

Supporting Information

Theoretical Insights into the Mechanism and Origin of Chemoselectivity in the Catalyst- and Directing Group-Dependent Oxidative Cyclization of Diynes with Pyridine *N*-oxides

Jia-Jie Chen,^a Jia-Yi Liu,^a Xi-Xi Cao,^a Jing-Xin Hu,^a Xin Lu,^b Wen-Bo Shen,^c Qing Sun,^{*a} Ren-Jie Song,^{*a} and Jin-Heng Li^{*a,d}

^aKey Laboratory of Jiangxi Province for Persistent Pollutants Control and Resources Recycle, Nanchang Hangkong University, Nanchang 330063, China

^bState Key Laboratory of Physical Chemistry of Solid Surface & Fujian Provincial Key Laboratory for Theoretical and Computational Chemistry, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

^cCollege of Sciences, Henan Agricultural University, Zhengzhou, Henan 450002, China

^dSchool of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 475004, China

****Correspondence:*** sunqing@nchu.edu.cn; srj0731@hmu.edu.cn; jhli@hnu.edu.cn

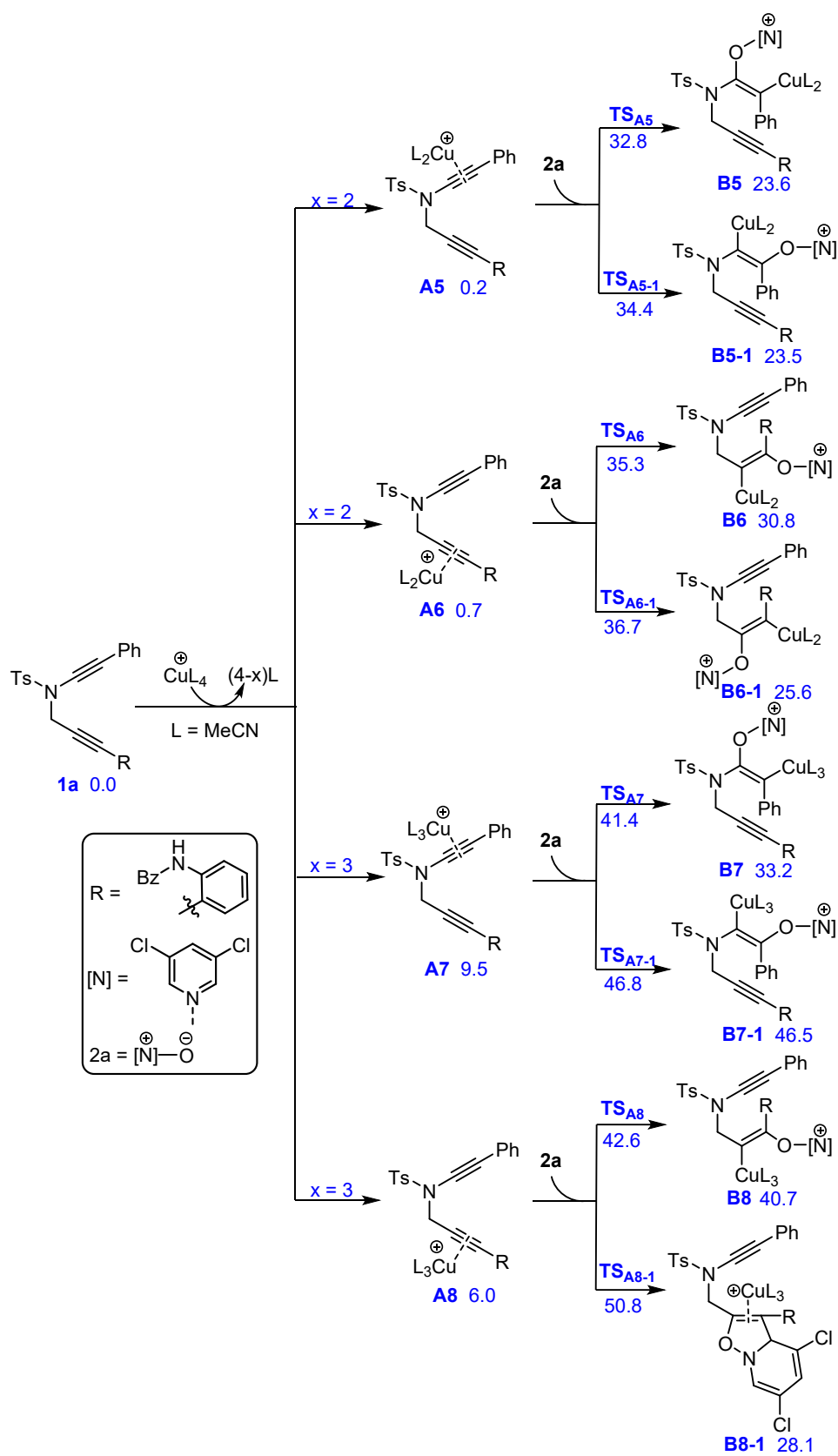


Figure S1. Relative free energies (ΔG , in kcal/mol) of the Cu(I)-bound precursors with two or three L ligands (L = CH₃CN), the transition states and intermediates of the nucleophilic attack of *N*-oxidant **2a** step.

Cartesian Coordinates and Thermochemical Data (Energies in Hartree)

1a

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.71834500 | 1.76353600 | 0.56376100 |
| C | 0.18961400 | 2.12765400 | -0.15608700 |
| N | 1.20565900 | 2.48466700 | -0.97064600 |
| C | 1.33075300 | 1.70372800 | -2.23206100 |
| C | 1.27539700 | 0.26904300 | -1.98623400 |
| C | 1.17439400 | -0.87937500 | -1.60487500 |
| C | 0.94920900 | -2.20698100 | -1.14008000 |
| C | 2.00477300 | -3.11722200 | -1.01696800 |
| C | -0.36345800 | -2.59802000 | -0.77328900 |
| C | 1.77826000 | -4.40400800 | -0.55070800 |
| H | 3.00483400 | -2.79013500 | -1.29621400 |
| C | -0.58176600 | -3.89601000 | -0.30416100 |
| C | 0.48421000 | -4.78292300 | -0.20028000 |
| H | 2.60388400 | -5.10542000 | -0.45961200 |
| H | -1.58507300 | -4.19212000 | -0.02266300 |
| S | 2.68422600 | 2.88596100 | -0.16598700 |
| O | 2.28662900 | 3.69964500 | 0.96962800 |
| O | 3.54858600 | 3.41129200 | -1.21211300 |
| C | 3.32176000 | 1.33995700 | 0.39573400 |
| C | 2.78367000 | 0.76029600 | 1.54584900 |
| C | 4.26640100 | 0.67538700 | -0.38276500 |
| C | 3.20533900 | -0.51018600 | 1.90943500 |
| H | 2.05197400 | 1.29597300 | 2.14616900 |
| C | 4.67806800 | -0.59264500 | 0.00374300 |
| H | 4.66843100 | 1.14530100 | -1.27714400 |
| C | 4.15129900 | -1.20499100 | 1.14548300 |
| H | 2.79254000 | -0.97871800 | 2.80136200 |

| | | | |
|---|-------------|-------------|-------------|
| H | 5.41747900 | -1.12365300 | -0.59379700 |
| C | 4.59865400 | -2.57184200 | 1.55700100 |
| H | 5.00963500 | -3.13354300 | 0.71105700 |
| H | 5.38443200 | -2.50898100 | 2.32125400 |
| H | 3.77315700 | -3.14711400 | 1.99069000 |
| H | 0.50659900 | 2.02000300 | -2.88280500 |
| H | 2.25995000 | 2.01091200 | -2.72509400 |
| C | -1.71948300 | 1.24524100 | 1.43918800 |
| C | -2.87746500 | 1.97592000 | 1.73983200 |
| C | -1.54373400 | -0.03096400 | 1.99998700 |
| C | -3.83668100 | 1.44022800 | 2.59035800 |
| H | -3.01543200 | 2.95968300 | 1.29617600 |
| C | -2.50977400 | -0.56234900 | 2.84373500 |
| H | -0.64144300 | -0.59249600 | 1.75793100 |
| C | -3.65561500 | 0.17358200 | 3.14198000 |
| H | -4.73375400 | 2.01119500 | 2.81935700 |
| H | -2.36984200 | -1.55324800 | 3.26960500 |
| H | -4.41076100 | -0.24302900 | 3.80479600 |
| N | -1.36588700 | -1.63664600 | -0.90841500 |
| H | -1.02369300 | -0.70897900 | -1.14018200 |
| C | -2.71389000 | -1.74751100 | -0.67157800 |
| O | -3.24760100 | -2.75361900 | -0.22307500 |
| C | -3.49418000 | -0.51686900 | -1.00064600 |
| C | -4.73178100 | -0.35128700 | -0.37454300 |
| C | -3.04742400 | 0.45259900 | -1.90547400 |
| C | -5.49865100 | 0.77992500 | -0.62399800 |
| H | -5.07208900 | -1.11676600 | 0.31914800 |
| C | -3.81928300 | 1.58026900 | -2.15971600 |
| H | -2.10924900 | 0.32206200 | -2.44408000 |
| C | -5.04179900 | 1.74912500 | -1.51409100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -6.45431000 | 0.90813100 | -0.12059100 |
| H | -3.46770300 | 2.32577100 | -2.86899100 |
| H | -5.64238100 | 2.63433100 | -1.71117300 |
| H | 0.29507100 | -5.78907300 | 0.16732400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1927.894051

Electronic Energy (0K) + ZPE = -1927.421460

Enthalpy (353K) = -1927.375949

Free Energy (353K) = -1927.506570

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1928.295309

Cu(CH₃CN)₄⁺

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| N | -1.85665700 | 0.35173400 | 0.71008100 |
| N | 1.23643100 | -0.49166800 | 1.54700400 |
| N | 0.70580600 | 1.64610700 | -0.91978900 |
| C | -2.93318500 | 0.54871400 | 1.08653600 |
| C | 1.92706800 | -0.77325200 | 2.43194900 |
| C | 1.10903600 | 2.60195300 | -1.43281000 |
| C | 2.78769200 | -1.12234000 | 3.53576600 |
| C | -4.27567400 | 0.79285900 | 1.55517300 |
| C | 1.61106600 | 3.79447900 | -2.07099600 |
| H | 2.42230100 | -2.03392300 | 4.01764100 |
| H | 3.80610200 | -1.29145300 | 3.17407900 |
| H | 2.79816800 | -0.30992700 | 4.26850300 |
| H | -4.85314500 | -0.13575300 | 1.52718100 |
| H | -4.24802400 | 1.16648200 | 2.58285500 |
| H | -4.76199300 | 1.53625000 | 0.91669600 |
| H | 1.79769300 | 4.56666300 | -1.31898200 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.54555700 | 3.57052000 | -2.59390800 |
| H | 0.87752000 | 4.16701600 | -2.79188400 |
| Cu | 0.01041800 | -0.00790600 | 0.01760000 |
| C | -0.09925800 | -3.47107100 | -3.04154500 |
| H | -0.47724600 | -3.09839200 | -3.99797100 |
| H | -0.74904700 | -4.27745800 | -2.68913800 |
| H | 0.91217400 | -3.86272400 | -3.18424500 |
| C | -0.07654300 | -2.40116500 | -2.07397400 |
| N | -0.05717300 | -1.54255400 | -1.29816900 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -728.001676

Electronic Energy (0K) + ZPE = -727.815870

Enthalpy (353K) = -727.787872

Free Energy (353K) = -727.887500

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -728.134954

CH₃CN

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| N | 1.43504300 | -0.00002600 | 0.00000700 |
| C | 0.27382000 | 0.00004800 | -0.00000100 |
| C | -1.17338400 | -0.00002600 | -0.00000800 |
| H | -1.54937500 | 0.22688600 | 1.00192900 |
| H | -1.54921600 | 0.75440900 | -0.69740800 |
| H | -1.54933100 | -0.98124300 | -0.30451900 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -132.665022

Electronic Energy (0K) + ZPE = -132.619896

Enthalpy (353K) = -132.614265

Free Energy (353K) = -132.647986

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -132.703132

A

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.17532200 | 2.53060900 | -1.17896100 |
| C | 0.79858500 | 2.03945900 | -1.71736500 |
| N | 1.90864500 | 1.49890400 | -2.25842100 |
| C | 1.76950300 | 0.16458700 | -2.85732200 |
| C | 1.41137300 | -0.89039900 | -1.89153000 |
| C | 1.26836100 | -1.97772100 | -1.32284200 |
| C | 1.16009000 | -3.23930200 | -0.66633100 |
| C | 2.31785800 | -3.96486800 | -0.34644300 |
| C | -0.11090200 | -3.73843800 | -0.30483000 |
| C | 2.21568900 | -5.16252200 | 0.34206500 |
| H | 3.28660300 | -3.56875700 | -0.64258100 |
| C | -0.19796200 | -4.93879500 | 0.39481500 |
| C | 0.95919100 | -5.63850500 | 0.71612100 |
| H | 3.11165900 | -5.72489300 | 0.58986700 |
| H | -1.17405800 | -5.32181600 | 0.67361000 |
| S | 3.37132400 | 1.85015400 | -1.38520800 |
| O | 3.44298500 | 3.29951200 | -1.35581100 |
| O | 4.38553100 | 1.04206200 | -2.04298800 |
| C | 3.09863400 | 1.25605800 | 0.25631300 |
| C | 2.49459000 | 2.09630300 | 1.19328700 |
| C | 3.46340800 | -0.05058900 | 0.57817600 |
| C | 2.24212800 | 1.60249900 | 2.46523500 |
| H | 2.24215300 | 3.12139600 | 0.93359100 |
| C | 3.20197300 | -0.52317300 | 1.85788000 |
| H | 3.96154800 | -0.67939400 | -0.15641500 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.57999700 | 0.28911800 | 2.81294900 |
| H | 1.77763700 | 2.24821300 | 3.20910400 |
| H | 3.49432400 | -1.53695000 | 2.12678300 |
| C | 2.26154500 | -0.23803300 | 4.17535500 |
| H | 2.90124600 | -1.08596500 | 4.43956200 |
| H | 2.37214200 | 0.53730600 | 4.94089100 |
| H | 1.22116700 | -0.58831900 | 4.21800100 |
| H | 0.99930100 | 0.24058300 | -3.63345500 |
| H | 2.71257400 | -0.09198100 | -3.35027400 |
| C | -1.27372900 | 3.14178300 | -0.50881600 |
| C | -2.53456600 | 2.52505600 | -0.47115200 |
| C | -1.08305700 | 4.36408100 | 0.15504500 |
| C | -3.58391700 | 3.13444700 | 0.20510200 |
| H | -2.68461200 | 1.57082000 | -0.97768000 |
| C | -2.13729400 | 4.95703700 | 0.83833300 |
| H | -0.10625800 | 4.84230500 | 0.12077900 |
| C | -3.39008900 | 4.34791300 | 0.86269400 |
| H | -4.55983800 | 2.65270500 | 0.22197900 |
| H | -1.98086800 | 5.90480900 | 1.34807700 |
| H | -4.21510900 | 4.81913500 | 1.39154100 |
| N | -1.24873200 | -3.00426700 | -0.67147800 |
| H | -1.16556200 | -2.46402500 | -1.52496200 |
| C | -2.27085900 | -2.67995300 | 0.19700400 |
| O | -2.32192100 | -3.12203200 | 1.33453500 |
| C | -3.28883900 | -1.72339800 | -0.33090900 |
| C | -4.15942700 | -1.15529300 | 0.60426700 |
| C | -3.40900200 | -1.37064800 | -1.67971100 |
| C | -5.12376200 | -0.23982100 | 0.20420300 |
| H | -4.06554400 | -1.45111700 | 1.64672300 |
| C | -4.37797700 | -0.45570600 | -2.07973000 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.78099000 | -1.82739700 | -2.44242400 |
| C | -5.23330800 | 0.11340400 | -1.13977700 |
| H | -5.79674500 | 0.19562100 | 0.93996700 |
| H | -4.47157100 | -0.19604400 | -3.13127800 |
| H | -5.99046600 | 0.82738300 | -1.45622000 |
| H | 0.87635900 | -6.57819700 | 1.25657300 |
| Cu | 0.34397100 | -0.42211000 | -0.22281000 |
| C | -2.27891700 | 1.30133700 | 2.96388400 |
| H | -2.16410100 | 2.38820700 | 2.88525200 |
| H | -2.01298500 | 0.97763400 | 3.97496400 |
| H | -3.32123200 | 1.03419700 | 2.75882100 |
| C | -1.41810600 | 0.66149700 | 2.00421900 |
| N | -0.71980200 | 0.15442000 | 1.23401200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2257.873704

Electronic Energy (0K) + ZPE = -2257.352492

Enthalpy (353K) = -2257.298856

Free Energy (353K) = -2257.446058

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2258.296426

2a (*Cu catalysis system*)

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.17599500 | -0.33676200 | 0.00093400 |
| C | -0.00005700 | -1.07494200 | 0.00073000 |
| C | -1.17611900 | -0.33655900 | 0.00074800 |
| C | -1.17992300 | 1.04400700 | -0.00006600 |
| C | 1.17995500 | 1.04391700 | 0.00012600 |
| H | -0.00023100 | -2.16018500 | 0.00081500 |
| H | 2.07358300 | 1.65700500 | -0.00042800 |

| | | | |
|----|-------------|-------------|-------------|
| N | 0.00015100 | 1.73498900 | -0.00016300 |
| O | 0.00019200 | 3.00046200 | -0.00006800 |
| H | -2.07334000 | 1.65740600 | -0.00065100 |
| Cl | -2.70832600 | -1.15700400 | -0.00034500 |
| Cl | 2.70822600 | -1.15716100 | -0.00041300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1242.358890

Electronic Energy (0K) + ZPE = -1242.285416

Enthalpy (353K) = -1242.274254

Free Energy (353K) = -1242.325673

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1242.501470

TS_A

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.74441300 | -1.97331700 | -1.54222900 |
| C | 0.54246900 | -1.78588300 | -1.53192700 |
| N | -0.79361700 | -1.62168800 | -1.47590200 |
| C | -1.31075600 | -0.23526900 | -1.45502100 |
| C | -0.83036400 | 0.56915900 | -0.29465800 |
| C | -1.24247100 | 1.58551400 | 0.37541100 |
| C | -0.88400300 | 2.53474800 | 1.41092800 |
| C | -1.69305800 | 2.68731100 | 2.54465100 |
| C | 0.31266000 | 3.28176900 | 1.31602100 |
| C | -1.31946700 | 3.52809900 | 3.58015700 |
| H | -2.62225100 | 2.12590300 | 2.60436800 |
| C | 0.67927400 | 4.13165900 | 2.36134900 |
| C | -0.12901700 | 4.24678900 | 3.48396400 |
| H | -1.95425500 | 3.62817900 | 4.45654900 |
| H | 1.59719800 | 4.70274900 | 2.27812700 |

| | | | |
|---|-------------|-------------|-------------|
| S | -1.59788000 | -2.78982800 | -0.47850900 |
| O | -1.23638300 | -4.08054300 | -1.03731500 |
| O | -2.98225900 | -2.34124300 | -0.42970300 |
| C | -0.85383900 | -2.62421100 | 1.11394800 |
| C | 0.29609900 | -3.35817200 | 1.40292600 |
| C | -1.36765700 | -1.69253600 | 2.01449900 |
| C | 0.94087900 | -3.13996300 | 2.61278600 |
| H | 0.66788500 | -4.09726100 | 0.69755900 |
| C | -0.70867800 | -1.49041700 | 3.21965000 |
| H | -2.27868800 | -1.14671200 | 1.77665800 |
| C | 0.45869700 | -2.19863800 | 3.52950700 |
| H | 1.83517100 | -3.71189000 | 2.85558400 |
| H | -1.10589700 | -0.77464500 | 3.93768300 |
| C | 1.19354500 | -1.93634000 | 4.80508000 |
| H | 0.52178500 | -1.57527600 | 5.59057000 |
| H | 1.70561500 | -2.83437700 | 5.16607800 |
| H | 1.95975000 | -1.16394900 | 4.65256600 |
| H | -0.96591200 | 0.22809400 | -2.38864400 |
| H | -2.39780800 | -0.32313100 | -1.52186700 |
| C | 3.14965000 | -2.19966700 | -1.49455000 |
| C | 4.04800300 | -1.19730800 | -1.89289200 |
| C | 3.64933100 | -3.41703200 | -1.00583800 |
| C | 5.41690900 | -1.41745500 | -1.81361100 |
| H | 3.66163900 | -0.25203200 | -2.27213900 |
| C | 5.02123300 | -3.62517600 | -0.92919600 |
| H | 2.95371300 | -4.19576300 | -0.69967700 |
| C | 5.90922400 | -2.62963500 | -1.33296600 |
| H | 6.10309700 | -0.63473100 | -2.13168600 |
| H | 5.39906300 | -4.57430400 | -0.55601800 |
| H | 6.98178300 | -2.79984000 | -1.27606000 |

| | | | |
|----|-------------|-------------|-------------|
| N | 1.10389400 | 3.15664800 | 0.16464100 |
| H | 0.60606600 | 2.86749200 | -0.66801000 |
| C | 2.47597400 | 3.05570800 | 0.15128000 |
| O | 3.15910300 | 3.23652100 | 1.14958700 |
| C | 3.09160500 | 2.70274200 | -1.16661900 |
| C | 4.48879400 | 2.68101700 | -1.21577200 |
| C | 2.36666100 | 2.39110400 | -2.32339300 |
| C | 5.15106100 | 2.37075600 | -2.39642700 |
| H | 5.04117500 | 2.92501700 | -0.31174500 |
| C | 3.03033700 | 2.07730900 | -3.50475100 |
| H | 1.27769500 | 2.39185100 | -2.33545600 |
| C | 4.42251000 | 2.06895100 | -3.54483900 |
| H | 6.23841500 | 2.36812600 | -2.42306200 |
| H | 2.45684400 | 1.84034000 | -4.39748200 |
| H | 4.93851900 | 1.82685800 | -4.47109100 |
| H | 0.16848900 | 4.91782100 | 4.28615900 |
| Cu | 0.89747300 | 0.15972800 | 0.50050700 |
| C | 5.10230500 | -0.66296000 | 1.74117700 |
| H | 5.37984500 | -1.62132500 | 1.28730800 |
| H | 5.25604300 | -0.71133500 | 2.82331400 |
| H | 5.73168500 | 0.12825200 | 1.32126800 |
| C | 3.72025500 | -0.38079800 | 1.45190800 |
| N | 2.61107900 | -0.15603800 | 1.21257900 |
| C | -5.27923700 | 0.67729500 | -2.14933600 |
| C | -5.76916500 | -0.30041800 | -1.29068800 |
| C | -5.26446000 | -0.32198700 | 0.00268600 |
| C | -4.30035900 | 0.58292300 | 0.40977100 |
| C | -4.30813600 | 1.57174400 | -1.73875200 |
| H | -6.52099000 | -1.01334600 | -1.61607900 |
| H | -3.87357400 | 2.34667400 | -2.36020100 |

| | | | |
|----|-------------|-------------|-------------|
| N | -3.83289000 | 1.49285500 | -0.47399500 |
| O | -2.90605000 | 2.34684900 | -0.10260800 |
| H | -3.87583500 | 0.61720200 | 1.40760500 |
| Cl | -5.83225300 | -1.48436000 | 1.14556300 |
| Cl | -5.87061800 | 0.78911900 | -3.77068500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.227311

Electronic Energy (0K) + ZPE = -3499.631489

Enthalpy (353K) = -3499.566430

Free Energy (353K) = -3499.741676

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.787913

B

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.97653800 | -2.05137200 | -1.46941400 |
| C | 0.78326800 | -1.82097900 | -1.51180400 |
| N | -0.54888500 | -1.63949000 | -1.48143400 |
| C | -1.09660900 | -0.27944500 | -1.69670400 |
| C | -0.78522200 | 0.70802200 | -0.60731300 |
| C | -1.59304400 | 1.75310200 | -0.37787300 |
| C | -1.41894000 | 2.91836200 | 0.51476800 |
| C | -2.50872600 | 3.40531900 | 1.25011100 |
| C | -0.18576600 | 3.60246500 | 0.63332000 |
| C | -2.38326700 | 4.46667500 | 2.13377900 |
| H | -3.48578300 | 2.94183100 | 1.12930200 |
| C | -0.06303600 | 4.67369500 | 1.52315000 |
| C | -1.14827400 | 5.09085100 | 2.28004000 |
| H | -3.24674500 | 4.80674800 | 2.69976100 |
| H | 0.89097600 | 5.18290700 | 1.59903200 |

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|---|-------------|-------------|-------------|
| S | -1.37466500 | -2.69782300 | -0.39792300 |
| O | -1.14123600 | -4.04016800 | -0.90379200 |
| O | -2.72483400 | -2.15284200 | -0.30548200 |
| C | -0.54532000 | -2.53079100 | 1.15319100 |
| C | 0.59677600 | -3.29206300 | 1.39146800 |
| C | -0.98000100 | -1.56897700 | 2.06596400 |
| C | 1.32197400 | -3.06629700 | 2.55508300 |
| H | 0.91308200 | -4.04890000 | 0.67814000 |
| C | -0.25207700 | -1.37153000 | 3.22960100 |
| H | -1.88060100 | -0.99277900 | 1.86908100 |
| C | 0.91624800 | -2.10228100 | 3.48182000 |
| H | 2.22269400 | -3.64804800 | 2.74653600 |
| H | -0.58545000 | -0.63047700 | 3.95445500 |
| C | 1.71536300 | -1.83564300 | 4.71747500 |
| H | 1.14021000 | -2.07714100 | 5.61995700 |
| H | 2.63790100 | -2.42468700 | 4.73654100 |
| H | 1.98110100 | -0.77315900 | 4.78745700 |
| H | -0.62302100 | 0.06876900 | -2.62614300 |
| H | -2.15545000 | -0.42595300 | -1.92953700 |
| C | 3.37039100 | -2.30514500 | -1.33264800 |
| C | 4.29844600 | -1.25742800 | -1.44232600 |
| C | 3.82856900 | -3.60076500 | -1.04491000 |
| C | 5.65510900 | -1.50809600 | -1.28207000 |
| H | 3.94443600 | -0.25084200 | -1.66144900 |
| C | 5.18696900 | -3.83692800 | -0.87229700 |
| H | 3.11174800 | -4.41588000 | -0.96741400 |
| C | 6.10478100 | -2.79531500 | -0.99297200 |
| H | 6.36466700 | -0.68794900 | -1.38000800 |
| H | 5.53162800 | -4.84444900 | -0.65064600 |
| H | 7.16754700 | -2.98736500 | -0.86543000 |

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|----|-------------|-------------|-------------|
| N | 0.88073300 | 3.25284300 | -0.21068600 |
| H | 0.61384500 | 2.68467600 | -1.00661700 |
| C | 2.21722200 | 3.29444500 | 0.09884600 |
| O | 2.64279400 | 3.70406000 | 1.17183600 |
| C | 3.14103100 | 2.79269200 | -0.96665000 |
| C | 4.48374800 | 2.63479800 | -0.60870400 |
| C | 2.74831800 | 2.50445100 | -2.27927900 |
| C | 5.41749300 | 2.19763100 | -1.53902200 |
| H | 4.77801200 | 2.87488000 | 0.41026900 |
| C | 3.68471200 | 2.06693600 | -3.21085700 |
| H | 1.72039300 | 2.65020300 | -2.60792600 |
| C | 5.01910100 | 1.91301800 | -2.84387700 |
| H | 6.46004300 | 2.08459300 | -1.24920300 |
| H | 3.37100100 | 1.85512900 | -4.23007800 |
| H | 5.74836400 | 1.57041900 | -3.57472400 |
| H | -1.03207100 | 5.92661700 | 2.96588800 |
| Cu | 0.81777100 | 0.42756600 | 0.41156400 |
| C | 4.78026700 | -0.69941400 | 2.12410100 |
| H | 4.89282600 | -1.76856900 | 1.91178300 |
| H | 4.87027700 | -0.52988600 | 3.20144400 |
| H | 5.56800100 | -0.14430900 | 1.60366500 |
| C | 3.49088900 | -0.25469500 | 1.66100200 |
| N | 2.45595100 | 0.09408900 | 1.27907600 |
| C | -5.65492100 | -0.09776000 | -1.88656700 |
| C | -5.90872200 | -0.73959900 | -0.67858100 |
| C | -5.06893800 | -0.46325900 | 0.39005300 |
| C | -4.00951900 | 0.41980100 | 0.25688300 |
| C | -4.59112000 | 0.77550800 | -2.01476100 |
| H | -6.73590500 | -1.43629500 | -0.57488000 |
| H | -4.32477900 | 1.30662200 | -2.92281600 |

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|----|-------------|-------------|-------------|
| N | -3.81551400 | 0.99886600 | -0.93759300 |
| O | -2.83532000 | 1.92964300 | -1.14223600 |
| H | -3.31659600 | 0.66098300 | 1.05706900 |
| Cl | -5.30896100 | -1.22504100 | 1.91533500 |
| Cl | -6.65609600 | -0.38462600 | -3.25967700 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.240403

Electronic Energy (0K) + ZPE = -3499.641639

Enthalpy (353K) = -3499.577354

Free Energy (353K) = -3499.748079

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.798324

A1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70235500 | -2.39007300 | -0.48207500 |
| C | -0.04871100 | -1.95057400 | -1.33542000 |
| N | -0.83579200 | -1.43159800 | -2.29779400 |
| C | -0.60992300 | -0.01140400 | -2.60833800 |
| C | -0.65056000 | 0.85962200 | -1.41835500 |
| C | -0.69392300 | 1.83286100 | -0.66288100 |
| C | -0.67102300 | 2.98142800 | 0.18299300 |
| C | -1.85953700 | 3.46200300 | 0.75141700 |
| C | 0.54178000 | 3.65585600 | 0.43477300 |
| C | -1.85029000 | 4.60673900 | 1.53311600 |
| H | -2.78544100 | 2.92572700 | 0.55085300 |
| C | 0.53517600 | 4.81165100 | 1.20793200 |
| C | -0.65321000 | 5.28577300 | 1.75262800 |
| H | -2.77711400 | 4.97403800 | 1.96588100 |
| H | 1.47479400 | 5.33011800 | 1.38497800 |

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|---|-------------|-------------|-------------|
| S | -2.48369500 | -1.98036200 | -2.33858800 |
| O | -2.41281500 | -3.37550500 | -1.94454500 |
| O | -2.97008000 | -1.57121800 | -3.64532100 |
| C | -3.29752300 | -1.03376200 | -1.09312900 |
| C | -3.13335100 | -1.39467200 | 0.24642400 |
| C | -4.00006200 | 0.11135300 | -1.46013700 |
| C | -3.68790000 | -0.58387300 | 1.22570800 |
| H | -2.59138400 | -2.29918900 | 0.51485700 |
| C | -4.54987900 | 0.90569600 | -0.46200400 |
| H | -4.11605500 | 0.37211600 | -2.50929300 |
| C | -4.39640500 | 0.57709500 | 0.88885500 |
| H | -3.56985400 | -0.85085000 | 2.27495600 |
| H | -5.10813900 | 1.80027700 | -0.73304800 |
| C | -4.97538200 | 1.44156200 | 1.96360800 |
| H | -5.39180600 | 2.36838900 | 1.55604000 |
| H | -5.77750600 | 0.91707300 | 2.49763900 |
| H | -4.21472300 | 1.70248000 | 2.70988400 |
| H | 0.37788600 | 0.07310400 | -3.07743100 |
| H | -1.35033300 | 0.30243900 | -3.35292500 |
| C | 1.56464800 | -3.00857600 | 0.47247700 |
| C | 2.46199500 | -2.24437600 | 1.23595900 |
| C | 1.50144800 | -4.39799300 | 0.66170800 |
| C | 3.28473800 | -2.86950000 | 2.16464500 |
| H | 2.49976700 | -1.16413600 | 1.09513100 |
| C | 2.32181900 | -5.00888500 | 1.60145300 |
| H | 0.80602300 | -4.98582400 | 0.06652500 |
| C | 3.21608000 | -4.24876800 | 2.35231900 |
| H | 3.98275800 | -2.27410400 | 2.74894500 |
| H | 2.26621800 | -6.08553200 | 1.74393200 |
| H | 3.86065100 | -4.73164400 | 3.08309800 |

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|----|-------------|-------------|-------------|
| N | 1.75438900 | 3.21319600 | -0.14517700 |
| H | 2.25930100 | 3.88667700 | -0.71121100 |
| C | 2.29208800 | 1.97323600 | 0.02022000 |
| O | 1.77432300 | 1.11779300 | 0.74517000 |
| C | 3.52386600 | 1.68252500 | -0.75886500 |
| C | 3.67552500 | 0.38392000 | -1.25472100 |
| C | 4.51648300 | 2.63729800 | -0.99683200 |
| C | 4.79927200 | 0.04947500 | -1.99928400 |
| H | 2.89700200 | -0.35370800 | -1.06217200 |
| C | 5.64866100 | 2.29221000 | -1.72615000 |
| H | 4.42782100 | 3.64274500 | -0.58783800 |
| C | 5.78800300 | 1.00257600 | -2.23249900 |
| H | 4.90620200 | -0.95743400 | -2.39537700 |
| H | 6.42708100 | 3.03198600 | -1.89574300 |
| H | 6.67229500 | 0.73823200 | -2.80768300 |
| H | -0.64157000 | 6.18734100 | 2.35967200 |
| Cu | -0.29553600 | 0.04108500 | 0.44265000 |
| C | 0.12752200 | -2.21651400 | 4.30159200 |
| H | 0.23586900 | -3.26261700 | 3.99673000 |
| H | -0.70376300 | -2.13166200 | 5.00770300 |
| H | 1.04997800 | -1.88538600 | 4.78835400 |
| C | -0.12437200 | -1.40423500 | 3.13890500 |
| N | -0.30919200 | -0.76487500 | 2.19288700 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2257.873805

Electronic Energy (0K) + ZPE = -2257.352650

Enthalpy (353K) = -2257.298988

Free Energy (353K) = -2257.446283

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2258.294328

TS_{A1}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 2.18358700 | 0.71544900 | -2.16352600 |
| C | 1.12218200 | 0.12359700 | -2.23063800 |
| N | -0.09697100 | -0.44453200 | -2.25263600 |
| C | -0.99903900 | -0.09554100 | -1.12875900 |
| C | -0.41269500 | -0.36206800 | 0.21520800 |
| C | -0.78084900 | -0.42053200 | 1.44517800 |
| C | -0.24291200 | -0.56217500 | 2.79395700 |
| C | 0.06556100 | -1.81711500 | 3.32447800 |
| C | -0.01472900 | 0.58797800 | 3.56810900 |
| C | 0.60734500 | -1.92242100 | 4.60072900 |
| H | -0.11842300 | -2.70490300 | 2.71999100 |
| C | 0.52263100 | 0.47891900 | 4.84294700 |
| C | 0.83493200 | -0.77686800 | 5.35909800 |
| H | 0.84916800 | -2.90284100 | 5.00472300 |
| H | 0.69604200 | 1.38330500 | 5.42142600 |
| S | -0.20380500 | -2.05168100 | -2.86758900 |
| O | 0.78389900 | -2.11497000 | -3.93067300 |
| O | -1.62096700 | -2.25731700 | -3.12614700 |
| C | 0.28987500 | -3.07774700 | -1.52003300 |
| C | 1.64621800 | -3.16309500 | -1.19842000 |
| C | -0.68536400 | -3.68012900 | -0.73034600 |
| C | 2.01819900 | -3.86555700 | -0.06163400 |
| H | 2.39670600 | -2.69369900 | -1.83130900 |
| C | -0.28984000 | -4.38237900 | 0.40143300 |
| H | -1.73528800 | -3.60441900 | -1.00471200 |
| C | 1.05945900 | -4.47642100 | 0.75689200 |
| H | 3.07191600 | -3.94003900 | 0.20362100 |

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|---|-------------|-------------|-------------|
| H | -1.04072300 | -4.86493700 | 1.02517200 |
| C | 1.48399300 | -5.21616800 | 1.98555100 |
| H | 0.62768800 | -5.48031300 | 2.61472300 |
| H | 2.00537000 | -6.14513700 | 1.72181300 |
| H | 2.18368200 | -4.61818600 | 2.58218300 |
| H | -1.19965400 | 0.98072600 | -1.23814000 |
| H | -1.93786100 | -0.62483900 | -1.32524300 |
| C | 3.43342300 | 1.39657400 | -2.09248000 |
| C | 3.71037500 | 2.24829700 | -1.00928900 |
| C | 4.40320200 | 1.20792900 | -3.08906900 |
| C | 4.93432600 | 2.90199100 | -0.93911700 |
| H | 2.96171000 | 2.38018600 | -0.22684300 |
| C | 5.62749400 | 1.85891400 | -3.00048900 |
| H | 4.18506200 | 0.55037300 | -3.92780600 |
| C | 5.89636300 | 2.70839100 | -1.92938400 |
| H | 5.14089000 | 3.56426100 | -0.10102200 |
| H | 6.37371200 | 1.70676700 | -3.77694000 |
| H | 6.85347500 | 3.22107200 | -1.86713600 |
| N | -0.36382200 | 1.85834200 | 3.02333900 |
| H | -1.34324100 | 2.11051000 | 3.10752600 |
| C | 0.31950800 | 2.37275500 | 1.95411900 |
| O | 1.43733600 | 1.97594000 | 1.63228900 |
| C | -0.40964500 | 3.40915600 | 1.16916600 |
| C | -0.14852500 | 3.47775600 | -0.20296400 |
| C | -1.35960700 | 4.26542400 | 1.73553000 |
| C | -0.84847600 | 4.37317700 | -1.00330400 |
| H | 0.59767300 | 2.81077800 | -0.63424500 |
| C | -2.04397800 | 5.17373000 | 0.93437200 |
| H | -1.54598200 | 4.25063800 | 2.80826700 |
| C | -1.79545900 | 5.22243300 | -0.43508700 |

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|----|-------------|-------------|-------------|
| H | -0.65186500 | 4.41165100 | -2.07215100 |
| H | -2.76987500 | 5.84823100 | 1.38199600 |
| H | -2.33895500 | 5.92671200 | -1.06086900 |
| H | 1.25614400 | -0.85947400 | 6.35793900 |
| Cu | 1.52737300 | -0.46294400 | 0.45320200 |
| C | 5.97449100 | -0.26971000 | 0.78068800 |
| H | 6.32993200 | -0.10635500 | -0.24227100 |
| H | 6.45557000 | -1.16199700 | 1.19187700 |
| H | 6.23622600 | 0.59749400 | 1.39467400 |
| C | 4.54382800 | -0.43937600 | 0.76737100 |
| N | 3.39359600 | -0.55979600 | 0.74261400 |
| C | -4.31281100 | 1.33837200 | -0.74210100 |
| C | -4.94384600 | 0.22585500 | -1.28501400 |
| C | -4.73545700 | -1.00137700 | -0.66344400 |
| C | -3.91151600 | -1.10609100 | 0.44235400 |
| C | -3.49482800 | 1.22523000 | 0.36971900 |
| H | -5.57912400 | 0.31184800 | -2.16208600 |
| H | -2.95785300 | 2.04954100 | 0.83477100 |
| N | -3.31364200 | 0.00689200 | 0.92212100 |
| O | -2.50161000 | -0.11466400 | 1.95227900 |
| H | -3.68894400 | -2.02691000 | 0.97148400 |
| Cl | -5.48647000 | -2.43124700 | -1.27427200 |
| Cl | -4.51082400 | 2.89483500 | -1.46300500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.223191

Electronic Energy (0K) + ZPE = -3499.627230

Enthalpy (353K) = -3499.562818

Free Energy (353K) = -3499.733835

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.783583

B1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 2.12612800 | 0.71917800 | -2.24360000 |
| C | 1.08150700 | 0.09535200 | -2.22570300 |
| N | -0.11711800 | -0.51224200 | -2.17424200 |
| C | -1.01152500 | -0.15427600 | -1.04066500 |
| C | -0.40120200 | -0.38743400 | 0.30964900 |
| C | -0.96225600 | -0.39551500 | 1.51105200 |
| C | -0.24805100 | -0.48982500 | 2.80847600 |
| C | 0.17384700 | -1.71645500 | 3.32508600 |
| C | 0.07537900 | 0.68711000 | 3.50179900 |
| C | 0.92586300 | -1.76711000 | 4.49458500 |
| H | -0.07223000 | -2.62979200 | 2.78327300 |
| C | 0.82995200 | 0.63783400 | 4.66676100 |
| C | 1.25853000 | -0.59101000 | 5.16225900 |
| H | 1.25535000 | -2.72711700 | 4.88580100 |
| H | 1.07777200 | 1.56698300 | 5.17526400 |
| S | -0.21607500 | -2.12337700 | -2.76369800 |
| O | 0.72616800 | -2.18709400 | -3.86796200 |
| O | -1.63885800 | -2.36346100 | -2.96228500 |
| C | 0.34942800 | -3.13226100 | -1.43279600 |
| C | 1.71999300 | -3.21136200 | -1.17975000 |
| C | -0.58262300 | -3.72086400 | -0.58306100 |
| C | 2.15053800 | -3.88681500 | -0.04752300 |
| H | 2.43562100 | -2.75150500 | -1.85833400 |
| C | -0.12967400 | -4.39750700 | 0.54236600 |
| H | -1.64537300 | -3.64986000 | -0.80574200 |
| C | 1.23576300 | -4.47692600 | 0.83392700 |
| H | 3.21628800 | -3.95119200 | 0.16765300 |

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|---|-------------|-------------|-------------|
| H | -0.84606300 | -4.86668000 | 1.21519000 |
| C | 1.72070000 | -5.17829700 | 2.06218900 |
| H | 0.90177800 | -5.38363900 | 2.75953900 |
| H | 2.19094500 | -6.13671000 | 1.80751700 |
| H | 2.47899300 | -4.57985900 | 2.58122000 |
| H | -1.22692800 | 0.91598300 | -1.18478400 |
| H | -1.93942700 | -0.69750600 | -1.25112600 |
| C | 3.36416300 | 1.42312200 | -2.21512400 |
| C | 3.64709100 | 2.30711000 | -1.15852400 |
| C | 4.32020800 | 1.22822400 | -3.22419800 |
| C | 4.85892400 | 2.98633800 | -1.12904400 |
| H | 2.91056100 | 2.44991000 | -0.36632600 |
| C | 5.53309400 | 1.90427900 | -3.17554900 |
| H | 4.09996100 | 0.54561700 | -4.04214700 |
| C | 5.80562800 | 2.78754000 | -2.13298000 |
| H | 5.06738000 | 3.67378100 | -0.31185600 |
| H | 6.26762800 | 1.74621800 | -3.96204400 |
| H | 6.75271200 | 3.32135100 | -2.10352500 |
| N | -0.36502900 | 1.93396100 | 2.96483900 |
| H | -1.36654400 | 2.09098100 | 2.99161200 |
| C | 0.31744100 | 2.52806500 | 1.93223900 |
| O | 1.48097300 | 2.25447100 | 1.66175900 |
| C | -0.48651600 | 3.48909500 | 1.12125600 |
| C | -0.19322400 | 3.58086300 | -0.24257000 |
| C | -1.54014400 | 4.23974500 | 1.65409000 |
| C | -0.96544800 | 4.38812200 | -1.07033600 |
| H | 0.63418000 | 2.99821600 | -0.64621700 |
| C | -2.29878300 | 5.06067900 | 0.82572200 |
| H | -1.75474500 | 4.21000500 | 2.72142900 |
| C | -2.01877900 | 5.12752000 | -0.53723400 |

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|----|-------------|-------------|-------------|
| H | -0.74304600 | 4.44255000 | -2.13338600 |
| H | -3.10847700 | 5.65221600 | 1.24633200 |
| H | -2.62195400 | 5.76013900 | -1.18476500 |
| H | 1.85046500 | -0.62853200 | 6.07351200 |
| Cu | 1.51505300 | -0.49371100 | 0.51331900 |
| C | 5.92947900 | 0.03092100 | 0.65425100 |
| H | 6.22844600 | 0.14407400 | -0.39350800 |
| H | 6.50136400 | -0.78293800 | 1.10946700 |
| H | 6.13800800 | 0.96324300 | 1.18832800 |
| C | 4.51932300 | -0.25744200 | 0.71751500 |
| N | 3.38344400 | -0.47599000 | 0.75318400 |
| C | -4.42799000 | 1.23237100 | -0.64441500 |
| C | -5.02894900 | 0.09498500 | -1.17401400 |
| C | -4.71570500 | -1.14423500 | -0.62178500 |
| C | -3.81757800 | -1.23618800 | 0.42809400 |
| C | -3.52232800 | 1.12807000 | 0.39900800 |
| H | -5.73177400 | 0.17374300 | -1.99956700 |
| H | -2.99368100 | 1.95846100 | 0.86547400 |
| N | -3.25552400 | -0.09948600 | 0.87483800 |
| O | -2.38543900 | -0.20210700 | 1.90879900 |
| H | -3.51142500 | -2.15536900 | 0.91913100 |
| Cl | -5.41900400 | -2.58477300 | -1.24655600 |
| Cl | -4.78461400 | 2.78963600 | -1.28262200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.228966

Electronic Energy (0K) + ZPE = -3499.630137

Enthalpy (353K) = -3499.565981

Free Energy (353K) = -3499.737619

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.788550

A2

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.98077800 | 2.62667300 | -0.04497500 |
| C | 0.14162900 | 2.76040900 | -0.49103200 |
| N | 1.39433600 | 2.90303100 | -0.96524400 |
| C | 1.79529900 | 2.06945000 | -2.11407200 |
| C | 1.71286600 | 0.62889600 | -1.84521700 |
| C | 1.83785200 | -0.56510200 | -1.55062800 |
| C | 2.24592900 | -1.89484900 | -1.20148200 |
| C | 3.59983200 | -2.25567700 | -1.23554200 |
| C | 1.28908900 | -2.83344200 | -0.79579100 |
| C | 3.98328500 | -3.53461000 | -0.85965300 |
| H | 4.33531000 | -1.52266900 | -1.55867000 |
| C | 1.68031600 | -4.10955300 | -0.41143900 |
| C | 3.02606900 | -4.45939900 | -0.44442900 |
| H | 5.03358500 | -3.81250200 | -0.88878400 |
| H | 0.92570300 | -4.82298800 | -0.08667400 |
| S | 2.60869200 | 3.29019100 | 0.21072500 |
| O | 1.98290800 | 4.27415800 | 1.07538200 |
| O | 3.79426800 | 3.60285300 | -0.57188700 |
| C | 2.85558800 | 1.78166700 | 1.08449900 |
| C | 1.86944600 | 1.34937000 | 1.97525500 |
| C | 3.96254200 | 0.99460400 | 0.77990700 |
| C | 1.98840600 | 0.08611400 | 2.53176500 |
| H | 1.02690900 | 1.98936900 | 2.22634100 |
| C | 4.07021400 | -0.25912100 | 1.36883400 |
| H | 4.72035500 | 1.35772600 | 0.08959400 |
| C | 3.07395700 | -0.74312100 | 2.22072000 |
| H | 1.21986000 | -0.27808200 | 3.21049800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 4.93217100 | -0.88586800 | 1.14529100 |
| C | 3.12009300 | -2.13891400 | 2.75134200 |
| H | 4.10069300 | -2.60231600 | 2.60139500 |
| H | 2.87717300 | -2.17173500 | 3.81973900 |
| H | 2.36519100 | -2.74767100 | 2.23238800 |
| H | 1.15688400 | 2.34769800 | -2.95980500 |
| H | 2.82497400 | 2.33617600 | -2.38115500 |
| C | -2.29873100 | 2.45916400 | 0.47447400 |
| C | -3.26106800 | 3.46781800 | 0.31319300 |
| C | -2.65298200 | 1.26979700 | 1.13329400 |
| C | -4.55003500 | 3.28869500 | 0.79960600 |
| H | -2.98365400 | 4.38848000 | -0.19542600 |
| C | -3.94495900 | 1.09575800 | 1.61188300 |
| H | -1.90393700 | 0.48659800 | 1.26363400 |
| C | -4.89462000 | 2.10388700 | 1.44645300 |
| H | -5.28874300 | 4.07674400 | 0.67396000 |
| H | -4.20984900 | 0.17094700 | 2.12044300 |
| H | -5.90405700 | 1.96642600 | 1.82730000 |
| N | -0.10312600 | -2.46287900 | -0.78776900 |
| H | -0.64960200 | -2.98980900 | -1.46710700 |
| C | -0.72107200 | -2.32368500 | 0.47448200 |
| O | -0.04869000 | -2.10956100 | 1.46626300 |
| C | -2.20386700 | -2.42393500 | 0.51297300 |
| C | -2.79957400 | -2.45196200 | 1.77919400 |
| C | -3.01159300 | -2.49663800 | -0.62726900 |
| C | -4.17788700 | -2.56121500 | 1.90434200 |
| H | -2.16183500 | -2.39471300 | 2.65772800 |
| C | -4.39303100 | -2.58491400 | -0.49924600 |
| H | -2.58291300 | -2.46878100 | -1.62728000 |
| C | -4.97715400 | -2.62053900 | 0.76436400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -4.63084900 | -2.59571600 | 2.89220300 |
| H | -5.01405600 | -2.63233800 | -1.39084700 |
| H | -6.05744000 | -2.69948500 | 0.86084500 |
| H | 3.32890500 | -5.45965300 | -0.14581500 |
| Cu | -0.16891600 | -0.29429500 | -1.59849000 |
| C | -4.46642700 | 0.90264700 | -2.18808800 |
| H | -4.55847500 | 1.92270500 | -2.57330900 |
| H | -4.91567300 | 0.85134400 | -1.18874800 |
| H | -4.98805400 | 0.21355700 | -2.85914100 |
| C | -3.07704200 | 0.53716600 | -2.09345500 |
| N | -1.96500000 | 0.23639300 | -1.99236200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2257.871381

Electronic Energy (0K) + ZPE = -2257.350010

Enthalpy (353K) = -2257.296864

Free Energy (353K) = -2257.441920

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2258.295094

TS_{A2}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.30658700 | -2.60241600 | 0.87166300 |
| C | 0.15657000 | -2.25714000 | 0.67330900 |
| N | -1.13554200 | -1.90248200 | 0.56023400 |
| C | -1.68277900 | -1.47328400 | -0.74177500 |
| C | -1.38591900 | -0.05697100 | -1.08419800 |
| C | -0.45697200 | 0.83605300 | -0.99469100 |
| C | -0.39448500 | 2.29548600 | -0.99048600 |
| C | -1.55253300 | 3.07435200 | -0.81900700 |
| C | 0.84247200 | 2.96994900 | -1.01110200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.48367400 | 4.44482200 | -0.62138400 |
| H | -2.51706300 | 2.57681000 | -0.84027000 |
| C | 0.91034000 | 4.34564600 | -0.79816300 |
| C | -0.24593100 | 5.08410300 | -0.58821300 |
| H | -2.39914100 | 5.01557600 | -0.48286500 |
| H | 1.88461900 | 4.82899400 | -0.81104100 |
| S | -1.89555300 | -1.37703500 | 2.01725000 |
| O | -1.56305300 | -2.38844900 | 3.00545100 |
| O | -3.27739300 | -1.11553100 | 1.63253500 |
| C | -1.10190100 | 0.13920200 | 2.44436800 |
| C | 0.22853100 | 0.11792700 | 2.87324700 |
| C | -1.79033500 | 1.33635700 | 2.28013800 |
| C | 0.87883800 | 1.32439700 | 3.07757300 |
| H | 0.74337300 | -0.82396900 | 3.04508300 |
| C | -1.12481300 | 2.53302700 | 2.51448800 |
| H | -2.83821200 | 1.32758700 | 1.99068700 |
| C | 0.22221500 | 2.54743800 | 2.88169700 |
| H | 1.92041400 | 1.32673900 | 3.39521400 |
| H | -1.65543600 | 3.47584000 | 2.39388400 |
| C | 0.96900200 | 3.83117000 | 3.04165400 |
| H | 0.30403500 | 4.69870500 | 2.98050800 |
| H | 1.50267700 | 3.86690400 | 3.99900600 |
| H | 1.72273800 | 3.90918500 | 2.24646700 |
| H | -1.26923800 | -2.16217400 | -1.48841300 |
| H | -2.75697100 | -1.66821400 | -0.70376300 |
| C | 2.66844600 | -2.94727500 | 1.11782300 |
| C | 3.11457500 | -4.26883900 | 0.96595500 |
| C | 3.58113500 | -1.95379500 | 1.51099100 |
| C | 4.44512400 | -4.58848700 | 1.20650200 |
| H | 2.40618100 | -5.03645900 | 0.66232900 |

| | | | |
|----|-------------|-------------|-------------|
| C | 4.90640600 | -2.28344900 | 1.76266700 |
| H | 3.23410100 | -0.92470100 | 1.61102900 |
| C | 5.34072600 | -3.59980400 | 1.60899400 |
| H | 4.78392700 | -5.61488000 | 1.08730000 |
| H | 5.60395300 | -1.51296200 | 2.08401000 |
| H | 6.37921100 | -3.85532300 | 1.80679300 |
| N | 2.04444400 | 2.26826000 | -1.29088900 |
| H | 2.13584900 | 1.84850900 | -2.20973200 |
| C | 3.10822200 | 2.20829500 | -0.42461100 |
| O | 3.03458700 | 2.59792800 | 0.73358900 |
| C | 4.35465700 | 1.60196500 | -0.97557800 |
| C | 5.23928800 | 1.01165200 | -0.06919700 |
| C | 4.67472100 | 1.62404200 | -2.33612000 |
| C | 6.41273500 | 0.41998400 | -0.52019500 |
| H | 4.99030700 | 1.02836400 | 0.99000100 |
| C | 5.85639300 | 1.04350500 | -2.78470300 |
| H | 4.02229700 | 2.12267800 | -3.05089400 |
| C | 6.72101500 | 0.43279800 | -1.87947300 |
| H | 7.09504500 | -0.04459000 | 0.18837200 |
| H | 6.10668600 | 1.07650200 | -3.84245300 |
| H | 7.64322800 | -0.02370600 | -2.23227300 |
| H | -0.18240500 | 6.15680000 | -0.42247500 |
| Cu | 1.16652400 | -0.24759000 | -1.07863900 |
| C | 4.82315400 | -2.63638700 | -2.11331000 |
| H | 4.53878100 | -3.67515000 | -2.30787900 |
| H | 5.47127700 | -2.59840400 | -1.22953600 |
| H | 5.36601000 | -2.24041300 | -2.97720300 |
| C | 3.64405100 | -1.84576000 | -1.86773200 |
| N | 2.70006100 | -1.21314000 | -1.65101200 |
| C | -5.90555100 | -1.36922700 | -1.89102000 |

| | | | |
|----|-------------|-------------|-------------|
| C | -6.51722700 | -0.97219200 | -0.70654100 |
| C | -5.86101600 | -0.02262200 | 0.06474600 |
| C | -4.64499700 | 0.50330900 | -0.33340800 |
| C | -4.68399400 | -0.84877500 | -2.27441400 |
| H | -7.47104000 | -1.39016900 | -0.39739500 |
| H | -4.14619700 | -1.12110000 | -3.17628100 |
| N | -4.08660400 | 0.07130200 | -1.48206100 |
| O | -2.91531500 | 0.55860900 | -1.85845000 |
| H | -4.08774300 | 1.25415400 | 0.21554400 |
| Cl | -6.53713700 | 0.51977500 | 1.55790500 |
| Cl | -6.66034500 | -2.54276500 | -2.91091000 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.215477

Electronic Energy (0K) + ZPE = -3499.619052

Enthalpy (353K) = -3499.554890

Free Energy (353K) = -3499.724602

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.775407

B2

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.47704500 | -2.85293800 | 0.56980700 |
| C | 0.34771600 | -2.43244400 | 0.39694600 |
| N | -0.93308400 | -2.02413600 | 0.35413400 |
| C | -1.55249900 | -1.54247600 | -0.89733400 |
| C | -1.52566300 | -0.04396200 | -1.08518000 |
| C | -0.51996000 | 0.81204300 | -0.86314800 |
| C | -0.62835000 | 2.28318900 | -0.79113600 |
| C | -1.83985200 | 2.93922000 | -0.49063900 |
| C | 0.52194200 | 3.10620100 | -0.83033900 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.90741400 | 4.29116500 | -0.19347000 |
| H | -2.76131500 | 2.36818400 | -0.46865800 |
| C | 0.45626900 | 4.46677300 | -0.52887900 |
| C | -0.74878500 | 5.06378900 | -0.19307000 |
| H | -2.86826900 | 4.74106500 | 0.04705200 |
| H | 1.37355600 | 5.04981800 | -0.56704100 |
| S | -1.66084500 | -1.70793200 | 1.87577500 |
| O | -1.21688400 | -2.77833200 | 2.75219200 |
| O | -3.07637300 | -1.52087200 | 1.57465800 |
| C | -0.97378900 | -0.17776800 | 2.43321400 |
| C | 0.39884400 | -0.09869900 | 2.68258900 |
| C | -1.79362600 | 0.93818900 | 2.55862400 |
| C | 0.95204500 | 1.13499200 | 2.98655200 |
| H | 1.02470100 | -0.98642000 | 2.63053700 |
| C | -1.22097300 | 2.16196200 | 2.88494400 |
| H | -2.86945700 | 0.85026200 | 2.42494900 |
| C | 0.15735200 | 2.28761000 | 3.06843600 |
| H | 2.02436200 | 1.21466700 | 3.16019500 |
| H | -1.85480300 | 3.04193000 | 2.98109300 |
| C | 0.78623500 | 3.61860000 | 3.32258800 |
| H | 0.03452000 | 4.39900400 | 3.47925300 |
| H | 1.44582800 | 3.58883100 | 4.19829400 |
| H | 1.40719200 | 3.89445900 | 2.45948000 |
| H | -1.01841800 | -2.06250100 | -1.70232500 |
| H | -2.57674100 | -1.92893200 | -0.91319200 |
| C | 2.84256800 | -3.20730000 | 0.78360800 |
| C | 3.30492200 | -4.50530500 | 0.51969400 |
| C | 3.74709700 | -2.24141300 | 1.25947500 |
| C | 4.64103500 | -4.82719500 | 0.72543600 |
| H | 2.60467500 | -5.25362000 | 0.15493500 |

| | | | |
|----|-------------|-------------|-------------|
| C | 5.07874200 | -2.57217000 | 1.47148800 |
| H | 3.39060400 | -1.22898200 | 1.45069400 |
| C | 5.52833600 | -3.86492800 | 1.20294900 |
| H | 4.99080400 | -5.83587400 | 0.51856500 |
| H | 5.76947600 | -1.81904600 | 1.84505700 |
| H | 6.57182900 | -4.12277000 | 1.36892500 |
| N | 1.79135300 | 2.58456700 | -1.19012500 |
| H | 1.86290300 | 2.07085400 | -2.06114500 |
| C | 2.87269600 | 2.58684000 | -0.34575900 |
| O | 2.81499500 | 2.99794100 | 0.80634100 |
| C | 4.13272800 | 2.02580900 | -0.91519800 |
| C | 5.03771500 | 1.44187900 | -0.02467700 |
| C | 4.44013700 | 2.07919900 | -2.27723700 |
| C | 6.22475200 | 0.89285300 | -0.49348600 |
| H | 4.79357600 | 1.42719800 | 1.03584000 |
| C | 5.63750500 | 1.54510000 | -2.74272100 |
| H | 3.76114700 | 2.56446500 | -2.97645600 |
| C | 6.52604100 | 0.94462700 | -1.85380000 |
| H | 6.92498600 | 0.43558100 | 0.20207700 |
| H | 5.88037100 | 1.60440700 | -3.80120000 |
| H | 7.46048300 | 0.52479300 | -2.22004100 |
| H | -0.78640500 | 6.12406400 | 0.04461400 |
| Cu | 1.19742600 | -0.06188100 | -0.95461700 |
| C | 4.87207300 | -2.26514900 | -2.30441900 |
| H | 4.57106700 | -3.26449200 | -2.63428800 |
| H | 5.54400200 | -2.35735800 | -1.44291700 |
| H | 5.39550900 | -1.75718700 | -3.12011400 |
| C | 3.70871000 | -1.50845100 | -1.91640100 |
| N | 2.77884400 | -0.90554400 | -1.58420000 |
| C | -5.92627700 | -1.10461700 | -2.01085200 |

| | | | |
|----|-------------|-------------|-------------|
| C | -6.44550900 | -0.90852900 | -0.73403300 |
| C | -5.65846100 | -0.24932600 | 0.20069400 |
| C | -4.39142600 | 0.20069000 | -0.13342900 |
| C | -4.65593100 | -0.66340500 | -2.33036800 |
| H | -7.44136600 | -1.25931100 | -0.47569300 |
| H | -4.17520700 | -0.77935700 | -3.29620900 |
| N | -3.94606400 | -0.03338700 | -1.37585400 |
| O | -2.72214100 | 0.44663400 | -1.77100200 |
| H | -3.72580800 | 0.72580900 | 0.54214200 |
| Cl | -6.23806000 | 0.03412000 | 1.79702300 |
| Cl | -6.85392100 | -1.90997300 | -3.21978400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.224283

Electronic Energy (0K) + ZPE = -3499.625804

Enthalpy (353K) = -3499.561812

Free Energy (353K) = -3499.730812

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.781662

A3

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.03549800 | -1.39892900 | 0.16397500 |
| C | 0.97896500 | -1.03672100 | 0.88535600 |
| N | 1.73725100 | -0.46174700 | 1.84267900 |
| C | 1.08190300 | 0.56575600 | 2.69744900 |
| C | 0.36916000 | 1.56061500 | 1.91291600 |
| C | -0.21490600 | 2.32085700 | 1.16744600 |
| C | -0.97963000 | 3.14470100 | 0.29241000 |
| C | -0.45208000 | 4.33940600 | -0.21067000 |
| C | -2.28198300 | 2.73226600 | -0.09017300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.18884100 | 5.12447900 | -1.08457400 |
| H | 0.54948300 | 4.63328000 | 0.09912800 |
| C | -3.01454800 | 3.52823200 | -0.97468900 |
| C | -2.46470200 | 4.70977800 | -1.46011600 |
| H | -0.77186700 | 6.05139700 | -1.47022700 |
| H | -4.00690500 | 3.21108000 | -1.27097600 |
| S | 3.38654400 | -0.18062000 | 1.39230700 |
| O | 3.72117800 | -1.34426400 | 0.56943300 |
| O | 4.08496600 | 0.08858400 | 2.63497300 |
| C | 3.33111200 | 1.26590200 | 0.39467100 |
| C | 2.88662200 | 1.15874900 | -0.92535500 |
| C | 3.60632900 | 2.49954400 | 0.98053100 |
| C | 2.71911000 | 2.31992100 | -1.66279000 |
| H | 2.68504900 | 0.18634900 | -1.37019200 |
| C | 3.43726500 | 3.64743800 | 0.21860700 |
| H | 3.94581300 | 2.55776500 | 2.01185300 |
| C | 2.98985400 | 3.57649200 | -1.10459900 |
| H | 2.37341400 | 2.25753300 | -2.69307200 |
| H | 3.65136400 | 4.61979600 | 0.65837700 |
| C | 2.81620200 | 4.81667300 | -1.92116700 |
| H | 2.70319200 | 5.70342600 | -1.28852800 |
| H | 3.69178100 | 4.98059200 | -2.56292200 |
| H | 1.94420600 | 4.74042000 | -2.58016300 |
| H | 0.39924000 | 0.02999200 | 3.36778900 |
| H | 1.85986000 | 1.00805700 | 3.33103000 |
| C | -1.03288200 | -1.53554500 | -0.77796100 |
| C | -1.76359700 | -2.72840900 | -0.88201600 |
| C | -1.34281800 | -0.44553800 | -1.60852200 |
| C | -2.79213200 | -2.82543500 | -1.80849800 |
| H | -1.51948400 | -3.56308900 | -0.22726300 |

| | | | |
|----|-------------|-------------|-------------|
| C | -2.37896600 | -0.55058400 | -2.52574300 |
| H | -0.76288100 | 0.47244400 | -1.51878500 |
| C | -3.10036600 | -1.73937800 | -2.62715500 |
| H | -3.36283800 | -3.74736800 | -1.88794400 |
| H | -2.62866200 | 0.29840000 | -3.15794100 |
| H | -3.91137100 | -1.81914800 | -3.34729700 |
| N | -2.74670400 | 1.53601000 | 0.45527900 |
| H | -2.07114400 | 1.06704200 | 1.04826300 |
| C | -3.90883900 | 0.85473900 | 0.19178300 |
| O | -4.75966900 | 1.24764900 | -0.59499900 |
| C | -4.05527200 | -0.43621300 | 0.93330400 |
| C | -5.02420400 | -1.32721200 | 0.46520900 |
| C | -3.28873700 | -0.78771000 | 2.05069100 |
| C | -5.21060100 | -2.55681700 | 1.08413800 |
| H | -5.62124000 | -1.03832500 | -0.39654800 |
| C | -3.47783600 | -2.01708300 | 2.67189200 |
| H | -2.55879400 | -0.09840300 | 2.47518900 |
| C | -4.43394300 | -2.90599800 | 2.18609600 |
| H | -5.96294000 | -3.24530100 | 0.70645000 |
| H | -2.88457800 | -2.27657900 | 3.54557400 |
| H | -4.58016500 | -3.86705400 | 2.67388000 |
| H | -3.05127400 | 5.31653400 | -2.14630900 |
| N | 2.47373100 | -4.02548200 | -1.11794600 |
| C | 2.94399300 | -4.90532300 | -1.70175800 |
| C | 3.52854700 | -5.99921400 | -2.43080900 |
| H | 2.94590800 | -6.90924700 | -2.25888600 |
| H | 3.53257300 | -5.76650700 | -3.49996600 |
| H | 4.55672500 | -6.15755900 | -2.09129900 |
| Cu | 1.72907000 | -2.58101600 | -0.15726600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2257.868137

Electronic Energy (0K) + ZPE = -2257.346982

Enthalpy (353K) = -2257.293033

Free Energy (353K) = -2257.443391

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2258.293617

TS_{A3}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 0.11367900 | -0.65209600 | 0.79127200 |
| C | -0.75034700 | -1.37764200 | 0.15172800 |
| N | -0.91298600 | -1.79309300 | -1.14938100 |
| C | -0.38618900 | -0.96000700 | -2.26505200 |
| C | -0.63997700 | 0.45680400 | -2.06495000 |
| C | -0.89516300 | 1.60378100 | -1.76108500 |
| C | -1.19555200 | 2.93989400 | -1.37267800 |
| C | -2.39824200 | 3.52322300 | -1.79417200 |
| C | -0.31558900 | 3.66854800 | -0.53513000 |
| C | -2.74723900 | 4.80444000 | -1.39962600 |
| H | -3.05091900 | 2.93730600 | -2.43895900 |
| C | -0.68120200 | 4.96017100 | -0.13984900 |
| C | -1.88118300 | 5.51292800 | -0.56995800 |
| H | -3.68368100 | 5.24461400 | -1.73308700 |
| H | -0.01994000 | 5.52062800 | 0.50860700 |
| S | -2.41200400 | -2.56928600 | -1.50308400 |
| O | -2.72767600 | -3.38152600 | -0.33101600 |
| O | -2.22816500 | -3.19092300 | -2.80504700 |
| C | -3.57207700 | -1.24580900 | -1.63656700 |
| C | -4.11284900 | -0.69431800 | -0.47327100 |
| C | -3.82444900 | -0.69132700 | -2.88951000 |

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|---|-------------|-------------|-------------|
| C | -4.89821900 | 0.44376500 | -0.57718400 |
| H | -3.92388200 | -1.15340200 | 0.49746400 |
| C | -4.62388400 | 0.44104700 | -2.97080500 |
| H | -3.40033100 | -1.13915800 | -3.78502700 |
| C | -5.16072400 | 1.02973900 | -1.82143000 |
| H | -5.32218400 | 0.88899400 | 0.32131800 |
| H | -4.82895900 | 0.88525700 | -3.94336900 |
| C | -6.01228500 | 2.25571800 | -1.91522800 |
| H | -5.79923800 | 2.82473600 | -2.82672400 |
| H | -7.07685200 | 1.98857800 | -1.93820200 |
| H | -5.86344200 | 2.91055300 | -1.04944300 |
| H | 0.68367000 | -1.16497000 | -2.36936300 |
| H | -0.84122900 | -1.32464100 | -3.19286400 |
| C | 0.24811000 | 0.25327200 | 1.91518900 |
| C | 1.43890000 | 0.37562500 | 2.64329800 |
| C | -0.85871900 | 1.03965600 | 2.28350200 |
| C | 1.50639600 | 1.23018600 | 3.73581100 |
| H | 2.32200200 | -0.18518000 | 2.34230200 |
| C | -0.78522300 | 1.89212500 | 3.37732200 |
| H | -1.77381700 | 0.97252100 | 1.69559700 |
| C | 0.39663400 | 1.98573900 | 4.10894500 |
| H | 2.43498700 | 1.31055100 | 4.29651300 |
| H | -1.64789200 | 2.49546800 | 3.64941700 |
| H | 0.45746500 | 2.65733600 | 4.96201100 |
| N | 0.90171200 | 3.07620500 | -0.17884800 |
| H | 1.10006600 | 2.17345600 | -0.60654500 |
| C | 1.81624700 | 3.53940400 | 0.74310200 |
| O | 1.59545300 | 4.46484600 | 1.51245300 |
| C | 3.12584700 | 2.82473800 | 0.74963600 |
| C | 3.84931600 | 2.81159900 | 1.94492900 |

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|----|-------------|-------------|-------------|
| C | 3.66591900 | 2.21933400 | -0.38686700 |
| C | 5.07077100 | 2.15497200 | 2.01846600 |
| H | 3.42962400 | 3.31186100 | 2.81470200 |
| C | 4.90081000 | 1.58145800 | -0.31912500 |
| H | 3.13787900 | 2.27378800 | -1.33802500 |
| C | 5.59582800 | 1.53342600 | 0.88660700 |
| H | 5.62023200 | 2.13360700 | 2.95678400 |
| H | 5.32684900 | 1.13003800 | -1.21385100 |
| H | 6.55680200 | 1.02669900 | 0.94021300 |
| H | -2.13787000 | 6.52026700 | -0.24971500 |
| N | -2.87115900 | -2.54538600 | 3.09679100 |
| C | -3.52088900 | -2.88298100 | 3.99157300 |
| C | -4.33017700 | -3.30091700 | 5.10595500 |
| H | -4.16648600 | -4.36478700 | 5.30181300 |
| H | -4.05892500 | -2.72401600 | 5.99516100 |
| H | -5.38698400 | -3.13522800 | 4.87604900 |
| Cu | -1.84224400 | -1.99431900 | 1.62840900 |
| C | 3.72905900 | -2.94044400 | -0.28472100 |
| C | 4.42882300 | -2.75622200 | -1.46931200 |
| C | 4.10646200 | -1.63377300 | -2.21992100 |
| C | 3.13314400 | -0.74536800 | -1.80204800 |
| C | 2.76554000 | -2.04035200 | 0.13866500 |
| H | 5.18980000 | -3.45918500 | -1.79496400 |
| H | 2.19682600 | -2.14588800 | 1.05630800 |
| N | 2.49259800 | -0.95935800 | -0.62751300 |
| O | 1.61565600 | -0.05846800 | -0.25573800 |
| H | 2.83066400 | 0.14074500 | -2.35100000 |
| Cl | 4.92133300 | -1.31072400 | -3.71008300 |
| Cl | 4.05465300 | -4.31802500 | 0.70918700 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.223131

Electronic Energy (0K) + ZPE = -3499.626160

Enthalpy (353K) = -3499.561789

Free Energy (353K) = -3499.734842

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.784545

B3

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.92867400 | -0.14298000 | 0.51097300 |
| C | -0.01249100 | -1.11363000 | 0.38581500 |
| N | -0.16747100 | -1.78809600 | -0.83801800 |
| C | -0.18276800 | -1.02600600 | -2.11518200 |
| C | -1.03965200 | 0.14982800 | -2.02734200 |
| C | -1.80055500 | 1.07774800 | -1.84259500 |
| C | -2.66611600 | 2.18145100 | -1.59334400 |
| C | -4.00408300 | 2.12614800 | -2.00183900 |
| C | -2.18486400 | 3.32983200 | -0.91784600 |
| C | -4.86810700 | 3.18101900 | -1.75238100 |
| H | -4.34273400 | 1.23230500 | -2.52212900 |
| C | -3.06522900 | 4.38606600 | -0.66503300 |
| C | -4.38877500 | 4.30409400 | -1.08241100 |
| H | -5.90441300 | 3.12771100 | -2.07651900 |
| H | -2.70071800 | 5.26164500 | -0.14253600 |
| S | -1.23803000 | -3.13290700 | -0.86766800 |
| O | -1.17053300 | -3.74832100 | 0.45396600 |
| O | -0.85555300 | -3.89390200 | -2.05024700 |
| C | -2.85946300 | -2.47123700 | -1.12467600 |
| C | -3.58137600 | -1.96171200 | -0.04432900 |
| C | -3.35857600 | -2.39844600 | -2.42401400 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.80459300 | -1.35214400 | -0.28308900 |
| H | -3.19972000 | -2.04606000 | 0.97183700 |
| C | -4.58943100 | -1.79369200 | -2.63961700 |
| H | -2.79161300 | -2.81450600 | -3.25291200 |
| C | -5.32481600 | -1.25600600 | -1.57843300 |
| H | -5.37380500 | -0.94539500 | 0.55105000 |
| H | -4.98766800 | -1.73159700 | -3.65100400 |
| C | -6.64972100 | -0.60437300 | -1.81833300 |
| H | -6.70648000 | -0.16600000 | -2.82087700 |
| H | -7.46336000 | -1.33725300 | -1.73879900 |
| H | -6.84801600 | 0.18026600 | -1.07996100 |
| H | 0.83766100 | -0.73928400 | -2.38567900 |
| H | -0.51888300 | -1.69843300 | -2.91191600 |
| C | 1.10926200 | 0.76462000 | 1.65357000 |
| C | 2.38425000 | 1.18523300 | 2.05665400 |
| C | -0.00532600 | 1.25508400 | 2.35140500 |
| C | 2.54032700 | 2.02950500 | 3.14983200 |
| H | 3.26684500 | 0.85002700 | 1.51332800 |
| C | 0.15415400 | 2.09142300 | 3.45146000 |
| H | -1.00526600 | 0.99316100 | 2.00457700 |
| C | 1.42802900 | 2.47861800 | 3.85858400 |
| H | 3.53974400 | 2.33786800 | 3.45021300 |
| H | -0.72409600 | 2.46211200 | 3.97556100 |
| H | 1.55307700 | 3.14236700 | 4.71089300 |
| N | -0.83308400 | 3.34054200 | -0.56352300 |
| H | -0.33568700 | 2.48210000 | -0.77869100 |
| C | -0.10550200 | 4.35701100 | 0.00735100 |
| O | -0.60747100 | 5.37986300 | 0.45431300 |
| C | 1.37263400 | 4.13936900 | 0.04109900 |
| C | 2.10536700 | 4.89345800 | 0.96244000 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.04839000 | 3.28112900 | -0.83188300 |
| C | 3.48843400 | 4.78735700 | 1.01878500 |
| H | 1.56844600 | 5.56428700 | 1.62892100 |
| C | 3.43501000 | 3.18033500 | -0.77769300 |
| H | 1.50807000 | 2.70669100 | -1.58423700 |
| C | 4.15676900 | 3.93108900 | 0.14564500 |
| H | 4.04818700 | 5.37544700 | 1.74238500 |
| H | 3.95637300 | 2.52111700 | -1.46965200 |
| H | 5.24117500 | 3.85390000 | 0.18174000 |
| H | -5.05517400 | 5.13870800 | -0.87626500 |
| N | -1.74265900 | -2.15533400 | 3.59592900 |
| C | -2.25578800 | -2.49395000 | 4.57541300 |
| C | -2.89729500 | -2.91548600 | 5.79370300 |
| H | -2.73736000 | -3.98746700 | 5.94279200 |
| H | -2.47695200 | -2.36636500 | 6.64139800 |
| H | -3.97127200 | -2.71597300 | 5.73180800 |
| Cu | -0.93130200 | -1.62448800 | 1.98529400 |
| C | 4.14241900 | -2.64516500 | -0.19555600 |
| C | 4.97986800 | -2.40838400 | -1.27693100 |
| C | 4.71020600 | -1.30296100 | -2.07729100 |
| C | 3.64193800 | -0.47096100 | -1.79767800 |
| C | 3.07098900 | -1.80856000 | 0.07785300 |
| H | 5.81589300 | -3.06788000 | -1.49409900 |
| H | 2.36973600 | -1.93659300 | 0.90077500 |
| N | 2.87442200 | -0.76092700 | -0.73261600 |
| O | 1.84930600 | 0.14986200 | -0.54574500 |
| H | 3.36428200 | 0.40680000 | -2.37488300 |
| Cl | 5.70253900 | -0.94601300 | -3.43974700 |
| Cl | 4.41112900 | -3.99920500 | 0.83697100 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.242935

Electronic Energy (0K) + ZPE = -3499.644652

Enthalpy (353K) = -3499.580019

Free Energy (353K) = -3499.756551

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.800849

A4

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.18921500 | -1.80669400 | -1.04833200 |
| C | 0.23301200 | -1.49979300 | -1.73302400 |
| N | -0.85187400 | -1.15964300 | -2.45805300 |
| C | -1.21953200 | 0.26709800 | -2.50226000 |
| C | -1.28172600 | 0.85475400 | -1.15108700 |
| C | -1.19839400 | 0.81456700 | 0.08761000 |
| C | -0.97604800 | 0.77674600 | 1.48967300 |
| C | -2.05905900 | 0.67538700 | 2.37887700 |
| C | 0.35512600 | 0.84779600 | 1.98339700 |
| C | -1.84135900 | 0.64470400 | 3.74439300 |
| H | -3.06522600 | 0.61673100 | 1.96735000 |
| C | 0.55624600 | 0.80908400 | 3.36671800 |
| C | -0.53250700 | 0.71172600 | 4.22367600 |
| H | -2.67896500 | 0.56751800 | 4.43220400 |
| H | 1.56604900 | 0.85706700 | 3.75389100 |
| S | -2.13026800 | -2.32885600 | -2.47940400 |
| O | -1.47125900 | -3.59167000 | -2.75694600 |
| O | -3.12435300 | -1.76953100 | -3.38245300 |
| C | -2.76891800 | -2.34484300 | -0.83540500 |
| C | -2.09869900 | -3.07333800 | 0.14864900 |
| C | -3.89784200 | -1.58288000 | -0.53963300 |

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|---|-------------|-------------|-------------|
| C | -2.57728300 | -3.02842700 | 1.45029900 |
| H | -1.22574400 | -3.67168100 | -0.10115000 |
| C | -4.36464900 | -1.56305600 | 0.76728900 |
| H | -4.40663600 | -1.02758000 | -1.32394800 |
| C | -3.71343300 | -2.27987500 | 1.77748700 |
| H | -2.06483800 | -3.58884600 | 2.23041900 |
| H | -5.25213200 | -0.98191900 | 1.01344300 |
| C | -4.23039300 | -2.26096600 | 3.18048400 |
| H | -4.81129100 | -1.35466500 | 3.38407100 |
| H | -4.89273700 | -3.11809000 | 3.35926000 |
| H | -3.41429400 | -2.32832200 | 3.90825800 |
| H | -0.46530000 | 0.78889400 | -3.10251400 |
| H | -2.17214800 | 0.36320500 | -3.03304800 |
| C | 2.28849800 | -2.15914500 | -0.20897000 |
| C | 3.55912500 | -2.40676500 | -0.74805800 |
| C | 2.10444900 | -2.22202300 | 1.18196700 |
| C | 4.62460300 | -2.70344100 | 0.09241300 |
| H | 3.69977800 | -2.35208700 | -1.82551800 |
| C | 3.17443800 | -2.51705200 | 2.01569600 |
| H | 1.11455800 | -2.03003600 | 1.59455800 |
| C | 4.43565000 | -2.75588000 | 1.47207500 |
| H | 5.60972500 | -2.88696600 | -0.33042600 |
| H | 3.02530200 | -2.55679100 | 3.09230900 |
| H | 5.27406100 | -2.98375300 | 2.12633100 |
| N | 1.38352100 | 0.93075500 | 1.05067300 |
| H | 1.11160200 | 0.71917200 | 0.09579900 |
| C | 2.73446800 | 1.10169100 | 1.27879600 |
| O | 3.21279800 | 1.23863900 | 2.39459700 |
| C | 3.58388100 | 1.09447900 | 0.05213500 |
| C | 4.95135700 | 0.87520300 | 0.23866300 |

| | | | |
|----|-------------|------------|-------------|
| C | 3.09128400 | 1.28470400 | -1.24401100 |
| C | 5.81134500 | 0.82549600 | -0.85051700 |
| H | 5.32185900 | 0.73495600 | 1.25124500 |
| C | 3.95399100 | 1.23967600 | -2.33296200 |
| H | 2.03618500 | 1.49233800 | -1.42343500 |
| C | 5.31300700 | 1.00462500 | -2.13858800 |
| H | 6.87221500 | 0.64404600 | -0.69542100 |
| H | 3.56431700 | 1.39230300 | -3.33653300 |
| H | 5.98473500 | 0.96625200 | -2.99308700 |
| H | -0.34961300 | 0.68308500 | 5.29533500 |
| Cu | -1.46105100 | 2.76754000 | -0.67591300 |
| C | -2.05890500 | 7.19745400 | -0.62859800 |
| H | -2.62080800 | 7.48943900 | -1.52095300 |
| H | -1.08865400 | 7.70274400 | -0.62966600 |
| H | -2.61950100 | 7.49034700 | 0.26418900 |
| C | -1.86212400 | 5.77291600 | -0.62877500 |
| N | -1.70424000 | 4.62782800 | -0.63020200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2257.865869

Electronic Energy (0K) + ZPE = -2257.343593

Enthalpy (353K) = -2257.290313

Free Energy (353K) = -2257.438392

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2258.294121

TS_{A4}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -1.31766400 | -2.15546400 | -1.77364600 |
| C | -1.71726900 | -1.02960300 | -2.00274800 |
| N | -2.15850800 | 0.21379100 | -2.24377100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.20665500 | 1.28491500 | -2.59938700 |
| C | -0.30861900 | 1.79353900 | -1.51611900 |
| C | -0.31198300 | 1.49430000 | -0.26255700 |
| C | -0.75743500 | 0.82928700 | 0.92609500 |
| C | -1.65078400 | 1.48498400 | 1.78822100 |
| C | -0.22021400 | -0.42684300 | 1.30401600 |
| C | -2.02411900 | 0.91112700 | 2.99260000 |
| H | -2.03188900 | 2.46038000 | 1.49176200 |
| C | -0.60892500 | -1.00238400 | 2.51666100 |
| C | -1.50217400 | -0.33336200 | 3.34538300 |
| H | -2.71690500 | 1.42691300 | 3.65329100 |
| H | -0.19807200 | -1.96420000 | 2.80202200 |
| S | -3.85095400 | 0.46676800 | -2.25485700 |
| O | -4.43546100 | -0.67962600 | -2.93254400 |
| O | -4.03142500 | 1.81745900 | -2.76785900 |
| C | -4.33555900 | 0.41575800 | -0.55746200 |
| C | -4.36958800 | -0.81332100 | 0.10525700 |
| C | -4.70108300 | 1.59757800 | 0.07853700 |
| C | -4.76705100 | -0.84094900 | 1.43228400 |
| H | -4.10430700 | -1.73179400 | -0.41316100 |
| C | -5.11775600 | 1.54174900 | 1.40358200 |
| H | -4.67373900 | 2.54073100 | -0.46122800 |
| C | -5.15264200 | 0.33024700 | 2.09718400 |
| H | -4.78856500 | -1.78902600 | 1.96793600 |
| H | -5.41536500 | 2.45711600 | 1.91263800 |
| C | -5.59404500 | 0.26939100 | 3.52508500 |
| H | -5.64414700 | 1.26606500 | 3.97564800 |
| H | -6.58994300 | -0.18422300 | 3.60811600 |
| H | -4.91312100 | -0.34946900 | 4.12232500 |
| H | -0.59316000 | 0.90534900 | -3.42671800 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.79178800 | 2.11544600 | -3.00755100 |
| C | -0.83614100 | -3.44156200 | -1.38640900 |
| C | -0.15799000 | -4.26186200 | -2.30003900 |
| C | -0.99945800 | -3.87611300 | -0.06058700 |
| C | 0.35290900 | -5.48693300 | -1.89112300 |
| H | -0.02951300 | -3.92141000 | -3.32543200 |
| C | -0.49418400 | -5.10642900 | 0.33814800 |
| H | -1.51847200 | -3.23090600 | 0.64782800 |
| C | 0.18417300 | -5.91212700 | -0.57486600 |
| H | 0.88705200 | -6.11304000 | -2.60231000 |
| H | -0.62348800 | -5.43600400 | 1.36658200 |
| H | 0.58484000 | -6.87255700 | -0.25854800 |
| N | 0.66059200 | -1.04829300 | 0.41547700 |
| H | 0.50488400 | -0.81549200 | -0.55847300 |
| C | 1.61907500 | -1.99057200 | 0.69985400 |
| O | 1.83476100 | -2.40156800 | 1.83223800 |
| C | 2.39817700 | -2.46973100 | -0.48086400 |
| C | 3.09019700 | -3.67440500 | -0.33213400 |
| C | 2.48033000 | -1.77746100 | -1.69512700 |
| C | 3.83439400 | -4.19329100 | -1.38371200 |
| H | 3.02488600 | -4.19665100 | 0.61952500 |
| C | 3.23253600 | -2.29453300 | -2.74386600 |
| H | 1.98058800 | -0.81815300 | -1.83772000 |
| C | 3.90508200 | -3.50467400 | -2.59225500 |
| H | 4.35997000 | -5.13739200 | -1.26138000 |
| H | 3.29620000 | -1.74827100 | -3.68195200 |
| H | 4.48900100 | -3.90821700 | -3.41629600 |
| H | -1.79418400 | -0.79544900 | 4.28614100 |
| Cu | 1.01518500 | 3.07148600 | -2.08479100 |
| C | 3.94213500 | 6.05451400 | -3.67318600 |

| | | | |
|----|------------|-------------|-------------|
| H | 3.39102100 | 6.86567600 | -4.15820100 |
| H | 4.60175900 | 5.57902700 | -4.40514400 |
| H | 4.54414100 | 6.46507700 | -2.85718300 |
| C | 3.01507100 | 5.08428200 | -3.15252400 |
| N | 2.26786000 | 4.30613100 | -2.73599200 |
| C | 2.12841400 | 1.48511600 | 3.70056700 |
| C | 3.16963900 | 0.62995300 | 3.36931900 |
| C | 3.49427100 | 0.50558400 | 2.02155200 |
| C | 2.78790500 | 1.19251600 | 1.05233300 |
| C | 1.42842000 | 2.17269800 | 2.72223100 |
| H | 3.71843500 | 0.08612600 | 4.13315600 |
| H | 0.61181700 | 2.85995100 | 2.91352600 |
| N | 1.77268700 | 2.00351300 | 1.42870900 |
| O | 1.06418400 | 2.61459200 | 0.49837600 |
| H | 2.97950800 | 1.13343400 | -0.01511400 |
| Cl | 4.79746600 | -0.51543600 | 1.52946300 |
| Cl | 1.66748800 | 1.70727300 | 5.35219200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.214347

Electronic Energy (0K) + ZPE = -3499.618718

Enthalpy (353K) = -3499.553697

Free Energy (353K) = -3499.729646

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.780116

B4

Number of imaginary frequencies: 0

| | | | |
|---|------------|-------------|-------------|
| C | 1.25397400 | 1.20939900 | -2.28884000 |
| C | 1.60459200 | 0.07951000 | -2.00793500 |
| N | 1.94534700 | -1.17728100 | -1.67896200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.88260500 | -2.22059600 | -1.67748400 |
| C | -0.03454900 | -2.31538200 | -0.50295600 |
| C | 0.08096700 | -1.63186500 | 0.63443300 |
| C | 0.96266600 | -0.58968100 | 1.20936200 |
| C | 2.01443000 | -0.97454600 | 2.04612600 |
| C | 0.62644900 | 0.77811800 | 1.12082500 |
| C | 2.71581600 | -0.03721300 | 2.79429500 |
| H | 2.25433500 | -2.03440900 | 2.12307100 |
| C | 1.34149200 | 1.72311900 | 1.86350900 |
| C | 2.36960700 | 1.30884300 | 2.70128400 |
| H | 3.52388100 | -0.35478300 | 3.44956100 |
| H | 1.06137900 | 2.76882500 | 1.80023700 |
| S | 3.58669400 | -1.61028600 | -1.94551500 |
| O | 4.02691900 | -0.95292300 | -3.16826400 |
| O | 3.62929900 | -3.06179400 | -1.82653000 |
| C | 4.44562100 | -0.88784800 | -0.58174300 |
| C | 4.61545500 | 0.49726600 | -0.53063500 |
| C | 4.97222800 | -1.72367000 | 0.39702600 |
| C | 5.30289000 | 1.04117000 | 0.54275300 |
| H | 4.22686600 | 1.13668200 | -1.32003800 |
| C | 5.67826700 | -1.15698400 | 1.45169100 |
| H | 4.83926100 | -2.80009800 | 0.32661900 |
| C | 5.84144900 | 0.22619600 | 1.54693700 |
| H | 5.43491000 | 2.12048400 | 0.60536200 |
| H | 6.10389100 | -1.79967600 | 2.22054900 |
| C | 6.55005900 | 0.84233000 | 2.71107200 |
| H | 7.05046000 | 0.08829600 | 3.32672200 |
| H | 7.29808600 | 1.57306500 | 2.38229100 |
| H | 5.84001400 | 1.38259500 | 3.35172600 |
| H | 0.28858700 | -2.07452300 | -2.59117500 |

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|----|-------------|-------------|-------------|
| H | 1.39070100 | -3.18384000 | -1.80129900 |
| C | 0.83531000 | 2.56109100 | -2.46773600 |
| C | -0.04142600 | 2.91115600 | -3.50570400 |
| C | 1.26042800 | 3.54914200 | -1.56471900 |
| C | -0.49107000 | 4.21958400 | -3.62803600 |
| H | -0.37285300 | 2.14387000 | -4.20264700 |
| C | 0.81708800 | 4.85815400 | -1.70185800 |
| H | 1.93356300 | 3.26901200 | -0.75501400 |
| C | -0.06266900 | 5.19441000 | -2.72931600 |
| H | -1.17947000 | 4.48056900 | -4.42865400 |
| H | 1.15162300 | 5.61782800 | -0.99915700 |
| H | -0.41565400 | 6.21832800 | -2.82906100 |
| N | -0.44392100 | 1.13024300 | 0.28250800 |
| H | -0.57478300 | 0.50647100 | -0.50373300 |
| C | -1.24903900 | 2.23676400 | 0.35510800 |
| O | -1.14792500 | 3.08292100 | 1.23571200 |
| C | -2.29784500 | 2.33125900 | -0.70816100 |
| C | -3.03553900 | 3.51705900 | -0.75164600 |
| C | -2.58290700 | 1.31770700 | -1.63177800 |
| C | -4.03177100 | 3.69606300 | -1.70250000 |
| H | -2.80469000 | 4.29489500 | -0.02807800 |
| C | -3.57839200 | 1.49869000 | -2.58526900 |
| H | -2.04168100 | 0.37011800 | -1.63207800 |
| C | -4.30332500 | 2.68716400 | -2.62309000 |
| H | -4.59545900 | 4.62556600 | -1.72865100 |
| H | -3.78983000 | 0.70676200 | -3.29983500 |
| H | -5.08135800 | 2.82524600 | -3.37046800 |
| H | 2.90851600 | 2.05252800 | 3.28506200 |
| Cu | -1.42238100 | -3.61178500 | -0.71018200 |
| C | -4.58418200 | -6.72462900 | -1.27721300 |

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|----|-------------|-------------|-------------|
| H | -4.10199000 | -7.70194100 | -1.37404400 |
| H | -5.14922900 | -6.50997200 | -2.18926100 |
| H | -5.26878100 | -6.74276700 | -0.42399900 |
| C | -3.58333500 | -5.70956300 | -1.07791800 |
| N | -2.77756300 | -4.89469900 | -0.92122800 |
| C | -2.22004600 | 0.70690600 | 3.49480000 |
| C | -3.39125900 | 0.94503500 | 2.78640200 |
| C | -3.69598000 | 0.11372300 | 1.71037900 |
| C | -2.83182500 | -0.90170000 | 1.34175300 |
| C | -1.37345200 | -0.32966900 | 3.13197000 |
| H | -4.05441800 | 1.76035300 | 3.06531200 |
| H | -0.44932600 | -0.58703800 | 3.64056900 |
| N | -1.71273000 | -1.07268300 | 2.06737100 |
| O | -0.85783000 | -2.07517400 | 1.69241400 |
| H | -2.97665600 | -1.58394800 | 0.50686400 |
| Cl | -5.14382000 | 0.34917200 | 0.80551800 |
| Cl | -1.77184300 | 1.71056400 | 4.81984500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.228620

Electronic Energy (0K) + ZPE = -3499.630024

Enthalpy (353K) = -3499.565676

Free Energy (353K) = -3499.738531

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.792850

A5

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.72076000 | -0.25473600 | 0.85944600 |
| C | 0.39633100 | -1.24617400 | 0.17750400 |
| N | -0.11769700 | -2.30975700 | -0.46437100 |

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|---|-------------|-------------|-------------|
| C | -0.60416300 | -2.09248900 | -1.85158400 |
| C | -1.52069000 | -0.96389200 | -1.91370300 |
| C | -2.22166800 | 0.01897400 | -1.78090700 |
| C | -2.89743600 | 1.25958400 | -1.60127400 |
| C | -4.29399300 | 1.33374000 | -1.56170800 |
| C | -2.12161900 | 2.43352800 | -1.41529400 |
| C | -4.92943200 | 2.54890700 | -1.35192300 |
| H | -4.86662500 | 0.41771000 | -1.69629100 |
| C | -2.77150700 | 3.65180400 | -1.20421500 |
| C | -4.16129300 | 3.69805400 | -1.17636300 |
| H | -6.01483200 | 2.59957900 | -1.32254600 |
| H | -2.17911600 | 4.54676500 | -1.05608000 |
| S | -0.97923100 | -3.45101200 | 0.52077700 |
| O | -0.19425500 | -3.54603800 | 1.73893000 |
| O | -1.19025500 | -4.59796500 | -0.34680100 |
| C | -2.51626000 | -2.65222500 | 0.84083300 |
| C | -2.56672900 | -1.66785800 | 1.82920200 |
| C | -3.60550800 | -2.91749200 | 0.01464900 |
| C | -3.73449900 | -0.93568800 | 1.97697200 |
| H | -1.70734500 | -1.47812500 | 2.46899700 |
| C | -4.76717900 | -2.17624500 | 0.18710800 |
| H | -3.54283900 | -3.68774900 | -0.75025800 |
| C | -4.84613100 | -1.17288700 | 1.15789500 |
| H | -3.78790000 | -0.15888700 | 2.73882600 |
| H | -5.62903700 | -2.37284700 | -0.44822000 |
| C | -6.09315800 | -0.36656800 | 1.33302300 |
| H | -6.77376500 | -0.48458100 | 0.48367900 |
| H | -6.63211600 | -0.67669900 | 2.23751200 |
| H | -5.86122500 | 0.69848800 | 1.44950800 |
| H | 0.28260300 | -1.91578300 | -2.47537300 |

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|---|-------------|-------------|-------------|
| H | -1.05609400 | -3.02898800 | -2.19702400 |
| C | 0.48505700 | 0.96319200 | 1.59386900 |
| C | 1.51660800 | 1.64959100 | 2.24456800 |
| C | -0.81797600 | 1.48708300 | 1.61832700 |
| C | 1.24932100 | 2.84201500 | 2.90571800 |
| H | 2.52625700 | 1.24477200 | 2.21613200 |
| C | -1.07783100 | 2.67915700 | 2.27851900 |
| H | -1.61438800 | 0.95183200 | 1.10231000 |
| C | -0.04356800 | 3.35981500 | 2.91961700 |
| H | 2.05468800 | 3.37380400 | 3.40654800 |
| H | -2.08807200 | 3.08232300 | 2.28628000 |
| H | -0.24700900 | 4.29742300 | 3.43163600 |
| N | -0.73519700 | 2.28044000 | -1.44845500 |
| H | -0.43449000 | 1.31595600 | -1.54436800 |
| C | 0.24893800 | 3.20351600 | -1.19678900 |
| O | 0.03041900 | 4.36998200 | -0.89982700 |
| C | 1.64106300 | 2.66284900 | -1.29938200 |
| C | 2.64978200 | 3.37696700 | -0.64774800 |
| C | 1.97469400 | 1.50270700 | -2.00862400 |
| C | 3.96528000 | 2.93033400 | -0.68226700 |
| H | 2.37970300 | 4.28288800 | -0.10985000 |
| C | 3.29301400 | 1.05783000 | -2.04654700 |
| H | 1.22076000 | 0.95173700 | -2.57139700 |
| C | 4.28903600 | 1.76980100 | -1.38162100 |
| H | 4.74192600 | 3.49241000 | -0.16795000 |
| H | 3.54495000 | 0.16418800 | -2.61419500 |
| H | 5.31960100 | 1.42171200 | -1.41500600 |
| H | -4.65039300 | 4.65527300 | -1.01026700 |
| N | 4.17284300 | -0.38334000 | 1.14671200 |
| C | 5.17027700 | 0.01464100 | 1.57679000 |

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|----|------------|-------------|-------------|
| C | 6.41106600 | 0.53536700 | 2.09214900 |
| H | 6.68199000 | 1.43925000 | 1.53655800 |
| H | 6.29935300 | 0.78475400 | 3.15141500 |
| H | 7.20462000 | -0.20889500 | 1.97847200 |
| Cu | 2.49490000 | -1.03100000 | 0.29905900 |
| C | 3.69717300 | -4.47617100 | -2.49508500 |
| H | 3.07980900 | -5.34266600 | -2.24022200 |
| H | 4.75182500 | -4.73438000 | -2.36213200 |
| H | 3.52247600 | -4.20445300 | -3.54024800 |
| C | 3.35425600 | -3.36870100 | -1.63905700 |
| N | 3.07875500 | -2.48012200 | -0.95140000 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2390.559106

Electronic Energy (0K) + ZPE = -2389.991419

Enthalpy (353K) = -2389.931119

Free Energy (353K) = -2390.096501

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2391.018720

TS_{A5}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.65081600 | -0.44963800 | 1.18339500 |
| C | -0.73677700 | 0.78390700 | 0.75201100 |
| N | -0.23323000 | 1.82116700 | 0.08046600 |
| C | 0.06097800 | 1.75000900 | -1.38045200 |
| C | 1.44870600 | 1.43201200 | -1.66715900 |
| C | 2.61857200 | 1.16645800 | -1.85703100 |
| C | 3.94069600 | 0.67029500 | -2.04500000 |
| C | 5.04207800 | 1.52821500 | -2.13680000 |
| C | 4.13249800 | -0.73395100 | -2.12882100 |

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|---|-------------|-------------|-------------|
| C | 6.32029800 | 1.01708500 | -2.30880500 |
| H | 4.87400800 | 2.60134300 | -2.07328500 |
| C | 5.42238900 | -1.23853000 | -2.30442000 |
| C | 6.49869100 | -0.36214200 | -2.39279800 |
| H | 7.17185900 | 1.68846600 | -2.37935200 |
| H | 5.56505400 | -2.31106600 | -2.36538700 |
| S | 0.24819500 | 3.27202200 | 0.92738200 |
| O | -0.81602900 | 3.56877000 | 1.87382000 |
| O | 0.58473000 | 4.20638900 | -0.13687100 |
| C | 1.69252700 | 2.80834600 | 1.81987400 |
| C | 1.55066200 | 2.28242100 | 3.10372200 |
| C | 2.93547800 | 2.90810000 | 1.19779700 |
| C | 2.68641200 | 1.84580300 | 3.76880700 |
| H | 0.57084000 | 2.22318900 | 3.57100900 |
| C | 4.05699200 | 2.46118400 | 1.88250500 |
| H | 3.02140100 | 3.32582000 | 0.19705400 |
| C | 3.94906200 | 1.91958300 | 3.16850200 |
| H | 2.59707900 | 1.43736800 | 4.77381600 |
| H | 5.03709400 | 2.53522000 | 1.41441800 |
| C | 5.15510200 | 1.39965400 | 3.88276000 |
| H | 6.08018900 | 1.80584000 | 3.46200700 |
| H | 5.12087200 | 1.63800200 | 4.95140600 |
| H | 5.20541600 | 0.30580300 | 3.80007600 |
| H | -0.60318200 | 0.97259700 | -1.78034700 |
| H | -0.22654700 | 2.70030700 | -1.84453500 |
| C | 0.61890300 | -1.19514400 | 1.30806500 |
| C | 0.56175300 | -2.56183400 | 1.62599900 |
| C | 1.88603200 | -0.62008900 | 1.11976700 |
| C | 1.71680900 | -3.32806200 | 1.73350100 |
| H | -0.41579200 | -3.02331500 | 1.77903200 |

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|----|-------------|-------------|-------------|
| C | 3.04214900 | -1.38217900 | 1.23324700 |
| H | 1.97122000 | 0.43632700 | 0.87589000 |
| C | 2.96348900 | -2.74072200 | 1.53488800 |
| H | 1.64162000 | -4.38787900 | 1.96825900 |
| H | 4.01198400 | -0.91264900 | 1.07246800 |
| H | 3.86994600 | -3.33701300 | 1.61368300 |
| N | 2.98899100 | -1.52180200 | -2.02377300 |
| H | 2.15692300 | -0.99282500 | -1.78926400 |
| C | 2.85768400 | -2.88545900 | -2.00551900 |
| O | 3.79604000 | -3.66425600 | -2.10841200 |
| C | 1.44737700 | -3.35682200 | -1.83331700 |
| C | 1.26279400 | -4.68457400 | -1.44188500 |
| C | 0.32718200 | -2.54093000 | -2.03166700 |
| C | -0.01490700 | -5.18560000 | -1.22711700 |
| H | 2.14146800 | -5.30904100 | -1.29780600 |
| C | -0.95174800 | -3.04342200 | -1.81891600 |
| H | 0.43063200 | -1.51467700 | -2.38551900 |
| C | -1.12487300 | -4.36360600 | -1.40933100 |
| H | -0.14666800 | -6.21888300 | -0.91490400 |
| H | -1.81807400 | -2.40164900 | -1.98098000 |
| H | -2.12617500 | -4.75531000 | -1.23950600 |
| H | 7.49758400 | -0.77072900 | -2.52835900 |
| N | -3.15683100 | -1.86025900 | 3.41208800 |
| C | -3.59677000 | -2.14547900 | 4.44412800 |
| C | -4.14328600 | -2.50260400 | 5.73030000 |
| H | -3.61945000 | -3.37939600 | 6.12255000 |
| H | -4.02092000 | -1.67047300 | 6.42972400 |
| H | -5.20760200 | -2.73548400 | 5.63161000 |
| Cu | -2.31089600 | -1.37746000 | 1.66075200 |
| C | -5.17602700 | -3.47605800 | -1.35147300 |

| | | | |
|----|-------------|-------------|-------------|
| H | -6.05836400 | -2.84834300 | -1.51035200 |
| H | -5.49617800 | -4.45887000 | -0.99286900 |
| H | -4.64672100 | -3.59514900 | -2.30249600 |
| C | -4.30610000 | -2.85740800 | -0.38056900 |
| N | -3.59630600 | -2.35314300 | 0.38457700 |
| C | -3.93230300 | 1.20176100 | -2.31997100 |
| C | -3.91045200 | 2.55225400 | -2.65473100 |
| C | -3.44451700 | 3.43856300 | -1.69243200 |
| C | -3.00971600 | 2.99343700 | -0.45293100 |
| C | -3.49349200 | 0.76543200 | -1.08672500 |
| H | -4.25093600 | 2.89975200 | -3.62607800 |
| H | -3.47547600 | -0.26988700 | -0.75924400 |
| N | -3.03912200 | 1.66962400 | -0.18852000 |
| O | -2.56477500 | 1.23511400 | 0.95789200 |
| H | -2.64682700 | 3.62796800 | 0.35062200 |
| Cl | -3.38532600 | 5.13491000 | -2.02068100 |
| Cl | -4.50448800 | 0.01860600 | -3.44737500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.899140

Electronic Energy (0K) + ZPE = -3632.256794

Enthalpy (353K) = -3632.185348

Free Energy (353K) = -3632.376373

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.495118

B5

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.23188400 | -1.60636100 | 0.67818600 |
| C | -1.00452500 | -1.45964300 | -0.42074300 |
| N | -0.44657100 | -1.45697600 | -1.71105000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.97955900 | -1.17589300 | -1.98046700 |
| C | 1.45778600 | 0.05201600 | -1.35701400 |
| C | 1.86167700 | 1.07405500 | -0.84065900 |
| C | 2.38526800 | 2.23633300 | -0.20442700 |
| C | 1.65261300 | 3.42809400 | -0.20366900 |
| C | 3.65604900 | 2.19340700 | 0.41968100 |
| C | 2.15478100 | 4.57107200 | 0.40077300 |
| H | 0.67746300 | 3.42831100 | -0.68824000 |
| C | 4.15436400 | 3.34913200 | 1.02685700 |
| C | 3.40578400 | 4.52164800 | 1.01053500 |
| H | 1.57422800 | 5.49109200 | 0.39475000 |
| H | 5.12643400 | 3.31525300 | 1.50365900 |
| S | -1.45343200 | -0.91615100 | -2.98933700 |
| O | -2.82180200 | -1.32682900 | -2.67155000 |
| O | -0.83660300 | -1.38987800 | -4.22167200 |
| C | -1.35094800 | 0.85102500 | -2.94246700 |
| C | -2.09284600 | 1.55289100 | -1.99262000 |
| C | -0.44406000 | 1.50182400 | -3.77664300 |
| C | -1.90909700 | 2.92346900 | -1.87829700 |
| H | -2.80416700 | 1.03231500 | -1.35441400 |
| C | -0.27269100 | 2.87316300 | -3.64278400 |
| H | 0.12272500 | 0.93975400 | -4.51494100 |
| C | -0.99313900 | 3.60167800 | -2.69073800 |
| H | -2.48582200 | 3.48311000 | -1.14271600 |
| H | 0.44009600 | 3.39021800 | -4.28289700 |
| C | -0.78682400 | 5.07606600 | -2.53975800 |
| H | 0.25418100 | 5.35402000 | -2.73997700 |
| H | -1.41402600 | 5.63581300 | -3.24564000 |
| H | -1.04925800 | 5.41435100 | -1.53013700 |
| H | 1.57880200 | -2.02377200 | -1.62916800 |

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|---|-------------|-------------|-------------|
| H | 1.12441800 | -1.14307400 | -3.06579200 |
| C | 1.13988300 | -2.04392900 | 0.98212400 |
| C | 1.66909900 | -3.19341200 | 0.37988000 |
| C | 1.92221700 | -1.36503800 | 1.92885600 |
| C | 2.95770700 | -3.62532500 | 0.68069000 |
| H | 1.05081500 | -3.75817700 | -0.31754700 |
| C | 3.20407400 | -1.80240300 | 2.23586000 |
| H | 1.52085400 | -0.47835100 | 2.41973600 |
| C | 3.72878700 | -2.93189700 | 1.60824900 |
| H | 3.35562000 | -4.51542100 | 0.19751200 |
| H | 3.80266500 | -1.25605600 | 2.96257500 |
| H | 4.73638900 | -3.26886800 | 1.84389300 |
| N | 4.34368900 | 0.97820300 | 0.36868900 |
| H | 3.79785100 | 0.20024900 | 0.01083200 |
| C | 5.64993100 | 0.71552900 | 0.70136600 |
| O | 6.37896500 | 1.51510200 | 1.27360800 |
| C | 6.13089300 | -0.64335900 | 0.30950200 |
| C | 7.21528700 | -1.16845500 | 1.01758000 |
| C | 5.57837700 | -1.37848500 | -0.74450800 |
| C | 7.72667500 | -2.41850500 | 0.69348900 |
| H | 7.64661200 | -0.57950600 | 1.82357500 |
| C | 6.10205400 | -2.62267400 | -1.07817800 |
| H | 4.75301500 | -0.97912500 | -1.33439800 |
| C | 7.17083000 | -3.14718200 | -0.35674000 |
| H | 8.56440500 | -2.82409100 | 1.25586200 |
| H | 5.67328500 | -3.18313700 | -1.90573500 |
| H | 7.57661800 | -4.12206300 | -0.61735400 |
| H | 3.81280200 | 5.40997700 | 1.48829800 |
| N | -4.00519800 | -3.24082200 | -0.23703900 |
| C | -4.46484600 | -4.30015300 | -0.32786000 |

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|----|-------------|-------------|-------------|
| C | -5.03585300 | -5.62051500 | -0.44549500 |
| H | -5.12332100 | -5.89066900 | -1.50202000 |
| H | -4.39356300 | -6.34956700 | 0.05716800 |
| H | -6.02914800 | -5.64064600 | 0.01200900 |
| Cu | -2.96849900 | -1.42650000 | -0.30246100 |
| C | -6.68540600 | 1.23489400 | 0.20392300 |
| H | -6.44493200 | 2.12647800 | 0.79222000 |
| H | -7.47424300 | 0.67163500 | 0.71158600 |
| H | -7.04370300 | 1.54270600 | -0.78288900 |
| C | -5.50910400 | 0.41155600 | 0.06330400 |
| N | -4.55862500 | -0.24330000 | -0.03314500 |
| C | -3.57802900 | 0.58496900 | 3.05477500 |
| C | -3.13001400 | 1.85567600 | 2.72504800 |
| C | -1.88861200 | 1.96857900 | 2.10547200 |
| C | -1.13001200 | 0.84736900 | 1.81513200 |
| C | -2.81278800 | -0.53234200 | 2.76452000 |
| H | -3.72703400 | 2.73628200 | 2.94705600 |
| H | -3.10041600 | -1.55740300 | 2.97740500 |
| N | -1.62557100 | -0.35265000 | 2.16607900 |
| O | -0.92441300 | -1.50355200 | 1.95863600 |
| H | -0.16657000 | 0.86208700 | 1.30929600 |
| Cl | -1.25865800 | 3.52714400 | 1.71261900 |
| Cl | -5.11858000 | 0.35991700 | 3.79702100 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.916711

Electronic Energy (0K) + ZPE = -3632.272618

Enthalpy (353K) = -3632.201100

Free Energy (353K) = -3632.392908

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.510838

TS_{A5-1}

Number of imaginary frequencies: 1

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|---|-------------|-------------|-------------|
| C | -0.20285600 | -1.40846500 | -0.15363800 |
| C | 0.70354800 | -1.28671200 | 0.76259300 |
| N | 0.45737800 | -0.99823400 | 2.10031400 |
| C | -0.88059700 | -0.53022900 | 2.51216400 |
| C | -1.32390700 | 0.64189500 | 1.76674100 |
| C | -1.65936700 | 1.60944200 | 1.11412100 |
| C | -2.12343300 | 2.70675400 | 0.33299700 |
| C | -1.38671200 | 3.89456500 | 0.27297900 |
| C | -3.34330100 | 2.59923400 | -0.37982000 |
| C | -1.83579500 | 4.96947200 | -0.47973900 |
| H | -0.45350500 | 3.94684100 | 0.83186600 |
| C | -3.78673400 | 3.68587800 | -1.13727700 |
| C | -3.03432500 | 4.85510000 | -1.17946800 |
| H | -1.25614500 | 5.88865400 | -0.52203500 |
| H | -4.71942400 | 3.60298900 | -1.68169700 |
| S | 1.76923100 | -0.41845900 | 3.02939000 |
| O | 2.92859200 | -1.21122200 | 2.62064600 |
| O | 1.31383200 | -0.44591400 | 4.41231700 |
| C | 2.02375100 | 1.25824700 | 2.53349300 |
| C | 2.80063500 | 1.53098800 | 1.40854300 |
| C | 1.38618200 | 2.27567800 | 3.24282900 |
| C | 2.93478000 | 2.85046100 | 0.99568300 |
| H | 3.31014100 | 0.72673600 | 0.87932700 |
| C | 1.53405700 | 3.58555900 | 2.81161100 |
| H | 0.79355700 | 2.04324300 | 4.12449800 |
| C | 2.30171100 | 3.89171100 | 1.68104800 |
| H | 3.55710100 | 3.08242100 | 0.13200200 |

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|---|-------------|-------------|-------------|
| H | 1.04734500 | 4.39104000 | 3.35947400 |
| C | 2.42015500 | 5.30733900 | 1.21330000 |
| H | 1.46670200 | 5.66012300 | 0.79636900 |
| H | 2.66968100 | 5.98011500 | 2.04187100 |
| H | 3.18407000 | 5.41584200 | 0.43684300 |
| H | -1.58089900 | -1.36186200 | 2.35368600 |
| H | -0.86490300 | -0.33961400 | 3.59059000 |
| C | -1.45304600 | -1.95561600 | -0.59012300 |
| C | -1.92189200 | -3.12060900 | 0.04406300 |
| C | -2.23244300 | -1.36377900 | -1.59948000 |
| C | -3.14080300 | -3.67826700 | -0.32352000 |
| H | -1.30687000 | -3.58002900 | 0.81757000 |
| C | -3.44254300 | -1.93042200 | -1.96717300 |
| H | -1.87125100 | -0.46632900 | -2.09752900 |
| C | -3.89399700 | -3.09148300 | -1.33661000 |
| H | -3.49862100 | -4.57733500 | 0.17302300 |
| H | -4.04274600 | -1.46752400 | -2.74759100 |
| H | -4.84394900 | -3.53219500 | -1.63126900 |
| N | -4.04022100 | 1.39424400 | -0.25993200 |
| H | -3.52527700 | 0.65666000 | 0.21062400 |
| C | -5.33382800 | 1.11144400 | -0.62379900 |
| O | -6.02513400 | 1.85742300 | -1.30462800 |
| C | -5.85097200 | -0.19730800 | -0.12190000 |
| C | -6.92884700 | -0.76177300 | -0.80941200 |
| C | -5.33974400 | -0.84683200 | 1.00694500 |
| C | -7.47521500 | -1.96789700 | -0.39082600 |
| H | -7.32670500 | -0.23715600 | -1.67483500 |
| C | -5.89548900 | -2.04886600 | 1.43107200 |
| H | -4.52735300 | -0.40780600 | 1.58621000 |
| C | -6.95843700 | -2.61358600 | 0.73091900 |

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|----|-------------|-------------|-------------|
| H | -8.30893300 | -2.40432200 | -0.93582500 |
| H | -5.49924600 | -2.54340700 | 2.31501100 |
| H | -7.39014000 | -3.55444600 | 1.06480700 |
| H | -3.39657600 | 5.69010400 | -1.77498000 |
| N | 2.07997100 | -4.07551900 | 0.05240900 |
| C | 1.60093900 | -5.09741100 | -0.20970400 |
| C | 1.00290100 | -6.36989700 | -0.53478500 |
| H | 1.01404700 | -7.02010600 | 0.34494400 |
| H | -0.03190700 | -6.22103400 | -0.85780800 |
| H | 1.56440900 | -6.85020200 | -1.34127100 |
| Cu | 2.49935900 | -2.04773400 | 0.35929100 |
| C | 6.99700000 | -1.72515800 | -0.31810200 |
| H | 7.32497900 | -0.68190100 | -0.35317000 |
| H | 7.29693900 | -2.22879100 | -1.24228200 |
| H | 7.47449100 | -2.22261100 | 0.53134700 |
| C | 5.56347900 | -1.78619800 | -0.17240000 |
| N | 4.41311100 | -1.83909900 | -0.05485600 |
| C | 3.59619700 | 0.42566600 | -2.67213300 |
| C | 3.17489600 | 1.74053400 | -2.53444500 |
| C | 1.84756700 | 1.94161000 | -2.17439900 |
| C | 0.98831100 | 0.87956200 | -1.95812800 |
| C | 2.73046300 | -0.63438100 | -2.46810400 |
| H | 3.84778000 | 2.57530700 | -2.70956400 |
| H | 2.99508500 | -1.68004100 | -2.58353900 |
| N | 1.44154000 | -0.38638000 | -2.13502000 |
| O | 0.63531400 | -1.39511500 | -1.97090100 |
| H | -0.05395700 | 0.98304900 | -1.67481600 |
| Cl | 1.23056000 | 3.54795500 | -2.00421100 |
| Cl | 5.23449800 | 0.07729700 | -3.11273600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.895149

Electronic Energy (0K) + ZPE = -3632.253276

Enthalpy (353K) = -3632.181884

Free Energy (353K) = -3632.371634

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.493394

B5-1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.21690700 | -1.41753300 | -0.82322200 |
| C | 0.99386400 | -1.40109600 | 0.28182000 |
| N | 0.44969500 | -1.50926300 | 1.57515700 |
| C | -0.97534300 | -1.27024500 | 1.88763000 |
| C | -1.48740900 | -0.01120600 | 1.36269000 |
| C | -1.91341100 | 1.02992200 | 0.90667700 |
| C | -2.45693400 | 2.21741500 | 0.33874000 |
| C | -1.71788500 | 3.40497800 | 0.35688300 |
| C | -3.74600200 | 2.20034100 | -0.24779100 |
| C | -2.23262500 | 4.56982100 | -0.19304800 |
| H | -0.72868500 | 3.38428800 | 0.81289600 |
| C | -4.25898500 | 3.37947200 | -0.79446100 |
| C | -3.50387200 | 4.54739600 | -0.76144000 |
| H | -1.64628100 | 5.48610700 | -0.17927000 |
| H | -5.24582600 | 3.36625300 | -1.24106100 |
| S | 1.48157800 | -1.02998700 | 2.85999000 |
| O | 2.82702500 | -1.51008600 | 2.54001700 |
| O | 0.84111600 | -1.48182900 | 4.08865900 |
| C | 1.47880600 | 0.74040900 | 2.82794300 |
| C | 2.32390000 | 1.41398300 | 1.94743800 |
| C | 0.55443800 | 1.42941500 | 3.61289300 |

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|---|-------------|-------------|-------------|
| C | 2.22781900 | 2.79639300 | 1.85122300 |
| H | 3.05268700 | 0.86557900 | 1.35328100 |
| C | 0.47562500 | 2.80993600 | 3.50128000 |
| H | -0.09008700 | 0.89048000 | 4.30320400 |
| C | 1.30094200 | 3.51235300 | 2.61473500 |
| H | 2.89034400 | 3.33473500 | 1.17429000 |
| H | -0.24225600 | 3.35852800 | 4.10912300 |
| C | 1.16520100 | 4.99511400 | 2.47122900 |
| H | 0.22259200 | 5.24841000 | 1.96512200 |
| H | 1.14077700 | 5.49076100 | 3.44846600 |
| H | 1.98552800 | 5.42296600 | 1.88612100 |
| H | -1.56624300 | -2.10057600 | 1.48444900 |
| H | -1.09893800 | -1.31960600 | 2.97450200 |
| C | -1.15844500 | -1.80533700 | -1.16971800 |
| C | -1.71172400 | -2.98998900 | -0.66377000 |
| C | -1.92394900 | -1.04036600 | -2.06364700 |
| C | -3.01035500 | -3.36669500 | -0.99365600 |
| H | -1.10381300 | -3.62822300 | -0.02303500 |
| C | -3.21635900 | -1.42144000 | -2.39869000 |
| H | -1.50158900 | -0.13144400 | -2.49180800 |
| C | -3.76820700 | -2.58269100 | -1.85795000 |
| H | -3.42581300 | -4.28579900 | -0.58541000 |
| H | -3.80187200 | -0.80615800 | -3.07940900 |
| H | -4.78358500 | -2.87713300 | -2.11626400 |
| N | -4.43249900 | 0.98362400 | -0.22839600 |
| H | -3.87314700 | 0.18815200 | 0.06507600 |
| C | -5.74599900 | 0.73235200 | -0.54003400 |
| O | -6.49554100 | 1.55824800 | -1.04438600 |
| C | -6.20498800 | -0.65184400 | -0.21765200 |
| C | -7.29167700 | -1.15238900 | -0.93951100 |

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|----|-------------|-------------|-------------|
| C | -5.62348700 | -1.43797700 | 0.78276000 |
| C | -7.77384000 | -2.43018400 | -0.68620000 |
| H | -7.74591100 | -0.52393600 | -1.70195800 |
| C | -6.11875200 | -2.71024200 | 1.04675200 |
| H | -4.79772200 | -1.05773400 | 1.38458200 |
| C | -7.18706600 | -3.21127600 | 0.30791200 |
| H | -8.61220800 | -2.81724200 | -1.26057700 |
| H | -5.66848000 | -3.31133600 | 1.83331900 |
| H | -7.56893000 | -4.20899800 | 0.51220300 |
| H | -3.92102700 | 5.45358000 | -1.19479600 |
| N | 3.60591700 | -3.56661600 | 0.07586400 |
| C | 3.82636200 | -4.70179500 | 0.14649300 |
| C | 4.10242700 | -6.11587400 | 0.23679500 |
| H | 4.19632800 | -6.40737700 | 1.28701100 |
| H | 3.28675600 | -6.68389500 | -0.21988300 |
| H | 5.03619000 | -6.34789700 | -0.28367200 |
| Cu | 2.95476000 | -1.54237100 | 0.17154800 |
| C | 7.15337900 | 0.21855100 | -0.19018900 |
| H | 7.13724100 | 1.29533200 | -0.38440800 |
| H | 7.69715600 | -0.28380500 | -0.99607800 |
| H | 7.66741900 | 0.03268700 | 0.75770300 |
| C | 5.80578300 | -0.29164900 | -0.12079800 |
| N | 4.72471300 | -0.70368800 | -0.06757100 |
| C | 3.67017400 | 0.94273600 | -2.79879100 |
| C | 3.22086600 | 2.18684800 | -2.38373100 |
| C | 1.93565000 | 2.27451600 | -1.85398600 |
| C | 1.14007100 | 1.14973600 | -1.71839400 |
| C | 2.86549300 | -0.17793000 | -2.66772600 |
| H | 3.84466600 | 3.07169900 | -2.47917000 |
| H | 3.14564000 | -1.18572900 | -2.95777400 |

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|----|------------|-------------|-------------|
| N | 1.64160100 | -0.02529800 | -2.14125000 |
| O | 0.90128700 | -1.16748600 | -2.09134100 |
| H | 0.13825500 | 1.14488800 | -1.29358200 |
| Cl | 1.30564900 | 3.81242000 | -1.39073800 |
| Cl | 5.25247500 | 0.74789500 | -3.45767700 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.915922

Electronic Energy (0K) + ZPE = -3632.272020

Enthalpy (353K) = -3632.200622

Free Energy (353K) = -3632.392584

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.510572

A6

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.20439700 | -2.11159600 | -1.42069100 |
| C | -0.55151900 | -1.33689100 | -1.97354700 |
| N | -1.38478900 | -0.45372700 | -2.55971300 |
| C | -1.12380500 | 0.98019300 | -2.32456300 |
| C | -0.96675900 | 1.27699800 | -0.89087900 |
| C | -0.97540000 | 1.05506200 | 0.33065200 |
| C | -0.92050100 | 0.63142500 | 1.69405000 |
| C | -1.96631700 | 0.89786000 | 2.58529800 |
| C | 0.25310300 | -0.01783400 | 2.15117700 |
| C | -1.86395500 | 0.52045200 | 3.91612700 |
| H | -2.85315500 | 1.40766700 | 2.21405600 |
| C | 0.33718100 | -0.40884700 | 3.48895200 |
| C | -0.71408800 | -0.13303700 | 4.35645700 |
| H | -2.67479800 | 0.73468200 | 4.60757700 |
| H | 1.23044900 | -0.91561100 | 3.83476400 |

| | | | |
|---|-------------|-------------|-------------|
| S | -3.03012200 | -0.95330600 | -2.73294500 |
| O | -2.95431700 | -2.33988500 | -3.15526400 |
| O | -3.63933800 | 0.06967800 | -3.56874000 |
| C | -3.71175300 | -0.86147000 | -1.10922200 |
| C | -3.44163500 | -1.88519900 | -0.19995400 |
| C | -4.46151100 | 0.25725300 | -0.75088000 |
| C | -3.94318800 | -1.77729600 | 1.08918000 |
| H | -2.86286700 | -2.75570900 | -0.50011400 |
| C | -4.96178200 | 0.33758500 | 0.54112400 |
| H | -4.65762100 | 1.04181000 | -1.47769700 |
| C | -4.71275200 | -0.67389700 | 1.47527800 |
| H | -3.74032400 | -2.56528100 | 1.81256800 |
| H | -5.55813100 | 1.20001300 | 0.83488800 |
| C | -5.27281000 | -0.58476300 | 2.85910600 |
| H | -5.37703800 | 0.45656500 | 3.18425400 |
| H | -6.27217300 | -1.03729200 | 2.90082000 |
| H | -4.64435400 | -1.11798700 | 3.58058600 |
| H | -0.20869100 | 1.24532500 | -2.86867200 |
| H | -1.93876500 | 1.55894300 | -2.77322800 |
| C | 1.08323400 | -3.00271600 | -0.73403500 |
| C | 2.23123800 | -3.50663300 | -1.36195000 |
| C | 0.82288400 | -3.34133200 | 0.60398100 |
| C | 3.10471500 | -4.32713100 | -0.65930600 |
| H | 2.43219600 | -3.23765200 | -2.39691400 |
| C | 1.70053000 | -4.16129300 | 1.29979000 |
| H | -0.06967000 | -2.94322500 | 1.08563100 |
| C | 2.84308600 | -4.65294800 | 0.66981500 |
| H | 3.99752200 | -4.70914600 | -1.14914900 |
| H | 1.49573900 | -4.41591600 | 2.33716200 |
| H | 3.53158300 | -5.29235300 | 1.21760400 |

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|----|-------------|-------------|-------------|
| N | 1.27125500 | -0.22506100 | 1.22058000 |
| H | 0.98073600 | -0.19535200 | 0.24833200 |
| C | 2.60627200 | -0.45242600 | 1.45668000 |
| O | 3.07825400 | -0.61815700 | 2.57296500 |
| C | 3.44720200 | -0.48706800 | 0.22447200 |
| C | 4.63480600 | -1.21999400 | 0.27985000 |
| C | 3.10729800 | 0.18588300 | -0.95504900 |
| C | 5.45767900 | -1.30637300 | -0.83591300 |
| H | 4.89059200 | -1.73048400 | 1.20565500 |
| C | 3.93793400 | 0.10731100 | -2.06730900 |
| H | 2.20420200 | 0.79716900 | -1.00910700 |
| C | 5.10877000 | -0.64502100 | -2.01129800 |
| H | 6.37288000 | -1.89190700 | -0.79084500 |
| H | 3.67252500 | 0.63887800 | -2.97840700 |
| H | 5.75399500 | -0.70998800 | -2.88438000 |
| H | -0.63175300 | -0.44075500 | 5.39628900 |
| N | 0.96920000 | 3.81368800 | -1.61349800 |
| C | 1.44105800 | 4.42948800 | -2.47148700 |
| C | 2.02948500 | 5.20001600 | -3.53703600 |
| H | 1.59841700 | 6.20547400 | -3.54455500 |
| H | 3.11018300 | 5.27388600 | -3.38385300 |
| H | 1.83211300 | 4.71570300 | -4.49789100 |
| Cu | 0.20130500 | 2.73357100 | -0.15190300 |
| C | 2.02517300 | 3.27246100 | 3.96384300 |
| H | 2.61571700 | 2.36127100 | 4.10328400 |
| H | 1.21562800 | 3.29175800 | 4.70017100 |
| H | 2.66773300 | 4.14607300 | 4.10602200 |
| C | 1.46844500 | 3.27641300 | 2.63520900 |
| N | 1.01778500 | 3.25964900 | 1.56952200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2390.555090

Electronic Energy (0K) + ZPE = -2389.986845

Enthalpy (353K) = -2389.926886

Free Energy (353K) = -2390.091955

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2391.018365

TS_{A6}

Number of imaginary frequencies: 1

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|---|-------------|-------------|-------------|
| C | -0.95819100 | -1.69365100 | -2.37240900 |
| C | -1.59461500 | -0.68831900 | -2.11932400 |
| N | -2.27944600 | 0.42741900 | -1.82862600 |
| C | -1.55894200 | 1.70678800 | -1.62498200 |
| C | -0.75886900 | 1.86234000 | -0.37432900 |
| C | -0.68428700 | 1.06536600 | 0.63629200 |
| C | -1.02193100 | -0.12772600 | 1.37053700 |
| C | -2.02854300 | -0.07690100 | 2.34597900 |
| C | -0.27385600 | -1.31983600 | 1.20959700 |
| C | -2.29584500 | -1.17369700 | 3.14891700 |
| H | -2.58179700 | 0.85222600 | 2.46849800 |
| C | -0.56135500 | -2.42900800 | 2.01152300 |
| C | -1.55712600 | -2.34504000 | 2.97604000 |
| H | -3.07486500 | -1.12000400 | 3.90607200 |
| H | 0.01796000 | -3.33670700 | 1.88551400 |
| S | -3.98545500 | 0.34838700 | -1.88995200 |
| O | -4.32423100 | -0.47312500 | -3.04197000 |
| O | -4.43896000 | 1.72898000 | -1.79331100 |
| C | -4.45696300 | -0.52370900 | -0.42858200 |
| C | -4.23261600 | -1.90032200 | -0.35470800 |
| C | -5.06855100 | 0.17222500 | 0.60864900 |

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|---|-------------|-------------|-------------|
| C | -4.62239700 | -2.57563000 | 0.79042600 |
| H | -3.77329500 | -2.43363000 | -1.18381000 |
| C | -5.47041500 | -0.53045600 | 1.73892300 |
| H | -5.23824900 | 1.24260200 | 0.52360200 |
| C | -5.25018500 | -1.90494100 | 1.84811400 |
| H | -4.44459300 | -3.64730500 | 0.86964300 |
| H | -5.95779200 | -0.00088700 | 2.55593400 |
| C | -5.67190100 | -2.66123800 | 3.06779600 |
| H | -5.94229900 | -1.98824800 | 3.88793900 |
| H | -6.54269200 | -3.29428700 | 2.85449700 |
| H | -4.87232200 | -3.32771800 | 3.41403100 |
| H | -0.90209000 | 1.83877000 | -2.49517600 |
| H | -2.30480200 | 2.50778400 | -1.67965900 |
| C | -0.19063500 | -2.88313200 | -2.54915600 |
| C | 0.71513300 | -2.99955400 | -3.61402400 |
| C | -0.28857900 | -3.92503200 | -1.61266700 |
| C | 1.51731000 | -4.12771200 | -3.72767000 |
| H | 0.79237200 | -2.18905900 | -4.33606700 |
| C | 0.50744500 | -5.05569200 | -1.74022800 |
| H | -0.98842600 | -3.82542300 | -0.78348800 |
| C | 1.41534700 | -5.15626500 | -2.79328300 |
| H | 2.22780800 | -4.20410500 | -4.54777400 |
| H | 0.42759400 | -5.85751200 | -1.00969100 |
| H | 2.04542900 | -6.03812500 | -2.88440600 |
| N | 0.72685000 | -1.33285100 | 0.23231400 |
| H | 0.55703800 | -0.71158500 | -0.55013800 |
| C | 1.86468400 | -2.09915800 | 0.20079300 |
| O | 2.13463800 | -2.93419900 | 1.05509900 |
| C | 2.78023100 | -1.82318600 | -0.94858200 |
| C | 3.79855900 | -2.75271800 | -1.17531600 |

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|----|-------------|-------------|-------------|
| C | 2.68649900 | -0.69782200 | -1.77704800 |
| C | 4.70116000 | -2.57167900 | -2.21531400 |
| H | 3.86093400 | -3.62065600 | -0.52333400 |
| C | 3.58895000 | -0.51905200 | -2.81927100 |
| H | 1.92214700 | 0.06522100 | -1.62249700 |
| C | 4.59637200 | -1.45480700 | -3.04065300 |
| H | 5.48631300 | -3.30462900 | -2.38509700 |
| H | 3.50879700 | 0.35834200 | -3.45669100 |
| H | 5.30190800 | -1.31141200 | -3.85588600 |
| H | -1.76367300 | -3.21284200 | 3.59906200 |
| Cu | 0.17455400 | 3.58957100 | -0.32119500 |
| C | 4.35987300 | 5.42477200 | -0.29323400 |
| H | 4.28411400 | 6.50551800 | -0.14128400 |
| H | 4.86139900 | 5.22956600 | -1.24588100 |
| H | 4.95029300 | 4.98877400 | 0.51844200 |
| C | 3.04293400 | 4.83839100 | -0.30665500 |
| N | 1.98659700 | 4.36334000 | -0.31521600 |
| C | 2.60818000 | -0.58663700 | 3.25036900 |
| C | 3.73872800 | -0.42754800 | 2.46113200 |
| C | 3.71533900 | 0.58318100 | 1.50582500 |
| C | 2.59523700 | 1.37215500 | 1.32722000 |
| C | 1.49564300 | 0.22215700 | 3.08157800 |
| H | 4.60985500 | -1.06329300 | 2.58944500 |
| H | 0.59424100 | 0.16199900 | 3.68217000 |
| N | 1.51361400 | 1.16796900 | 2.11617600 |
| O | 0.42816700 | 1.88944900 | 1.90914000 |
| H | 2.50243900 | 2.16570100 | 0.59184100 |
| Cl | 5.09590100 | 0.86768900 | 0.50268200 |
| Cl | 2.55126900 | -1.81610500 | 4.46075800 |
| C | -2.64340100 | 7.23345000 | -1.03454800 |

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|---|-------------|------------|-------------|
| H | -2.07854700 | 8.12625300 | -1.31836900 |
| H | -3.22950200 | 7.45045000 | -0.13664800 |
| H | -3.32270800 | 6.96425300 | -1.84859000 |
| C | -1.73749900 | 6.14155000 | -0.77296800 |
| N | -1.00934100 | 5.26569200 | -0.56279100 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.890725

Electronic Energy (0K) + ZPE = -3632.248939

Enthalpy (353K) = -3632.177293

Free Energy (353K) = -3632.368693

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.490385

B6

Number of imaginary frequencies: 0

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|---|-------------|-------------|-------------|
| C | -1.12363700 | -1.16626700 | -2.40522500 |
| C | -1.59328500 | -0.16882800 | -1.89111200 |
| N | -2.07591300 | 0.94108000 | -1.30931200 |
| C | -1.14543000 | 2.08363500 | -1.08712600 |
| C | -0.21703400 | 2.04821500 | 0.07988500 |
| C | -0.24227100 | 1.15830400 | 1.07007400 |
| C | -0.97380700 | -0.07917500 | 1.43204400 |
| C | -2.03252600 | -0.01075500 | 2.34269900 |
| C | -0.47582200 | -1.34759300 | 1.06612500 |
| C | -2.57948000 | -1.16270800 | 2.89519900 |
| H | -2.40371600 | 0.97075900 | 2.63506900 |
| C | -1.02752800 | -2.50644100 | 1.61866300 |
| C | -2.06561900 | -2.40704400 | 2.53675000 |
| H | -3.39730500 | -1.09005300 | 3.60907000 |
| H | -0.61877900 | -3.47221900 | 1.34049400 |

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|---|-------------|-------------|-------------|
| S | -3.76320600 | 1.20758500 | -1.47951000 |
| O | -4.15302600 | 0.76727700 | -2.81156000 |
| O | -3.98526500 | 2.58747600 | -1.06276100 |
| C | -4.48668400 | 0.11978600 | -0.29218200 |
| C | -4.47681500 | -1.25620500 | -0.53074300 |
| C | -5.08136100 | 0.65986900 | 0.84267300 |
| C | -5.05320300 | -2.09536900 | 0.40895300 |
| H | -4.03516300 | -1.66134500 | -1.43824400 |
| C | -5.67557700 | -0.20023100 | 1.75873100 |
| H | -5.08539100 | 1.73526000 | 0.99978600 |
| C | -5.65946100 | -1.58233400 | 1.56328600 |
| H | -5.04363400 | -3.17210200 | 0.24541700 |
| H | -6.15290800 | 0.20850400 | 2.64775200 |
| C | -6.25229900 | -2.51335000 | 2.57244600 |
| H | -6.76791300 | -1.97118900 | 3.37126000 |
| H | -6.96676000 | -3.20280800 | 2.10721500 |
| H | -5.47040000 | -3.13179400 | 3.03286400 |
| H | -0.56705000 | 2.20986900 | -2.01417100 |
| H | -1.77020200 | 2.97964000 | -1.00040900 |
| C | -0.56204200 | -2.40444900 | -2.83785700 |
| C | 0.34126800 | -2.45396300 | -3.90982700 |
| C | -0.87404400 | -3.58640300 | -2.14604100 |
| C | 0.92776200 | -3.65998700 | -4.27238500 |
| H | 0.58254700 | -1.53737600 | -4.44454900 |
| C | -0.29005600 | -4.78931200 | -2.52005900 |
| H | -1.57406800 | -3.54021500 | -1.31249300 |
| C | 0.61431000 | -4.82778200 | -3.57998900 |
| H | 1.63415200 | -3.68887800 | -5.09898300 |
| H | -0.53614300 | -5.70026800 | -1.97927000 |
| H | 1.07589900 | -5.77003100 | -3.86638600 |

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|----|-------------|-------------|-------------|
| N | 0.58460800 | -1.39277200 | 0.14289800 |
| H | 0.53147900 | -0.69522200 | -0.58827600 |
| C | 1.58082700 | -2.32606700 | 0.04922800 |
| O | 1.68908400 | -3.27633000 | 0.81605300 |
| C | 2.56716800 | -2.07860900 | -1.04776100 |
| C | 3.44223900 | -3.12268200 | -1.35764200 |
| C | 2.67373800 | -0.86846200 | -1.74495000 |
| C | 4.39456300 | -2.97183600 | -2.35774100 |
| H | 3.35301800 | -4.05407000 | -0.80363600 |
| C | 3.62597500 | -0.71936300 | -2.74673700 |
| H | 2.02976000 | -0.01791200 | -1.51607500 |
| C | 4.48539000 | -1.77059800 | -3.05645800 |
| H | 5.06530000 | -3.79394400 | -2.59594700 |
| H | 3.70082600 | 0.22379400 | -3.28293400 |
| H | 5.22943200 | -1.65099900 | -3.84076000 |
| H | -2.48056800 | -3.31462100 | 2.97040000 |
| Cu | 1.09517800 | 3.44874100 | 0.02853000 |
| C | 4.66692000 | 6.15557100 | -0.25304100 |
| H | 4.56028900 | 6.98164800 | 0.45637900 |
| H | 4.72253700 | 6.55915400 | -1.26835800 |
| H | 5.58784600 | 5.60795500 | -0.03189900 |
| C | 3.53376400 | 5.27299600 | -0.14402900 |
| N | 2.62118600 | 4.56734400 | -0.06017600 |
| C | 2.56615800 | -1.36012100 | 3.24120600 |
| C | 3.71500800 | -1.21444600 | 2.47343300 |
| C | 3.81699000 | -0.10732600 | 1.63516300 |
| C | 2.78084100 | 0.80464600 | 1.54661400 |
| C | 1.54126900 | -0.42995300 | 3.16096700 |
| H | 4.51729000 | -1.94579100 | 2.52876600 |
| H | 0.62107200 | -0.46778000 | 3.73596500 |

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|----|-------------|-------------|-------------|
| N | 1.69026100 | 0.59397300 | 2.30529400 |
| O | 0.66178400 | 1.49228200 | 2.19704900 |
| H | 2.75751200 | 1.68661200 | 0.90637300 |
| Cl | 5.23173600 | 0.13627300 | 0.67973300 |
| Cl | 2.37387700 | -2.71119500 | 4.28948800 |
| C | -2.93557200 | 5.85923300 | -1.27703600 |
| H | -3.03200400 | 6.32023900 | -2.26436500 |
| H | -3.39241900 | 6.51629600 | -0.53124600 |
| H | -3.46226800 | 4.89748900 | -1.27838600 |
| C | -1.54029700 | 5.64645500 | -0.96251100 |
| N | -0.42289000 | 5.45155700 | -0.70938400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.901844

Electronic Energy (0K) + ZPE = -3632.257883

Enthalpy (353K) = -3632.186302

Free Energy (353K) = -3632.377153

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.500339

TS_{A6-1}

Number of imaginary frequencies: 1

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|---|-------------|-------------|-------------|
| C | -0.97335900 | -2.20457900 | -1.54792900 |
| C | -1.59083400 | -1.30161400 | -2.08031600 |
| N | -2.40780200 | -0.39353500 | -2.64576600 |
| C | -2.08809700 | 1.06047800 | -2.57890600 |
| C | -1.09731200 | 1.35941300 | -1.56615700 |
| C | -0.63433900 | 1.55337300 | -0.41490800 |
| C | -1.36338900 | 1.79968400 | 0.84747900 |
| C | -2.23088400 | 2.89783200 | 0.92230600 |
| C | -1.20876100 | 0.96434500 | 1.96733300 |

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|---|-------------|-------------|-------------|
| C | -2.91846600 | 3.18005500 | 2.09448900 |
| H | -2.33835900 | 3.53554500 | 0.04615300 |
| C | -1.93046900 | 1.23959200 | 3.13118900 |
| C | -2.76400400 | 2.34824100 | 3.20118300 |
| H | -3.57846900 | 4.04317000 | 2.14011700 |
| H | -1.82139800 | 0.57867700 | 3.98476700 |
| S | -4.09016600 | -0.78595300 | -2.54839600 |
| O | -4.17986000 | -2.19630000 | -2.87878000 |
| O | -4.75407800 | 0.22906000 | -3.35154800 |
| C | -4.48675000 | -0.54091700 | -0.84574100 |
| C | -4.11880800 | -1.51559800 | 0.08427500 |
| C | -5.11374400 | 0.64038500 | -0.45383400 |
| C | -4.38903400 | -1.29042800 | 1.42627200 |
| H | -3.65041000 | -2.44158500 | -0.24090000 |
| C | -5.38610400 | 0.83697500 | 0.89332700 |
| H | -5.39763700 | 1.38322900 | -1.19527300 |
| C | -5.03592700 | -0.12243400 | 1.84854000 |
| H | -4.11014100 | -2.04183000 | 2.16372900 |
| H | -5.88601000 | 1.74994300 | 1.21324200 |
| C | -5.38238500 | 0.07714800 | 3.28948000 |
| H | -5.42248200 | 1.14071700 | 3.54853600 |
| H | -6.37040200 | -0.34971300 | 3.50729300 |
| H | -4.66357700 | -0.41903600 | 3.95063300 |
| H | -1.80750100 | 1.42232200 | -3.57134800 |
| H | -2.99545300 | 1.60962900 | -2.28313300 |
| C | -0.32070300 | -3.29634700 | -0.89926800 |
| C | 0.59424600 | -4.10823400 | -1.58691400 |
| C | -0.62974800 | -3.59295300 | 0.43924900 |
| C | 1.18252800 | -5.19233200 | -0.94753800 |
| H | 0.82385900 | -3.88810500 | -2.62782400 |

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|----|-------------|-------------|-------------|
| C | -0.05469500 | -4.69083400 | 1.06474800 |
| H | -1.32838500 | -2.95163300 | 0.97644000 |
| C | 0.85390900 | -5.48960100 | 0.37387300 |
| H | 1.89282000 | -5.81537500 | -1.48645600 |
| H | -0.30419000 | -4.91610900 | 2.09929000 |
| H | 1.31112100 | -6.34394500 | 0.86817700 |
| N | -0.34444900 | -0.15331900 | 1.90048800 |
| H | -0.29987800 | -0.66164500 | 1.02232300 |
| C | 0.54847900 | -0.46746300 | 2.89647800 |
| O | 0.57531000 | 0.12317900 | 3.96896100 |
| C | 1.50621500 | -1.57878600 | 2.61882400 |
| C | 1.95313700 | -2.30596700 | 3.72640900 |
| C | 2.03339400 | -1.85973800 | 1.35400000 |
| C | 2.89726800 | -3.31329200 | 3.57681500 |
| H | 1.54876400 | -2.06272200 | 4.70609300 |
| C | 3.00096400 | -2.84994200 | 1.21224400 |
| H | 1.71580500 | -1.29420800 | 0.47539000 |
| C | 3.42878100 | -3.58090600 | 2.31775600 |
| H | 3.22620100 | -3.88232400 | 4.44312000 |
| H | 3.41652000 | -3.06243500 | 0.23062200 |
| H | 4.17783700 | -4.36014600 | 2.19527600 |
| H | -3.30402800 | 2.55397400 | 4.12255800 |
| N | 1.21150400 | 4.14741800 | 0.14563100 |
| C | 1.12369000 | 5.30168900 | 0.14086200 |
| C | 1.01371800 | 6.73951700 | 0.13668800 |
| H | 0.94417700 | 7.10718900 | 1.16457000 |
| H | 1.89465500 | 7.17716400 | -0.34190300 |
| H | 0.11813600 | 7.04150500 | -0.41420500 |
| Cu | 1.21698800 | 2.09032500 | 0.17200800 |
| C | 4.39775000 | 0.45450600 | 2.97313100 |

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|----|------------|-------------|-------------|
| H | 3.89635500 | 0.31856100 | 3.93708000 |
| H | 5.23466200 | 1.14823000 | 3.09631500 |
| H | 4.77497500 | -0.51210800 | 2.62348700 |
| C | 3.45538100 | 0.98128500 | 2.01897500 |
| N | 2.68542600 | 1.39318500 | 1.25949300 |
| C | 3.31417000 | -0.69494600 | -2.27098800 |
| C | 4.18028200 | 0.31550000 | -1.86316000 |
| C | 3.68647100 | 1.61050600 | -1.89849800 |
| C | 2.39503000 | 1.88466900 | -2.32576400 |
| C | 2.01807600 | -0.42732600 | -2.66622300 |
| H | 5.19860000 | 0.10062400 | -1.55309300 |
| H | 1.29708800 | -1.17128200 | -2.99135800 |
| N | 1.58995600 | 0.86199400 | -2.72036800 |
| O | 0.39881100 | 1.11580800 | -3.12500100 |
| H | 1.97910400 | 2.88106900 | -2.43762600 |
| Cl | 4.68151700 | 2.93836900 | -1.40710900 |
| Cl | 3.86669900 | -2.33551100 | -2.34171800 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.888816

Electronic Energy (0K) + ZPE = -3632.247181

Enthalpy (353K) = -3632.175773

Free Energy (353K) = -3632.363709

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.491325

B6-1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -1.15519100 | -2.12591800 | -1.30363400 |
| C | -1.66158000 | -1.15422300 | -1.83407900 |
| N | -2.33774800 | -0.17104400 | -2.45546300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.92974000 | 1.26169100 | -2.30658800 |
| C | -0.53976600 | 1.37797800 | -1.80441900 |
| C | -0.08649800 | 1.63312500 | -0.58643900 |
| C | -1.06648000 | 1.94250300 | 0.47705800 |
| C | -1.79682500 | 3.14171500 | 0.45488700 |
| C | -1.21844100 | 1.10092500 | 1.59511900 |
| C | -2.63417100 | 3.49930000 | 1.50539000 |
| H | -1.67393100 | 3.80789900 | -0.39921100 |
| C | -2.07328500 | 1.45138300 | 2.63866400 |
| C | -2.77288900 | 2.65213700 | 2.60223100 |
| H | -3.17983800 | 4.43983700 | 1.46565700 |
| H | -2.17578400 | 0.77384400 | 3.48198800 |
| S | -4.04250800 | -0.42553400 | -2.52606000 |
| O | -4.22727500 | -1.79559700 | -2.97157600 |
| O | -4.55343600 | 0.69829400 | -3.29566300 |
| C | -4.55134800 | -0.27542100 | -0.84216100 |
| C | -4.41177500 | -1.37395000 | 0.00939700 |
| C | -5.01882400 | 0.95175000 | -0.37677900 |
| C | -4.74763800 | -1.22605800 | 1.34652100 |
| H | -4.06212200 | -2.32957000 | -0.37380300 |
| C | -5.35889200 | 1.07216300 | 0.96475900 |
| H | -5.12927300 | 1.79199200 | -1.05838600 |
| C | -5.22723200 | -0.00723400 | 1.84222000 |
| H | -4.64776200 | -2.07395900 | 2.02282100 |
| H | -5.73162900 | 2.02351200 | 1.34061400 |
| C | -5.59989600 | 0.12236700 | 3.28506400 |
| H | -5.77564100 | 1.16581200 | 3.56532300 |
| H | -6.51673000 | -0.44052800 | 3.50219000 |
| H | -4.81708800 | -0.28559200 | 3.93540700 |
| H | -2.05453500 | 1.74139300 | -3.28259600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.59130600 | 1.75598100 | -1.58446200 |
| C | -0.60131400 | -3.28585400 | -0.68193900 |
| C | 0.26830900 | -4.13106300 | -1.38824400 |
| C | -0.94032600 | -3.60370300 | 0.64359200 |
| C | 0.79457500 | -5.26152900 | -0.77608700 |
| H | 0.51733400 | -3.89555100 | -2.42152600 |
| C | -0.42126900 | -4.74229700 | 1.24494700 |
| H | -1.61285500 | -2.94400500 | 1.19063100 |
| C | 0.44981200 | -5.56939900 | 0.53871700 |
| H | 1.47175700 | -5.90865700 | -1.32920700 |
| H | -0.68726700 | -4.97985800 | 2.27250000 |
| H | 0.86204400 | -6.45624100 | 1.01489200 |
| N | -0.46158800 | -0.09585400 | 1.66499600 |
| H | -0.37034400 | -0.63620500 | 0.81038800 |
| C | 0.37336000 | -0.38003900 | 2.71489600 |
| O | 0.37651600 | 0.26615700 | 3.75626100 |
| C | 1.29892400 | -1.53891200 | 2.53219900 |
| C | 1.69716700 | -2.22145400 | 3.68445700 |
| C | 1.83479300 | -1.91037000 | 1.29490000 |
| C | 2.60079000 | -3.27413900 | 3.60496800 |
| H | 1.28634700 | -1.91007100 | 4.64209200 |
| C | 2.76292800 | -2.94425400 | 1.22100700 |
| H | 1.55479800 | -1.37513600 | 0.38463800 |
| C | 3.14073200 | -3.63216000 | 2.37199600 |
| H | 2.89127500 | -3.80992200 | 4.50565600 |
| H | 3.18741700 | -3.22284000 | 0.25896000 |
| H | 3.85751200 | -4.44772900 | 2.30584400 |
| H | -3.43018600 | 2.92008600 | 3.42665400 |
| N | 2.02854700 | 4.06774000 | 0.32609500 |
| C | 1.60372600 | 5.11403500 | 0.59580100 |

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|----|------------|-------------|-------------|
| C | 1.07149600 | 6.41385300 | 0.93209400 |
| H | 1.68997800 | 6.88374200 | 1.70227500 |
| H | 1.05887700 | 7.05300900 | 0.04437200 |
| H | 0.05011000 | 6.30708400 | 1.31046600 |
| Cu | 1.66139900 | 1.83658700 | 0.21262100 |
| C | 4.36536500 | 0.27848400 | 3.44917800 |
| H | 3.72402300 | 0.29110900 | 4.33663100 |
| H | 5.26752000 | 0.86490600 | 3.64676000 |
| H | 4.64597900 | -0.75542400 | 3.22301600 |
| C | 3.64088500 | 0.83904000 | 2.33727400 |
| N | 3.03954500 | 1.27852800 | 1.45136600 |
| C | 3.14949800 | -0.95570800 | -2.37440500 |
| C | 4.12316500 | -0.00654100 | -2.06108800 |
| C | 3.75882500 | 1.33139500 | -2.04442100 |
| C | 2.45127400 | 1.71402500 | -2.33414900 |
| C | 1.85160500 | -0.57042400 | -2.65215200 |
| H | 5.14509400 | -0.30976300 | -1.84823100 |
| H | 1.02960800 | -1.24018100 | -2.89345000 |
| N | 1.57548500 | 0.74570300 | -2.66045100 |
| O | 0.30982900 | 1.10979400 | -2.96227100 |
| H | 2.10650800 | 2.74063800 | -2.41266700 |
| Cl | 4.90718000 | 2.55644100 | -1.65742500 |
| Cl | 3.55822000 | -2.62938800 | -2.46961000 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3632.916773

Electronic Energy (0K) + ZPE = -3632.271583

Enthalpy (353K) = -3632.200742

Free Energy (353K) = -3632.386434

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3633.514173

A7

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.05981000 | -0.11802400 | 0.84500000 |
| C | 0.55710100 | -0.82692200 | -0.03468100 |
| N | 1.09331600 | -1.65306900 | -0.92366600 |
| C | 0.58109500 | -1.81292300 | -2.31475900 |
| C | -0.74963400 | -1.25483700 | -2.42623300 |
| C | -1.85249500 | -0.75103900 | -2.47980100 |
| C | -3.05878100 | 0.00686400 | -2.48378000 |
| C | -4.26101300 | -0.52343700 | -2.96342900 |
| C | -3.02042200 | 1.33643500 | -1.98868800 |
| C | -5.41707500 | 0.24424400 | -2.96949900 |
| H | -4.26745800 | -1.54462500 | -3.33743700 |
| C | -4.19311200 | 2.09632200 | -1.98719200 |
| C | -5.37276800 | 1.54880400 | -2.48164900 |
| H | -6.34599700 | -0.17083900 | -3.35145700 |
| H | -4.16194900 | 3.11078200 | -1.60769800 |
| S | 2.56227800 | -2.44214800 | -0.48341400 |
| O | 2.74793100 | -3.45433300 | -1.51327500 |
| O | 2.43158200 | -2.80070400 | 0.91733900 |
| C | 3.76794800 | -1.16875900 | -0.65028100 |
| C | 4.35215800 | -0.94213000 | -1.89662400 |
| C | 4.06261600 | -0.37597800 | 0.45597300 |
| C | 5.25436600 | 0.10296400 | -2.02311100 |
| H | 4.11593600 | -1.58265400 | -2.74329600 |
| C | 4.96654100 | 0.66770800 | 0.30342500 |
| H | 3.60190300 | -0.58070000 | 1.41976000 |
| C | 5.56922800 | 0.92386500 | -0.93166600 |
| H | 5.72944200 | 0.29071100 | -2.98459900 |

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|---|-------------|-------------|-------------|
| H | 5.21008500 | 1.29639400 | 1.15833600 |
| C | 6.51447300 | 2.06908500 | -1.10746100 |
| H | 6.08548300 | 2.82228700 | -1.78142400 |
| H | 6.74126800 | 2.55687400 | -0.15453100 |
| H | 7.45684300 | 1.73961700 | -1.56047900 |
| H | 1.27147200 | -1.31369700 | -3.01052500 |
| H | 0.58157900 | -2.88342400 | -2.55018100 |
| C | -0.10563200 | 1.01575300 | 1.71671700 |
| C | 1.02308200 | 1.56503900 | 2.34220800 |
| C | -1.37017200 | 1.56563600 | 1.96921400 |
| C | 0.88200300 | 2.63923800 | 3.21236000 |
| H | 2.00582500 | 1.14385200 | 2.13417900 |
| C | -1.49720400 | 2.65638100 | 2.82027200 |
| H | -2.24631600 | 1.13269300 | 1.48929100 |
| C | -0.37504500 | 3.19070300 | 3.45064100 |
| H | 1.76243300 | 3.05740400 | 3.69546000 |
| H | -2.48008000 | 3.08693600 | 2.99761900 |
| H | -0.47973800 | 4.03755200 | 4.12477700 |
| N | -1.78541000 | 1.80629600 | -1.54329200 |
| H | -1.04431900 | 1.11443800 | -1.56595500 |
| C | -1.43610700 | 3.05266100 | -1.08468500 |
| O | -2.24062300 | 3.95101700 | -0.87735200 |
| C | 0.02897200 | 3.22634800 | -0.84062000 |
| C | 0.41651200 | 4.27666400 | -0.00547800 |
| C | 1.01166100 | 2.41088000 | -1.41561800 |
| C | 1.75917900 | 4.49242700 | 0.27809800 |
| H | -0.35538700 | 4.91088200 | 0.42429300 |
| C | 2.35461600 | 2.62787900 | -1.13147300 |
| H | 0.74876800 | 1.61597200 | -2.11396100 |
| C | 2.73023200 | 3.66334400 | -0.27854700 |

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|----|-------------|-------------|-------------|
| H | 2.04870200 | 5.30564300 | 0.93975900 |
| H | 3.11248200 | 1.99142600 | -1.58636300 |
| H | 3.78256600 | 3.82933000 | -0.05420100 |
| H | -6.27387400 | 2.15814300 | -2.48237400 |
| N | -0.89013200 | -3.57046700 | 0.38701900 |
| N | -3.22041900 | -1.20481500 | 0.85734200 |
| C | -0.45714600 | -4.51265900 | -0.12807400 |
| C | -4.33921000 | -0.94044500 | 0.71874500 |
| C | 0.10989900 | -5.66979100 | -0.77719400 |
| C | -5.73250700 | -0.60632400 | 0.55080800 |
| H | 1.13969200 | -5.44603400 | -1.07825900 |
| H | 0.11377900 | -6.52000800 | -0.08870400 |
| H | -0.47755300 | -5.92760500 | -1.66340400 |
| H | -6.21049200 | -1.32828600 | -0.11807200 |
| H | -6.23693500 | -0.62658600 | 1.52139100 |
| H | -5.82074800 | 0.39597700 | 0.11892800 |
| Cu | -1.31506500 | -1.78991400 | 1.20759000 |
| C | -0.61699200 | -1.08748400 | 5.70570000 |
| H | -0.39530500 | -0.01538600 | 5.71986100 |
| H | 0.24408600 | -1.63699900 | 6.09693700 |
| H | -1.48667900 | -1.28293700 | 6.33965600 |
| C | -0.89086900 | -1.50021500 | 4.35046800 |
| N | -1.10764600 | -1.81405500 | 3.25674200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2523.235055

Electronic Energy (0K) + ZPE = -2522.620719

Enthalpy (353K) = -2522.553743

Free Energy (353K) = -2522.732716

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2523.729673

TS_{A7}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 0.64766300 | -0.31971400 | 1.37044800 |
| C | 0.39346500 | 0.88410100 | 0.93519600 |
| N | -0.41240800 | 1.68521800 | 0.25065300 |
| C | -0.51662300 | 1.65137000 | -1.24308200 |
| C | -0.19953200 | 0.33336100 | -1.74803600 |
| C | 0.09394800 | -0.79474600 | -2.08962800 |
| C | 0.25281100 | -2.16729700 | -2.43686800 |
| C | 1.47656800 | -2.67449100 | -2.88652600 |
| C | -0.86007300 | -3.03756900 | -2.29977200 |
| C | 1.60924400 | -4.01760500 | -3.20870500 |
| H | 2.31933500 | -1.99001200 | -2.97965100 |
| C | -0.71535000 | -4.38893300 | -2.62272200 |
| C | 0.51041500 | -4.86358100 | -3.07481100 |
| H | 2.56158800 | -4.40360500 | -3.56414100 |
| H | -1.56704600 | -5.04970300 | -2.51181600 |
| S | -0.95455400 | 3.15982000 | 1.01386600 |
| O | -0.34555700 | 4.25390500 | 0.26412400 |
| O | -0.69701800 | 2.97143900 | 2.42955500 |
| C | -2.69886700 | 3.19109100 | 0.73237600 |
| C | -3.20244900 | 3.86140700 | -0.38371900 |
| C | -3.54435200 | 2.63186100 | 1.68886200 |
| C | -4.57693300 | 3.95489200 | -0.54145800 |
| H | -2.52662800 | 4.32158200 | -1.10079700 |
| C | -4.91703100 | 2.73922300 | 1.51152000 |
| H | -3.13527800 | 2.15042700 | 2.57390500 |
| C | -5.45171000 | 3.39837700 | 0.40035000 |
| H | -4.98513100 | 4.47873400 | -1.40418000 |

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|---|-------------|-------------|-------------|
| H | -5.58917100 | 2.31111900 | 2.25302000 |
| C | -6.92989300 | 3.49464700 | 0.19609200 |
| H | -7.23548800 | 2.92930900 | -0.69449400 |
| H | -7.48462100 | 3.10356100 | 1.05467300 |
| H | -7.23918500 | 4.53332200 | 0.02980600 |
| H | -1.55140000 | 1.91735000 | -1.50232600 |
| H | 0.13807600 | 2.41664200 | -1.68300500 |
| C | -0.50647100 | -1.24052600 | 1.48090200 |
| C | -1.76678300 | -0.81003600 | 1.92421000 |
| C | -0.34814900 | -2.59259300 | 1.14114200 |
| C | -2.82970100 | -1.69938800 | 2.02723700 |
| H | -1.89712000 | 0.22992500 | 2.21690200 |
| C | -1.41845500 | -3.47690900 | 1.22305200 |
| H | 0.62628200 | -2.93862100 | 0.79576900 |
| C | -2.66084300 | -3.03689100 | 1.67410100 |
| H | -3.79938700 | -1.34190600 | 2.37164300 |
| H | -1.28250500 | -4.51662100 | 0.92898400 |
| H | -3.49437800 | -3.73276800 | 1.74690700 |
| N | -2.04315500 | -2.46995000 | -1.83706300 |
| H | -1.94024600 | -1.51272600 | -1.51757500 |
| C | -3.26703000 | -3.05100700 | -1.61910100 |
| O | -3.49710700 | -4.24288200 | -1.77385200 |
| C | -4.31196400 | -2.09070000 | -1.15223500 |
| C | -5.41424200 | -2.61464100 | -0.47336100 |
| C | -4.22524400 | -0.70953600 | -1.35728300 |
| C | -6.39522800 | -1.76990100 | 0.03103800 |
| H | -5.47787600 | -3.69187500 | -0.33679100 |
| C | -5.21052300 | 0.13322600 | -0.85946800 |
| H | -3.40773700 | -0.27826700 | -1.93462500 |
| C | -6.29006100 | -0.39272000 | -0.15398000 |

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|----|-------------|-------------|-------------|
| H | -7.24326300 | -2.18503500 | 0.57052100 |
| H | -5.13430500 | 1.20592800 | -1.02790900 |
| H | -7.05540900 | 0.27183600 | 0.24351500 |
| H | 0.60568700 | -5.91811100 | -3.32380800 |
| N | 4.09366500 | -0.09811400 | 2.51781500 |
| N | 3.43411600 | -2.14142900 | 0.22892800 |
| C | 4.95510200 | 0.50391300 | 3.00381200 |
| C | 4.02959700 | -2.71464100 | -0.58358600 |
| C | 6.02593600 | 1.25493400 | 3.61551600 |
| C | 4.78120400 | -3.42832200 | -1.58973900 |
| H | 5.61760200 | 2.12632400 | 4.13592400 |
| H | 6.55702400 | 0.62555300 | 4.33565800 |
| H | 6.72989100 | 1.59365400 | 2.84991500 |
| H | 5.84199200 | -3.17105700 | -1.51327800 |
| H | 4.66267300 | -4.50657400 | -1.44495000 |
| H | 4.41707000 | -3.16229800 | -2.58818400 |
| Cu | 2.44451600 | -1.05164000 | 1.73979500 |
| C | 1.24606000 | -4.44046300 | 4.76277900 |
| H | 0.23071500 | -4.65767200 | 4.41619200 |
| H | 1.19847700 | -4.05710600 | 5.78612000 |
| H | 1.83316500 | -5.36322900 | 4.75326700 |
| C | 1.85113700 | -3.45700500 | 3.89544600 |
| N | 2.32369600 | -2.66626200 | 3.19140000 |
| C | 3.20924600 | 3.83986700 | -1.63731800 |
| C | 3.74149900 | 2.84825700 | -2.45177300 |
| C | 3.66870500 | 1.54380100 | -1.98047000 |
| C | 3.09239800 | 1.24425300 | -0.76130100 |
| C | 2.61585700 | 3.53640500 | -0.42534400 |
| H | 4.19836000 | 3.08316300 | -3.40873300 |
| H | 2.15466100 | 4.25981300 | 0.23766900 |

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|----|------------|------------|-------------|
| N | 2.56028200 | 2.24582700 | -0.01940100 |
| O | 1.98126300 | 1.97390000 | 1.12433600 |
| H | 3.01761000 | 0.24558700 | -0.33572700 |
| Cl | 4.31866400 | 0.24108900 | -2.92124000 |
| Cl | 3.25967400 | 5.49663200 | -2.13680200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.573463

Electronic Energy (0K) + ZPE = -3764.884920

Enthalpy (353K) = -3764.806849

Free Energy (353K) = -3765.012207

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.206057

B7

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.77555500 | -0.19030300 | 1.39848900 |
| C | 0.62487400 | 1.05156400 | 0.91591900 |
| N | -0.48047300 | 1.65443800 | 0.27034800 |
| C | -0.58976000 | 1.58599900 | -1.21198000 |
| C | -0.24887600 | 0.26243400 | -1.69759100 |
| C | 0.05665200 | -0.85666200 | -2.05855800 |
| C | 0.22278300 | -2.22764200 | -2.41136000 |
| C | 1.44276000 | -2.72473300 | -2.88097800 |
| C | -0.87988300 | -3.10816900 | -2.25711400 |
| C | 1.58238200 | -4.06650300 | -3.20683100 |
| H | 2.27856800 | -2.03359500 | -2.98647400 |
| C | -0.72859700 | -4.45806300 | -2.58338900 |
| C | 0.49361100 | -4.92221200 | -3.05601800 |
| H | 2.53247400 | -4.44349800 | -3.57767200 |
| H | -1.57262800 | -5.12631600 | -2.45878400 |

| | | | |
|---|-------------|-------------|-------------|
| S | -1.03344900 | 3.11449700 | 0.94765700 |
| O | -0.45534600 | 4.22832400 | 0.18914600 |
| O | -0.78233700 | 3.00262500 | 2.37787000 |
| C | -2.78338100 | 3.12446700 | 0.66768700 |
| C | -3.29660700 | 3.77152900 | -0.45703700 |
| C | -3.62595400 | 2.57774900 | 1.63379100 |
| C | -4.67246100 | 3.85350600 | -0.61533400 |
| H | -2.62490200 | 4.22463300 | -1.18247200 |
| C | -5.00009300 | 2.67488100 | 1.45887900 |
| H | -3.21581600 | 2.11386400 | 2.52750100 |
| C | -5.54229700 | 3.30949700 | 0.33739600 |
| H | -5.08497300 | 4.35948300 | -1.48678200 |
| H | -5.66749500 | 2.25632300 | 2.21036700 |
| C | -7.02204000 | 3.38586800 | 0.13242700 |
| H | -7.32974600 | 2.74742200 | -0.70698100 |
| H | -7.57193000 | 3.06202800 | 1.02177700 |
| H | -7.33697000 | 4.40600900 | -0.11629300 |
| H | -1.63295000 | 1.81100200 | -1.47901800 |
| H | 0.03315700 | 2.34956800 | -1.70585400 |
| C | -0.40054500 | -1.06651300 | 1.51827300 |
| C | -1.63119700 | -0.60944000 | 2.01880300 |
| C | -0.29389300 | -2.42649300 | 1.18477400 |
| C | -2.71130500 | -1.47130400 | 2.16790700 |
| H | -1.71645400 | 0.43094700 | 2.32427400 |
| C | -1.38016200 | -3.28547200 | 1.31250200 |
| H | 0.66070500 | -2.80148200 | 0.81253400 |
| C | -2.59305800 | -2.81361600 | 1.81029300 |
| H | -3.65341000 | -1.09085100 | 2.56173100 |
| H | -1.28073200 | -4.32999400 | 1.01923800 |
| H | -3.43903100 | -3.48897300 | 1.92264800 |

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|----|-------------|-------------|-------------|
| N | -2.06188000 | -2.54998200 | -1.78014400 |
| H | -1.96396500 | -1.59016700 | -1.46533200 |
| C | -3.26706400 | -3.14903700 | -1.51271400 |
| O | -3.47782600 | -4.34881200 | -1.63081800 |
| C | -4.31805800 | -2.19670200 | -1.04457900 |
| C | -5.39415100 | -2.72117700 | -0.32519600 |
| C | -4.26361700 | -0.82131900 | -1.29355300 |
| C | -6.38106300 | -1.88066700 | 0.17438800 |
| H | -5.43239600 | -3.79465800 | -0.15374300 |
| C | -5.25634600 | 0.01647600 | -0.80260300 |
| H | -3.46543200 | -0.39266600 | -1.89915800 |
| C | -6.30926700 | -0.50840600 | -0.05739200 |
| H | -7.20779600 | -2.29517700 | 0.74646000 |
| H | -5.20491900 | 1.08478400 | -1.00483800 |
| H | -7.07909800 | 0.15338600 | 0.33626200 |
| H | 0.59374600 | -5.97566600 | -3.30762800 |
| N | 4.25873100 | 0.01403300 | 2.44422000 |
| N | 3.53047200 | -2.07738800 | 0.23653300 |
| C | 5.14713700 | 0.60780400 | 2.89132500 |
| C | 4.07230500 | -2.69241000 | -0.58355000 |
| C | 6.25253400 | 1.34603100 | 3.45520600 |
| C | 4.76174600 | -3.45963100 | -1.59539000 |
| H | 5.88167800 | 2.24211900 | 3.96156600 |
| H | 6.78432600 | 0.72169900 | 4.17927800 |
| H | 6.94608800 | 1.64321000 | 2.66330700 |
| H | 5.83524800 | -3.25262700 | -1.55156800 |
| H | 4.59558100 | -4.52813600 | -1.42697200 |
| H | 4.38443000 | -3.19560200 | -2.58940200 |
| Cu | 2.55574600 | -0.92369300 | 1.78020300 |
| C | 1.42515600 | -4.33642100 | 4.76908200 |

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|----|------------|-------------|-------------|
| H | 0.40312800 | -4.52861400 | 4.42751500 |
| H | 1.39285500 | -3.96976200 | 5.79910500 |
| H | 1.99471900 | -5.26971700 | 4.73937700 |
| C | 2.04174300 | -3.34929000 | 3.91391700 |
| N | 2.52439500 | -2.55436800 | 3.22096700 |
| C | 3.16177100 | 3.81298100 | -1.68102700 |
| C | 3.69102800 | 2.80708000 | -2.48182300 |
| C | 3.54138600 | 1.48880500 | -2.06457700 |
| C | 2.87591000 | 1.18472300 | -0.89037200 |
| C | 2.49312400 | 3.50292200 | -0.50878600 |
| H | 4.21287000 | 3.04597600 | -3.40518500 |
| H | 2.02485100 | 4.22023900 | 0.15838000 |
| N | 2.37622300 | 2.20815000 | -0.17771400 |
| O | 1.75135900 | 1.95210600 | 1.02557200 |
| H | 2.71664300 | 0.18240900 | -0.48764700 |
| Cl | 4.20705600 | 0.19825700 | -2.99961200 |
| Cl | 3.31484900 | 5.46860300 | -2.13576300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.588859

Electronic Energy (0K) + ZPE = -3764.898511

Enthalpy (353K) = -3764.820469

Free Energy (353K) = -3765.027095

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.219567

TS_{A7-1}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.14294900 | -0.06246500 | -1.02164300 |
| C | -1.01429200 | -0.38141800 | -0.07091100 |
| N | -1.02943600 | -0.06626500 | 1.25182800 |

| | | | |
|---|-------------|-------------|------------|
| C | 0.07223200 | 0.60782600 | 1.97644300 |
| C | 1.29727300 | -0.17175100 | 1.88950300 |
| C | 2.26876400 | -0.86984500 | 1.67807000 |
| C | 3.43280600 | -1.63226400 | 1.36924700 |
| C | 3.45678300 | -3.01513000 | 1.58667000 |
| C | 4.55941300 | -0.99252900 | 0.79514900 |
| C | 4.57118900 | -3.76716600 | 1.24387500 |
| H | 2.57864200 | -3.48639100 | 2.02361100 |
| C | 5.67560900 | -1.75903100 | 0.44865900 |
| C | 5.67305300 | -3.13110200 | 0.67616000 |
| H | 4.58156900 | -4.83988300 | 1.41911600 |
| H | 6.53521600 | -1.26740900 | 0.00971000 |
| S | -2.36385200 | -0.55893800 | 2.19053500 |
| O | -1.85812500 | -0.97216800 | 3.49747400 |
| O | -3.14819900 | -1.49016100 | 1.39110300 |
| C | -3.26730000 | 0.95231300 | 2.36878500 |
| C | -3.49041100 | 1.50074600 | 3.62421000 |
| C | -3.73145200 | 1.57288600 | 1.20742500 |
| C | -4.20370600 | 2.69317400 | 3.71352500 |
| H | -3.11343200 | 1.00309000 | 4.51433300 |
| C | -4.43591100 | 2.75863000 | 1.31652400 |
| H | -3.52822000 | 1.12798600 | 0.23425500 |
| C | -4.68532800 | 3.33480700 | 2.57125300 |
| H | -4.38858300 | 3.13568300 | 4.69070700 |
| H | -4.80244100 | 3.25433200 | 0.41763100 |
| C | -5.45429900 | 4.61456500 | 2.66636300 |
| H | -5.52757900 | 4.96638700 | 3.69993500 |
| H | -4.98193100 | 5.40345900 | 2.06855500 |
| H | -6.47235800 | 4.48960600 | 2.27721000 |
| H | 0.23338600 | 1.59988000 | 1.53062600 |

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|---|-------------|-------------|-------------|
| H | -0.22773300 | 0.76897800 | 3.01823700 |
| C | 0.82184700 | 1.00365100 | -1.32572900 |
| C | 0.49946800 | 2.33079100 | -1.00750800 |
| C | 2.04075700 | 0.73122700 | -1.95758200 |
| C | 1.38236700 | 3.36262200 | -1.31294600 |
| H | -0.45803400 | 2.54235300 | -0.52796000 |
| C | 2.91884600 | 1.76392900 | -2.26389200 |
| H | 2.29008400 | -0.30099700 | -2.20313400 |
| C | 2.58979900 | 3.08069300 | -1.94574300 |
| H | 1.12822300 | 4.38907300 | -1.05658200 |
| H | 3.86976000 | 1.54278100 | -2.74576600 |
| H | 3.28361800 | 3.88608800 | -2.17842800 |
| N | 4.48326600 | 0.39164700 | 0.62622100 |
| H | 3.56906900 | 0.78946800 | 0.81715900 |
| C | 5.47501300 | 1.27186900 | 0.27083300 |
| O | 6.58115400 | 0.92692000 | -0.12432100 |
| C | 5.10156100 | 2.71250900 | 0.39887900 |
| C | 5.83296300 | 3.63107800 | -0.35853600 |
| C | 4.09182300 | 3.17292800 | 1.25055400 |
| C | 5.54592900 | 4.98803400 | -0.28588600 |
| H | 6.62536200 | 3.25990300 | -1.00431700 |
| C | 3.81418500 | 4.53319100 | 1.33147900 |
| H | 3.53319800 | 2.48175700 | 1.88202600 |
| C | 4.53438900 | 5.44086300 | 0.55917000 |
| H | 6.11400300 | 5.69559400 | -0.88526600 |
| H | 3.03608500 | 4.88563900 | 2.00450700 |
| H | 4.31343400 | 6.50398400 | 0.62250500 |
| H | 6.55263900 | -3.70981600 | 0.40243300 |
| N | -0.22511700 | -3.23629500 | 0.98399200 |
| N | 1.76454500 | -2.89725600 | -1.49961800 |

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|----|-------------|-------------|-------------|
| C | -0.66315300 | -3.67617300 | 1.96184800 |
| C | 2.68130500 | -3.41902300 | -1.97560200 |
| C | -1.21564100 | -4.23044600 | 3.17415900 |
| C | 3.82712600 | -4.06813400 | -2.56366600 |
| H | -2.27135900 | -3.95323600 | 3.25504500 |
| H | -1.12475100 | -5.32070200 | 3.16145900 |
| H | -0.67816400 | -3.83314100 | 4.04020700 |
| H | 4.12147300 | -4.92525600 | -1.95025900 |
| H | 3.57942800 | -4.41499200 | -3.57131800 |
| H | 4.66178000 | -3.36269800 | -2.62076200 |
| Cu | 0.28809400 | -1.99243700 | -0.52142400 |
| C | -3.18193500 | -4.54130400 | -0.10913600 |
| H | -3.28236700 | -3.62670000 | 0.48970500 |
| H | -2.78255500 | -5.34595300 | 0.51692900 |
| H | -4.16754800 | -4.84023500 | -0.47882700 |
| C | -2.29018200 | -4.28661900 | -1.21943700 |
| N | -1.57768100 | -4.05105600 | -2.10781800 |
| C | -3.59821200 | 1.68343900 | -2.88950500 |
| C | -4.60843300 | 0.85985300 | -2.38690400 |
| C | -4.25908500 | -0.41719700 | -1.98442000 |
| C | -2.94244900 | -0.86046500 | -2.06523200 |
| C | -2.29907300 | 1.23464200 | -2.98505900 |
| H | -5.63493500 | 1.21062600 | -2.32083300 |
| H | -1.46283500 | 1.81527600 | -3.36072400 |
| N | -2.02105700 | -0.03198100 | -2.59599700 |
| O | -0.75185500 | -0.41847400 | -2.55848200 |
| H | -2.60894000 | -1.86276400 | -1.82330000 |
| Cl | -5.44774200 | -1.49506000 | -1.34335800 |
| Cl | -3.96731000 | 3.29542400 | -3.40069000 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.569608

Electronic Energy (0K) + ZPE = -3764.880198

Enthalpy (353K) = -3764.802972

Free Energy (353K) = -3765.005438

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.200387

B7-1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.20721600 | -0.07568100 | -1.08821700 |
| C | -1.06947900 | -0.38351400 | -0.10964400 |
| N | -1.04641200 | -0.01787100 | 1.20226100 |
| C | 0.07044300 | 0.66475600 | 1.89606100 |
| C | 1.28794800 | -0.12828900 | 1.82767300 |
| C | 2.25237200 | -0.84289600 | 1.64022100 |
| C | 3.40821500 | -1.62916100 | 1.36154500 |
| C | 3.40412100 | -3.00850300 | 1.60155900 |
| C | 4.55453400 | -1.01890400 | 0.79486000 |
| C | 4.50850000 | -3.78649400 | 1.28551700 |
| H | 2.51134000 | -3.45657400 | 2.03309700 |
| C | 5.66035600 | -1.81163500 | 0.47458400 |
| C | 5.62899200 | -3.17985300 | 0.72215300 |
| H | 4.49651800 | -4.85638000 | 1.47724200 |
| H | 6.53483300 | -1.34319000 | 0.03985800 |
| S | -2.34622300 | -0.50476400 | 2.19359800 |
| O | -1.79511400 | -0.91992500 | 3.48203600 |
| O | -3.17056100 | -1.43185900 | 1.43034900 |
| C | -3.23019300 | 1.01399100 | 2.40782000 |
| C | -3.39841600 | 1.55717500 | 3.67418300 |
| C | -3.73580100 | 1.64429400 | 1.26892200 |

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|---|-------------|-------------|-------------|
| C | -4.09723400 | 2.75466300 | 3.79981700 |
| H | -2.98915600 | 1.05096900 | 4.54508400 |
| C | -4.42530900 | 2.83536000 | 1.41469500 |
| H | -3.57724600 | 1.20413400 | 0.28442300 |
| C | -4.61846400 | 3.40674800 | 2.68146800 |
| H | -4.23884900 | 3.19241400 | 4.78632100 |
| H | -4.82564200 | 3.34104800 | 0.53632600 |
| C | -5.36825100 | 4.69459900 | 2.81397300 |
| H | -5.43142200 | 5.01989800 | 3.85687400 |
| H | -4.88536000 | 5.49232100 | 2.23635500 |
| H | -6.38922400 | 4.59624100 | 2.42521900 |
| H | 0.23810100 | 1.64088900 | 1.42033600 |
| H | -0.21860100 | 0.86216400 | 2.93483400 |
| C | 0.77719900 | 0.98935700 | -1.36134300 |
| C | 0.45703200 | 2.31966700 | -1.05657300 |
| C | 2.00925700 | 0.70808200 | -1.96263600 |
| C | 1.35511100 | 3.34467700 | -1.34075100 |
| H | -0.51071400 | 2.54114000 | -0.60285900 |
| C | 2.90287800 | 1.73352900 | -2.24954300 |
| H | 2.25864800 | -0.32650500 | -2.19854500 |
| C | 2.57658900 | 3.05319800 | -1.94141400 |
| H | 1.10036400 | 4.37352400 | -1.09468800 |
| H | 3.86263000 | 1.50393200 | -2.70946500 |
| H | 3.28210000 | 3.85302900 | -2.15784000 |
| N | 4.50781300 | 0.36445100 | 0.60723000 |
| H | 3.60175300 | 0.78390600 | 0.79154600 |
| C | 5.52164900 | 1.21777900 | 0.24838400 |
| O | 6.62250200 | 0.84253100 | -0.13385700 |
| C | 5.18219700 | 2.66851400 | 0.35435300 |
| C | 5.94793300 | 3.55918300 | -0.40260700 |

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|----|-------------|-------------|-------------|
| C | 4.17275900 | 3.16482300 | 1.18578400 |
| C | 5.69581000 | 4.92389900 | -0.34874200 |
| H | 6.73968400 | 3.16015200 | -1.03228100 |
| C | 3.93001500 | 4.53267500 | 1.24820300 |
| H | 3.58496500 | 2.49536100 | 1.81421200 |
| C | 4.68506800 | 5.41254400 | 0.47708700 |
| H | 6.29074200 | 5.60945800 | -0.94760500 |
| H | 3.15145800 | 4.91261600 | 1.90557700 |
| H | 4.49118100 | 6.48168300 | 0.52577700 |
| H | 6.50093100 | -3.77879600 | 0.46820700 |
| N | -0.24879300 | -3.21103500 | 1.01780700 |
| N | 1.72748800 | -2.91347500 | -1.48224200 |
| C | -0.67049200 | -3.64580100 | 2.00507800 |
| C | 2.64354000 | -3.44257600 | -1.95157900 |
| C | -1.20150300 | -4.19396900 | 3.22964300 |
| C | 3.78905900 | -4.10042300 | -2.53059300 |
| H | -2.25520100 | -3.91530500 | 3.32999500 |
| H | -1.11219500 | -5.28438400 | 3.22018100 |
| H | -0.64731600 | -3.79351200 | 4.08365300 |
| H | 4.07620100 | -4.95570000 | -1.91122600 |
| H | 3.54489100 | -4.45142900 | -3.53767200 |
| H | 4.62745500 | -3.39938000 | -2.58707000 |
| Cu | 0.25421500 | -1.99362500 | -0.51107200 |
| C | -3.20383700 | -4.49843100 | -0.04079700 |
| H | -3.30004200 | -3.56393100 | 0.52771600 |
| H | -2.79705600 | -5.27972900 | 0.60965000 |
| H | -4.19211100 | -4.81148400 | -0.39116000 |
| C | -2.32207000 | -4.27994400 | -1.16670600 |
| N | -1.61780400 | -4.07109100 | -2.06827800 |
| C | -3.63501200 | 1.64064500 | -2.96656800 |

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|----|-------------|-------------|-------------|
| C | -4.63954400 | 0.83599700 | -2.42103300 |
| C | -4.29097700 | -0.42534700 | -1.97369100 |
| C | -2.97444900 | -0.87256300 | -2.04700000 |
| C | -2.33565100 | 1.19013600 | -3.04905400 |
| H | -5.66609500 | 1.18787200 | -2.36361200 |
| H | -1.50018800 | 1.75660100 | -3.44782800 |
| N | -2.06099800 | -0.06060500 | -2.61370200 |
| O | -0.78178800 | -0.44542000 | -2.54847300 |
| H | -2.64268400 | -1.86900700 | -1.78329300 |
| Cl | -5.47618600 | -1.47916800 | -1.28927400 |
| Cl | -4.01574400 | 3.22435900 | -3.55051200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.569596

Electronic Energy (0K) + ZPE = -3764.879604

Enthalpy (353K) = -3764.801751

Free Energy (353K) = -3765.006259

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.199966

A8

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 2.11841200 | -1.43257800 | -1.37884000 |
| C | 1.08312700 | -1.34694800 | -2.01013600 |
| N | -0.07821100 | -1.27707000 | -2.69165600 |
| C | -0.86039500 | -0.03109000 | -2.57381100 |
| C | -1.26582000 | 0.23370400 | -1.18568100 |
| C | -1.48316000 | 0.02557300 | 0.01099200 |
| C | -1.56861500 | -0.23922200 | 1.40854200 |
| C | -2.79751100 | -0.48518700 | 2.03122800 |
| C | -0.38083100 | -0.19080700 | 2.17677300 |

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|---|-------------|-------------|-------------|
| C | -2.85730700 | -0.68409400 | 3.40301400 |
| H | -3.69807000 | -0.50474700 | 1.42036200 |
| C | -0.44993700 | -0.41123400 | 3.55258000 |
| C | -1.68262600 | -0.64813800 | 4.15340100 |
| H | -3.81276500 | -0.87052300 | 3.88642900 |
| H | 0.46030000 | -0.37858200 | 4.14037700 |
| S | -0.92736200 | -2.77317800 | -2.86613500 |
| O | 0.06058300 | -3.70169000 | -3.38647700 |
| O | -2.12462400 | -2.43027300 | -3.61844900 |
| C | -1.37517000 | -3.26008700 | -1.23010500 |
| C | -0.40061800 | -3.80860700 | -0.39285700 |
| C | -2.67929700 | -3.04821500 | -0.79061800 |
| C | -0.74887100 | -4.13045200 | 0.91024600 |
| H | 0.60574200 | -3.99357800 | -0.76031600 |
| C | -3.00881900 | -3.39757800 | 0.51274000 |
| H | -3.42231800 | -2.62471300 | -1.46214700 |
| C | -2.05189300 | -3.92885500 | 1.38198300 |
| H | -0.00042800 | -4.55519000 | 1.57779300 |
| H | -4.02751400 | -3.25040600 | 0.86792700 |
| C | -2.40012200 | -4.28127200 | 2.79294200 |
| H | -3.41767200 | -3.96968100 | 3.04962500 |
| H | -2.32623100 | -5.36393700 | 2.95577500 |
| H | -1.70515200 | -3.80639900 | 3.49646500 |
| H | -0.22576400 | 0.77892300 | -2.95400400 |
| H | -1.72670500 | -0.10388800 | -3.23933600 |
| C | 3.32480100 | -1.54993300 | -0.62414500 |
| C | 4.54192000 | -1.08318100 | -1.14091200 |
| C | 3.29534300 | -2.12441300 | 0.65705300 |
| C | 5.70304100 | -1.18242400 | -0.38522400 |
| H | 4.56239800 | -0.63946700 | -2.13404600 |

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|---|-------------|-------------|-------------|
| C | 4.46209300 | -2.22872100 | 1.40217800 |
| H | 2.34691200 | -2.48030100 | 1.05650500 |
| C | 5.66631300 | -1.75516900 | 0.88421000 |
| H | 6.64222800 | -0.81119700 | -0.78915100 |
| H | 4.43250200 | -2.67703000 | 2.39247800 |
| H | 6.57834300 | -1.83291300 | 1.47161400 |
| N | 0.80843500 | 0.11501400 | 1.50557600 |
| H | 0.79347300 | -0.04314000 | 0.50111900 |
| C | 1.84975900 | 0.87519200 | 1.98676100 |
| O | 2.03258700 | 1.09112900 | 3.17854800 |
| C | 2.73113400 | 1.45143000 | 0.93054700 |
| C | 4.07071600 | 1.69080200 | 1.24429000 |
| C | 2.23900900 | 1.82095100 | -0.32673500 |
| C | 4.91671000 | 2.26371700 | 0.30307400 |
| H | 4.43858200 | 1.41057000 | 2.22906400 |
| C | 3.08586100 | 2.40325800 | -1.26339900 |
| H | 1.18418100 | 1.68287400 | -0.57148200 |
| C | 4.42584500 | 2.61984200 | -0.95179700 |
| H | 5.96313900 | 2.43213600 | 0.54681000 |
| H | 2.69713400 | 2.69126500 | -2.23848300 |
| H | 5.08893300 | 3.07122000 | -1.68634900 |
| H | -1.72182200 | -0.81347300 | 5.22761600 |
| N | -0.75125300 | 3.36985400 | -1.88151100 |
| N | -1.07920700 | 2.94964400 | 1.36289600 |
| C | -0.27300600 | 4.08238100 | -2.65771300 |
| C | -0.78942500 | 3.14001500 | 2.46769500 |
| C | 0.33130200 | 4.96818800 | -3.62158300 |
| C | -0.40309200 | 3.34212300 | 3.84269500 |
| H | 0.71315900 | 4.39057200 | -4.46859100 |
| H | -0.41103600 | 5.68596200 | -3.98251000 |

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|----|-------------|------------|-------------|
| H | 1.15805900 | 5.51128900 | -3.15410500 |
| H | 0.48705900 | 2.73558400 | 4.04872000 |
| H | -0.17758400 | 4.39763400 | 4.02020600 |
| H | -1.21579400 | 3.02843700 | 4.50492100 |
| Cu | -1.52977200 | 2.18851800 | -0.47009200 |
| C | -6.22096800 | 2.87953000 | -0.49686400 |
| H | -6.63476200 | 2.55363300 | 0.46176900 |
| H | -6.67621400 | 2.29467100 | -1.30127400 |
| H | -6.45578000 | 3.93744100 | -0.64654400 |
| C | -4.79001600 | 2.69134700 | -0.50244000 |
| N | -3.64133800 | 2.54375000 | -0.50757500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2523.235552

Electronic Energy (0K) + ZPE = -2522.621210

Enthalpy (353K) = -2522.554283

Free Energy (353K) = -2522.737084

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2523.731427

TS_{A8}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -1.65825700 | -0.99716800 | -2.44770600 |
| C | -1.77933800 | 0.15734900 | -2.08564200 |
| N | -1.86949400 | 1.42805100 | -1.66525900 |
| C | -0.62778600 | 2.18785000 | -1.36296500 |
| C | 0.08100400 | 1.89233100 | -0.08107100 |
| C | -0.34190000 | 1.15766700 | 0.89039900 |
| C | -1.26955100 | 0.21855200 | 1.47479700 |
| C | -2.21583400 | 0.65021700 | 2.41386300 |
| C | -1.15318500 | -1.16670400 | 1.19799100 |

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|---|-------------|-------------|-------------|
| C | -3.03605600 | -0.25689100 | 3.06626000 |
| H | -2.27764100 | 1.71469300 | 2.63196900 |
| C | -1.99271000 | -2.07637900 | 1.84959500 |
| C | -2.91587400 | -1.61761000 | 2.78035200 |
| H | -3.76535600 | 0.09119800 | 3.79440900 |
| H | -1.88844200 | -3.13511700 | 1.64043300 |
| S | -3.38868700 | 2.19746000 | -1.80037900 |
| O | -3.97971100 | 1.75838300 | -3.05619200 |
| O | -3.13218200 | 3.60917700 | -1.54913600 |
| C | -4.34920200 | 1.53308000 | -0.47491200 |
| C | -4.78159700 | 0.20671500 | -0.54489500 |
| C | -4.67969500 | 2.35141300 | 0.59954300 |
| C | -5.54238600 | -0.29930000 | 0.49627400 |
| H | -4.53552500 | -0.41411300 | -1.40333400 |
| C | -5.46385400 | 1.82834700 | 1.62169800 |
| H | -4.33526400 | 3.38189900 | 0.62848300 |
| C | -5.89749800 | 0.50179300 | 1.58943900 |
| H | -5.87535600 | -1.33587900 | 0.46500800 |
| H | -5.73493500 | 2.45857700 | 2.46722300 |
| C | -6.72356900 | -0.06960100 | 2.69803100 |
| H | -6.74346500 | 0.59220300 | 3.57008000 |
| H | -7.76028200 | -0.22804100 | 2.37467100 |
| H | -6.33697400 | -1.04679000 | 3.01272900 |
| H | 0.05388300 | 2.01786100 | -2.20790600 |
| H | -0.89063400 | 3.25082900 | -1.39058800 |
| C | -1.52819500 | -2.38494000 | -2.74958300 |
| C | -0.70509100 | -2.81865800 | -3.80002800 |
| C | -2.19170300 | -3.33714900 | -1.95899500 |
| C | -0.54477500 | -4.17599300 | -4.04664700 |
| H | -0.18783400 | -2.07937200 | -4.40847100 |

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|---|-------------|-------------|-------------|
| C | -2.03579000 | -4.69240600 | -2.21947600 |
| H | -2.82045600 | -2.99585900 | -1.13710500 |
| C | -1.21048900 | -5.11427900 | -3.26013700 |
| H | 0.10313700 | -4.50410700 | -4.85638100 |
| H | -2.55308800 | -5.42378400 | -1.60273100 |
| H | -1.08426300 | -6.17648700 | -3.45716000 |
| N | -0.18368300 | -1.55562300 | 0.27082400 |
| H | 0.11099500 | -0.80990800 | -0.34760800 |
| C | 0.44197200 | -2.76834700 | 0.14419500 |
| O | 0.18206400 | -3.73614200 | 0.84868600 |
| C | 1.49189200 | -2.82620700 | -0.92162900 |
| C | 2.05322500 | -4.08065200 | -1.17498500 |
| C | 1.93238100 | -1.72187800 | -1.66259500 |
| C | 3.02240700 | -4.23824300 | -2.15755800 |
| H | 1.70415200 | -4.92835500 | -0.59042200 |
| C | 2.89493800 | -1.88267100 | -2.65258700 |
| H | 1.54158800 | -0.71618400 | -1.49694700 |
| C | 3.44115800 | -3.13935500 | -2.90361700 |
| H | 3.44707900 | -5.22116900 | -2.34719500 |
| H | 3.21762700 | -1.01824600 | -3.23043300 |
| H | 4.19300700 | -3.26062700 | -3.68042700 |
| H | -3.55518100 | -2.33712100 | 3.28795700 |
| N | 3.44960000 | 1.71354000 | -1.09707300 |
| N | 2.96268000 | 3.67899600 | 1.34122500 |
| C | 4.39961100 | 1.20723500 | -1.52780000 |
| C | 3.51226800 | 4.25216300 | 2.18388200 |
| C | 5.58629300 | 0.57607800 | -2.05645600 |
| C | 4.19411400 | 4.97081000 | 3.23396400 |
| H | 5.38317600 | -0.47781600 | -2.27526400 |
| H | 5.89518900 | 1.07955900 | -2.97758900 |

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|----|------------|-------------|-------------|
| H | 6.39780400 | 0.64219800 | -1.32495400 |
| H | 4.19038300 | 4.37913200 | 4.15395400 |
| H | 5.22884900 | 5.16966100 | 2.94016600 |
| H | 3.68650700 | 5.92192500 | 3.42025100 |
| Cu | 1.88613000 | 2.75184300 | -0.13540800 |
| C | 1.31352800 | 6.48399500 | -3.03153700 |
| H | 0.41287400 | 7.00402400 | -2.69201400 |
| H | 1.16204700 | 6.14343200 | -4.05998100 |
| H | 2.15836000 | 7.17844400 | -3.00587800 |
| C | 1.57842700 | 5.35277000 | -2.17373800 |
| N | 1.78850500 | 4.44451200 | -1.48522000 |
| C | 1.56919900 | -2.06332500 | 3.36572500 |
| C | 2.70364200 | -2.36404100 | 2.62454000 |
| C | 3.22268400 | -1.35912500 | 1.81482200 |
| C | 2.61633800 | -0.12081100 | 1.72901200 |
| C | 0.96802000 | -0.81799300 | 3.28323700 |
| H | 3.16990800 | -3.34392200 | 2.67703500 |
| H | 0.08844000 | -0.51904600 | 3.84378600 |
| N | 1.49454400 | 0.11096400 | 2.45314800 |
| O | 0.86992100 | 1.26056500 | 2.30646400 |
| H | 2.95348900 | 0.70390900 | 1.10528700 |
| Cl | 4.64560700 | -1.65409300 | 0.87400200 |
| Cl | 0.85316100 | -3.25362300 | 4.39137400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.569748

Electronic Energy (0K) + ZPE = -3764.880867

Enthalpy (353K) = -3764.802833

Free Energy (353K) = -3765.008692

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.203877

B8

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 1.69719500 | -0.94368400 | 2.36181200 |
| C | 1.82701900 | 0.18281800 | 1.92302900 |
| N | 1.89550300 | 1.42379900 | 1.41497800 |
| C | 0.61086900 | 2.17092500 | 1.20749000 |
| C | -0.21100000 | 1.90431000 | -0.00678400 |
| C | 0.16357600 | 1.15272400 | -1.03815600 |
| C | 1.27485200 | 0.24775500 | -1.41317500 |
| C | 2.28184400 | 0.69032500 | -2.27465600 |
| C | 1.20956600 | -1.12690200 | -1.09623600 |
| C | 3.20321500 | -0.19688800 | -2.81858300 |
| H | 2.31504300 | 1.74802700 | -2.53303300 |
| C | 2.14083600 | -2.01956800 | -1.63491900 |
| C | 3.12372400 | -1.55042400 | -2.49818400 |
| H | 3.97584900 | 0.16372100 | -3.49448900 |
| H | 2.06408200 | -3.07472500 | -1.39543500 |
| S | 3.36643800 | 2.26311500 | 1.66846900 |
| O | 3.86707600 | 1.90725800 | 2.99000300 |
| O | 3.08733600 | 3.65390500 | 1.33452400 |
| C | 4.46110400 | 1.58425500 | 0.45897400 |
| C | 4.95015000 | 0.28665400 | 0.62346100 |
| C | 4.83865400 | 2.37381700 | -0.62129000 |
| C | 5.81609300 | -0.22141500 | -0.33178000 |
| H | 4.66516100 | -0.31125500 | 1.48633000 |
| C | 5.72418800 | 1.84991200 | -1.55617100 |
| H | 4.44968900 | 3.38387600 | -0.72160800 |
| C | 6.21613500 | 0.54972700 | -1.43079300 |
| H | 6.19754800 | -1.23618500 | -0.22651500 |

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|---|-------------|-------------|-------------|
| H | 6.03253100 | 2.45871800 | -2.40449900 |
| C | 7.14520400 | -0.02745500 | -2.45146800 |
| H | 7.28536200 | 0.65053400 | -3.29933000 |
| H | 8.13111900 | -0.23388300 | -2.01642100 |
| H | 6.76353300 | -0.98268700 | -2.83396700 |
| H | 0.00312500 | 1.99249600 | 2.10726200 |
| H | 0.86875000 | 3.23652100 | 1.22578600 |
| C | 1.54630200 | -2.31266700 | 2.73114900 |
| C | 0.68729400 | -2.68462800 | 3.77675600 |
| C | 2.21801500 | -3.31055000 | 2.00675500 |
| C | 0.49657400 | -4.02641000 | 4.08047200 |
| H | 0.16638200 | -1.90990300 | 4.33608200 |
| C | 2.03038100 | -4.64972500 | 2.32340700 |
| H | 2.87685500 | -3.01489000 | 1.19079300 |
| C | 1.16759000 | -5.01033600 | 3.35680600 |
| H | -0.17908300 | -4.30641800 | 4.88561900 |
| H | 2.55331800 | -5.41707000 | 1.75711100 |
| H | 1.01705700 | -6.06030200 | 3.59755200 |
| N | 0.17646200 | -1.53818900 | -0.24051700 |
| H | -0.15302900 | -0.80914300 | 0.37886000 |
| C | -0.41496900 | -2.76637600 | -0.14104300 |
| O | -0.11298900 | -3.72190600 | -0.84747900 |
| C | -1.49495300 | -2.85800100 | 0.89276400 |
| C | -2.03167800 | -4.12647000 | 1.12713700 |
| C | -1.98663700 | -1.76659300 | 1.62038700 |
| C | -3.02803000 | -4.30950900 | 2.07795400 |
| H | -1.64191000 | -4.96418400 | 0.55389300 |
| C | -2.97538500 | -1.95229800 | 2.57911100 |
| H | -1.61189700 | -0.75208800 | 1.47234500 |
| C | -3.49866200 | -3.22258800 | 2.81046000 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.43335500 | -5.30319700 | 2.25352200 |
| H | -3.33562900 | -1.09764000 | 3.14904100 |
| H | -4.27199900 | -3.36394600 | 3.56236200 |
| H | 3.83841600 | -2.25363900 | -2.92104100 |
| Cu | -1.97721700 | 2.76926200 | 0.13233000 |
| C | -5.71113000 | 0.48741500 | 2.01769400 |
| H | -6.51130100 | 0.54791500 | 1.27331000 |
| H | -6.04860500 | 0.96449800 | 2.94272700 |
| H | -5.48666800 | -0.56549300 | 2.21927800 |
| C | -4.53047600 | 1.15721900 | 1.52265200 |
| N | -3.58653100 | 1.69887000 | 1.12113800 |
| C | -1.52421000 | -2.09249700 | -3.37968500 |
| C | -2.68495900 | -2.37580000 | -2.67004600 |
| C | -3.19746700 | -1.39326100 | -1.82773000 |
| C | -2.54595800 | -0.18331000 | -1.67553500 |
| C | -0.89329100 | -0.86527100 | -3.24401500 |
| H | -3.18140100 | -3.33744100 | -2.77226000 |
| H | 0.00459600 | -0.56618600 | -3.77630600 |
| N | -1.42184000 | 0.02284800 | -2.38534700 |
| O | -0.76685500 | 1.20825200 | -2.20806900 |
| H | -2.85494800 | 0.62457800 | -1.01412900 |
| Cl | -4.65145200 | -1.67191700 | -0.94047200 |
| Cl | -0.82261900 | -3.26893700 | -4.42310600 |
| C | -4.43551300 | 4.64673200 | -3.35415400 |
| H | -5.51244900 | 4.62483200 | -3.16349800 |
| H | -4.22305200 | 4.09868300 | -4.27684800 |
| H | -4.11650900 | 5.68605000 | -3.47641200 |
| C | -3.72635000 | 4.04588400 | -2.24912000 |
| N | -3.15599100 | 3.56665100 | -1.36207200 |
| C | -1.61250000 | 6.45926700 | 3.07926100 |

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|---|-------------|------------|------------|
| H | -0.66526900 | 6.31857900 | 3.60821000 |
| H | -2.42306700 | 6.53174000 | 3.81040800 |
| H | -1.56566600 | 7.38921400 | 2.50517400 |
| C | -1.84915400 | 5.34561800 | 2.19044300 |
| N | -2.03931400 | 4.45172400 | 1.47744100 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.577900

Electronic Energy (0K) + ZPE = -3764.887025

Enthalpy (353K) = -3764.809322

Free Energy (353K) = -3765.013136

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.210729

TS_{A8-1}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.96774700 | -2.46170400 | -1.33164800 |
| C | 0.98908100 | -1.93964000 | -1.83144100 |
| N | -0.07166800 | -1.32784800 | -2.37903300 |
| C | -0.13886800 | 0.13820600 | -2.44178900 |
| C | -0.72175500 | 0.76736700 | -1.20744900 |
| C | -0.90249200 | 0.58237500 | 0.07252800 |
| C | -0.71304400 | -0.28552900 | 1.21952300 |
| C | -1.85343600 | -0.73853900 | 1.90161200 |
| C | 0.55166100 | -0.67904200 | 1.71733100 |
| C | -1.75968000 | -1.51826700 | 3.04472500 |
| H | -2.83125900 | -0.46918500 | 1.50907100 |
| C | 0.64110200 | -1.45124900 | 2.87669800 |
| C | -0.50683300 | -1.86304300 | 3.54342800 |
| H | -2.66567800 | -1.84657100 | 3.55018900 |
| H | 1.62398900 | -1.73229600 | 3.24314900 |

| | | | |
|---|-------------|-------------|-------------|
| S | -1.44386400 | -2.27604400 | -2.77343200 |
| O | -0.94475700 | -3.38670000 | -3.56813600 |
| O | -2.40152600 | -1.32224400 | -3.31682800 |
| C | -2.05656700 | -2.91636300 | -1.24533800 |
| C | -1.30493200 | -3.86090700 | -0.54109700 |
| C | -3.30606400 | -2.50268300 | -0.79466700 |
| C | -1.81487500 | -4.36684600 | 0.64356200 |
| H | -0.34366500 | -4.20268400 | -0.91664300 |
| C | -3.80687700 | -3.03977200 | 0.38510700 |
| H | -3.88267400 | -1.78217200 | -1.37015600 |
| C | -3.07132200 | -3.97152800 | 1.12059500 |
| H | -1.23451800 | -5.09386800 | 1.20990000 |
| H | -4.78592400 | -2.72418600 | 0.74484000 |
| C | -3.60897500 | -4.55661700 | 2.38757400 |
| H | -4.45234100 | -3.97640900 | 2.77618800 |
| H | -3.96099700 | -5.58309600 | 2.22235500 |
| H | -2.83234300 | -4.60693300 | 3.16006300 |
| H | 0.88805400 | 0.48183800 | -2.61528900 |
| H | -0.72659900 | 0.41936400 | -3.31879500 |
| C | 3.06176700 | -3.00591400 | -0.59449900 |
| C | 4.35880600 | -3.00895600 | -1.12750400 |
| C | 2.85257200 | -3.46632200 | 0.71550900 |
| C | 5.42731300 | -3.44773000 | -0.35578400 |
| H | 4.51730800 | -2.64882300 | -2.14187000 |
| C | 3.92443600 | -3.90975500 | 1.47815700 |
| H | 1.84299100 | -3.45303400 | 1.12508800 |
| C | 5.21278500 | -3.89618400 | 0.94575600 |
| H | 6.43278400 | -3.43659400 | -0.77007500 |
| H | 3.75666700 | -4.26064100 | 2.49401400 |
| H | 6.05233400 | -4.23577800 | 1.54807100 |

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|----|-------------|-------------|-------------|
| N | 1.71129800 | -0.32436500 | 0.99908300 |
| H | 1.66300700 | -0.48304000 | -0.00300300 |
| C | 2.91753100 | 0.02676600 | 1.54065800 |
| O | 3.09368400 | 0.15815800 | 2.74739300 |
| C | 4.02261100 | 0.25500800 | 0.56019700 |
| C | 5.32983200 | 0.20498500 | 1.05112100 |
| C | 3.81421200 | 0.51897500 | -0.79761500 |
| C | 6.41029100 | 0.40273900 | 0.20051500 |
| H | 5.47981200 | 0.00259900 | 2.10891000 |
| C | 4.89518000 | 0.72865300 | -1.64708700 |
| H | 2.80595500 | 0.57586400 | -1.20759700 |
| C | 6.19472500 | 0.66611700 | -1.15044400 |
| H | 7.42385100 | 0.35034100 | 0.59101100 |
| H | 4.72091800 | 0.93475400 | -2.70125800 |
| H | 7.03976300 | 0.82303900 | -1.81695000 |
| H | -0.41896300 | -2.46601600 | 4.44430900 |
| N | 1.61961700 | 3.01327200 | -1.55477100 |
| N | 1.01654500 | 2.60239800 | 1.66846800 |
| C | 2.31788500 | 3.51276700 | -2.33002400 |
| C | 1.31585200 | 2.62426800 | 2.78598200 |
| C | 3.19465900 | 4.13510400 | -3.29061100 |
| C | 1.68006100 | 2.64449500 | 4.18066000 |
| H | 3.15835800 | 3.58730800 | -4.23680500 |
| H | 2.88205100 | 5.16930800 | -3.46226300 |
| H | 4.22022800 | 4.12841300 | -2.90921500 |
| H | 2.76269100 | 2.76654800 | 4.27649600 |
| H | 1.17315200 | 3.47070000 | 4.68737000 |
| H | 1.38816400 | 1.69665900 | 4.64270400 |
| Cu | 0.48380800 | 2.13399400 | -0.18395500 |
| C | 0.11048300 | 7.21398500 | -0.29751500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.07539300 | 7.69287500 | 0.68524900 |
| H | -0.58086400 | 7.73058900 | -0.96961900 |
| H | 1.12547500 | 7.29904100 | -0.69713500 |
| C | -0.26025600 | 5.82111400 | -0.18222000 |
| N | -0.55541900 | 4.70234400 | -0.09026500 |
| C | -4.90245500 | 0.78329900 | -0.49130200 |
| C | -4.77585000 | 1.26010800 | 0.83333300 |
| C | -3.63538400 | 1.94658500 | 1.14936000 |
| C | -2.61634700 | 2.17502300 | 0.19740600 |
| C | -3.94074200 | 1.03037700 | -1.43019500 |
| H | -5.55712500 | 1.08073300 | 1.56671200 |
| H | -3.95060500 | 0.66173900 | -2.45171700 |
| N | -2.88810600 | 1.83741300 | -1.09740500 |
| O | -1.83064000 | 1.84189900 | -1.89112700 |
| H | -1.87333500 | 2.95211500 | 0.34527000 |
| Cl | -3.34110300 | 2.52841600 | 2.75719500 |
| Cl | -6.30523000 | -0.14332100 | -0.93393600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.560179

Electronic Energy (0K) + ZPE = -3764.870384

Enthalpy (353K) = -3764.792835

Free Energy (353K) = -3764.997117

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.192892

B8-1

Number of imaginary frequencies: 0

| | | | |
|---|-------------|------------|-------------|
| C | -0.06633500 | 3.01637800 | -1.31154200 |
| C | 0.35399100 | 1.96076900 | -1.74404300 |
| N | 0.81863500 | 0.78413800 | -2.18853100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.02765500 | -0.41320600 | -2.19078600 |
| C | 0.20187300 | -1.31097000 | -1.00366000 |
| C | 0.29350600 | -1.08862700 | 0.34730900 |
| C | 0.44369900 | 0.21023100 | 1.06247900 |
| C | 1.72663600 | 0.53939700 | 1.51947700 |
| C | -0.59072600 | 1.13263200 | 1.30376600 |
| C | 1.96592600 | 1.69496900 | 2.25066600 |
| H | 2.55398500 | -0.12663400 | 1.28704300 |
| C | -0.35547500 | 2.28039400 | 2.05927200 |
| C | 0.91387000 | 2.55477000 | 2.54876800 |
| H | 2.97709200 | 1.91720400 | 2.58665200 |
| H | -1.17459800 | 2.97658000 | 2.22519900 |
| S | 2.38598000 | 0.74229500 | -2.90005100 |
| O | 2.40366900 | 1.74465600 | -3.95328600 |
| O | 2.59951000 | -0.66736000 | -3.19408900 |
| C | 3.46113500 | 1.26668800 | -1.60504500 |
| C | 3.59381600 | 2.63078700 | -1.33918800 |
| C | 4.15246900 | 0.30912800 | -0.86913800 |
| C | 4.42083100 | 3.02697700 | -0.29946700 |
| H | 3.06585100 | 3.36722800 | -1.94048800 |
| C | 4.98657700 | 0.73075800 | 0.15882400 |
| H | 4.03747900 | -0.75028900 | -1.09140500 |
| C | 5.12673800 | 2.08763900 | 0.46305300 |
| H | 4.53074800 | 4.08682000 | -0.07468600 |
| H | 5.53494200 | -0.00841400 | 0.74217700 |
| C | 6.02225800 | 2.53811800 | 1.57275200 |
| H | 6.24977300 | 1.72016600 | 2.26382100 |
| H | 6.97527800 | 2.91145900 | 1.17636500 |
| H | 5.56868700 | 3.35926100 | 2.13938900 |
| H | -1.06423700 | -0.06064600 | -2.23417800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.15580200 | -0.99537600 | -3.09849300 |
| C | -0.50599400 | 4.21790700 | -0.68498500 |
| C | -1.86180700 | 4.57721100 | -0.68978300 |
| C | 0.41690700 | 5.02217000 | 0.00270700 |
| C | -2.28430700 | 5.71023900 | -0.00511500 |
| H | -2.57855100 | 3.95787700 | -1.22654300 |
| C | -0.01224300 | 6.16226600 | 0.66749800 |
| H | 1.46398800 | 4.72375900 | 0.02491500 |
| C | -1.36322500 | 6.50603700 | 0.67158800 |
| H | -3.33892600 | 5.97570000 | -0.00439800 |
| H | 0.70934100 | 6.78066200 | 1.19651900 |
| H | -1.69751100 | 7.39380500 | 1.20326700 |
| N | -1.85369900 | 0.96005000 | 0.67731800 |
| H | -1.85071100 | 1.01953900 | -0.33581300 |
| C | -3.06902000 | 1.07142200 | 1.31218200 |
| O | -3.17316100 | 1.15998200 | 2.52682400 |
| C | -4.25319100 | 0.96130200 | 0.40996300 |
| C | -5.41933600 | 0.42364500 | 0.96040000 |
| C | -4.23639000 | 1.33286700 | -0.93853900 |
| C | -6.54664200 | 0.23585300 | 0.17058100 |
| H | -5.42172800 | 0.15042700 | 2.01354600 |
| C | -5.37246800 | 1.16317600 | -1.72287200 |
| H | -3.35094500 | 1.78388400 | -1.38876800 |
| C | -6.52479300 | 0.60659600 | -1.17211900 |
| H | -7.44615500 | -0.19508400 | 0.60352800 |
| H | -5.35944200 | 1.47177500 | -2.76564200 |
| H | -7.41029100 | 0.46989500 | -1.78882600 |
| H | 1.08559600 | 3.46208700 | 3.12330700 |
| N | -2.97665600 | -1.94659300 | -1.45250500 |
| N | -2.38022300 | -1.82175200 | 1.93925000 |

| | | | |
|----|-------------|-------------|-------------|
| C | -3.73262900 | -2.17015800 | -2.29919000 |
| C | -2.62674200 | -1.66291300 | 3.05851500 |
| C | -4.67293200 | -2.45110200 | -3.35422500 |
| C | -2.92400700 | -1.45928000 | 4.45351500 |
| H | -4.18655600 | -2.33631500 | -4.32733300 |
| H | -5.04386000 | -3.47546100 | -3.25391100 |
| H | -5.51590300 | -1.75634700 | -3.28757700 |
| H | -3.95095100 | -1.09775800 | 4.56212000 |
| H | -2.80822700 | -2.39885100 | 5.00172700 |
| H | -2.23741700 | -0.71113600 | 4.86192300 |
| Cu | -1.78939800 | -1.58056400 | 0.05720400 |
| C | -0.73969500 | -5.35209100 | -2.17698900 |
| H | 0.34320100 | -5.49012500 | -2.10357900 |
| H | -0.94771400 | -4.57423300 | -2.91843700 |
| H | -1.19698300 | -6.28999900 | -2.50571400 |
| C | -1.27741300 | -4.96161000 | -0.89160100 |
| N | -1.72226500 | -4.64515400 | 0.13452000 |
| C | 3.53749700 | -2.93592900 | 0.48997800 |
| C | 3.07313700 | -2.72000200 | 1.84674600 |
| C | 1.76870900 | -2.48996200 | 2.03331200 |
| C | 0.76560400 | -2.46970600 | 0.91983900 |
| C | 2.67598000 | -3.06569300 | -0.53168000 |
| H | 3.77669600 | -2.73934700 | 2.67500000 |
| H | 2.96547800 | -3.22826600 | -1.56624500 |
| N | 1.29891400 | -3.15062500 | -0.27650400 |
| O | 0.58743600 | -2.57845400 | -1.37699600 |
| H | -0.11842200 | -3.03741400 | 1.24703800 |
| Cl | 1.10619000 | -2.18143800 | 3.60991500 |
| Cl | 5.25620200 | -3.07399100 | 0.22223900 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3765.607289

Electronic Energy (0K) + ZPE = -3764.913473

Enthalpy (353K) = -3764.836890

Free Energy (353K) = -3765.035220

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3766.192892

TS_B

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 2.26154300 | -1.73460700 | -1.77972400 |
| C | 1.04593700 | -1.70867600 | -1.76295400 |
| N | -0.29527900 | -1.73112000 | -1.67073900 |
| C | -1.03586300 | -0.45637800 | -1.76034300 |
| C | -0.79124500 | 0.49326500 | -0.63024900 |
| C | -1.74408700 | 1.49015100 | -0.44941200 |
| C | -1.73844800 | 2.49048200 | 0.66076200 |
| C | -2.90625500 | 2.68670700 | 1.40704100 |
| C | -0.61830000 | 3.29328800 | 0.96111400 |
| C | -2.95756700 | 3.58502800 | 2.46371100 |
| H | -3.79905800 | 2.11651100 | 1.16283100 |
| C | -0.67406800 | 4.20380500 | 2.02103900 |
| C | -1.82963700 | 4.33609800 | 2.77708300 |
| H | -3.87591800 | 3.69994500 | 3.03401000 |
| H | 0.19557500 | 4.81533000 | 2.23317100 |
| S | -0.91609700 | -2.97968000 | -0.64692600 |
| O | -0.54066600 | -4.22845400 | -1.28777100 |
| O | -2.31574400 | -2.62831900 | -0.43837700 |
| C | -0.02391800 | -2.83905400 | 0.87183700 |
| C | 1.21839800 | -3.46038300 | 0.97701200 |
| C | -0.52815500 | -2.04187400 | 1.90131400 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.97451800 | -3.25683300 | 2.12465100 |
| H | 1.58621400 | -4.09407100 | 0.17398300 |
| C | 0.23656700 | -1.86423400 | 3.04462500 |
| H | -1.51015500 | -1.58186600 | 1.81616400 |
| C | 1.50269900 | -2.45145900 | 3.16469900 |
| H | 2.95103200 | -3.73066500 | 2.21398400 |
| H | -0.14652600 | -1.25086600 | 3.85871000 |
| C | 2.33068000 | -2.20457900 | 4.38531200 |
| H | 1.87775700 | -2.67076700 | 5.26940500 |
| H | 3.34287000 | -2.60672400 | 4.27462800 |
| H | 2.40378000 | -1.13057800 | 4.59742300 |
| H | -0.68752600 | 0.02383300 | -2.68795400 |
| H | -2.08687600 | -0.70819500 | -1.93756000 |
| C | 3.68309800 | -1.76572700 | -1.70938800 |
| C | 4.42748000 | -0.57496600 | -1.73192200 |
| C | 4.35298400 | -2.99215100 | -1.57259100 |
| C | 5.81261900 | -0.61916200 | -1.63470800 |
| H | 3.91154400 | 0.38014500 | -1.83421300 |
| C | 5.73744000 | -3.02215800 | -1.46150400 |
| H | 3.77742900 | -3.91556800 | -1.56217300 |
| C | 6.47219800 | -1.83883700 | -1.49549500 |
| H | 6.37934800 | 0.30991600 | -1.66377400 |
| H | 6.24643700 | -3.97744500 | -1.35574600 |
| H | 7.55640900 | -1.86721500 | -1.41685600 |
| N | 0.52263300 | 3.23249300 | 0.13752400 |
| H | 0.37148500 | 2.86985900 | -0.79555600 |
| C | 1.82384600 | 3.37654600 | 0.55137500 |
| O | 2.13059400 | 3.60502800 | 1.71481700 |
| C | 2.86352100 | 3.21554100 | -0.51133400 |
| C | 4.18793900 | 3.09741100 | -0.07798600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.59028400 | 3.19507000 | -1.88340900 |
| C | 5.22039800 | 2.95146100 | -0.99464800 |
| H | 4.38748400 | 3.13446700 | 0.99046800 |
| C | 3.62588200 | 3.04939800 | -2.80145900 |
| H | 1.57747800 | 3.33053100 | -2.25979700 |
| C | 4.94048100 | 2.92473100 | -2.35990700 |
| H | 6.24733600 | 2.86413300 | -0.64553500 |
| H | 3.40472600 | 3.04470700 | -3.86593400 |
| H | 5.74784500 | 2.81265500 | -3.08041500 |
| H | -1.85327700 | 5.04923800 | 3.59767000 |
| Cu | 0.81920500 | 0.30194200 | 0.35686500 |
| C | 4.94612900 | -0.36452900 | 1.93388500 |
| H | 5.18599700 | -1.41357800 | 1.72851500 |
| H | 5.05828200 | -0.16782300 | 3.00468600 |
| H | 5.63466800 | 0.27799300 | 1.37427100 |
| C | 3.59328400 | -0.09142800 | 1.52224800 |
| N | 2.50741000 | 0.12237300 | 1.18597200 |
| C | -6.33679700 | 0.19192100 | -1.37086900 |
| C | -6.31648600 | -0.81905600 | -0.41399800 |
| C | -5.13825600 | -1.04813200 | 0.28756400 |
| C | -4.01485900 | -0.27561400 | 0.01765700 |
| C | -5.19829700 | 0.95066400 | -1.61359700 |
| H | -7.20357100 | -1.41568800 | -0.21981600 |
| H | -5.13270200 | 1.75695000 | -2.34018800 |
| N | -4.12223400 | 0.66370500 | -0.89751500 |
| O | -2.74307200 | 1.58519400 | -1.31951600 |
| H | -3.04611200 | -0.39415200 | 0.51431300 |
| Cl | -5.05188900 | -2.28108900 | 1.49059000 |
| Cl | -7.77823300 | 0.52034900 | -2.26479600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3500.225122

Electronic Energy (0K) + ZPE = -3499.628537

Enthalpy (353K) = -3499.564795

Free Energy (353K) = -3499.733395

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3500.782782

[N] (*Cu catalysis system*)

Number of imaginary frequencies: 0

| | | | |
|----|-------------|-------------|-------------|
| C | 1.17991300 | -0.01061700 | -0.00005100 |
| C | -0.00000100 | -0.74065100 | -0.00006700 |
| C | -1.17991800 | -0.01059900 | -0.00003800 |
| C | -1.14650100 | 1.38061400 | -0.00000400 |
| C | 1.14649700 | 1.38061100 | -0.00002000 |
| H | -0.00002000 | -1.82748600 | -0.00006000 |
| H | 2.07429700 | 1.95191400 | 0.00007700 |
| N | 0.00000700 | 2.05648800 | 0.00001800 |
| H | -2.07428600 | 1.95193800 | 0.00006200 |
| Cl | -2.71554600 | -0.83729300 | 0.00002400 |
| Cl | 2.71554700 | -0.83729100 | 0.00002800 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1167.231701

Electronic Energy (0K) + ZPE = -1167.162272

Enthalpy (353K) = -1167.152324

Free Energy (353K) = -1167.200977

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1167.348389

C

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 3.30070100 | 0.20200000 | -1.25934900 |
| C | 2.73021500 | -0.85599000 | -1.43665000 |
| N | 2.06676200 | -2.01362000 | -1.62440300 |
| C | 0.67017600 | -1.91324000 | -2.06249500 |
| C | -0.19916100 | -1.07197000 | -1.23450100 |
| C | -1.60393800 | -0.95118900 | -1.61318600 |
| C | -2.68109600 | -1.74052500 | -0.98671700 |
| C | -2.54891400 | -3.13089300 | -0.89739300 |
| C | -3.87406500 | -1.13248400 | -0.55333300 |
| C | -3.60030600 | -3.91591800 | -0.44260300 |
| H | -1.62668800 | -3.61119700 | -1.21962900 |
| C | -4.92210500 | -1.92629700 | -0.09802600 |
| C | -4.79194500 | -3.31009500 | -0.05648000 |
| H | -3.49082600 | -4.99576700 | -0.39630800 |
| H | -5.83634600 | -1.44364900 | 0.24061500 |
| S | 2.37172500 | -3.26116300 | -0.45014500 |
| O | 3.80496400 | -3.22677600 | -0.23044900 |
| O | 1.69685700 | -4.43104400 | -0.98935300 |
| C | 1.51624200 | -2.70333400 | 0.98636200 |
| C | 2.09577800 | -1.70080700 | 1.76906600 |
| C | 0.23151300 | -3.17888200 | 1.24467100 |
| C | 1.35678200 | -1.16354000 | 2.81140200 |
| H | 3.10697700 | -1.35332000 | 1.56786500 |
| C | -0.48993100 | -2.62313900 | 2.29540400 |
| H | -0.19082500 | -3.97822900 | 0.64011100 |
| C | 0.05155800 | -1.59980300 | 3.07796000 |
| H | 1.79254500 | -0.38128100 | 3.43116300 |
| H | -1.49438900 | -2.98622700 | 2.50776300 |
| C | -0.73956100 | -0.95922000 | 4.17231800 |
| H | -1.68823300 | -1.47686700 | 4.34219700 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.17671700 | -0.94449900 | 5.11288700 |
| H | -0.96478000 | 0.08548200 | 3.91895600 |
| H | 0.64567200 | -1.44437400 | -3.06547600 |
| H | 0.27861500 | -2.92756600 | -2.22955000 |
| C | 3.95482600 | 1.43956600 | -1.00020400 |
| C | 3.43813000 | 2.63760800 | -1.51986400 |
| C | 5.10085600 | 1.47599800 | -0.19081600 |
| C | 4.06656600 | 3.84451500 | -1.24139600 |
| H | 2.54549700 | 2.60708600 | -2.14244000 |
| C | 5.71869300 | 2.69002900 | 0.08392400 |
| H | 5.49928800 | 0.54662700 | 0.21120700 |
| C | 5.20694100 | 3.87571600 | -0.44019800 |
| H | 3.66359300 | 4.76704400 | -1.65320200 |
| H | 6.60963900 | 2.70894200 | 0.70733200 |
| H | 5.69815600 | 4.82228500 | -0.22743300 |
| N | -4.03472300 | 0.26857800 | -0.54640500 |
| H | -4.90980400 | 0.63285200 | -0.90572900 |
| C | -3.13510200 | 1.13880100 | -0.00564800 |
| O | -2.07469200 | 0.75553800 | 0.49146100 |
| C | -3.49133600 | 2.57987800 | -0.07055600 |
| C | -2.43890700 | 3.49888000 | -0.10578300 |
| C | -4.81166000 | 3.03846400 | -0.07960100 |
| C | -2.70358100 | 4.86019700 | -0.17537200 |
| H | -1.41577700 | 3.12734700 | -0.09069200 |
| C | -5.07292400 | 4.40258800 | -0.13373700 |
| H | -5.64367200 | 2.34004000 | -0.00810100 |
| C | -4.02098700 | 5.31310100 | -0.18871800 |
| H | -1.88203100 | 5.57142400 | -0.21816600 |
| H | -6.10107900 | 4.75570600 | -0.12784700 |
| H | -4.22874600 | 6.37952100 | -0.23696200 |

| | | | |
|----|-------------|-------------|-------------|
| H | -5.62216500 | -3.91529500 | 0.29870500 |
| Cu | 0.33785400 | 0.21924900 | 0.01085000 |
| C | 2.32865900 | 3.73337500 | 1.95928600 |
| H | 3.40128700 | 3.57485600 | 1.79893000 |
| H | 2.12686200 | 3.81744400 | 3.03133100 |
| H | 2.02325000 | 4.65788500 | 1.45947200 |
| C | 1.59712600 | 2.62219400 | 1.41020600 |
| N | 1.01474700 | 1.72671000 | 0.96652700 |
| O | -1.75558400 | -0.07785300 | -2.46380600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2333.039134

Electronic Energy (0K) + ZPE = -2332.515180

Enthalpy (353K) = -2332.460128

Free Energy (353K) = -2332.612874

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2333.480447

TS_C

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.44119500 | -1.78153700 | 0.56391700 |
| C | -1.60856800 | -2.29374200 | 0.26362800 |
| N | -2.23347200 | -2.25883700 | -0.89715100 |
| C | -1.54919000 | -1.52469400 | -2.00266100 |
| C | -0.29883600 | -0.94209000 | -1.56673500 |
| C | 0.48684100 | -0.07879700 | -2.38836900 |
| C | 0.31955900 | 1.30168000 | -1.79062000 |
| C | -0.91484500 | 1.97973600 | -1.90382100 |
| C | 1.42786700 | 1.94491900 | -1.17745400 |
| C | -1.05554600 | 3.26543100 | -1.39813000 |
| H | -1.74542200 | 1.48381400 | -2.40503900 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.26145600 | 3.23126800 | -0.66353100 |
| C | 0.03380000 | 3.87631500 | -0.78019700 |
| H | -2.00106500 | 3.79188200 | -1.49677300 |
| H | 2.10113200 | 3.73214200 | -0.19458600 |
| S | -3.98388400 | -2.20845700 | -0.87644400 |
| O | -4.40059500 | -3.25123000 | 0.03961700 |
| O | -4.37328800 | -2.21049900 | -2.27634100 |
| C | -4.24200500 | -0.61399600 | -0.16527900 |
| C | -4.20025900 | -0.48740000 | 1.22269000 |
| C | -4.31125500 | 0.50221500 | -0.99990100 |
| C | -4.20150000 | 0.78635300 | 1.77504900 |
| H | -4.16305200 | -1.36921000 | 1.85757800 |
| C | -4.31237500 | 1.76511000 | -0.42396200 |
| H | -4.37454300 | 0.38236900 | -2.07965500 |
| C | -4.22723700 | 1.92605900 | 0.96457000 |
| H | -4.16946300 | 0.89970800 | 2.85723200 |
| H | -4.37424000 | 2.64581200 | -1.06163400 |
| C | -4.11842000 | 3.29435300 | 1.55691900 |
| H | -3.09691800 | 3.68075600 | 1.42312900 |
| H | -4.79301500 | 4.00232600 | 1.06283900 |
| H | -4.33899100 | 3.29359400 | 2.62917000 |
| H | -1.30924900 | -2.21338100 | -2.83358100 |
| H | -2.26766700 | -0.80514100 | -2.42300000 |
| C | 0.76832600 | -2.17489300 | 1.25074700 |
| C | 1.77931100 | -1.24855400 | 1.54849000 |
| C | 0.93918900 | -3.51853500 | 1.62724700 |
| C | 2.93621500 | -1.65492100 | 2.19720000 |
| H | 1.64967300 | -0.20156700 | 1.26919100 |
| C | 2.09249500 | -3.91609200 | 2.28702800 |
| H | 0.15425700 | -4.23693700 | 1.40098500 |

| | | | |
|----|-------------|-------------|-------------|
| C | 3.09398600 | -2.98844000 | 2.56845500 |
| H | 3.71453200 | -0.92802500 | 2.41867500 |
| H | 2.21456600 | -4.95636900 | 2.57833700 |
| H | 3.99916400 | -3.30566800 | 3.08068500 |
| N | 2.64684200 | 1.27041100 | -1.15243100 |
| H | 2.78886000 | 0.58466500 | -1.88673500 |
| C | 3.58140600 | 1.35220300 | -0.13621900 |
| O | 3.35897600 | 1.97031600 | 0.89537200 |
| C | 4.85562200 | 0.61874800 | -0.37092700 |
| C | 5.70518300 | 0.45748500 | 0.72859800 |
| C | 5.24405700 | 0.11553800 | -1.61738200 |
| C | 6.91201600 | -0.21397700 | 0.59194100 |
| H | 5.40047300 | 0.87112600 | 1.68712400 |
| C | 6.45499100 | -0.55269100 | -1.75264100 |
| H | 4.62954700 | 0.26028800 | -2.50383500 |
| C | 7.28714000 | -0.72267400 | -0.64960200 |
| H | 7.56420000 | -0.33843100 | 1.45289000 |
| H | 6.75216500 | -0.93580800 | -2.72562600 |
| H | 8.23353500 | -1.24700200 | -0.75986400 |
| H | -0.06597400 | 4.88596500 | -0.38896400 |
| Cu | -0.55287200 | 0.21649200 | 0.08561300 |
| C | -1.05357300 | 2.74091800 | 3.88130000 |
| H | -1.93188800 | 2.39933700 | 4.43739200 |
| H | -1.16854400 | 3.80025400 | 3.63304900 |
| H | -0.16278800 | 2.61163900 | 4.50346500 |
| C | -0.91078700 | 1.96878200 | 2.67396200 |
| N | -0.79537400 | 1.34421500 | 1.70771500 |
| O | 1.26577800 | -0.34684700 | -3.29426000 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2333.000815

Electronic Energy (0K) + ZPE = -2332.476333

Enthalpy (353K) = -2332.423167

Free Energy (353K) = -2332.568083

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2333.439838

D

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.50428100 | -1.52029000 | 0.45313300 |
| C | -1.77661700 | -2.22043100 | 0.11930600 |
| N | -1.99236900 | -1.89118200 | -1.14277800 |
| C | -1.04594400 | -0.94924700 | -1.76010900 |
| C | -0.13281000 | -0.69389800 | -0.61207500 |
| C | 1.23213000 | -0.09349400 | -0.85062200 |
| C | 1.43745000 | 1.35519900 | -0.85385100 |
| C | 0.32553800 | 2.21406300 | -0.93478000 |
| C | 2.74262600 | 1.92708400 | -0.77674800 |
| C | 0.46143200 | 3.58778500 | -0.92339100 |
| H | -0.67335400 | 1.78981600 | -1.02285100 |
| C | 2.86511300 | 3.32396300 | -0.75342200 |
| C | 1.74233000 | 4.13208800 | -0.82696400 |
| H | -0.41330800 | 4.22815000 | -0.99478900 |
| H | 3.85246400 | 3.76010800 | -0.67670100 |
| S | -3.53828400 | -2.18379000 | -1.90924200 |
| O | -3.99779300 | -3.47600400 | -1.44461900 |
| O | -3.29531000 | -1.90993100 | -3.31557200 |
| C | -4.49265200 | -0.88844300 | -1.18803500 |
| C | -5.14302200 | -1.12290800 | 0.02389700 |
| C | -4.50024100 | 0.36445000 | -1.79696300 |
| C | -5.81791900 | -0.07265600 | 0.62625400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -5.12492100 | -2.11063100 | 0.47765300 |
| C | -5.18457300 | 1.40157500 | -1.17422000 |
| H | -3.99833000 | 0.52074700 | -2.74927500 |
| C | -5.84967900 | 1.19934100 | 0.03908100 |
| H | -6.34073200 | -0.23867100 | 1.56665900 |
| H | -5.21422200 | 2.38340500 | -1.64300000 |
| C | -6.60855400 | 2.30833300 | 0.69520200 |
| H | -6.39920600 | 3.27519300 | 0.22697100 |
| H | -7.68895400 | 2.13055000 | 0.62125400 |
| H | -6.37451600 | 2.37361600 | 1.76446400 |
| H | -0.50674900 | -1.41760400 | -2.59623800 |
| H | -1.55861900 | -0.06013700 | -2.15256100 |
| C | 0.23120100 | -1.80719900 | 1.70065200 |
| C | 1.30495000 | -1.01359000 | 2.13485000 |
| C | -0.15233700 | -2.90778500 | 2.47905300 |
| C | 1.97799200 | -1.31912200 | 3.30886200 |
| H | 1.61931800 | -0.13928500 | 1.56680600 |
| C | 0.53062000 | -3.21484300 | 3.64960600 |
| H | -0.98473600 | -3.52446000 | 2.15027300 |
| C | 1.59561500 | -2.42316000 | 4.06841900 |
| H | 2.80595700 | -0.69279300 | 3.63145100 |
| H | 0.22766500 | -4.07848200 | 4.23652300 |
| H | 2.12756000 | -2.66332700 | 4.98585400 |
| N | 3.84526200 | 1.08659200 | -0.72638100 |
| H | 3.61828700 | 0.10154600 | -0.84156900 |
| C | 5.16287000 | 1.41172300 | -0.47027400 |
| O | 5.53957700 | 2.53571500 | -0.17250800 |
| C | 6.11530800 | 0.26682300 | -0.56530300 |
| C | 7.36023400 | 0.42904400 | 0.04967800 |
| C | 5.83817900 | -0.92115500 | -1.25044100 |

| | | | |
|----|-------------|-------------|-------------|
| C | 8.30571500 | -0.58597700 | 0.00208300 |
| H | 7.56780700 | 1.36272200 | 0.56650500 |
| C | 6.78985200 | -1.93316000 | -1.30363600 |
| H | 4.89429900 | -1.06494200 | -1.77418900 |
| C | 8.02076300 | -1.77009600 | -0.67420200 |
| H | 9.26785000 | -0.45412600 | 0.49128100 |
| H | 6.56984600 | -2.85030900 | -1.84452000 |
| H | 8.76136400 | -2.56555300 | -0.71569900 |
| H | 1.87395100 | 5.21156800 | -0.81652900 |
| Cu | -1.36744000 | 0.29976200 | 0.91134100 |
| C | -3.45450500 | 3.96798100 | 2.42717500 |
| H | -4.11930000 | 3.71327100 | 3.25800900 |
| H | -4.03503700 | 4.42930700 | 1.62246600 |
| H | -2.69704100 | 4.67568200 | 2.77747600 |
| C | -2.81083900 | 2.77737100 | 1.93991600 |
| N | -2.29468800 | 1.82128100 | 1.54504600 |
| O | 2.11700500 | -0.92738900 | -1.03489300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2333.099670

Electronic Energy (0K) + ZPE = -2332.571172

Enthalpy (353K) = -2332.517871

Free Energy (353K) = -2332.667218

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2333.538492

E

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -0.49820200 | 1.01474200 | -0.12119100 |
| C | -1.80281000 | 0.82372200 | 0.50853100 |
| N | -1.70307200 | -0.27958700 | 1.23893000 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.39807300 | -0.93182300 | 1.15389800 |
| C | 0.32001400 | -0.01193100 | 0.24047600 |
| C | 1.79186000 | -0.14972000 | -0.01625000 |
| C | 2.26289900 | -1.22885200 | -0.88360900 |
| C | 1.31421900 | -1.94359000 | -1.63639400 |
| C | 3.64208400 | -1.56562800 | -1.00583700 |
| C | 1.68396500 | -2.97347400 | -2.47865700 |
| H | 0.26561900 | -1.65866700 | -1.56795300 |
| C | 4.00223000 | -2.62350000 | -1.85227100 |
| C | 3.03498200 | -3.30861500 | -2.57103800 |
| H | 0.93692300 | -3.50868800 | -3.05754900 |
| H | 5.04662600 | -2.89424900 | -1.93577400 |
| S | -3.00140500 | -0.99501000 | 2.16819100 |
| O | -3.94190600 | 0.08227700 | 2.41608900 |
| O | -2.31183800 | -1.68048900 | 3.24508400 |
| C | -3.68737100 | -2.15511600 | 1.04070000 |
| C | -4.69015900 | -1.73491700 | 0.16781800 |
| C | -3.19692100 | -3.46067600 | 1.02990300 |
| C | -5.20799000 | -2.65271800 | -0.73383100 |
| H | -5.06645000 | -0.71473700 | 0.20362500 |
| C | -3.73246000 | -4.35878800 | 0.11934700 |
| H | -2.42242500 | -3.76816300 | 1.72842400 |
| C | -4.74106400 | -3.97153600 | -0.77082900 |
| H | -5.99530000 | -2.34642900 | -1.41974400 |
| H | -3.36696400 | -5.38367900 | 0.09798900 |
| C | -5.32852000 | -4.96223400 | -1.72319200 |
| H | -4.56975600 | -5.65975100 | -2.09346600 |
| H | -6.10016600 | -5.56216100 | -1.22352800 |
| H | -5.80002300 | -4.46824400 | -2.57848800 |
| H | 0.06976400 | -0.99597500 | 2.14560900 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.18938700 | 2.14682200 | -1.00515700 |
| C | -0.71758100 | 3.41650400 | -0.73822800 |
| C | 0.64048700 | 1.97923900 | -2.11955500 |
| C | -0.41527600 | 4.49365800 | -1.56299500 |
| H | -1.35354700 | 3.56154000 | 0.13552800 |
| C | 0.94075900 | 3.05770400 | -2.94309000 |
| H | 1.03380900 | 0.99209800 | -2.35910200 |
| C | 0.41459000 | 4.31692900 | -2.66714200 |
| H | -0.82435900 | 5.47594300 | -1.33836600 |
| H | 1.58226100 | 2.91118100 | -3.80873500 |
| H | 0.65010300 | 5.15951900 | -3.31297500 |
| N | 4.57522200 | -0.82905400 | -0.28926300 |
| H | 4.16499700 | -0.07613000 | 0.26010100 |
| C | 5.93550700 | -1.03020800 | -0.18594700 |
| O | 6.52565000 | -1.97581800 | -0.68866200 |
| C | 6.65676900 | 0.00346800 | 0.61390200 |
| C | 7.92282900 | -0.33936300 | 1.09734500 |
| C | 6.14901600 | 1.28218200 | 0.86622500 |
| C | 8.66151100 | 0.57084700 | 1.84069800 |
| H | 8.31168300 | -1.33134500 | 0.88112400 |
| C | 6.89450900 | 2.19538100 | 1.60323500 |
| H | 5.18412400 | 1.59299600 | 0.46877700 |
| C | 8.14731100 | 1.84021500 | 2.09565000 |
| H | 9.64135900 | 0.29197400 | 2.22092300 |
| H | 6.49697100 | 3.19054100 | 1.78710600 |
| H | 8.72649800 | 2.55640000 | 2.67407600 |
| H | 3.34743300 | -4.12018400 | -3.22435700 |
| O | 2.51290300 | 0.65302800 | 0.57529400 |
| H | -0.49331800 | -1.95489200 | 0.76020600 |
| Cu | -3.33867500 | 1.90963200 | 0.29771600 |

| | | | |
|---|-------------|------------|-------------|
| C | -6.92813800 | 4.49729000 | -0.34415000 |
| H | -6.83334200 | 5.02947800 | -1.29523200 |
| H | -6.99795100 | 5.22350600 | 0.47142800 |
| H | -7.83407500 | 3.88427800 | -0.35997300 |
| C | -5.77770300 | 3.65690900 | -0.14273200 |
| N | -4.85189900 | 2.98366300 | 0.01880200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2333.151871

Electronic Energy (0K) + ZPE = -2332.623781

Enthalpy (353K) = -2332.569801

Free Energy (353K) = -2332.724593

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2333.588321

F

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.55346900 | 1.38278700 | -0.84263900 |
| C | 1.69152500 | 1.25575700 | -1.64900800 |
| N | 1.65985900 | -0.01708000 | -2.21950700 |
| C | 0.60892100 | -0.72835700 | -1.69477100 |
| C | -0.10704100 | 0.08862600 | -0.85870100 |
| C | -1.43340100 | -0.22664200 | -0.27067700 |
| C | -1.62520600 | -1.52260300 | 0.40565500 |
| C | -0.50161100 | -2.25719600 | 0.82461100 |
| C | -2.92279300 | -2.04426000 | 0.68185500 |
| C | -0.62298200 | -3.47820400 | 1.46183600 |
| H | 0.48963000 | -1.83950500 | 0.66427200 |
| C | -3.03224800 | -3.29443000 | 1.30591800 |
| C | -1.89768700 | -3.99470800 | 1.68523300 |
| H | 0.26186400 | -4.02193300 | 1.78153400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.01858200 | -3.70042400 | 1.48999600 |
| S | 3.08485000 | -0.76372800 | -2.85882800 |
| O | 3.73647200 | 0.27637500 | -3.63000100 |
| O | 2.61349700 | -1.99779400 | -3.45530800 |
| C | 3.99487000 | -1.08683100 | -1.38600200 |
| C | 4.95153900 | -0.16475300 | -0.96803100 |
| C | 3.67346400 | -2.21401800 | -0.63023900 |
| C | 5.60432500 | -0.38906900 | 0.23634300 |
| H | 5.18488400 | 0.70466300 | -1.57858600 |
| C | 4.33142300 | -2.40995700 | 0.57536700 |
| H | 2.92984600 | -2.92738600 | -0.98049200 |
| C | 5.30144000 | -1.50451200 | 1.02428400 |
| H | 6.35871300 | 0.31716300 | 0.57814700 |
| H | 4.09668300 | -3.28477800 | 1.17924000 |
| C | 6.00906800 | -1.73689500 | 2.32044500 |
| H | 5.33857700 | -2.17406100 | 3.06862300 |
| H | 6.83828100 | -2.44346300 | 2.18513700 |
| H | 6.43445000 | -0.81051500 | 2.72095900 |
| H | 0.44240400 | -1.76260300 | -1.97577100 |
| C | 0.08813100 | 2.64531400 | -0.23482900 |
| C | 0.25592800 | 3.85129500 | -0.92412400 |
| C | -0.48412200 | 2.66162800 | 1.04428000 |
| C | -0.14112800 | 5.05112000 | -0.34370700 |
| H | 0.67896800 | 3.84486900 | -1.92692500 |
| C | -0.87814100 | 3.86223800 | 1.61967100 |
| H | -0.60944200 | 1.72969200 | 1.59423600 |
| C | -0.70729600 | 5.05977500 | 0.92749500 |
| H | -0.01352000 | 5.98173200 | -0.89144900 |
| H | -1.31918400 | 3.86385000 | 2.61357800 |
| H | -1.01936900 | 5.99854300 | 1.37884300 |

| | | | |
|----|-------------|-------------|-------------|
| N | -4.03834300 | -1.28988800 | 0.33763900 |
| H | -3.80484200 | -0.36671600 | -0.02420700 |
| C | -5.36718100 | -1.64905800 | 0.37796700 |
| O | -5.76627800 | -2.77203000 | 0.65427600 |
| C | -6.31548200 | -0.54647200 | 0.03858200 |
| C | -7.60247400 | -0.91469100 | -0.36319000 |
| C | -5.98940300 | 0.81015300 | 0.13801200 |
| C | -8.54226800 | 0.05474100 | -0.68593200 |
| H | -7.84749000 | -1.97238200 | -0.42081000 |
| C | -6.93522300 | 1.77955800 | -0.17625800 |
| H | -5.00801300 | 1.12728700 | 0.48731200 |
| C | -8.20906600 | 1.40435300 | -0.59390100 |
| H | -9.53790500 | -0.24111100 | -1.00807200 |
| H | -6.67688600 | 2.83213000 | -0.08864500 |
| H | -8.94529900 | 2.16537500 | -0.84233900 |
| H | -2.01609200 | -4.95750800 | 2.17729300 |
| O | -2.32618500 | 0.61440200 | -0.39660600 |
| Cu | 2.29490200 | 1.07825400 | 0.37892800 |
| C | 4.18888500 | 1.03400600 | 4.43484600 |
| H | 3.61727700 | 1.70083800 | 5.08751400 |
| H | 5.22077500 | 1.39229800 | 4.37120900 |
| H | 4.17936100 | 0.02399700 | 4.85518300 |
| C | 3.59758600 | 1.02206200 | 3.12269800 |
| N | 3.12307400 | 1.01731800 | 2.06818000 |
| H | 2.34806400 | 2.02562100 | -2.04503800 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2333.177082

Electronic Energy (0K) + ZPE = -2332.648113

Enthalpy (353K) = -2332.594910

Free Energy (353K) = -2332.743893

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2333.615002

3a

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 0.93496000 | 1.78078300 | -0.32722800 |
| C | 2.10551800 | 1.68049100 | -1.03399100 |
| N | 2.19762200 | 0.39749200 | -1.54870300 |
| C | 1.13264400 | -0.34889500 | -1.11748100 |
| C | 0.31408300 | 0.47144600 | -0.37261600 |
| C | -0.98319100 | 0.04449600 | 0.17883800 |
| C | -1.12370700 | -1.34969500 | 0.67190600 |
| C | 0.00447300 | -2.04242400 | 1.13843200 |
| C | -2.38851100 | -2.00013600 | 0.72604700 |
| C | -0.07651900 | -3.34419700 | 1.60403000 |
| H | 0.96161200 | -1.52881100 | 1.15672500 |
| C | -2.45574400 | -3.32649000 | 1.17108200 |
| C | -1.31256900 | -3.98420100 | 1.60096000 |
| H | 0.81301900 | -3.85162800 | 1.96787200 |
| H | -3.41648600 | -3.82582600 | 1.17987800 |
| S | 3.61687200 | -0.26755400 | -2.25250900 |
| O | 4.23988200 | 0.83250500 | -2.96500000 |
| O | 3.16926300 | -1.47063300 | -2.93009500 |
| C | 4.58384800 | -0.69097100 | -0.84131900 |
| C | 5.52079600 | 0.22283500 | -0.36566600 |
| C | 4.35006000 | -1.90705600 | -0.20102100 |
| C | 6.24443300 | -0.10175300 | 0.77307900 |
| H | 5.68423900 | 1.16516800 | -0.88287100 |
| C | 5.08316300 | -2.20743900 | 0.93717300 |
| H | 3.61280700 | -2.60689000 | -0.58899300 |

| | | | |
|---|-------------|-------------|-------------|
| C | 6.03879700 | -1.31516800 | 1.43779300 |
| H | 6.98398200 | 0.59833800 | 1.15725800 |
| H | 4.91581100 | -3.15285200 | 1.45007500 |
| C | 6.84371000 | -1.66610000 | 2.64822600 |
| H | 6.28013400 | -2.30941400 | 3.33197000 |
| H | 7.75108400 | -2.21365700 | 2.36167200 |
| H | 7.16259400 | -0.77101600 | 3.19215300 |
| H | 1.01947100 | -1.38413700 | -1.41439800 |
| C | 0.54321400 | 3.01528600 | 0.37806700 |
| C | -0.73953300 | 3.56871100 | 0.28456800 |
| C | 1.51469100 | 3.70011400 | 1.12192400 |
| C | -1.03923700 | 4.76695200 | 0.92357900 |
| H | -1.49821300 | 3.04763800 | -0.29053100 |
| C | 1.21356600 | 4.89915200 | 1.75746800 |
| H | 2.51241900 | 3.27309000 | 1.21217900 |
| C | -0.06705400 | 5.43660400 | 1.66180600 |
| H | -2.04076800 | 5.18348600 | 0.83802500 |
| H | 1.98065300 | 5.41116500 | 2.33459000 |
| H | -0.30681400 | 6.37265100 | 2.16160500 |
| N | -3.52819100 | -1.29204500 | 0.34900200 |
| H | -3.35027700 | -0.30021000 | 0.20146700 |
| C | -4.79278800 | -1.76817700 | 0.10409500 |
| O | -5.09502300 | -2.95471000 | 0.10703600 |
| C | -5.80495100 | -0.70852900 | -0.18964500 |
| C | -6.96686200 | -1.10265800 | -0.85855900 |
| C | -5.65708400 | 0.62655600 | 0.19998100 |
| C | -7.95558000 | -0.17464700 | -1.15659700 |
| H | -7.07521900 | -2.14702800 | -1.14111300 |
| C | -6.65263700 | 1.55254200 | -0.09055500 |
| H | -4.78113400 | 0.95288700 | 0.75862700 |

| | | | |
|---|-------------|-------------|-------------|
| C | -7.79908900 | 1.15565800 | -0.77344400 |
| H | -8.85165200 | -0.48827700 | -1.68711200 |
| H | -6.53419500 | 2.58682000 | 0.22349900 |
| H | -8.57471000 | 1.88309800 | -1.00210800 |
| H | -1.39723600 | -5.00934400 | 1.95499600 |
| O | -1.93270000 | 0.83483800 | 0.19632000 |
| H | 2.86411600 | 2.42293000 | -1.24907900 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2003.204222

Electronic Energy (0K) + ZPE = -2002.724196

Enthalpy (353K) = -2002.678743

Free Energy (353K) = -2002.813340

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2003.614949

1b

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -5.13298400 | 1.75734600 | 0.32055300 |
| C | -3.90434200 | 1.21065200 | 0.66711200 |
| C | -3.43148200 | 0.06396500 | 0.00953300 |
| C | -4.21290400 | -0.51433000 | -1.00398000 |
| C | -5.43325800 | 0.04826500 | -1.35234400 |
| C | -5.89913400 | 1.18210100 | -0.69065400 |
| H | -5.49242200 | 2.64308600 | 0.84019100 |
| H | -3.84860900 | -1.40469000 | -1.51222800 |
| H | -6.02806300 | -0.40560900 | -2.14218500 |
| H | -6.85853400 | 1.61700500 | -0.96234400 |
| C | -2.17509500 | -0.51033600 | 0.35930300 |
| C | -1.11205100 | -1.02738700 | 0.63915400 |
| N | 0.05054500 | -1.60019400 | 0.99588800 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.64626400 | -1.22173200 | 2.29822900 |
| C | 0.99632000 | 0.19092900 | 2.38618200 |
| C | 1.26788700 | 1.36950400 | 2.43893500 |
| C | 1.61017400 | 2.77846800 | 2.49190300 |
| S | 1.10865000 | -2.11978200 | -0.25785100 |
| O | 0.23751700 | -2.53860500 | -1.34191300 |
| O | 2.02646200 | -3.04844300 | 0.38424800 |
| C | 1.99968100 | -0.67018800 | -0.73498800 |
| C | 1.36434200 | 0.28483200 | -1.53039400 |
| C | 3.28913800 | -0.47304800 | -0.25075500 |
| C | 2.04131600 | 1.45575900 | -1.83193300 |
| H | 0.36103700 | 0.10982500 | -1.91170300 |
| C | 3.95305400 | 0.70379300 | -0.57438200 |
| H | 3.76539700 | -1.23182500 | 0.36523700 |
| C | 3.33974600 | 1.68476000 | -1.35773900 |
| H | 1.56011900 | 2.21081300 | -2.45200400 |
| H | 4.96580800 | 0.86620300 | -0.20950800 |
| C | 4.03999700 | 2.96631300 | -1.68114900 |
| H | 5.08841000 | 2.94825000 | -1.36634700 |
| H | 4.00960000 | 3.17742200 | -2.75703100 |
| H | 3.55435400 | 3.81380400 | -1.17925400 |
| H | -0.08649100 | -1.49484100 | 3.06741000 |
| H | 1.51844100 | -1.86781500 | 2.45363600 |
| H | -3.29871900 | 1.66223300 | 1.45022400 |
| H | 1.53568000 | 3.16806100 | 3.51420700 |
| H | 2.63443200 | 2.95376300 | 2.14009100 |
| H | 0.93550800 | 3.37059100 | 1.86181300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1336.824658

Electronic Energy (0K) + ZPE = -1336.513229

Enthalpy (333K) = -1336.485162

Free Energy (333K) = -1336.576895

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1337.083643

AuPPh₃NTf₂

Number of imaginary frequencies: 0

| | | | |
|----|-------------|-------------|-------------|
| C | 2.76741200 | 2.20360800 | 0.80126800 |
| F | 1.50297200 | 2.56160400 | 0.96243800 |
| F | 3.10410500 | 1.35255300 | 1.75564900 |
| F | 3.53410100 | 3.27690300 | 0.87593500 |
| S | 3.03765300 | 1.44421900 | -0.87306700 |
| O | 4.47735500 | 1.33221500 | -1.01013000 |
| O | 2.26310100 | 2.27238700 | -1.78201000 |
| N | 2.28264300 | -0.00961500 | -0.68074900 |
| O | 4.19262600 | -1.44450800 | -1.69551900 |
| O | 1.96871100 | -2.45246600 | -1.04889600 |
| S | 3.02165200 | -1.47096600 | -0.84208300 |
| C | 3.63653500 | -1.82075900 | 0.86496300 |
| F | 4.59885500 | -0.97819600 | 1.19028200 |
| F | 2.63874000 | -1.70977400 | 1.73045600 |
| F | 4.10291900 | -3.05717400 | 0.89080400 |
| Au | 0.15181900 | -0.03871400 | -0.30917000 |
| P | -2.12617700 | -0.06436900 | 0.03018200 |
| C | -3.02374700 | -0.28845100 | -1.53660700 |
| C | -2.48031300 | 0.26454300 | -2.70112200 |
| C | -4.25094300 | -0.95522300 | -1.58877400 |
| C | -3.16441800 | 0.15695600 | -3.90640700 |
| H | -1.51928500 | 0.77850600 | -2.65989300 |
| C | -4.92717200 | -1.06537700 | -2.79948100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.68055400 | -1.38910700 | -0.68702300 |
| C | -4.38577900 | -0.50987100 | -3.95546500 |
| H | -2.73823500 | 0.58729300 | -4.80967100 |
| H | -5.87976400 | -1.58867100 | -2.83883200 |
| H | -4.91627800 | -0.60098100 | -4.90073300 |
| C | -2.65537800 | -1.40563300 | 1.14108100 |
| C | -3.74023000 | -1.25373900 | 2.00941700 |
| C | -1.97528300 | -2.62672900 | 1.08240800 |
| C | -4.13857300 | -2.31832800 | 2.81180800 |
| H | -4.27632500 | -0.30696600 | 2.05929400 |
| C | -2.38132900 | -3.68780600 | 1.88308100 |
| H | -1.12608900 | -2.74461500 | 0.40865700 |
| C | -3.46077600 | -3.53245900 | 2.74902500 |
| H | -4.98106600 | -2.19698700 | 3.48881700 |
| H | -1.84858500 | -4.63469000 | 1.83583700 |
| H | -3.77306900 | -4.36119300 | 3.38060200 |
| C | -2.73360800 | 1.48691700 | 0.76706000 |
| C | -3.81373000 | 2.18927000 | 0.22948300 |
| C | -2.09086500 | 1.96737700 | 1.91457600 |
| C | -4.24525900 | 3.36600700 | 0.83638000 |
| H | -4.32056200 | 1.82352500 | -0.66178000 |
| C | -2.53110000 | 3.13761400 | 2.51917400 |
| H | -1.24823900 | 1.41829500 | 2.33702700 |
| C | -3.60697200 | 3.83904700 | 1.97771900 |
| H | -5.08463900 | 3.91267400 | 0.41277000 |
| H | -2.03013400 | 3.50660200 | 3.41119300 |
| H | -3.94603700 | 4.75944700 | 2.44788500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2998.343001

Electronic Energy (0K) + ZPE = -2998.011873

Enthalpy (333K) = -2997.969974

Free Energy (333K) = -2998.097357

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2998.864499

NTf₂⁻

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -2.11755700 | 0.72145200 | 0.21327700 |
| F | -2.41995400 | 0.74108000 | 1.50293800 |
| F | -1.33108400 | 1.75293500 | -0.06202400 |
| F | -3.23774300 | 0.83928900 | -0.49098000 |
| S | -1.29099700 | -0.85633700 | -0.24685200 |
| O | -1.00510900 | -0.71552500 | -1.67119200 |
| O | -2.23198900 | -1.88426700 | 0.18500800 |
| N | -0.03676900 | -0.78136700 | 0.75587100 |
| O | 1.79269700 | -1.64900300 | -0.86333900 |
| O | 2.30055100 | -1.03320100 | 1.52119000 |
| S | 1.50078700 | -0.84464400 | 0.31740600 |
| C | 1.89943000 | 0.88205700 | -0.19092800 |
| F | 1.20420100 | 1.23730700 | -1.26108000 |
| F | 1.63001500 | 1.72576300 | 0.79658900 |
| F | 3.19459900 | 0.96142300 | -0.47737400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1826.867423

Electronic Energy (0K) + ZPE = -1826.811210

Enthalpy (333K) = -1826.793766

Free Energy (333K) = -1826.858618

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1827.223710

A'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -2.47931800 | 4.86886400 | -1.07784500 |
| C | -2.04255900 | 3.59797400 | -0.72580600 |
| C | -2.95665200 | 2.63345500 | -0.27987500 |
| C | -4.31776000 | 2.96751500 | -0.19422400 |
| C | -4.74729000 | 4.23857100 | -0.54491400 |
| C | -3.83011500 | 5.19088000 | -0.98695100 |
| H | -1.76232700 | 5.60895900 | -1.42519300 |
| H | -5.03134100 | 2.22153800 | 0.15044000 |
| H | -5.80326600 | 4.48888600 | -0.47473200 |
| H | -4.17111900 | 6.18645200 | -1.26205700 |
| C | -2.51200700 | 1.29890400 | 0.08552800 |
| C | -2.99393800 | 0.19135100 | 0.46682000 |
| N | -3.34768400 | -0.99559300 | 0.83628800 |
| C | -3.32209200 | -1.42298600 | 2.26904300 |
| C | -2.05992000 | -1.09567600 | 2.90513200 |
| C | -1.03096000 | -0.77118000 | 3.45593000 |
| C | 0.18970000 | -0.38219100 | 4.13608400 |
| S | -3.63701200 | -2.21069100 | -0.43150800 |
| O | -4.50105100 | -3.18499300 | 0.20895300 |
| O | -4.05741900 | -1.42985300 | -1.57770200 |
| C | -2.04274600 | -2.90090300 | -0.71545600 |
| C | -1.65387700 | -4.02597200 | 0.01090200 |
| C | -1.21228100 | -2.32114600 | -1.67728000 |
| C | -0.41019800 | -4.58432900 | -0.24686300 |
| H | -2.32349300 | -4.47552700 | 0.74012800 |
| C | 0.02697900 | -2.89939100 | -1.91486400 |
| H | -1.54191400 | -1.45894300 | -2.25380600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.44406600 | -4.03605300 | -1.21089600 |
| H | -0.10020500 | -5.47377800 | 0.29881800 |
| H | 0.68137000 | -2.46838500 | -2.67223900 |
| C | 1.78884400 | -4.63460200 | -1.46826700 |
| H | 1.81954500 | -5.69439800 | -1.19431800 |
| H | 2.56062700 | -4.12358200 | -0.87518800 |
| H | 2.07778400 | -4.53955400 | -2.52091000 |
| H | -3.52935600 | -2.49894700 | 2.28570900 |
| H | -4.16318400 | -0.92908300 | 2.76961000 |
| Au | -0.40734600 | 0.74311300 | 0.11020300 |
| P | 1.91939100 | 0.48949300 | -0.02628100 |
| H | 0.96754800 | -1.15009600 | 4.04330600 |
| H | 0.58576900 | 0.55503500 | 3.72482300 |
| H | 0.00286500 | -0.21903800 | 5.20430600 |
| H | -0.98630400 | 3.33799500 | -0.79814300 |
| C | 2.43372200 | -0.11512900 | -1.66556500 |
| C | 3.52812800 | -0.96827800 | -1.83162300 |
| C | 1.71623200 | 0.32348200 | -2.78428700 |
| C | 3.89715600 | -1.38091600 | -3.10916600 |
| H | 4.09473200 | -1.31074800 | -0.96635600 |
| C | 2.09305100 | -0.08657400 | -4.05804700 |
| H | 0.85770500 | 0.98441700 | -2.65226100 |
| C | 3.18073200 | -0.94287200 | -4.21938100 |
| H | 4.74681200 | -2.04811400 | -3.23515200 |
| H | 1.53287400 | 0.25571200 | -4.92512400 |
| H | 3.47025900 | -1.26983800 | -5.21558200 |
| C | 2.61950300 | -0.66472000 | 1.19658700 |
| C | 3.73550800 | -0.34394200 | 1.97228900 |
| C | 2.00634800 | -1.91528900 | 1.34213200 |
| C | 4.23406400 | -1.27038300 | 2.88499200 |

| | | | |
|---|------------|-------------|-------------|
| H | 4.21948900 | 0.62553800 | 1.86808800 |
| C | 2.51628400 | -2.84030000 | 2.24549400 |
| H | 1.12960000 | -2.16620100 | 0.74072200 |
| C | 3.62936200 | -2.51593100 | 3.02008400 |
| H | 5.10165300 | -1.01589100 | 3.48938300 |
| H | 2.04077800 | -3.81330500 | 2.35263400 |
| H | 4.02365600 | -3.23702200 | 3.73253000 |
| C | 2.75746400 | 2.08787500 | 0.21694000 |
| C | 3.97777800 | 2.37097200 | -0.40418100 |
| C | 2.17929200 | 3.02940000 | 1.07584700 |
| C | 4.61204900 | 3.58542600 | -0.16469900 |
| H | 4.43473300 | 1.64372900 | -1.07391900 |
| C | 2.82090100 | 4.23981200 | 1.31502800 |
| H | 1.22261200 | 2.81357000 | 1.55372000 |
| C | 4.03535200 | 4.51768400 | 0.69356100 |
| H | 5.55951800 | 3.80380700 | -0.65195500 |
| H | 2.36769500 | 4.96962800 | 1.98189800 |
| H | 4.53326900 | 5.46740400 | 0.87587400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2508.293342

Electronic Energy (0K) + ZPE = -2507.706661

Enthalpy (333K) = -2507.654878

Free Energy (333K) = -2507.800188

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2508.722291

2a (Au catalysis system)

Number of imaginary frequencies: 0

| | | | |
|---|------------|-------------|------------|
| C | 1.17618600 | -0.33546200 | 0.00004100 |
| C | 0.00016900 | -1.07464900 | 0.00010300 |

| | | | |
|----|-------------|-------------|-------------|
| C | -1.17568300 | -0.33640500 | 0.00002900 |
| C | -1.18012300 | 1.04429500 | 0.00001200 |
| C | 1.18012000 | 1.04473500 | 0.00004800 |
| H | 0.00095500 | -2.15989400 | 0.00008800 |
| H | 2.07263500 | 1.65948500 | -0.00002400 |
| N | -0.00056400 | 1.73543900 | 0.00021000 |
| O | -0.00055100 | 2.99983100 | -0.00014700 |
| H | -2.07279900 | 1.65883500 | -0.00014900 |
| Cl | -2.70968300 | -1.15784400 | -0.00004100 |
| Cl | 2.70989200 | -1.15746400 | -0.00005400 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1242.374667

Electronic Energy (0K) + ZPE = -1242.301227

Enthalpy (333K) = -1242.291097

Free Energy (333K) = -1242.338619

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1242.516989

TS_A'

Number of imaginary frequencies: 1

| | | | |
|---|------------|------------|-------------|
| C | 1.01628300 | 4.80024800 | 0.96170400 |
| C | 0.84423300 | 3.43484200 | 0.76728000 |
| C | 1.36879800 | 2.80083000 | -0.36946400 |
| C | 2.03346500 | 3.57951200 | -1.32854300 |
| C | 2.17699400 | 4.94956100 | -1.14249800 |
| C | 1.67932600 | 5.56309500 | 0.00434800 |
| H | 0.61811900 | 5.27108500 | 1.85791900 |
| H | 2.43111400 | 3.10476500 | -2.22082900 |
| H | 2.68642100 | 5.54180300 | -1.89981700 |
| H | 1.80133800 | 6.63446900 | 0.14783300 |

| | | | |
|----|-------------|-------------|-------------|
| C | 1.16530900 | 1.35914100 | -0.54510400 |
| C | 1.96451800 | 0.41502900 | -0.94321000 |
| N | 2.13978800 | -0.86258600 | -1.23486500 |
| C | 1.95414800 | -1.35306000 | -2.62489300 |
| C | 0.61152800 | -1.10093000 | -3.12101600 |
| C | -0.48513800 | -0.83533100 | -3.56193100 |
| C | -1.79089800 | -0.51316900 | -4.10651200 |
| S | 2.56807900 | -1.98982500 | 0.01964800 |
| O | 3.41114000 | -2.97887000 | -0.63451900 |
| O | 3.06753000 | -1.16299500 | 1.10586300 |
| C | 1.05257300 | -2.75201100 | 0.50551300 |
| C | 0.64240200 | -3.92012400 | -0.13578700 |
| C | 0.32048700 | -2.19736900 | 1.55636100 |
| C | -0.52021600 | -4.54324500 | 0.29539900 |
| H | 1.23775900 | -4.35249300 | -0.93633800 |
| C | -0.83705200 | -2.84203900 | 1.97182600 |
| H | 0.66909700 | -1.30055800 | 2.06436900 |
| C | -1.27254600 | -4.01987100 | 1.35352100 |
| H | -0.84420200 | -5.46433400 | -0.18641100 |
| H | -1.40959300 | -2.43055000 | 2.80252200 |
| C | -2.53379200 | -4.69043400 | 1.79313700 |
| H | -2.50788800 | -5.76778200 | 1.59734800 |
| H | -3.39783400 | -4.28477300 | 1.24749300 |
| H | -2.72393300 | -4.53586300 | 2.86092100 |
| H | 2.20417100 | -2.42014200 | -2.63557000 |
| H | 2.70229900 | -0.84770900 | -3.25038600 |
| Au | -0.81286000 | 0.65243200 | -0.18997000 |
| P | -3.10776100 | 0.29038900 | 0.18846300 |
| H | -2.50975500 | -1.32564500 | -3.94357600 |
| H | -2.19517100 | 0.39541500 | -3.64182800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.72903900 | -0.33020200 | -5.18607800 |
| H | 0.30858300 | 2.83996600 | 1.50688600 |
| C | -3.50089700 | -0.27686800 | 1.87693100 |
| C | -4.52869300 | -1.18603200 | 2.14053800 |
| C | -2.75313200 | 0.25169300 | 2.93568000 |
| C | -4.80148100 | -1.56413300 | 3.45279900 |
| H | -5.11989300 | -1.59928100 | 1.32408000 |
| C | -3.03348800 | -0.12423600 | 4.24423700 |
| H | -1.94721400 | 0.95827800 | 2.73107800 |
| C | -4.05491800 | -1.03658100 | 4.50220900 |
| H | -5.60063000 | -2.27428800 | 3.65331400 |
| H | -2.44974500 | 0.28954600 | 5.06334800 |
| H | -4.26907000 | -1.33641000 | 5.52560000 |
| C | -3.87346700 | -0.91530800 | -0.94493800 |
| C | -5.06589600 | -0.65994700 | -1.62548700 |
| C | -3.21979900 | -2.14032500 | -1.12557100 |
| C | -5.59959900 | -1.62526900 | -2.47600300 |
| H | -5.58114900 | 0.29028300 | -1.49614900 |
| C | -3.76344000 | -3.10538000 | -1.96524400 |
| H | -2.28209100 | -2.33824800 | -0.60208200 |
| C | -4.95345300 | -2.84602400 | -2.64377800 |
| H | -6.52644200 | -1.42050700 | -3.00707500 |
| H | -3.25424600 | -4.05816200 | -2.09737500 |
| H | -5.37511000 | -3.59730400 | -3.30781600 |
| C | -4.00915800 | 1.86127000 | -0.02755700 |
| C | -5.23574400 | 2.09535100 | 0.60256000 |
| C | -3.46388100 | 2.83982800 | -0.86633700 |
| C | -5.90931300 | 3.29323400 | 0.38948600 |
| H | -5.66754300 | 1.34167300 | 1.26005100 |
| C | -4.14360800 | 4.03464700 | -1.07899400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.49842800 | 2.66637100 | -1.34514700 |
| C | -5.36479100 | 4.26113900 | -0.45082800 |
| H | -6.86170100 | 3.47157800 | 0.88358700 |
| H | -3.71328100 | 4.79265300 | -1.72948100 |
| H | -5.89266900 | 5.19844900 | -0.61212600 |
| C | 6.36499900 | -0.78856600 | -0.19873000 |
| C | 6.60604200 | -0.18666300 | 1.02778600 |
| C | 5.81992500 | 0.91051300 | 1.36106000 |
| C | 4.83433200 | 1.37341300 | 0.51164000 |
| C | 5.37847900 | -0.31754300 | -1.04855700 |
| H | 7.37855600 | -0.55414200 | 1.69680700 |
| H | 5.15522300 | -0.73364600 | -2.02486100 |
| N | 4.63384500 | 0.74580100 | -0.67127900 |
| O | 3.69541400 | 1.17987900 | -1.47086200 |
| H | 4.18601400 | 2.21942700 | 0.71531200 |
| Cl | 6.06695300 | 1.72944000 | 2.86715700 |
| Cl | 7.29753300 | -2.15816900 | -0.69940600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3750.668668

Electronic Energy (0K) + ZPE = -3750.007223

Enthalpy (333K) = -3749.945576

Free Energy (333K) = -3750.112501

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3751.234608

B'

Number of imaginary frequencies: 0

| | | | |
|---|------------|------------|-------------|
| C | 1.22343700 | 4.72058800 | 1.08632500 |
| C | 1.04548700 | 3.35850200 | 0.87316600 |
| C | 1.41126700 | 2.76545900 | -0.34590500 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.92323800 | 3.59023000 | -1.35834700 |
| C | 2.07193900 | 4.95808000 | -1.15238800 |
| C | 1.73295100 | 5.52751600 | 0.07170400 |
| H | 0.94852900 | 5.15605700 | 2.04492400 |
| H | 2.19328600 | 3.15406700 | -2.31816100 |
| H | 2.46076600 | 5.58196900 | -1.95485100 |
| H | 1.85681900 | 6.59630500 | 0.23209400 |
| C | 1.20801400 | 1.31423400 | -0.53286400 |
| C | 2.18621400 | 0.50563700 | -0.95400300 |
| N | 2.16265700 | -0.86989600 | -1.17980700 |
| C | 1.96505300 | -1.37654000 | -2.55144200 |
| C | 0.63056400 | -1.11129600 | -3.07388800 |
| C | -0.45513300 | -0.85215100 | -3.54506500 |
| C | -1.75237000 | -0.53436900 | -4.11338900 |
| S | 2.48955400 | -1.96570900 | 0.06549900 |
| O | 3.33745300 | -3.00140200 | -0.51759400 |
| O | 2.97549700 | -1.15587100 | 1.17766300 |
| C | 0.96522300 | -2.72785300 | 0.54632000 |
| C | 0.56087800 | -3.90336200 | -0.08325500 |
| C | 0.22738200 | -2.17417400 | 1.59218300 |
| C | -0.60120900 | -4.52952600 | 0.34786900 |
| H | 1.16245000 | -4.34044900 | -0.87663600 |
| C | -0.92918000 | -2.81975600 | 2.01045200 |
| H | 0.56991700 | -1.27110700 | 2.09314700 |
| C | -1.35994500 | -4.00232200 | 1.39866500 |
| H | -0.91967700 | -5.45530800 | -0.12910700 |
| H | -1.50572500 | -2.40384800 | 2.83645400 |
| C | -2.62351000 | -4.67196500 | 1.83504000 |
| H | -2.59161300 | -5.75211100 | 1.65510700 |
| H | -3.48378600 | -4.27807800 | 1.27496100 |

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|----|-------------|-------------|-------------|
| H | -2.82544600 | -4.50400100 | 2.89873700 |
| H | 2.18937300 | -2.45004800 | -2.55356300 |
| H | 2.72134000 | -0.91130500 | -3.20120600 |
| Au | -0.74794100 | 0.64687100 | -0.20044700 |
| P | -3.06557000 | 0.30370400 | 0.15754300 |
| H | -2.47157900 | -1.34883300 | -3.96137400 |
| H | -2.16859000 | 0.37269600 | -3.65610500 |
| H | -1.67520500 | -0.35249300 | -5.19225500 |
| H | 0.62142800 | 2.73284900 | 1.65920500 |
| C | -3.48843400 | -0.22414000 | 1.85371700 |
| C | -4.51897400 | -1.12662600 | 2.12809700 |
| C | -2.75632800 | 0.33349500 | 2.90875800 |
| C | -4.81051200 | -1.46905100 | 3.44634700 |
| H | -5.09886200 | -1.56181000 | 1.31486300 |
| C | -3.05480000 | -0.00683400 | 4.22308100 |
| H | -1.94820000 | 1.03560900 | 2.69574700 |
| C | -4.07954400 | -0.91243500 | 4.49168900 |
| H | -5.61243100 | -2.17391500 | 3.65482900 |
| H | -2.48319700 | 0.43019500 | 5.03877000 |
| H | -4.30856100 | -1.18394400 | 5.51981800 |
| C | -3.85147200 | -0.90921800 | -0.95700800 |
| C | -5.04350500 | -0.65323800 | -1.63839500 |
| C | -3.20962400 | -2.14227500 | -1.12448700 |
| C | -5.58821000 | -1.62442600 | -2.47510700 |
| H | -5.55009500 | 0.30318700 | -1.52074100 |
| C | -3.76391800 | -3.11347900 | -1.95035300 |
| H | -2.27266300 | -2.34112500 | -0.60050900 |
| C | -4.95341600 | -2.85299900 | -2.62904500 |
| H | -6.51468100 | -1.41816700 | -3.00640900 |
| H | -3.26316800 | -4.07219600 | -2.07167700 |

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|----|-------------|-------------|-------------|
| H | -5.38354400 | -3.60915900 | -3.28211700 |
| C | -3.96046100 | 1.87703300 | -0.08684700 |
| C | -5.18959500 | 2.12788000 | 0.53194100 |
| C | -3.40628300 | 2.84052100 | -0.93695500 |
| C | -5.85681400 | 3.32514200 | 0.29630000 |
| H | -5.62879300 | 1.38692000 | 1.19898100 |
| C | -4.07939100 | 4.03508700 | -1.17272200 |
| H | -2.43783600 | 2.65617300 | -1.40515600 |
| C | -5.30333700 | 4.27726000 | -0.55615400 |
| H | -6.81125400 | 3.51544400 | 0.78208700 |
| H | -3.64137500 | 4.78093400 | -1.83220100 |
| H | -5.82616500 | 5.21416400 | -0.73568900 |
| C | 6.33038800 | -0.77180800 | -0.30505900 |
| C | 6.58282000 | -0.19946600 | 0.93569100 |
| C | 5.75160500 | 0.82638100 | 1.37450300 |
| C | 4.69284300 | 1.25575600 | 0.59544300 |
| C | 5.27122000 | -0.32952300 | -1.08107100 |
| H | 7.41063200 | -0.54457000 | 1.54913300 |
| H | 5.01543400 | -0.71693200 | -2.06220000 |
| N | 4.50359300 | 0.65505800 | -0.59029200 |
| O | 3.46164700 | 1.08918800 | -1.36627800 |
| H | 3.99347500 | 2.04063300 | 0.86817100 |
| Cl | 6.02299200 | 1.57883800 | 2.90228400 |
| Cl | 7.31754700 | -2.05096200 | -0.90427300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3750.682798

Electronic Energy (0K) + ZPE = -3750.019567

Enthalpy (333K) = -3749.957957

Free Energy (333K) = -3750.125773

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3751.246795

A1'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -6.55668900 | -4.43320000 | 0.48196700 |
| C | -5.47161700 | -3.68723700 | 0.04144400 |
| C | -5.49564900 | -2.28698100 | 0.13316200 |
| C | -6.62232500 | -1.65435300 | 0.68207800 |
| C | -7.69524500 | -2.41059500 | 1.13408300 |
| C | -7.66838500 | -3.79950000 | 1.03193200 |
| H | -6.53180400 | -5.51771600 | 0.40076500 |
| H | -6.64190300 | -0.56836600 | 0.74990000 |
| H | -8.56187400 | -1.91182400 | 1.56251600 |
| H | -8.51417900 | -4.38800500 | 1.38046600 |
| C | -4.39297700 | -1.50962800 | -0.32689200 |
| C | -3.47067500 | -0.82918000 | -0.72856400 |
| N | -2.47140600 | -0.04840600 | -1.17889900 |
| C | -1.55196500 | -0.56964800 | -2.19686600 |
| C | -0.69176500 | -1.65401700 | -1.69292000 |
| C | -0.20186000 | -2.72103400 | -1.31895300 |
| C | 0.25275100 | -4.05308100 | -0.95316100 |
| S | -1.93439000 | 1.20470800 | -0.11749200 |
| O | -1.70475200 | 0.64616500 | 1.20860600 |
| O | -0.84362000 | 1.84475400 | -0.84326300 |
| C | -3.35226800 | 2.25284600 | -0.06211600 |
| C | -4.15823300 | 2.24830700 | 1.07097300 |
| C | -3.64276000 | 3.05031700 | -1.16967500 |
| C | -5.27855300 | 3.07068800 | 1.09312000 |
| H | -3.91109600 | 1.61408800 | 1.91861300 |
| C | -4.76305600 | 3.86218500 | -1.12439500 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.00019700 | 3.03544200 | -2.04755800 |
| C | -5.59613500 | 3.88474100 | 0.00348100 |
| H | -5.91849200 | 3.08035100 | 1.97365500 |
| H | -5.00500500 | 4.49484100 | -1.97704700 |
| C | -6.79879300 | 4.77297200 | 0.02328800 |
| H | -7.37227700 | 4.66293400 | 0.94907000 |
| H | -7.46609000 | 4.55150300 | -0.81908300 |
| H | -6.50983200 | 5.82736700 | -0.07257000 |
| H | -0.96427800 | 0.26515700 | -2.58957100 |
| H | -2.16443000 | -0.95902500 | -3.01899900 |
| Au | 1.27361300 | -1.03483100 | -0.66615800 |
| P | 3.10492700 | 0.10459300 | 0.22341400 |
| H | -4.59776900 | -4.17890600 | -0.38116900 |
| H | 0.35292500 | -4.14750700 | 0.13373300 |
| H | -0.47424900 | -4.79636600 | -1.30040400 |
| H | 1.22247300 | -4.27741400 | -1.41164900 |
| C | 2.87545700 | 0.47018900 | 1.98975000 |
| C | 1.61102100 | 0.90112600 | 2.40634000 |
| C | 3.91603900 | 0.35694300 | 2.91483500 |
| C | 1.39158200 | 1.21877200 | 3.74073400 |
| H | 0.79715300 | 0.98659600 | 1.68519700 |
| C | 3.68686700 | 0.67193300 | 4.25123300 |
| H | 4.90304300 | 0.02408400 | 2.59713800 |
| C | 2.42861700 | 1.10071300 | 4.66344900 |
| H | 0.40583500 | 1.55003400 | 4.05997600 |
| H | 4.49598000 | 0.58004000 | 4.97221700 |
| H | 2.25402800 | 1.34116900 | 5.70983900 |
| C | 4.62534300 | -0.88147100 | 0.06982700 |
| C | 5.86995000 | -0.28242800 | -0.14151900 |
| C | 4.53360400 | -2.27105500 | 0.20879000 |

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|---|------------|-------------|-------------|
| C | 7.01368600 | -1.07171000 | -0.21242100 |
| H | 5.94836100 | 0.79864000 | -0.24821300 |
| C | 5.68065300 | -3.05286800 | 0.14285100 |
| H | 3.56062500 | -2.73952000 | 0.36910500 |
| C | 6.91951700 | -2.45304400 | -0.07028700 |
| H | 7.98128600 | -0.60405100 | -0.37912300 |
| H | 5.60697500 | -4.13246400 | 0.25123200 |
| H | 7.81591000 | -3.06634700 | -0.12824300 |
| C | 3.39342700 | 1.69113300 | -0.61593600 |
| C | 3.84259400 | 2.81476700 | 0.08259000 |
| C | 3.18218500 | 1.76496900 | -1.99716400 |
| C | 4.08028200 | 4.00335900 | -0.60059000 |
| H | 4.00783300 | 2.76370600 | 1.15789100 |
| C | 3.42634800 | 2.95372700 | -2.67396000 |
| H | 2.82517500 | 0.88892000 | -2.54007100 |
| C | 3.87261600 | 4.07282200 | -1.97491100 |
| H | 4.42676600 | 4.87803700 | -0.05506800 |
| H | 3.25975700 | 3.00934700 | -3.74721800 |
| H | 4.05553400 | 5.00528500 | -2.50420800 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2508.276594

Electronic Energy (0K) + ZPE = -2507.690933

Enthalpy (333K) = -2507.638222

Free Energy (333K) = -2507.791743

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2508.706992

TS_{A1'}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|------------|
| C | -1.74365500 | -0.13157800 | 4.83484300 |
|---|-------------|-------------|------------|

| | | | |
|---|-------------|-------------|-------------|
| C | -1.57404300 | 0.11222400 | 3.47880700 |
| C | -1.49045000 | 1.43113900 | 3.00273800 |
| C | -1.57148600 | 2.49548000 | 3.91350400 |
| C | -1.72428200 | 2.24091700 | 5.27035400 |
| C | -1.81471300 | 0.93052700 | 5.73381700 |
| H | -1.81133000 | -1.15604000 | 5.19443000 |
| H | -1.50684900 | 3.51720500 | 3.54472200 |
| H | -1.77938100 | 3.07161500 | 5.97057000 |
| H | -1.93985200 | 0.73645200 | 6.79680300 |
| C | -1.29871100 | 1.67122000 | 1.61087100 |
| C | -1.10303500 | 1.82905600 | 0.42137900 |
| N | -0.88478200 | 1.97844700 | -0.89442300 |
| C | -1.49303900 | 1.01811400 | -1.82482100 |
| C | -1.08024500 | -0.39412200 | -1.57599100 |
| C | -1.70875700 | -1.49869000 | -1.67104700 |
| C | -1.86161200 | -2.94494100 | -1.68088300 |
| S | 0.49513800 | 2.90168300 | -1.35584400 |
| O | 1.54364300 | 2.67742200 | -0.37128300 |
| O | 0.70645500 | 2.58618900 | -2.76221600 |
| C | -0.09298100 | 4.56019200 | -1.19036300 |
| C | 0.21047200 | 5.28242700 | -0.04130200 |
| C | -0.89132900 | 5.09359900 | -2.20232800 |
| C | -0.29153300 | 6.57232600 | 0.08654300 |
| H | 0.83330700 | 4.84519300 | 0.73526400 |
| C | -1.37978800 | 6.38102800 | -2.05385800 |
| H | -1.12004200 | 4.51191000 | -3.09293200 |
| C | -1.08841600 | 7.13852500 | -0.91108100 |
| H | -0.05850200 | 7.15167300 | 0.97818700 |
| H | -1.99988300 | 6.81545400 | -2.83664700 |
| C | -1.61553300 | 8.53221900 | -0.78228400 |

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|----|-------------|-------------|-------------|
| H | -1.46707400 | 8.93190300 | 0.22597700 |
| H | -2.68649300 | 8.57607100 | -1.01424300 |
| H | -1.11155600 | 9.20730200 | -1.48639700 |
| H | -1.20807300 | 1.31463400 | -2.83981900 |
| H | -2.58298300 | 1.10743800 | -1.74263400 |
| Au | 0.87292000 | -0.85484100 | -0.83226100 |
| P | 3.00960100 | -1.31114300 | 0.02991200 |
| H | -1.50140800 | -0.71246300 | 2.77009100 |
| H | -0.88877400 | -3.40166600 | -1.46125800 |
| H | -2.57132900 | -3.29482700 | -0.92134500 |
| H | -2.18405400 | -3.30040700 | -2.66598600 |
| C | 3.13717600 | -0.96253900 | 1.81515600 |
| C | 2.54232900 | 0.20795500 | 2.29993300 |
| C | 3.82002300 | -1.81025200 | 2.69163900 |
| C | 2.62970600 | 0.52398000 | 3.65086200 |
| H | 2.01685500 | 0.87551300 | 1.61502900 |
| C | 3.90104600 | -1.48915200 | 4.04357100 |
| H | 4.29040100 | -2.72036000 | 2.32195500 |
| C | 3.30496500 | -0.32655600 | 4.52296100 |
| H | 2.15873900 | 1.43102300 | 4.02438000 |
| H | 4.43133100 | -2.15200500 | 4.72365800 |
| H | 3.36522100 | -0.08249800 | 5.58132700 |
| C | 3.42620700 | -3.07599700 | -0.16848200 |
| C | 4.65309900 | -3.50524800 | -0.67743300 |
| C | 2.46597800 | -4.01983800 | 0.21768400 |
| C | 4.91542900 | -4.86790500 | -0.79839000 |
| H | 5.40709800 | -2.78116800 | -0.98108500 |
| C | 2.73665400 | -5.37729100 | 0.10346700 |
| H | 1.50773900 | -3.68537000 | 0.61855800 |
| C | 3.96176600 | -5.80169000 | -0.40829300 |

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|----|-------------|-------------|-------------|
| H | 5.87169600 | -5.19771200 | -1.19799100 |
| H | 1.98970600 | -6.10597800 | 0.41019400 |
| H | 4.17109100 | -6.86480600 | -0.50413300 |
| C | 4.33052700 | -0.35970900 | -0.78139700 |
| C | 5.52866100 | -0.06816400 | -0.12174000 |
| C | 4.14604100 | 0.05239800 | -2.10488800 |
| C | 6.53379600 | 0.62561300 | -0.78650300 |
| H | 5.67786600 | -0.38362400 | 0.91026000 |
| C | 5.15603200 | 0.74298700 | -2.76557300 |
| H | 3.20496700 | -0.16260100 | -2.61306000 |
| C | 6.34809300 | 1.02967200 | -2.10608500 |
| H | 7.46385900 | 0.85352300 | -0.27076300 |
| H | 5.00750100 | 1.06549400 | -3.79352600 |
| H | 7.13522000 | 1.57588400 | -2.62122600 |
| C | -6.41554400 | -2.85595600 | -1.11465300 |
| C | -6.51154500 | -2.43364400 | 0.20510800 |
| C | -5.56480200 | -1.51628300 | 0.64188000 |
| C | -4.57639400 | -1.04157200 | -0.20143300 |
| C | -5.41869700 | -2.38722800 | -1.95084200 |
| H | -7.29149200 | -2.80117800 | 0.86551100 |
| H | -5.29251600 | -2.67958500 | -2.98750000 |
| N | -4.52310600 | -1.48605700 | -1.48050300 |
| O | -3.60503000 | -1.03794100 | -2.28742400 |
| H | -3.81673700 | -0.32118300 | 0.08438200 |
| Cl | -5.60688000 | -0.93399100 | 2.27234000 |
| Cl | -7.55023400 | -4.00034300 | -1.74928500 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3750.652242

Electronic Energy (0K) + ZPE = -3749.991703

Enthalpy (333K) = -3749.929310

Free Energy (333K) = -3750.103823

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3751.219227

B1'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -1.72396100 | -0.51079000 | 4.97419500 |
| C | -1.58016500 | -0.23161200 | 3.62173000 |
| C | -1.60926400 | 1.09748600 | 3.16683900 |
| C | -1.77497400 | 2.13544800 | 4.09659500 |
| C | -1.90085000 | 1.84643000 | 5.44926700 |
| C | -1.88027200 | 0.52585100 | 5.89193600 |
| H | -1.70404800 | -1.54345100 | 5.31591500 |
| H | -1.79779900 | 3.16521800 | 3.74557600 |
| H | -2.02204200 | 2.65845200 | 6.16306200 |
| H | -1.98478700 | 0.30450500 | 6.95180100 |
| C | -1.44967500 | 1.37628400 | 1.77861400 |
| C | -1.27070400 | 1.56812400 | 0.59076100 |
| N | -1.08367700 | 1.73880300 | -0.72378900 |
| C | -1.59115900 | 0.72014600 | -1.66548500 |
| C | -0.98178600 | -0.63071600 | -1.41256900 |
| C | -1.70106700 | -1.74060000 | -1.59960900 |
| C | -1.33719700 | -3.17633600 | -1.46904800 |
| S | -0.08030200 | 3.02751400 | -1.23208800 |
| O | 0.95941500 | 3.18892200 | -0.22801300 |
| O | 0.24476400 | 2.73884900 | -2.62186600 |
| C | -1.15208400 | 4.43414700 | -1.15939100 |
| C | -1.18798400 | 5.20298700 | -0.00008900 |
| C | -1.97602200 | 4.71665400 | -2.24834700 |
| C | -2.06300000 | 6.28085500 | 0.05991300 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.53441400 | 4.96823200 | 0.83661900 |
| C | -2.83943200 | 5.79782800 | -2.16744300 |
| H | -1.93117300 | 4.10690800 | -3.14813500 |
| C | -2.89640200 | 6.59477200 | -1.01668300 |
| H | -2.09672300 | 6.89401600 | 0.95889400 |
| H | -3.48262800 | 6.03716800 | -3.01311600 |
| C | -3.82238200 | 7.76846500 | -0.96234600 |
| H | -3.90921700 | 8.17226200 | 0.05159600 |
| H | -4.82676300 | 7.50128000 | -1.31226300 |
| H | -3.46559300 | 8.57800400 | -1.61275900 |
| H | -1.33165000 | 1.06569200 | -2.67311100 |
| H | -2.68761700 | 0.72318200 | -1.59204800 |
| Au | 1.00867000 | -0.73110000 | -0.77414700 |
| P | 3.26058700 | -0.82296300 | -0.03455500 |
| H | -1.44253400 | -1.03617300 | 2.89928200 |
| H | -0.28049100 | -3.26119500 | -1.19834400 |
| H | -1.91875400 | -3.69166700 | -0.69111500 |
| H | -1.49469300 | -3.71410800 | -2.41383600 |
| C | 3.42454900 | -0.73080000 | 1.78142800 |
| C | 2.54693300 | 0.10985200 | 2.47535000 |
| C | 4.39851300 | -1.44552800 | 2.48436800 |
| C | 2.64488000 | 0.23615800 | 3.85638500 |
| H | 1.78776200 | 0.66949800 | 1.92802000 |
| C | 4.48950600 | -1.31929500 | 3.86742700 |
| H | 5.08875400 | -2.10026900 | 1.95382000 |
| C | 3.61422600 | -0.48124500 | 4.55261500 |
| H | 1.95809300 | 0.89048100 | 4.38967100 |
| H | 5.24831900 | -1.87833400 | 4.41059400 |
| H | 3.68667100 | -0.38821700 | 5.63406100 |
| C | 4.10310000 | -2.36880400 | -0.52224700 |

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|---|-------------|-------------|-------------|
| C | 5.35491600 | -2.38245700 | -1.14036300 |
| C | 3.45048800 | -3.57907000 | -0.25562900 |
| C | 5.94577500 | -3.59492200 | -1.48845200 |
| H | 5.87380400 | -1.44893000 | -1.35169400 |
| C | 4.04789700 | -4.78589900 | -0.59647200 |
| H | 2.47509300 | -3.57342900 | 0.23287700 |
| C | 5.29568700 | -4.79396400 | -1.21714000 |
| H | 6.92016300 | -3.59888700 | -1.97188300 |
| H | 3.53727700 | -5.72217700 | -0.38209000 |
| H | 5.76068300 | -5.73868200 | -1.49026900 |
| C | 4.27213900 | 0.53685100 | -0.70580100 |
| C | 5.35597900 | 1.07540500 | -0.00659100 |
| C | 3.95609800 | 1.02439800 | -1.97840000 |
| C | 6.11465800 | 2.09150700 | -0.57864700 |
| H | 5.60884000 | 0.70154900 | 0.98490200 |
| C | 4.72003500 | 2.03677300 | -2.54767200 |
| H | 3.10432600 | 0.61037000 | -2.51946800 |
| C | 5.79755200 | 2.57139700 | -1.84669100 |
| H | 6.95525100 | 2.51107500 | -0.03047100 |
| H | 4.46680700 | 2.41503300 | -3.53547400 |
| H | 6.39041700 | 3.36927600 | -2.28862000 |
| C | -5.80317900 | -3.64885900 | -1.22708000 |
| C | -6.01494100 | -3.28167100 | 0.09694200 |
| C | -5.17550200 | -2.32567400 | 0.65935500 |
| C | -4.16053400 | -1.75283000 | -0.08708600 |
| C | -4.77665000 | -3.07823500 | -1.96213800 |
| H | -6.81526700 | -3.73302100 | 0.67766700 |
| H | -4.53705900 | -3.31480700 | -2.99456600 |
| N | -4.00833700 | -2.16084400 | -1.35703600 |
| O | -3.04530900 | -1.57014400 | -2.13447900 |

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|----|-------------|-------------|-------------|
| H | -3.46513600 | -1.00155200 | 0.27931700 |
| Cl | -5.38656700 | -1.82398400 | 2.29476200 |
| Cl | -6.80473600 | -4.83330800 | -1.97818600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3750.672334

Electronic Energy (0K) + ZPE = -3750.008284

Enthalpy (333K) = -3749.946585

Free Energy (333K) = -3750.117832

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3751.236145

A2'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -4.18356700 | -4.79170900 | 2.62078800 |
| C | -3.69575300 | -3.72269400 | 1.88023400 |
| C | -2.63822000 | -3.91059400 | 0.97933300 |
| C | -2.08178000 | -5.19161900 | 0.83199300 |
| C | -2.57258900 | -6.25444700 | 1.57457900 |
| C | -3.62265000 | -6.05649600 | 2.47011900 |
| H | -5.00464600 | -4.63665800 | 3.31654800 |
| H | -1.26474500 | -5.34224500 | 0.12888400 |
| H | -2.13677100 | -7.24342100 | 1.45428200 |
| H | -4.00529000 | -6.89294900 | 3.05049900 |
| C | -2.11806700 | -2.80293100 | 0.19556800 |
| C | -1.23412100 | -2.58451000 | -0.68627700 |
| N | -0.42353400 | -2.24281900 | -1.63351800 |
| C | 0.94981700 | -1.74904700 | -1.37881900 |
| C | 0.95604100 | -0.63916200 | -0.42118700 |
| C | 0.71561800 | 0.21743100 | 0.43063400 |
| C | 0.36623300 | 1.20148500 | 1.43951000 |

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|----|-------------|-------------|-------------|
| S | -1.01653800 | -2.33135400 | -3.32352800 |
| O | 0.20172300 | -2.46596200 | -4.10044400 |
| O | -2.03517100 | -3.35949200 | -3.27779300 |
| C | -1.74928000 | -0.75566800 | -3.59533400 |
| C | -0.94999800 | 0.28556900 | -4.06509900 |
| C | -3.12075700 | -0.59597500 | -3.37740200 |
| C | -1.54619700 | 1.51116300 | -4.32811400 |
| H | 0.11003500 | 0.13395700 | -4.25506300 |
| C | -3.69069700 | 0.63761400 | -3.65359500 |
| H | -3.73121600 | -1.42816500 | -3.03265800 |
| C | -2.91827800 | 1.70435200 | -4.13361500 |
| H | -0.94031300 | 2.32964600 | -4.71211400 |
| H | -4.76166200 | 0.77872100 | -3.51359300 |
| C | -3.56156100 | 3.02073500 | -4.42580300 |
| H | -2.82642900 | 3.77995500 | -4.71114400 |
| H | -4.11747000 | 3.38988400 | -3.55461600 |
| H | -4.28704700 | 2.92764400 | -5.24411300 |
| H | 1.38445400 | -1.45052100 | -2.33883000 |
| H | 1.55268000 | -2.58319100 | -1.00056000 |
| Au | -2.89827100 | -0.78289600 | 0.38921000 |
| P | -3.95108600 | 1.26586300 | 0.83966600 |
| Au | 3.07100300 | 0.02604800 | 0.12386500 |
| P | 5.37897900 | 0.28682000 | 0.32662400 |
| H | -4.13438300 | -2.73037800 | 1.98931000 |
| H | 0.88850300 | 2.15011000 | 1.26881700 |
| H | -0.71373500 | 1.39901000 | 1.40307700 |
| H | 0.62025400 | 0.83828400 | 2.44190200 |
| C | -5.47046100 | 1.48332600 | -0.13733000 |
| C | -5.88193100 | 2.73840500 | -0.59434500 |
| C | -6.25273500 | 0.35278100 | -0.40035900 |

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|---|-------------|-------------|-------------|
| C | -7.06830900 | 2.85712200 | -1.31256200 |
| H | -5.27985500 | 3.62313900 | -0.39020000 |
| C | -7.44094000 | 0.47963500 | -1.11041400 |
| H | -5.92558800 | -0.62670000 | -0.04778300 |
| C | -7.84561000 | 1.73125400 | -1.56964500 |
| H | -7.38648100 | 3.83373300 | -1.67004400 |
| H | -8.04680200 | -0.40025600 | -1.31383100 |
| H | -8.77135400 | 1.82866800 | -2.13216100 |
| C | -2.90187100 | 2.71732100 | 0.50782500 |
| C | -2.73127700 | 3.74433300 | 1.43845300 |
| C | -2.23521700 | 2.77533300 | -0.72287100 |
| C | -1.89894700 | 4.82035200 | 1.13846400 |
| H | -3.24399600 | 3.70966100 | 2.39792400 |
| C | -1.41611700 | 3.85711300 | -1.02064800 |
| H | -2.36138700 | 1.97037600 | -1.45080800 |
| C | -1.24480700 | 4.87898400 | -0.08738700 |
| H | -1.76752200 | 5.61715500 | 1.86686600 |
| H | -0.90435300 | 3.90443500 | -1.97966400 |
| H | -0.59845400 | 5.72247900 | -0.31921100 |
| C | -4.43767300 | 1.34037300 | 2.59210100 |
| C | -5.51233000 | 2.12835600 | 3.01706300 |
| C | -3.69547600 | 0.61318300 | 3.52941700 |
| C | -5.83504300 | 2.18856400 | 4.36837900 |
| H | -6.09683400 | 2.69667700 | 2.29465400 |
| C | -4.02122200 | 0.67999100 | 4.87978600 |
| H | -2.86689500 | -0.01504700 | 3.19687000 |
| C | -5.09099200 | 1.46639900 | 5.29792300 |
| H | -6.67270600 | 2.80001600 | 4.69550600 |
| H | -3.44477500 | 0.10995500 | 5.60470800 |
| H | -5.34977200 | 1.51294600 | 6.35331200 |

| | | | |
|---|------------|-------------|-------------|
| C | 5.80614500 | 1.97403700 | 0.84996500 |
| C | 6.94830700 | 2.62007700 | 0.37008400 |
| C | 4.98311600 | 2.61060100 | 1.78610600 |
| C | 7.26212400 | 3.89658700 | 0.82683700 |
| H | 7.59489700 | 2.12867700 | -0.35539600 |
| C | 5.30651500 | 3.88243300 | 2.24290500 |
| H | 4.09017900 | 2.10533100 | 2.15868200 |
| C | 6.44429100 | 4.52554200 | 1.76076300 |
| H | 8.14997900 | 4.39977200 | 0.45130800 |
| H | 4.66718000 | 4.37500200 | 2.97178400 |
| H | 6.69293500 | 5.52385600 | 2.11355700 |
| C | 6.23381100 | -0.02247800 | -1.24798200 |
| C | 7.44090300 | -0.72379700 | -1.30110400 |
| C | 5.67307800 | 0.49517900 | -2.42145000 |
| C | 8.07893500 | -0.90702200 | -2.52458300 |
| H | 7.88568400 | -1.12598700 | -0.39232100 |
| C | 6.31933300 | 0.31422800 | -3.63780200 |
| H | 4.73204900 | 1.04510400 | -2.37939200 |
| C | 7.52039400 | -0.39010500 | -3.68921900 |
| H | 9.01688800 | -1.45575700 | -2.56478600 |
| H | 5.88271900 | 0.71823700 | -4.54814900 |
| H | 8.02179700 | -0.53764800 | -4.64302400 |
| C | 6.07633500 | -0.85855100 | 1.55203900 |
| C | 7.12477600 | -0.48166300 | 2.39503100 |
| C | 5.56690100 | -2.16076100 | 1.60696000 |
| C | 7.65754900 | -1.40647100 | 3.28809200 |
| H | 7.52776800 | 0.52908600 | 2.35539800 |
| C | 6.10845900 | -3.08079600 | 2.49609000 |
| H | 4.74600900 | -2.45022800 | 0.94922500 |
| C | 7.15158000 | -2.70186900 | 3.33817800 |

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|---|------------|-------------|------------|
| H | 8.47184800 | -1.11223700 | 3.94593500 |
| H | 5.71264200 | -4.09283500 | 2.53713400 |
| H | 7.56997900 | -3.42044900 | 4.03926300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3679.730641

Electronic Energy (0K) + ZPE = -3678.868148

Enthalpy (333K) = -3678.792458

Free Energy (333K) = -3678.994158

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3680.335591

TS_{B'}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.13304700 | 4.69026400 | 1.41799100 |
| C | 0.83756900 | 3.39355700 | 1.02260300 |
| C | 1.66097000 | 2.68411600 | 0.12158000 |
| C | 2.78506000 | 3.36640500 | -0.39555700 |
| C | 3.06296500 | 4.67205500 | -0.01904100 |
| C | 2.24765800 | 5.33748400 | 0.89440900 |
| H | 0.48368900 | 5.19989000 | 2.12605000 |
| H | 3.42849700 | 2.88083600 | -1.12046700 |
| H | 3.92549600 | 5.17845700 | -0.44687000 |
| H | 2.47553500 | 6.36017400 | 1.18663600 |
| C | 1.27846400 | 1.30328300 | -0.18759900 |
| C | 2.12213400 | 0.36894200 | -0.76260400 |
| N | 1.77515500 | -1.00482700 | -0.87409600 |
| C | 1.73219300 | -1.58908200 | -2.22807700 |
| C | 0.62924500 | -1.02602700 | -2.99514500 |
| C | -0.29703400 | -0.54538100 | -3.60996200 |
| C | -1.41427900 | 0.02052700 | -4.34316400 |

| | | | |
|----|-------------|-------------|-------------|
| S | 2.11847300 | -2.06864500 | 0.39355500 |
| O | 3.11460900 | -3.03066500 | -0.07082100 |
| O | 2.40361100 | -1.23315300 | 1.55642000 |
| C | 0.59944400 | -2.93575400 | 0.67882900 |
| C | 0.36820300 | -4.15979900 | 0.05614800 |
| C | -0.33293300 | -2.38378700 | 1.55720400 |
| C | -0.82439600 | -4.82802900 | 0.30803200 |
| H | 1.11915000 | -4.59746300 | -0.59758000 |
| C | -1.51268500 | -3.07226800 | 1.80253700 |
| H | -0.12516600 | -1.44112700 | 2.06019200 |
| C | -1.77961400 | -4.29797800 | 1.18086800 |
| H | -1.01079000 | -5.78853600 | -0.16971000 |
| H | -2.24205700 | -2.65677400 | 2.49746900 |
| C | -3.07082400 | -5.00939400 | 1.43426700 |
| H | -2.97969300 | -6.08815200 | 1.26771100 |
| H | -3.85773300 | -4.64284900 | 0.76010100 |
| H | -3.42603900 | -4.84615400 | 2.45820700 |
| H | 1.61204300 | -2.67493200 | -2.13556700 |
| H | 2.69291700 | -1.43404100 | -2.74029600 |
| Au | -0.74206200 | 0.76419400 | -0.02043600 |
| P | -3.09508100 | 0.46161300 | 0.03062500 |
| H | -2.25032600 | -0.68798500 | -4.40248100 |
| H | -1.78204900 | 0.93250700 | -3.85533700 |
| H | -1.12660000 | 0.28696700 | -5.36726300 |
| H | -0.04436000 | 2.89501300 | 1.42592600 |
| C | -3.74378700 | -0.16964900 | 1.61645000 |
| C | -4.72091000 | -1.16487400 | 1.68797600 |
| C | -3.23110600 | 0.38548800 | 2.79528200 |
| C | -5.17733700 | -1.60279100 | 2.92913100 |
| H | -5.12928000 | -1.60008700 | 0.77678700 |

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|---|-------------|-------------|-------------|
| C | -3.69451200 | -0.05006100 | 4.03098600 |
| H | -2.46521400 | 1.16116800 | 2.74195800 |
| C | -4.66538500 | -1.04792600 | 4.09819600 |
| H | -5.93658900 | -2.38036000 | 2.97980400 |
| H | -3.29355400 | 0.38557000 | 4.94338000 |
| H | -5.02291300 | -1.39313800 | 5.06573000 |
| C | -3.71884600 | -0.66886700 | -1.25702400 |
| C | -4.88748200 | -0.42036500 | -1.98103500 |
| C | -2.98680500 | -1.83627800 | -1.50200300 |
| C | -5.31984800 | -1.33553100 | -2.93685800 |
| H | -5.46257000 | 0.48659800 | -1.80247900 |
| C | -3.42710900 | -2.75223000 | -2.45095200 |
| H | -2.07276500 | -2.02859500 | -0.93699700 |
| C | -4.59360700 | -2.49997300 | -3.17077200 |
| H | -6.22911100 | -1.13676500 | -3.49971500 |
| H | -2.85356800 | -3.65920400 | -2.63194100 |
| H | -4.93621900 | -3.21257200 | -3.91782300 |
| C | -3.93485900 | 2.06112300 | -0.22674900 |
| C | -5.23052200 | 2.29702200 | 0.24466900 |
| C | -3.26392700 | 3.06316100 | -0.93640800 |
| C | -5.84828200 | 3.51873300 | -0.00029000 |
| H | -5.75925300 | 1.52455800 | 0.80228800 |
| C | -3.88735000 | 4.28266700 | -1.18126700 |
| H | -2.24624900 | 2.88652500 | -1.28885200 |
| C | -5.17822000 | 4.50985200 | -0.71319300 |
| H | -6.85578900 | 3.69742900 | 0.36851200 |
| H | -3.36006300 | 5.05891700 | -1.73125900 |
| H | -5.66333200 | 5.46546300 | -0.89989200 |
| C | 6.83895300 | -0.35850400 | -0.72649400 |
| C | 6.95313800 | -0.26254400 | 0.65753000 |

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|----|------------|-------------|-------------|
| C | 5.84320500 | 0.14339700 | 1.38917700 |
| C | 4.65432200 | 0.44973800 | 0.73887100 |
| C | 5.63597900 | -0.05701900 | -1.35137800 |
| H | 7.88918900 | -0.50187800 | 1.15568400 |
| H | 5.46443900 | -0.11265900 | -2.42378200 |
| N | 4.63000500 | 0.32306100 | -0.57639200 |
| O | 3.23652200 | 0.71345500 | -1.39070700 |
| H | 3.73512600 | 0.75096700 | 1.24062600 |
| Cl | 5.91718900 | 0.27129900 | 3.11040300 |
| Cl | 8.18512800 | -0.86729300 | -1.68447600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -3750.665898

Electronic Energy (0K) + ZPE = -3750.004520

Enthalpy (333K) = -3749.943037

Free Energy (333K) = -3750.111154

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -3751.229894

[N] (*Au catalysis system*)

Number of imaginary frequencies: 0

| | | | |
|----|-------------|-------------|-------------|
| C | 1.18060100 | -0.00916300 | -0.00006800 |
| C | 0.00000900 | -0.73929800 | -0.00003100 |
| C | -1.18044400 | -0.01043700 | -0.00001800 |
| C | -1.14690700 | 1.38160600 | 0.00006400 |
| C | 1.14733500 | 1.38173600 | -0.00016300 |
| H | 0.00106800 | -1.82621100 | -0.00002000 |
| H | 2.07368700 | 1.95550600 | -0.00014800 |
| N | -0.00043400 | 2.05433900 | 0.00007900 |
| H | -2.07403600 | 1.95469600 | 0.00020500 |
| Cl | -2.71662900 | -0.83789300 | -0.00000800 |

| | | | |
|----|------------|-------------|------------|
| Cl | 2.71655600 | -0.83805000 | 0.00005000 |
|----|------------|-------------|------------|

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1167.245319

Electronic Energy (0K) + ZPE = -1167.175884

Enthalpy (333K) = -1167.166853

Free Energy (333K) = -1167.211861

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1167.361999

C'

Number of imaginary frequencies: 0

| | | | |
|---|------------|-------------|-------------|
| C | 2.49097300 | 4.57471300 | -1.69302200 |
| C | 1.92609100 | 3.39925400 | -1.23376500 |
| C | 2.74444400 | 2.31136900 | -0.84699500 |
| C | 4.15311600 | 2.45238700 | -0.92310400 |
| C | 4.71058700 | 3.63219000 | -1.37208600 |
| C | 3.88011600 | 4.68893700 | -1.75889800 |
| H | 1.85989500 | 5.40477100 | -1.99836300 |
| H | 4.79489300 | 1.62838100 | -0.61629000 |
| H | 5.79019500 | 3.74142500 | -1.42648300 |
| H | 4.32553100 | 5.61473200 | -2.11625300 |
| C | 2.14273700 | 1.11873900 | -0.36290700 |
| C | 2.92647000 | -0.13499300 | -0.35372100 |
| N | 3.23899800 | -0.80321200 | 0.80256000 |
| C | 2.87577300 | -0.32910700 | 2.15519900 |
| C | 2.63171600 | 1.10056600 | 2.18613100 |
| C | 2.41771700 | 2.28878900 | 2.30843000 |
| C | 2.14826100 | 3.70788300 | 2.37205100 |
| S | 3.66937200 | -2.48800600 | 0.66972500 |
| O | 3.79834900 | -2.90728400 | 2.05683000 |

| | | | |
|----|-------------|-------------|-------------|
| O | 4.78794500 | -2.60288100 | -0.24347600 |
| C | 2.21227100 | -3.20964100 | -0.02292700 |
| C | 1.13394900 | -3.46755400 | 0.82649400 |
| C | 2.15230100 | -3.48866100 | -1.38470700 |
| C | -0.02193400 | -4.00995700 | 0.28732400 |
| H | 1.20447000 | -3.26910000 | 1.89387800 |
| C | 0.98399100 | -4.03580800 | -1.90177600 |
| H | 3.00462200 | -3.27974300 | -2.02463400 |
| C | -0.11599400 | -4.29981700 | -1.08072300 |
| H | -0.86769700 | -4.22846300 | 0.93789600 |
| H | 0.92510300 | -4.26424200 | -2.96451800 |
| C | -1.37233200 | -4.89300300 | -1.63390800 |
| H | -2.25580800 | -4.33435500 | -1.29939300 |
| H | -1.36913900 | -4.90460000 | -2.72873300 |
| H | -1.50157800 | -5.92702100 | -1.28826200 |
| H | 1.98349500 | -0.86881400 | 2.50550200 |
| H | 3.69644100 | -0.58519100 | 2.83290800 |
| O | 3.13151900 | -0.57830500 | -1.47773200 |
| Au | 0.11095000 | 0.75104500 | -0.14759800 |
| P | -2.21526100 | 0.34827100 | 0.07377400 |
| H | 2.12315200 | 4.04958600 | 3.41389900 |
| H | 2.92679000 | 4.28268200 | 1.85562800 |
| H | 1.17555900 | 3.94736700 | 1.92257200 |
| H | 0.84465600 | 3.28408500 | -1.16966400 |
| C | -3.13959900 | 1.84572000 | 0.55527600 |
| C | -4.07239900 | 1.85183200 | 1.59399100 |
| C | -2.89844100 | 3.01905700 | -0.17018400 |
| C | -4.75532100 | 3.02526000 | 1.90475200 |
| H | -4.27136700 | 0.94335900 | 2.16034900 |
| C | -3.58716900 | 4.18450000 | 0.14052700 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.17897100 | 3.01437500 | -0.99029300 |
| C | -4.51369000 | 4.18844500 | 1.18154700 |
| H | -5.48086400 | 3.02641200 | 2.71504700 |
| H | -3.39898300 | 5.09238900 | -0.42808400 |
| H | -5.04910300 | 5.10259300 | 1.42815500 |
| C | -2.60231700 | -0.91473400 | 1.32715400 |
| C | -3.62024900 | -1.85506200 | 1.15133300 |
| C | -1.86650400 | -0.90041800 | 2.51841800 |
| C | -3.89990500 | -2.77111800 | 2.16178500 |
| H | -4.19704900 | -1.87636300 | 0.22823000 |
| C | -2.15358600 | -1.81396000 | 3.52591600 |
| H | -1.07540900 | -0.16180100 | 2.65882900 |
| C | -3.16977400 | -2.75029100 | 3.34660300 |
| H | -4.69285400 | -3.50214400 | 2.02140000 |
| H | -1.58203200 | -1.79740500 | 4.45108500 |
| H | -3.39135100 | -3.46744100 | 4.13370800 |
| C | -2.93649300 | -0.20222400 | -1.50339100 |
| C | -4.29622800 | -0.04341100 | -1.79136900 |
| C | -2.09515700 | -0.81754900 | -2.43556000 |
| C | -4.80643500 | -0.51332600 | -2.99655400 |
| H | -4.95577600 | 0.44484500 | -1.07441300 |
| C | -2.61176800 | -1.29180500 | -3.63664500 |
| H | -1.03071500 | -0.91229600 | -2.21497200 |
| C | -3.96686800 | -1.13926000 | -3.91550600 |
| H | -5.86353600 | -0.38904900 | -3.21998800 |
| H | -1.95308000 | -1.77149800 | -4.35733900 |
| H | -4.37115600 | -1.50342700 | -4.85735700 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.494865

Electronic Energy (0K) + ZPE = -2582.902093

Enthalpy (333K) = -2582.850034

Free Energy (333K) = -2582.994588

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2583.942206

TS_{C'}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | -2.94224300 | 4.25776000 | 1.72688600 |
| C | -2.29597000 | 3.18300600 | 1.13340800 |
| C | -3.02119600 | 2.05170600 | 0.71761400 |
| C | -4.42017600 | 2.03903000 | 0.89232600 |
| C | -5.06314700 | 3.11684400 | 1.47541800 |
| C | -4.32415800 | 4.22457500 | 1.89587800 |
| H | -2.37160200 | 5.12239100 | 2.05611600 |
| H | -4.99859800 | 1.17866600 | 0.55812400 |
| H | -6.14195700 | 3.09978400 | 1.60765100 |
| H | -4.83274700 | 5.06773600 | 2.35795900 |
| C | -2.33322200 | 0.93143500 | 0.10365200 |
| C | -2.91605700 | -0.42689000 | 0.30777700 |
| N | -3.12055400 | -1.20867900 | -0.80756400 |
| C | -2.86643800 | -0.63535700 | -2.13191600 |
| C | -2.77762500 | 0.81536300 | -1.98398400 |
| C | -2.76395900 | 2.01836100 | -2.21762500 |
| C | -2.69622700 | 3.44912400 | -2.30651800 |
| S | -3.20996700 | -2.92571600 | -0.65211700 |
| O | -3.22308100 | -3.37614600 | -2.03582000 |
| O | -4.30075900 | -3.24484900 | 0.24647800 |
| C | -1.66018200 | -3.34068000 | 0.08775600 |
| C | -0.52635500 | -3.37902100 | -0.72622100 |
| C | -1.58850500 | -3.60815200 | 1.45130700 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.69452800 | -3.69960900 | -0.15349700 |
| H | -0.60112700 | -3.18857600 | -1.79495400 |
| C | -0.35472100 | -3.93384700 | 2.00273100 |
| H | -2.48378800 | -3.56732500 | 2.06505600 |
| C | 0.79840400 | -3.98884500 | 1.21422200 |
| H | 1.58592800 | -3.74766400 | -0.77863600 |
| H | -0.28570100 | -4.15533700 | 3.06653700 |
| C | 2.11957600 | -4.37557500 | 1.79887700 |
| H | 2.91354800 | -3.67911600 | 1.50043700 |
| H | 2.08795600 | -4.41556300 | 2.89242400 |
| H | 2.42370000 | -5.36793200 | 1.43989200 |
| H | -1.93043600 | -1.02649000 | -2.55662500 |
| H | -3.68252800 | -0.89293100 | -2.81461700 |
| O | -3.04581800 | -0.81936700 | 1.45492400 |
| Au | -0.23945100 | 0.75155400 | -0.02025100 |
| P | 2.11643700 | 0.52493500 | -0.09206600 |
| H | -2.90307000 | 3.76116700 | -3.33905900 |
| H | -3.45420500 | 3.91858100 | -1.66609200 |
| H | -1.69848500 | 3.82028500 | -2.03865500 |
| H | -1.21544000 | 3.19425400 | 0.99245100 |
| C | 2.65861200 | -0.59451500 | -1.42304500 |
| C | 3.76746500 | -1.43595600 | -1.30174100 |
| C | 1.93084200 | -0.57602000 | -2.61926700 |
| C | 4.13794700 | -2.25478400 | -2.36493400 |
| H | 4.34296500 | -1.45871600 | -0.37826100 |
| C | 2.30614500 | -1.39384100 | -3.67881800 |
| H | 1.06573800 | 0.08199000 | -2.71692100 |
| C | 3.40801600 | -2.23618600 | -3.55000800 |
| H | 4.99979400 | -2.91041300 | -2.26450400 |
| H | 1.73569200 | -1.37697000 | -4.60465700 |

| | | | |
|---|------------|-------------|-------------|
| H | 3.69794000 | -2.88087300 | -4.37660700 |
| C | 2.95865300 | 2.11732000 | -0.38445300 |
| C | 2.60501400 | 3.19404600 | 0.43839000 |
| C | 3.92253800 | 2.29089100 | -1.37897600 |
| C | 3.21475200 | 4.43026000 | 0.26812100 |
| H | 1.85782600 | 3.05723300 | 1.22168100 |
| C | 4.52582900 | 3.53494400 | -1.54879400 |
| H | 4.20796300 | 1.45895300 | -2.02093600 |
| C | 4.17339000 | 4.60170800 | -0.72904600 |
| H | 2.94006600 | 5.26272300 | 0.91195100 |
| H | 5.27644800 | 3.66693000 | -2.32482600 |
| H | 4.64673400 | 5.57141900 | -0.86585800 |
| C | 2.77145100 | -0.09325600 | 1.49012500 |
| C | 4.13231500 | 0.00000200 | 1.80635300 |
| C | 1.88335400 | -0.65696900 | 2.41214700 |
| C | 4.59744900 | -0.49060200 | 3.02079100 |
| H | 4.82786300 | 0.46187600 | 1.10608700 |
| C | 2.35317800 | -1.13833500 | 3.63065700 |
| H | 0.81878500 | -0.70510000 | 2.17691200 |
| C | 3.70949600 | -1.06023700 | 3.93138900 |
| H | 5.65572400 | -0.42007800 | 3.26137200 |
| H | 1.65588400 | -1.57306400 | 4.34393200 |
| H | 4.07716500 | -1.43573700 | 4.88372300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.491903

Electronic Energy (0K) + ZPE = -2582.901527

Enthalpy (333K) = -2582.849626

Free Energy (333K) = -2582.993628

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2583.938747

D'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 2.62410700 | 4.64579700 | -0.77205700 |
| C | 2.47288900 | 3.42663500 | -0.12199300 |
| C | 2.67149000 | 2.21173000 | -0.79153400 |
| C | 2.99262800 | 2.25188200 | -2.15443200 |
| C | 3.13869200 | 3.47375300 | -2.80421000 |
| C | 2.96067600 | 4.67390500 | -2.12228400 |
| H | 2.47032100 | 5.57241800 | -0.22339600 |
| H | 3.13791900 | 1.32203300 | -2.69616000 |
| H | 3.40467100 | 3.48320400 | -3.85929600 |
| H | 3.08110900 | 5.62360700 | -2.63812000 |
| C | 2.51974500 | 0.93545400 | -0.03919600 |
| C | 2.95216400 | -0.37434700 | -0.58914900 |
| N | 3.31386600 | -1.19710600 | 0.49851600 |
| C | 3.13834400 | -0.55473900 | 1.79098200 |
| C | 2.95282500 | 0.90593400 | 1.37198800 |
| C | 3.24794100 | 1.86684700 | 2.18439900 |
| C | 3.49926600 | 2.77308700 | 3.23339800 |
| S | 3.28883400 | -2.90264300 | 0.39374600 |
| O | 3.45167400 | -3.32864100 | 1.77685300 |
| O | 4.24045700 | -3.29555000 | -0.62672400 |
| C | 1.64723600 | -3.27540400 | -0.14640300 |
| C | 0.62844900 | -3.35963700 | 0.80405100 |
| C | 1.39225700 | -3.45427500 | -1.50398700 |
| C | -0.66543800 | -3.62214600 | 0.37611500 |
| H | 0.84682900 | -3.24321200 | 1.86406600 |
| C | 0.08976800 | -3.71663700 | -1.90950100 |
| H | 2.20226600 | -3.39442500 | -2.22493500 |

| | | | |
|----|-------------|-------------|-------------|
| C | -0.95538400 | -3.79809200 | -0.98329500 |
| H | -1.46973000 | -3.69918900 | 1.10774600 |
| H | -0.12180800 | -3.86635800 | -2.96727300 |
| C | -2.36135200 | -4.04091100 | -1.43183300 |
| H | -2.92746200 | -3.09769000 | -1.45750400 |
| H | -2.39804900 | -4.46821000 | -2.43981300 |
| H | -2.89315300 | -4.71444800 | -0.74931800 |
| H | 2.22801000 | -0.88998900 | 2.30842700 |
| H | 4.00245400 | -0.69778700 | 2.44351000 |
| O | 2.96880400 | -0.74245600 | -1.74715100 |
| Au | 0.33805800 | 0.60566100 | 0.05982800 |
| P | -1.99989900 | 0.45627500 | 0.13930500 |
| H | 3.85664800 | 2.08353000 | 4.03114800 |
| H | 4.33015100 | 3.46161300 | 3.04029300 |
| H | 2.60703100 | 3.27392700 | 3.62849100 |
| H | 2.13453100 | 3.42465700 | 0.91870800 |
| C | -2.73700100 | 2.05412400 | 0.61698100 |
| C | -3.84566400 | 2.14165200 | 1.46239100 |
| C | -2.16880000 | 3.22006900 | 0.08968800 |
| C | -4.38130800 | 3.38802900 | 1.77468900 |
| H | -4.29318500 | 1.23965600 | 1.87752700 |
| C | -2.71261200 | 4.46063700 | 0.39986000 |
| H | -1.29795400 | 3.15267500 | -0.56513500 |
| C | -3.81738200 | 4.54442600 | 1.24461800 |
| H | -5.24316200 | 3.45331400 | 2.43490300 |
| H | -2.26890300 | 5.36389900 | -0.01265500 |
| H | -4.23809200 | 5.51627100 | 1.49295600 |
| C | -2.59654200 | -0.76379400 | 1.35403000 |
| C | -3.64262100 | -1.64888400 | 1.08569300 |
| C | -1.96681200 | -0.79278800 | 2.60489700 |

| | | | |
|---|-------------|-------------|-------------|
| C | -4.05042500 | -2.55803300 | 2.05934400 |
| H | -4.14016300 | -1.63703500 | 0.11738900 |
| C | -2.38243600 | -1.69569000 | 3.57543000 |
| H | -1.14551300 | -0.10530300 | 2.81502300 |
| C | -3.42304700 | -2.58202700 | 3.30100900 |
| H | -4.86260200 | -3.24855400 | 1.84305800 |
| H | -1.89170900 | -1.71236700 | 4.54588900 |
| H | -3.74431500 | -3.29341800 | 4.05839200 |
| C | -2.69960700 | 0.02555500 | -1.48389300 |
| C | -4.04644500 | 0.25972100 | -1.78485300 |
| C | -1.86465000 | -0.55709400 | -2.44322900 |
| C | -4.55297800 | -0.10815000 | -3.02596300 |
| H | -4.69954400 | 0.72884900 | -1.04944900 |
| C | -2.37633500 | -0.91930600 | -3.68577000 |
| H | -0.81029000 | -0.72299300 | -2.21397500 |
| C | -3.71965600 | -0.69837300 | -3.97418600 |
| H | -5.60046900 | 0.07208800 | -3.25623300 |
| H | -1.72212100 | -1.37088500 | -4.42850500 |
| H | -4.11956200 | -0.97949100 | -4.94588200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.512850

Electronic Energy (0K) + ZPE = -2582.922261

Enthalpy (333K) = -2582.870314

Free Energy (333K) = -2583.015524

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2583.957993

TS_{D'}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|------------|
| C | -0.13144700 | -5.25231400 | 0.89226800 |
|---|-------------|-------------|------------|

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69380700 | -4.35038800 | 0.22650300 |
| C | 1.13027800 | -3.17548000 | 0.86489600 |
| C | 0.77586500 | -2.95683000 | 2.21176100 |
| C | -0.02915400 | -3.86889500 | 2.87048700 |
| C | -0.49368000 | -5.01182400 | 2.21116400 |
| H | -0.45853000 | -6.15823200 | 0.38815900 |
| H | 1.12263000 | -2.05656200 | 2.71240300 |
| H | -0.30725200 | -3.68995500 | 3.90642600 |
| H | -1.12023500 | -5.72572300 | 2.74084100 |
| C | 1.84418700 | -2.16815900 | 0.10466900 |
| C | 2.84743000 | -1.21288600 | 0.64776500 |
| N | 3.46220300 | -0.63914200 | -0.47018300 |
| C | 2.97776300 | -1.16965100 | -1.73369900 |
| C | 1.84770700 | -2.08301800 | -1.29945800 |
| C | 1.00166800 | -2.78945500 | -2.16154800 |
| C | 1.49590400 | -3.40682100 | -3.38158500 |
| S | 4.40210800 | 0.78912300 | -0.40008200 |
| O | 4.74950100 | 1.03083900 | -1.79220000 |
| O | 5.42527900 | 0.58899400 | 0.60669900 |
| C | 3.26137100 | 2.02538700 | 0.14200800 |
| C | 2.46243200 | 2.66041500 | -0.80728200 |
| C | 3.19338000 | 2.35826600 | 1.49467600 |
| C | 1.59078400 | 3.65736500 | -0.38716200 |
| H | 2.54713900 | 2.41043400 | -1.86292500 |
| C | 2.30877700 | 3.35073100 | 1.89125800 |
| H | 3.83217800 | 1.85503700 | 2.21526400 |
| C | 1.50236000 | 4.01961600 | 0.96078400 |
| H | 0.98928600 | 4.18668900 | -1.12390400 |
| H | 2.25011900 | 3.62898800 | 2.94281700 |
| C | 0.57757900 | 5.10494700 | 1.41254800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 0.06875300 | 5.58429700 | 0.56994800 |
| H | -0.19063000 | 4.71393400 | 2.09250900 |
| H | 1.12149700 | 5.88009100 | 1.96650500 |
| H | 2.65659300 | -0.37804300 | -2.41989900 |
| H | 3.74597100 | -1.77549100 | -2.23586300 |
| O | 3.06906300 | -0.93355900 | 1.80675100 |
| Au | 0.00807100 | -0.68976200 | -0.52579900 |
| P | -1.94129300 | 0.50286300 | -0.12307900 |
| H | 1.50759600 | -2.53770000 | -4.07596000 |
| H | 2.52105700 | -3.80317100 | -3.35368500 |
| H | 0.80021100 | -4.11939300 | -3.83523900 |
| H | 1.07550400 | -4.60233300 | -0.76372700 |
| C | -3.37957700 | -0.53817000 | -0.52687100 |
| C | -4.53585600 | -0.00850100 | -1.10480800 |
| C | -3.31684200 | -1.90040800 | -0.21300200 |
| C | -5.62082900 | -0.84082500 | -1.36506300 |
| H | -4.59353000 | 1.05076200 | -1.35134500 |
| C | -4.40523000 | -2.72437500 | -0.46966900 |
| H | -2.40906900 | -2.31291200 | 0.23044500 |
| C | -5.55623800 | -2.19425800 | -1.04860800 |
| H | -6.51912800 | -0.42784900 | -1.81803100 |
| H | -4.35104000 | -3.78287900 | -0.22588100 |
| H | -6.40525900 | -2.84108700 | -1.25803300 |
| C | -2.10780300 | 2.01590500 | -1.11420300 |
| C | -2.62685100 | 3.19907800 | -0.58412900 |
| C | -1.75192800 | 1.95063900 | -2.46679400 |
| C | -2.79729500 | 4.30764700 | -1.40944100 |
| H | -2.90236500 | 3.25886800 | 0.46756500 |
| C | -1.92971800 | 3.05904400 | -3.28498900 |
| H | -1.34270800 | 1.02588000 | -2.87654700 |

| | | | |
|---|-------------|------------|-------------|
| C | -2.45286100 | 4.23745100 | -2.75564800 |
| H | -3.20211200 | 5.22847400 | -0.99599800 |
| H | -1.65671400 | 3.00539500 | -4.33631300 |
| H | -2.58883900 | 5.10580900 | -3.39625100 |
| C | -2.08123400 | 0.93447300 | 1.63706700 |
| C | -3.32902800 | 1.11216500 | 2.24418100 |
| C | -0.91262200 | 1.09092000 | 2.38857200 |
| C | -3.39922000 | 1.45410500 | 3.59023600 |
| H | -4.24475500 | 0.98397100 | 1.66832900 |
| C | -0.98895200 | 1.43653000 | 3.73340400 |
| H | 0.05916300 | 0.94066500 | 1.91411800 |
| C | -2.23231900 | 1.61625400 | 4.33310000 |
| H | -4.36979700 | 1.59031200 | 4.06140500 |
| H | -0.07602900 | 1.55737300 | 4.31249800 |
| H | -2.29341400 | 1.87832000 | 5.38696800 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.503056

Electronic Energy (0K) + ZPE = -2582.910945

Enthalpy (333K) = -2582.860682

Free Energy (333K) = -2582.999089

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2583.947162

E'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|------------|
| C | -0.92104300 | -2.67883800 | 2.25711800 |
| C | -0.01861200 | -2.48421200 | 1.21917700 |
| C | 1.10455500 | -1.64579400 | 1.39820900 |
| C | 1.30675000 | -1.03205100 | 2.65194600 |
| C | 0.38725300 | -1.21553900 | 3.67016200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -0.72552400 | -2.03710500 | 3.47659900 |
| H | -1.76621600 | -3.34926000 | 2.11989800 |
| H | 2.17488500 | -0.39836400 | 2.80289300 |
| H | 0.53556100 | -0.71906500 | 4.62609300 |
| H | -1.43052000 | -2.19286200 | 4.29004700 |
| C | 2.04018100 | -1.43309100 | 0.32777200 |
| C | 3.51584400 | -1.30865600 | 0.57765100 |
| N | 4.09892200 | -1.28841500 | -0.67609400 |
| C | 3.14296800 | -1.38109900 | -1.76671800 |
| C | 1.82101600 | -1.38428500 | -1.03725400 |
| C | 0.58701100 | -1.24558600 | -1.70802700 |
| C | 0.56705500 | -1.47863800 | -3.16402600 |
| S | 5.79153200 | -1.14510800 | -0.93550000 |
| O | 5.90756000 | -1.15315900 | -2.38508100 |
| O | 6.44588500 | -2.15469400 | -0.12574100 |
| C | 6.16065300 | 0.46350200 | -0.31227900 |
| C | 5.96657000 | 1.56217300 | -1.14659100 |
| C | 6.63060100 | 0.60715300 | 0.99226800 |
| C | 6.25128600 | 2.82924100 | -0.65676000 |
| H | 5.61478700 | 1.42904800 | -2.16711300 |
| C | 6.91128400 | 1.88221300 | 1.45810900 |
| H | 6.76984200 | -0.26544700 | 1.62396000 |
| C | 6.72541100 | 3.00823100 | 0.64646700 |
| H | 6.11113500 | 3.69693800 | -1.29874300 |
| H | 7.28538700 | 2.01276500 | 2.47249700 |
| C | 7.03578300 | 4.37163800 | 1.17690500 |
| H | 6.86152700 | 5.15078700 | 0.42795600 |
| H | 6.41983800 | 4.60204800 | 2.05550600 |
| H | 8.08214800 | 4.43955100 | 1.50012100 |
| H | 3.23944400 | -0.53305800 | -2.45700200 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.29031400 | -2.30568200 | -2.34122300 |
| O | 4.09269700 | -1.22415600 | 1.64098800 |
| Au | -1.14825200 | -0.50562400 | -0.85385600 |
| P | -3.18060800 | 0.47723300 | -0.09809000 |
| H | 0.69865500 | -0.48615700 | -3.63429200 |
| H | 1.35273100 | -2.13892700 | -3.55126500 |
| H | -0.41631500 | -1.81783300 | -3.50810800 |
| H | -0.12135400 | -3.04802200 | 0.29458900 |
| C | -3.19581500 | 0.81283200 | 1.69364500 |
| C | -4.24870400 | 0.42696400 | 2.52576100 |
| C | -2.08935400 | 1.47863200 | 2.23641200 |
| C | -4.19704500 | 0.71277600 | 3.88784700 |
| H | -5.11149300 | -0.09559000 | 2.11643600 |
| C | -2.05104200 | 1.77481800 | 3.59344200 |
| H | -1.25782700 | 1.76934800 | 1.59225000 |
| C | -3.10382400 | 1.38794400 | 4.42063300 |
| H | -5.01856500 | 0.40838500 | 4.53240800 |
| H | -1.19184400 | 2.29704100 | 4.00869000 |
| H | -3.06910300 | 1.61173600 | 5.48453700 |
| C | -4.60736200 | -0.59705600 | -0.45610700 |
| C | -5.90445600 | -0.08882200 | -0.58299500 |
| C | -4.38485200 | -1.97168000 | -0.58672700 |
| C | -6.96537300 | -0.95259300 | -0.83180600 |
| H | -6.08584500 | 0.98125900 | -0.48564800 |
| C | -5.44976400 | -2.83189100 | -0.83236200 |
| H | -3.36928100 | -2.36316800 | -0.50641600 |
| C | -6.73861000 | -2.32153600 | -0.95552400 |
| H | -7.97273100 | -0.55503500 | -0.93178200 |
| H | -5.27123300 | -3.89971100 | -0.93626200 |
| H | -7.57113000 | -2.99269600 | -1.15458800 |

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|---|-------------|------------|-------------|
| C | -3.53107100 | 2.07167000 | -0.91227000 |
| C | -4.09051200 | 3.15364800 | -0.22786900 |
| C | -3.24889100 | 2.18448400 | -2.27837900 |
| C | -4.36310200 | 4.33757700 | -0.90730900 |
| H | -4.31528100 | 3.07474800 | 0.83490400 |
| C | -3.52948400 | 3.36660200 | -2.95306200 |
| H | -2.80851400 | 1.34155300 | -2.81259900 |
| C | -4.08351700 | 4.44438200 | -2.26632000 |
| H | -4.79680000 | 5.17855300 | -0.37103600 |
| H | -3.30889200 | 3.44940900 | -4.01489100 |
| H | -4.29599100 | 5.37213300 | -2.79295300 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.557577

Electronic Energy (0K) + ZPE = -2582.964416

Enthalpy (333K) = -2582.912784

Free Energy (333K) = -2583.061086

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2584.000794

TS_{E'}

Number of imaginary frequencies: 1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.15231500 | -3.77274200 | -1.16527000 |
| C | -0.07905000 | -3.45044600 | -0.53763500 |
| C | -1.07372500 | -2.71773900 | -1.26279700 |
| C | -0.87159000 | -2.42508800 | -2.62280800 |
| C | 0.32811500 | -2.77149400 | -3.20956100 |
| C | 1.34527800 | -3.43019600 | -2.48196400 |
| H | 1.90458300 | -4.33428800 | -0.61549600 |
| H | -1.63043200 | -1.87758200 | -3.17575800 |
| H | 0.50532000 | -2.51636100 | -4.25190000 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.27336000 | -3.69286500 | -2.98391000 |
| C | -2.06772800 | -2.16437800 | -0.41414000 |
| C | -3.41501800 | -1.61687000 | -0.61651000 |
| N | -3.87383800 | -1.34643800 | 0.68496400 |
| C | -2.89426000 | -1.65495100 | 1.73116300 |
| C | -1.72224200 | -2.09215600 | 0.91019200 |
| C | -0.39563900 | -2.40247500 | 1.31216700 |
| C | -0.14978000 | -3.17530200 | 2.55927000 |
| S | -5.32696400 | -0.52152100 | 1.00933900 |
| O | -5.31345200 | -0.35980000 | 2.45635600 |
| O | -6.40709600 | -1.23093300 | 0.34938400 |
| C | -5.08520200 | 1.04836500 | 0.23382900 |
| C | -4.26842400 | 1.98731500 | 0.86550000 |
| C | -5.68696800 | 1.31217100 | -0.99125700 |
| C | -4.05497600 | 3.20837700 | 0.24607400 |
| H | -3.81952300 | 1.77022500 | 1.83265100 |
| C | -5.46645000 | 2.54642300 | -1.59063900 |
| H | -6.31333600 | 0.56154700 | -1.46492200 |
| C | -4.65057900 | 3.50657800 | -0.98717800 |
| H | -3.42253800 | 3.95365600 | 0.72667300 |
| H | -5.93556200 | 2.76888000 | -2.54745400 |
| C | -4.42621400 | 4.84083100 | -1.62480100 |
| H | -4.97897900 | 5.62595000 | -1.09202800 |
| H | -3.36740800 | 5.12505600 | -1.59490600 |
| H | -4.75689700 | 4.85407700 | -2.66836400 |
| H | -2.67034200 | -0.77757900 | 2.35054400 |
| H | -3.25038200 | -2.45757700 | 2.39180100 |
| O | -4.02124600 | -1.40040200 | -1.64419800 |
| Au | 1.06449100 | -0.98418300 | 0.70792100 |
| P | 2.58537900 | 0.70065100 | 0.11156700 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.26856100 | -2.45990700 | 3.39013500 |
| H | -0.85581600 | -3.99872900 | 2.72795600 |
| H | 0.87802400 | -3.54692500 | 2.61836300 |
| H | -0.42430800 | -4.15288300 | 0.22778300 |
| C | 3.57419000 | 1.31328800 | 1.51324400 |
| C | 2.93702700 | 1.45977300 | 2.75066100 |
| C | 4.92085100 | 1.66119500 | 1.37894000 |
| C | 3.64084000 | 1.95509200 | 3.84166500 |
| H | 1.88670900 | 1.18473100 | 2.85546900 |
| C | 5.62205700 | 2.15054200 | 2.47711700 |
| H | 5.42383000 | 1.55179200 | 0.41920600 |
| C | 4.98417400 | 2.29716200 | 3.70527600 |
| H | 3.14250200 | 2.06763500 | 4.80178400 |
| H | 6.67096400 | 2.41768700 | 2.37078600 |
| H | 5.53679700 | 2.67695300 | 4.56173000 |
| C | 1.71444200 | 2.14013400 | -0.58406200 |
| C | 2.26155300 | 3.42566000 | -0.52488500 |
| C | 0.48218000 | 1.93690400 | -1.21496100 |
| C | 1.58109400 | 4.49517200 | -1.09668400 |
| H | 3.22032700 | 3.59110700 | -0.03471500 |
| C | -0.19238000 | 3.00963700 | -1.78817700 |
| H | 0.05058200 | 0.93445400 | -1.25179400 |
| C | 0.35714800 | 4.28749800 | -1.72778900 |
| H | 2.00790000 | 5.49428700 | -1.04819200 |
| H | -1.15094200 | 2.84752500 | -2.27663200 |
| H | -0.17036500 | 5.12764800 | -2.17416900 |
| C | 3.77396000 | 0.13060700 | -1.14603600 |
| C | 4.43010300 | -1.08524800 | -0.91571900 |
| C | 4.05048100 | 0.86060500 | -2.30346700 |
| C | 5.36010900 | -1.55896900 | -1.83205000 |

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|---|------------|-------------|-------------|
| H | 4.20764000 | -1.66103400 | -0.01554500 |
| C | 4.97763700 | 0.37575300 | -3.22283200 |
| H | 3.54640400 | 1.80723100 | -2.49109900 |
| C | 5.63215300 | -0.82864300 | -2.98764300 |
| H | 5.87002400 | -2.50191400 | -1.64802400 |
| H | 5.18903600 | 0.94537000 | -4.12490100 |
| H | 6.35565700 | -1.20331600 | -3.70824200 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.539469

Electronic Energy (0K) + ZPE = -2582.946403

Enthalpy (333K) = -2582.896003

Free Energy (333K) = -2583.036792

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2583.983082

F'

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | -1.11145500 | -4.40437200 | 0.44368300 |
| C | 0.20490500 | -3.95379000 | -0.06909900 |
| C | 1.14885000 | -3.40790600 | 0.96703300 |
| C | 0.96429300 | -3.73702400 | 2.33816000 |
| C | -0.21704500 | -4.30411700 | 2.71134900 |
| C | -1.27374600 | -4.59873900 | 1.76815700 |
| H | -1.89113600 | -4.66278100 | -0.27126500 |
| H | 1.71095100 | -3.44829000 | 3.07343300 |
| H | -0.39928700 | -4.51001800 | 3.76400400 |
| H | -2.21116600 | -4.99382900 | 2.15209400 |
| C | 1.97510800 | -2.52309600 | 0.32332100 |
| C | 3.07633800 | -1.61122300 | 0.61211300 |
| N | 3.37652200 | -1.02550100 | -0.64422700 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.54127800 | -1.50066600 | -1.76726800 |
| C | 1.54099100 | -2.34181700 | -1.03676700 |
| C | 0.40535400 | -3.09218800 | -1.31389800 |
| C | -0.16857600 | -3.43762000 | -2.64770600 |
| S | 4.44219600 | 0.28023100 | -0.84003400 |
| O | 4.45071500 | 0.50887500 | -2.27852600 |
| O | 5.67094500 | -0.01437300 | -0.12736600 |
| C | 3.60140800 | 1.62150000 | -0.04792500 |
| C | 2.63242300 | 2.31762800 | -0.76997600 |
| C | 3.90770800 | 1.95645400 | 1.26813800 |
| C | 1.96685500 | 3.36987600 | -0.15661000 |
| H | 2.43013000 | 2.06504200 | -1.80916000 |
| C | 3.23350200 | 3.01669800 | 1.86080300 |
| H | 4.66794100 | 1.40120100 | 1.81060500 |
| C | 2.25992200 | 3.73846000 | 1.16229800 |
| H | 1.21702700 | 3.93096200 | -0.71516500 |
| H | 3.47439200 | 3.29894200 | 2.88454400 |
| C | 1.53446800 | 4.87248300 | 1.81486400 |
| H | 1.24051000 | 5.63648200 | 1.08638400 |
| H | 0.61574900 | 4.52198900 | 2.30490100 |
| H | 2.14646400 | 5.35135300 | 2.58704500 |
| H | 2.09928500 | -0.66506000 | -2.32231500 |
| H | 3.13812800 | -2.09939300 | -2.46779800 |
| O | 3.61719600 | -1.33726300 | 1.66299700 |
| Au | -0.44467800 | -0.97573600 | -0.70532000 |
| P | -1.89658700 | 0.73453600 | -0.06954400 |
| H | 0.11760000 | -2.69614800 | -3.40266900 |
| H | 0.19782000 | -4.41678900 | -2.98714800 |
| H | -1.26377300 | -3.49061300 | -2.62055400 |
| H | 0.69270500 | -4.90151200 | -0.40276000 |

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|---|-------------|-------------|-------------|
| C | -3.62829800 | 0.26654500 | -0.38192600 |
| C | -4.06744900 | -0.97493200 | 0.09476100 |
| C | -4.51195500 | 1.10202000 | -1.06748200 |
| C | -5.38188100 | -1.37233200 | -0.11077600 |
| H | -3.37885600 | -1.62474300 | 0.63676800 |
| C | -5.82706300 | 0.69316600 | -1.27665600 |
| H | -4.18114700 | 2.07064500 | -1.43829200 |
| C | -6.26109000 | -0.53905000 | -0.80068000 |
| H | -5.72107200 | -2.33524700 | 0.26401200 |
| H | -6.51329000 | 1.34485500 | -1.81246400 |
| H | -7.28877200 | -0.85387200 | -0.96719900 |
| C | -1.59941300 | 2.28991600 | -0.95962600 |
| C | -1.78043700 | 3.53188000 | -0.34549500 |
| C | -1.22394300 | 2.22321900 | -2.30630300 |
| C | -1.58326400 | 4.69929800 | -1.07752100 |
| H | -2.07283200 | 3.59178400 | 0.70185800 |
| C | -1.03070800 | 3.39272900 | -3.03228600 |
| H | -1.08240700 | 1.25211700 | -2.78301300 |
| C | -1.20874200 | 4.63029800 | -2.41689600 |
| H | -1.72154700 | 5.66550500 | -0.59743600 |
| H | -0.73709900 | 3.33894500 | -4.07797900 |
| H | -1.05245500 | 5.54519800 | -2.98385300 |
| C | -1.75795900 | 1.07088200 | 1.71197800 |
| C | -2.85612900 | 1.51799400 | 2.45334700 |
| C | -0.51869700 | 0.89685700 | 2.33771900 |
| C | -2.70955800 | 1.79109500 | 3.80916200 |
| H | -3.82419100 | 1.65456600 | 1.97298500 |
| C | -0.37742900 | 1.17580900 | 3.69239000 |
| H | 0.33932200 | 0.54869000 | 1.75923300 |
| C | -1.47361500 | 1.61993800 | 4.42738000 |

| | | | |
|---|-------------|------------|------------|
| H | -3.56520300 | 2.13659200 | 4.38461300 |
| H | 0.58837300 | 1.03990300 | 4.17372600 |
| H | -1.36512000 | 1.83031200 | 5.48901600 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -2583.571203

Electronic Energy (0K) + ZPE = -2582.975991

Enthalpy (333K) = -2582.925693

Free Energy (333K) = -2583.064300

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -2584.016041

4a

Number of imaginary frequencies: 0

| | | | |
|---|-------------|-------------|-------------|
| C | 5.07187900 | 0.81278700 | 0.82849900 |
| C | 3.80672500 | 0.28150900 | 0.63954200 |
| C | 2.91802300 | 0.87843600 | -0.28108600 |
| C | 3.28615800 | 2.00507600 | -1.00663600 |
| C | 4.56138100 | 2.53255200 | -0.80627300 |
| C | 5.44418000 | 1.94467600 | 0.09831500 |
| H | 5.76739600 | 0.36046800 | 1.53465700 |
| H | 2.59717800 | 2.46118500 | -1.71419700 |
| H | 4.87156500 | 3.41358400 | -1.36448100 |
| H | 6.43529100 | 2.37176500 | 0.23718200 |
| C | 1.70155200 | 0.07844600 | -0.24886900 |
| C | 0.38861700 | 0.03537100 | -0.89658500 |
| N | -0.22265900 | -1.11107000 | -0.33688100 |
| C | 0.61414000 | -1.78628000 | 0.66638500 |
| C | 1.82648900 | -0.93325600 | 0.63072800 |
| C | 3.16916000 | -0.93426500 | 1.29136900 |
| C | 3.94900600 | -2.23050900 | 1.07478200 |

| | | | |
|---|-------------|-------------|-------------|
| S | -1.78033700 | -1.63705400 | -0.72773900 |
| O | -1.97054700 | -2.82348200 | 0.09712500 |
| O | -1.89220600 | -1.71943300 | -2.17391700 |
| C | -2.83240200 | -0.34308800 | -0.13598300 |
| C | -3.21171900 | -0.34772400 | 1.20644200 |
| C | -3.25356800 | 0.65607900 | -1.00680600 |
| C | -4.02677700 | 0.67090600 | 1.67353600 |
| H | -2.88526900 | -1.14631800 | 1.86897700 |
| C | -4.07229500 | 1.66719600 | -0.51814000 |
| H | -2.94076300 | 0.63950300 | -2.04680800 |
| C | -4.46783900 | 1.69189000 | 0.82139200 |
| H | -4.33608400 | 0.67811700 | 2.71790100 |
| H | -4.41192900 | 2.45339600 | -1.19032700 |
| C | -5.34912900 | 2.77905700 | 1.35066100 |
| H | -6.28382400 | 2.36898400 | 1.75394800 |
| H | -4.86118200 | 3.31824900 | 2.17258300 |
| H | -5.60747700 | 3.50772400 | 0.57557200 |
| H | 0.12373400 | -1.79812300 | 1.64930600 |
| H | 0.81364100 | -2.82738400 | 0.37888500 |
| O | -0.12318500 | 0.77635500 | -1.71016500 |
| H | 4.06984000 | -2.43806700 | 0.00454800 |
| H | 4.94669100 | -2.16298500 | 1.52275300 |
| H | 3.43424400 | -3.08225700 | 1.53467900 |
| H | 3.05697400 | -0.76816300 | 2.37483100 |

SMD-M06/6-31G(d,p)/SDD

Electronic Energy (0K) = -1412.166716

Electronic Energy (0K) + ZPE = -1411.846417

Enthalpy (333K) = -1411.819599

Free Energy (333K) = -1411.907369

SMD-M06/6-311++G(d,p)/SDD

Electronic Energy (0K) = -1412.435738