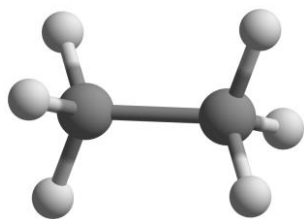
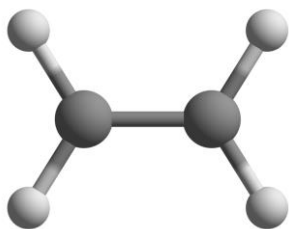


Optimized structures at B97-3c level.



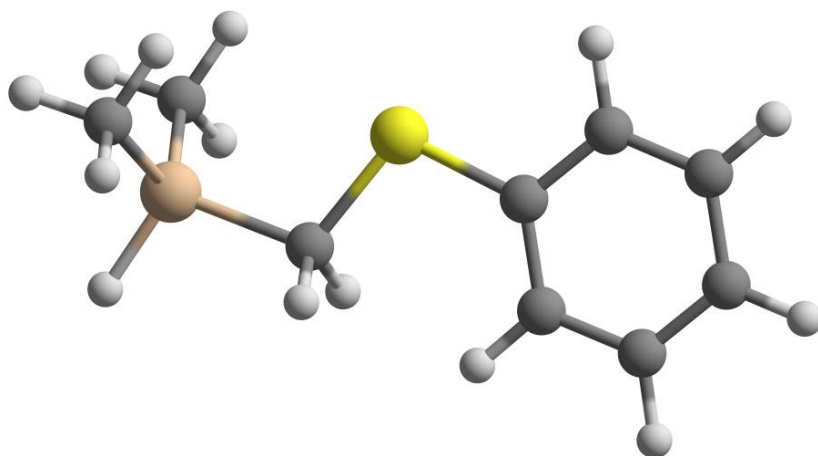
Final Gibbs free energy ... -79.73656094 Eh

6	0.000000000	-1.092924000	-0.716703000
1	0.000000000	-0.078785000	-1.115510000
1	0.878274000	-1.599994000	-1.115595000
1	-0.878274000	-1.599994000	-1.115595000
6	0.000000000	-1.092883000	0.801848000
1	-0.878274000	-0.585814000	1.200740000
1	0.000000000	-2.107022000	1.200655000
1	0.878274000	-0.585814000	1.200740000

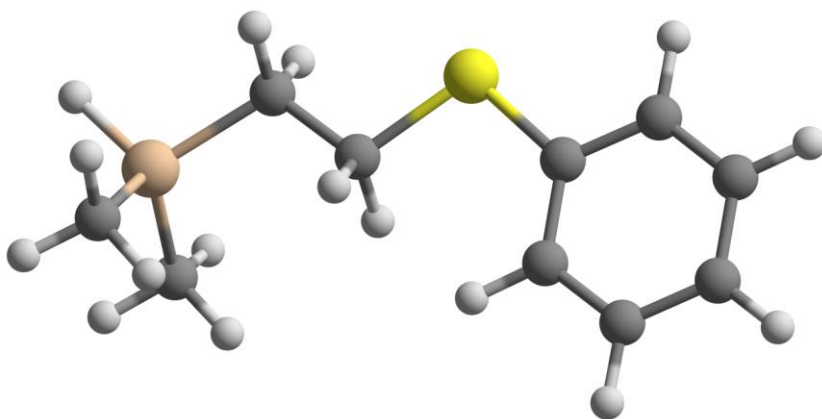


Final Gibbs free energy ... -78.51771632 Eh

6	1.054102000	-0.871072000	-0.451423000
6	1.054102000	-0.871072000	0.872209000
1	1.054102000	0.048568000	-1.022609000
1	1.054102000	-1.790712000	-1.022609000
1	1.054102000	0.048569000	1.443395000
1	1.054102000	-1.790712000	1.443395000

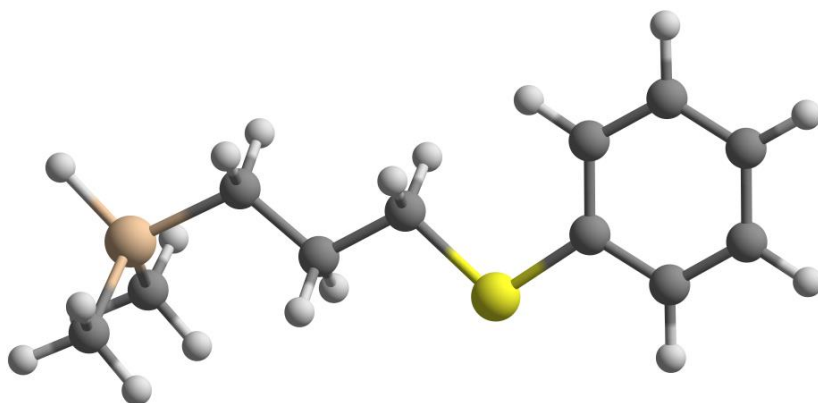


Final Gibbs free energy ... -1038.64922682 Eh			
16	2.306255000	-1.847854000	-1.327360000
14	4.044988000	-4.267708000	-1.931778000
6	2.854988000	-0.489273000	1.064656000
1	3.656378000	-1.186523000	1.256681000
6	2.080026000	-0.598716000	-0.086058000
6	3.687012000	-2.851051000	-0.719858000
1	4.579397000	-2.234620000	-0.610856000
1	3.443746000	-3.272115000	0.255868000
6	2.559591000	-5.403310000	-2.048527000
1	2.760077000	-6.254020000	-2.698703000
1	1.694968000	-4.875261000	-2.447882000
1	2.281360000	-5.793587000	-1.070423000
6	1.050987000	0.320335000	-0.305985000
1	0.443284000	0.242219000	-1.198418000
6	2.601144000	0.524648000	1.978686000
1	3.212280000	0.597200000	2.868930000
6	4.527726000	-3.580897000	-3.606249000
1	5.379494000	-2.906522000	-3.528956000
1	3.706332000	-3.020781000	-4.050659000
1	4.799211000	-4.378381000	-4.296938000
6	1.580588000	1.436195000	1.760905000
1	1.387609000	2.223804000	2.476410000
6	0.807338000	1.326351000	0.611249000
1	0.006285000	2.029885000	0.426054000
1	5.196903000	-5.007500000	-1.343179000

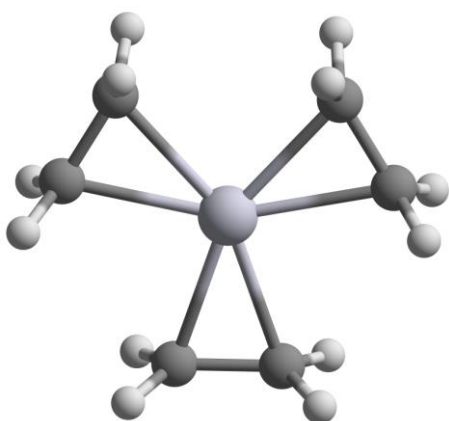


Final Gibbs free energy ... -1077.91484942 Eh

16	2.146584000	-1.716135000	-1.266990000
6	3.133566000	0.077014000	0.654081000
1	4.010259000	-0.542169000	0.766947000
6	2.122940000	-0.270998000	-0.240309000
6	3.721980000	-2.541543000	-0.838219000
1	4.540885000	-1.854091000	-1.042196000
1	3.717857000	-2.764147000	0.227328000
6	1.004342000	0.559267000	-0.355109000
1	0.212959000	0.298753000	-1.046178000
6	3.021925000	1.232780000	1.415244000
1	3.815977000	1.487824000	2.105030000
6	1.912305000	2.054294000	1.299686000
1	1.831384000	2.953202000	1.895423000
6	0.904093000	1.708145000	0.407988000
1	0.030272000	2.337998000	0.304764000
6	3.860864000	-3.810011000	-1.657928000
1	3.015590000	-4.473463000	-1.465828000
1	3.827072000	-3.572475000	-2.722861000
14	5.461267000	-4.754654000	-1.302890000
1	5.458128000	-5.966526000	-2.169888000
6	6.955892000	-3.699124000	-1.728826000
1	7.024198000	-2.821944000	-1.085680000
1	7.881344000	-4.261207000	-1.608210000
1	6.918094000	-3.349041000	-2.759769000
6	5.525888000	-5.287324000	0.497496000
1	5.590446000	-4.430135000	1.167477000
1	4.641788000	-5.858606000	0.778211000
1	6.395633000	-5.914316000	0.690736000

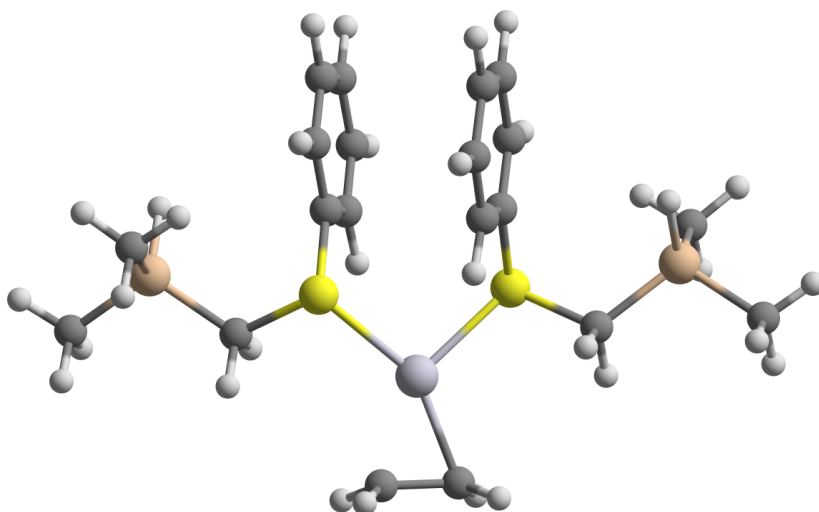


Final Gibbs free energy ... -1117.18155548 Eh			
16	-0.948166000	0.702101000	-0.498745000
14	3.730418000	2.536686000	1.949897000
6	-2.866821000	-0.183683000	-2.182814000
1	-3.412182000	-0.378941000	-1.268412000
6	-1.582068000	0.362961000	-2.118941000
6	0.735619000	1.332868000	-0.810544000
1	1.302067000	0.583452000	-1.361768000
1	0.676498000	2.235982000	-1.416512000
6	1.411433000	1.632704000	0.516227000
1	0.810600000	2.358398000	1.066576000
1	1.425819000	0.724390000	1.120536000
6	3.885760000	0.979145000	2.989592000
1	4.475611000	1.160545000	3.887307000
1	4.370410000	0.175479000	2.436213000
1	2.909939000	0.615336000	3.310449000
6	-0.891535000	0.606651000	-3.304298000
1	0.101315000	1.029341000	-3.290381000
6	-3.442275000	-0.477516000	-3.405420000
1	-4.437768000	-0.900678000	-3.434453000
6	2.829233000	3.877464000	2.909730000
1	1.836384000	3.549125000	3.216320000
1	2.707374000	4.782336000	2.315275000
1	3.373954000	4.150492000	3.812818000
6	-2.752622000	-0.235316000	-4.587331000
1	-3.204292000	-0.466702000	-5.542263000
6	-1.478961000	0.306284000	-4.525940000
1	-0.927925000	0.501722000	-5.436697000
1	5.096524000	3.025500000	1.604677000
6	2.830488000	2.161358000	0.331498000
1	3.425647000	1.438948000	-0.233417000
1	2.813672000	3.071662000	-0.273754000



Final Gibbs free energy ... -355.24139878 Eh

78	1.175048000	-0.477243000	-0.255318000
6	3.173126000	-1.282401000	0.146642000
6	3.228217000	0.106092000	0.241056000
1	3.641591000	0.691738000	-0.568015000
1	3.243910000	0.586568000	1.209214000
1	3.544054000	-1.783696000	-0.736247000
1	3.144552000	-1.889101000	1.040753000
6	0.668635000	-2.596181000	-0.502003000
6	-0.480369000	-1.839357000	-0.716307000
1	1.218222000	-3.002595000	-1.339314000
1	0.813667000	-3.113081000	0.436209000
1	-0.830916000	-1.653017000	-1.721661000
1	-1.234652000	-1.763825000	0.054213000
6	0.829936000	1.685497000	-0.197196000
6	-0.371924000	1.054022000	-0.508385000
1	1.010115000	2.051588000	0.803737000
1	1.411108000	2.164661000	-0.972423000
1	-1.133656000	0.927249000	0.247980000
1	-0.731206000	1.039033000	-1.527777000

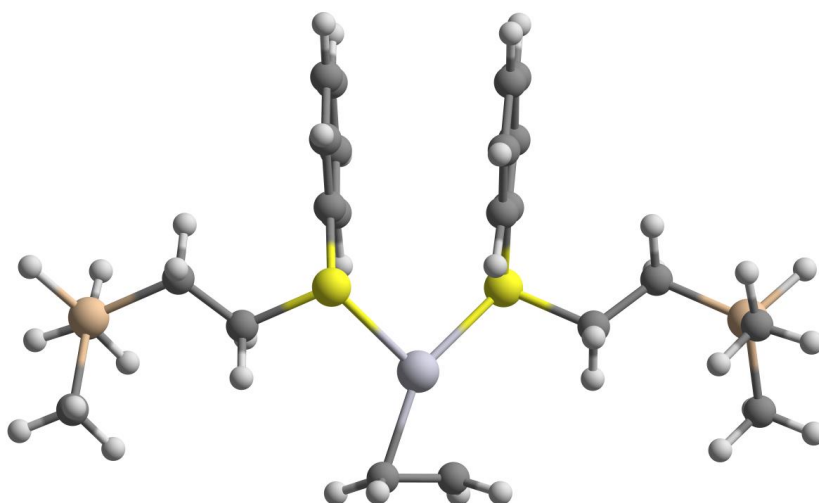


Final Gibbs free energy ... -2275.49702906 Eh

78	1.626062000	-0.176546000	0.159724000
16	0.218766000	1.077348000	-1.276500000

14	-2.259053000	3.010046000	-1.048976000
6	-1.611841000	-1.005575000	-1.320313000
1	-1.345996000	-1.144009000	-0.281301000
6	-0.997385000	0.004254000	-2.051203000
6	-0.888075000	2.047450000	-0.171320000
1	-1.276532000	1.378264000	0.593228000
1	-0.208093000	2.731679000	0.335708000
6	-3.113753000	4.090273000	0.230053000
1	-3.936675000	4.649570000	-0.214145000
1	-2.423169000	4.812215000	0.665639000
1	-3.525461000	3.494978000	1.044196000
6	-1.283252000	0.167147000	-3.398397000
1	-0.781063000	0.939251000	-3.963337000
6	-2.528955000	-1.838801000	-1.939167000
1	-3.007533000	-2.624832000	-1.370074000
6	-1.530618000	4.048701000	-2.429021000
1	-0.995770000	3.431875000	-3.148024000
1	-0.823390000	4.779313000	-2.036599000
1	-2.306220000	4.593303000	-2.966162000
6	-2.822217000	-1.676579000	-3.287954000
1	-3.533894000	-2.333585000	-3.770305000
6	-2.193804000	-0.677994000	-4.015814000
1	-2.406259000	-0.557159000	-5.069604000
6	2.794504000	-0.321920000	1.880442000
6	2.134566000	0.950206000	1.837644000
1	2.712019000	1.839934000	1.611154000
1	1.302100000	1.137739000	2.508033000
1	3.860450000	-0.371877000	1.683381000
1	2.451939000	-1.074104000	2.582650000
1	-3.247169000	2.051570000	-1.606904000
16	1.725039000	-2.197095000	-1.073998000
14	3.917400000	-4.246616000	-2.039676000
6	2.288457000	-0.799120000	-3.403225000
1	2.883556000	-0.155373000	-2.770263000
6	1.607141000	-1.870172000	-2.837408000
6	3.480857000	-2.741514000	-0.981721000
1	4.113263000	-1.884138000	-1.200708000
1	3.624174000	-2.966273000	0.074943000
6	5.680235000	-4.748344000	-1.622194000
1	5.998927000	-5.601408000	-2.220547000
1	5.774751000	-5.029079000	-0.573334000
1	6.381902000	-3.936622000	-1.810575000
6	0.794916000	-2.676170000	-3.620885000
1	0.249699000	-3.490914000	-3.166255000
6	2.171292000	-0.552438000	-4.761017000
1	2.702883000	0.280537000	-5.201872000
6	2.719919000	-5.645873000	-1.689228000
1	1.692440000	-5.349206000	-1.888963000
1	2.773465000	-5.952123000	-0.644546000
1	2.941245000	-6.518865000	-2.302098000
6	1.363064000	-1.360763000	-5.551463000

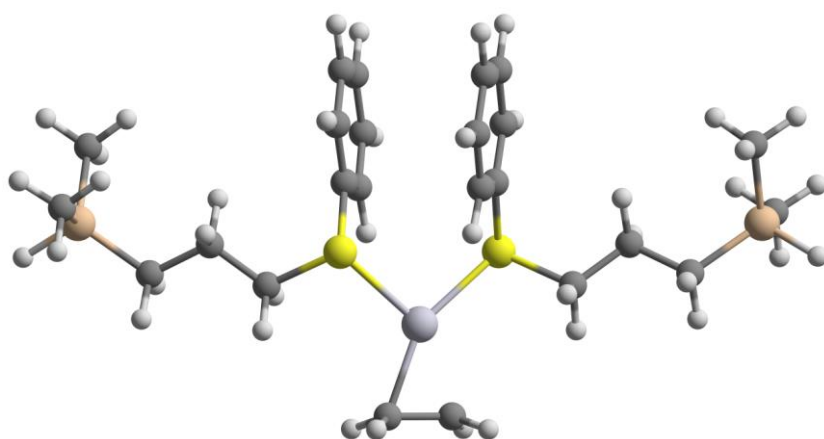
1	1.267960000	-1.161364000	-6.610690000
6	0.671153000	-2.416404000	-4.978095000
1	0.028024000	-3.039062000	-5.585459000
1	3.850979000	-3.872156000	-3.475597000



Final Gibbs free energy ... -2354.03430456 Eh

78	1.823203000	0.099963000	0.067695000
16	0.514314000	1.262089000	-1.530524000
6	-1.441459000	-0.693132000	-1.324828000
1	-1.153761000	-0.746374000	-0.283732000
6	-0.788110000	0.200961000	-2.165835000
6	-0.529622000	2.430893000	-0.540792000
1	-1.028111000	1.832488000	0.216809000
1	0.208512000	3.048264000	-0.035004000
6	-1.108524000	0.253266000	-3.514881000
1	-0.584075000	0.942107000	-4.161735000
6	-2.421256000	-1.527602000	-1.837451000
1	-2.926793000	-2.225081000	-1.182690000
6	-2.741592000	-1.481974000	-3.189057000
1	-3.499899000	-2.142198000	-3.588863000
6	-2.081618000	-0.594526000	-4.025325000
1	-2.318745000	-0.562693000	-5.080374000
6	2.989785000	0.073290000	1.795978000
6	2.435568000	1.380281000	1.595891000
1	3.081627000	2.185075000	1.262691000
1	1.628721000	1.716079000	2.239231000
1	4.047005000	-0.086471000	1.610394000
1	2.593246000	-0.555843000	2.585301000
16	1.748061000	-2.057969000	-0.914412000
6	2.411016000	-0.965513000	-3.376847000
1	3.041818000	-0.292064000	-2.812949000
6	1.664023000	-1.925761000	-2.703250000
6	3.478068000	-2.704745000	-0.757867000
1	4.129733000	-1.937189000	-1.165704000
1	3.634930000	-2.725774000	0.317605000
6	0.811368000	-2.766229000	-3.404703000
1	0.225088000	-3.499422000	-2.869261000

6	2.309183000	-0.857926000	-4.754103000
1	2.889068000	-0.108646000	-5.276678000
6	1.452893000	-1.694687000	-5.459888000
1	1.367497000	-1.600914000	-6.534438000
6	0.702134000	-2.643444000	-4.782758000
1	0.025160000	-3.289644000	-5.325399000
6	3.687545000	-4.051508000	-1.403900000
1	3.035694000	-4.796017000	-0.943678000
1	3.407501000	-4.006631000	-2.457834000
14	5.484314000	-4.633879000	-1.304958000
1	5.555020000	-5.983399000	-1.935189000
6	6.591857000	-3.454002000	-2.259796000
1	6.624485000	-2.470560000	-1.791523000
1	7.615271000	-3.823962000	-2.309860000
1	6.239967000	-3.319383000	-3.282109000
6	6.043918000	-4.762886000	0.483830000
1	6.041609000	-3.789126000	0.973128000
1	5.394274000	-5.421512000	1.059363000
1	7.056370000	-5.159028000	0.553409000
6	-1.493143000	3.238391000	-1.373819000
1	-0.948096000	3.828791000	-2.112528000
1	-2.149281000	2.571584000	-1.935909000
14	-2.578313000	4.386752000	-0.334115000
1	-3.438874000	5.160930000	-1.274168000
6	-1.520000000	5.583750000	0.654045000
1	-0.895394000	5.059651000	1.377075000
1	-0.860665000	6.162138000	0.007697000
1	-2.136407000	6.290019000	1.209104000
6	-3.677715000	3.379723000	0.809381000
1	-4.385671000	4.016875000	1.338281000
1	-4.252971000	2.637982000	0.256190000
1	-3.094187000	2.849129000	1.561294000

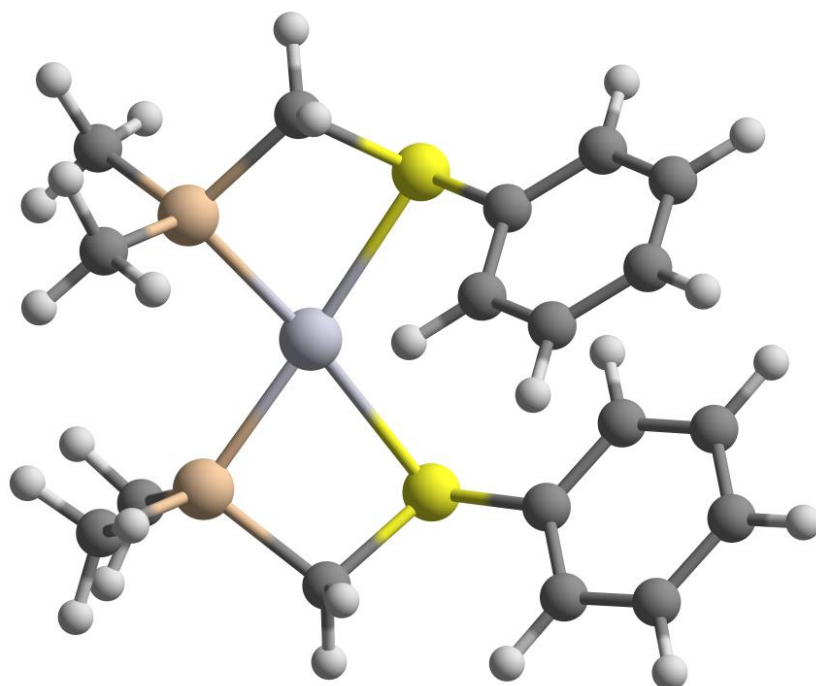


Final Gibbs free energy ... -2432.56640988 Eh

78	1.874453000	0.150119000	0.076271000
16	0.504321000	1.300933000	-1.480948000
6	-1.398171000	-0.708463000	-1.279825000
1	-1.102443000	-0.763168000	-0.241083000
6	-0.777018000	0.211928000	-2.116396000

6	-0.545173000	2.425407000	-0.463593000
1	-1.042071000	1.820350000	0.290812000
1	0.176299000	3.059734000	0.046719000
6	-1.105679000	0.265610000	-3.463463000
1	-0.604091000	0.973986000	-4.107566000
6	-2.357116000	-1.565952000	-1.794253000
1	-2.838518000	-2.283234000	-1.142704000
6	-2.687346000	-1.517481000	-3.143226000
1	-3.429338000	-2.195220000	-3.544315000
6	-2.057367000	-0.604839000	-3.975711000
1	-2.300807000	-0.571509000	-5.029291000
6	3.077187000	0.134672000	1.779353000
6	2.494372000	1.431631000	1.599869000
1	3.117387000	2.250422000	1.257071000
1	1.693922000	1.748011000	2.260551000
1	4.132528000	-0.005237000	1.569541000
1	2.708057000	-0.507571000	2.571427000
16	1.817227000	-2.002015000	-0.922748000
6	2.447867000	-0.876108000	-3.379792000
1	3.069519000	-0.197105000	-2.812327000
6	1.723332000	-1.856729000	-2.711650000
6	3.539236000	-2.643818000	-0.768823000
1	4.209513000	-1.890759000	-1.175595000
1	3.703715000	-2.683082000	0.305807000
6	0.880988000	-2.705440000	-3.415717000
1	0.309962000	-3.453012000	-2.883509000
6	2.335706000	-0.757620000	-4.755575000
1	2.898569000	0.007043000	-5.274446000
6	1.491640000	-1.604011000	-5.464365000
1	1.398691000	-1.502278000	-6.537569000
6	0.762149000	-2.572684000	-4.791880000
1	0.093386000	-3.225654000	-5.336674000
6	3.738544000	-3.992221000	-1.423782000
1	3.024962000	-4.701534000	-1.001418000
1	3.496997000	-3.909163000	-2.483639000
6	-1.528315000	3.229181000	-1.284775000
1	-0.978655000	3.795757000	-2.038403000
1	-2.177289000	2.543479000	-1.830050000
6	5.165682000	-4.507678000	-1.254414000
1	5.407546000	-4.599488000	-0.192426000
1	5.873080000	-3.778431000	-1.658125000
6	-2.370127000	4.166159000	-0.422161000
1	-2.911877000	3.589544000	0.332186000
1	-1.721515000	4.848499000	0.133314000
14	-3.618694000	5.184655000	-1.406095000
1	-4.389469000	6.026183000	-0.445517000
14	5.477098000	-6.168039000	-2.096858000
1	6.902162000	-6.543285000	-1.865914000
6	4.373710000	-7.499453000	-1.359638000
1	3.320003000	-7.288765000	-1.541121000
1	4.589449000	-8.475553000	-1.792953000

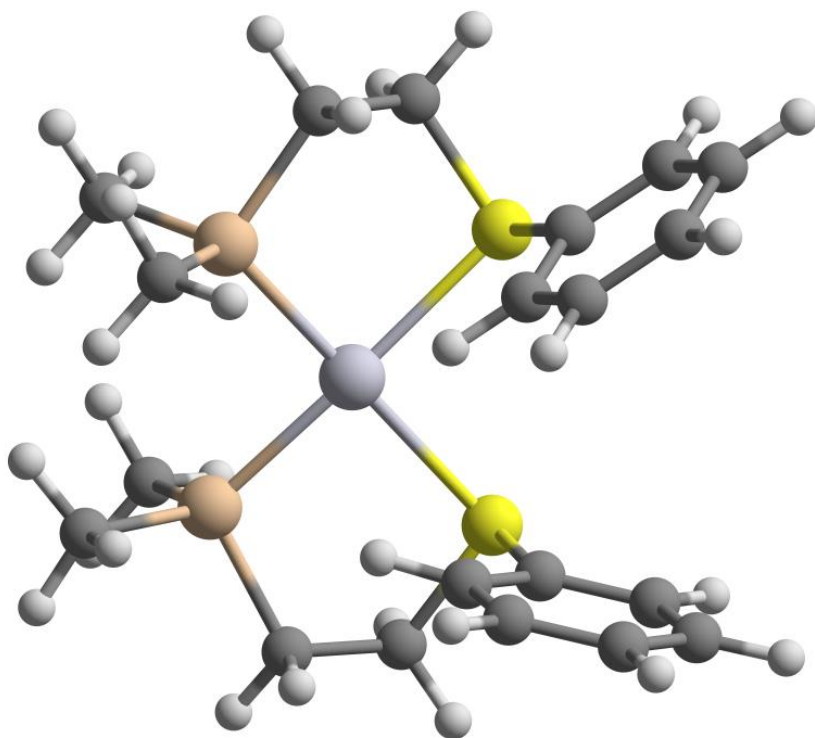
1	4.511861000	-7.582076000	-0.282041000
6	5.178165000	-6.026273000	-3.947382000
1	5.788516000	-5.240492000	-4.391408000
1	5.419401000	-6.957350000	-4.459146000
1	4.136087000	-5.794580000	-4.166243000
6	-2.732180000	6.311223000	-2.621847000
1	-3.437288000	6.935585000	-3.169550000
1	-2.032926000	6.974501000	-2.113737000
1	-2.166796000	5.737617000	-3.355928000
6	-4.813847000	4.054284000	-2.316057000
1	-5.315164000	3.370060000	-1.632169000
1	-5.585070000	4.626912000	-2.830169000
1	-4.301271000	3.451434000	-3.065289000



Final Gibbs free energy ... -2195.82798882 Eh

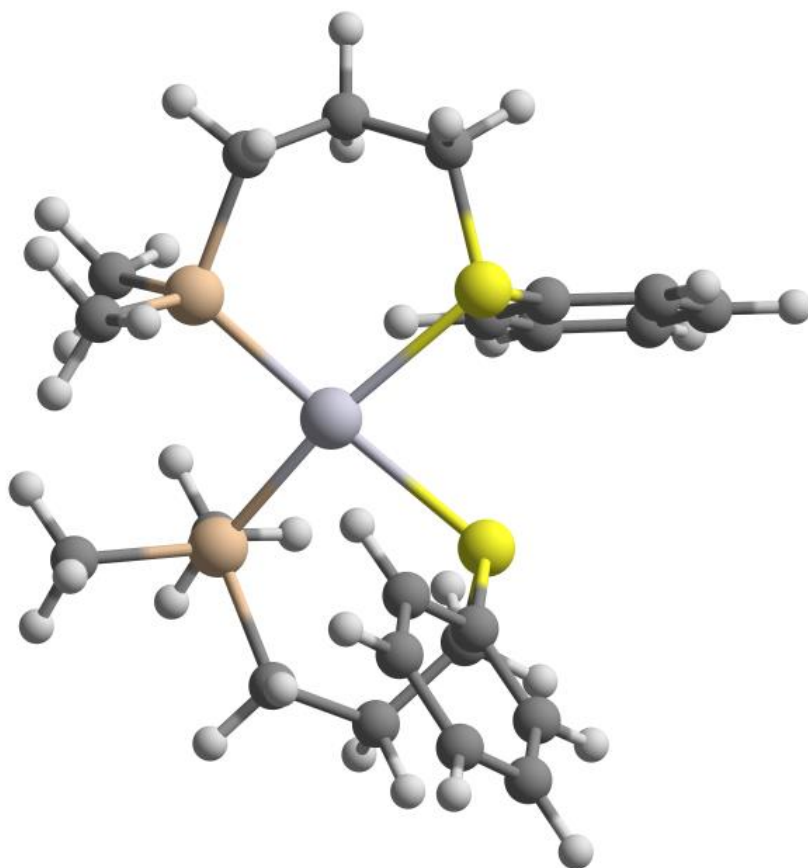
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16	0.069336000	2.011835000	-1.493810000
16	0.106028000	-2.160944000	-1.376147000
14	-2.397941000	-1.860326000	-0.029906000
14	-2.502375000	1.701961000	-0.123094000
6	-1.145581000	3.017914000	-0.488590000
1	-0.621630000	3.328369000	0.412163000
1	-1.405703000	3.909312000	-1.056313000
6	2.355390000	-2.769091000	0.180141000
1	1.762392000	-3.509867000	0.696283000
6	1.800002000	-2.004140000	-0.837255000
6	-0.822031000	-2.980141000	-0.016171000
1	-0.884532000	-4.054176000	-0.179274000
1	-0.295024000	-2.787341000	0.915449000
6	-2.964557000	1.846970000	1.699477000
1	-3.739963000	1.131150000	1.966425000
1	-3.341183000	2.844395000	1.932887000

1	-2.105945000	1.651261000	2.340067000
6	-3.655345000	-2.595080000	-1.226238000
1	-4.514456000	-1.933526000	-1.334881000
1	-4.021569000	-3.564750000	-0.884203000
1	-3.221939000	-2.724643000	-2.216617000
6	1.549219000	2.033411000	-0.482583000
6	1.605412000	1.309805000	0.704618000
1	0.739197000	0.736967000	1.010505000
6	2.662350000	2.734014000	-0.929956000
1	2.610382000	3.289284000	-1.856423000
6	-4.033037000	2.075741000	-1.157898000
1	-3.790118000	2.104596000	-2.218849000
1	-4.482157000	3.032177000	-0.884017000
1	-4.788407000	1.302082000	-1.020475000
6	2.583890000	-1.071604000	-1.513836000
1	2.145065000	-0.466631000	-2.295441000
6	3.686782000	-2.584596000	0.528985000
1	4.112685000	-3.180883000	1.325259000
6	3.832289000	2.714717000	-0.182409000
1	4.699402000	3.259749000	-0.531257000
6	3.888745000	2.000733000	1.005235000
1	4.804065000	1.980535000	1.581592000
6	-3.142263000	-1.876638000	1.701237000
1	-2.459518000	-1.449278000	2.433210000
1	-3.389789000	-2.891915000	2.015236000
1	-4.062078000	-1.293527000	1.731662000
6	2.773846000	1.300484000	1.446801000
1	2.821288000	0.725010000	2.361267000
6	4.467793000	-1.653116000	-0.137361000
1	5.502688000	-1.509934000	0.142198000
6	3.910763000	-0.902054000	-1.164107000
1	4.504618000	-0.160627000	-1.680157000



Final Gibbs free energy ... -2274.39219099 Eh			
78	0.957708000	-0.235249000	-0.675878000
16	-0.665744000	-1.642329000	-1.896876000
16	0.252620000	1.778009000	-1.943139000
14	2.740364000	1.000514000	0.121012000
14	1.447899000	-2.051954000	0.663382000
6	-0.108157000	-3.333942000	-1.387701000
1	-0.888983000	-4.022099000	-1.710343000
1	0.769127000	-3.501945000	-2.011064000
6	0.216180000	-3.414707000	0.079734000
1	0.622239000	-4.405254000	0.303921000
1	-0.703904000	-3.320898000	0.658860000
6	-1.033753000	2.312905000	0.474794000
1	-0.185124000	1.842959000	0.948102000
6	-1.074679000	2.407331000	-0.913616000
6	1.616211000	2.994485000	-1.612870000
1	2.310905000	2.799736000	-2.428862000
1	1.178371000	3.978159000	-1.775405000
6	2.280064000	2.828251000	-0.270922000
1	1.638479000	3.223247000	0.517108000
1	3.189522000	3.436553000	-0.253574000
6	1.063441000	-1.842722000	2.504337000
1	1.752028000	-1.161444000	2.997140000
1	1.122467000	-2.804395000	3.018264000
1	0.055570000	-1.453957000	2.648592000
6	4.306274000	0.641528000	-0.883518000
1	4.650482000	-0.378995000	-0.728030000
1	5.117807000	1.315996000	-0.602787000
1	4.126287000	0.756991000	-1.951894000
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6	-2.371036000	-0.892066000	0.154832000

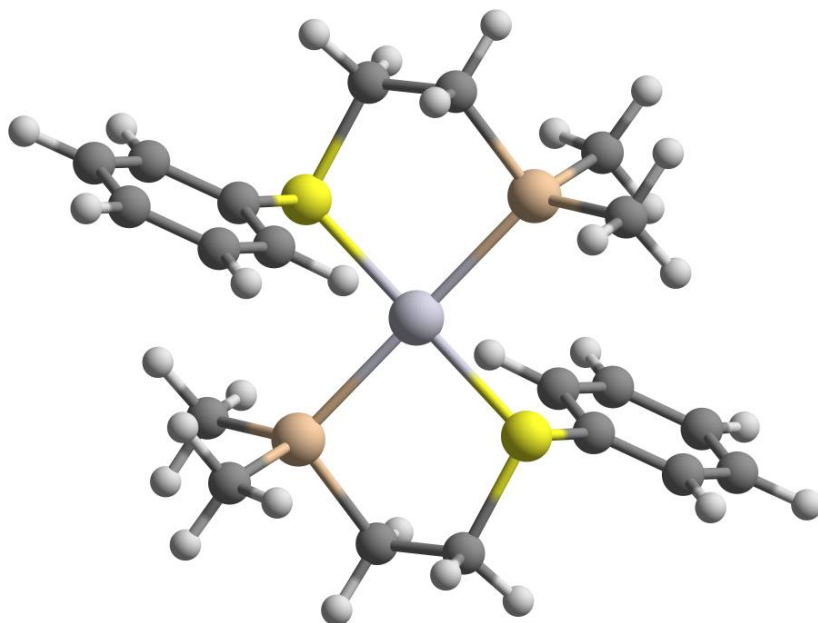
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6	-3.370784000	-2.105844000	-1.671553000
1	-3.273105000	-2.599917000	-2.628841000
6	3.182591000	-2.794374000	0.523872000
1	3.433136000	-3.021203000	-0.511999000
1	3.261788000	-3.717827000	1.100343000
1	3.942712000	-2.109072000	0.895616000
6	-2.193380000	2.941171000	-1.542170000
1	-2.222080000	3.001298000	-2.621310000
6	-2.102707000	2.773265000	1.226301000
1	-2.066129000	2.700337000	2.305269000
6	-4.607862000	-2.012379000	-1.051870000
1	-5.478503000	-2.445798000	-1.525706000
6	-4.731543000	-1.351240000	0.163130000
1	-5.700072000	-1.270223000	0.638494000
6	3.239503000	1.012319000	1.943786000
1	2.388203000	1.215827000	2.592222000
1	3.988884000	1.784887000	2.125807000
1	3.669940000	0.062812000	2.257110000
6	-3.613311000	-0.788716000	0.761439000
1	-3.703800000	-0.264808000	1.703241000
6	-3.221525000	3.307534000	0.600914000
1	-4.058855000	3.655238000	1.191273000
6	-3.267046000	3.385599000	-0.782932000
1	-4.138917000	3.793634000	-1.276310000



Final Gibbs free energy ... -2352.91043522 Eh

78	0.319090000	-0.321538000	-0.720455000
16	-1.525354000	-1.590447000	-1.901976000
16	-0.643187000	1.529720000	-2.156331000
14	2.180179000	0.947715000	-0.184407000
14	1.011322000	-2.037382000	0.665670000
6	-1.599598000	-3.403180000	-1.582602000
1	-2.421485000	-3.519735000	-0.877185000
1	-1.907491000	-3.846257000	-2.527247000
6	-0.020713000	-3.624163000	0.390630000
1	0.551594000	-4.418726000	0.877349000
1	-0.950650000	-3.549356000	0.961121000
6	-1.758529000	2.346922000	0.208936000
1	-1.424763000	1.381775000	0.571960000
6	-1.455318000	2.715331000	-1.096547000
6	0.794841000	2.450230000	-2.827577000
1	1.412677000	1.637020000	-3.201178000
1	0.455794000	3.023076000	-3.688116000
6	1.785664000	2.796987000	-0.445027000
1	0.913523000	3.011709000	0.172401000
1	2.602465000	3.368571000	0.003068000
6	0.725214000	-1.682917000	2.503680000
1	1.323860000	-0.857544000	2.876395000
1	0.956423000	-2.564678000	3.105345000
1	-0.321442000	-1.431479000	2.675680000
6	3.600229000	0.516591000	-1.371502000
1	3.969189000	-0.493021000	-1.204668000
1	4.438010000	1.204186000	-1.236725000
1	3.289696000	0.573400000	-2.414388000
6	-0.795776000	-1.589177000	-3.542488000
6	0.583116000	-1.666854000	-3.716040000
1	1.221057000	-1.725041000	-2.844894000
6	-1.633282000	-1.459438000	-4.643516000
1	-2.701522000	-1.380738000	-4.496240000
6	2.795211000	-2.640674000	0.438488000
1	2.960992000	-2.995009000	-0.579494000
1	2.999815000	-3.473327000	1.114297000
1	3.535660000	-1.869849000	0.634672000
6	-1.839997000	3.959813000	-1.582375000
1	-1.625368000	4.235506000	-2.605839000
6	-2.440835000	3.231664000	1.029576000
1	-2.671365000	2.944865000	2.046861000
6	-1.091604000	-1.416153000	-5.920560000
1	-1.745242000	-1.311572000	-6.776168000
6	0.282340000	-1.498188000	-6.098261000
1	0.702352000	-1.458945000	-7.094598000
6	2.912573000	0.954397000	1.560940000
1	2.181733000	1.309346000	2.286730000
1	3.765427000	1.635170000	1.593143000
1	3.260991000	-0.019112000	1.894602000
6	1.116767000	-1.621698000	-4.995399000
1	2.188920000	-1.680321000	-5.127742000

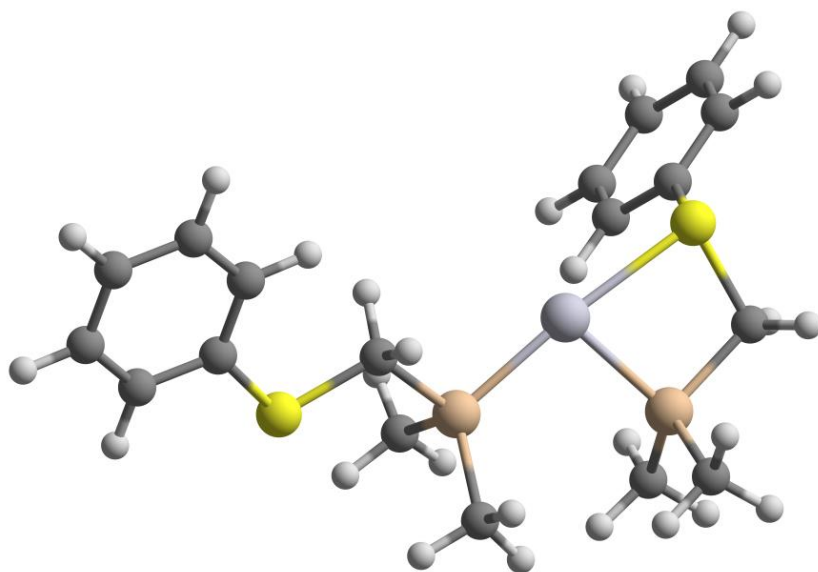
6	-2.807875000	4.484432000	0.557914000
1	-3.331313000	5.176472000	1.203820000
6	-2.502746000	4.846480000	-0.747383000
1	-2.791167000	5.819338000	-1.122701000
6	1.552718000	3.335998000	-1.852404000
1	2.513582000	3.542376000	-2.330857000
1	1.041357000	4.298442000	-1.791915000
6	-0.341850000	-4.041490000	-1.039303000
1	-0.504467000	-5.122750000	-1.094008000
1	0.492948000	-3.837357000	-1.713123000



Final Gibbs free energy ... -2274.36470297 Eh

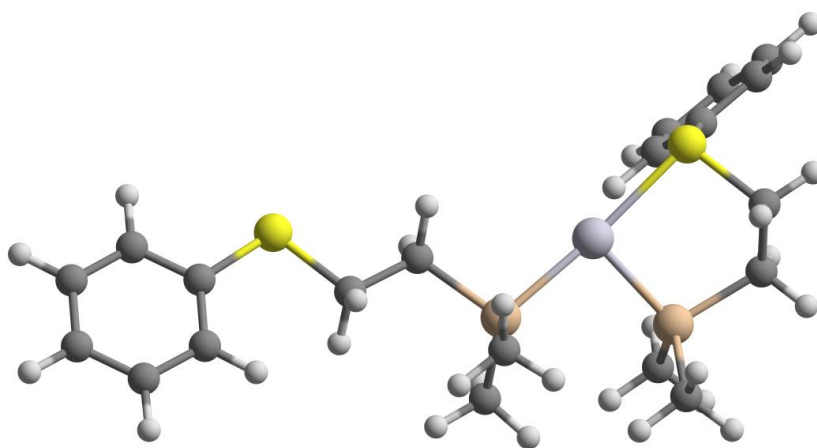
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16	1.481502000	-2.203131000	0.578432000
16	0.379282000	1.467739000	-1.883878000
14	2.868458000	0.854962000	0.119028000
14	-1.005625000	-1.590681000	-1.427207000
6	0.160427000	-3.517986000	0.297001000
1	0.661171000	-4.464167000	0.497800000
1	-0.551063000	-3.330358000	1.099981000
6	-0.476862000	-3.404409000	-1.056685000
1	-1.346492000	-4.066223000	-1.097928000
1	0.217660000	-3.742147000	-1.827559000
6	-1.261400000	2.011995000	0.301640000
1	-0.632120000	1.316736000	0.839717000
6	-0.995797000	2.260324000	-1.039045000
6	1.699462000	2.783285000	-1.602237000
1	2.409939000	2.597457000	-2.406524000
1	1.197605000	3.729311000	-1.801020000
6	2.338722000	2.668841000	-0.249509000
1	1.645480000	3.006679000	0.522467000
1	3.208506000	3.330539000	-0.209447000
6	-1.441312000	-1.501309000	-3.268262000
1	-1.804647000	-0.506791000	-3.528818000

1	-2.217946000	-2.217762000	-3.543077000
1	-0.568497000	-1.697058000	-3.890985000
6	4.483911000	0.562363000	-0.834253000
1	4.846812000	-0.451798000	-0.669824000
1	5.272366000	1.251522000	-0.524085000
1	4.343526000	0.675632000	-1.909560000
6	2.856170000	-2.998364000	-0.264523000
6	3.125258000	-2.749257000	-1.604317000
1	2.499044000	-2.051665000	-2.142958000
6	3.663530000	-3.857581000	0.470263000
1	3.457302000	-4.028627000	1.518268000
6	-2.623373000	-1.296292000	-0.478530000
1	-2.486130000	-1.406622000	0.597461000
1	-3.410281000	-1.986962000	-0.789329000
1	-2.986600000	-0.282887000	-0.646851000
6	-1.807223000	3.116244000	-1.773127000
1	-1.603545000	3.286848000	-2.821696000
6	-2.340504000	2.634179000	0.909344000
1	-2.551258000	2.438266000	1.951985000
6	4.739124000	-4.481612000	-0.145600000
1	5.371616000	-5.146720000	0.426771000
6	5.009882000	-4.241145000	-1.485098000
1	5.853728000	-4.722269000	-1.961195000
6	3.308978000	0.764798000	1.958806000
1	2.438434000	0.960825000	2.584589000
1	4.087058000	1.480537000	2.231388000
1	3.672501000	-0.230106000	2.217715000
6	4.203727000	-3.374099000	-2.210531000
1	4.417161000	-3.177666000	-3.252528000
6	-3.150890000	3.497814000	0.184518000
1	-3.995337000	3.976787000	0.661715000
6	-2.883586000	3.737570000	-1.155786000
1	-3.519306000	4.400079000	-1.727593000



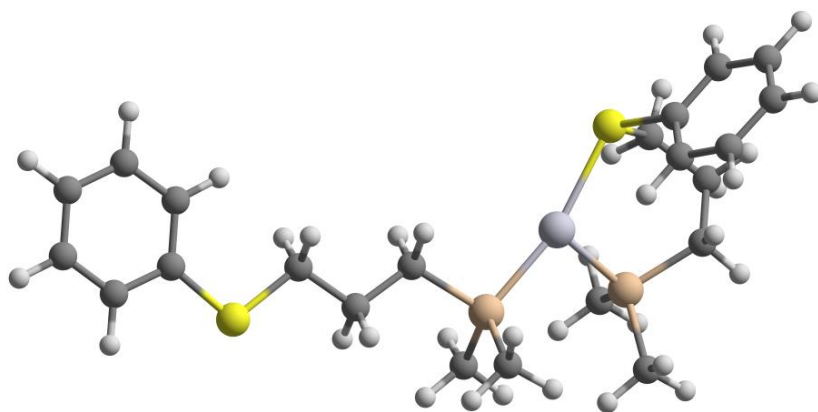
Final Gibbs free energy ... -2195.81145631 Eh

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16	-0.160390000	-3.887503000	-0.207874000
14	-0.936112000	-0.949740000	0.305626000
14	-2.033987000	2.300643000	0.186019000
6	-1.233376000	3.985040000	-0.241426000
1	-1.040857000	4.624053000	0.616258000
1	-1.756135000	4.571503000	-0.994254000
6	1.454031000	-4.352430000	-2.453588000
1	1.482604000	-3.287464000	-2.627643000
6	0.743020000	-4.872853000	-1.375206000
6	0.049582000	-2.181470000	-0.784616000
1	1.107583000	-1.917963000	-0.768826000
1	-0.307910000	-2.090142000	-1.809731000
6	-2.485981000	2.227312000	2.005874000
1	-2.886699000	1.251010000	2.271671000
1	-3.245193000	2.973644000	2.245845000
1	-1.617555000	2.411780000	2.634763000
6	-2.758020000	-1.400627000	0.118443000
1	-3.396527000	-0.791371000	0.756803000
1	-2.917386000	-2.442894000	0.394702000
1	-3.094021000	-1.274575000	-0.909267000
6	1.545536000	4.026230000	0.348312000
6	1.644934000	3.292354000	1.526194000
1	1.051952000	2.393052000	1.636825000
6	2.322797000	5.163300000	0.161219000
1	2.241129000	5.724108000	-0.759526000
6	-3.554991000	2.063369000	-0.885708000
1	-3.299451000	2.137773000	-1.940819000
1	-4.297738000	2.831682000	-0.661471000
1	-4.018669000	1.093800000	-0.725080000
6	0.726719000	-6.256409000	-1.176730000
1	0.176228000	-6.671130000	-0.341848000
6	2.133455000	-5.203100000	-3.315070000
1	2.680751000	-4.782123000	-4.148735000
6	3.197036000	5.569509000	1.159870000
1	3.803419000	6.453106000	1.013180000
6	3.291295000	4.846941000	2.340454000
1	3.973677000	5.165674000	3.116955000
6	-0.444314000	-1.245934000	2.104803000
1	0.631073000	-1.137017000	2.239187000
1	-0.719321000	-2.247966000	2.435132000
1	-0.931074000	-0.528790000	2.764449000
6	2.514862000	3.709623000	2.521163000
1	2.593210000	3.137923000	3.436130000
6	2.116359000	-6.574698000	-3.117590000
1	2.647518000	-7.232354000	-3.792246000
6	1.407424000	-7.094673000	-2.040907000
1	1.383209000	-8.163476000	-1.872242000



Final Gibbs free energy ... -2274.35701491 Eh			
78	0.782592000	-0.590971000	-0.576577000
16	-0.821925000	-1.880843000	-1.967163000
16	1.893994000	5.242501000	0.171833000
14	2.401429000	0.750221000	0.385139000
14	1.375537000	-2.462220000	0.546105000
6	0.005777000	-3.522821000	-1.766877000
1	-0.650128000	-4.264009000	-2.220804000
1	0.894701000	-3.432000000	-2.388344000
6	0.344064000	-3.826007000	-0.327365000
1	0.882278000	-4.776924000	-0.279692000
1	-0.578013000	-3.968400000	0.237840000
6	4.504719000	6.054375000	0.804186000
1	4.803667000	5.018368000	0.846482000
6	3.189082000	6.405681000	0.505158000
6	2.698233000	3.607738000	0.373386000
1	3.521650000	3.538462000	-0.333333000
1	3.102963000	3.548415000	1.381904000
6	1.682402000	2.511175000	0.125233000
1	1.290816000	2.599389000	-0.890052000
1	0.828645000	2.627719000	0.794585000
6	0.857987000	-2.488772000	2.354042000
1	1.405246000	-1.767508000	2.953637000
1	1.038602000	-3.480632000	2.774328000
1	-0.203935000	-2.274017000	2.457300000
6	4.043722000	0.663204000	-0.553161000
1	4.456801000	-0.343257000	-0.531173000
1	4.791519000	1.333670000	-0.126312000
1	3.910499000	0.933487000	-1.600217000
6	-2.316884000	-2.157202000	-1.012997000
6	-2.482772000	-1.544514000	0.222659000
1	-1.689284000	-0.915884000	0.606171000
6	-3.318337000	-2.969222000	-1.534571000
1	-3.194517000	-3.423542000	-2.508348000
6	3.194586000	-2.923557000	0.402710000
1	3.518648000	-2.937570000	-0.636362000
1	3.362396000	-3.917219000	0.822913000
1	3.836212000	-2.227045000	0.937614000
6	2.845662000	7.760252000	0.457751000

1	1.827138000	8.045536000	0.227388000
6	5.450667000	7.040231000	1.050464000
1	6.467163000	6.748510000	1.281254000
6	-4.476231000	-3.185939000	-0.803607000
1	-5.253372000	-3.820687000	-1.207591000
6	-4.644870000	-2.578500000	0.433847000
1	-5.552620000	-2.743842000	0.998382000
6	2.804828000	0.604765000	2.226464000
1	1.909962000	0.706447000	2.838686000
1	3.505329000	1.383454000	2.531462000
1	3.266694000	-0.350571000	2.470349000
6	-3.650737000	-1.754617000	0.941365000
1	-3.778560000	-1.276913000	1.903344000
6	5.107390000	8.381785000	1.002670000
1	5.849249000	9.144802000	1.195406000
6	3.796489000	8.733760000	0.703654000
1	3.510399000	9.776690000	0.662098000



Final Gibbs free energy ... -2352.88764281 Eh			
78	-0.077439000	0.224205000	-0.205022000
16	-2.276864000	-6.568445000	1.741407000
16	-1.227110000	2.070442000	-1.367556000
14	2.054257000	0.960539000	-0.415322000
14	0.524152000	-1.779147000	0.777207000
6	-2.365275000	-4.926640000	0.945598000
1	-2.544028000	-5.055077000	-0.120961000
1	-3.197948000	-4.368495000	1.371319000
6	-1.074429000	-2.803084000	0.519994000
1	-1.920885000	-2.226635000	0.904352000
1	-1.245275000	-2.904749000	-0.554506000
6	-1.296614000	3.381585000	1.047520000
1	-0.993880000	2.426182000	1.457076000
6	-1.443311000	3.512111000	-0.328128000
6	0.070581000	2.613804000	-2.555053000
1	0.376457000	1.669236000	-2.998389000
1	-0.409828000	3.202797000	-3.333364000
6	1.875090000	2.835389000	-0.681555000
1	1.316124000	3.210743000	0.175469000
1	2.875448000	3.267123000	-0.582122000
6	0.811354000	-1.657860000	2.644249000

1	1.651772000	-1.008586000	2.879371000
1	1.019609000	-2.635829000	3.080969000
1	-0.065493000	-1.248741000	3.145485000
6	2.931890000	0.205855000	-1.904416000
1	3.122877000	-0.854355000	-1.761866000
1	3.892638000	0.702051000	-2.058940000
1	2.351664000	0.311350000	-2.819030000
6	-3.856685000	-7.293132000	1.397585000
6	-4.078327000	-8.577285000	1.904039000
1	-3.299724000	-9.070043000	2.472146000
6	-4.868755000	-6.671629000	0.668150000
1	-4.729491000	-5.681302000	0.262711000
6	1.946213000	-2.787631000	0.045868000
1	1.803666000	-2.953286000	-1.021191000
1	2.016175000	-3.763288000	0.528433000
1	2.908722000	-2.296633000	0.177567000
6	-1.810379000	4.733042000	-0.882536000
1	-1.949048000	4.826014000	-1.951047000
6	-1.512103000	4.479197000	1.867228000
1	-1.396000000	4.375968000	2.937649000
6	-6.074852000	-7.325210000	0.454004000
1	-6.849540000	-6.826936000	-0.114439000
6	-6.292257000	-8.597656000	0.957249000
1	-7.234117000	-9.101110000	0.786784000
6	3.167189000	0.785834000	1.093554000
1	2.702812000	1.225788000	1.974363000
1	4.113240000	1.302002000	0.919713000
1	3.396900000	-0.251311000	1.324751000
6	-5.283448000	-9.218680000	1.684043000
1	-5.435683000	-10.212509000	2.084411000
6	-1.857232000	5.705937000	1.317898000
1	-2.016378000	6.562373000	1.959001000
6	-2.002711000	5.830545000	-0.057303000
1	-2.278988000	6.782603000	-0.490214000
6	1.251378000	3.369687000	-1.967157000
1	2.004613000	3.389689000	-2.758652000
1	0.952770000	4.407965000	-1.815450000
6	-1.061441000	-4.181793000	1.175027000
1	-0.887647000	-4.085759000	2.247201000
1	-0.235969000	-4.774471000	0.779250000