	-4.610845000
6	0.811210000	-1.735158000	1.132592000
6	0.088490000	-1.934426000	-0.181265000
6	-0.459088000	-3.167549000	-0.513708000
6	-1.125324000	-3.356712000	-1.731450000
6	-1.243714000	-2.313295000	-2.637933000
6	-0.682959000	-1.059005000	-2.329926000
6	-0.020938000	-0.869328000	-1.103685000
1	2.295944000	-2.506955000	-2.083011000
1	3.241633000	-1.640334000	-4.213296000
1	6.841294000	-0.514230000	-2.164885000

1	5.887106000	-1.361638000	-0.021848000
1	2.771924000	0.497616000	-1.397215000
1	3.713236000	2.446224000	-2.913209000
1	3.719821000	4.744306000	-1.626085000
1	6.616764000	-0.960092000	-4.856755000
1	5.888241000	0.607313000	-4.514390000
1	4.984619000	-0.600027000	-5.446101000
1	0.771678000	-2.654142000	1.720793000
1	0.316438000	-0.960840000	1.723414000
1	-0.348373000	-3.997578000	0.178093000
1	-1.539574000	-4.331343000	-1.969221000
1	-1.742554000	-2.460931000	-3.589985000
1	-0.694700000	-0.258651000	-3.065053000
1	0.471807000	0.081023000	-0.908028000
7	-4.587130000	1.699691000	0.137217000
6	-5.795616000	1.739701000	0.813665000
6	-6.057181000	0.471460000	1.207445000
7	-4.996849000	-0.307142000	0.770848000
6	-3.949924000	2.835500000	-0.459354000
6	-3.654631000	2.817551000	-1.820937000
6	-3.001879000	3.912622000	-2.383522000
6	-2.660204000	5.008971000	-1.590607000
6	-2.977250000	5.017577000	-0.233307000
6	-3.624913000	3.926103000	0.342131000
6	-4.900742000	-1.721989000	0.981051000
6	-5.968707000	-2.528309000	0.598281000
6	-5.882658000	-3.903259000	0.798921000
6	-4.738266000	-4.458904000	1.367603000
6	-3.678757000	-3.637846000	1.750196000
6	-3.757134000	-2.260020000	1.566477000
1	-6.349966000	2.657007000	0.936366000
1	-6.880673000	0.050322000	1.762709000
1	-2.765305000	3.910628000	-3.442407000
1	-2.712299000	5.869998000	0.383029000
1	-6.709683000	-4.539414000	0.501754000
1	-2.792911000	-4.066934000	2.207145000
6	-4.090034000	0.444288000	0.110266000
79	-2.344620000	-0.146871000	-0.704823000

1	-2.150483000	5.858010000	-2.033698000
1	-4.674147000	-5.531504000	1.518543000
1	-3.936351000	1.958760000	-2.422263000
1	-3.862954000	3.907828000	1.401393000
1	-2.952302000	-1.604155000	1.884238000
1	-6.846000000	-2.081938000	0.140234000
6	4.648695000	0.770462000	2.390248000
6	3.953092000	1.333784000	3.611739000
6	2.452336000	1.073673000	3.525093000
8	1.891464000	1.912764000	2.503642000
1	4.142548000	2.410334000	3.674416000
7	4.054526000	0.092371000	1.488082000
6	1.697664000	1.266012000	4.812102000
1	1.818092000	2.295091000	5.158818000
1	0.637748000	1.062478000	4.645593000
1	2.083499000	0.587643000	5.575927000
6	6.113954000	1.048852000	2.261033000
1	6.652276000	0.612883000	3.109474000
1	6.503807000	0.635707000	1.329952000
1	6.293394000	2.128677000	2.284069000
8	2.273769000	-0.242426000	3.039681000
1	-1.087687000	2.691270000	0.439246000
1	-1.122421000	2.670520000	-1.083746000
8	-0.633640000	2.316993000	-0.327655000
1	4.377738000	0.871445000	4.510626000
1	0.826040000	0.945411000	1.035348000

Zero-point correction= 0.736166 (Hartree/Particle)

Thermal correction to Energy= 0.784807

Thermal correction to Enthalpy= 0.785751

Thermal correction to Gibbs Free Energy= 0.649503

Sum of electronic and zero-point Energies= -3073.386304

Sum of electronic and thermal Energies= -3073.337664

Sum of electronic and thermal Enthalpies= -3073.336719

Sum of electronic and thermal Free Energies= -3073.472968

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6	4.344600000	0.303039000	-0.528307000
6	5.024394000	1.453643000	-0.130139000
6	6.228730000	1.318234000	0.546749000

6	6.763550000	0.054731000	0.824489000
6	6.065485000	-1.079103000	0.396607000
6	4.857332000	-0.969116000	-0.282867000
16	2.816330000	0.520206000	-1.407456000
8	2.759817000	-0.479534000	-2.479678000
8	2.701790000	1.929770000	-1.743643000
7	1.475002000	0.217137000	-0.425439000
6	1.037518000	-1.106275000	-0.222039000
6	-0.475222000	-1.385931000	-0.186064000
6	-0.844586000	-2.199041000	1.017911000
6	-0.319958000	-2.130793000	2.279764000
6	-1.035806000	-2.931189000	3.227369000
6	-2.083508000	-3.596135000	2.670038000
16	-2.228301000	-3.249521000	0.979753000
6	8.057783000	-0.070352000	1.579228000
6	1.069932000	1.309985000	0.489498000
6	2.132972000	1.675882000	1.501758000
6	2.506807000	3.010332000	1.650731000
6	3.475297000	3.372393000	2.586877000
6	4.082804000	2.396881000	3.372557000
6	3.717079000	1.057950000	3.223096000
6	2.745402000	0.699296000	2.295005000
1	4.613225000	2.433213000	-0.346474000
1	6.765574000	2.208602000	0.862210000
1	6.477650000	-2.065200000	0.590974000
1	4.322013000	-1.854611000	-0.604504000
1	0.542649000	-1.522050000	2.530663000
1	-0.765602000	-3.011916000	4.273826000
1	-2.770781000	-4.289086000	3.136710000
1	7.899600000	0.136743000	2.643045000
1	8.794979000	0.648975000	1.212923000
1	8.475238000	-1.075256000	1.489491000
1	0.782429000	2.180880000	-0.105136000
1	0.179882000	0.946035000	1.010481000
1	2.042672000	3.765031000	1.020047000
1	3.760402000	4.414528000	2.693488000
1	4.843235000	2.675359000	4.095734000
1	4.195381000	0.292480000	3.826604000

1	2.488100000	-0.349517000	2.161317000
7	-4.547979000	1.710553000	0.213422000
6	-5.108665000	2.978581000	0.180917000
6	-4.136748000	3.819987000	-0.239337000
7	-3.013235000	3.040295000	-0.462194000
6	-5.271917000	0.534925000	0.595611000
6	-4.752314000	-0.326706000	1.558430000
6	-5.476136000	-1.464911000	1.906276000
6	-6.707952000	-1.726154000	1.309849000
6	-7.220878000	-0.848090000	0.356538000
6	-6.502143000	0.286550000	-0.008314000
6	-1.756531000	3.547233000	-0.924526000
6	-1.151671000	4.594952000	-0.238039000
6	0.076422000	5.078056000	-0.689141000
6	0.690937000	4.505799000	-1.800800000
6	0.069194000	3.458941000	-2.481223000
6	-1.163645000	2.979668000	-2.051657000
1	-6.132656000	3.158095000	0.468971000
1	-4.138776000	4.884185000	-0.414973000
1	-5.071032000	-2.145127000	2.648887000
1	-8.178025000	-1.048207000	-0.113722000
1	0.556478000	5.895431000	-0.160574000
1	0.546051000	3.013309000	-3.347208000
6	-3.254514000	1.737826000	-0.184357000
79	-1.874890000	0.212417000	-0.240749000
1	-7.268855000	-2.612734000	1.587002000
1	1.654856000	4.871907000	-2.138447000
1	-3.797845000	-0.106073000	2.027291000
1	-6.881104000	0.969085000	-0.762853000
1	-1.668650000	2.177479000	-2.579787000
1	-1.630959000	5.016227000	0.640453000
6	1.653872000	-3.376890000	-0.125898000
6	0.722357000	-3.976502000	-0.898671000
6	-0.173894000	-3.254238000	-1.791032000
8	-0.774841000	-2.132342000	-1.424910000
1	0.674617000	-5.058956000	-0.946376000
7	1.931893000	-2.018933000	-0.169175000
6	-1.006745000	-4.054199000	-2.742137000

1	-1.766243000	-4.579790000	-2.153367000
1	-1.500561000	-3.392963000	-3.454017000
1	-0.394185000	-4.786874000	-3.267421000
6	2.588013000	-4.144188000	0.753763000
1	2.327248000	-5.202614000	0.783428000
1	3.611654000	-4.031740000	0.381544000
1	2.556707000	-3.734561000	1.768762000
8	1.024515000	-2.588675000	-3.099941000
1	1.952593000	-2.926473000	-2.927897000
1	1.105455000	-1.621558000	-3.016856000
8	3.529828000	-3.152281000	-2.582490000
1	4.048820000	-3.631402000	-3.244590000
1	3.801079000	-2.222053000	-2.649253000

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6	4.331278000	0.302133000	-0.578524000
6	5.002032000	1.445524000	-0.144787000
6	6.209468000	1.300519000	0.524238000
6	6.759857000	0.034218000	0.756156000
6	6.074686000	-1.091348000	0.288370000
6	4.860615000	-0.970903000	-0.379031000
16	2.786224000	0.532925000	-1.426498000
8	2.700689000	-0.464295000	-2.503039000
8	2.687719000	1.944082000	-1.762456000
7	1.456373000	0.241001000	-0.437001000
6	1.035826000	-1.094437000	-0.208349000
6	-0.473798000	-1.389327000	-0.224445000
6	-0.876134000	-2.190532000	0.977817000
6	-0.438978000	-2.067224000	2.269515000
6	-1.173195000	-2.884418000	3.188865000
6	-2.150195000	-3.612242000	2.583014000
16	-2.198197000	-3.311893000	0.876990000
6	8.057114000	-0.101506000	1.503678000
6	1.086472000	1.322573000	0.505649000
6	2.153344000	1.624001000	1.534331000
6	2.558280000	2.942369000	1.737108000
6	3.534008000	3.243475000	2.687203000
6	4.117651000	2.222658000	3.432516000
6	3.719701000	0.900014000	3.230074000

6	2.740232000	0.601716000	2.288705000
1	4.580281000	2.427569000	-0.326071000
1	6.735783000	2.185676000	0.870824000
1	6.498881000	-2.078800000	0.446135000
1	4.330261000	-1.851953000	-0.719834000
1	0.373539000	-1.407182000	2.558119000
1	-0.967849000	-2.928716000	4.252286000
1	-2.835103000	-4.324162000	3.023832000
1	8.797953000	0.612175000	1.133298000
1	8.466349000	-1.109506000	1.411348000
1	7.906403000	0.107394000	2.568172000
1	0.833657000	2.217566000	-0.068920000
1	0.177607000	0.978337000	1.007858000
1	2.111669000	3.732414000	1.137456000
1	3.843528000	4.273366000	2.836580000
1	4.883858000	2.452472000	4.166634000
1	4.178992000	0.100244000	3.803123000
1	2.453497000	-0.433538000	2.114916000
7	-4.530884000	1.723464000	0.217896000
6	-5.087697000	2.993689000	0.209925000
6	-4.112061000	3.840088000	-0.191155000
7	-2.990547000	3.061154000	-0.427057000
6	-5.257326000	0.543827000	0.581875000
6	-4.741524000	-0.329620000	1.536214000
6	-5.468564000	-1.469848000	1.870116000
6	-6.699127000	-1.722453000	1.267193000
6	-7.207918000	-0.833205000	0.322195000
6	-6.486451000	0.304541000	-0.027759000
6	-1.730848000	3.573961000	-0.874364000
6	-1.123956000	4.604343000	-0.163684000
6	0.107030000	5.092929000	-0.601216000
6	0.721616000	4.543667000	-1.724289000
6	0.097941000	3.513913000	-2.428661000
6	-1.136712000	3.028716000	-2.011704000
1	-6.111726000	3.170597000	0.499481000
1	-4.110040000	4.907607000	-0.345329000
1	-5.068093000	-2.158030000	2.607680000
1	-8.164226000	-1.026480000	-0.152648000

1	0.588766000	5.896892000	-0.053884000
1	0.575749000	3.085035000	-3.302465000
6	-3.236257000	1.753669000	-0.176452000
79	-1.862782000	0.219474000	-0.260112000
1	-7.262366000	-2.610833000	1.533635000
1	1.687198000	4.914177000	-2.052481000
1	-3.788190000	-0.115131000	2.010365000
1	-6.862813000	0.996589000	-0.774920000
1	-1.641881000	2.237754000	-2.556218000
1	-1.603861000	5.007958000	0.722723000
6	1.644920000	-3.347324000	-0.034217000
6	0.770511000	-3.944648000	-0.856513000
6	-0.020710000	-3.199708000	-1.883438000
8	-0.763555000	-2.113571000	-1.461119000
1	0.622837000	-5.017927000	-0.810436000
7	1.950526000	-1.981084000	-0.111660000
6	-0.902607000	-4.083545000	-2.731266000
1	-1.634793000	-4.571866000	-2.083722000
1	-1.424621000	-3.476522000	-3.472943000
1	-0.304439000	-4.845825000	-3.234262000
6	2.456736000	-4.078059000	0.987889000
1	2.218334000	-5.142360000	0.997103000
1	3.523673000	-3.944557000	0.780909000
1	2.259821000	-3.658069000	1.980374000
8	0.987871000	-2.603986000	-2.891236000
1	2.030952000	-2.867368000	-2.763403000
1	0.918848000	-1.628576000	-2.914709000
8	3.378459000	-3.063390000	-2.669417000
1	3.762142000	-3.644674000	-3.346166000
1	3.751496000	-2.172354000	-2.797355000

Zero-point correction= 0.733975 (Hartree/Particle)

Thermal correction to Energy= 0.782932

Thermal correction to Enthalpy= 0.783876

Thermal correction to Gibbs Free Energy= 0.648886

Sum of electronic and zero-point Energies= -3073.336205

Sum of electronic and thermal Energies= -3073.287249

Sum of electronic and thermal Enthalpies= -3073.286305

Sum of electronic and thermal Free Energies= -3073.421295

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6	4.407074000	0.164509000	-0.391872000
6	5.245930000	1.251643000	-0.184098000
6	6.385958000	1.070160000	0.593646000
6	6.684987000	-0.174111000	1.156552000
6	5.823273000	-1.251823000	0.912252000
6	4.682030000	-1.093780000	0.137762000
16	2.946596000	0.368468000	-1.378130000
8	3.054159000	-0.565721000	-2.505372000
8	2.780568000	1.786546000	-1.680685000
7	1.694432000	-0.122253000	-0.349302000
6	0.846205000	-1.205659000	-0.905721000
6	-0.453360000	-1.480395000	-0.093584000
6	-0.224071000	-2.117535000	1.236330000
6	0.943607000	-2.354983000	1.912711000
6	0.739521000	-2.897482000	3.218879000
6	-0.578361000	-3.078363000	3.511915000
16	-1.594167000	-2.561573000	2.218391000
6	7.890163000	-0.343185000	2.040744000
6	1.169472000	0.959091000	0.513031000
6	2.234173000	1.595173000	1.381596000
6	2.574393000	2.935531000	1.207484000
6	3.537132000	3.532469000	2.020820000
6	4.173322000	2.786069000	3.009088000
6	3.836329000	1.443158000	3.189793000
6	2.867039000	0.854547000	2.384777000
1	4.998551000	2.220972000	-0.604132000
1	7.048693000	1.911647000	0.775840000
1	6.051074000	-2.224114000	1.340445000
1	3.995121000	-1.916700000	-0.045943000
1	1.917686000	-2.155899000	1.481900000
1	1.544351000	-3.153672000	3.897720000
1	-1.014527000	-3.496467000	4.409413000
1	8.704985000	0.315174000	1.730047000
1	8.248924000	-1.375007000	2.028874000
1	7.638310000	-0.091076000	3.076937000
1	0.657467000	1.731734000	-0.075352000
1	0.441232000	0.483827000	1.172306000

1	2.090707000	3.502414000	0.416216000
1	3.793918000	4.577529000	1.876157000
1	4.929055000	3.246091000	3.638626000
1	4.328550000	0.858092000	3.961104000
1	2.600344000	-0.189904000	2.525860000
7	-4.556520000	1.633821000	0.266687000
6	-5.160996000	2.853168000	0.001080000
6	-4.217246000	3.633467000	-0.574693000
7	-3.067696000	2.864199000	-0.653749000
6	-5.217950000	0.535050000	0.902792000
6	-4.628500000	-0.074230000	2.007753000
6	-5.279557000	-1.142670000	2.618005000
6	-6.510852000	-1.583093000	2.136157000
6	-7.095062000	-0.954715000	1.038084000
6	-6.449173000	0.108817000	0.412424000
6	-1.813553000	3.325575000	-1.170398000
6	-1.225196000	4.448051000	-0.598670000
6	0.014554000	4.876567000	-1.070750000
6	0.657632000	4.176028000	-2.088433000
6	0.051566000	3.056686000	-2.659142000
6	-1.195336000	2.631982000	-2.210755000
1	-6.189898000	3.048915000	0.259800000
1	-4.252451000	4.647792000	-0.939975000
1	-4.826388000	-1.621803000	3.479745000
1	-8.053235000	-1.295635000	0.660175000
1	0.483481000	5.748492000	-0.626245000
1	0.553392000	2.512742000	-3.452151000
6	-3.264989000	1.630230000	-0.135110000
79	-1.867324000	0.117971000	-0.058474000
1	-7.016716000	-2.412640000	2.619128000
1	1.634263000	4.496173000	-2.435928000
1	-3.679570000	0.293424000	2.385201000
1	-6.886311000	0.597809000	-0.452838000
1	-1.691739000	1.775230000	-2.657441000
1	-1.725603000	4.965213000	0.214250000
6	1.449387000	-3.429258000	-1.568481000
6	0.238073000	-3.651757000	-2.384636000
6	-1.015706000	-3.260985000	-1.886070000

8	-1.280190000	-2.452399000	-0.913434000
1	0.191434000	-4.600827000	-2.918233000
7	1.728763000	-2.359506000	-0.936644000
6	-2.265351000	-3.831101000	-2.475524000
1	-2.994774000	-3.033408000	-2.632789000
1	-2.059953000	-4.350997000	-3.410479000
1	-2.693084000	-4.538685000	-1.757283000
6	2.444713000	-4.553020000	-1.564624000
1	3.334392000	-4.277531000	-0.997725000
1	1.993238000	-5.452199000	-1.133595000
1	2.729297000	-4.796429000	-2.594479000
8	0.406167000	-0.849579000	-2.203519000
1	-0.253730000	-0.141317000	-2.102011000
1	1.736998000	-1.416568000	-3.636106000
8	1.343688000	-2.122166000	-4.203486000
1	0.667056000	-2.807636000	-3.432102000
1	2.069566000	-2.640980000	-4.593326000

Zero-point correction= 0.729660 (Hartree/Particle)

Thermal correction to Energy= 0.778488

Thermal correction to Enthalpy= 0.779432

Thermal correction to Gibbs Free Energy= 0.644317

Sum of electronic and zero-point Energies= -3073.311810

Sum of electronic and thermal Energies= -3073.262982

Sum of electronic and thermal Enthalpies= -3073.262038

Sum of electronic and thermal Free Energies= -3073.397153

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6	4.495064000	-0.231706000	-0.719279000
6	4.679871000	0.813419000	0.186230000
6	5.587865000	0.631468000	1.219897000
6	6.309061000	-0.563827000	1.348262000
6	6.113160000	-1.579563000	0.406202000
6	5.204134000	-1.424660000	-0.634291000
16	3.335814000	-0.014081000	-2.025174000
8	3.365023000	-1.170698000	-2.913045000
8	3.484763000	1.307038000	-2.602994000
7	1.793058000	0.056447000	-1.206580000
6	1.347208000	-1.043771000	-0.537704000
6	0.210298000	-1.067454000	0.438141000

6	0.750752000	-0.671168000	1.786547000
6	2.055586000	-0.550279000	2.185492000
6	2.198917000	-0.137885000	3.545040000
6	0.999185000	0.026063000	4.169633000
16	-0.320005000	-0.296478000	3.106421000
6	7.293652000	-0.735351000	2.470800000
6	1.052857000	1.336610000	-1.370256000
6	1.445311000	2.455943000	-0.431845000
6	2.300307000	3.473487000	-0.868578000
6	2.628381000	4.532476000	-0.024546000
6	2.096348000	4.591775000	1.262405000
6	1.223200000	3.595801000	1.695507000
6	0.893899000	2.538925000	0.849352000
1	4.117368000	1.739217000	0.095634000
1	5.737846000	1.426640000	1.944229000
1	6.672580000	-2.506438000	0.492307000
1	5.041087000	-2.210546000	-1.364176000
1	2.899148000	-0.758766000	1.535551000
1	3.155406000	0.013921000	4.031859000
1	0.809873000	0.303623000	5.198349000
1	8.223464000	-0.202047000	2.246187000
1	7.537550000	-1.788255000	2.625860000
1	6.898066000	-0.325283000	3.403507000
1	1.196380000	1.646777000	-2.405918000
1	-0.000304000	1.084108000	-1.240957000
1	2.708357000	3.431733000	-1.873155000
1	3.294632000	5.314226000	-0.376299000
1	2.352596000	5.417092000	1.919627000
1	0.787630000	3.643666000	2.689216000
1	0.189687000	1.782879000	1.181954000
7	-4.692817000	0.265187000	-0.001698000
6	-5.724391000	1.168799000	-0.202710000
6	-5.143313000	2.361328000	-0.471590000
7	-3.774578000	2.147700000	-0.437086000
6	-4.887025000	-1.112813000	0.343266000
6	-4.402163000	-1.589456000	1.559251000
6	-4.600313000	-2.927752000	1.887556000
6	-5.281744000	-3.770886000	1.010893000

6	-5.766790000	-3.277613000	-0.199228000
6	-5.570225000	-1.941541000	-0.541008000
6	-2.793184000	3.169998000	-0.659391000
6	-2.681132000	4.203997000	0.264390000
6	-1.728320000	5.198485000	0.054179000
6	-0.903668000	5.151965000	-1.067909000
6	-1.028743000	4.109171000	-1.985316000
6	-1.978766000	3.110159000	-1.787347000
1	-6.760386000	0.878781000	-0.122446000
1	-5.564273000	3.330638000	-0.688543000
1	-4.224510000	-3.308266000	2.831687000
1	-6.295948000	-3.933158000	-0.883103000
1	-1.626490000	6.004105000	0.773834000
1	-0.387269000	4.074405000	-2.860370000
6	-3.486860000	0.859330000	-0.147479000
79	-1.645471000	-0.004570000	0.043270000
1	-5.436693000	-4.813058000	1.271183000
1	-0.157261000	5.924074000	-1.224112000
1	-3.888277000	-0.914016000	2.236248000
1	-5.932922000	-1.542681000	-1.483403000
1	-2.098398000	2.296383000	-2.496459000
1	-3.326540000	4.217678000	1.137402000
6	1.885418000	-3.400681000	-0.593898000
6	0.573876000	-4.066671000	-0.923379000
6	-0.595182000	-3.110229000	-0.679768000
8	-0.221117000	-2.424232000	0.546684000
1	0.480843000	-4.929278000	-0.257231000
7	2.092070000	-2.134363000	-0.639458000
6	-1.903668000	-3.817439000	-0.393678000
1	-1.838175000	-4.398697000	0.528965000
1	-2.689372000	-3.062809000	-0.288346000
1	-2.157231000	-4.481627000	-1.224701000
6	3.026278000	-4.297014000	-0.246673000
1	3.252347000	-4.938210000	-1.106996000
1	3.910413000	-3.728204000	0.037335000
1	2.727584000	-4.956407000	0.573645000
8	-0.778091000	-2.233224000	-1.743027000
1	0.802296000	-2.510116000	-4.496621000

1	-0.085446000	-2.356296000	-2.434376000
8	1.098749000	-2.648850000	-3.587108000
1	0.602705000	-4.447715000	-1.951063000
1	1.921326000	-2.141813000	-3.487941000

Zero-point correction= 0.736095 (Hartree/Particle)

Thermal correction to Energy= 0.784957

Thermal correction to Enthalpy= 0.785901

Thermal correction to Gibbs Free Energy= 0.651834

Sum of electronic and zero-point Energies= -3073.356825

Sum of electronic and thermal Energies= -3073.307963

Sum of electronic and thermal Enthalpies= -3073.307019

Sum of electronic and thermal Free Energies= -3073.441086

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6	4.415885000	0.018275000	-0.347533000
6	4.485114000	1.221398000	0.353113000
6	5.172413000	1.240381000	1.561197000
6	5.791871000	0.088052000	2.058584000
6	5.722269000	-1.095306000	1.312019000
6	5.035064000	-1.142198000	0.106861000
16	3.477794000	-0.016660000	-1.838169000
8	3.771472000	-1.240730000	-2.582564000
8	3.614080000	1.253627000	-2.526272000
7	1.831362000	-0.023322000	-1.300890000
6	1.259302000	-1.174999000	-0.800398000
6	0.088588000	-1.188871000	0.199417000
6	0.636736000	-1.206468000	1.597044000
6	1.716539000	-0.552892000	2.127406000
6	1.868496000	-0.769060000	3.532762000
6	0.909369000	-1.586845000	4.046773000
16	-0.192890000	-2.115827000	2.825006000
6	6.541259000	0.114891000	3.361737000
6	1.052055000	1.193032000	-1.650152000
6	1.397983000	2.387901000	-0.792094000
6	2.074975000	3.478646000	-1.343128000
6	2.424021000	4.569216000	-0.549063000
6	2.094370000	4.580614000	0.805701000
6	1.401207000	3.504323000	1.358092000
6	1.052153000	2.415184000	0.561646000

1	4.009706000	2.120336000	-0.030178000
1	5.227099000	2.166049000	2.126371000
1	6.208655000	-1.992112000	1.685043000
1	4.973650000	-2.054179000	-0.475438000
1	2.389843000	0.061871000	1.539748000
1	2.669638000	-0.337993000	4.122575000
1	0.792943000	-1.934461000	5.064447000
1	6.300921000	-0.763918000	3.966148000
1	6.304761000	1.012191000	3.937241000
1	7.621131000	0.102641000	3.180441000
1	1.227827000	1.415410000	-2.703990000
1	0.002639000	0.914285000	-1.534932000
1	2.347182000	3.458842000	-2.394342000
1	2.956054000	5.407591000	-0.988421000
1	2.370668000	5.427766000	1.426038000
1	1.131178000	3.510221000	2.409841000
1	0.518005000	1.574802000	0.997694000
7	-4.664742000	0.350564000	0.307619000
6	-5.712663000	1.257981000	0.299794000
6	-5.161447000	2.479042000	0.112149000
7	-3.794219000	2.278836000	0.000635000
6	-4.831107000	-1.063321000	0.462881000
6	-4.087211000	-1.747795000	1.421483000
6	-4.239694000	-3.126276000	1.539354000
6	-5.140278000	-3.806077000	0.721115000
6	-5.892181000	-3.105871000	-0.220289000
6	-5.737654000	-1.728722000	-0.357692000
6	-2.850202000	3.328581000	-0.241036000
6	-2.716783000	4.346735000	0.697819000
6	-1.809258000	5.374056000	0.453750000
6	-1.052462000	5.377471000	-0.716717000
6	-1.200938000	4.352288000	-1.649345000
6	-2.103941000	3.318546000	-1.416051000
1	-6.736744000	0.949837000	0.441465000
1	-5.601938000	3.460706000	0.035381000
1	-3.661010000	-3.665297000	2.282602000
1	-6.595807000	-3.631184000	-0.857780000
1	-1.690573000	6.168877000	1.182799000

1	-0.615651000	4.357328000	-2.563113000
6	-3.474729000	0.972276000	0.122583000
79	-1.627685000	0.060622000	0.098188000
1	-5.260720000	-4.879966000	0.821306000
1	-0.343635000	6.178185000	-0.900929000
1	-3.405700000	-1.202107000	2.066522000
1	-6.301448000	-1.174176000	-1.101732000
1	-2.244244000	2.518554000	-2.136840000
1	-3.310654000	4.323976000	1.606437000
6	1.967861000	-3.434950000	-0.813068000
6	0.707394000	-3.982809000	-1.444462000
6	-0.372091000	-2.911442000	-1.396303000
8	-0.472239000	-2.511541000	-0.042728000
1	0.376677000	-4.847795000	-0.862097000
7	2.176523000	-2.192423000	-0.595133000
6	-1.721914000	-3.312383000	-1.932527000
1	-2.113142000	-4.142606000	-1.339465000
1	-2.405963000	-2.462501000	-1.854749000
1	-1.640546000	-3.626507000	-2.976367000
6	3.028299000	-4.424201000	-0.454348000
1	3.428314000	-4.869424000	-1.372679000
1	3.834649000	-3.950758000	0.104889000
1	2.594907000	-5.236423000	0.136319000
8	0.126339000	-1.759175000	-2.096460000
1	1.502205000	-2.011023000	-4.844205000
1	0.702007000	-2.018903000	-2.918315000
8	1.675899000	-2.376017000	-3.963614000
1	0.915318000	-4.328456000	-2.464432000
1	2.551544000	-2.044327000	-3.686509000

Zero-point correction= 0.734669 (Hartree/Particle)

Thermal correction to Energy= 0.782535

Thermal correction to Enthalpy= 0.783479

Thermal correction to Gibbs Free Energy= 0.651267

Sum of electronic and zero-point Energies= -3073.346794

Sum of electronic and thermal Energies= -3073.298928

Sum of electronic and thermal Enthalpies= -3073.297984

Sum of electronic and thermal Free Energies= -3073.430195

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6	3.477607000	0.011687000	-2.095526000
6	4.632447000	0.699330000	-2.459192000
6	5.715114000	-0.022665000	-2.953303000
6	5.651139000	-1.412340000	-3.091094000
6	4.466579000	-2.072231000	-2.736238000
6	3.376187000	-1.371040000	-2.241228000
16	2.125375000	0.919677000	-1.393534000
8	0.876257000	0.241878000	-1.730593000
8	2.336927000	2.318334000	-1.744677000
7	2.242360000	0.841610000	0.273075000
6	1.544333000	-0.191721000	0.945368000
6	0.694417000	0.157400000	1.935886000
6	0.211697000	1.476361000	2.315611000
6	-0.511039000	1.750197000	3.454990000
6	-0.969798000	3.094573000	3.507081000
6	-0.598000000	3.812426000	2.406023000
16	0.319090000	2.876701000	1.292129000
6	6.815558000	-2.189089000	-3.640630000
6	3.435917000	1.434337000	0.931590000
6	4.271373000	0.406569000	1.657413000
6	4.066864000	0.193639000	3.022355000
6	4.795986000	-0.777907000	3.705374000
6	5.737375000	-1.546146000	3.024936000
6	5.948453000	-1.338087000	1.662331000
6	5.218398000	-0.368012000	0.981733000
1	4.680721000	1.778687000	-2.359344000
1	6.622606000	0.502350000	-3.236840000
1	4.401272000	-3.150589000	-2.853518000
1	2.458160000	-1.880751000	-1.971146000
1	-0.704661000	1.004995000	4.216925000
1	-1.545551000	3.507801000	4.326342000
1	-0.795295000	4.854563000	2.190028000
1	6.983595000	-3.103620000	-3.065491000
1	7.730661000	-1.593517000	-3.627212000
1	6.620592000	-2.485764000	-4.676741000
1	4.016393000	1.945445000	0.158493000
1	3.084025000	2.197924000	1.633169000
1	3.329461000	0.794154000	3.550851000

1	4.628544000	-0.933497000	4.766664000
1	6.306736000	-2.303958000	3.554293000
1	6.684770000	-1.930962000	1.128251000
1	5.388273000	-0.208208000	-0.079697000
6	0.975573000	-2.413573000	0.534258000
6	-0.419674000	-2.309493000	1.016427000
6	-0.716471000	-1.672960000	2.196440000
8	0.190054000	-0.844648000	2.774126000
1	-1.106898000	-3.094297000	0.707223000
7	1.868701000	-1.488624000	0.565182000
6	-1.908058000	-1.926015000	3.050881000
1	-1.560440000	-2.358256000	3.996267000
1	-2.408611000	-0.980628000	3.281028000
1	-2.598689000	-2.616757000	2.566406000
6	1.355794000	-3.760950000	-0.004172000
1	1.154584000	-4.541779000	0.736165000
1	0.751434000	-3.989652000	-0.889497000
1	2.413606000	-3.772738000	-0.268862000
7	-4.494500000	-0.296250000	-1.114837000
6	-5.405922000	0.547521000	-1.723246000
6	-4.792430000	1.746838000	-1.846195000
7	-3.519633000	1.600484000	-1.317786000
6	-4.775989000	-1.660176000	-0.773029000
6	-4.735859000	-2.051871000	0.563190000
6	-5.002360000	-3.380132000	0.884733000
6	-5.318945000	-4.293960000	-0.119790000
6	-5.372310000	-3.881934000	-1.449903000
6	-5.098182000	-2.557833000	-1.785396000
6	-2.579007000	2.684434000	-1.285408000
6	-2.953728000	3.859023000	-0.637817000
6	-2.094374000	4.953297000	-0.673935000
6	-0.878688000	4.864477000	-1.350758000
6	-0.513278000	3.676938000	-1.981777000
6	-1.362999000	2.573670000	-1.951554000
1	-6.395625000	0.216780000	-1.996570000
1	-5.127295000	2.682080000	-2.266324000
1	-4.977564000	-3.696430000	1.922646000
1	-5.621300000	-4.591429000	-2.232003000

1	-2.378332000	5.874188000	-0.174562000
1	0.441883000	3.596406000	-2.487837000
6	-3.327141000	0.343638000	-0.866068000
79	-1.765328000	-0.578818000	0.055120000
1	-5.531810000	-5.327047000	0.135066000
1	-0.213901000	5.721961000	-1.383427000
1	-4.507764000	-1.319613000	1.332258000
1	-5.121863000	-2.221399000	-2.817387000
1	-1.088685000	1.643734000	-2.439112000
1	-3.907304000	3.910051000	-0.120969000

Zero-point correction= 0.682010 (Hartree/Particle)

Thermal correction to Energy= 0.727653

Thermal correction to Enthalpy= 0.728597

Thermal correction to Gibbs Free Energy= 0.597878

Sum of electronic and zero-point Energies= -2920.601222

Sum of electronic and thermal Energies= -2920.555579

Sum of electronic and thermal Enthalpies= -2920.554635

Sum of electronic and thermal Free Energies= -2920.685354

B-TSa6-C

6	3.298754000	-1.639966000	-1.898481000
6	4.597415000	-1.356751000	-2.322737000
6	5.552380000	-2.363502000	-2.265433000
6	5.224640000	-3.644216000	-1.803542000
6	3.909626000	-3.900040000	-1.401789000
6	2.939924000	-2.904368000	-1.441745000
16	2.096051000	-0.338822000	-1.911069000
8	0.758670000	-0.912308000	-1.947189000
8	2.510766000	0.618137000	-2.930069000
7	2.240552000	0.494676000	-0.451427000
6	1.559224000	0.022914000	0.685732000
6	1.088509000	0.970270000	1.609715000
6	0.954000000	2.405179000	1.417888000
6	1.254129000	3.383384000	2.333881000
6	0.949652000	4.690399000	1.857730000
6	0.411656000	4.675116000	0.602238000
16	0.260473000	3.078517000	-0.023390000
6	6.270829000	-4.723841000	-1.765600000
6	3.372302000	1.437400000	-0.300400000

6	4.221287000	1.142086000	0.915030000
6	4.601665000	2.187167000	1.756749000
6	5.417756000	1.944805000	2.861067000
6	5.848017000	0.650279000	3.137612000
6	5.460531000	-0.400781000	2.306127000
6	4.652544000	-0.157575000	1.199894000
1	4.851288000	-0.371622000	-2.700868000
1	6.568470000	-2.156252000	-2.589329000
1	3.641429000	-4.892826000	-1.052172000
1	1.922363000	-3.095392000	-1.121741000
1	1.684982000	3.163084000	3.304082000
1	1.128595000	5.598918000	2.419787000
1	0.100561000	5.517478000	-0.002280000
1	7.176959000	-4.370624000	-1.265247000
1	6.553683000	-5.018393000	-2.781459000
1	5.907604000	-5.611098000	-1.243149000
1	3.973153000	1.368299000	-1.210802000
1	2.993325000	2.462829000	-0.255372000
1	4.252844000	3.195438000	1.546127000
1	5.709038000	2.767323000	3.506937000
1	6.477978000	0.456468000	4.000218000
1	5.788328000	-1.413306000	2.520464000
1	4.345142000	-0.983614000	0.561778000
6	0.424796000	-1.850769000	1.495824000
6	-0.528438000	-1.119402000	2.244714000
6	-0.255976000	0.172201000	2.734388000
8	1.059651000	0.515971000	2.937917000
1	-1.431398000	-1.613985000	2.603715000
7	1.417402000	-1.296185000	0.800176000
6	-1.258870000	1.067255000	3.378156000
1	-1.007540000	1.172221000	4.438700000
1	-1.218141000	2.066265000	2.929563000
1	-2.267116000	0.664052000	3.270517000
6	0.270528000	-3.338345000	1.341201000
1	1.197999000	-3.834322000	1.642554000
1	-0.548458000	-3.722418000	1.951473000
1	0.084696000	-3.590098000	0.292441000
7	-4.670879000	-0.504305000	-0.715590000

6	-5.545506000	0.029539000	-1.646337000
6	-4.853362000	0.970981000	-2.327745000
7	-3.571544000	0.982848000	-1.801215000
6	-5.030065000	-1.531733000	0.218907000
6	-4.932642000	-1.283113000	1.586016000
6	-5.275750000	-2.292341000	2.481326000
6	-5.724395000	-3.525043000	2.008935000
6	-5.832999000	-3.752074000	0.638249000
6	-5.482689000	-2.753988000	-0.267538000
6	-2.537545000	1.846445000	-2.294024000
6	-2.771426000	3.218200000	-2.318062000
6	-1.797154000	4.058341000	-2.852480000
6	-0.611989000	3.523719000	-3.355778000
6	-0.390166000	2.148077000	-3.314475000
6	-1.355109000	1.297686000	-2.780362000
1	-6.568007000	-0.305437000	-1.723099000
1	-5.136704000	1.619060000	-3.141995000
1	-5.205048000	-2.108805000	3.548485000
1	-6.185339000	-4.709567000	0.269593000
1	-1.969768000	5.129444000	-2.877943000
1	0.537803000	1.729448000	-3.689628000
6	-3.451722000	0.075467000	-0.809775000
79	-1.905978000	-0.369917000	0.402061000
1	-5.995664000	-4.307533000	2.710076000
1	0.141608000	4.181777000	-3.776697000
1	-4.602083000	-0.309160000	1.933988000
1	-5.547217000	-2.918403000	-1.338859000
1	-1.193300000	0.225428000	-2.746703000
1	-3.701768000	3.615640000	-1.923969000

Zero-point correction= 0.680767 (Hartree/Particle)

Thermal correction to Energy= 0.724930

Thermal correction to Enthalpy= 0.725874

Thermal correction to Gibbs Free Energy= 0.599558

Sum of electronic and zero-point Energies= -2920.587065

Sum of electronic and thermal Energies= -2920.542901

Sum of electronic and thermal Enthalpies= -2920.541957

Sum of electronic and thermal Free Energies= -2920.668274

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6	0.835164000	2.757634000	-1.855405000
6	-0.507659000	2.598907000	-1.518370000
6	-1.249512000	3.727741000	-1.189403000
6	-0.666577000	4.999002000	-1.193826000
6	0.683533000	5.124520000	-1.546235000
6	1.445030000	4.011552000	-1.878607000
16	1.784316000	1.314118000	-2.220245000
8	2.887355000	1.656211000	-3.100238000
8	0.872856000	0.235507000	-2.556459000
7	2.518611000	0.913820000	-0.715611000
6	1.720967000	0.360382000	0.291503000
6	0.843686000	-0.791944000	0.002709000
6	1.322509000	-1.901770000	-0.728584000
6	0.538888000	-2.975491000	-1.170070000
6	1.265520000	-3.974277000	-1.828099000
6	2.608478000	-3.660603000	-1.907668000
16	3.000633000	-2.178306000	-1.178111000
6	-1.469163000	6.214884000	-0.820952000
6	3.552838000	1.888037000	-0.275029000
6	4.692392000	1.185772000	0.419168000
6	5.467788000	0.266272000	-0.291527000
6	6.546610000	-0.363943000	0.319878000
6	6.861452000	-0.073142000	1.647983000
6	6.093772000	0.846021000	2.358368000
6	5.007346000	1.470068000	1.746206000
1	-0.964825000	1.613043000	-1.533519000
1	-2.301129000	3.619635000	-0.937271000
1	1.139974000	6.109945000	-1.569585000
1	2.486275000	4.114861000	-2.168206000
1	-0.533672000	-3.007353000	-0.999464000
1	0.836723000	-4.878179000	-2.241673000
1	3.386304000	-4.247323000	-2.382260000
1	-2.541184000	6.014014000	-0.879114000
1	-1.232681000	7.056978000	-1.476679000
1	-1.238515000	6.524838000	0.204159000
1	3.926298000	2.370907000	-1.179113000
1	3.098340000	2.642466000	0.372530000
1	5.221193000	0.054526000	-1.329650000

1	7.145539000	-1.076302000	-0.239196000
1	7.704828000	-0.561777000	2.125991000
1	6.335885000	1.074443000	3.391802000
1	4.398795000	2.180132000	2.300042000
7	-3.986166000	-1.711518000	-0.034380000
6	-5.345671000	-1.453377000	-0.039229000
6	-5.486479000	-0.145812000	0.277879000
7	-4.206777000	0.359601000	0.463600000
6	-3.393967000	-2.989889000	-0.307992000
6	-2.720302000	-3.658379000	0.712885000
6	-2.124506000	-4.886574000	0.438130000
6	-2.206567000	-5.433737000	-0.842421000
6	-2.886163000	-4.754175000	-1.852172000
6	-3.485426000	-3.523623000	-1.589324000
6	-3.934237000	1.716464000	0.825276000
6	-4.695651000	2.735913000	0.257006000
6	-4.472222000	4.052221000	0.653569000
6	-3.483957000	4.347401000	1.591143000
6	-2.718308000	3.319651000	2.138621000
6	-2.946827000	1.997192000	1.768202000
1	-6.073816000	-2.223387000	-0.240141000
1	-6.368426000	0.458484000	0.420332000
1	-1.601807000	-5.417665000	1.226945000
1	-2.949696000	-5.178028000	-2.848880000
1	-5.068610000	4.847963000	0.218858000
1	-1.953006000	3.539624000	2.876325000
6	-3.274563000	-0.600540000	0.263382000
79	-1.221322000	-0.585558000	0.223061000
1	-1.741360000	-6.391722000	-1.051826000
1	-3.314276000	5.374777000	1.896791000
1	-2.673289000	-3.219035000	1.704957000
1	-4.009169000	-2.975383000	-2.366462000
1	-2.385011000	1.186179000	2.221636000
1	-5.450081000	2.504255000	-0.488364000
6	1.072758000	0.246021000	2.415163000
6	0.995029000	-1.137141000	2.384669000
6	2.125014000	-2.062410000	2.069440000
8	3.266205000	-1.681519000	1.902712000

1	0.202449000	-1.597443000	2.973679000
7	1.757025000	0.929866000	1.468222000
6	1.747807000	-3.522550000	2.051508000
1	0.761261000	-3.669183000	1.601565000
1	2.504443000	-4.096934000	1.514122000
1	1.698232000	-3.881665000	3.086010000
6	0.336574000	1.077153000	3.416384000
1	1.067974000	1.526163000	4.098780000
1	-0.193114000	1.895384000	2.920121000
1	-0.358150000	0.474253000	4.002763000

Zero-point correction= 0.680030 (Hartree/Particle)

Thermal correction to Energy= 0.725235

Thermal correction to Enthalpy= 0.726180

Thermal correction to Gibbs Free Energy= 0.599404

Sum of electronic and zero-point Energies= -2920.566016

Sum of electronic and thermal Energies= -2920.520811

Sum of electronic and thermal Enthalpies= -2920.519867

Sum of electronic and thermal Free Energies= -2920.646642

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6	4.318474000	-1.364336000	0.754092000
6	4.798448000	-1.934099000	-0.419710000
6	5.926508000	-1.372974000	-1.010852000
6	6.562069000	-0.260953000	-0.448050000
6	6.056793000	0.279239000	0.742737000
6	4.936492000	-0.266845000	1.353550000
16	2.881640000	-2.023435000	1.543263000
8	3.055771000	-1.977391000	2.986874000
8	2.481160000	-3.269871000	0.918252000
7	1.719963000	-0.775910000	1.244300000
6	1.497862000	-0.361918000	-0.041831000
6	0.976122000	0.862617000	-0.498118000
6	1.017907000	2.152178000	0.225765000
6	0.088935000	3.159376000	0.209383000
6	0.505099000	4.325116000	0.918483000
6	1.751257000	4.194311000	1.454966000
16	2.444835000	2.659179000	1.096721000
6	7.748092000	0.369547000	-1.123699000
6	0.918330000	-0.284451000	2.375504000

6	-0.445441000	-0.938761000	2.450059000
6	-0.692715000	-2.197524000	1.897892000
6	-1.965410000	-2.759817000	1.973431000
6	-3.000117000	-2.073659000	2.605918000
6	-2.754719000	-0.821096000	3.168606000
6	-1.484801000	-0.254057000	3.085524000
1	4.292683000	-2.787784000	-0.858385000
1	6.318982000	-1.805084000	-1.926698000
1	6.549293000	1.134772000	1.195830000
1	4.551038000	0.145737000	2.281506000
1	-0.868028000	3.064516000	-0.295912000
1	-0.102049000	5.216487000	1.022965000
1	2.306571000	4.912253000	2.044243000
1	7.429401000	1.237769000	-1.711462000
1	8.237546000	-0.331895000	-1.802584000
1	8.478936000	0.720631000	-0.391184000
1	1.492926000	-0.472550000	3.284099000
1	0.806284000	0.796924000	2.283221000
1	0.100080000	-2.738881000	1.387490000
1	-2.146230000	-3.733648000	1.527467000
1	-3.991313000	-2.513464000	2.664934000
1	-3.554379000	-0.282005000	3.668084000
1	-1.298824000	0.730688000	3.509025000
7	-4.137692000	0.948678000	-0.474268000
6	-5.427451000	0.506355000	-0.712235000
6	-5.337241000	-0.819892000	-0.961488000
7	-3.992519000	-1.152836000	-0.877194000
6	-3.793540000	2.301406000	-0.137801000
6	-3.904197000	3.290932000	-1.109643000
6	-3.568458000	4.601638000	-0.776732000
6	-3.131639000	4.907011000	0.511388000
6	-3.026377000	3.903079000	1.473764000
6	-3.359696000	2.589808000	1.153229000
6	-3.497516000	-2.487048000	-1.035212000
6	-4.215922000	-3.533589000	-0.461411000
6	-3.738146000	-4.834963000	-0.585395000
6	-2.544211000	-5.083140000	-1.260410000
6	-1.839728000	-4.027502000	-1.836338000

6	-2.320095000	-2.724098000	-1.740093000
1	-6.275306000	1.172389000	-0.677364000
1	-6.092828000	-1.549621000	-1.205630000
1	-3.649568000	5.382241000	-1.525927000
1	-2.685254000	4.141453000	2.476102000
1	-4.291976000	-5.652292000	-0.135316000
1	-0.918236000	-4.217268000	-2.377404000
6	-3.248643000	-0.062704000	-0.577140000
79	-1.242147000	0.177091000	-0.403590000
1	-2.874426000	5.930277000	0.766261000
1	-2.167109000	-6.097055000	-1.343530000
1	-4.243501000	3.030738000	-2.107688000
1	-3.288519000	1.791538000	1.885915000
1	-1.795418000	-1.900535000	-2.214262000
1	-5.124054000	-3.326710000	0.096540000
6	1.706831000	-0.593418000	-2.191529000
6	1.259778000	0.823760000	-2.009611000
6	2.404275000	1.823202000	-2.327271000
8	2.142761000	2.863257000	-2.880168000
1	0.420050000	1.089792000	-2.657799000
7	1.872379000	-1.230261000	-1.076322000
6	3.798706000	1.432701000	-1.912952000
1	4.221804000	0.797137000	-2.701213000
1	4.414752000	2.327014000	-1.810132000
1	3.814088000	0.854214000	-0.984125000
6	1.912294000	-1.224508000	-3.519047000
1	0.935780000	-1.380355000	-3.993196000
1	2.485256000	-0.564725000	-4.177641000
1	2.415834000	-2.185979000	-3.413961000

Zero-point correction= 0.681655 (Hartree/Particle)

Thermal correction to Energy= 0.727407

Thermal correction to Enthalpy= 0.728352

Thermal correction to Gibbs Free Energy= 0.599351

Sum of electronic and zero-point Energies= -2920.630243

Sum of electronic and thermal Energies= -2920.584491

Sum of electronic and thermal Enthalpies= -2920.583547

Sum of electronic and thermal Free Energies= -2920.712547

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6	-4.416507000	0.256670000	-0.876425000
6	-4.536877000	-0.603866000	-1.964760000
6	-5.765225000	-1.206776000	-2.202524000
6	-6.863636000	-0.965927000	-1.368509000
6	-6.712116000	-0.088550000	-0.289580000
6	-5.494496000	0.531788000	-0.036496000
16	-2.877352000	1.070716000	-0.553338000
8	-3.175699000	2.330218000	0.110974000
8	-2.074509000	1.073715000	-1.774397000
7	-2.028177000	0.176576000	0.601852000
6	-1.316026000	-0.948470000	0.179421000
6	-0.151752000	-1.552669000	0.735523000
6	0.265132000	-1.571695000	2.162633000
6	1.378997000	-1.073121000	2.781046000
6	1.484230000	-1.447600000	4.154171000
6	0.450499000	-2.235835000	4.563914000
16	-0.663503000	-2.531458000	3.284995000
6	-8.178108000	-1.651085000	-1.620657000
6	-2.291023000	0.453501000	2.022964000
6	-1.189970000	1.214628000	2.727131000
6	-0.399685000	2.151703000	2.060290000
6	0.609803000	2.827360000	2.745892000
6	0.821028000	2.587779000	4.102878000
6	0.012899000	1.673815000	4.776531000
6	-0.984944000	0.988166000	4.088846000
1	-3.682657000	-0.791818000	-2.604399000
1	-5.876774000	-1.874356000	-3.052098000
1	-7.562287000	0.122505000	0.352383000
1	-5.390815000	1.235045000	0.783406000
1	2.111739000	-0.457040000	2.269388000
1	2.291342000	-1.134272000	4.805562000
1	0.271031000	-2.649657000	5.547720000
1	-9.014546000	-1.044131000	-1.266483000
1	-8.214517000	-2.608670000	-1.089916000
1	-8.318165000	-1.856884000	-2.684410000
1	-3.220235000	1.027071000	2.074092000
1	-2.477616000	-0.498205000	2.525779000
1	-0.569525000	2.355274000	1.004574000

1	1.223714000	3.550801000	2.217350000
1	1.607774000	3.115534000	4.632994000
1	0.170266000	1.480551000	5.833369000
1	-1.596211000	0.253757000	4.608413000
7	3.796036000	1.082265000	-1.314185000
6	4.517842000	2.177975000	-1.756735000
6	3.691247000	3.244756000	-1.658801000
7	2.485457000	2.768812000	-1.169010000
6	4.302010000	-0.257678000	-1.295871000
6	4.665414000	-0.849486000	-2.504257000
6	5.143061000	-2.159243000	-2.498854000
6	5.254621000	-2.858623000	-1.298311000
6	4.897528000	-2.248669000	-0.096442000
6	4.417413000	-0.941059000	-0.087049000
6	1.331376000	3.595730000	-0.975609000
6	1.456137000	4.758374000	-0.220147000
6	0.339739000	5.572506000	-0.048909000
6	-0.878368000	5.222007000	-0.628416000
6	-0.983756000	4.057466000	-1.386420000
6	0.125278000	3.236569000	-1.569590000
1	5.540596000	2.090821000	-2.088496000
1	3.833739000	4.285712000	-1.903662000
1	5.421081000	-2.631809000	-3.434959000
1	4.996177000	-2.788263000	0.839908000
1	0.421822000	6.477157000	0.544534000
1	-1.929710000	3.777813000	-1.835735000
6	2.542735000	1.437805000	-0.950732000
79	1.133177000	0.171052000	-0.221464000
1	5.624453000	-3.878521000	-1.298308000
1	-1.746904000	5.857449000	-0.488772000
1	4.562086000	-0.291249000	-3.430045000
1	4.144354000	-0.446163000	0.840488000
1	0.057104000	2.330766000	-2.163365000
1	2.410286000	5.007546000	0.235142000
6	-1.062677000	-2.703748000	-1.071478000
6	0.036605000	-2.756047000	-0.145510000
6	0.738322000	-4.030903000	0.199677000
8	0.413636000	-5.074510000	-0.337690000

1	0.859199000	-2.426883000	-1.183221000
7	-1.778354000	-1.599326000	-0.928228000
6	1.921380000	-3.971404000	1.135010000
1	1.585449000	-4.037210000	2.175763000
1	2.571205000	-4.822350000	0.922800000
1	2.468081000	-3.032772000	1.020199000
6	-1.330216000	-3.647299000	-2.193213000
1	-1.711762000	-4.590991000	-1.793891000
1	-2.061584000	-3.212622000	-2.876612000
1	-0.410395000	-3.888320000	-2.733181000
8	1.508121000	-2.181926000	-2.286882000
1	2.376862000	-1.783574000	-2.103144000
1	0.928906000	-1.476287000	-2.733678000
8	-0.118114000	-0.438807000	-3.271335000
1	-0.611659000	-0.729551000	-4.052433000
1	-0.788858000	-0.138318000	-2.630087000

Zero-point correction= 0.726504 (Hartree/Particle)

Thermal correction to Energy= 0.776609

Thermal correction to Enthalpy= 0.777553

Thermal correction to Gibbs Free Energy= 0.640557

Sum of electronic and zero-point Energies= -3073.379792

Sum of electronic and thermal Energies= -3073.329687

Sum of electronic and thermal Enthalpies= -3073.328743

Sum of electronic and thermal Free Energies= -3073.465739

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6	-4.719000000	1.385044000	-0.013950000
6	-4.933116000	0.738132000	-1.232068000
6	-5.909995000	-0.245699000	-1.297098000
6	-6.669077000	-0.586757000	-0.169411000
6	-6.432153000	0.085611000	1.033472000
6	-5.455279000	1.072172000	1.125153000
16	-3.426086000	2.581717000	0.103247000
8	-3.664924000	3.449473000	1.242677000
8	-3.193502000	3.155047000	-1.214560000
7	-2.022247000	1.689671000	0.490339000
6	-1.538340000	0.797654000	-0.475706000
6	-1.142219000	-0.552122000	-0.364380000
6	-1.620333000	-1.464523000	0.700665000

6	-0.951951000	-2.124550000	1.694596000
6	-1.803320000	-2.931458000	2.508052000
6	-3.108128000	-2.873015000	2.114895000
16	-3.319410000	-1.844481000	0.751872000
6	-7.710992000	-1.667058000	-0.261351000
6	-1.790061000	1.415358000	1.923694000
6	-0.335120000	1.545668000	2.304916000
6	0.452875000	2.586548000	1.807273000
6	1.770561000	2.730383000	2.233858000
6	2.314206000	1.833637000	3.153969000
6	1.529577000	0.797716000	3.656808000
6	0.208581000	0.655752000	3.233325000
1	-4.361777000	1.015206000	-2.112730000
1	-6.093987000	-0.754583000	-2.239158000
1	-7.022644000	-0.164262000	1.909920000
1	-5.278291000	1.597798000	2.058195000
1	0.117759000	-2.025210000	1.843585000
1	-1.459084000	-3.522904000	3.348230000
1	-3.960603000	-3.376550000	2.551805000
1	-8.376276000	-1.495185000	-1.112113000
1	-8.313853000	-1.714584000	0.647635000
1	-7.237179000	-2.643071000	-0.409431000
1	-2.361962000	2.167377000	2.469706000
1	-2.173431000	0.431845000	2.208489000
1	0.030148000	3.284520000	1.088180000
1	2.374703000	3.545491000	1.846729000
1	3.342784000	1.949994000	3.483046000
1	1.941111000	0.102120000	4.382219000
1	-0.410283000	-0.145302000	3.629390000
7	3.895598000	-1.547906000	0.162102000
6	5.266671000	-1.367353000	0.122472000
6	5.474340000	-0.035075000	0.024963000
7	4.223849000	0.566020000	0.002264000
6	3.266414000	-2.832922000	0.273351000
6	3.419708000	-3.751277000	-0.761368000
6	2.836902000	-5.010440000	-0.637180000
6	2.106044000	-5.334944000	0.504743000
6	1.957311000	-4.402301000	1.530370000

6	2.545179000	-3.143823000	1.423111000
6	4.048954000	1.985925000	-0.087406000
6	4.891346000	2.811584000	0.654939000
6	4.744303000	4.192759000	0.557612000
6	3.756294000	4.740531000	-0.260067000
6	2.916742000	3.901485000	-0.989868000
6	3.067369000	2.520038000	-0.915148000
1	5.953232000	-2.197976000	0.173579000
1	6.384323000	0.538860000	-0.049844000
1	2.950835000	-5.734980000	-1.436561000
1	1.392175000	-4.656050000	2.421418000
1	5.397255000	4.839574000	1.134331000
1	2.141853000	4.303487000	-1.633961000
6	3.243223000	-0.365084000	0.086780000
79	1.224649000	-0.223881000	-0.047248000
1	1.651594000	-6.316037000	0.596442000
1	3.642242000	5.817636000	-0.326933000
1	3.988448000	-3.478872000	-1.645407000
1	2.462034000	-2.411171000	2.220950000
1	2.428010000	1.870645000	-1.500372000
1	5.640185000	2.381647000	1.312778000
6	-1.030971000	0.130205000	-2.569139000
6	-0.811574000	-0.953036000	-1.741727000
6	-0.217386000	-2.216884000	-2.219952000
8	0.433739000	-2.212017000	-3.262296000
1	2.727929000	0.002760000	-2.669385000
7	-1.441182000	1.166614000	-1.778193000
6	-0.375490000	-3.477477000	-1.420536000
1	-1.413674000	-3.628814000	-1.111573000
1	-0.024024000	-4.322460000	-2.013643000
1	0.228682000	-3.403712000	-0.507588000
6	-0.991469000	0.271135000	-4.055539000
1	-1.236604000	-0.683933000	-4.522267000
1	-1.724060000	1.020409000	-4.365875000
1	-0.015976000	0.587184000	-4.428723000
8	2.023550000	0.207538000	-3.299030000
1	1.480817000	-0.601526000	-3.344766000
1	1.092586000	1.838598000	-3.111196000

8	0.611051000	2.677973000	-2.994366000
1	0.914660000	3.236878000	-3.720897000
1	-1.534227000	2.121846000	-2.111206000

Zero-point correction= 0.734848 (Hartree/Particle)

Thermal correction to Energy= 0.785902

Thermal correction to Enthalpy= 0.786846

Thermal correction to Gibbs Free Energy= 0.647404

Sum of electronic and zero-point Energies= -3073.423245

Sum of electronic and thermal Energies= -3073.372192

Sum of electronic and thermal Enthalpies= -3073.371248

Sum of electronic and thermal Free Energies= -3073.510689

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6	-4.549167000	-1.137960000	-0.995610000
6	-5.296320000	-0.259771000	-0.211576000
6	-6.331697000	0.447395000	-0.807059000
6	-6.631259000	0.281611000	-2.166151000
6	-5.867446000	-0.612472000	-2.922351000
6	-4.825292000	-1.331196000	-2.345600000
16	-3.254906000	-2.070151000	-0.227356000
8	-2.853246000	-3.129582000	-1.142444000
8	-3.659724000	-2.392922000	1.133472000
7	-2.023251000	-0.909394000	-0.089632000
6	-1.159451000	-0.987138000	1.017756000
6	-0.594384000	0.156351000	1.683168000
6	-1.060539000	1.550609000	1.640173000
6	-0.411177000	2.646466000	2.152634000
6	-1.170366000	3.847410000	2.051612000
6	-2.382362000	3.650430000	1.459053000
16	-2.626218000	2.000371000	1.024234000
6	-7.778132000	1.029047000	-2.788007000
6	-1.537812000	-0.281914000	-1.330290000
6	-0.348287000	-0.949023000	-1.993926000
6	0.142057000	-2.197737000	-1.607670000
6	1.263223000	-2.735869000	-2.239529000
6	1.892260000	-2.042451000	-3.270729000
6	1.398174000	-0.800407000	-3.669307000
6	0.285752000	-0.257766000	-3.032037000
1	-5.077616000	-0.143994000	0.845703000

1	-6.924835000	1.133551000	-0.209340000
1	-6.092932000	-0.751604000	-3.975560000
1	-4.235663000	-2.031331000	-2.928819000
1	0.584640000	2.587251000	2.580500000
1	-0.820953000	4.813796000	2.394305000
1	-3.151846000	4.380021000	1.244135000
1	-8.720926000	0.506951000	-2.591812000
1	-7.658767000	1.107358000	-3.870781000
1	-7.866751000	2.034459000	-2.369095000
1	-2.381953000	-0.231580000	-2.025350000
1	-1.285589000	0.758533000	-1.095860000
1	-0.347547000	-2.753726000	-0.815402000
1	1.643470000	-3.702699000	-1.922574000
1	2.759361000	-2.470190000	-3.764185000
1	1.875585000	-0.257579000	-4.479614000
1	-0.098532000	0.711005000	-3.345665000
7	3.400499000	2.029163000	-0.992760000
6	4.635834000	2.059386000	-1.618629000
6	5.132989000	0.803239000	-1.550770000
7	4.193004000	0.037039000	-0.877386000
6	2.538935000	3.165783000	-0.844058000
6	3.041076000	4.321982000	-0.255830000
6	2.196963000	5.419350000	-0.097714000
6	0.869733000	5.350881000	-0.515522000
6	0.381766000	4.186343000	-1.107334000
6	1.218513000	3.088724000	-1.283442000
6	4.355814000	-1.361828000	-0.614569000
6	4.839741000	-2.175041000	-1.635841000
6	5.002183000	-3.537361000	-1.401310000
6	4.676133000	-4.078391000	-0.159465000
6	4.201321000	-3.251208000	0.856684000
6	4.046192000	-1.884499000	0.638692000
1	5.032713000	2.962566000	-2.054881000
1	6.065389000	0.386954000	-1.898147000
1	2.578819000	6.325151000	0.361457000
1	-0.650763000	4.132077000	-1.438366000
1	5.374000000	-4.175948000	-2.195833000
1	3.967529000	-3.665912000	1.831929000

6	3.123771000	0.788136000	-0.533603000
79	1.439328000	0.292693000	0.461628000
1	0.213563000	6.204915000	-0.381214000
1	4.799667000	-5.141425000	0.019567000
1	4.072250000	4.353926000	0.082766000
1	0.864990000	2.180073000	-1.761611000
1	3.702342000	-1.227492000	1.431691000
1	5.064296000	-1.746205000	-2.607570000
6	-0.018466000	-1.856991000	2.632120000
6	0.147441000	-0.435106000	2.759529000
6	-1.121177000	-1.115672000	4.115542000
8	-0.610299000	-1.305038000	5.163160000
1	0.807078000	0.070079000	3.455766000
7	-0.818966000	-2.147377000	1.567409000
6	-2.537533000	-0.779495000	3.793894000
1	-3.146138000	-1.219376000	4.586532000
1	-2.636075000	0.311105000	3.829804000
1	-2.867262000	-1.154538000	2.826219000
6	0.822495000	-2.920097000	3.255710000
1	1.667184000	-3.123628000	2.588329000
1	1.213233000	-2.596394000	4.221074000
1	0.247279000	-3.840644000	3.374524000

Zero-point correction= 0.679470 (Hartree/Particle)

Thermal correction to Energy= 0.725180

Thermal correction to Enthalpy= 0.726124

Thermal correction to Gibbs Free Energy= 0.596164

Sum of electronic and zero-point Energies= -2920.595824

Sum of electronic and thermal Energies= -2920.550115

Sum of electronic and thermal Enthalpies= -2920.549171

Sum of electronic and thermal Free Energies= -2920.679131

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6	4.713371000	0.744689000	-1.161685000
6	5.363364000	0.551179000	0.057837000
6	6.510136000	-0.228117000	0.082719000
6	7.018481000	-0.804802000	-1.091073000
6	6.349730000	-0.581993000	-2.296805000
6	5.193876000	0.193481000	-2.343895000
16	3.277477000	1.776255000	-1.205524000

8	2.899369000	1.975399000	-2.598774000
8	3.483604000	2.920822000	-0.331570000
7	2.135491000	0.783967000	-0.420525000
6	1.106893000	1.440104000	0.273825000
6	0.481144000	0.866865000	1.513120000
6	1.020634000	-0.186780000	2.377864000
6	0.382013000	-0.763050000	3.450335000
6	1.207434000	-1.666467000	4.172179000
6	2.462224000	-1.760336000	3.639319000
16	2.657895000	-0.757208000	2.259756000
6	8.261552000	-1.649690000	-1.037619000
6	1.819064000	-0.515341000	-1.051294000
6	0.572792000	-0.556811000	-1.912083000
6	0.009773000	0.572252000	-2.513102000
6	-1.161535000	0.454094000	-3.261827000
6	-1.763870000	-0.790466000	-3.440409000
6	-1.187588000	-1.922735000	-2.866840000
6	-0.035065000	-1.802547000	-2.095993000
1	4.982366000	1.010934000	0.964568000
1	7.029174000	-0.387361000	1.023717000
1	6.738882000	-1.015576000	-3.213020000
1	4.675390000	0.373381000	-3.280099000
1	-0.649760000	-0.542089000	3.704906000
1	0.884622000	-2.221641000	5.044460000
1	3.292346000	-2.366028000	3.978993000
1	8.591455000	-1.934443000	-2.038687000
1	8.079580000	-2.564551000	-0.464523000
1	9.075420000	-1.112613000	-0.542250000
1	2.699410000	-0.813158000	-1.630195000
1	1.718273000	-1.258950000	-0.254030000
1	0.477817000	1.543343000	-2.392286000
1	-1.599170000	1.340598000	-3.711757000
1	-2.671565000	-0.879353000	-4.030520000
1	-1.642154000	-2.898970000	-3.009683000
1	0.399160000	-2.683978000	-1.627862000
7	-2.959142000	-2.652611000	-0.244756000
6	-4.060531000	-3.071903000	-0.975364000
6	-4.778345000	-1.963691000	-1.272752000

7	-4.100200000	-0.894961000	-0.713616000
6	-1.897868000	-3.519047000	0.171088000
6	-1.231963000	-3.287790000	1.373237000
6	-0.145678000	-4.089255000	1.714516000
6	0.247772000	-5.135220000	0.882617000
6	-0.455521000	-5.385828000	-0.293822000
6	-1.526143000	-4.574583000	-0.659904000
6	-4.520641000	0.473577000	-0.805578000
6	-4.616642000	1.065945000	-2.060971000
6	-5.008430000	2.399731000	-2.148440000
6	-5.298640000	3.121995000	-0.992100000
6	-5.205976000	2.511223000	0.257595000
6	-4.815191000	1.178482000	0.358772000
1	-4.248732000	-4.113192000	-1.183828000
1	-5.714270000	-1.835190000	-1.793680000
1	0.384369000	-3.896703000	2.642175000
1	-0.162814000	-6.205513000	-0.941538000
1	-5.082412000	2.874010000	-3.121437000
1	-5.440566000	3.070753000	1.157301000
6	-2.975534000	-1.307391000	-0.094347000
79	-1.570514000	-0.073633000	0.708146000
1	1.092807000	-5.758644000	1.155218000
1	-5.601931000	4.161387000	-1.064733000
1	-1.562004000	-2.499285000	2.040905000
1	-2.050419000	-4.747604000	-1.594388000
1	-4.747295000	0.682685000	1.322287000
1	-4.372713000	0.490500000	-2.948695000
6	-0.433879000	2.916696000	0.859561000
6	-0.525995000	1.755153000	1.819555000
6	-0.050715000	4.177364000	1.691993000
8	-0.725819000	4.457902000	2.654809000
1	-1.063341000	1.806709000	2.760070000
7	0.608381000	2.560128000	-0.085752000
6	1.103881000	4.997882000	1.203110000
1	0.934718000	5.280281000	0.159064000
1	1.212628000	5.884283000	1.827983000
1	2.018669000	4.396877000	1.213951000
6	-1.718906000	3.279903000	0.100097000

1	-2.021222000	2.445551000	-0.542167000
1	-2.514390000	3.494508000	0.816595000
1	-1.543459000	4.162027000	-0.521831000

Zero-point correction= 0.683246 (Hartree/Particle)

Thermal correction to Energy= 0.728448

Thermal correction to Enthalpy= 0.729392

Thermal correction to Gibbs Free Energy= 0.602057

Sum of electronic and zero-point Energies= -2920.628216

Sum of electronic and thermal Energies= -2920.583014

Sum of electronic and thermal Enthalpies= -2920.582069

Sum of electronic and thermal Free Energies= -2920.709405

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6	5.010294000	-0.653852000	0.889084000
6	5.508581000	-0.617697000	-0.413645000
6	6.662825000	0.108793000	-0.665201000
6	7.323832000	0.795061000	0.364367000
6	6.800311000	0.737556000	1.657662000
6	5.643463000	0.011416000	1.932556000
16	3.544289000	-1.595069000	1.206773000
8	3.438595000	-1.776009000	2.650935000
8	3.540093000	-2.759712000	0.328176000
7	2.311355000	-0.590105000	0.673257000
6	1.296293000	-1.147469000	-0.137214000
6	0.791943000	-0.598973000	-1.329697000
6	1.271937000	0.547175000	-2.086445000
6	0.658071000	1.120444000	-3.174764000
6	1.410361000	2.182750000	-3.749391000
6	2.585706000	2.401977000	-3.088345000
16	2.794731000	1.323135000	-1.765182000
6	8.581816000	1.564762000	0.069062000
6	1.945060000	0.555920000	1.533655000
6	0.624660000	0.385451000	2.252759000
6	0.299799000	-0.801445000	2.917530000
6	-0.924822000	-0.928914000	3.566792000
6	-1.830904000	0.132533000	3.574307000
6	-1.506802000	1.320477000	2.924751000
6	-0.285933000	1.442515000	2.259456000
1	5.003889000	-1.157142000	-1.209696000

1	7.066040000	0.142350000	-1.673549000
1	7.307048000	1.259897000	2.463675000
1	5.246688000	-0.049563000	2.940841000
1	-0.304958000	0.784762000	-3.545365000
1	1.092677000	2.757395000	-4.611041000
1	3.346117000	3.141859000	-3.301029000
1	9.375508000	0.890931000	-0.268841000
1	8.938435000	2.095938000	0.953791000
1	8.414581000	2.294244000	-0.728969000
1	2.760788000	0.706727000	2.248468000
1	1.900670000	1.452063000	0.905842000
1	1.006763000	-1.625529000	2.917054000
1	-1.169327000	-1.855493000	4.077248000
1	-2.783521000	0.032248000	4.085996000
1	-2.206181000	2.151890000	2.928065000
1	-0.038949000	2.365208000	1.737357000
7	-3.368941000	2.447181000	0.203887000
6	-4.620341000	2.865114000	0.633711000
6	-5.413604000	1.770308000	0.647473000
7	-4.629769000	0.710012000	0.223069000
6	-2.222355000	3.302118000	0.135055000
6	-1.302773000	3.164766000	-0.902756000
6	-0.150852000	3.947696000	-0.899432000
6	0.060146000	4.886033000	0.109603000
6	-0.889591000	5.046287000	1.117120000
6	-2.031135000	4.249699000	1.139549000
6	-5.095406000	-0.641077000	0.117650000
6	-5.670544000	-1.242658000	1.232971000
6	-6.120518000	-2.556968000	1.134194000
6	-5.987488000	-3.255898000	-0.063955000
6	-5.413944000	-2.638129000	-1.174236000
6	-4.970560000	-1.320775000	-1.091877000
1	-4.835236000	3.898663000	0.855062000
1	-6.457618000	1.646623000	0.889038000
1	0.572830000	3.829205000	-1.700964000
1	-0.737785000	5.781195000	1.900563000
1	-6.568056000	-3.035654000	1.998840000
1	-5.320718000	-3.176045000	-2.112043000

6	-3.367825000	1.114828000	-0.040306000
79	-1.855938000	-0.072588000	-0.669194000
1	0.956479000	5.497373000	0.105037000
1	-6.335993000	-4.281120000	-0.134107000
1	-1.486226000	2.461035000	-1.708224000
1	-2.753161000	4.348664000	1.944198000
1	-4.540827000	-0.817437000	-1.952375000
1	-5.749323000	-0.690405000	2.164590000
6	-0.293737000	-2.517106000	-0.760226000
6	-0.309783000	-1.441410000	-1.695872000
6	1.476422000	-3.624179000	-1.250304000
8	2.044700000	-3.077191000	-2.094078000
1	-0.765243000	-1.483373000	-2.680381000
7	0.669639000	-2.286025000	0.204139000
6	1.444994000	-4.951877000	-0.606882000
1	0.693778000	-5.561620000	-1.117340000
1	2.434776000	-5.391751000	-0.750217000
1	1.202216000	-4.850027000	0.448425000
6	-1.356871000	-3.562365000	-0.569058000
1	-2.244449000	-3.106758000	-0.117613000
1	-1.654644000	-4.001830000	-1.525202000
1	-1.019742000	-4.350642000	0.104820000

Zero-point correction= 0.680702 (Hartree/Particle)

Thermal correction to Energy= 0.726139

Thermal correction to Enthalpy= 0.727083

Thermal correction to Gibbs Free Energy= 0.598801

Sum of electronic and zero-point Energies= -2920.591070

Sum of electronic and thermal Energies= -2920.545633

Sum of electronic and thermal Enthalpies= -2920.544689

Sum of electronic and thermal Free Energies= -2920.672970

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6	4.959647000	-0.897549000	0.074446000
6	5.043549000	-1.503032000	-1.178559000
6	5.937269000	-0.985468000	-2.106501000
6	6.732125000	0.127095000	-1.802210000
6	6.629284000	0.705382000	-0.532436000
6	5.746058000	0.199720000	0.415626000
16	3.755936000	-1.478231000	1.226473000
8	4.192551000	-1.129385000	2.571609000

8	3.412097000	-2.852642000	0.884878000
7	2.352438000	-0.594597000	0.967584000
6	1.402022000	-1.056913000	0.054628000
6	1.022728000	-0.502726000	-1.145917000
6	1.534481000	0.663063000	-1.857654000
6	0.890391000	1.306864000	-2.888291000
6	1.635884000	2.392088000	-3.428183000
6	2.839513000	2.556114000	-2.804769000
16	3.085016000	1.389255000	-1.563925000
6	7.670411000	0.688545000	-2.834715000
6	2.179081000	0.730465000	1.613000000
6	1.163987000	0.672629000	2.723019000
6	1.545522000	0.424945000	4.042942000
6	0.578081000	0.288900000	5.035578000
6	-0.775331000	0.401897000	4.714744000
6	-1.160046000	0.663610000	3.400610000
6	-0.189477000	0.801281000	2.409118000
1	4.430908000	-2.367437000	-1.413235000
1	6.024784000	-1.451321000	-3.084026000
1	7.253655000	1.557535000	-0.280639000
1	5.676598000	0.639979000	1.405360000
1	-0.092693000	1.011841000	-3.240827000
1	1.292375000	3.020895000	-4.240613000
1	3.605649000	3.293866000	-3.002989000
1	8.216889000	-0.111112000	-3.341762000
1	8.390755000	1.375454000	-2.386088000
1	7.109997000	1.236558000	-3.599821000
1	3.154665000	1.053494000	1.981970000
1	1.853568000	1.438955000	0.845598000
1	2.600474000	0.316235000	4.281503000
1	0.877817000	0.092723000	6.060417000
1	-1.527268000	0.293626000	5.490246000
1	-2.212242000	0.771092000	3.150436000
1	-0.477917000	1.019538000	1.380712000
7	-3.361536000	2.296013000	0.229288000
6	-4.618572000	2.808625000	0.506697000
6	-5.510075000	1.842026000	0.186203000
7	-4.774588000	0.763313000	-0.278911000

6	-2.133271000	2.992810000	0.469473000
6	-1.136431000	2.995785000	-0.504097000
6	0.084014000	3.604565000	-0.222662000
6	0.287219000	4.231211000	1.006990000
6	-0.733465000	4.254210000	1.955422000
6	-1.948872000	3.626915000	1.694850000
6	-5.348266000	-0.476197000	-0.711942000
6	-6.259220000	-1.124235000	0.116857000
6	-6.815956000	-2.329285000	-0.303836000
6	-6.457001000	-2.877085000	-1.533716000
6	-5.546411000	-2.214253000	-2.354617000
6	-4.991606000	-1.002939000	-1.951078000
1	-4.755631000	3.812277000	0.877195000
1	-6.588288000	1.824922000	0.217952000
1	0.867263000	3.600160000	-0.977062000
1	-0.578849000	4.740423000	2.912919000
1	-7.524887000	-2.842898000	0.337072000
1	-5.275630000	-2.631859000	-3.318913000
6	-3.451331000	1.031569000	-0.243168000
79	-1.917946000	-0.184829000	-0.762151000
1	1.238444000	4.707722000	1.221484000
1	-6.890451000	-3.818435000	-1.855351000
1	-1.316065000	2.531837000	-1.469070000
1	-2.734706000	3.601223000	2.444009000
1	-4.301056000	-0.460792000	-2.589668000
1	-6.515437000	-0.694991000	1.080650000
6	-0.281569000	-2.350792000	-0.739451000
6	-0.086768000	-1.294200000	-1.631978000
6	0.661452000	-3.137597000	1.399678000
8	0.455920000	-4.293991000	1.143591000
1	-0.446574000	-1.305130000	-2.655816000
7	0.595196000	-2.186310000	0.301723000
6	0.831202000	-2.607528000	2.788798000
1	0.035023000	-1.884730000	2.994805000
1	0.756592000	-3.454979000	3.469625000
1	1.784455000	-2.103561000	2.943043000
6	-1.212240000	-3.506729000	-0.912443000
1	-1.794535000	-3.699859000	-0.008762000

1	-1.894740000	-3.277056000	-1.733327000
1	-0.653618000	-4.414624000	-1.148999000

Zero-point correction= 0.683026 (Hartree/Particle)

Thermal correction to Energy= 0.728375

Thermal correction to Enthalpy= 0.729319

Thermal correction to Gibbs Free Energy= 0.598728

Sum of electronic and zero-point Energies= -2920.661337

Sum of electronic and thermal Energies= -2920.615987

Sum of electronic and thermal Enthalpies= -2920.615043

Sum of electronic and thermal Free Energies= -2920.745635

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6	4.714858000	-1.186935000	0.254505000
6	5.158367000	-1.607226000	-0.993749000
6	6.305354000	-1.025004000	-1.520945000
6	6.997054000	-0.031194000	-0.819942000
6	6.520197000	0.369848000	0.434369000
6	5.381704000	-0.205696000	0.984073000
16	3.308551000	-1.972438000	0.983139000
8	3.618394000	-2.307316000	2.366870000
8	2.821676000	-3.024834000	0.104676000
7	2.164547000	-0.709978000	1.108654000
6	1.781998000	-0.040513000	-0.045138000
6	0.921025000	1.121442000	-0.110075000
6	0.680521000	2.145161000	0.934211000
6	-0.485982000	2.650297000	1.442662000
6	-0.281442000	3.725960000	2.360119000
6	1.037496000	4.021970000	2.536719000
16	2.051318000	3.010443000	1.578758000
6	8.219472000	0.614546000	-1.412366000
6	1.449080000	-0.540461000	2.382717000
6	0.066389000	-1.152628000	2.396362000
6	-0.185875000	-2.387002000	1.789224000
6	-1.451625000	-2.962641000	1.868416000
6	-2.479225000	-2.308197000	2.547448000
6	-2.234064000	-1.076067000	3.151991000
6	-0.966198000	-0.500199000	3.074661000
1	4.609960000	-2.370049000	-1.535444000
1	6.670606000	-1.347722000	-2.491548000

1	7.053138000	1.137136000	0.988275000
1	5.019141000	0.101306000	1.961003000
1	-1.466270000	2.269937000	1.168598000
1	-1.085283000	4.245677000	2.867748000
1	1.475676000	4.770541000	3.183994000
1	8.734081000	-0.066030000	-2.094457000
1	8.918201000	0.925514000	-0.632180000
1	7.940456000	1.507824000	-1.981810000
1	2.070575000	-1.003031000	3.151347000
1	1.394110000	0.522926000	2.617962000
1	0.604726000	-2.899594000	1.245299000
1	-1.635586000	-3.921513000	1.391898000
1	-3.466000000	-2.758648000	2.605890000
1	-3.029177000	-0.560997000	3.682823000
1	-0.773973000	0.462070000	3.543963000
7	-4.128720000	0.541446000	-0.554150000
6	-5.388610000	-0.005087000	-0.721777000
6	-5.208913000	-1.335678000	-0.887079000
7	-3.842823000	-1.569999000	-0.810706000
6	-3.853892000	1.934567000	-0.349409000
6	-3.098161000	2.620325000	-1.297620000
6	-2.787231000	3.958559000	-1.073560000
6	-3.238751000	4.597236000	0.081730000
6	-4.007748000	3.900801000	1.012958000
6	-4.318593000	2.558083000	0.803653000
6	-3.257257000	-2.871856000	-0.918928000
6	-3.910880000	-3.947807000	-0.321964000
6	-3.350614000	-5.218558000	-0.411994000
6	-2.140673000	-5.407269000	-1.077838000
6	-1.498937000	-4.322076000	-1.671902000
6	-2.060498000	-3.049493000	-1.608622000
1	-6.279149000	0.603540000	-0.730312000
1	-5.914943000	-2.127631000	-1.079776000
1	-2.200064000	4.499800000	-1.809258000
1	-4.361281000	4.398836000	1.909950000
1	-3.855761000	-6.058278000	0.053636000
1	-0.562211000	-4.465072000	-2.200735000
6	-3.174924000	-0.415022000	-0.597329000

79	-1.220594000	0.020421000	-0.314648000
1	-2.995583000	5.640773000	0.254569000
1	-1.701888000	-6.397681000	-1.139194000
1	-2.762040000	2.108277000	-2.194010000
1	-4.899892000	1.993212000	1.526288000
1	-1.578684000	-2.205668000	-2.092353000
1	-4.835981000	-3.789419000	0.223658000
6	1.748744000	0.440462000	-2.169390000
6	0.943466000	1.455554000	-1.514132000
6	0.364107000	2.656291000	-2.216044000
8	-0.363619000	2.487557000	-3.172985000
1	0.481656000	0.375491000	-2.254325000
7	2.209017000	-0.446383000	-1.235353000
6	0.771074000	4.006789000	-1.707190000
1	1.846944000	4.037330000	-1.513019000
1	0.493037000	4.760107000	-2.445151000
1	0.254261000	4.210684000	-0.761906000
6	2.284189000	0.459322000	-3.569946000
1	1.691133000	1.112315000	-4.211312000
1	3.313945000	0.824944000	-3.541443000
1	2.285345000	-0.550753000	-3.982694000

Zero-point correction= 0.678481 (Hartree/Particle)

Thermal correction to Energy= 0.724118

Thermal correction to Enthalpy= 0.725062

Thermal correction to Gibbs Free Energy= 0.595516

Sum of electronic and zero-point Energies= -2920.587492

Sum of electronic and thermal Energies= -2920.541855

Sum of electronic and thermal Enthalpies= -2920.540911

Sum of electronic and thermal Free Energies= -2920.670457

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6	-4.699286000	0.872114000	0.851591000
6	-5.107560000	1.829839000	-0.067902000
6	-6.123396000	1.499801000	-0.961235000
6	-6.716512000	0.234301000	-0.943508000
6	-6.274661000	-0.709661000	-0.004867000
6	-5.272253000	-0.398004000	0.902005000
16	-3.438752000	1.264570000	2.026267000
8	-3.813062000	0.749047000	3.337714000

8	-3.078033000	2.670032000	1.909609000
7	-2.171460000	0.238536000	1.527688000
6	-1.740291000	0.339402000	0.205814000
6	-1.021343000	-0.790588000	-0.480309000
6	-0.959217000	-2.155537000	0.076240000
6	0.099931000	-2.904484000	0.510601000
6	-0.297296000	-4.170495000	1.035605000
6	-1.647045000	-4.354777000	0.992566000
16	-2.461683000	-2.996061000	0.318525000
6	-7.825140000	-0.114836000	-1.897671000
6	-1.262215000	-0.291303000	2.564868000
6	0.097549000	0.369931000	2.561144000
6	0.231807000	1.735010000	2.287591000
6	1.483068000	2.344108000	2.346717000
6	2.610795000	1.597168000	2.686686000
6	2.483344000	0.236137000	2.955753000
6	1.232827000	-0.378800000	2.882913000
1	-4.631281000	2.804403000	-0.086385000
1	-6.458191000	2.236188000	-1.685910000
1	-6.730190000	-1.695683000	0.017196000
1	-4.939320000	-1.123131000	1.638586000
1	1.126432000	-2.553218000	0.474153000
1	0.396472000	-4.904428000	1.427021000
1	-2.218599000	-5.217465000	1.309516000
1	-7.929469000	0.639586000	-2.679962000
1	-8.779115000	-0.184963000	-1.364749000
1	-7.645469000	-1.084827000	-2.369696000
1	-1.762439000	-0.130753000	3.522818000
1	-1.164281000	-1.372095000	2.439004000
1	-0.646106000	2.324507000	2.032393000
1	1.574238000	3.405067000	2.133733000
1	3.586103000	2.073343000	2.740528000
1	3.358638000	-0.347342000	3.225749000
1	1.133978000	-1.442783000	3.089102000
7	4.101144000	-0.605941000	0.012697000
6	5.318702000	-0.043622000	0.349936000
6	5.191495000	1.291228000	0.159676000
7	3.897551000	1.510545000	-0.283808000

6	3.813103000	-2.009713000	0.056631000
6	3.423619000	-2.661236000	-1.111903000
6	3.123713000	-4.020249000	-1.059691000
6	3.224286000	-4.713912000	0.145775000
6	3.628479000	-4.051014000	1.303434000
6	3.926104000	-2.690246000	1.265206000
6	3.361542000	2.806582000	-0.570307000
6	3.704647000	3.871501000	0.259783000
6	3.183583000	5.134171000	-0.006319000
6	2.318111000	5.324813000	-1.081540000
6	1.988317000	4.252178000	-1.907677000
6	2.518978000	2.987963000	-1.664886000
1	6.160936000	-0.644796000	0.655128000
1	5.905817000	2.092968000	0.262428000
1	2.820271000	-4.537469000	-1.964313000
1	3.711314000	-4.590130000	2.241419000
1	3.445763000	5.966637000	0.638121000
1	1.328172000	4.398917000	-2.756377000
6	3.218431000	0.345721000	-0.360105000
79	1.244547000	0.003770000	-0.708659000
1	2.992394000	-5.773541000	0.180832000
1	1.905934000	6.308965000	-1.278484000
1	3.366033000	-2.106886000	-2.044118000
1	4.237751000	-2.158483000	2.158580000
1	2.293845000	2.153567000	-2.322340000
1	4.353307000	3.708111000	1.115222000
6	-1.498344000	1.019252000	-1.889161000
6	-0.828844000	-0.336640000	-1.771838000
6	-0.343736000	-1.069933000	-2.996451000
8	-0.188375000	-0.422921000	-4.013333000
1	-0.804799000	1.799348000	-2.226233000
7	-1.972003000	1.342309000	-0.554824000
6	-0.078317000	-2.546032000	-2.925753000
1	-0.979445000	-3.079081000	-2.604937000
1	0.234553000	-2.895174000	-3.910046000
1	0.702177000	-2.755311000	-2.187070000
6	-2.695000000	0.962981000	-2.850892000
1	-2.354270000	0.786794000	-3.871778000

1	-3.379873000	0.163329000	-2.551209000
1	-3.226277000	1.915759000	-2.805829000

Zero-point correction= 0.683316 (Hartree/Particle)

Thermal correction to Energy= 0.728585

Thermal correction to Enthalpy= 0.729529

Thermal correction to Gibbs Free Energy= 0.601659

Sum of electronic and zero-point Energies= -2920.631985

Sum of electronic and thermal Energies= -2920.586715

Sum of electronic and thermal Enthalpies= -2920.585771

Sum of electronic and thermal Free Energies= -2920.713641

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6	4.849657000	-0.899890000	0.754095000
6	5.014685000	-1.890333000	-0.207897000
6	5.948921000	-1.685391000	-1.219270000
6	6.707419000	-0.512700000	-1.272628000
6	6.518634000	0.463746000	-0.283894000
6	5.593971000	0.279582000	0.734305000
16	3.682241000	-1.134710000	2.059382000
8	4.177676000	-0.530538000	3.290581000
8	3.282426000	-2.536685000	2.091292000
7	2.412605000	-0.136950000	1.570240000
6	1.913274000	-0.278005000	0.265100000
6	1.319877000	0.750963000	-0.483909000
6	1.261305000	2.147247000	-0.042134000
6	0.164689000	2.917280000	0.242969000
6	0.513447000	4.210215000	0.735426000
6	1.862837000	4.393029000	0.816737000
16	2.733454000	3.000231000	0.301500000
6	7.704699000	-0.286406000	-2.375491000
6	1.525137000	0.421796000	2.611057000
6	0.142058000	-0.189115000	2.611299000
6	-0.042926000	-1.556357000	2.376697000
6	-1.318328000	-2.114653000	2.448390000
6	-2.415455000	-1.315044000	2.770304000
6	-2.238422000	0.048990000	2.990193000
6	-0.965436000	0.612969000	2.897984000
1	4.421837000	-2.797567000	-0.161001000
1	6.093144000	-2.450181000	-1.976533000

1	7.111204000	1.373703000	-0.311870000
1	5.456022000	1.029178000	1.507547000
1	-0.854554000	2.558419000	0.121909000
1	-0.210575000	4.964306000	1.019427000
1	2.402565000	5.272825000	1.142083000
1	7.326611000	0.454782000	-3.087553000
1	7.906278000	-1.208969000	-2.923826000
1	8.648312000	0.096351000	-1.977482000
1	2.019130000	0.256085000	3.572023000
1	1.456164000	1.505179000	2.474101000
1	0.817083000	-2.184933000	2.152961000
1	-1.454314000	-3.177470000	2.268391000
1	-3.407192000	-1.751660000	2.846226000
1	-3.092386000	0.674363000	3.235718000
1	-0.825566000	1.679413000	3.062713000
7	-4.091972000	0.837445000	0.161296000
6	-5.298809000	0.389964000	0.671137000
6	-5.286009000	-0.959773000	0.560023000
7	-4.070581000	-1.303134000	-0.012666000
6	-3.695789000	2.210537000	0.059861000
6	-3.340729000	2.723714000	-1.186712000
6	-2.930519000	4.050975000	-1.279036000
6	-2.887905000	4.851340000	-0.137635000
6	-3.252642000	4.325259000	1.100567000
6	-3.658235000	2.996624000	1.207244000
6	-3.648861000	-2.648228000	-0.261368000
6	-3.950759000	-3.633351000	0.675868000
6	-3.527444000	-4.940063000	0.448754000
6	-2.802836000	-5.255033000	-0.698834000
6	-2.520726000	-4.263166000	-1.635983000
6	-2.951249000	-2.955494000	-1.428733000
1	-6.055096000	1.071612000	1.027991000
1	-6.035110000	-1.699338000	0.796063000
1	-2.654818000	4.460814000	-2.245352000
1	-3.219670000	4.946837000	1.989308000
1	-3.756360000	-5.709365000	1.178712000
1	-1.978289000	-4.508216000	-2.543287000
6	-3.327129000	-0.198778000	-0.239232000

79	-1.409327000	-0.059653000	-0.830663000
1	-2.571823000	5.886787000	-0.213800000
1	-2.468798000	-6.273361000	-0.868027000
1	-3.392508000	2.088539000	-2.066184000
1	-3.938453000	2.569820000	2.165245000
1	-2.765746000	-2.186161000	-2.171485000
1	-4.498757000	-3.380233000	1.577983000
6	1.153000000	-1.255526000	-1.575812000
6	0.794884000	0.142734000	-1.661913000
6	0.381507000	0.777281000	-2.961923000
8	0.077701000	0.061772000	-3.898607000
1	0.608036000	-1.833715000	-0.569842000
7	1.869372000	-1.465635000	-0.369934000
6	0.366772000	2.276861000	-3.076195000
1	1.310420000	2.710206000	-2.733615000
1	0.186312000	2.540445000	-4.118781000
1	-0.429983000	2.692027000	-2.449414000
6	1.247680000	-2.274110000	-2.672823000
1	0.291372000	-2.398811000	-3.178102000
1	1.980833000	-1.938788000	-3.412183000
1	1.576491000	-3.225269000	-2.250066000

Zero-point correction= 0.678840 (Hartree/Particle)

Thermal correction to Energy= 0.723853

Thermal correction to Enthalpy= 0.724797

Thermal correction to Gibbs Free Energy= 0.599306

Sum of electronic and zero-point Energies= -2920.582792

Sum of electronic and thermal Energies= -2920.537780

Sum of electronic and thermal Enthalpies= -2920.536835

Sum of electronic and thermal Free Energies= -2920.662326

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6	4.937647000	-0.912997000	0.502411000
6	5.029943000	-1.781533000	-0.579952000
6	6.056765000	-1.599675000	-1.500006000
6	6.981567000	-0.562407000	-1.351247000
6	6.870493000	0.286627000	-0.241455000
6	5.861548000	0.113532000	0.696562000
16	3.609654000	-1.118499000	1.653958000
8	4.164163000	-0.870189000	2.977342000

8	2.939344000	-2.380676000	1.335190000
7	2.468484000	0.073491000	1.332341000
6	1.125050000	-0.314806000	0.948778000
6	0.656611000	-0.006167000	-0.449070000
6	1.438091000	0.721626000	-1.390553000
6	0.872359000	1.444816000	-2.442169000
6	1.806681000	2.128433000	-3.238929000
6	3.095382000	1.893109000	-2.820394000
16	3.181247000	0.890647000	-1.447423000
6	8.103010000	-0.378242000	-2.335730000
6	2.623735000	1.379423000	2.041168000
6	1.752943000	2.447280000	1.422153000
6	2.298395000	3.378014000	0.534395000
6	1.483533000	4.313473000	-0.097220000
6	0.112154000	4.326342000	0.154461000
6	-0.438755000	3.418310000	1.057227000
6	0.382930000	2.494299000	1.699759000
1	4.315682000	-2.588622000	-0.702263000
1	6.138714000	-2.274262000	-2.347053000
1	7.594875000	1.084763000	-0.106176000
1	5.802986000	0.757062000	1.568539000
1	-0.200455000	1.467285000	-2.600420000
1	1.553155000	2.749328000	-4.088518000
1	4.008566000	2.272186000	-3.263928000
1	9.034286000	-0.788068000	-1.930431000
1	8.275070000	0.681420000	-2.541434000
1	7.892677000	-0.890070000	-3.277054000
1	2.375855000	1.253228000	3.100270000
1	3.674574000	1.668543000	1.966502000
1	3.365942000	3.361672000	0.332628000
1	1.917786000	5.030309000	-0.787220000
1	-0.524455000	5.053405000	-0.339847000
1	-1.506565000	3.434384000	1.263616000
1	-0.045173000	1.797235000	2.417297000
6	-2.339332000	-0.956803000	2.665301000
6	-1.128518000	-1.084729000	3.536003000
6	0.138454000	-1.070873000	3.071331000
8	-2.622607000	-1.820291000	1.850589000

1	-1.313062000	-1.179003000	4.604202000
7	0.215161000	-0.778837000	1.706801000
6	-3.188677000	0.266789000	2.834203000
1	-2.681467000	1.086738000	2.304771000
1	-4.171836000	0.106395000	2.385497000
1	-3.277124000	0.556423000	3.884596000
6	1.304930000	-1.345101000	3.974333000
1	1.862804000	-2.213509000	3.614347000
1	1.999073000	-0.506613000	4.038570000
1	0.936910000	-1.567213000	4.977452000
8	1.138213000	-2.038274000	-1.031971000
1	0.386381000	-2.499244000	-0.567861000
1	1.916668000	-2.321201000	-0.523235000
8	-0.714983000	-3.304243000	0.374612000
1	-1.345959000	-3.843222000	-0.121012000
1	-1.259178000	-2.716179000	0.930044000
79	-1.405655000	-0.073964000	-0.670006000
6	-3.466569000	-0.174282000	-0.706351000
7	-4.354125000	0.801786000	-0.402048000
7	-4.213042000	-1.301585000	-0.766008000
6	-5.632754000	0.288012000	-0.243361000
6	-4.043303000	2.193015000	-0.285740000
6	-5.541884000	-1.042195000	-0.472217000
6	-3.707208000	-2.601636000	-1.073805000
1	-6.480023000	0.917595000	-0.020716000
6	-4.505331000	2.902632000	0.820041000
6	-3.327728000	2.823384000	-1.301647000
1	-6.294585000	-1.814823000	-0.492972000
6	-2.876645000	-2.776122000	-2.179287000
6	-4.074178000	-3.678114000	-0.269271000
6	-4.247552000	4.269090000	0.905113000
1	-5.055681000	2.387755000	1.601984000
6	-3.074016000	4.188147000	-1.203532000
1	-3.003030000	2.251734000	-2.165178000
6	-2.397447000	-4.050282000	-2.473343000
1	-2.614268000	-1.924521000	-2.798855000
6	-3.603680000	-4.950886000	-0.582962000
1	-4.700509000	-3.511562000	0.601209000

6	-3.533123000	4.912513000	-0.104143000
1	-4.604435000	4.828462000	1.763724000
1	-2.528177000	4.687801000	-1.997357000
6	-2.763243000	-5.139084000	-1.681098000
1	-1.744711000	-4.191979000	-3.328352000
1	-3.882190000	-5.793860000	0.040460000
1	-3.337109000	5.977842000	-0.035792000
1	-2.391757000	-6.130985000	-1.916356000

Zero-point correction= 0.731708 (Hartree/Particle)

Thermal correction to Energy= 0.781687

Thermal correction to Enthalpy= 0.782631

Thermal correction to Gibbs Free Energy= 0.647822

Sum of electronic and zero-point Energies= -3073.309690

Sum of electronic and thermal Energies= -3073.259711

Sum of electronic and thermal Enthalpies= -3073.258766

Sum of electronic and thermal Free Energies= -3073.393576

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6	2.644456000	-1.594127000	-2.053730000
6	3.690691000	-1.156291000	-2.865189000
6	4.884454000	-1.864678000	-2.839892000
6	5.042149000	-2.989488000	-2.019187000
6	3.963516000	-3.412442000	-1.235072000
6	2.757065000	-2.722014000	-1.245109000
16	1.166981000	-0.641946000	-1.940303000
8	0.078026000	-1.490700000	-1.503285000
8	1.019469000	0.163469000	-3.142168000
7	1.538910000	0.490144000	-0.690160000
6	1.045231000	0.560365000	0.608958000
6	0.026935000	-0.376183000	1.221299000
6	0.581174000	-1.756641000	1.408023000
6	-0.007650000	-2.962570000	1.148608000
6	0.791765000	-4.081001000	1.535407000
6	1.980311000	-3.706689000	2.092501000
16	2.140512000	-1.994857000	2.164594000
6	6.357151000	-3.717192000	-1.986853000
6	2.485049000	1.554628000	-1.095685000
6	3.834240000	1.499813000	-0.408186000
6	4.569899000	2.682964000	-0.311372000

6	5.827956000	2.686674000	0.285908000
6	6.360707000	1.506628000	0.801927000
6	5.629249000	0.324309000	0.710489000
6	4.373374000	0.320158000	0.106484000
1	3.572851000	-0.285244000	-3.502358000
1	5.712286000	-1.540826000	-3.464129000
1	4.065388000	-4.293606000	-0.607768000
1	1.918933000	-3.054648000	-0.639373000
1	-0.980273000	-3.037168000	0.673838000
1	0.494661000	-5.114466000	1.402517000
1	2.769554000	-4.341260000	2.474467000
1	7.129618000	-3.087254000	-1.533733000
1	6.690315000	-3.963267000	-2.999056000
1	6.287335000	-4.641004000	-1.409421000
1	2.611821000	1.485264000	-2.177507000
1	2.004292000	2.519578000	-0.904361000
1	4.149958000	3.608477000	-0.698714000
1	6.387400000	3.614436000	0.356485000
1	7.337848000	1.509766000	1.274521000
1	6.032257000	-0.601295000	1.110718000
1	3.812033000	-0.607957000	0.054504000
7	-3.895719000	1.266717000	-1.507692000
6	-5.222994000	1.275398000	-1.907408000
6	-5.780323000	0.146525000	-1.411164000
7	-4.777529000	-0.519135000	-0.721879000
6	-2.941254000	2.290554000	-1.805014000
6	-3.270479000	3.620963000	-1.565407000
6	-2.321025000	4.608840000	-1.819125000
6	-1.054934000	4.264619000	-2.290024000
6	-0.743352000	2.928103000	-2.537799000
6	-1.690916000	1.934751000	-2.308762000
6	-4.952128000	-1.763819000	-0.038984000
6	-4.036314000	-2.793685000	-0.247615000
6	-4.201055000	-3.994516000	0.436719000
6	-5.275899000	-4.164827000	1.307348000
6	-6.192555000	-3.131696000	1.493672000
6	-6.032721000	-1.921126000	0.823745000
1	-5.630376000	2.061091000	-2.524173000

1	-6.775323000	-0.259568000	-1.504868000
1	-2.570007000	5.648742000	-1.633273000
1	0.229373000	2.645770000	-2.929095000
1	-3.492186000	-4.800772000	0.278049000
1	-7.029970000	-3.261314000	2.171253000
6	-3.616505000	0.171165000	-0.762920000
79	-1.822098000	-0.195154000	0.164819000
1	-0.316724000	5.038670000	-2.473326000
1	-5.402786000	-5.104608000	1.834748000
1	-4.248860000	3.874420000	-1.168443000
1	-1.466046000	0.895223000	-2.527144000
1	-6.729030000	-1.101982000	0.975423000
1	-3.218871000	-2.655284000	-0.948735000
6	1.840559000	2.527886000	2.019851000
6	1.021079000	3.709923000	2.096969000
6	-0.330843000	3.763453000	1.918437000
8	-1.129960000	2.714503000	1.760286000
1	1.530108000	4.624893000	2.374320000
7	1.504226000	1.503171000	1.331412000
6	-1.083644000	5.050584000	1.925124000
1	-1.644270000	5.137232000	0.988826000
1	-1.810630000	5.045714000	2.742831000
1	-0.416068000	5.905043000	2.028020000
6	3.153194000	2.529185000	2.746612000
1	2.944849000	2.499055000	3.819029000
1	3.758407000	1.664299000	2.475840000
1	3.684553000	3.455997000	2.513974000
8	-0.207296000	0.209641000	2.543284000
1	1.133378000	0.304979000	3.882033000
1	-1.000384000	-0.228833000	2.888826000
8	1.842058000	0.446465000	4.528487000
1	2.171990000	-0.438565000	4.720936000
1	-0.712833000	1.862000000	2.018827000

Zero-point correction= 0.733352 (Hartree/Particle)

Thermal correction to Energy= 0.784274

Thermal correction to Enthalpy= 0.785219

Thermal correction to Gibbs Free Energy= 0.642969

Sum of electronic and zero-point Energies= -3073.348309

Sum of electronic and thermal Energies= -3073.297387

Sum of electronic and thermal Enthalpies= -3073.296443
Sum of electronic and thermal Free Energies= -3073.438692

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6	-4.539206000	0.863110000	0.159455000
6	-5.537595000	1.048193000	-0.787583000
6	-6.697356000	0.282593000	-0.697106000
6	-6.858925000	-0.663052000	0.317491000
6	-5.833894000	-0.818413000	1.262685000
6	-4.681755000	-0.045220000	1.205915000
16	-3.161384000	1.975184000	0.120675000
8	-3.214474000	2.768881000	1.346368000
8	-3.138077000	2.689710000	-1.149525000
7	-1.750868000	1.017744000	0.316985000
6	-1.553938000	-0.077222000	-0.560716000
6	-0.385110000	-0.998690000	-0.267302000
6	-0.574697000	-1.686636000	1.062055000
6	-1.755137000	-2.113657000	1.614647000
6	-1.582475000	-2.815984000	2.843464000
6	-0.267842000	-2.919678000	3.200746000
16	0.763013000	-2.157259000	2.055819000
6	-8.108407000	-1.495027000	0.415804000
6	-0.648365000	1.799922000	0.928228000
6	-0.174837000	1.326601000	2.281994000
6	-1.054444000	0.800446000	3.227784000
6	-0.591452000	0.423087000	4.485434000
6	0.753058000	0.588391000	4.817978000
6	1.630775000	1.137346000	3.886515000
6	1.167892000	1.500539000	2.623289000
1	-5.403630000	1.770627000	-1.585931000
1	-7.484368000	0.418643000	-1.433129000
1	-5.951697000	-1.544510000	2.062618000
1	-3.903775000	-0.157405000	1.954673000
1	-2.717057000	-1.934314000	1.143714000
1	-2.396433000	-3.219906000	3.434363000
1	0.150648000	-3.391935000	4.080013000
1	-8.786736000	-1.289671000	-0.414595000
1	-8.638956000	-1.286881000	1.350401000
1	-7.868538000	-2.562478000	0.410379000

1	0.183853000	1.851510000	0.222387000
1	-1.010266000	2.825089000	1.038967000
1	-2.104359000	0.686666000	2.973781000
1	-1.283464000	0.002802000	5.209204000
1	1.111355000	0.294119000	5.799719000
1	2.677554000	1.278281000	4.139130000
1	1.853734000	1.924329000	1.891795000
6	-0.409130000	-1.528052000	-3.134350000
6	-1.834910000	-1.681835000	-3.317787000
6	-2.721972000	-1.126450000	-2.452657000
8	0.032633000	-0.287212000	-3.072056000
1	-2.169775000	-2.410376000	-4.046594000
7	-2.447840000	-0.206578000	-1.471177000
6	0.528129000	-2.571076000	-3.646620000
1	0.610200000	-2.440385000	-4.731179000
1	1.517568000	-2.453565000	-3.197192000
1	0.146022000	-3.570603000	-3.438515000
6	-4.182112000	-1.460862000	-2.555973000
1	-4.745715000	-0.573582000	-2.857634000
1	-4.353618000	-2.258776000	-3.280238000
1	-4.555184000	-1.771119000	-1.574268000
8	-0.366998000	-2.049902000	-1.266134000
1	1.000401000	-0.265807000	-2.940756000
1	-1.157591000	-2.648836000	-1.152633000
8	-2.459628000	-3.644862000	-0.891294000
1	-2.336544000	-4.178468000	-0.092586000
1	-2.669503000	-4.266651000	-1.602759000
79	1.550062000	-0.088779000	-0.428664000
6	3.395187000	0.819569000	-0.592958000
7	4.646668000	0.326542000	-0.454752000
7	3.569162000	2.152025000	-0.757997000
6	5.591740000	1.340572000	-0.516269000
6	4.956579000	-1.048246000	-0.205674000
6	4.910041000	2.494360000	-0.706093000
6	2.484100000	3.080303000	-0.880450000
1	6.649359000	1.140482000	-0.445644000
6	5.867240000	-1.364270000	0.798883000
6	4.346997000	-2.043393000	-0.966015000

1	5.246520000	3.511859000	-0.829783000
6	1.564813000	2.930258000	-1.916103000
6	2.341720000	4.083406000	0.074155000
6	6.165489000	-2.701548000	1.046588000
1	6.322264000	-0.573774000	1.387584000
6	4.641614000	-3.377165000	-0.698292000
1	3.660567000	-1.769858000	-1.760360000
6	0.463617000	3.780485000	-1.973674000
1	1.713976000	2.155433000	-2.661479000
6	1.245802000	4.940157000	-0.003092000
1	3.069945000	4.174308000	0.874712000
6	5.550047000	-3.708055000	0.305302000
1	6.871631000	-2.954198000	1.830653000
1	4.167885000	-4.157328000	-1.285283000
6	0.302287000	4.782601000	-1.017223000
1	-0.268047000	3.658420000	-2.765348000
1	1.122492000	5.719353000	0.741586000
1	5.780403000	-4.748924000	0.507433000
1	-0.560938000	5.438654000	-1.061775000

Zero-point correction= 0.733643 (Hartree/Particle)

Thermal correction to Energy= 0.783020

Thermal correction to Enthalpy= 0.783964

Thermal correction to Gibbs Free Energy= 0.647852

Sum of electronic and zero-point Energies= -3073.323452

Sum of electronic and thermal Energies= -3073.274075

Sum of electronic and thermal Enthalpies= -3073.273131

Sum of electronic and thermal Free Energies= -3073.409243

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6	0.389776000	2.852456000	-0.515863000
6	0.719694000	3.593354000	0.618034000
6	2.015973000	4.071644000	0.743620000
6	2.974776000	3.836112000	-0.253257000
6	2.604395000	3.110350000	-1.388266000
6	1.311732000	2.613606000	-1.529327000
16	-1.281604000	2.316781000	-0.730754000
8	-2.148994000	3.462818000	-0.499944000
8	-1.353289000	1.570920000	-1.982264000
7	-1.621032000	1.241403000	0.542229000

6	-1.097462000	-0.072439000	0.449041000
6	0.403326000	-0.218807000	0.406394000
6	1.105636000	0.428733000	1.398577000
6	0.599236000	1.079327000	2.564757000
6	1.589831000	1.620043000	3.358683000
6	2.860340000	1.438143000	2.801344000
16	2.864857000	0.558803000	1.373182000
6	4.384955000	4.325400000	-0.078301000
6	-2.947430000	1.390885000	1.207658000
6	-4.182697000	0.952318000	0.439943000
6	-4.821827000	-0.245852000	0.775073000
6	-5.984728000	-0.640420000	0.120346000
6	-6.527117000	0.160931000	-0.883572000
6	-5.907075000	1.362449000	-1.214176000
6	-4.747403000	1.760431000	-0.551050000
1	-0.021703000	3.782414000	1.389620000
1	2.292467000	4.641729000	1.626310000
1	3.332720000	2.933475000	-2.173978000
1	1.021421000	2.068235000	-2.420757000
1	-0.457351000	1.103669000	2.796036000
1	1.423293000	2.142118000	4.291714000
1	3.795044000	1.806926000	3.210549000
1	4.963480000	3.602819000	0.509249000
1	4.409862000	5.278386000	0.455646000
1	4.885476000	4.446769000	-1.041286000
1	-2.854640000	0.800511000	2.122951000
1	-3.024486000	2.444635000	1.480158000
1	-4.394318000	-0.873345000	1.552070000
1	-6.468024000	-1.573628000	0.393222000
1	-7.431945000	-0.146509000	-1.398893000
1	-6.330133000	2.001003000	-1.983600000
1	-4.283884000	2.708895000	-0.799562000
6	-1.527874000	-2.391397000	0.584580000
6	-1.037348000	-2.986902000	1.692270000
6	-0.775853000	-2.317507000	2.977438000
8	-1.095838000	-1.158602000	3.215633000
1	-0.832294000	-4.051326000	1.640149000
7	-1.894671000	-1.051786000	0.519416000

6	-0.094595000	-3.166497000	4.021745000
1	0.086930000	-2.578403000	4.921651000
1	-0.718791000	-4.032628000	4.265042000
1	0.852219000	-3.549468000	3.627104000
6	-1.875883000	-3.148911000	-0.664464000
1	-2.956822000	-3.095949000	-0.833053000
1	-1.387838000	-2.694909000	-1.533737000
1	-1.569105000	-4.192522000	-0.584038000
78	1.223060000	-1.389668000	-0.945955000
17	2.225967000	-2.863075000	-2.628127000
17	2.322507000	-2.598547000	0.781876000
6	0.411841000	-0.639859000	-2.453624000
8	-0.007096000	-0.334310000	-3.460646000

Zero-point correction= 0.454605 (Hartree/Particle)

Thermal correction to Energy= 0.492644

Thermal correction to Enthalpy= 0.493588

Thermal correction to Gibbs Free Energy= 0.380263

Sum of electronic and zero-point Energies= -3250.262006

Sum of electronic and thermal Energies= -3250.223967

Sum of electronic and thermal Enthalpies= -3250.223023

Sum of electronic and thermal Free Energies= -3250.336347

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6	1.338830000	2.719998000	-0.683327000
6	1.961340000	3.150784000	0.485043000
6	3.308101000	2.860795000	0.662119000
6	4.029926000	2.152141000	-0.305685000
6	3.381477000	1.767216000	-1.485688000
6	2.039576000	2.063573000	-1.693197000
16	-0.331475000	3.194002000	-0.984101000
8	-0.452598000	3.570927000	-2.387323000
8	-0.760652000	4.139962000	0.035941000
7	-1.337686000	1.806789000	-0.784018000
6	-0.918799000	0.467694000	-0.777743000
6	-0.055632000	-0.060884000	0.353456000
6	0.161361000	0.724447000	1.510931000
6	-0.648272000	1.727211000	2.061229000
6	-0.120611000	2.282050000	3.231359000
6	1.087801000	1.705962000	3.579769000

16	1.553249000	0.456508000	2.537128000
6	5.472074000	1.797298000	-0.078204000
6	-2.658967000	2.058836000	-1.433594000
6	-3.742914000	1.316828000	-0.692914000
6	-4.358859000	0.198386000	-1.254326000
6	-5.333588000	-0.499645000	-0.543196000
6	-5.694162000	-0.084079000	0.737191000
6	-5.090498000	1.041085000	1.298570000
6	-4.123864000	1.740804000	0.582361000
1	1.398799000	3.691844000	1.239145000
1	3.808241000	3.183791000	1.570846000
1	3.940561000	1.246745000	-2.258264000
1	1.546128000	1.805405000	-2.625863000
1	-1.597806000	2.006054000	1.626381000
1	-0.593982000	3.069771000	3.803427000
1	1.713187000	1.964842000	4.426089000
1	5.950822000	2.506036000	0.601018000
1	6.026987000	1.776597000	-1.018896000
1	5.545801000	0.801089000	0.372097000
1	-2.840913000	3.134568000	-1.367083000
1	-2.619648000	1.775745000	-2.487793000
1	-4.068983000	-0.125514000	-2.250250000
1	-5.807878000	-1.369125000	-0.988624000
1	-6.448378000	-0.631497000	1.294449000
1	-5.379206000	1.376183000	2.289894000
1	-3.662807000	2.629572000	1.008683000
6	-1.521495000	-1.661314000	-1.708088000
6	-2.022229000	-2.405435000	-0.683069000
6	-2.388033000	-1.877416000	0.619852000
8	-1.899313000	-0.841958000	1.093323000
1	-2.298410000	-3.433967000	-0.891065000
7	-1.400455000	-0.288940000	-1.690932000
6	-3.370798000	-2.663015000	1.439980000
1	-3.691517000	-2.081395000	2.304054000
1	-4.228781000	-2.976408000	0.841623000
1	-2.850251000	-3.565600000	1.784105000
6	-1.284170000	-2.265918000	-3.060496000
1	-0.281487000	-2.020549000	-3.423126000

1	-1.393849000	-3.350118000	-3.028213000
1	-1.996359000	-1.846437000	-3.778223000
78	1.125190000	-1.617038000	-0.029224000
17	2.651246000	-3.468738000	-0.543626000
17	0.532394000	-2.673536000	2.023426000
6	1.649230000	-1.023237000	-1.704113000
8	1.985154000	-0.801198000	-2.766275000

Zero-point correction= 0.454589 (Hartree/Particle)

Thermal correction to Energy= 0.491383

Thermal correction to Enthalpy= 0.492327

Thermal correction to Gibbs Free Energy= 0.384734

Sum of electronic and zero-point Energies= -3250.253394

Sum of electronic and thermal Energies= -3250.216600

Sum of electronic and thermal Enthalpies= -3250.215656

Sum of electronic and thermal Free Energies= -3250.323249

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6	-3.651701000	0.108095000	-0.900718000
6	-4.104324000	-0.980641000	-0.157058000
6	-5.087462000	-0.765176000	0.800821000
6	-5.634968000	0.507098000	1.002163000
6	-5.175927000	1.572731000	0.218468000
6	-4.182428000	1.385023000	-0.733880000
16	-2.439206000	-0.160974000	-2.158730000
8	-2.315204000	1.011651000	-3.001234000
8	-2.671068000	-1.468449000	-2.743922000
7	-0.889738000	-0.359615000	-1.330353000
6	-0.392786000	0.720715000	-0.686303000
6	1.059863000	0.889624000	-0.131464000
6	1.006500000	1.563794000	1.219415000
6	0.023966000	1.536749000	2.172153000
6	0.417580000	2.161668000	3.395903000
6	1.682373000	2.661717000	3.343229000
16	2.428190000	2.365479000	1.815935000
6	-6.722724000	0.719489000	2.017815000
6	-0.413041000	-1.757267000	-1.272315000
6	-1.094635000	-2.540663000	-0.177988000
6	-1.734203000	-3.744854000	-0.471913000
6	-2.391811000	-4.452751000	0.533743000

6	-2.416623000	-3.957321000	1.835845000
6	-1.770457000	-2.758075000	2.136086000
6	-1.111417000	-2.055694000	1.131865000
1	-3.704701000	-1.976573000	-0.320865000
1	-5.439101000	-1.602311000	1.396871000
1	-5.600008000	2.562838000	0.359550000
1	-3.819821000	2.208853000	-1.339392000
1	-0.951541000	1.089427000	2.013121000
1	-0.223187000	2.240004000	4.265587000
1	2.224974000	3.200578000	4.108644000
1	-7.705523000	0.598245000	1.549524000
1	-6.678657000	1.726887000	2.438206000
1	-6.650590000	-0.006780000	2.830457000
1	-0.591972000	-2.205968000	-2.247550000
1	0.662975000	-1.737260000	-1.131319000
1	-1.731694000	-4.115371000	-1.493293000
1	-2.893491000	-5.385738000	0.296712000
1	-2.936414000	-4.503674000	2.616555000
1	-1.783512000	-2.369538000	3.149647000
1	-0.625658000	-1.109582000	1.361668000
6	-0.909045000	3.028000000	-0.350164000
6	0.227014000	3.681470000	-0.871493000
6	1.361936000	3.047089000	-1.309361000
8	1.667899000	1.773664000	-1.102297000
1	0.193694000	4.760888000	-0.965627000
7	-1.176852000	1.748413000	-0.541725000
6	2.440013000	3.740001000	-2.066950000
1	2.151988000	4.760866000	-2.313926000
1	3.359240000	3.744025000	-1.472769000
1	2.644700000	3.179244000	-2.984348000
6	-1.963771000	3.836725000	0.334444000
1	-2.560936000	4.360469000	-0.422002000
1	-2.624033000	3.193543000	0.917289000
1	-1.501909000	4.590987000	0.975172000
78	2.388824000	-0.698506000	-0.033221000
17	2.776970000	-0.617435000	-2.404799000
17	4.051575000	-2.494457000	0.195643000
6	2.127989000	-0.919279000	1.779844000

8	2.002688000	-1.089576000	2.896842000
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Zero-point correction= 0.456846 (Hartree/Particle)

Thermal correction to Energy= 0.493816

Thermal correction to Enthalpy= 0.494760

Thermal correction to Gibbs Free Energy= 0.385807

Sum of electronic and zero-point Energies= -3250.275210

Sum of electronic and thermal Energies= -3250.238240

Sum of electronic and thermal Enthalpies= -3250.237296

Sum of electronic and thermal Free Energies= -3250.346249

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6	-3.411686000	0.976465000	0.610084000
6	-3.355844000	2.030026000	-0.299369000
6	-4.207658000	2.004731000	-1.398239000
6	-5.118987000	0.958922000	-1.579326000
6	-5.180917000	-0.058722000	-0.618088000
6	-4.331238000	-0.059719000	0.480245000
16	-2.312073000	1.022765000	1.991705000
8	-2.773907000	0.119340000	3.039658000
8	-2.081249000	2.418114000	2.329675000
7	-0.753617000	0.519574000	1.368931000
6	-0.556257000	-0.804730000	1.019549000
6	0.534094000	-1.207555000	-0.055210000
6	-0.193779000	-1.422214000	-1.365505000
6	-1.315320000	-0.806897000	-1.849481000
6	-1.595391000	-1.148797000	-3.208659000
6	-0.686659000	-2.020615000	-3.726247000
16	0.530105000	-2.436987000	-2.577133000
6	-6.016805000	0.917863000	-2.784651000
6	0.337441000	1.440767000	1.740831000
6	0.552501000	2.586087000	0.779670000
6	1.386543000	3.633382000	1.177899000
6	1.653040000	4.691406000	0.314020000
6	1.084260000	4.718104000	-0.959104000
6	0.251239000	3.678088000	-1.360997000
6	-0.010202000	2.616214000	-0.495099000
1	-2.666415000	2.854466000	-0.151069000
1	-4.171204000	2.815923000	-2.119387000
1	-5.906828000	-0.858824000	-0.733351000

1	-4.372233000	-0.842253000	1.228269000
1	-1.932332000	-0.135709000	-1.261659000
1	-2.445414000	-0.766870000	-3.761867000
1	-0.666155000	-2.465517000	-4.712305000
1	-6.102565000	1.902051000	-3.249517000
1	-7.016521000	0.566462000	-2.516928000
1	-5.615525000	0.225251000	-3.532536000
1	0.124747000	1.829314000	2.738321000
1	1.243056000	0.844375000	1.849848000
1	1.829707000	3.616080000	2.170681000
1	2.305134000	5.497551000	0.635478000
1	1.291503000	5.543690000	-1.632560000
1	-0.191143000	3.683550000	-2.353037000
1	-0.644371000	1.795054000	-0.822058000
6	-1.823481000	-2.795450000	0.849288000
6	-0.788431000	-3.774910000	0.790989000
6	0.548599000	-3.579891000	0.615428000
8	1.167155000	-2.436471000	0.330901000
1	-1.097981000	-4.807318000	0.898112000
7	-1.706196000	-1.504152000	1.019190000
6	1.540661000	-4.689850000	0.703522000
1	2.040019000	-4.815650000	-0.262282000
1	2.307701000	-4.418206000	1.436177000
1	1.065135000	-5.623901000	0.999237000
6	-3.235647000	-3.300661000	0.746412000
1	-3.795711000	-3.026872000	1.645207000
1	-3.720788000	-2.818747000	-0.108877000
1	-3.272723000	-4.381523000	0.614079000
8	0.379242000	-1.500315000	2.586243000
1	1.347363000	-1.398750000	2.465112000
1	0.101593000	-0.922630000	3.351731000
8	-0.424757000	0.134747000	4.478895000
1	-0.090860000	0.061346000	5.383420000
1	-1.391283000	0.067383000	4.520351000
78	2.221855000	-0.024732000	-0.387402000
17	4.253754000	1.267357000	-0.908278000
17	3.255318000	-0.757464000	1.696241000
6	1.591969000	0.594750000	-1.997260000

8	1.271400000	0.977088000	-3.019227000
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Zero-point correction= 0.507528 (Hartree/Particle)

Thermal correction to Energy= 0.548115

Thermal correction to Enthalpy= 0.549059

Thermal correction to Gibbs Free Energy= 0.435222

Sum of electronic and zero-point Energies= -3403.029893

Sum of electronic and thermal Energies= -3402.989307

Sum of electronic and thermal Enthalpies= -3402.988363

Sum of electronic and thermal Free Energies= -3403.102200

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6	-3.602377000	0.077915000	-0.719886000
6	-4.075826000	-1.143720000	-0.249841000
6	-5.101469000	-1.140240000	0.690538000
6	-5.660930000	0.056837000	1.144474000
6	-5.176344000	1.268279000	0.629837000
6	-4.147116000	1.290380000	-0.299102000
16	-2.341511000	0.069060000	-1.963995000
8	-2.259583000	1.390004000	-2.584465000
8	-2.554258000	-1.076175000	-2.828654000
7	-0.817550000	-0.266557000	-1.195147000
6	-0.338725000	0.685027000	-0.333615000
6	1.102547000	0.750238000	0.283840000
6	0.928393000	0.955581000	1.775545000
6	-0.032127000	0.496150000	2.635415000
6	0.244703000	0.814020000	4.001217000
6	1.402428000	1.518050000	4.146945000
16	2.174657000	1.808853000	2.632593000
6	-6.773106000	0.060742000	2.155670000
6	-0.320034000	-1.643202000	-1.434808000
6	-1.080694000	-2.681768000	-0.649288000
6	-1.776022000	-3.700473000	-1.301236000
6	-2.499313000	-4.637210000	-0.563910000
6	-2.534206000	-4.556093000	0.827018000
6	-1.825578000	-3.549367000	1.483515000
6	-1.096634000	-2.621528000	0.745757000
1	-3.666003000	-2.080270000	-0.614679000
1	-5.475241000	-2.086600000	1.069768000
1	-5.613115000	2.204654000	0.965779000

1	-3.769017000	2.227415000	-0.693660000
1	-0.922288000	-0.032113000	2.312091000
1	-0.399437000	0.540085000	4.828072000
1	1.840873000	1.904357000	5.057634000
1	-7.046529000	-0.954564000	2.448807000
1	-7.661142000	0.554385000	1.749313000
1	-6.477449000	0.612300000	3.053394000
1	-0.364906000	-1.837508000	-2.504962000
1	0.726382000	-1.658931000	-1.147344000
1	-1.767638000	-3.742368000	-2.386657000
1	-3.041913000	-5.424948000	-1.077055000
1	-3.105390000	-5.280145000	1.399665000
1	-1.839386000	-3.489831000	2.567372000
1	-0.542894000	-1.833960000	1.252794000
6	-0.857887000	2.813541000	0.529005000
6	0.099164000	3.609808000	-0.090525000
6	1.193749000	2.942731000	-0.919891000
8	1.822969000	1.878524000	-0.214232000
1	0.348334000	4.548418000	0.399207000
7	-1.176682000	1.605243000	0.021356000
6	2.317715000	3.912033000	-1.231777000
1	2.771338000	4.286558000	-0.311223000
1	3.080360000	3.399819000	-1.824130000
1	1.919421000	4.752606000	-1.805283000
6	-1.715069000	3.334808000	1.635237000
1	-1.873108000	4.410733000	1.534886000
1	-2.669525000	2.807866000	1.674085000
1	-1.183773000	3.158542000	2.578837000
8	0.616376000	2.436483000	-2.099523000
1	-0.864683000	3.913687000	-1.091704000
1	1.266696000	1.820872000	-2.488316000
8	-1.634993000	3.945323000	-2.049234000
1	-1.149222000	4.322615000	-2.805295000
1	-1.769659000	2.987210000	-2.268105000
78	2.495058000	-0.731615000	-0.089018000
17	4.340750000	-2.358618000	-0.462639000
17	2.618546000	-0.028533000	-2.431935000
6	2.378310000	-1.433617000	1.599797000

8	2.338778000	-1.908450000	2.633267000
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Zero-point correction= 0.508751 (Hartree/Particle)

Thermal correction to Energy= 0.549415

Thermal correction to Enthalpy= 0.550359

Thermal correction to Gibbs Free Energy= 0.436253

Sum of electronic and zero-point Energies= -3403.034448

Sum of electronic and thermal Energies= -3402.993785

Sum of electronic and thermal Enthalpies= -3402.992840

Sum of electronic and thermal Free Energies= -3403.106946

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6	-3.447205000	0.144873000	-1.124936000
6	-4.372966000	-0.894634000	-1.196914000
6	-5.642746000	-0.697353000	-0.671610000
6	-5.997409000	0.519884000	-0.078503000
6	-5.055954000	1.553328000	-0.048810000
6	-3.779015000	1.378869000	-0.571610000
16	-1.814856000	-0.151902000	-1.761100000
8	-1.374050000	1.059228000	-2.455632000
8	-1.851197000	-1.419582000	-2.469793000
7	-0.726284000	-0.393872000	-0.504389000
6	-0.081578000	0.709534000	0.100023000
6	1.441091000	0.601637000	0.401920000
6	1.644282000	0.685619000	1.890599000
6	0.848028000	0.214567000	2.897841000
6	1.442369000	0.363063000	4.190218000
6	2.673071000	0.942673000	4.133863000
16	3.132787000	1.324324000	2.513784000
6	-7.359787000	0.692920000	0.534029000
6	-0.751910000	-1.723536000	0.143420000
6	-2.052521000	-2.018962000	0.860245000
6	-2.671998000	-3.255993000	0.689700000
6	-3.864725000	-3.544848000	1.353231000
6	-4.448176000	-2.593753000	2.185806000
6	-3.836688000	-1.349858000	2.353025000
6	-2.645123000	-1.064662000	1.694682000
1	-4.096909000	-1.840640000	-1.649608000
1	-6.369248000	-1.504232000	-0.714531000
1	-5.325367000	2.509039000	0.391727000

1	-3.050512000	2.180710000	-0.527555000
1	-0.125086000	-0.236046000	2.727875000
1	0.965449000	0.055666000	5.113180000
1	3.335194000	1.189809000	4.953085000
1	-7.423696000	0.135084000	1.474834000
1	-8.139935000	0.306207000	-0.127193000
1	-7.571493000	1.742522000	0.748340000
1	-0.536444000	-2.485020000	-0.609119000
1	0.066612000	-1.734918000	0.865891000
1	-2.224014000	-3.991155000	0.026005000
1	-4.340236000	-4.510427000	1.211212000
1	-5.379816000	-2.814624000	2.697736000
1	-4.294155000	-0.599161000	2.990691000
1	-2.192241000	-0.080678000	1.797503000
6	-0.278413000	2.911866000	0.926759000
6	0.837913000	3.509819000	0.494854000
6	1.738007000	2.902045000	-0.536207000
8	2.223859000	1.642269000	-0.217639000
1	1.139819000	4.465281000	0.909411000
7	-0.792271000	1.731798000	0.365937000
6	2.933518000	3.762851000	-0.870098000
1	3.522482000	3.927690000	0.034830000
1	3.547133000	3.256350000	-1.617586000
1	2.597090000	4.724875000	-1.261761000
6	-1.166197000	3.475670000	1.991987000
1	-0.773933000	4.417921000	2.376810000
1	-2.173407000	3.633850000	1.593287000
1	-1.247455000	2.759507000	2.817243000
8	0.982946000	2.732659000	-1.819095000
1	-0.030615000	3.139911000	-1.875408000
1	1.114749000	1.811801000	-2.192003000
8	-1.273825000	3.633207000	-1.967085000
1	-1.383723000	4.361464000	-2.599593000
1	-1.777457000	2.864960000	-2.299267000
78	2.352349000	-1.029083000	-0.489265000
17	3.531020000	-2.912722000	-1.596177000
17	1.771694000	-0.085862000	-2.669638000
6	2.813724000	-1.789424000	1.109159000

8	3.112676000	-2.295630000	2.083698000
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Zero-point correction= 0.508327 (Hartree/Particle)

Thermal correction to Energy= 0.548381

Thermal correction to Enthalpy= 0.549325

Thermal correction to Gibbs Free Energy= 0.435875

Sum of electronic and zero-point Energies= -3403.045885

Sum of electronic and thermal Energies= -3403.005830

Sum of electronic and thermal Enthalpies= -3403.004886

Sum of electronic and thermal Free Energies= -3403.118336

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6	-3.602377000	0.077915000	-0.719886000
6	-4.075826000	-1.143720000	-0.249841000
6	-5.101469000	-1.140240000	0.690538000
6	-5.660930000	0.056837000	1.144474000
6	-5.176344000	1.268279000	0.629837000
6	-4.147116000	1.290380000	-0.299102000
16	-2.341511000	0.069060000	-1.963995000
8	-2.259583000	1.390004000	-2.584465000
8	-2.554258000	-1.076175000	-2.828654000
7	-0.817550000	-0.266557000	-1.195147000
6	-0.338725000	0.685027000	-0.333615000
6	1.102547000	0.750238000	0.283840000
6	0.928393000	0.955581000	1.775545000
6	-0.032127000	0.496150000	2.635415000
6	0.244703000	0.814020000	4.001217000
6	1.402428000	1.518050000	4.146945000
16	2.174657000	1.808853000	2.632593000
6	-6.773106000	0.060742000	2.155670000
6	-0.320034000	-1.643202000	-1.434808000
6	-1.080694000	-2.681768000	-0.649288000
6	-1.776022000	-3.700473000	-1.301236000
6	-2.499313000	-4.637210000	-0.563910000
6	-2.534206000	-4.556093000	0.827018000
6	-1.825578000	-3.549367000	1.483515000
6	-1.096634000	-2.621528000	0.745757000
1	-3.666003000	-2.080270000	-0.614679000
1	-5.475241000	-2.086600000	1.069768000
1	-5.613115000	2.204654000	0.965779000

1	-3.769017000	2.227415000	-0.693660000
1	-0.922288000	-0.032113000	2.312091000
1	-0.399437000	0.540085000	4.828072000
1	1.840873000	1.904357000	5.057634000
1	-7.046529000	-0.954564000	2.448807000
1	-7.661142000	0.554385000	1.749313000
1	-6.477449000	0.612300000	3.053394000
1	-0.364906000	-1.837508000	-2.504962000
1	0.726382000	-1.658931000	-1.147344000
1	-1.767638000	-3.742368000	-2.386657000
1	-3.041913000	-5.424948000	-1.077055000
1	-3.105390000	-5.280145000	1.399665000
1	-1.839386000	-3.489831000	2.567372000
1	-0.542894000	-1.833960000	1.252794000
6	-0.857887000	2.813541000	0.529005000
6	0.099164000	3.609808000	-0.090525000
6	1.193749000	2.942731000	-0.919891000
8	1.822969000	1.878524000	-0.214232000
1	0.348334000	4.548418000	0.399207000
7	-1.176682000	1.605243000	0.021356000
6	2.317715000	3.912033000	-1.231777000
1	2.771338000	4.286558000	-0.311223000
1	3.080360000	3.399819000	-1.824130000
1	1.919421000	4.752606000	-1.805283000
6	-1.715069000	3.334808000	1.635237000
1	-1.873108000	4.410733000	1.534886000
1	-2.669525000	2.807866000	1.674085000
1	-1.183773000	3.158542000	2.578837000
8	0.616376000	2.436483000	-2.099523000
1	-0.864683000	3.913687000	-1.091704000
1	1.266696000	1.820872000	-2.488316000
8	-1.634993000	3.945323000	-2.049234000
1	-1.149222000	4.322615000	-2.805295000
1	-1.769659000	2.987210000	-2.268105000
78	2.495058000	-0.731615000	-0.089018000
17	4.340750000	-2.358618000	-0.462639000
17	2.618546000	-0.028533000	-2.431935000
6	2.378310000	-1.433617000	1.599797000

8	2.338778000	-1.908450000	2.633267000
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Zero-point correction= 0.505412 (Hartree/Particle)

Thermal correction to Energy= 0.545207

Thermal correction to Enthalpy= 0.546151

Thermal correction to Gibbs Free Energy= 0.433167

Sum of electronic and zero-point Energies= -3403.018714

Sum of electronic and thermal Energies= -3402.978919

Sum of electronic and thermal Enthalpies= -3402.977975

Sum of electronic and thermal Free Energies= -3403.090959

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6	-3.477053000	0.524685000	-1.030496000
6	-4.277032000	-0.615338000	-0.944358000
6	-5.492188000	-0.517369000	-0.282074000
6	-5.917924000	0.696760000	0.273578000
6	-5.095785000	1.822209000	0.154917000
6	-3.870020000	1.749755000	-0.497324000
16	-1.971521000	0.442624000	-1.943741000
8	-1.539905000	1.785610000	-2.280612000
8	-2.085053000	-0.583456000	-2.960635000
7	-0.732143000	-0.191386000	-0.877942000
6	-0.228996000	0.579062000	0.087961000
6	1.128077000	0.271963000	0.774078000
6	0.838857000	-0.689675000	1.909193000
6	1.062550000	-2.037296000	2.004112000
6	0.531745000	-2.610805000	3.198200000
6	-0.081593000	-1.687466000	3.991012000
16	-0.018105000	-0.108047000	3.309458000
6	-7.238500000	0.775240000	0.987581000
6	-0.371390000	-1.610438000	-1.092265000
6	-1.482806000	-2.519307000	-0.615147000
6	-1.985616000	-3.491565000	-1.481037000
6	-3.020450000	-4.331201000	-1.072640000
6	-3.563178000	-4.198883000	0.204164000
6	-3.064187000	-3.229041000	1.073033000
6	-2.029431000	-2.392110000	0.665492000
1	-3.959357000	-1.554031000	-1.389308000
1	-6.127590000	-1.395079000	-0.203871000
1	-5.422805000	2.769799000	0.572948000

1	-3.227155000	2.620590000	-0.596719000
1	1.587363000	-2.608069000	1.244731000
1	0.613541000	-3.660795000	3.450897000
1	-0.542038000	-1.836270000	4.959090000
1	-8.039973000	0.364724000	0.366783000
1	-7.490776000	1.805688000	1.245117000
1	-7.210314000	0.188397000	1.911330000
1	-0.162818000	-1.760584000	-2.149307000
1	0.552289000	-1.793218000	-0.543844000
1	-1.573708000	-3.577466000	-2.482765000
1	-3.407791000	-5.080509000	-1.755807000
1	-4.374805000	-4.846745000	0.520353000
1	-3.486081000	-3.117040000	2.067026000
1	-1.665909000	-1.622176000	1.342661000
6	-0.824138000	2.661123000	1.194452000
6	0.423863000	3.501345000	1.159302000
6	1.568225000	2.695588000	0.579310000
8	1.539257000	1.474236000	1.381622000
1	0.649731000	3.767684000	2.197149000
7	-1.004760000	1.533624000	0.595057000
6	2.943270000	3.299113000	0.749419000
1	3.167248000	3.440856000	1.808653000
1	3.689647000	2.621882000	0.319180000
1	2.992570000	4.262115000	0.235902000
6	-1.962504000	3.198298000	1.992635000
1	-2.338451000	4.082836000	1.462793000
1	-2.759027000	2.462012000	2.096426000
1	-1.611222000	3.528827000	2.973901000
8	1.230473000	2.491734000	-0.755455000
1	0.230461000	4.425066000	0.605018000
1	1.956189000	2.095943000	-1.267287000
8	-1.359982000	4.270995000	-1.057898000
1	-2.010651000	4.340998000	-1.768356000
1	-0.790109000	3.543743000	-1.352149000
78	2.755410000	-0.368209000	-0.386690000
17	4.867011000	-1.082707000	-1.454178000
17	1.873825000	0.091951000	-2.583803000
6	3.641558000	-0.600067000	1.209577000

8	4.253402000	-0.704418000	2.161685000
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Zero-point correction= 0.510218 (Hartree/Particle)

Thermal correction to Energy= 0.551032

Thermal correction to Enthalpy= 0.551977

Thermal correction to Gibbs Free Energy= 0.436766

Sum of electronic and zero-point Energies= -3403.051034

Sum of electronic and thermal Energies= -3403.010220

Sum of electronic and thermal Enthalpies= -3403.009276

Sum of electronic and thermal Free Energies= -3403.124487

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6	3.504321000	-0.981946000	-0.825223000
6	4.317939000	0.070911000	-1.235448000
6	5.559942000	0.226636000	-0.629072000
6	5.994144000	-0.656048000	0.363531000
6	5.162498000	-1.722724000	0.732285000
6	3.918429000	-1.896011000	0.143746000
16	1.947725000	-1.219991000	-1.628547000
8	1.526784000	-2.598082000	-1.401772000
8	2.031838000	-0.681023000	-2.972791000
7	0.741583000	-0.243037000	-0.872966000
6	0.187121000	-0.666672000	0.287421000
6	-1.091577000	-0.007321000	0.892035000
6	-0.711774000	1.202410000	1.707393000
6	-0.805920000	2.528721000	1.378042000
6	-0.266273000	3.394250000	2.374855000
6	0.216795000	2.709903000	3.450455000
16	0.026758000	1.009184000	3.270751000
6	7.329703000	-0.478943000	1.030821000
6	0.495416000	1.080816000	-1.486813000
6	1.647144000	2.031771000	-1.254562000
6	2.131474000	2.777658000	-2.330348000
6	3.187915000	3.669695000	-2.154026000
6	3.770244000	3.819234000	-0.897019000
6	3.291397000	3.075644000	0.181134000
6	2.236555000	2.184901000	0.004606000
1	3.988569000	0.759063000	-2.007935000
1	6.200306000	1.048798000	-0.934392000
1	5.500378000	-2.427678000	1.486964000

1	3.281984000	-2.730910000	0.415361000
1	-1.250608000	2.881065000	0.453136000
1	-0.251983000	4.474066000	2.292651000
1	0.652111000	3.109844000	4.356925000
1	7.199565000	-0.253898000	2.094185000
1	7.896123000	0.334967000	0.574592000
1	7.921839000	-1.396231000	0.963792000
1	0.307110000	0.941127000	-2.549130000
1	-0.423565000	1.466237000	-1.046541000
1	1.685607000	2.646778000	-3.312847000
1	3.558892000	4.240662000	-2.999547000
1	4.595800000	4.510358000	-0.758089000
1	3.746128000	3.181730000	1.161336000
1	1.897495000	1.584182000	0.846134000
6	0.867314000	-2.193976000	2.002169000
6	-0.374278000	-3.045288000	2.033317000
6	-1.470510000	-2.334721000	1.254298000
8	-1.534762000	-1.004030000	1.809394000
1	-0.668410000	-3.188608000	3.078236000
7	1.066051000	-1.229730000	1.180894000
6	-2.831644000	-2.983359000	1.304401000
1	-3.180793000	-3.034635000	2.338403000
1	-3.535964000	-2.393242000	0.710841000
1	-2.776782000	-3.996814000	0.897630000
6	1.927442000	-2.491743000	3.009222000
1	2.208202000	-3.549211000	2.950082000
1	2.801660000	-1.858304000	2.858192000
1	1.519666000	-2.328058000	4.012954000
8	-1.025242000	-2.136872000	-0.054802000
1	-0.160173000	-4.034130000	1.609752000
1	-0.997137000	-2.905448000	-0.748592000
8	-0.997839000	-3.686962000	-1.986459000
1	-1.474633000	-3.042538000	-2.539795000
1	-0.066843000	-3.603558000	-2.253025000
78	-2.727808000	0.345125000	-0.365863000
17	-4.907972000	0.771945000	-1.492341000
17	-1.969767000	-0.625992000	-2.479284000
6	-3.531773000	1.087745000	1.101682000

8	-4.088458000	1.536529000	1.986366000
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Zero-point correction= 0.508298 (Hartree/Particle)

Thermal correction to Energy= 0.547984

Thermal correction to Enthalpy= 0.548928

Thermal correction to Gibbs Free Energy= 0.435602

Sum of electronic and zero-point Energies= -3403.041262

Sum of electronic and thermal Energies= -3403.001576

Sum of electronic and thermal Enthalpies= -3403.000632

Sum of electronic and thermal Free Energies= -3403.113957

C-P2

6	-2.611563000	-1.508415000	-1.743666000
6	-2.729395000	-2.762251000	-1.148483000
6	-3.983405000	-3.173953000	-0.715231000
6	-5.105840000	-2.352612000	-0.871510000
6	-4.957041000	-1.113022000	-1.505312000
6	-3.711201000	-0.676660000	-1.938096000
16	-1.011053000	-0.871296000	-2.118229000
8	-1.103756000	0.133773000	-3.162407000
8	-0.098225000	-2.005584000	-2.304977000
7	-0.483736000	-0.102739000	-0.718235000
6	-0.313600000	1.327163000	-0.752647000
6	0.347941000	1.936822000	0.522270000
6	-0.494215000	2.214250000	1.719643000
6	-0.334456000	1.611974000	2.936912000
6	-1.299862000	2.029206000	3.899189000
6	-2.158112000	2.960912000	3.393951000
16	-1.821751000	3.325697000	1.744739000
6	-6.441893000	-2.783147000	-0.333043000
6	-0.427614000	-0.929673000	0.498429000
6	-1.672630000	-0.981712000	1.364930000
6	-1.701566000	-1.922836000	2.397740000
6	-2.796964000	-1.999878000	3.253587000
6	-3.878833000	-1.136668000	3.083491000
6	-3.853102000	-0.198830000	2.053910000
6	-2.755325000	-0.119821000	1.198083000
1	-1.856735000	-3.395746000	-1.020213000
1	-4.093551000	-4.144547000	-0.240333000
1	-5.826460000	-0.477818000	-1.648080000

1	-3.585633000	0.296376000	-2.402766000
1	0.446593000	0.881769000	3.127279000
1	-1.347522000	1.656887000	4.915121000
1	-2.976551000	3.459456000	3.896447000
1	-6.583503000	-3.861365000	-0.440533000
1	-7.260645000	-2.267318000	-0.839347000
1	-6.505059000	-2.546694000	0.735208000
1	-0.147761000	-1.939398000	0.177369000
1	0.421991000	-0.594797000	1.103207000
1	-0.859886000	-2.599788000	2.529905000
1	-2.806777000	-2.736008000	4.051891000
1	-4.734211000	-1.194620000	3.749617000
1	-4.689468000	0.480030000	1.912143000
1	-2.740514000	0.616456000	0.399532000
6	-1.464202000	3.151035000	-1.656788000
6	-0.155712000	3.801516000	-2.037152000
6	0.997018000	3.004831000	-1.444078000
8	0.939309000	3.117015000	-0.016508000
1	-0.131277000	4.828011000	-1.657307000
7	-1.542648000	2.016829000	-1.074970000
6	2.353157000	3.378039000	-1.976692000
1	2.590329000	4.402899000	-1.682875000
1	3.116699000	2.706003000	-1.581639000
1	2.351218000	3.312374000	-3.066908000
6	-2.718307000	3.900991000	-1.976294000
1	-2.757278000	4.125138000	-3.047459000
1	-3.596366000	3.321822000	-1.687739000
1	-2.720372000	4.859104000	-1.445392000
8	0.734326000	1.628464000	-1.690166000
1	-0.076714000	3.848217000	-3.129148000
1	1.136169000	1.245456000	0.842772000
8	2.342786000	-0.591065000	-1.912499000
1	1.701035000	-1.310719000	-2.111406000
1	1.831800000	0.250193000	-1.955432000
78	3.072124000	-0.922812000	0.041713000
17	3.832560000	-1.408368000	2.185237000
17	2.474926000	-3.176467000	-0.349477000
6	3.593864000	0.823063000	0.393833000

8	3.934832000	1.861042000	0.696677000
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Zero-point correction= 0.513610 (Hartree/Particle)

Thermal correction to Energy= 0.552801

Thermal correction to Enthalpy= 0.553745

Thermal correction to Gibbs Free Energy= 0.440338

Sum of electronic and zero-point Energies= -3403.073324

Sum of electronic and thermal Energies= -3403.034133

Sum of electronic and thermal Enthalpies= -3403.033189

Sum of electronic and thermal Free Energies= -3403.146597

C-TSb4

6	-3.674677000	1.242145000	-0.375597000
6	-4.023506000	0.831758000	-1.657390000
6	-5.133275000	0.006886000	-1.806170000
6	-5.878762000	-0.407715000	-0.697199000
6	-5.504164000	0.036008000	0.578903000
6	-4.406403000	0.866341000	0.751477000
16	-2.297436000	2.319121000	-0.145866000
8	-2.616051000	3.260193000	0.917854000
8	-1.822376000	2.829973000	-1.416560000
7	-1.087989000	1.288246000	0.570175000
6	-0.637251000	0.216493000	-0.177274000
6	0.422031000	-0.696430000	0.391994000
6	0.283370000	-1.178430000	1.709170000
6	1.306773000	-1.586832000	2.577476000
6	0.853538000	-1.948660000	3.850242000
6	-0.517592000	-1.837329000	3.963213000
16	-1.266313000	-1.276459000	2.547488000
6	-7.046130000	-1.340684000	-0.858606000
6	-0.352364000	1.883361000	1.722434000
6	0.876251000	2.674164000	1.336612000
6	0.770504000	3.898240000	0.670063000
6	1.917729000	4.599375000	0.309698000
6	3.179553000	4.089354000	0.617833000
6	3.292119000	2.879843000	1.297817000
6	2.141956000	2.177806000	1.658591000
1	-3.431454000	1.145720000	-2.510178000
1	-5.424269000	-0.323639000	-2.798858000
1	-6.084933000	-0.270916000	1.443896000

1	-4.119171000	1.216239000	1.738532000
1	2.346601000	-1.587420000	2.276723000
1	1.492004000	-2.279965000	4.658628000
1	-1.121408000	-2.071691000	4.832229000
1	-7.395129000	-1.364607000	-1.892852000
1	-7.877591000	-1.046167000	-0.213091000
1	-6.755956000	-2.358810000	-0.576328000
1	-1.074527000	2.511165000	2.242915000
1	-0.072076000	1.083760000	2.403253000
1	-0.208810000	4.308387000	0.437104000
1	1.827215000	5.547981000	-0.210102000
1	4.071534000	4.637766000	0.331922000
1	4.270157000	2.478718000	1.545658000
1	2.224362000	1.229390000	2.186223000
6	-0.601117000	-1.104612000	-1.960094000
6	-0.506553000	-2.271401000	-1.220204000
6	-1.480508000	-2.824262000	-0.236160000
8	-1.154951000	-3.784900000	0.436051000
1	0.161527000	-3.038353000	-1.605786000
7	-1.045810000	0.058633000	-1.403929000
6	-2.887730000	-2.278766000	-0.196636000
1	-3.362207000	-2.470906000	-1.165320000
1	-3.442352000	-2.789755000	0.591075000
1	-2.922019000	-1.199771000	-0.033162000
6	-0.109482000	-1.003028000	-3.368286000
1	0.367224000	-1.928678000	-3.690964000
1	-0.968541000	-0.799120000	-4.018489000
1	0.583974000	-0.163754000	-3.477196000
78	2.217193000	-0.653314000	-0.519392000
17	2.623861000	-2.952263000	-0.007453000
17	4.406123000	-0.505428000	-1.588247000
6	2.008651000	1.079088000	-1.152684000
8	1.926363000	2.088063000	-1.665018000

Zero-point correction= 0.454587 (Hartree/Particle)

Thermal correction to Energy= 0.491403

Thermal correction to Enthalpy= 0.492348

Thermal correction to Gibbs Free Energy= 0.385203

Sum of electronic and zero-point Energies= -3250.250738

Sum of electronic and thermal Energies= -3250.213921

Sum of electronic and thermal Enthalpies= -3250.212977
Sum of electronic and thermal Free Energies= -3250.320121

C-TSc4

6	3.285754000	-0.178197000	1.553426000
6	2.968556000	-1.499492000	1.871841000
6	3.857869000	-2.500878000	1.512705000
6	5.053045000	-2.201603000	0.843899000
6	5.354017000	-0.865465000	0.566117000
6	4.477197000	0.155490000	0.919697000
16	2.112869000	1.096876000	1.902567000
8	2.835345000	2.347573000	2.081192000
8	1.242212000	0.587994000	2.966273000
7	1.114040000	1.305555000	0.542923000
6	-0.224586000	0.776200000	0.626488000
6	-0.494201000	-0.622367000	0.138082000
6	0.516310000	-1.484573000	-0.390344000
6	0.401459000	-2.872449000	-0.482056000
6	1.480004000	-3.481930000	-1.137467000
6	2.383711000	-2.551083000	-1.605906000
16	1.975752000	-0.957287000	-1.192886000
6	5.980978000	-3.312263000	0.437670000
6	1.275634000	2.554213000	-0.270706000
6	2.302508000	2.445169000	-1.368352000
6	3.625189000	2.827984000	-1.136192000
6	4.578496000	2.718228000	-2.147008000
6	4.208551000	2.242735000	-3.403431000
6	2.883065000	1.885435000	-3.649592000
6	1.934277000	1.988027000	-2.636076000
1	2.043318000	-1.748066000	2.380296000
1	3.621277000	-3.534771000	1.748424000
1	6.284647000	-0.618975000	0.063771000
1	4.716545000	1.190491000	0.703108000
1	-0.431943000	-3.415097000	-0.052371000
1	1.582745000	-4.548881000	-1.288544000
1	3.270367000	-2.736987000	-2.200675000
1	6.281878000	-3.903497000	1.307746000
1	6.879920000	-2.924894000	-0.045615000
1	5.479042000	-3.992018000	-0.258639000

1	0.288995000	2.743951000	-0.701741000
1	1.527945000	3.388091000	0.385921000
1	3.902622000	3.218894000	-0.160082000
1	5.605787000	3.013489000	-1.956106000
1	4.949161000	2.160830000	-4.193098000
1	2.587438000	1.528892000	-4.631393000
1	0.900242000	1.702425000	-2.818921000
6	-3.689086000	2.654368000	0.505583000
6	-2.566683000	3.286245000	1.261293000
6	-1.408428000	2.668374000	1.572911000
8	-4.105387000	1.542255000	0.791568000
1	-2.709223000	4.321648000	1.560999000
7	-1.255492000	1.397172000	1.020768000
6	-4.319391000	3.480851000	-0.575874000
1	-4.657460000	4.437710000	-0.164931000
1	-3.567588000	3.703766000	-1.340407000
1	-5.156350000	2.944143000	-1.022883000
6	-0.415276000	3.267586000	2.528617000
1	-0.247629000	2.570799000	3.354933000
1	0.556250000	3.483045000	2.082184000
1	-0.820180000	4.197379000	2.931011000
8	-0.642341000	-1.335611000	2.185766000
1	-1.496378000	-0.898219000	2.449835000
1	0.036404000	-0.856492000	2.692099000
8	-2.957881000	-0.128811000	2.749463000
1	-3.752533000	-0.586862000	3.053071000
1	-3.244647000	0.477130000	2.035029000
78	-2.334843000	-0.985987000	-0.514022000
17	-1.757717000	0.623425000	-2.226783000
17	-4.521517000	-1.446889000	-1.529191000
6	-2.788780000	-2.252749000	0.746063000
8	-3.116304000	-3.054860000	1.481138000

Zero-point correction= 0.505618 (Hartree/Particle)

Thermal correction to Energy= 0.547457

Thermal correction to Enthalpy= 0.548401

Thermal correction to Gibbs Free Energy= 0.430071

Sum of electronic and zero-point Energies= -3403.001599

Sum of electronic and thermal Energies= -3402.959760

Sum of electronic and thermal Enthalpies= -3402.958815

Sum of electronic and thermal Free Energies= -3403.077145