# Supporting Information

# Mechanistic Study on Cu(I) Catalyzed Carboxylation of C-F Bond with $CO_2$: A DFT Study

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## 1. Complete Gaussian 16 reference.

Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

## 2. Energy profiles about the generation of catalyst species A and B.

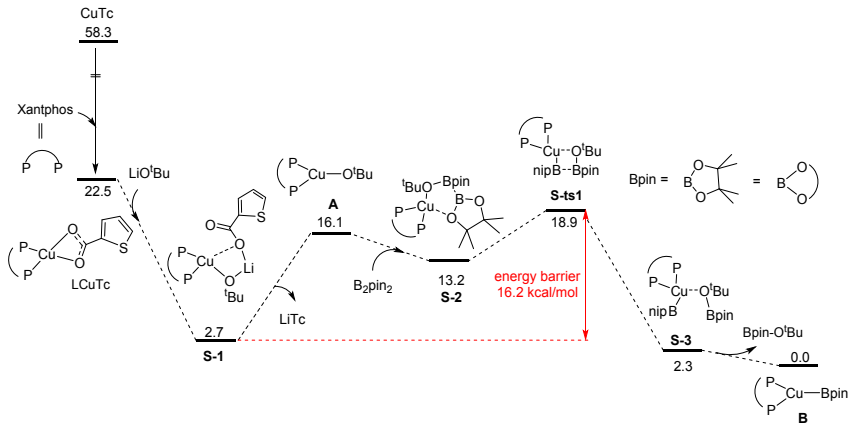


**Fig. S1** Energy profiles about the generation of catalyst species **A** and **B**. For clarity, LCuBpin (**B**) was set as the energy reference point. The relative free energies are given in kcal/mol.

First, coordination of Xantphos to CuTc generates LCuTc (L= Xantphos), from which the ligand exchange occurs via a coordination-dissociation mode (LCuTc + LiO$^t$Bu→**S-1**→**A** + LiTc). All efforts in locating the transition states for formation of **S-1** were failed, but the partial optimization (Fig. S2) by fixing the Cu-O(O$^t$Bu) bond at different distances indicates the easiness of this elementary step. From **A**, the approaching of Bpin-Bpin generates the intermediate **S-2** with two groups of Lewis acid-base interactions (i.e. Cu-O(Bpin) and O(O$^t$Bu)-B). Thereafter, the dissociation of Bpin-O$^t$Bu occurs via the transition state of **S-ts1**, resulting in the formation of the intermediate LCuBpin (**B**). The free energy barrier for this step is 6.7 kcal/mol. And the maximum activation barrier for the formation of **B** is 16.2 kcal/mol (**S-1**→**S-ts1**).

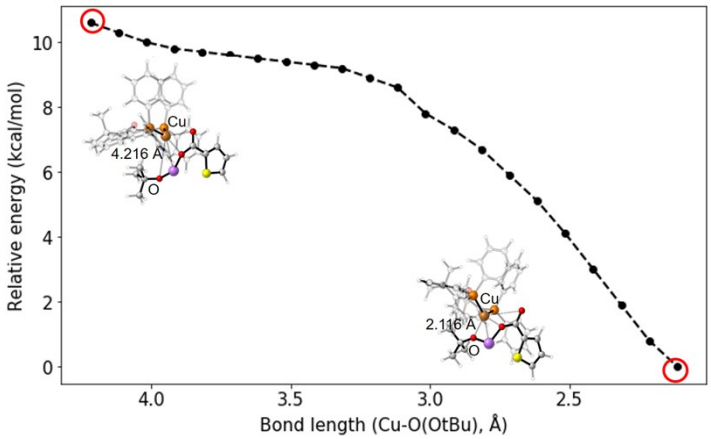


**Fig. S2** The energy changes along with the approaching of LiO$^t$Bu to CuTc. The partial optimization is conducted by fixing the Cu-O(O$^t$Bu) bond at different distances.

## 3. The energy changes along with the dissociation of Cu-F bond.

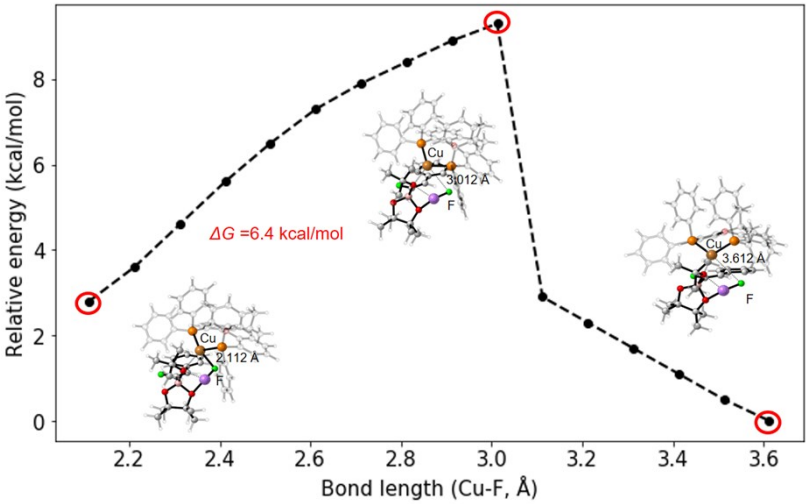


**Fig. S3** The energy changes along with the dissociation of Cu-F bond. The partial optimization is conducted by fixing the Cu-F bond at different distances.

From the starting point to the highest point, it needs to experience a maximum barriers of 6.4 kcal/mol by fixing the Cu-F bond at different distances, indicating that the process can easily occur.

## 4. Energy profiles about the transmetalation process without considering the role of the lithium salt.

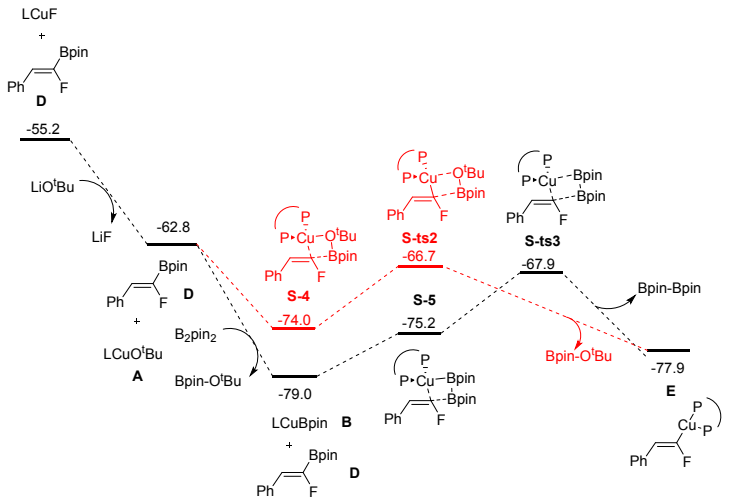


**Fig. S4** Energy profiles for transmetalation process on **D** without considering the role of the lithium salt. The relative free energies are given in kcal/mol.

By comparing with considering the role of the lithium salt pathway, the process coordinated by the lithium salt is actually favored.

## 5. Cartesian coordinates and electronic energies.

### 1a

Total electronic energy = -508.206846

Thermal corrections to Gibbs free energy = 0.085095

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.32318800 | 1.33587200 | 0.00004400 |
| C | -0.31814300 | 0.35179500 | -0.00016300 |
| C | -0.71245800 | -0.99965000 | -0.00017100 |
| C | -2.06196100 | -1.34232700 | -0.00008600 |
| C | -3.04898500 | -0.35424700 | 0.00006200 |
| C | -2.67170600 | 0.98914900 | 0.00014200 |
| H | -1.03652200 | 2.38448800 | 0.00012900 |
| H | 0.03641500 | -1.78153700 | -0.00023600 |
| H | -2.34414800 | -2.39155300 | -0.00012200 |
| H | -4.09972300 | -0.62906500 | 0.00014600 |
| H | -3.42753500 | 1.76951500 | 0.00028600 |
| C | 1.07584000 | 0.80058000 | -0.00015700 |
| H | 1.25207600 | 1.87111400 | -0.00027300 |
| C | 2.18327600 | 0.06072100 | 0.00002300 |
| F | 3.40913700 | 0.56924000 | -0.00001300 |
| F | 2.24457200 | -1.26638600 | 0.00022400 |

### 2a

Total electronic energy = -604.593428
Thermal corrections to Gibbs free energy = 0.093988
No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 3.04706300 | 1.21234200 | 0.00009400 |
| C | 1.66789500 | 1.02618800 | 0.00010100 |
| C | 1.12304500 | -0.27413500 | -0.00002500 |
| C | 2.01033600 | -1.36776900 | -0.00012700 |
| C | 3.38895500 | -1.17717600 | -0.00013100 |
| C | 3.91392600 | 0.11637800 | -0.00001800 |
| H | 3.44928200 | 2.22165100 | 0.00018400 |
| H | 1.00649000 | 1.88212900 | 0.00018400 |
| H | 1.60308800 | -2.37557000 | -0.00022500 |
| H | 4.05324800 | -2.03679300 | -0.00020500 |
| H | 4.98932000 | 0.27004200 | -0.00000700 |
| C | -0.30774400 | -0.55738500 | -0.00003100 |
| H | -0.60079500 | -1.60240400 | -0.00007900 |
| C | -1.34982700 | 0.28977200 | 0.00000500 |
| C | -2.77100300 | -0.15180400 | 0.00003100 |
| O | -3.68974900 | 0.72882300 | -0.00043400 |
| O | -3.02860700 | -1.40403300 | 0.00043800 |
| Li | -4.77918900 | -0.77625300 | -0.00014700 |
| F | -1.19467800 | 1.63032500 | 0.00012900 |

**A**

Total electronic energy = -2694.171986
Thermal corrections to Gibbs free energy = 0.646201
No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 1.85194500 | -0.38203500 | -0.14352700 |
| P | -1.91931200 | -0.00783200 | -0.06755600 |
| C | 1.94803500 | -0.15895700 | 1.67664800 |
| C | 3.28279500 | -1.45435300 | -0.52187800 |
| C | 2.34476000 | 1.26260200 | -0.78723600 |
| C | -1.90135000 | -0.08766000 | 1.76436800 |
| C | -2.05998800 | 1.78171200 | -0.48420700 |
| C | -3.58002600 | -0.64325500 | -0.50321300 |
| C | 2.45598000 | 0.99260000 | 2.28962000 |
| C | 1.46739100 | -1.20565500 | 2.47796100 |
| C | 3.09355100 | -2.46846400 | -1.47333000 |

| | | | |
|---|---|---|---|
| C | 4.52838900 | -1.30384700 | 0.10679600 |
| C | 1.41092200 | 2.29527300 | -0.65561000 |
| C | 3.52965900 | 1.55080600 | -1.47564400 |
| C | -2.17159100 | -1.32928100 | 2.36351500 |
| C | -1.54124200 | 0.99695900 | 2.57155400 |
| C | -3.23647000 | 2.37863500 | -0.95993700 |
| C | -0.90305600 | 2.56913700 | -0.47398300 |
| C | -3.71025800 | -1.33418800 | -1.71562300 |
| C | -4.70785400 | -0.45269900 | 0.30925300 |
| H | 2.82946100 | 1.81020100 | 1.68149300 |
| C | 2.48457900 | 1.09493300 | 3.68156800 |
| C | 1.50742600 | -1.10535100 | 3.86600600 |
| H | 1.05800600 | -2.09598700 | 2.01091400 |
| C | 4.15908500 | -3.31065600 | -1.80198200 |
| H | 2.10276100 | -2.61968800 | -1.90501500 |
| C | 5.58519200 | -2.14787000 | -0.22865600 |
| H | 4.66385600 | -0.53300000 | 0.86057300 |
| O | 0.24456500 | 1.98161900 | 0.01648700 |
| C | 1.58969500 | 3.58163500 | -1.16395300 |
| H | 4.27649400 | 0.77482500 | -1.60279100 |
| C | 3.73810200 | 2.82400800 | -2.00858400 |
| H | -2.44331800 | -2.17976400 | 1.74426700 |
| C | -2.10510800 | -1.47250000 | 3.74728900 |
| H | -1.31825900 | 1.95820900 | 2.12302600 |
| C | -1.46308200 | 0.84571900 | 3.95611600 |
| H | -4.15446000 | 1.80344200 | -0.99059400 |
| C | -3.22360500 | 3.69401000 | -1.42160300 |
| C | -0.84999600 | 3.88318500 | -0.94750000 |
| H | -2.82742000 | -1.51972700 | -2.32100500 |
| C | -4.95683100 | -1.81543200 | -2.11780700 |
| H | -4.60833100 | 0.07074800 | 1.25544700 |
| C | -5.95034700 | -0.94074800 | -0.09232100 |
| H | 2.87970400 | 1.99420500 | 4.14670500 |
| C | 2.01414500 | 0.04641100 | 4.47184300 |
| H | 1.12456900 | -1.91904500 | 4.47412300 |
| C | 5.40106900 | -3.14989900 | -1.18702700 |
| H | 4.01051000 | -4.10066900 | -2.53307800 |
| H | 6.54920400 | -2.02989100 | 0.25878200 |
| C | 0.49596200 | 4.61173300 | -0.86396700 |
| C | 2.77970400 | 3.82930100 | -1.85614800 |
| H | 4.65648800 | 3.03666700 | -2.54763700 |
| H | -2.32561200 | -2.43541900 | 4.19966000 |
| C | -1.74985200 | -0.38421600 | 4.54750400 |
| H | -1.17277300 | 1.69198300 | 4.57179400 |

| | | | |
|---|---|---|---|
| C | -2.04009700 | 4.43590900 | -1.42735200 |
| H | -4.14058400 | 4.14207300 | -1.79244100 |
| H | -5.04806800 | -2.35739300 | -3.05455800 |
| C | -6.07615800 | -1.61930200 | -1.30800700 |
| H | -6.81996400 | -0.79365000 | 0.54220800 |
| H | 2.03538200 | 0.12776800 | 5.55506300 |
| H | 6.22537900 | -3.80992800 | -1.44390700 |
| C | 0.69063200 | 5.10793500 | 0.59446900 |
| C | 0.55984800 | 5.81303700 | -1.81456900 |
| H | 2.96694900 | 4.81022200 | -2.27903700 |
| H | -1.68902300 | -0.49757100 | 5.62616000 |
| H | -2.05087800 | 5.45068200 | -1.80950400 |
| H | -7.04478700 | -2.00210500 | -1.61721600 |
| H | 0.65954700 | 4.27270400 | 1.30038900 |
| H | -0.10098100 | 5.81635600 | 0.86249000 |
| H | 1.66013300 | 5.60788700 | 0.69672000 |
| H | 1.52331900 | 6.32324400 | -1.72479100 |
| H | -0.21090000 | 6.54718300 | -1.56214400 |
| H | 0.42313500 | 5.50924500 | -2.85738500 |
| Cu | -0.18997600 | -1.20557200 | -0.83827300 |
| O | -0.04934900 | -2.82811400 | -1.81315400 |
| C | -0.37709600 | -4.07974600 | -1.28296600 |
| C | 0.26171700 | -5.15743200 | -2.18200800 |
| H | 0.01893600 | -6.17513400 | -1.84973300 |
| H | -0.09097400 | -5.03198500 | -3.21148800 |
| H | 1.35223100 | -5.04597300 | -2.18132700 |
| C | -1.90509700 | -4.28301700 | -1.25283600 |
| H | -2.37239500 | -3.52391400 | -0.61510700 |
| H | -2.31688400 | -4.16939300 | -2.26196900 |
| H | -2.18676800 | -5.27389200 | -0.87192400 |
| C | 0.17052300 | -4.23544800 | 0.15396600 |
| H | 1.25044700 | -4.05034300 | 0.16550500 |
| H | -0.31120200 | -3.50016000 | 0.81375400 |
| H | -0.01517100 | -5.23486500 | 0.56989600 |

**B**

Total electronic energy =-2872.372609

Thermal corrections to Gibbs free energy = 0.697388

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 2.89827700 | 0.16828800 | -0.07521600 |
| O | 3.57934500 | -0.74443000 | 0.73995500 |

| | | | |
|---|---|---|---|
| O | 3.81342500 | 1.10559300 | -0.57026000 |
| C | 5.00754500 | -0.53210900 | 0.61151200 |
| C | 5.07937300 | 0.95053100 | 0.11777800 |
| C | 5.51487400 | -1.54028600 | -0.42767100 |
| C | 5.66832200 | -0.79768200 | 1.96057300 |
| C | 6.21125900 | 1.25428100 | -0.85855300 |
| C | 5.08637800 | 1.96928700 | 1.26459500 |
| H | 6.60171600 | -1.48693400 | -0.55458600 |
| H | 5.03778500 | -1.37467000 | -1.39809800 |
| H | 5.25814400 | -2.55030400 | -0.09155100 |
| H | 6.74340100 | -0.58467800 | 1.91995700 |
| H | 5.54046200 | -1.85089500 | 2.23137000 |
| H | 5.22089800 | -0.19096200 | 2.75062100 |
| H | 7.18883000 | 1.08162700 | -0.39245000 |
| H | 6.16183300 | 2.30478400 | -1.16377100 |
| H | 6.13862700 | 0.63912100 | -1.75799300 |
| H | 6.03875300 | 1.97105800 | 1.80621100 |
| H | 4.27841600 | 1.76346100 | 1.97283300 |
| H | 4.92379300 | 2.96898800 | 0.84885400 |
| Cu | 0.93455700 | 0.11749500 | -0.47677000 |
| P | -0.27797300 | -1.84802600 | -0.65401300 |
| P | -0.54322600 | 1.89999800 | -0.45041300 |
| C | -1.85911200 | -1.94115000 | -1.57889600 |
| C | 0.65599700 | -3.32040300 | -1.22154300 |
| C | -0.76663500 | -2.32566100 | 1.05216400 |
| C | -2.04698600 | 1.92194300 | -1.50982000 |
| C | -1.17864100 | 2.09902800 | 1.26819900 |
| C | 0.20332000 | 3.53823000 | -0.80498500 |
| C | -3.00527500 | -2.57875400 | -1.08684100 |
| C | -1.91081500 | -1.31346000 | -2.83205300 |
| C | 2.02428100 | -3.37804200 | -0.90753300 |
| C | 0.06584600 | -4.37004600 | -1.93825300 |
| C | -1.43866000 | -1.36639900 | 1.81534400 |
| C | -0.43146200 | -3.53036600 | 1.68101700 |
| C | -1.89251000 | 2.24683200 | -2.86810000 |
| C | -3.31090700 | 1.53388600 | -1.04776600 |
| C | -1.07055200 | 3.27547700 | 2.02154100 |
| C | -1.65967400 | 0.96138600 | 1.92536200 |
| C | 1.60159600 | 3.64099000 | -0.81739000 |
| C | -0.57676000 | 4.68196800 | -1.04264800 |
| H | -2.97715900 | -3.06307400 | -0.11570000 |
| C | -4.18086900 | -2.59205400 | -1.83886400 |
| C | -3.07947100 | -1.34196800 | -3.58872400 |
| H | -1.03636800 | -0.78706400 | -3.20425600 |

| | | | |
|---|---|---|---|
| C | 2.78244600 | -4.48032400 | -1.30122600 |
| H | 2.48763300 | -2.56329600 | -0.35814000 |
| C | 0.83346000 | -5.46476200 | -2.33815500 |
| H | -0.99031300 | -4.32952700 | -2.18514500 |
| O | -1.76277600 | -0.18963000 | 1.16990500 |
| C | -1.76957500 | -1.52928500 | 3.16071600 |
| H | 0.09546900 | -4.29625100 | 1.12250700 |
| C | -0.74931000 | -3.73068400 | 3.02522800 |
| H | -0.91821400 | 2.54986700 | -3.24186900 |
| C | -2.98244900 | 2.20886600 | -3.73492300 |
| H | -3.45132500 | 1.26945000 | -0.00656700 |
| C | -4.39765800 | 1.48471700 | -1.92058600 |
| H | -0.68917500 | 4.17666200 | 1.55526700 |
| C | -1.42157800 | 3.28189600 | 3.37138600 |
| C | -2.01014100 | 0.92759600 | 3.27703800 |
| H | 2.21409900 | 2.75990800 | -0.65007300 |
| C | 2.20704100 | 4.87699700 | -1.05654700 |
| H | -1.65989200 | 4.60419600 | -1.04702100 |
| C | 0.03339400 | 5.91192400 | -1.28029600 |
| H | -5.06609300 | -3.08576800 | -1.44674300 |
| C | -4.21831900 | -1.97890200 | -3.09184200 |
| H | -3.10916800 | -0.84362500 | -4.55220800 |
| C | 2.19154700 | -5.52257100 | -2.01924400 |
| H | 3.84016100 | -4.51795000 | -1.05501900 |
| H | 0.36972100 | -6.27261400 | -2.89783800 |
| C | -2.54648500 | -0.39486400 | 3.83754500 |
| C | -1.40476600 | -2.73929800 | 3.75982300 |
| H | -0.47901700 | -4.66510300 | 3.50801500 |
| H | -2.84867700 | 2.47732200 | -4.77948000 |
| C | -4.24049000 | 1.82753100 | -3.26326000 |
| H | -5.37017500 | 1.17677700 | -1.54717500 |
| C | -1.87871500 | 2.11889800 | 3.99594300 |
| H | -1.32851600 | 4.19855700 | 3.94619300 |
| H | 3.29132700 | 4.94591400 | -1.06972600 |
| C | 1.42819900 | 6.01098700 | -1.28602500 |
| H | -0.57694300 | 6.79225200 | -1.46290900 |
| H | -5.13461500 | -1.98808500 | -3.67557900 |
| H | 2.78758600 | -6.37554600 | -2.33234900 |
| C | -4.03884400 | -0.52398600 | 3.42921300 |
| C | -2.43826900 | -0.45626800 | 5.36589000 |
| H | -1.63141300 | -2.91624400 | 4.80553400 |
| H | -5.09008500 | 1.79244400 | -3.93938000 |
| H | -2.13135800 | 2.14650700 | 5.05020300 |
| H | 1.90275700 | 6.97025400 | -1.47469000 |

| | | | |
|---|---|---|---|
| H | -4.15120000 | -0.49392800 | 2.34135800 |
| H | -4.62227900 | 0.29753900 | 3.85949400 |
| H | -4.44843800 | -1.47407600 | 3.78985800 |
| H | -2.84461000 | -1.39929500 | 5.74309400 |
| H | -3.02214700 | 0.34584100 | 5.82687400 |
| H | -1.39942900 | -0.36686700 | 5.69933100 |

**B1**

Total electronic energy = -3380.611614

Thermal corrections to Gibbs free energy = 0.811182

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | -1.24682000 | 1.04839000 | -1.60373000 |
| O | -1.36107100 | 2.42329600 | -1.46860800 |
| O | -2.43064400 | 0.50642000 | -2.08059000 |
| C | -2.60490800 | 2.85364200 | -2.08379400 |
| C | -3.45646200 | 1.53841900 | -2.06079300 |
| C | -2.25333100 | 3.32328000 | -3.49897900 |
| C | -3.17086000 | 4.00618300 | -1.26121600 |
| C | -4.36866500 | 1.33408300 | -3.26463200 |
| C | -4.24275000 | 1.35377400 | -0.76054100 |
| H | -3.12756300 | 3.72253700 | -4.02450000 |
| H | -1.83020300 | 2.50441000 | -4.08823300 |
| H | -1.49972400 | 4.11404200 | -3.43152600 |
| H | -4.15501800 | 4.31025100 | -1.63679400 |
| H | -2.49946000 | 4.86833100 | -1.33007600 |
| H | -3.26045400 | 3.73615500 | -0.20692500 |
| H | -5.11416800 | 2.13518100 | -3.33109300 |
| H | -4.90081500 | 0.38263300 | -3.16246600 |
| H | -3.80021300 | 1.30591800 | -4.19665600 |
| H | -5.09407000 | 2.04136100 | -0.70197500 |
| H | -3.60221700 | 1.51689000 | 0.10909700 |
| H | -4.61606200 | 0.32758200 | -0.71323400 |
| Cu | 0.35902200 | -0.01098800 | -1.05573400 |
| P | 1.13344800 | 1.21304200 | 0.79614400 |
| P | -0.50005200 | -2.01699100 | -0.28258900 |
| C | 2.16374100 | 0.40991200 | 2.08615900 |
| C | 2.08694400 | 2.71404400 | 0.33507900 |
| C | -0.28213300 | 1.93617900 | 1.72733300 |
| C | 0.43550700 | -3.00524800 | 0.94367000 |
| C | -2.16028600 | -1.89509200 | 0.48941100 |
| C | -0.77981800 | -3.17209400 | -1.67560000 |

| | | | |
|---|---|---|---|
| C | 1.67366000 | 0.06778400 | 3.35242100 |
| C | 3.47205600 | 0.03300900 | 1.73898700 |
| C | 1.66402300 | 3.41958300 | -0.80392900 |
| C | 3.21227700 | 3.16073000 | 1.03871700 |
| C | -1.33135200 | 1.09682200 | 2.11139900 |
| C | -0.43607400 | 3.30616500 | 1.96986500 |
| C | 1.82347700 | -2.82967600 | 0.99870600 |
| C | -0.17735900 | -3.92337700 | 1.80792900 |
| C | -3.29638400 | -2.61549700 | 0.10636700 |
| C | -2.31268800 | -0.93244000 | 1.48960300 |
| C | -1.52555100 | -2.70067600 | -2.77101000 |
| C | -0.21907400 | -4.45473100 | -1.72341200 |
| H | 0.66769000 | 0.34906700 | 3.64150500 |
| C | 2.47575900 | -0.63419400 | 4.25331900 |
| C | 4.27722800 | -0.64652900 | 2.64884600 |
| H | 3.86607100 | 0.27916900 | 0.76148200 |
| C | 2.37301100 | 4.53891700 | -1.23683200 |
| H | 0.78034800 | 3.09389900 | -1.34114100 |
| C | 3.92457400 | 4.27576400 | 0.59446400 |
| H | 3.54489700 | 2.63078900 | 1.92396000 |
| O | -1.16951500 | -0.25045300 | 1.85726800 |
| C | -2.51167200 | 1.54488400 | 2.71113000 |
| H | 0.34949300 | 3.99194000 | 1.67482300 |
| C | -1.60738000 | 3.79296300 | 2.54939600 |
| H | 2.29641000 | -2.09773400 | 0.35480300 |
| C | 2.59263500 | -3.57388800 | 1.89213700 |
| H | -1.25428200 | -4.05850600 | 1.77548300 |
| C | 0.59190900 | -4.65732200 | 2.71008600 |
| H | -3.21704200 | -3.36606900 | -0.67233800 |
| C | -4.53048100 | -2.34390900 | 0.69998500 |
| C | -3.53297500 | -0.61450400 | 2.08507500 |
| H | -1.94776300 | -1.70022300 | -2.74475600 |
| C | -1.71771000 | -3.51618500 | -3.88417200 |
| H | 0.35962200 | -4.82407500 | -0.88317400 |
| C | -0.40399400 | -5.26027400 | -2.84910600 |
| H | 2.07929500 | -0.89812400 | 5.22989900 |
| C | 3.78021700 | -0.98814900 | 3.90874300 |
| H | 5.28912200 | -0.91696900 | 2.36021600 |
| C | 3.51142900 | 4.96357300 | -0.54730200 |
| H | 2.04066300 | 5.07307400 | -2.12275300 |
| H | 4.80261600 | 4.60562200 | 1.14315600 |
| C | -3.53431800 | 0.48848500 | 3.14703700 |
| C | -2.63736000 | 2.92250800 | 2.91385500 |
| H | -1.72043900 | 4.85960200 | 2.71881400 |

| | | | |
|---|---|---|---|
| H | 3.66566100 | -3.41932400 | 1.93044200 |
| C | 1.97807500 | -4.48605200 | 2.75049200 |
| H | 0.11025500 | -5.36352000 | 3.38107600 |
| C | -4.65007000 | -1.34717800 | 1.67145600 |
| H | -5.40918200 | -2.90500200 | 0.39577800 |
| H | -2.29730300 | -3.14631200 | -4.72544200 |
| C | -1.15525900 | -4.79488100 | -3.92849100 |
| H | 0.03723300 | -6.25286700 | -2.87852300 |
| H | 4.40346000 | -1.52943100 | 4.61520700 |
| H | 4.07029800 | 5.82790800 | -0.89553800 |
| C | -3.04997800 | -0.12560600 | 4.48786600 |
| C | -4.93098300 | 1.09026000 | 3.34437200 |
| H | -3.53853900 | 3.32423100 | 3.36378100 |
| H | 2.57535400 | -5.05758200 | 3.45570400 |
| H | -5.62381300 | -1.13897500 | 2.10094700 |
| H | -1.29876600 | -5.42313900 | -4.80327800 |
| H | -2.05761000 | -0.57251900 | 4.37680500 |
| H | -3.74283300 | -0.90755100 | 4.81799200 |
| H | -2.99625800 | 0.64794100 | 5.26191700 |
| H | -4.91365500 | 1.86011600 | 4.12132600 |
| H | -5.63780300 | 0.32394400 | 3.67556500 |
| H | -5.31008000 | 1.53654300 | 2.41932100 |
| C | 4.13977100 | -1.50392400 | -1.42854800 |
| C | 3.34312900 | -0.42516100 | -1.87011600 |
| C | 3.91190000 | 0.86567800 | -1.82366400 |
| C | 5.20099400 | 1.05974900 | -1.33461000 |
| C | 5.97095600 | -0.01777100 | -0.88672300 |
| C | 5.42999100 | -1.30479100 | -0.94542700 |
| H | 3.72970300 | -2.50979500 | -1.46926700 |
| H | 3.33805200 | 1.71873800 | -2.15494300 |
| H | 5.59898300 | 2.06973900 | -1.29393200 |
| H | 6.97506700 | 0.14208600 | -0.50480700 |
| H | 6.01438600 | -2.15915100 | -0.61342100 |
| C | 1.99523700 | -0.71974000 | -2.35349000 |
| H | 1.75060400 | -1.76768100 | -2.49570700 |
| C | 1.06745100 | 0.15789600 | -2.93320400 |
| F | 0.22492200 | -0.32650300 | -3.88131800 |
| F | 1.42341000 | 1.41809500 | -3.29084300 |

**B1’**

Total electronic energy =-3380.603363

Thermal corrections to Gibbs free energy = 0.809689

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 1.38430900 | 1.19448300 | 0.28103100 |
| O | 1.94097000 | 0.82453800 | 1.50066900 |
| O | 1.64091200 | 2.54068400 | 0.03757600 |
| C | 2.77435300 | 1.90076800 | 1.99990800 |
| C | 2.21198700 | 3.14514600 | 1.22845400 |
| C | 4.21714600 | 1.54846800 | 1.62195600 |
| C | 2.61877300 | 1.95199500 | 3.51670200 |
| C | 3.26128300 | 4.16172800 | 0.79217300 |
| C | 1.05909800 | 3.84015200 | 1.95796900 |
| H | 4.93019200 | 2.29167500 | 1.99554800 |
| H | 4.33135600 | 1.46367800 | 0.53795900 |
| H | 4.46977100 | 0.57978700 | 2.06589800 |
| H | 3.18901300 | 2.78437100 | 3.94572500 |
| H | 2.98953700 | 1.01828900 | 3.95091200 |
| H | 1.57031300 | 2.05434300 | 3.80419000 |
| H | 3.77532600 | 4.59426300 | 1.65853700 |
| H | 2.77637000 | 4.97668200 | 0.24429200 |
| H | 4.00389000 | 3.70495600 | 0.13434000 |
| H | 1.40526400 | 4.38381800 | 2.84413900 |
| H | 0.29737600 | 3.11909600 | 2.26272600 |
| H | 0.58527000 | 4.55265500 | 1.27617500 |
| Cu | 0.42457500 | -0.08179700 | -0.94478300 |
| P | 0.29030500 | -1.96375200 | 0.33697400 |
| P | -1.69957200 | 0.93910000 | -1.11122600 |
| C | -1.07373000 | -3.15878300 | 0.06851200 |
| C | 1.82503800 | -2.95664400 | 0.23700400 |
| C | 0.17259200 | -1.61328400 | 2.13846200 |
| C | -3.24121300 | 0.00588500 | -1.47854900 |
| C | -2.10858800 | 1.83460300 | 0.44317900 |
| C | -1.67742100 | 2.31085800 | -2.33240500 |
| C | -1.50409500 | -4.03639800 | 1.07469900 |
| C | -1.72138100 | -3.16611200 | -1.17331500 |
| C | 3.03507200 | -2.31147200 | 0.54299700 |
| C | 1.84302000 | -4.28628100 | -0.19844500 |
| C | -0.76321700 | -0.66012500 | 2.54556600 |
| C | 1.02583800 | -2.13681900 | 3.11469000 |
| C | -3.38181400 | -0.60272600 | -2.73796900 |
| C | -4.22654700 | -0.22104400 | -0.50875800 |
| C | -2.48757800 | 3.18064500 | 0.50432500 |
| C | -1.94524700 | 1.15459500 | 1.65429200 |
| C | -0.53997400 | 3.13982300 | -2.33097200 |
| C | -2.70342600 | 2.55980900 | -3.25245800 |

| | | | |
|---|---|---|---|
| H | -1.01319800 | -4.02714400 | 2.04315900 |
| C | -2.56497800 | -4.90914300 | 0.83899300 |
| C | -2.78073100 | -4.04270600 | -1.40760200 |
| H | -1.40668100 | -2.47671000 | -1.94785200 |
| C | 4.24045500 | -3.00057700 | 0.43450800 |
| H | 3.02070900 | -1.27273100 | 0.85853700 |
| C | 3.05668500 | -4.96545400 | -0.32546100 |
| H | 0.91241700 | -4.78810200 | -0.44245300 |
| O | -1.60814600 | -0.17800900 | 1.56646000 |
| C | -0.85506100 | -0.16586800 | 3.84693400 |
| H | 1.76947400 | -2.87499000 | 2.83719300 |
| C | 0.95492100 | -1.67729600 | 4.43007800 |
| H | -2.61479300 | -0.46330500 | -3.49060800 |
| C | -4.49201900 | -1.39392400 | -3.02371800 |
| H | -4.14085200 | 0.23887400 | 0.46925300 |
| C | -5.32384500 | -1.03647000 | -0.78882700 |
| H | -2.62079000 | 3.74018100 | -0.41462900 |
| C | -2.66252100 | 3.80714300 | 1.73802000 |
| C | -2.10781600 | 1.75020800 | 2.90787600 |
| H | 0.24810400 | 2.97713100 | -1.60089100 |
| C | -0.43669500 | 4.18741300 | -3.24515000 |
| H | -3.59272600 | 1.93926000 | -3.25467400 |
| C | -2.58844100 | 3.60506000 | -4.17125400 |
| H | -2.89517200 | -5.58318100 | 1.62482800 |
| C | -3.20508400 | -4.91245900 | -0.40302800 |
| H | -3.28592300 | -4.02720200 | -2.36769900 |
| C | 4.25564700 | -4.32713800 | -0.00510100 |
| H | 5.17025500 | -2.49220500 | 0.67308500 |
| H | 3.06268200 | -5.99546300 | -0.67136100 |
| C | -1.94977000 | 0.86279700 | 4.14651800 |
| C | 0.03363100 | -0.69226500 | 4.78985000 |
| H | 1.62875200 | -2.08242000 | 5.17932600 |
| H | -4.59004700 | -1.84491100 | -4.00766400 |
| C | -5.46462400 | -1.62068700 | -2.04697100 |
| H | -6.07366800 | -1.20744700 | -0.02128700 |
| C | -2.46782000 | 3.10145500 | 2.92725700 |
| H | -2.94695200 | 4.85446300 | 1.77507600 |
| H | 0.44474300 | 4.82309700 | -3.23273000 |
| C | -1.45499500 | 4.41850200 | -4.17326700 |
| H | -3.39009000 | 3.78465200 | -4.88253900 |
| H | -4.03727800 | -5.58748600 | -0.58335700 |
| H | 5.19818400 | -4.85922800 | -0.10079000 |
| C | -3.28387800 | 0.09904700 | 4.36273300 |
| C | -1.63238400 | 1.68656200 | 5.40130800 |

| | | | |
|---|---|---|---|
| H | 0.00853400 | -0.33888100 | 5.81474500 |
| H | -6.32299600 | -2.24976400 | -2.26521700 |
| H | -2.60117100 | 3.61226300 | 3.87442400 |
| H | -1.36736900 | 5.23015200 | -4.89024000 |
| H | -3.53499300 | -0.50241700 | 3.48389900 |
| H | -4.10157400 | 0.80593200 | 4.54291000 |
| H | -3.20074100 | -0.57196300 | 5.22487400 |
| H | -1.54644500 | 1.03828500 | 6.27796200 |
| H | -2.43727200 | 2.39630300 | 5.61305900 |
| H | -0.69705900 | 2.24461700 | 5.28864300 |
| C | 3.56045300 | 1.56880700 | -2.43584100 |
| C | 2.96868700 | 0.29148400 | -2.47773800 |
| C | 3.79476000 | -0.83087200 | -2.29688100 |
| C | 5.16073300 | -0.67334300 | -2.07089500 |
| C | 5.73710900 | 0.59706900 | -2.02897500 |
| C | 4.92568400 | 1.72014500 | -2.21682400 |
| H | 2.92754100 | 2.44349300 | -2.54728400 |
| H | 3.36711700 | -1.82386200 | -2.31314900 |
| H | 5.77575900 | -1.55689200 | -1.92424000 |
| H | 6.80288600 | 0.71266200 | -1.85317900 |
| H | 5.35759200 | 2.71723900 | -2.18847000 |
| C | 1.52082500 | 0.21909000 | -2.72395500 |
| H | 1.05743300 | 1.13071700 | -3.08899000 |
| C | 0.71064100 | -0.90798000 | -2.83975400 |
| F | -0.37377000 | -0.87266500 | -3.67078000 |
| F | 1.21150400 | -2.16902300 | -2.87005500 |

**B2**

Total electronic energy = -3061.019022

Thermal corrections to Gibbs free energy = 0.704368

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 2.71215500 | 0.26480500 | 0.73760500 |
| O | 3.29053100 | -0.41620300 | 1.80890600 |
| O | 3.69568100 | 1.03571500 | 0.09788300 |
| C | 4.73325000 | -0.27386800 | 1.75317900 |
| C | 4.91485600 | 1.01600100 | 0.88301700 |
| C | 5.27838800 | -1.54016800 | 1.08037700 |
| C | 5.26954100 | -0.17124800 | 3.17793500 |
| C | 6.10594300 | 0.99078200 | -0.07015500 |
| C | 4.92623700 | 2.30895000 | 1.70739500 |
| H | 6.37335800 | -1.54340100 | 1.04412300 |

| | | | |
|---|---|---|---|
| H | 4.89141500 | -1.64349300 | 0.06350700 |
| H | 4.95232400 | -2.41025800 | 1.65998200 |
| H | 6.35329100 | -0.00331400 | 3.17867500 |
| H | 5.07013000 | -1.10584100 | 3.71215300 |
| H | 4.78920400 | 0.63986100 | 3.72924600 |
| H | 7.04998900 | 0.90191400 | 0.48053700 |
| H | 6.13553200 | 1.92249000 | -0.64504200 |
| H | 6.03125400 | 0.16105600 | -0.77598500 |
| H | 5.84293100 | 2.41110700 | 2.29847000 |
| H | 4.06608000 | 2.34912500 | 2.38222800 |
| H | 4.86074300 | 3.16225600 | 1.02421700 |
| Cu | 0.83569500 | 0.14714000 | 0.05024300 |
| P | -0.25719900 | -1.82842000 | -0.43316500 |
| P | -0.63886100 | 1.88918500 | -0.29817200 |
| C | -1.49449400 | -1.94638300 | -1.78058700 |
| C | 0.83928900 | -3.27012300 | -0.72029500 |
| C | -1.20678400 | -2.33275700 | 1.05571300 |
| C | -1.75613300 | 1.86590400 | -1.75797600 |
| C | -1.75601000 | 2.07506600 | 1.15432500 |
| C | 0.13285200 | 3.54611800 | -0.45708300 |
| C | -2.72460600 | -2.60160200 | -1.64016600 |
| C | -1.18094900 | -1.33029200 | -3.00115400 |
| C | 2.07822800 | -3.28379600 | -0.05896500 |
| C | 0.49491200 | -4.33521100 | -1.56384000 |
| C | -2.09463400 | -1.39541000 | 1.59233400 |
| C | -1.03828500 | -3.53480000 | 1.75283100 |
| C | -1.19319200 | 2.15916200 | -3.01147100 |
| C | -3.10486300 | 1.49730700 | -1.68905100 |
| C | -1.89039300 | 3.24606000 | 1.91216500 |
| C | -2.38891000 | 0.92503200 | 1.63911500 |
| C | 1.49796400 | 3.67713800 | -0.17037900 |
| C | -0.60015300 | 4.67410400 | -0.86140000 |
| H | -2.97797200 | -3.07662800 | -0.69750900 |
| C | -3.62397900 | -2.64528600 | -2.70633600 |
| C | -2.07331200 | -1.38986300 | -4.06870400 |
| H | -0.24599200 | -0.78845500 | -3.10641500 |
| C | 2.95252100 | -4.35522200 | -0.23656100 |
| H | 2.35469800 | -2.45175600 | 0.58173100 |
| C | 1.37850500 | -5.39985400 | -1.74511900 |
| H | -0.45963100 | -4.32851300 | -2.08043800 |
| O | -2.24819100 | -0.22145300 | 0.88211500 |
| C | -2.79584600 | -1.57682000 | 2.78462000 |
| H | -0.35455400 | -4.28398500 | 1.36855400 |
| C | -1.72641400 | -3.75329700 | 2.94735000 |

| | | | |
|---|---|---|---|
| H | -0.14458200 | 2.43368600 | -3.07969100 |
| C | -1.97300100 | 2.11218800 | -4.16441400 |
| H | -3.55559900 | 1.25935000 | -0.73268900 |
| C | -3.87915800 | 1.43708500 | -2.84799300 |
| H | -1.40457000 | 4.15682700 | 1.58129400 |
| C | -2.61806200 | 3.23503800 | 3.10212800 |
| C | -3.11350800 | 0.87307100 | 2.83188500 |
| H | 2.07499700 | 2.80185100 | 0.10995500 |
| C | 2.11634200 | 4.92549400 | -0.27258500 |
| H | -1.65349500 | 4.57244400 | -1.10597500 |
| C | 0.02054500 | 5.91751000 | -0.95886100 |
| H | -4.57762000 | -3.15259100 | -2.58671700 |
| C | -3.29764400 | -2.04491500 | -3.92294600 |
| H | -1.82395900 | -0.90118200 | -5.00496400 |
| C | 2.60693400 | -5.41219700 | -1.08125100 |
| H | 3.91078800 | -4.35431100 | 0.27480900 |
| H | 1.10694100 | -6.21936500 | -2.40506300 |
| C | -3.76079600 | -0.46452300 | 3.20992200 |
| C | -2.59020800 | -2.78303800 | 3.46215200 |
| H | -1.58489000 | -4.68519800 | 3.48659400 |
| H | -1.52698500 | 2.35437100 | -5.12537700 |
| C | -3.32015800 | 1.75144600 | -4.08628500 |
| H | -4.92331900 | 1.14510800 | -2.77973400 |
| C | -3.21661500 | 2.05985900 | 3.56292400 |
| H | -2.71084000 | 4.14775500 | 3.68322100 |
| H | 3.17666700 | 5.01655200 | -0.05328500 |
| C | 1.38124600 | 6.04483200 | -0.66172700 |
| H | -0.55333300 | 6.78609800 | -1.27029400 |
| H | -3.99890400 | -2.07813700 | -4.75214600 |
| H | 3.29476800 | -6.24077700 | -1.22650800 |
| C | -5.06792700 | -0.62061400 | 2.38682500 |
| C | -4.09792300 | -0.53679700 | 4.70404500 |
| H | -3.10506100 | -2.97371500 | 4.39744000 |
| H | -3.92745200 | 1.70890300 | -4.98611000 |
| H | -3.76354200 | 2.07423000 | 4.49926100 |
| H | 1.86509000 | 7.01455600 | -0.74215300 |
| H | -4.86166700 | -0.58341000 | 1.31307200 |
| H | -5.76860500 | 0.18520000 | 2.63199900 |
| H | -5.54356700 | -1.58174800 | 2.61149300 |
| H | -4.57478800 | -1.49130400 | 4.94538700 |
| H | -4.80792500 | 0.24909600 | 4.97804400 |
| H | -3.20228500 | -0.42870600 | 5.32413500 |
| C | 2.85131100 | -0.30350300 | -2.41154000 |
| O | 2.02897500 | 0.46765700 | -2.73240300 |

| | | | |
|---|---|---|---|
| O | 3.67381300 | -1.09692600 | -2.16892700 |

**$B_2Pin_2$**

Total electronic energy = -822.689504

Thermal corrections to Gibbs free energy = 0.318358

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | -0.84904900 | -0.00001400 | -0.00001500 |
| O | -1.61045800 | -1.03382900 | -0.48980300 |
| O | -1.61043300 | 1.03381000 | 0.48979100 |
| C | -2.99424200 | -0.58091300 | -0.52716300 |
| C | -2.99423000 | 0.58092100 | 0.52716000 |
| B | 0.84904600 | -0.00001500 | -0.00001600 |
| O | 1.61043900 | 0.49011800 | -1.03367100 |
| O | 1.61043200 | -0.49013600 | 1.03365400 |
| C | 2.99423900 | 0.52732600 | -0.58076800 |
| C | 2.99423000 | -0.52733200 | 0.58077200 |
| C | 3.25689000 | -1.95816600 | 0.10015600 |
| H | 4.30069300 | -2.09774900 | -0.19938600 |
| H | 3.03417500 | -2.65181200 | 0.91624700 |
| H | 2.61261900 | -2.21346300 | -0.74654900 |
| C | 3.90062300 | 0.19122400 | -1.75947300 |
| H | 3.81310900 | 0.96945000 | -2.52395500 |
| H | 4.94813000 | 0.14290300 | -1.44078700 |
| H | 3.62923200 | -0.76295600 | -2.21564500 |
| C | 3.25687700 | 1.95815900 | -0.10013600 |
| H | 4.30066700 | 2.09773400 | 0.19945600 |
| H | 3.03420700 | 2.65180600 | -0.91623700 |
| H | 2.61256500 | 2.21346000 | 0.74653600 |
| C | -3.25684900 | -0.10068500 | -1.95814000 |
| H | -3.03417700 | -0.91698800 | -2.65154900 |
| H | -4.30063300 | 0.19888000 | -2.09782600 |
| H | -2.61252200 | 0.74590700 | -2.21366600 |
| C | -3.90063000 | 1.75952400 | 0.19075200 |
| H | -4.94813000 | 1.44080600 | 0.14250500 |
| H | -3.81313600 | 2.52420800 | 0.96878100 |
| H | -3.62924000 | 2.21545700 | -0.76354400 |
| C | -3.25683600 | 0.10068100 | 1.95813300 |
| H | -3.03410700 | 0.91695800 | 2.65155500 |
| H | -4.30063500 | -0.19882800 | 2.09782800 |
| H | -2.61255300 | -0.74595200 | 2.21363000 |
| C | -3.90066000 | -1.75949300 | -0.19072700 |

| | | | |
|---|---|---|---|
| H | -4.94815400 | -1.44075300 | -0.14247300 |
| H | -3.81319000 | -2.52419100 | -0.96874400 |
| H | -3.62926500 | -2.21541200 | 0.76357400 |
| C | 3.90060600 | -0.19120200 | 1.75947600 |
| H | 3.81312000 | -0.96942800 | 2.52395900 |
| H | 4.94810800 | -0.14284700 | 1.44078300 |
| H | 3.62918000 | 0.76297100 | 2.21564500 |

**Bpin-O$^t$Bu**

Total electronic energy = -644.516584

Thermal corrections to Gibbs free energy = 0.269167

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 0.75554900 | -1.30258900 | 0.56000300 |
| O | 0.16355800 | 0.73166700 | -0.34549400 |
| C | 1.97794600 | -0.70924200 | 0.05929500 |
| C | 1.58650800 | 0.80817500 | -0.07035700 |
| B | -0.27628500 | -0.47568200 | 0.17174100 |
| C | 2.27428100 | -1.36555700 | -1.29358500 |
| H | 3.22704500 | -1.02327600 | -1.71028300 |
| H | 2.32422600 | -2.44957000 | -1.15589800 |
| H | 1.48083500 | -1.15140300 | -2.01651600 |
| C | 3.10319400 | -0.99961300 | 1.04590700 |
| H | 3.29511500 | -2.07657000 | 1.07761600 |
| H | 4.02759200 | -0.49731600 | 0.73917000 |
| H | 2.84410600 | -0.67313300 | 2.05519000 |
| C | 2.26457100 | 1.55592100 | -1.21198600 |
| H | 1.91595200 | 2.59333800 | -1.23224600 |
| H | 3.35186000 | 1.56496400 | -1.07663300 |
| H | 2.03576600 | 1.10270800 | -2.17873200 |
| C | 1.74536300 | 1.58127800 | 1.24276300 |
| H | 2.79905400 | 1.74333300 | 1.49118100 |
| H | 1.25987900 | 2.55663400 | 1.14128500 |
| H | 1.27045400 | 1.04819600 | 2.07218900 |
| O | -1.56364200 | -0.86350600 | 0.30648000 |
| C | -2.71207700 | -0.03824200 | -0.00481500 |
| C | -2.69297200 | 1.22237100 | 0.86683200 |
| H | -2.65381000 | 0.94638000 | 1.92618600 |
| H | -1.82407900 | 1.84212400 | 0.63237300 |
| H | -3.59945500 | 1.81431500 | 0.69941400 |
| C | -2.70200200 | 0.31177800 | -1.49687300 |
| H | -3.60636100 | 0.87017900 | -1.76261200 |

| | | | |
|---|---|---|---|
| H | -1.83010100 | 0.92149100 | -1.74667400 |
| H | -2.67506600 | -0.60389200 | -2.09743100 |
| C | -3.91960500 | -0.91267300 | 0.33712300 |
| H | -3.90460000 | -1.83034800 | -0.25948500 |
| H | -3.89857600 | -1.19174100 | 1.39541600 |
| H | -4.85336700 | -0.37776700 | 0.13405200 |

**Bpin-OtBu+LiF**

Total electronic energy = -752.023544

Thermal corrections to Gibbs free energy = 0.271687

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | -0.74395200 | 0.59516200 | -1.16500500 |
| O | -0.30614900 | -1.15844400 | 0.27457000 |
| C | -2.04413600 | 0.20521000 | -0.61464000 |
| C | -1.63038700 | -0.64523000 | 0.65063200 |
| B | 0.20482700 | -0.24439300 | -0.59302500 |
| C | -2.74312400 | -0.61193900 | -1.69991300 |
| H | -3.75065400 | -0.90472400 | -1.38906000 |
| H | -2.82437900 | -0.00624200 | -2.60739000 |
| H | -2.17612100 | -1.51612700 | -1.94169400 |
| C | -2.81490700 | 1.47875800 | -0.29214300 |
| H | -3.06061900 | 2.00594400 | -1.22016500 |
| H | -3.75401100 | 1.24065200 | 0.21897700 |
| H | -2.22123000 | 2.14213600 | 0.34071700 |
| C | -2.53491400 | -1.83489300 | 0.93823700 |
| H | -2.15941900 | -2.37332500 | 1.81340500 |
| H | -3.55257600 | -1.49568300 | 1.16020800 |
| H | -2.57220200 | -2.53194000 | 0.09815900 |
| C | -1.42290300 | 0.20880500 | 1.90489400 |
| H | -2.38077400 | 0.57756800 | 2.28673300 |
| H | -0.96937800 | -0.41811200 | 2.67927000 |
| H | -0.76094900 | 1.06171400 | 1.70870300 |
| O | 1.49059200 | 0.07425900 | -0.89716600 |
| C | 2.65577300 | -0.33393800 | -0.09529700 |
| C | 2.40264100 | -0.00772500 | 1.38008200 |
| H | 1.98615100 | 1.00142200 | 1.47648500 |
| H | 1.69545800 | -0.71512300 | 1.82049100 |
| H | 3.34474700 | -0.07293100 | 1.93517700 |
| C | 2.88894000 | -1.82519800 | -0.33062800 |
| H | 3.77072600 | -2.15947900 | 0.22650500 |
| H | 2.02754000 | -2.40627300 | 0.01236300 |

| | | | |
|---|---|---|---|
| H | 3.05330400 | -2.02952300 | -1.39406900 |
| C | 3.80034200 | 0.51028600 | -0.65161100 |
| H | 3.90938600 | 0.35011200 | -1.72934300 |
| H | 3.61245700 | 1.57412200 | -0.46818300 |
| H | 4.74184300 | 0.24188900 | -0.16222100 |
| Li | 0.55754700 | 2.03324000 | -0.72176900 |
| F | 0.49733800 | 2.51150400 | 0.82538900 |

**Bpin-F**

Total electronic energy = -511.276600

Thermal corrections to Gibbs free energy = 0.151470

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 0.85463400 | 1.07081400 | 0.42639900 |
| O | 0.85482500 | -1.07069500 | -0.42630800 |
| C | -0.52410000 | 0.78604000 | 0.05259700 |
| C | -0.52421600 | -0.78602200 | -0.05256100 |
| B | 1.58900900 | 0.00007800 | 0.00009800 |
| C | -0.76600900 | 1.47717800 | -1.29217100 |
| H | -1.80528000 | 1.36992500 | -1.61819500 |
| H | -0.54276400 | 2.54285900 | -1.18795700 |
| H | -0.11367800 | 1.06710200 | -2.06946400 |
| C | -1.44736700 | 1.35921000 | 1.12020700 |
| H | -1.36590100 | 2.45039500 | 1.12984000 |
| H | -2.48998100 | 1.09710000 | 0.90873200 |
| H | -1.18803100 | 0.99125600 | 2.11491600 |
| C | -1.44719200 | -1.35933500 | -1.12028400 |
| H | -1.36550300 | -2.45050400 | -1.12993200 |
| H | -2.48989800 | -1.09746100 | -0.90895300 |
| H | -1.18782700 | -0.99131200 | -2.11495700 |
| C | -0.76588900 | -1.47724400 | 1.29216100 |
| H | -1.80514600 | -1.37010900 | 1.61828300 |
| H | -0.54255400 | -2.54289500 | 1.18785700 |
| H | -0.11354800 | -1.06718000 | 2.06944800 |
| F | 2.91533800 | 0.00005600 | -0.00005900 |

**C**

Total electronic energy = -3380.663141

Thermal corrections to Gibbs free energy = 0.810388

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.00854700 | 1.74488600 | 2.12362400 |
| C | 0.07063200 | 2.63526300 | 2.63832600 |
| B | 1.42280300 | 1.81091200 | 2.69836600 |
| O | 2.50293600 | 2.13278100 | 1.91397300 |
| O | 1.61846700 | 0.67430000 | 3.44591100 |
| C | 3.58806700 | 1.23062400 | 2.25829600 |
| C | 2.82716300 | 0.03467100 | 2.93888700 |
| C | 4.50246000 | 1.99571200 | 3.21827400 |
| C | 4.33372700 | 0.87064700 | 0.97781100 |
| C | 3.55615200 | -0.61377100 | 4.10895000 |
| C | 2.37955000 | -1.02830700 | 1.93660900 |
| H | 5.38620900 | 1.40810000 | 3.48730800 |
| H | 3.97050700 | 2.26870800 | 4.13458600 |
| H | 4.83364100 | 2.91786700 | 2.73169200 |
| H | 5.12836300 | 0.14404300 | 1.18168500 |
| H | 4.79480400 | 1.77010500 | 0.55797800 |
| H | 3.66493500 | 0.45490600 | 0.22325700 |
| H | 4.50392200 | -1.05298900 | 3.77776100 |
| H | 2.93763600 | -1.41465100 | 4.52610200 |
| H | 3.76123200 | 0.10595900 | 4.90392900 |
| H | 3.22677900 | -1.57305400 | 1.50997900 |
| H | 1.81200500 | -0.57657500 | 1.11691500 |
| H | 1.72926300 | -1.75014300 | 2.43529900 |
| H | -1.21330300 | 1.01448800 | 2.90901000 |
| Cu | -0.41021400 | 0.62929000 | 0.54687200 |
| P | 0.40016800 | 1.17528900 | -1.49720500 |
| P | -1.23884400 | -1.54425000 | 0.60745700 |
| C | -0.93784800 | 0.83246600 | -2.69940400 |
| C | 0.85516100 | 2.91016800 | -1.87014000 |
| C | 1.87933600 | 0.25555400 | -2.08930900 |
| C | -2.50046400 | -1.98768300 | -0.64231200 |
| C | -0.00063000 | -2.89263500 | 0.45912200 |
| C | -2.03783300 | -1.93351800 | 2.20959600 |
| C | -0.84474300 | -0.11129000 | -3.72676500 |
| C | -2.13321200 | 1.54917800 | -2.52412800 |
| C | 1.55848000 | 3.63187900 | -0.89569900 |
| C | 0.55102200 | 3.51638000 | -3.09783200 |
| C | 1.93697400 | -1.12915600 | -1.89313000 |
| C | 3.03421600 | 0.88409100 | -2.57514600 |
| C | -3.51867200 | -1.05741800 | -0.89532200 |
| C | -2.49115000 | -3.20490300 | -1.33637000 |
| C | 0.13629700 | -3.95606500 | 1.35964000 |
| C | 0.94961300 | -2.78428400 | -0.56047600 |

| | | | |
|---|---|---|---|
| C | -1.36705300 | -1.54026700 | 3.38031900 |
| C | -3.28908400 | -2.55394100 | 2.31012700 |
| H | 0.07363400 | -0.67053500 | -3.87098900 |
| C | -1.93335900 | -0.33262800 | -4.57262600 |
| C | -3.20536100 | 1.34390800 | -3.38694000 |
| H | -2.22703500 | 2.26193200 | -1.70981100 |
| C | 1.94783500 | 4.94732700 | -1.14923100 |
| H | 1.79326000 | 3.17399800 | 0.05687400 |
| C | 0.93804300 | 4.83342100 | -3.34263900 |
| H | 0.00682800 | 2.96229700 | -3.85546800 |
| O | 0.78349900 | -1.73206800 | -1.43645000 |
| C | 3.08114300 | -1.90025600 | -2.11291600 |
| H | 3.03018800 | 1.95587300 | -2.73601100 |
| C | 4.19258900 | 0.14449800 | -2.81092300 |
| H | -3.52646000 | -0.10577000 | -0.37372100 |
| C | -4.52421300 | -1.35378400 | -1.81268800 |
| H | -1.70814800 | -3.93157500 | -1.14542100 |
| C | -3.48916300 | -3.48783200 | -2.26893700 |
| H | -0.58310000 | -4.07162100 | 2.16278800 |
| C | 1.21154200 | -4.83775400 | 1.24545400 |
| C | 2.04027500 | -3.64364300 | -0.70305300 |
| H | -0.40841900 | -1.03412400 | 3.31507100 |
| C | -1.94012700 | -1.77321800 | 4.62904400 |
| H | -3.81604000 | -2.85491300 | 1.41077500 |
| C | -3.86427800 | -2.77468000 | 3.56296700 |
| H | -1.85716400 | -1.07447200 | -5.36273000 |
| C | -3.11005400 | 0.39870300 | -4.41107300 |
| H | -4.12245200 | 1.90690300 | -3.23863800 |
| C | 1.63601500 | 5.55115000 | -2.36832600 |
| H | 2.48172800 | 5.50231900 | -0.38326100 |
| H | 0.69343000 | 5.29914200 | -4.29339400 |
| C | 2.97411400 | -3.41340700 | -1.89502400 |
| C | 4.22029200 | -1.23116700 | -2.57116500 |
| H | 5.08446700 | 0.64428300 | -3.17662700 |
| H | -5.30678200 | -0.62461700 | -1.99912300 |
| C | -4.51038700 | -2.56587200 | -2.50446700 |
| H | -3.47210300 | -4.43246600 | -2.80583900 |
| C | 2.15902200 | -4.67762500 | 0.23129200 |
| H | 1.31616000 | -5.65425500 | 1.95367000 |
| H | -1.41609800 | -1.45822200 | 5.52678700 |
| C | -3.19215300 | -2.38630300 | 4.72278200 |
| H | -4.83890200 | -3.25006000 | 3.63100500 |
| H | -3.95335900 | 0.22455100 | -5.07337700 |
| H | 1.93106600 | 6.57948400 | -2.55859600 |

| | | | |
|---|---|---|---|
| C | 2.31021300 | -4.03501000 | -3.15338800 |
| C | 4.34794300 | -4.06071700 | -1.68065700 |
| H | 5.13643900 | -1.78265200 | -2.75086800 |
| H | -5.28885700 | -2.78911000 | -3.22882700 |
| H | 2.99141300 | -5.36984800 | 0.16943600 |
| H | -3.64452000 | -2.55392500 | 5.69611900 |
| H | 1.32371300 | -3.59691400 | -3.33174700 |
| H | 2.18748400 | -5.11572300 | -3.02180100 |
| H | 2.93215000 | -3.85548900 | -4.03722600 |
| H | 4.98826500 | -3.90734700 | -2.55396500 |
| H | 4.24882400 | -5.14201500 | -1.54934300 |
| H | 4.85414500 | -3.64853800 | -0.80158100 |
| C | -2.27005400 | 2.25540400 | 1.53638000 |
| C | -3.45359700 | 1.49899600 | 1.71276200 |
| C | -2.36123500 | 3.38897100 | 0.69236300 |
| C | -4.64359000 | 1.83425900 | 1.07038300 |
| H | -3.42257700 | 0.62943400 | 2.36450800 |
| C | -3.55758300 | 3.72561500 | 0.06183500 |
| H | -1.48210000 | 3.99941500 | 0.53444900 |
| C | -4.70762800 | 2.94780000 | 0.22869100 |
| H | -5.52763400 | 1.22139600 | 1.23306400 |
| H | -3.58772500 | 4.60698400 | -0.57528600 |
| H | -5.63597200 | 3.21568400 | -0.26820300 |
| F | 0.28067100 | 3.74777300 | 1.81574000 |
| F | -0.23798100 | 3.19527800 | 3.89300600 |

**C'**

Total electronic energy = -3380.655720

Thermal corrections to Gibbs free energy = 0.810122

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.46782900 | 0.15349300 | 1.09872600 |
| C | -3.40689900 | 0.46841200 | -0.09106400 |
| H | -3.25838900 | 1.53641100 | -0.28121300 |
| B | -2.79961100 | -0.28338500 | -1.33005400 |
| O | -2.62222700 | -1.64536800 | -1.41857000 |
| O | -2.31144800 | 0.37583300 | -2.43931500 |
| C | -2.15425200 | -1.95436500 | -2.75906400 |
| C | -1.55695800 | -0.57885200 | -3.23516800 |
| C | -3.38730200 | -2.39009100 | -3.55554200 |
| C | -1.14504200 | -3.09236800 | -2.67138900 |
| C | -1.77418500 | -0.25933200 | -4.70965000 |

| | | | |
|---|---|---|---|
| C | -0.08236100 | -0.39252200 | -2.86624100 |
| H | -3.12476800 | -2.69315800 | -4.57414100 |
| H | -4.12705000 | -1.58552900 | -3.60731700 |
| H | -3.85107300 | -3.24155600 | -3.04875300 |
| H | -0.74499100 | -3.33033400 | -3.66352600 |
| H | -1.63233900 | -3.98753100 | -2.27301100 |
| H | -0.31153800 | -2.84419200 | -2.01417700 |
| H | -1.27195600 | -0.99890600 | -5.34335000 |
| H | -1.35219600 | 0.72485600 | -4.93637900 |
| H | -2.83545200 | -0.24103600 | -4.96560800 |
| H | 0.57132600 | -1.05962300 | -3.43659400 |
| H | 0.08205500 | -0.57865300 | -1.80149100 |
| H | 0.21385300 | 0.64070300 | -3.07020200 |
| Cu | -0.55406000 | 0.05062500 | 0.61479600 |
| P | 0.89703200 | -1.67832300 | 0.90320300 |
| P | 0.50045400 | 2.04726600 | 0.18682200 |
| C | 1.98017200 | -1.32438500 | 2.33890000 |
| C | 0.15814800 | -3.30291700 | 1.30858900 |
| C | 2.08304600 | -2.10049600 | -0.43511400 |
| C | 1.20758700 | 2.41855500 | 1.83184700 |
| C | 1.85312100 | 2.30610000 | -1.03272700 |
| C | -0.58651600 | 3.48164900 | -0.15967000 |
| C | 3.36474800 | -1.53092100 | 2.33172800 |
| C | 1.36668000 | -0.80822500 | 3.48998600 |
| C | -1.16827900 | -3.54537800 | 0.92740000 |
| C | 0.88816600 | -4.30393900 | 1.96810500 |
| C | 2.84362600 | -1.06114600 | -0.98153600 |
| C | 2.20500000 | -3.36584400 | -1.02371000 |
| C | 0.31370900 | 2.43563700 | 2.91812900 |
| C | 2.57424200 | 2.61242400 | 2.05680900 |
| C | 1.92276400 | 3.41461800 | -1.88943400 |
| C | 2.74843700 | 1.25719400 | -1.27042700 |
| C | -1.52312800 | 3.34894100 | -1.19665700 |
| C | -0.51354900 | 4.68611800 | 0.55173900 |
| H | 3.84941200 | -1.92840700 | 1.44583200 |
| C | 4.12573600 | -1.22565000 | 3.46093000 |
| C | 2.12838900 | -0.51460500 | 4.61825400 |
| H | 0.29527500 | -0.62845600 | 3.49528300 |
| C | -1.74891200 | -4.78813800 | 1.18869100 |
| H | -1.74790300 | -2.76489500 | 0.44970400 |
| C | 0.30198600 | -5.54088600 | 2.22824000 |
| H | 1.91015100 | -4.10919800 | 2.28070700 |
| O | 2.68696300 | 0.18288800 | -0.40484200 |
| C | 3.71375100 | -1.21830000 | -2.06198900 |

| | | | |
|---|---|---|---|
| H | 1.62915300 | -4.19558500 | -0.62958600 |
| C | 3.04392200 | -3.55276200 | -2.12303300 |
| H | -0.74422700 | 2.24686600 | 2.75293000 |
| C | 0.78853500 | 2.68588300 | 4.20361000 |
| H | 3.26916300 | 2.59014600 | 1.22342400 |
| C | 3.04477400 | 2.83717600 | 3.35120100 |
| H | 1.24577000 | 4.24776500 | -1.73932000 |
| C | 2.82693100 | 3.43173000 | -2.95039900 |
| C | 3.64740200 | 1.22935400 | -2.33957900 |
| H | -1.59783400 | 2.41596100 | -1.74654800 |
| C | -2.37406200 | 4.40747000 | -1.51236300 |
| H | 0.20652300 | 4.79659500 | 1.35571700 |
| C | -1.37241900 | 5.74021400 | 0.23685000 |
| H | 5.20036900 | -1.38648900 | 3.44530100 |
| C | 3.50936100 | -0.71959800 | 4.60555700 |
| H | 1.64465700 | -0.10708600 | 5.50013500 |
| C | -1.01736200 | -5.78497900 | 1.83447900 |
| H | -2.77993000 | -4.96765200 | 0.89744900 |
| H | 0.86976600 | -6.31192800 | 2.74180500 |
| C | 4.54778900 | -0.00186400 | -2.47487900 |
| C | 3.79214000 | -2.49100100 | -2.63668300 |
| H | 3.12141000 | -4.53512200 | -2.57922700 |
| H | 0.09139300 | 2.70917100 | 5.03666600 |
| C | 2.15359000 | 2.88614400 | 4.42333300 |
| H | 4.10858600 | 2.97939900 | 3.51947000 |
| C | 3.67041800 | 2.34305500 | -3.18369700 |
| H | 2.86705900 | 4.29386200 | -3.60946800 |
| H | -3.10092100 | 4.29071700 | -2.31128900 |
| C | -2.30347300 | 5.60324100 | -0.79424800 |
| H | -1.31346300 | 6.66844800 | 0.79851200 |
| H | 4.10302600 | -0.47994600 | 5.48329400 |
| H | -1.47506700 | -6.74835300 | 2.04234800 |
| C | 5.72163400 | 0.13848900 | -1.46811900 |
| C | 5.11716300 | -0.14663500 | -3.89105600 |
| H | 4.44444400 | -2.66230700 | -3.48586200 |
| H | 2.52249400 | 3.06913400 | 5.42875200 |
| H | 4.34884100 | 2.36795300 | -4.02926800 |
| H | -2.97444400 | 6.42347800 | -1.03387300 |
| H | 5.34982300 | 0.24066000 | -0.44441000 |
| H | 6.32037600 | 1.02421600 | -1.70728000 |
| H | 6.36688200 | -0.74579800 | -1.51383300 |
| H | 5.76763100 | -1.02369500 | -3.95675000 |
| H | 5.73032800 | 0.72102700 | -4.15107800 |
| H | 4.32204200 | -0.24624500 | -4.63713900 |

| | | | |
|---|---|---|---|
| F | -2.93004600 | -1.03990000 | 1.69097400 |
| F | -2.73335400 | 1.13124000 | 2.09449000 |
| C | -4.87741400 | 0.22622100 | 0.17749800 |
| C | -5.71129100 | 1.29683800 | 0.52413400 |
| C | -5.43339000 | -1.06006400 | 0.12012000 |
| C | -7.06447900 | 1.09554100 | 0.79705600 |
| H | -5.28873300 | 2.29685200 | 0.58129800 |
| C | -6.78557400 | -1.26455000 | 0.39233200 |
| H | -4.79778100 | -1.89910800 | -0.14113400 |
| C | -7.60811800 | -0.18822900 | 0.73099400 |
| H | -7.69387400 | 1.94140300 | 1.06230000 |
| H | -7.19896500 | -2.26895900 | 0.34153400 |
| H | -8.66212900 | -0.34881100 | 0.94200700 |

**C1**

Total electronic energy = -3380.649425

Thermal corrections to Gibbs free energy =0.811055

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.84311300 | 1.43179100 | 0.18241900 |
| C | -2.55975100 | 1.35316600 | -1.12896800 |
| B | -4.10170800 | 0.95905700 | -1.18431800 |
| O | -5.07864300 | 1.80669800 | -0.75263500 |
| O | -4.57097800 | -0.22286500 | -1.68932300 |
| C | -6.34999500 | 1.25468500 | -1.19649100 |
| C | -6.00421600 | -0.26555800 | -1.42164200 |
| C | -6.71288000 | 1.99197600 | -2.48899100 |
| C | -7.39394900 | 1.52426500 | -0.11942600 |
| C | -6.69071200 | -0.91143400 | -2.61997500 |
| C | -6.20684100 | -1.12576600 | -0.17152900 |
| H | -7.69143300 | 1.68116500 | -2.86900100 |
| H | -5.96327900 | 1.81715800 | -3.26670700 |
| H | -6.74367900 | 3.06627100 | -2.28562900 |
| H | -8.35276600 | 1.06532800 | -0.38582300 |
| H | -7.54758900 | 2.60324000 | -0.02130500 |
| H | -7.07566000 | 1.13803100 | 0.85066800 |
| H | -7.77948800 | -0.89469000 | -2.49770900 |
| H | -6.37567800 | -1.95665600 | -2.70263200 |
| H | -6.43410100 | -0.40566500 | -3.55294000 |
| H | -7.27168300 | -1.27761300 | 0.03325100 |
| H | -5.73905700 | -0.67415000 | 0.70548700 |
| H | -5.74077800 | -2.10250500 | -0.33257700 |

| | | | |
|---|---|---|---|
| H | -1.63141800 | 2.48425400 | 0.38237700 |
| Cu | -0.04311500 | 0.52158700 | -0.14905400 |
| P | 0.34957000 | -1.71916500 | 0.11855600 |
| P | 1.83468700 | 1.80134100 | -0.03491400 |
| C | 0.89927200 | -1.95392700 | 1.85345200 |
| C | -1.09735100 | -2.83828900 | -0.03228400 |
| C | 1.61076100 | -2.60017400 | -0.89590300 |
| C | 2.55640200 | 1.54882100 | 1.63192800 |
| C | 3.26145900 | 1.52736400 | -1.15454500 |
| C | 1.57457100 | 3.61152100 | -0.13496900 |
| C | 2.19790900 | -2.34118200 | 2.20145600 |
| C | -0.02615700 | -1.65656800 | 2.86669300 |
| C | -2.02711800 | -2.56727000 | -1.04618600 |
| C | -1.30950000 | -3.92956800 | 0.82142300 |
| C | 2.82186200 | -1.95988100 | -1.18011300 |
| C | 1.38615300 | -3.84430800 | -1.50199300 |
| C | 1.66813600 | 1.35875200 | 2.70107200 |
| C | 3.93593400 | 1.52124200 | 1.87230600 |
| C | 3.89454700 | 2.51399600 | -1.92060100 |
| C | 3.68746200 | 0.20602600 | -1.32512100 |
| C | 0.48628500 | 4.07914900 | -0.88561500 |
| C | 2.41642200 | 4.53040100 | 0.50894900 |
| H | 2.92487200 | -2.56912800 | 1.42989500 |
| C | 2.56313100 | -2.43822500 | 3.54509500 |
| C | 0.33672300 | -1.77648500 | 4.20520600 |
| H | -1.03035500 | -1.34123900 | 2.61051100 |
| C | -3.15319600 | -3.37536900 | -1.20238500 |
| H | -1.90253400 | -1.69429600 | -1.67647900 |
| C | -2.44100200 | -4.73081600 | 0.66806100 |
| H | -0.59987300 | -4.14125700 | 1.61451000 |
| O | 3.04471300 | -0.74705000 | -0.56004900 |
| C | 3.78786100 | -2.47159900 | -2.05142000 |
| H | 0.46005400 | -4.37309800 | -1.30827100 |
| C | 2.33199900 | -4.38834300 | -2.36965700 |
| H | 0.59671200 | 1.34572000 | 2.52331500 |
| C | 2.15472200 | 1.16323100 | 3.99125100 |
| H | 4.63092400 | 1.65637600 | 1.04920700 |
| C | 4.41975600 | 1.31263800 | 3.16452900 |
| H | 3.59027200 | 3.54972800 | -1.81632700 |
| C | 4.89771900 | 2.16235000 | -2.82511300 |
| C | 4.68944100 | -0.18073500 | -2.21531600 |
| H | -0.19454200 | 3.37580600 | -1.35409200 |
| C | 0.25437000 | 5.45083100 | -1.00125700 |
| H | 3.24928100 | 4.17127800 | 1.10624200 |

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|---|---|---|---|
| C | 2.17991400 | 5.89928700 | 0.39228100 |
| H | 3.57638000 | -2.73157300 | 3.80508700 |
| C | 1.63361900 | -2.16529100 | 4.54888600 |
| H | -0.39759200 | -1.55062400 | 4.97302300 |
| C | -3.36438400 | -4.45592500 | -0.34407000 |
| H | -3.87351900 | -3.13480800 | -1.97801300 |
| H | -2.60268900 | -5.56880900 | 1.34061000 |
| C | 5.07637300 | -1.66248400 | -2.23516700 |
| C | 3.51736400 | -3.70489700 | -2.64990100 |
| H | 2.14202300 | -5.34947300 | -2.83802600 |
| H | 1.45657400 | 1.00453200 | 4.80643900 |
| C | 3.53061400 | 1.13703400 | 4.22560900 |
| H | 5.49181700 | 1.28800100 | 3.34098600 |
| C | 5.28940400 | 0.82970700 | -2.97412200 |
| H | 5.37871900 | 2.93260400 | -3.42062700 |
| H | -0.59538600 | 5.80347900 | -1.57855000 |
| C | 1.09977100 | 6.36077100 | -0.36526600 |
| H | 2.83435600 | 6.60583000 | 0.89546900 |
| H | 1.92118900 | -2.24728600 | 5.59355200 |
| H | -4.24754000 | -5.07893000 | -0.45742600 |
| C | 5.99806900 | -1.93548100 | -1.01563300 |
| C | 5.81952100 | -2.04655600 | -3.52025000 |
| H | 4.23302800 | -4.14185800 | -3.33752700 |
| H | 3.90838400 | 0.97021200 | 5.23053600 |
| H | 6.06957600 | 0.58202500 | -3.68549200 |
| H | 0.91362000 | 7.42788000 | -0.45035100 |
| H | 5.50065000 | -1.66427900 | -0.07978700 |
| H | 6.91848200 | -1.34687100 | -1.09836800 |
| H | 6.26204100 | -2.99789100 | -0.97123100 |
| H | 6.10929300 | -3.10117900 | -3.49842600 |
| H | 6.74262300 | -1.46779800 | -3.61846300 |
| H | 5.20397600 | -1.87306000 | -4.40877500 |
| C | -2.40709400 | 0.78331400 | 1.38191100 |
| C | -2.17887100 | 1.35281700 | 2.65666200 |
| C | -3.11925300 | -0.43571800 | 1.35735200 |
| C | -2.61725900 | 0.73783500 | 3.82561200 |
| H | -1.64755000 | 2.30068500 | 2.71447300 |
| C | -3.57466200 | -1.04245600 | 2.52736600 |
| H | -3.29162000 | -0.93281800 | 0.41223300 |
| C | -3.32412300 | -0.46910200 | 3.77654700 |
| H | -2.41610900 | 1.21072800 | 4.78435400 |
| H | -4.10908300 | -1.98680500 | 2.45539600 |
| H | -3.67044500 | -0.94780500 | 4.68794500 |
| F | -2.42850100 | 2.58570800 | -1.77943100 |

| | | | |
|---|---|---|---|
| F | -1.88392500 | 0.45942800 | -2.03416800 |

**C2**

Total electronic energy = -3569.297762

Thermal corrections to Gibbs free energy = 0.818861

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.11289100 | 1.99878500 | 0.29543100 |
| P | -1.13363400 | -1.55871800 | 1.08623100 |
| O | -2.50651600 | 0.52346400 | -0.31236500 |
| C | -1.28961100 | 2.39145100 | -1.07058400 |
| C | -1.11638800 | 3.40355000 | -2.02258400 |
| H | -0.27771500 | 4.08466600 | -1.93964800 |
| C | -2.00281100 | 3.51893500 | -3.09368800 |
| H | -1.85507300 | 4.30285600 | -3.83051000 |
| C | -3.07416100 | 2.63403200 | -3.23278500 |
| H | -3.74332800 | 2.74112400 | -4.07911800 |
| C | -3.28247400 | 1.61114200 | -2.30432400 |
| C | -2.37317700 | 1.52507700 | -1.25015400 |
| C | -3.00116800 | -0.68563600 | -0.75889400 |
| C | -2.48867800 | -1.82172500 | -0.12737100 |
| C | -2.99211300 | -3.06510400 | -0.52051300 |
| H | -2.61781300 | -3.96872300 | -0.05218600 |
| C | -3.95271500 | -3.13762100 | -1.53055300 |
| H | -4.33394500 | -4.10590600 | -1.84091300 |
| C | -4.41939600 | -1.98056000 | -2.15701400 |
| H | -5.15213800 | -2.06743500 | -2.95143200 |
| C | -3.95163800 | -0.71903800 | -1.77554200 |
| C | -4.45157300 | 0.61962700 | -2.32840500 |
| C | -5.54697200 | 1.15159000 | -1.36496100 |
| H | -6.39360500 | 0.45671200 | -1.33413200 |
| H | -5.90636300 | 2.13074300 | -1.70075800 |
| H | -5.15552100 | 1.25828500 | -0.34832500 |
| C | -5.04453900 | 0.46960700 | -3.73478200 |
| H | -4.29654200 | 0.09067000 | -4.43613000 |
| H | -5.42184500 | 1.42890300 | -4.10119300 |
| H | -5.89507500 | -0.21818300 | -3.72277600 |
| C | -0.92630900 | 2.69747500 | 1.79317700 |
| C | -0.11371500 | 3.03899600 | 2.88710600 |
| H | 0.96256700 | 2.91583700 | 2.81756800 |
| C | -0.67647400 | 3.55219500 | 4.05328600 |
| H | -0.03304300 | 3.82610500 | 4.88522800 |

| | | | |
|---|---|---|---|
| C | -2.06006100 | 3.71424800 | 4.15281400 |
| H | -2.49994100 | 4.11193100 | 5.06311700 |
| C | -2.87434100 | 3.35372900 | 3.07959400 |
| H | -3.95252100 | 3.46482900 | 3.15198800 |
| C | -2.31334500 | 2.85116000 | 1.90552100 |
| H | -2.95947500 | 2.58432200 | 1.07792900 |
| C | 1.23051900 | 3.22509500 | 0.04677200 |
| C | 2.51155000 | 2.77737600 | -0.29946000 |
| H | 2.70331300 | 1.71269500 | -0.38009600 |
| C | 3.54033800 | 3.69981000 | -0.50963200 |
| H | 4.53126900 | 3.35196100 | -0.78338000 |
| C | 3.30333100 | 5.06645300 | -0.36750100 |
| H | 4.10734900 | 5.77833800 | -0.53228200 |
| C | 2.03203600 | 5.51818900 | -0.00368200 |
| H | 1.84398400 | 6.58120700 | 0.11883200 |
| C | 1.00357900 | 4.60260100 | 0.20536600 |
| H | 0.01908900 | 4.95304700 | 0.49987300 |
| C | -2.01907100 | -0.80374500 | 2.50870100 |
| C | -1.26230300 | -0.16939300 | 3.50246000 |
| H | -0.18893700 | -0.06863200 | 3.38224900 |
| C | -1.88040400 | 0.36113200 | 4.63212700 |
| H | -1.28244900 | 0.85910300 | 5.38808300 |
| C | -3.26694100 | 0.28665100 | 4.77050300 |
| H | -3.74993200 | 0.71415600 | 5.64462300 |
| C | -4.03176700 | -0.32225500 | 3.77506500 |
| H | -5.11266000 | -0.37639900 | 3.87348300 |
| C | -3.41131300 | -0.86933400 | 2.65148700 |
| H | -4.00863200 | -1.35236600 | 1.88473900 |
| C | -0.80802500 | -3.26293900 | 1.68166100 |
| C | 0.20375000 | -3.99826200 | 1.04992900 |
| H | 0.79766800 | -3.53455200 | 0.27245500 |
| C | 0.45309600 | -5.31670600 | 1.43234800 |
| H | 1.23995500 | -5.87792100 | 0.93636300 |
| C | -0.29485400 | -5.90546300 | 2.45287400 |
| H | -0.09487600 | -6.93015200 | 2.75420400 |
| C | -1.29808700 | -5.17274400 | 3.09162000 |
| H | -1.88045600 | -5.62549100 | 3.88955100 |
| C | -1.55681100 | -3.85731500 | 2.70806200 |
| H | -2.33817500 | -3.29339900 | 3.20657400 |
| Cu | 0.39608000 | -0.26154400 | -0.04571200 |
| C | 1.39457300 | -0.56727200 | -1.77596800 |
| H | 1.84339900 | 0.40071200 | -2.03375500 |
| C | 0.29033600 | -0.86090700 | -2.73840500 |
| C | -1.81261200 | -1.36637000 | -4.57313000 |

| | | | |
|---|---|---|---|
| C | -0.22610900 | 0.15587600 | -3.56158400 |
| C | -0.29147000 | -2.14103300 | -2.85267700 |
| C | -1.31900100 | -2.38796300 | -3.75653700 |
| C | -1.25997900 | -0.08999800 | -4.46375500 |
| H | 0.19714200 | 1.15467600 | -3.49254900 |
| H | 0.08394300 | -2.94490400 | -2.22963100 |
| H | -1.74390900 | -3.38612900 | -3.82003700 |
| H | -1.62718800 | 0.72140500 | -5.08667700 |
| H | -2.61096400 | -1.56606600 | -5.28312200 |
| C | 2.50387700 | -1.56793500 | -1.74721500 |
| B | 3.86125600 | -1.06735900 | -1.09609100 |
| O | 3.93557900 | -0.46845500 | 0.13977900 |
| C | 5.35283700 | -0.39463100 | 0.48872600 |
| C | 6.03647300 | -0.43761700 | -0.92371900 |
| O | 5.07309200 | -1.19058000 | -1.71018000 |
| C | 7.37685700 | -1.16103700 | -0.97113600 |
| H | 7.28340700 | -2.20034200 | -0.65062200 |
| H | 8.11045600 | -0.65865600 | -0.33053700 |
| H | 7.75869800 | -1.15617500 | -1.99641500 |
| C | 6.14955600 | 0.93859600 | -1.58515300 |
| H | 5.18373500 | 1.45116700 | -1.58439200 |
| H | 6.45700500 | 0.80713700 | -2.62640800 |
| H | 6.88679700 | 1.57144500 | -1.08064300 |
| C | 5.59253000 | 0.87775800 | 1.29082900 |
| H | 5.06489400 | 0.81846000 | 2.24727200 |
| H | 5.22729000 | 1.76222400 | 0.76744700 |
| H | 6.66103400 | 1.00474300 | 1.49741400 |
| C | 5.66639000 | -1.63087900 | 1.33653300 |
| H | 6.70852800 | -1.62741300 | 1.67078100 |
| H | 5.48053600 | -2.55125400 | 0.77540800 |
| H | 5.02234600 | -1.64299000 | 2.21919400 |
| C | 2.30234200 | -0.69274300 | 2.39469100 |
| O | 2.24810200 | 0.47432800 | 2.49164500 |
| O | 2.35239600 | -1.85916900 | 2.36998900 |
| F | 2.14889300 | -2.75022800 | -1.03190000 |
| F | 2.79781500 | -2.06524900 | -3.01962500 |

**$CO_2$**

Total electronic energy = -188.636269

Thermal corrections to Gibbs free energy =-0.009098

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| O | 0.00000000 | 0.00000000 | 1.16956600 |
| O | 0.00000000 | 0.00000000 | -1.16956600 |

**CuTc**

Total electronic energy =-938.460100

Thermal corrections to Gibbs free energy = 0.035562

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 2.77615300 | -0.03229000 | -0.00011100 |
| O | 0.96515900 | -1.03336700 | 0.00041700 |
| O | 1.11564000 | 1.19222000 | -0.00013700 |
| C | 0.41829100 | 0.12165400 | 0.00023600 |
| C | -1.04543400 | 0.22224400 | 0.00028000 |
| C | -1.80572900 | 1.36951500 | 0.00018200 |
| S | -2.04433800 | -1.20608100 | -0.00009400 |
| C | -3.20132700 | 1.10387000 | -0.00006100 |
| H | -1.35638700 | 2.35502700 | 0.00034100 |
| C | -3.47791000 | -0.24184600 | -0.00020900 |
| H | -3.96623900 | 1.87209300 | -0.00008300 |
| H | -4.45015600 | -0.71684400 | -0.00035300 |

**D**

Total electronic energy = -819.714470

Thermal corrections to Gibbs free energy = 0.254449

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 5.01427400 | 1.03481800 | -0.09049800 |
| C | 3.62292900 | 0.99798900 | -0.08660400 |
| C | 2.94143600 | -0.23095900 | 0.02782900 |
| C | 3.70686200 | -1.40788700 | 0.13660900 |
| C | 5.09808700 | -1.36679600 | 0.13243500 |
| C | 5.75896900 | -0.14241700 | 0.01858900 |
| H | 5.52233600 | 1.99115500 | -0.17956300 |
| H | 3.05603600 | 1.91492500 | -0.17181400 |
| H | 3.19467400 | -2.36272200 | 0.22550500 |
| H | 5.66626800 | -2.28887800 | 0.21785400 |
| H | 6.84466500 | -0.10522200 | 0.01478100 |
| C | 1.48651900 | -0.35461100 | 0.03948200 |
| H | 1.09866400 | -1.36657600 | 0.13068400 |

| | | | |
|---|---|---|---|
| C | 0.52789900 | 0.58659300 | -0.04381000 |
| F | 0.85621700 | 1.90614800 | -0.16565300 |
| C | -2.90590400 | -0.93115400 | -0.10804500 |
| C | -3.23323300 | 0.58941100 | 0.12385200 |
| B | -0.99130800 | 0.28251000 | -0.01357600 |
| O | -1.47902200 | -0.98653500 | 0.17792000 |
| O | -1.96152100 | 1.23152800 | -0.17942400 |
| C | -4.30023500 | 1.16675300 | -0.79834300 |
| H | -5.25783500 | 0.65590400 | -0.64760800 |
| H | -4.44193200 | 2.22881300 | -0.57640800 |
| H | -4.01558300 | 1.07556500 | -1.84846200 |
| C | -3.55285200 | 0.92210600 | 1.58428100 |
| H | -3.55852700 | 2.00907200 | 1.70618000 |
| H | -4.53286800 | 0.53401900 | 1.87955800 |
| H | -2.79628800 | 0.50876500 | 2.25824600 |
| C | -3.07840500 | -1.37054900 | -1.56518300 |
| H | -2.63663700 | -2.36348500 | -1.69025000 |
| H | -4.13484200 | -1.42287100 | -1.84689800 |
| H | -2.56927500 | -0.68355600 | -2.24803700 |
| C | -3.62647400 | -1.89543100 | 0.82629600 |
| H | -4.71144900 | -1.82616500 | 0.68987100 |
| H | -3.32050700 | -2.92215200 | 0.60300700 |
| H | -3.39120800 | -1.69162000 | 1.87280700 |

**D’**

Total electronic energy = -819.707520

Thermal corrections to Gibbs free energy = 0.253286

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -3.25408500 | -1.80694700 | 0.27993600 |
| C | -2.29130000 | -0.80119900 | 0.29781600 |
| C | -2.65224000 | 0.53731500 | 0.05008900 |
| C | -4.01098400 | 0.81929000 | -0.19789600 |
| C | -4.97005900 | -0.18903200 | -0.21672600 |
| C | -4.59472200 | -1.51186600 | 0.02143900 |
| H | -2.95374100 | -2.83302000 | 0.47550200 |
| H | -1.26035100 | -1.05123300 | 0.50645100 |
| H | -4.30956900 | 1.84811100 | -0.38261700 |
| H | -6.00933600 | 0.05859800 | -0.41408400 |
| H | -5.33889900 | -2.30326400 | 0.01153100 |
| C | -1.73280000 | 1.67568600 | 0.04081500 |
| H | -2.23213400 | 2.64344500 | -0.00866400 |

| | | | |
|---|---|---|---|
| C | -0.38847500 | 1.77838900 | 0.05241400 |
| F | 0.07710100 | 3.07073000 | 0.02168500 |
| C | 2.03253500 | -1.13140800 | -0.11368600 |
| C | 2.97870700 | 0.11315200 | 0.03464100 |
| B | 0.80548400 | 0.78070900 | 0.03509000 |
| O | 2.07466000 | 1.22268000 | -0.22306700 |
| O | 0.73751800 | -0.57205000 | 0.25651500 |
| C | 4.12227300 | 0.17424400 | -0.97083900 |
| H | 4.70951600 | 1.08209100 | -0.80342500 |
| H | 4.78662100 | -0.68902600 | -0.85240700 |
| H | 3.75313700 | 0.19484200 | -1.99814200 |
| C | 2.34034600 | -2.29544200 | 0.81937800 |
| H | 1.61703300 | -3.10046200 | 0.65635800 |
| H | 3.34165000 | -2.69292700 | 0.62016800 |
| H | 2.28482200 | -1.99569900 | 1.86772700 |
| C | 1.89667600 | -1.62249700 | -1.55762500 |
| H | 2.80986800 | -2.12017800 | -1.89871700 |
| H | 1.07035500 | -2.33713200 | -1.61363400 |
| H | 1.67604400 | -0.79420300 | -2.23762800 |
| C | 3.50871600 | 0.30291900 | 1.45910400 |
| H | 3.97600500 | 1.28898100 | 1.53313000 |
| H | 2.69767700 | 0.25624100 | 2.19228000 |
| H | 4.25503200 | -0.45594000 | 1.71481700 |

**D1**

Total electronic energy = -1060.452849

Thermal corrections to Gibbs free energy = 0.375954

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 1.42904700 | 1.34062900 | -0.77174200 |
| C | 1.42092500 | 2.70459300 | -0.31692900 |
| C | 1.73917200 | 2.77934800 | 1.18038400 |
| H | 1.79176300 | 3.82788500 | 1.49523400 |
| H | 0.96748700 | 2.27769300 | 1.76603500 |
| H | 2.69599700 | 2.29630800 | 1.39463400 |
| C | 0.05832700 | 3.34167700 | -0.62063200 |
| H | -0.17921800 | 3.24174700 | -1.68649700 |
| H | -0.73166400 | 2.86189400 | -0.04157300 |
| H | 0.06949300 | 4.40896300 | -0.37115300 |
| C | 2.52137500 | 3.40405900 | -1.12360100 |
| H | 3.49158500 | 2.93274500 | -0.93048400 |
| H | 2.30807900 | 3.34283000 | -2.19998600 |

| | | | |
|---|---|---|---|
| H | 2.59352900 | 4.46440800 | -0.85953800 |
| C | -5.14821200 | 0.41553800 | 0.97083600 |
| C | -3.76148600 | 0.41900500 | 0.84170400 |
| C | -3.13050800 | -0.34943100 | -0.15793600 |
| C | -3.95017200 | -1.11376400 | -1.01093800 |
| C | -5.33618800 | -1.11542800 | -0.87964700 |
| C | -5.94513300 | -0.34799100 | 0.11473800 |
| H | -5.61112900 | 1.01568500 | 1.75005500 |
| H | -3.15862600 | 1.01230600 | 1.51516100 |
| H | -3.48224000 | -1.71492100 | -1.78730400 |
| H | -5.94127300 | -1.71662300 | -1.55337600 |
| H | -7.02628100 | -0.34564100 | 0.22216700 |
| C | -1.68182300 | -0.39860300 | -0.36848200 |
| H | -1.34970800 | -1.04508600 | -1.17683500 |
| C | -0.67610300 | 0.21220000 | 0.27749100 |
| F | -0.98427000 | 1.04084800 | 1.33967100 |
| C | 2.60384700 | -1.29678500 | 0.74369000 |
| C | 1.88102800 | -2.03488100 | -0.44020500 |
| B | 0.89763900 | 0.10715600 | -0.03438300 |
| O | 1.66641800 | -0.29282600 | 1.11403400 |
| O | 1.18669900 | -0.95004000 | -1.09126000 |
| C | 2.81213500 | -2.69837900 | -1.45128300 |
| H | 3.41213900 | -3.48087700 | -0.97409500 |
| H | 2.22682200 | -3.16558000 | -2.25121800 |
| H | 3.50266400 | -1.97763300 | -1.90272200 |
| C | 0.82996400 | -3.03945000 | 0.04326500 |
| H | 0.22720000 | -3.36400400 | -0.81114200 |
| H | 1.29436700 | -3.92287200 | 0.49295300 |
| H | 0.16099400 | -2.57791400 | 0.77285100 |
| C | 3.92193900 | -0.62811400 | 0.31241100 |
| H | 4.25493900 | 0.02850500 | 1.12167000 |
| H | 4.71272400 | -1.35982100 | 0.11286100 |
| H | 3.78893200 | -0.00260000 | -0.57618100 |
| C | 2.86854500 | -2.18482700 | 1.95931300 |
| H | 3.50823500 | -3.03691100 | 1.70004500 |
| H | 3.37576300 | -1.60108700 | 2.73408400 |
| H | 1.93311100 | -2.55843300 | 2.38031600 |
| Li | 1.70381800 | 0.35364100 | -2.22480500 |

**D2**

Total electronic energy = -1008.357752

Thermal corrections to Gibbs free energy = 0.259246

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -5.10200900 | -0.74061400 | -0.42135200 |
| C | -3.71523100 | -0.62334300 | -0.41527200 |
| C | -3.10199400 | 0.57279700 | 0.00973900 |
| C | -3.92929700 | 1.63408200 | 0.42413900 |
| C | -5.31579600 | 1.51286400 | 0.41647500 |
| C | -5.90888800 | 0.32235300 | -0.00734200 |
| H | -5.55737600 | -1.66998400 | -0.75211200 |
| H | -3.10034300 | -1.45220700 | -0.73805400 |
| H | -3.46972100 | 2.56192000 | 0.75540300 |
| H | -5.93297700 | 2.34592900 | 0.74098600 |
| H | -6.99060600 | 0.22290900 | -0.01506000 |
| C | -1.65648600 | 0.77563400 | 0.04796200 |
| H | -1.32463400 | 1.74811500 | 0.40466500 |
| C | -0.64709900 | -0.04652900 | -0.28756700 |
| F | -0.90620800 | -1.30724600 | -0.76182000 |
| C | 2.72484100 | 1.57622200 | 0.04351200 |
| C | 3.11326200 | 0.06175500 | -0.14052600 |
| B | 0.85528500 | 0.31015800 | -0.17812200 |
| O | 1.29872100 | 1.50114800 | 0.33298200 |
| O | 1.85724000 | -0.52879700 | -0.58720500 |
| C | 4.17356300 | -0.20809000 | -1.20125000 |
| H | 5.12047900 | 0.27272100 | -0.93160600 |
| H | 4.34715400 | -1.28562400 | -1.27820100 |
| H | 3.86260200 | 0.15469400 | -2.18282300 |
| C | 3.48662400 | -0.63094900 | 1.17295700 |
| H | 3.57772500 | -1.70650300 | 0.99452000 |
| H | 4.44462700 | -0.26656100 | 1.55655300 |
| H | 2.71893700 | -0.47814000 | 1.93633600 |
| C | 2.86650200 | 2.39729400 | -1.24132600 |
| H | 2.39088700 | 3.37118700 | -1.09314500 |
| H | 3.91738800 | 2.56024900 | -1.50025900 |
| H | 2.37261900 | 1.90261000 | -2.08323000 |
| C | 3.41601900 | 2.28095100 | 1.20428000 |
| H | 4.50154900 | 2.29445800 | 1.05640000 |
| H | 3.06796800 | 3.31663400 | 1.26498100 |
| H | 3.19754700 | 1.79310600 | 2.15628600 |
| C | 0.86238700 | -3.01098600 | 0.52799300 |
| O | 1.12774500 | -3.62723100 | -0.42795600 |
| O | 0.60844900 | -2.43408700 | 1.51478100 |

**D3**

Total electronic energy = -3621.454965

Thermal corrections to Gibbs free energy = 0.929601
No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 1.28802100 | 2.21047400 | 0.08606200 |
| P | 1.32195100 | -1.55111100 | -0.87761400 |
| C | 2.33863600 | 2.82429100 | -1.27942900 |
| C | 0.12781400 | 3.58587000 | 0.43199000 |
| C | 2.42451800 | 2.18042600 | 1.52674100 |
| C | 2.30929100 | -1.02617400 | -2.33978200 |
| C | 2.54262800 | -2.17739300 | 0.34215300 |
| C | 0.45845200 | -3.00658100 | -1.54791400 |
| C | 3.46813300 | 3.62494000 | -1.05782100 |
| C | 1.98303300 | 2.48302900 | -2.59120600 |
| C | -0.65490100 | 3.53741900 | 1.60229400 |
| C | -0.12559800 | 4.58548500 | -0.51672400 |
| C | 3.21660700 | 1.03610800 | 1.69308100 |
| C | 2.50872100 | 3.17405600 | 2.50909900 |
| C | 1.62935100 | -0.88586700 | -3.56090900 |
| C | 3.67443600 | -0.72606900 | -2.28274900 |
| C | 2.66419200 | -3.52299800 | 0.70610200 |
| C | 3.28174600 | -1.23767200 | 1.07390400 |
| C | -0.93343000 | -3.05563700 | -1.43713800 |
| C | 1.13973600 | -4.01409200 | -2.25295100 |
| H | 3.75338200 | 3.88644900 | -0.04353300 |
| C | 4.22717600 | 4.07917500 | -2.13535900 |
| C | 2.73491000 | 2.95208500 | -3.66754500 |
| H | 1.13019700 | 1.83756900 | -2.76703800 |
| C | -1.66651800 | 4.47405700 | 1.80932200 |
| H | -0.48466100 | 2.74872900 | 2.32739200 |
| C | -1.14903000 | 5.51314500 | -0.30773700 |
| H | 0.46945900 | 4.63513600 | -1.42271600 |
| O | 3.13925200 | 0.08440300 | 0.69664200 |
| C | 4.05338200 | 0.82507100 | 2.79054100 |
| H | 1.90937600 | 4.07294000 | 2.41325800 |
| C | 3.33406200 | 2.99586000 | 3.61928400 |
| H | 0.57190600 | -1.12634100 | -3.62107700 |
| C | 2.30688400 | -0.46207000 | -4.70162400 |
| H | 4.21759400 | -0.83253500 | -1.35165100 |
| C | 4.34886600 | -0.29446500 | -3.42585000 |
| H | 2.07628200 | -4.27342700 | 0.19125000 |
| C | 3.49690500 | -3.88861200 | 1.76393700 |
| C | 4.11941100 | -1.56826800 | 2.13985600 |

| | | | |
|---|---|---|---|
| H | -1.45989900 | -2.28037500 | -0.89417600 |
| C | -1.64618900 | -4.10400400 | -2.02344800 |
| H | 2.21879500 | -3.96179700 | -2.36706000 |
| C | 0.42781500 | -5.06571500 | -2.82137700 |
| H | 5.10412900 | 4.69511400 | -1.95618200 |
| C | 3.85844900 | 3.74793700 | -3.44142100 |
| H | 2.45344700 | 2.67612700 | -4.67843900 |
| C | -1.92240300 | 5.46036900 | 0.85146300 |
| H | -2.26056700 | 4.42846900 | 2.71784300 |
| H | -1.33889800 | 6.27849100 | -1.05497200 |
| C | 4.91771400 | -0.44053800 | 2.80270000 |
| C | 4.09076500 | 1.83077200 | 3.76187500 |
| H | 3.38697500 | 3.76751800 | 4.38128300 |
| H | 1.77042000 | -0.36811400 | -5.64180700 |
| C | 3.67017700 | -0.16370200 | -4.63655200 |
| H | 5.40838900 | -0.06230000 | -3.36712700 |
| C | 4.21111800 | -2.92331600 | 2.47603400 |
| H | 3.57858200 | -4.93403400 | 2.04553100 |
| H | -2.72491600 | -4.11935600 | -1.92705800 |
| C | -0.96720300 | -5.10754800 | -2.70988800 |
| H | 0.95555500 | -5.84683900 | -3.36157300 |
| H | 4.45031400 | 4.10443500 | -4.27984600 |
| H | -2.72078100 | 6.17927000 | 1.00962300 |
| C | 6.17370800 | -0.16718900 | 1.93140200 |
| C | 5.36425100 | -0.81506700 | 4.22216400 |
| H | 4.72034600 | 1.71366800 | 4.63677400 |
| H | 4.19898300 | 0.16890800 | -5.52520200 |
| H | 4.84381900 | -3.23411100 | 3.29983100 |
| H | -1.52064000 | -5.92500700 | -3.16376300 |
| H | 5.89013600 | 0.11116700 | 0.91170500 |
| H | 6.80276900 | -1.06274400 | 1.88178600 |
| H | 6.76046600 | 0.65318200 | 2.35914400 |
| H | 5.95694600 | -0.01033200 | 4.66622100 |
| H | 6.00449000 | -1.70153800 | 4.20447200 |
| H | 4.50730200 | -1.01681800 | 4.87258900 |
| Cu | 0.26559600 | 0.11511400 | 0.10237000 |
| O | -3.05208300 | 0.70328700 | -0.73377700 |
| C | -3.00736300 | 0.88227500 | -2.14907100 |
| C | -3.94376100 | 2.03035000 | -2.55609600 |
| H | -3.88706300 | 2.21802500 | -3.63546000 |
| H | -4.97171400 | 1.77733900 | -2.28994300 |
| H | -3.65796500 | 2.94976600 | -2.03202500 |
| C | -3.39612300 | -0.40738000 | -2.88256000 |
| H | -2.71130500 | -1.22032300 | -2.62735600 |

| | | | |
|---|---|---|---|
| H | -4.40842100 | -0.71362200 | -2.60926800 |
| H | -3.35800100 | -0.24995000 | -3.96708800 |
| C | -1.55799800 | 1.25846500 | -2.47557200 |
| H | -1.27810400 | 2.17887700 | -1.95110000 |
| H | -0.87994200 | 0.45800300 | -2.15319700 |
| H | -1.41795100 | 1.41778700 | -3.55146700 |
| C | -1.87496300 | -5.56254400 | 1.28089300 |
| C | -2.65145800 | -4.41751800 | 1.11334100 |
| C | -2.19835800 | -3.17042900 | 1.57700000 |
| C | -0.95475700 | -3.11705400 | 2.23648200 |
| C | -0.18099100 | -4.26292900 | 2.40327100 |
| C | -0.63460700 | -5.49296700 | 1.91918000 |
| H | -2.24007800 | -6.51628600 | 0.90813400 |
| H | -3.61037200 | -4.47657400 | 0.61226300 |
| H | -0.59597200 | -2.15341300 | 2.58982400 |
| H | 0.77948400 | -4.19356300 | 2.90561700 |
| H | -0.03279000 | -6.38912700 | 2.04638800 |
| C | -2.91341500 | -1.90932100 | 1.36972200 |
| H | -2.68514300 | -1.12379000 | 2.08182600 |
| C | -3.68460900 | -1.51503000 | 0.34372200 |
| F | -3.97714600 | -2.44186400 | -0.64208700 |
| C | -6.33007100 | 0.62157200 | 0.57689400 |
| C | -5.36834800 | 1.45445800 | 1.50049000 |
| B | -4.15078500 | 0.01577100 | 0.05182600 |
| O | -5.47453800 | 0.20861600 | -0.48803800 |
| O | -4.13075600 | 0.74129300 | 1.37038700 |
| C | -5.16605400 | 2.89068500 | 0.99715900 |
| H | -6.05784200 | 3.50822100 | 1.15219200 |
| H | -4.33854800 | 3.34919300 | 1.55045700 |
| H | -4.91056000 | 2.90059300 | -0.06386900 |
| C | -5.76131400 | 1.47572600 | 2.97598900 |
| H | -5.04020100 | 2.07555100 | 3.54338300 |
| H | -6.75405600 | 1.92084600 | 3.11301000 |
| H | -5.76538900 | 0.46805800 | 3.39614900 |
| C | -7.48729400 | 1.42510000 | -0.01369600 |
| H | -8.09951000 | 0.77298700 | -0.64529800 |
| H | -8.12881500 | 1.83468300 | 0.77570300 |
| H | -7.12317600 | 2.24844000 | -0.63287100 |
| C | -6.87634200 | -0.62973000 | 1.28466800 |
| H | -7.62279600 | -0.37982700 | 2.04708700 |
| H | -7.34772700 | -1.27174800 | 0.53401600 |
| H | -6.06822400 | -1.19668500 | 1.75474000 |
| F | -0.87310000 | 0.54641500 | 1.61537400 |
| Li | -2.33898900 | 1.19686800 | 0.95559900 |

**D4**

Total electronic energy =-3621.455343

Thermal corrections to Gibbs free energy = 0.935777

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 1.19715200 | 1.45898400 | -1.30936700 |
| P | 0.40437000 | -2.14884300 | -0.16376500 |
| C | 2.50942200 | 0.76274800 | -2.38848300 |
| C | 0.67437600 | 2.96611100 | -2.21007200 |
| C | 2.15278600 | 2.06643200 | 0.12999400 |
| C | 1.60185400 | -2.78831300 | -1.40836800 |
| C | 1.34664900 | -2.15146100 | 1.41596000 |
| C | -0.71772100 | -3.59129700 | -0.02073300 |
| C | 3.85708600 | 1.11564800 | -2.24314700 |
| C | 2.13884900 | -0.10832600 | -3.42159400 |
| C | -0.27319500 | 3.80882600 | -1.60764900 |
| C | 1.12139700 | 3.24851000 | -3.50956800 |
| C | 2.67787500 | 1.09002700 | 0.98157000 |
| C | 2.36933400 | 3.40621700 | 0.46778900 |
| C | 1.07614300 | -3.29213900 | -2.60947000 |
| C | 2.98824200 | -2.78247000 | -1.22414600 |
| C | 1.12445100 | -3.05636100 | 2.46187800 |
| C | 2.27060700 | -1.12461500 | 1.64125700 |
| C | -2.10052100 | -3.38238800 | 0.02047800 |
| C | -0.21557500 | -4.90393600 | 0.01427500 |
| H | 4.15452000 | 1.79154600 | -1.44808400 |
| C | 4.81691100 | 0.60501400 | -3.11716600 |
| C | 3.09541800 | -0.59898100 | -4.30785700 |
| H | 1.10222600 | -0.40597400 | -3.52889200 |
| C | -0.75791600 | 4.91886500 | -2.29948400 |
| H | -0.65992200 | 3.64639600 | -0.60365100 |
| C | 0.62046400 | 4.35408000 | -4.19879100 |
| H | 1.85461100 | 2.60729400 | -3.98595900 |
| O | 2.45854200 | -0.22452400 | 0.61282100 |
| C | 3.39934700 | 1.37171400 | 2.13950500 |
| H | 1.97025600 | 4.19089500 | -0.16517200 |
| C | 3.07041700 | 3.72461600 | 1.63140900 |
| H | 0.00013600 | -3.31019500 | -2.76081500 |
| C | 1.91998500 | -3.80071000 | -3.59343300 |
| H | 3.41426000 | -2.39782600 | -0.30557100 |
| C | 3.83260500 | -3.28179300 | -2.21677700 |

| | | | |
|---|---|---|---|
| H | 0.39887600 | -3.85160500 | 2.33754600 |
| C | 1.81387200 | -2.92041700 | 3.66687300 |
| C | 2.98461800 | -0.96457800 | 2.83064500 |
| H | -2.51964000 | -2.38683000 | -0.00332600 |
| C | -2.97039000 | -4.47195400 | 0.10584600 |
| H | 0.85576200 | -5.07415100 | -0.03789100 |
| C | -1.08673400 | -5.98658800 | 0.10496200 |
| H | 5.86033700 | 0.88114300 | -2.99167500 |
| C | 4.43710600 | -0.24694900 | -4.15508600 |
| H | 2.79483900 | -1.27531200 | -5.10105800 |
| C | -0.32008000 | 5.19171300 | -3.59700800 |
| H | -1.48658300 | 5.55521100 | -1.80626700 |
| H | 0.97137300 | 4.56083300 | -5.20633300 |
| C | 3.99868200 | 0.18230400 | 2.89625700 |
| C | 3.57691300 | 2.72052200 | 2.45976700 |
| H | 3.21869600 | 4.76615600 | 1.89954300 |
| H | 1.49762600 | -4.20100000 | -4.51112500 |
| C | 3.30327300 | -3.79845300 | -3.39837700 |
| H | 4.90754500 | -3.26713900 | -2.06163900 |
| C | 2.73755200 | -1.88819500 | 3.84821200 |
| H | 1.62870000 | -3.62383900 | 4.47309100 |
| H | -4.04073000 | -4.28878600 | 0.13379800 |
| C | -2.46845500 | -5.77140500 | 0.15061900 |
| H | -0.69047700 | -6.99788600 | 0.13445600 |
| H | 5.18434900 | -0.64053500 | -4.83851900 |
| H | -0.70747600 | 6.05156100 | -4.13699700 |
| C | 5.27642800 | -0.26659600 | 2.13451700 |
| C | 4.37937200 | 0.54285300 | 4.33625300 |
| H | 4.11218200 | 2.99546300 | 3.36148200 |
| H | 3.96335600 | -4.19229100 | -4.16603000 |
| H | 3.25759600 | -1.80021700 | 4.79554400 |
| H | -3.14659200 | -6.61802200 | 0.21610900 |
| H | 5.04739800 | -0.52001300 | 1.09495100 |
| H | 5.71528400 | -1.14711800 | 2.61688300 |
| H | 6.01729700 | 0.54053100 | 2.13424700 |
| H | 5.12787500 | 1.34085600 | 4.34394800 |
| H | 4.82913700 | -0.31641700 | 4.84299500 |
| H | 3.50782800 | 0.87555300 | 4.90493900 |
| Cu | -0.35649400 | -0.04590400 | -0.61971200 |
| O | -2.37561200 | 0.20738900 | -1.20244600 |
| C | -2.87133100 | 0.28432700 | -2.55766800 |
| C | -3.43914300 | 1.68535500 | -2.81865800 |
| H | -3.71898500 | 1.79515600 | -3.87305800 |
| H | -4.31936500 | 1.87611000 | -2.20511900 |

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|---|---|---|---|
| H | -2.68041000 | 2.44024400 | -2.58512400 |
| C | -3.89941100 | -0.82048800 | -2.82651400 |
| H | -3.46132700 | -1.80014600 | -2.60939200 |
| H | -4.78163600 | -0.71352300 | -2.19743500 |
| H | -4.20602000 | -0.79690500 | -3.87882200 |
| C | -1.65657800 | 0.06347200 | -3.46460400 |
| H | -0.93143300 | 0.87244600 | -3.34246900 |
| H | -1.17281200 | -0.89084700 | -3.22540500 |
| H | -1.96274200 | 0.03983000 | -4.51636200 |
| C | 0.71461000 | 0.74818600 | 4.84648600 |
| C | 0.02809100 | 0.40437500 | 3.68413600 |
| C | -0.36642200 | 1.40322800 | 2.77645700 |
| C | -0.04029300 | 2.74582400 | 3.05803300 |
| C | 0.65206300 | 3.07791600 | 4.21808400 |
| C | 1.02900200 | 2.08113900 | 5.12136300 |
| H | 1.00770400 | -0.03517400 | 5.53990600 |
| H | -0.20709900 | -0.63169700 | 3.48226500 |
| H | -0.38559900 | 3.51191100 | 2.36827700 |
| H | 0.89015100 | 4.11831800 | 4.42197700 |
| H | 1.55885700 | 2.34093900 | 6.03439500 |
| C | -1.17977600 | 1.17293300 | 1.57845300 |
| H | -1.30433200 | 2.06981300 | 0.97730700 |
| C | -1.96571500 | 0.13126500 | 1.21903200 |
| F | -1.90633000 | -1.00697900 | 2.00040700 |
| C | -5.18673000 | -0.56442700 | 0.97685300 |
| C | -5.35082800 | 0.97975900 | 0.67705200 |
| B | -3.14939000 | 0.15979800 | 0.05763300 |
| O | -4.08190000 | -0.93934200 | 0.16162100 |
| O | -4.02668200 | 1.37427900 | 0.26999300 |
| C | -6.31975800 | 1.27689800 | -0.47372900 |
| H | -7.35548800 | 1.06352900 | -0.18951800 |
| H | -6.25516200 | 2.33907100 | -0.73619700 |
| H | -6.07962700 | 0.69545600 | -1.36538900 |
| C | -5.75665900 | 1.81940000 | 1.89184000 |
| H | -5.86439500 | 2.87286000 | 1.60176400 |
| H | -6.72200700 | 1.49416800 | 2.29513400 |
| H | -5.01030600 | 1.75854200 | 2.68721000 |
| C | -6.38918900 | -1.41452400 | 0.56183800 |
| H | -6.18378900 | -2.46431800 | 0.79645300 |
| H | -7.29429700 | -1.11815700 | 1.10413500 |
| H | -6.58248700 | -1.34215300 | -0.51057400 |
| C | -4.86948800 | -0.85636500 | 2.45376100 |
| H | -5.74519100 | -0.68953100 | 3.09029700 |
| H | -4.56892000 | -1.90415600 | 2.54175300 |

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|---|---|---|---|
| H | -4.04681500 | -0.24716900 | 2.83013900 |
| Li | -3.22651800 | 3.01813400 | 0.49011800 |
| F | -2.00180700 | 4.07821600 | 0.71171300 |

**D5**

Total electronic energy = -3621.454006

Thermal corrections to Gibbs free energy = 0.930176

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 0.71098400 | -1.28191800 | -1.63167800 |
| P | 1.93401400 | 0.22079400 | 1.66610500 |
| C | 2.42306800 | -1.91252700 | -1.84595200 |
| C | -0.32284700 | -2.60802500 | -2.37017500 |
| C | 0.68260500 | 0.16946700 | -2.75469900 |
| C | 3.62442700 | -0.49222300 | 1.58737200 |
| C | 2.14954200 | 1.96731200 | 1.12231100 |
| C | 1.65090100 | 0.37927200 | 3.47276200 |
| C | 3.15294300 | -1.66535600 | -3.01614200 |
| C | 3.00119800 | -2.68570500 | -0.83129400 |
| C | -1.64598800 | -2.35296200 | -2.77153600 |
| C | 0.14955500 | -3.93054500 | -2.35892500 |
| C | 1.32919800 | 1.32118600 | -2.27724400 |
| C | -0.03182600 | 0.27466900 | -3.95055200 |
| C | 3.90422400 | -1.65546800 | 2.32419900 |
| C | 4.61830400 | 0.03731900 | 0.75547800 |
| C | 2.18855300 | 3.04739100 | 2.01096300 |
| C | 2.09140600 | 2.25617200 | -0.24762800 |
| C | 0.32458100 | 0.37146700 | 3.93051800 |
| C | 2.69489300 | 0.52190200 | 4.39974400 |
| H | 2.71422100 | -1.06377800 | -3.80595000 |
| C | 4.43801600 | -2.18519100 | -3.16728900 |
| C | 4.27670300 | -3.22454400 | -0.99295500 |
| H | 2.45611900 | -2.85721800 | 0.08925900 |
| C | -2.46690600 | -3.41567000 | -3.15269200 |
| H | -2.05022900 | -1.33797000 | -2.81587700 |
| C | -0.68741800 | -4.98501500 | -2.72551200 |
| H | 1.17178200 | -4.14205900 | -2.06437200 |
| O | 2.05235200 | 1.17439300 | -1.10501800 |
| C | 1.25077400 | 2.56582800 | -2.89799800 |

| | | | |
|---|---|---|---|
| H | -0.55492000 | -0.58590500 | -4.34601100 |
| C | -0.11586600 | 1.50270600 | -4.60708900 |
| H | 3.14272000 | -2.07987700 | 2.97300600 |
| C | 5.15985000 | -2.25421500 | 2.25303300 |
| H | 4.41731900 | 0.92928200 | 0.17305800 |
| C | 5.86929000 | -0.57438900 | 0.67207100 |
| H | 2.21742700 | 2.86207300 | 3.07870400 |
| C | 2.14715000 | 4.35527100 | 1.53044700 |
| C | 2.04666600 | 3.55319100 | -0.76272600 |
| H | -0.49168600 | 0.29264500 | 3.22146600 |
| C | 0.05066800 | 0.50013700 | 5.29300900 |
| H | 3.72434400 | 0.53119900 | 4.05685200 |
| C | 2.41657600 | 0.64543100 | 5.76064800 |
| H | 4.99783600 | -1.98230300 | -4.07625500 |
| C | 4.99951600 | -2.97074200 | -2.15878200 |
| H | 4.71343800 | -3.81719500 | -0.19658200 |
| C | -2.00137100 | -4.73131800 | -3.12136000 |
| H | -3.48276300 | -3.20305400 | -3.47276800 |
| H | -0.30638000 | -6.00265100 | -2.70870700 |
| C | 2.02966400 | 3.73396900 | -2.28461600 |
| C | 0.50265300 | 2.63538500 | -4.08097700 |
| H | -0.69780800 | 1.58095200 | -5.51942000 |
| H | 5.36698500 | -3.14315200 | 2.84280400 |
| C | 6.14785500 | -1.71435500 | 1.42544900 |
| H | 6.62861500 | -0.15392100 | 0.01897900 |
| C | 2.06787200 | 4.60385600 | 0.15979600 |
| H | 2.16393200 | 5.18705300 | 2.22811300 |
| H | -0.98045600 | 0.49388200 | 5.63489100 |
| C | 1.09404200 | 0.63234400 | 6.21020700 |
| H | 3.23267600 | 0.75388300 | 6.46972800 |
| H | 5.99947400 | -3.37836600 | -2.27873900 |
| H | -2.65319000 | -5.55138300 | -3.41040200 |
| C | 3.49307100 | 3.65714700 | -2.79512100 |
| C | 1.42405200 | 5.08801000 | -2.68191000 |
| H | 0.40154300 | 3.58141900 | -4.60082500 |
| H | 7.12567800 | -2.18369000 | 1.36532500 |
| H | 2.02054600 | 5.62915000 | -0.18870200 |
| H | 0.87936200 | 0.72642200 | 7.27107200 |
| H | 3.94733300 | 2.69694800 | -2.53102700 |
| H | 4.09472700 | 4.45762600 | -2.35008400 |
| H | 3.51991100 | 3.75983100 | -3.88565800 |
| H | 1.42579100 | 5.20968900 | -3.76849800 |
| H | 2.01647800 | 5.91219500 | -2.27448100 |
| H | 0.39554600 | 5.18588700 | -2.31957600 |

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|---|---|---|---|
| Cu | 0.10200000 | -0.35913800 | 0.35973500 |
| O | -1.69885300 | -2.25502800 | 0.91785800 |
| C | -1.32667600 | -3.38494600 | 1.75781000 |
| C | -2.09289300 | -4.62617500 | 1.28976100 |
| H | -1.75141400 | -5.50911800 | 1.84120300 |
| H | -3.16648800 | -4.50869400 | 1.45473400 |
| H | -1.91359500 | -4.79282600 | 0.22207500 |
| C | -1.60853000 | -3.04165900 | 3.22257400 |
| H | -1.05941700 | -2.13914800 | 3.51075800 |
| H | -2.67565300 | -2.87143200 | 3.38250100 |
| H | -1.28444600 | -3.86307000 | 3.87116700 |
| C | 0.17105800 | -3.57273100 | 1.52613200 |
| H | 0.36238000 | -3.80892200 | 0.47597500 |
| H | 0.71317900 | -2.65645400 | 1.78351400 |
| H | 0.55313900 | -4.39120800 | 2.14562800 |
| C | -3.90197200 | 4.71394800 | 1.32904300 |
| C | -3.03824300 | 3.62136000 | 1.27464700 |
| C | -2.30678300 | 3.34498500 | 0.10283900 |
| C | -2.47614700 | 4.20361500 | -1.00140400 |
| C | -3.34201100 | 5.29223600 | -0.94345600 |
| C | -4.06104600 | 5.55447400 | 0.22504000 |
| H | -4.45424800 | 4.91155700 | 2.24443300 |
| H | -2.91698500 | 2.98050500 | 2.13766900 |
| H | -1.93205200 | 3.98777200 | -1.91798700 |
| H | -3.45955100 | 5.93436300 | -1.81248400 |
| H | -4.73780900 | 6.40302600 | 0.27428200 |
| C | -1.38439100 | 2.21508600 | -0.05089700 |
| H | -0.75917700 | 2.27402600 | -0.94072200 |
| C | -1.18842000 | 1.08785600 | 0.67131400 |
| F | -2.00650400 | 0.97799500 | 1.81993600 |
| C | -5.16660200 | -1.32918200 | 1.17463800 |
| C | -4.73995600 | -0.71504800 | -0.20455700 |
| B | -2.97378600 | -1.80822700 | 0.78309300 |
| O | -4.08028200 | -2.26024300 | 1.46127400 |
| O | -3.28008400 | -0.80910800 | -0.11832900 |
| C | -5.14703700 | -1.54404000 | -1.42256200 |
| H | -6.22622500 | -1.48670200 | -1.59777800 |
| H | -4.61836400 | -1.13247800 | -2.28702900 |
| H | -4.86438100 | -2.59451800 | -1.29981200 |
| C | -5.11882300 | 0.74766200 | -0.40979900 |
| H | -4.76407600 | 1.07554100 | -1.39189800 |
| H | -6.20825300 | 0.86231100 | -0.38145500 |
| H | -4.67921600 | 1.39518900 | 0.35160500 |
| C | -6.47205200 | -2.11107600 | 1.14113500 |

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|---|---|---|---|
| H | -6.68406200 | -2.51993800 | 2.13409700 |
| H | -7.30316600 | -1.45657000 | 0.85676000 |
| H | -6.42171200 | -2.94008500 | 0.43203600 |
| C | -5.17115200 | -0.30038300 | 2.30845400 |
| H | -6.00457900 | 0.40146300 | 2.20574100 |
| H | -5.27658200 | -0.82575700 | 3.26294100 |
| H | -4.23674300 | 0.26644600 | 2.32347800 |
| Li | -2.30379000 | 0.41726200 | -1.21906300 |
| F | -2.78461800 | 0.39036000 | -2.79963600 |

**E**

Total electronic energy = -2869.394288

Thermal corrections to Gibbs free energy = 0.631928

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.61471700 | 0.63603000 | -0.86267600 |
| C | -3.66212100 | -0.21065800 | -0.73048000 |
| Cu | -0.72314000 | 0.21552200 | -0.88563200 |
| P | 0.05595100 | -1.84158700 | -0.31897200 |
| P | 0.67903000 | 1.92092800 | -0.29237700 |
| C | 0.01302800 | -1.86917700 | 1.51674000 |
| C | -1.00570800 | -3.25787500 | -0.79139300 |
| C | 1.74903300 | -2.43521000 | -0.70731500 |
| C | 0.37880700 | 1.97678300 | 1.51738900 |
| C | 2.50998100 | 1.94811100 | -0.48289600 |
| C | 0.17403600 | 3.59244200 | -0.83722800 |
| C | 1.03375900 | -2.42619300 | 2.29680900 |
| C | -1.09641400 | -1.28328000 | 2.14629600 |
| C | -1.78541600 | -3.14125100 | -1.95001000 |
| C | -1.08318800 | -4.42880200 | -0.02344200 |
| C | 2.80807900 | -1.55363200 | -0.46464700 |
| C | 2.05741800 | -3.66838300 | -1.29475300 |
| C | -0.93342000 | 2.25697900 | 1.93800800 |
| C | 1.36027000 | 1.68088500 | 2.46871900 |
| C | 3.24194300 | 3.06082500 | -0.92088800 |
| C | 3.20879600 | 0.74527800 | -0.32677200 |
| C | -0.50730100 | 3.71277400 | -2.05430100 |
| C | 0.42505500 | 4.74025800 | -0.07040100 |
| H | 1.89688000 | -2.87865900 | 1.81917900 |
| C | 0.94755300 | -2.39790000 | 3.68937200 |
| C | -1.18067200 | -1.26563900 | 3.53664300 |
| H | -1.88237600 | -0.83250700 | 1.54658600 |

| | | | |
|---|---|---|---|
| C | -2.62513400 | -4.18493300 | -2.34180100 |
| H | -1.75166100 | -2.21999600 | -2.52520500 |
| C | -1.92281300 | -5.47010800 | -0.41594600 |
| H | -0.49549600 | -4.51537700 | 0.88568500 |
| O | 2.48034800 | -0.34310300 | 0.11331800 |
| C | 4.13968100 | -1.83263000 | -0.77582000 |
| H | 1.26307400 | -4.37850100 | -1.49709400 |
| C | 3.37662200 | -3.97483000 | -1.63172400 |
| H | -1.70722400 | 2.45210800 | 1.20167200 |
| C | -1.24122800 | 2.26651000 | 3.29612800 |
| H | 2.37338800 | 1.45523700 | 2.15407000 |
| C | 1.03987500 | 1.67559100 | 3.82701400 |
| H | 2.73856200 | 4.01018500 | -1.06304800 |
| C | 4.60284500 | 2.94494000 | -1.20187800 |
| C | 4.56784900 | 0.59026500 | -0.61163100 |
| H | -0.73771000 | 2.81923900 | -2.62680800 |
| C | -0.91424300 | 4.96671700 | -2.51130800 |
| H | 0.93016500 | 4.64764200 | 0.88665800 |
| C | 0.01587200 | 5.99178500 | -0.52687300 |
| H | 1.74619400 | -2.82920600 | 4.28699100 |
| C | -0.15927300 | -1.81917700 | 4.31083200 |
| H | -2.03702100 | -0.79995600 | 4.01402300 |
| C | -2.69385000 | -5.34930100 | -1.57543200 |
| H | -3.23322700 | -4.08195000 | -3.23581100 |
| H | -1.98214100 | -6.37274700 | 0.18578300 |
| C | 5.18717800 | -0.79044100 | -0.37192500 |
| C | 4.40711400 | -3.06685800 | -1.37675600 |
| H | 3.60535800 | -4.93013600 | -2.09460800 |
| H | -2.25615900 | 2.48959400 | 3.61334500 |
| C | -0.25676200 | 1.97518300 | 4.24362000 |
| H | 1.80676500 | 1.43699100 | 4.55853800 |
| C | 5.25860500 | 1.72028500 | -1.05769700 |
| H | 5.15652200 | 3.81365400 | -1.54543100 |
| H | -1.44918700 | 5.05069700 | -3.45282300 |
| C | -0.65157800 | 6.10587500 | -1.74976700 |
| H | 0.21111600 | 6.87687000 | 0.07224500 |
| H | -0.22300900 | -1.79304900 | 5.39513300 |
| H | -3.35385600 | -6.15865100 | -1.87472100 |
| C | 5.45621800 | -0.94512900 | 1.14966600 |
| C | 6.50508400 | -0.97152200 | -1.13422700 |
| H | 5.42451400 | -3.32923000 | -1.64526200 |
| H | -0.50249500 | 1.97268400 | 5.30194600 |
| H | 6.31430000 | 1.65119200 | -1.29569600 |
| H | -0.97579100 | 7.08137300 | -2.10145300 |

| | | | |
|---|---|---|---|
| H | 4.53314000 | -0.82898600 | 1.72517400 |
| H | 6.17075000 | -0.18593400 | 1.48629200 |
| H | 5.87064500 | -1.93708900 | 1.36101100 |
| H | 6.93416000 | -1.95733200 | -0.93233200 |
| H | 7.24368600 | -0.23324800 | -0.80857500 |
| H | 6.36344500 | -0.86847800 | -2.21490300 |
| H | -3.38178600 | -1.26068700 | -0.78818400 |
| F | -2.94021000 | 2.00403900 | -0.79422700 |
| C | -5.09496200 | 0.01772100 | -0.52385000 |
| C | -5.93930700 | -1.10943900 | -0.45639400 |
| C | -5.69030200 | 1.28818500 | -0.37503100 |
| C | -7.31044700 | -0.98280000 | -0.25244000 |
| H | -5.49934800 | -2.09819000 | -0.56857600 |
| C | -7.06253500 | 1.41141600 | -0.17056300 |
| H | -5.06747400 | 2.17051100 | -0.42250000 |
| C | -7.88305400 | 0.28250100 | -0.10771100 |
| H | -7.93350600 | -1.87268100 | -0.20616300 |
| H | -7.49643700 | 2.40232400 | -0.05929200 |
| H | -8.95284400 | 0.38750000 | 0.05165200 |

**E1**

Total electronic energy =-3058.037300

Thermal corrections to Gibbs free energy = 0.637029

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.50839800 | 0.79810700 | -0.26848100 |
| C | -3.61064500 | 0.03344900 | -0.45146500 |
| Cu | -0.63483000 | 0.34936700 | -0.51048800 |
| P | -0.07298300 | -1.81746500 | -0.03683300 |
| P | 1.03639200 | 1.84322000 | -0.13260000 |
| C | -0.13190200 | -1.79031400 | 1.79695100 |
| C | -1.32101500 | -3.08294600 | -0.48108500 |
| C | 1.51314400 | -2.65113900 | -0.45241200 |
| C | 1.23055500 | 1.80756000 | 1.69264600 |
| C | 2.74807800 | 1.62316400 | -0.75962700 |
| C | 0.67349400 | 3.60373400 | -0.47333500 |
| C | 0.99349500 | -2.00626800 | 2.59917000 |
| C | -1.35770200 | -1.46065200 | 2.40062800 |
| C | -1.95771900 | -2.96620000 | -1.72472300 |
| C | -1.66764000 | -4.13947000 | 0.37296100 |
| C | 2.68423000 | -1.88546400 | -0.44358300 |
| C | 1.61098400 | -3.97026200 | -0.91608000 |

| | | | |
|---|---|---|---|
| C | 0.05263200 | 1.83349400 | 2.45710300 |
| C | 2.47076700 | 1.73283200 | 2.33626300 |
| C | 3.48794800 | 2.59914100 | -1.43941400 |
| C | 3.32640400 | 0.35578200 | -0.62564300 |
| C | -0.33345500 | 3.90888100 | -1.39639800 |
| C | 1.34784800 | 4.64432300 | 0.18394300 |
| H | 1.94624400 | -2.25537600 | 2.14477700 |
| C | 0.89500500 | -1.90293600 | 3.98735600 |
| C | -1.45379600 | -1.37827800 | 3.78735100 |
| H | -2.22641400 | -1.25730300 | 1.78159800 |
| C | -2.92670800 | -3.89381000 | -2.10899500 |
| H | -1.71303700 | -2.13498200 | -2.37791200 |
| C | -2.63896900 | -5.06319200 | -0.01201600 |
| H | -1.18715300 | -4.22829600 | 1.34221600 |
| O | 2.57584200 | -0.59537700 | 0.03665000 |
| C | 3.91940300 | -2.34685100 | -0.90502500 |
| H | 0.72535100 | -4.59529200 | -0.94080100 |
| C | 2.83154600 | -4.46804200 | -1.37092400 |
| H | -0.91292000 | 1.88860800 | 1.96209900 |
| C | 0.12500600 | 1.78735300 | 3.84726300 |
| H | 3.38564400 | 1.71279000 | 1.75279400 |
| C | 2.53546900 | 1.68125400 | 3.72942000 |
| H | 3.07288000 | 3.59255000 | -1.56762700 |
| C | 4.74459300 | 2.29144000 | -1.96231200 |
| C | 4.58723100 | 0.01816600 | -1.12072500 |
| H | -0.88555300 | 3.10750200 | -1.87442200 |
| C | -0.65125900 | 5.23898100 | -1.67549400 |
| H | 2.11076700 | 4.41072100 | 0.92117200 |
| C | 1.03008600 | 5.97143400 | -0.09687400 |
| H | 1.77685200 | -2.06336400 | 4.60110800 |
| C | -0.32762600 | -1.59698300 | 4.58414100 |
| H | -2.40767600 | -1.12976600 | 4.24422200 |
| C | -3.27018800 | -4.94126700 | -1.25239900 |
| H | -3.42088000 | -3.78873800 | -3.07055600 |
| H | -2.90699300 | -5.87528800 | 0.65805600 |
| C | 5.11053900 | -1.38823700 | -0.81178800 |
| C | 3.97238900 | -3.66181400 | -1.37579000 |
| H | 2.89438900 | -5.48964100 | -1.73367200 |
| H | -0.79034700 | 1.79600500 | 4.43086700 |
| C | 1.36410800 | 1.70749000 | 4.48608900 |
| H | 3.50249200 | 1.62038800 | 4.22158100 |
| C | 5.28961000 | 1.01512800 | -1.80498300 |
| H | 5.30630000 | 3.05321100 | -2.49461600 |
| H | -1.44063700 | 5.46433200 | -2.38649400 |

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|---|---|---|---|
| C | 0.03147500 | 6.26954300 | -1.02936700 |
| H | 1.55376500 | 6.77351900 | 0.41587400 |
| H | -0.40139800 | -1.52009800 | 5.66534700 |
| H | -4.03214800 | -5.65751000 | -1.54673100 |
| C | 5.62618500 | -1.39665300 | 0.65304200 |
| C | 6.25422100 | -1.79711400 | -1.74759400 |
| H | 4.90704600 | -4.06637400 | -1.74822700 |
| H | 1.41506300 | 1.66006400 | 5.57030300 |
| H | 6.27010600 | 0.80182000 | -2.21620200 |
| H | -0.21990200 | 7.30509600 | -1.24127800 |
| H | 4.83461100 | -1.10370300 | 1.34911800 |
| H | 6.45946800 | -0.69407400 | 0.76434100 |
| H | 5.97205800 | -2.39958500 | 0.92646600 |
| H | 6.62690800 | -2.79257800 | -1.48923300 |
| H | 7.09833900 | -1.10856300 | -1.64760700 |
| H | 5.93478100 | -1.80626900 | -2.79468100 |
| H | -3.39234100 | -0.95010600 | -0.86071900 |
| F | -2.74119200 | 2.06656000 | 0.28509200 |
| C | -5.03278100 | 0.27333600 | -0.19271800 |
| C | -5.93566400 | -0.77532500 | -0.46288700 |
| C | -5.56266300 | 1.48035400 | 0.30902100 |
| C | -7.30310700 | -0.63286100 | -0.24499200 |
| H | -5.54414400 | -1.71485700 | -0.84758900 |
| C | -6.93169800 | 1.61974800 | 0.52419200 |
| H | -4.89247200 | 2.30098300 | 0.52428700 |
| C | -7.81148400 | 0.56946400 | 0.25088200 |
| H | -7.97349000 | -1.46078500 | -0.46248500 |
| H | -7.31610400 | 2.56087400 | 0.90999500 |
| H | -8.87816000 | 0.68656400 | 0.42208400 |
| C | -2.44013600 | 1.03957400 | -3.29376700 |
| O | -2.05061800 | -0.04584400 | -3.50109300 |
| O | -2.81434500 | 2.14054500 | -3.17465500 |

**F**

Total electronic energy = -3058.061450

Thermal corrections to Gibbs free energy = 0.641870

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.19573900 | 0.30351600 | -0.68846100 |
| P | -1.20542100 | 1.92806800 | -0.10675000 |
| P | -0.28649700 | -1.80615100 | -0.06790200 |
| C | -1.49560200 | 1.87244400 | 1.70047100 |

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|---|---|---|---|
| C | -0.68125400 | 3.64859100 | -0.43486600 |
| C | -2.89593800 | 1.82200700 | -0.81077600 |
| C | -0.36793400 | -1.89829900 | 1.76153500 |
| C | -1.87683300 | -2.51993100 | -0.64828200 |
| C | 0.96066200 | -3.07793300 | -0.48269700 |
| C | -2.74928100 | 2.10580500 | 2.27926700 |
| C | -0.39943000 | 1.55743100 | 2.51754100 |
| C | 0.36335000 | 3.84581100 | -1.34937300 |
| C | -1.26190800 | 4.75336300 | 0.20582900 |
| C | -3.54161700 | 0.58087100 | -0.75023400 |
| C | -3.55853100 | 2.86356800 | -1.47137900 |
| C | 0.82037200 | -1.65276200 | 2.46996200 |
| C | -1.55139200 | -2.14646100 | 2.46416500 |
| C | -2.00980800 | -3.80022400 | -1.20225600 |
| C | -3.00902600 | -1.69543200 | -0.65585200 |
| C | 1.86544700 | -2.80043400 | -1.51716800 |
| C | 1.05900900 | -4.29030000 | 0.21759700 |
| H | -3.60327800 | 2.33515600 | 1.64903400 |
| C | -2.90594000 | 2.02922900 | 3.66353800 |
| C | -0.56079200 | 1.49275000 | 3.90016400 |
| H | 0.56669800 | 1.34520600 | 2.06726900 |
| C | 0.80512200 | 5.13917100 | -1.63509600 |
| H | 0.84077500 | 2.98583700 | -1.81290400 |
| C | -0.81765800 | 6.04218900 | -0.08284000 |
| H | -2.05094900 | 4.59994100 | 0.93654300 |
| O | -2.87080700 | -0.43756200 | -0.10105000 |
| C | -4.79348200 | 0.32991800 | -1.31438100 |
| H | -3.08704600 | 3.83755500 | -1.54216200 |
| C | -4.80838200 | 2.64462300 | -2.05238100 |
| H | 1.72812300 | -1.40779300 | 1.92743500 |
| C | 0.82074000 | -1.68933900 | 3.86186400 |
| H | -2.47488900 | -2.33389800 | 1.92679800 |
| C | -1.54834800 | -2.15885100 | 3.86008700 |
| H | -1.15344000 | -4.46474200 | -1.22313700 |
| C | -3.22490700 | -4.20862000 | -1.75096900 |
| C | -4.23857900 | -2.07064700 | -1.20343200 |
| H | 1.82087900 | -1.84369300 | -2.02980800 |
| C | 2.84745500 | -3.73370300 | -1.85507100 |
| H | 0.37632600 | -4.49549900 | 1.03712000 |
| C | 2.03819800 | -5.22020500 | -0.12592900 |
| H | -3.88238800 | 2.20533700 | 4.10681400 |
| C | -1.81183300 | 1.72455200 | 4.47471500 |
| H | 0.28756200 | 1.23579700 | 4.52590100 |
| C | 0.21377500 | 6.23562100 | -1.00669700 |

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|---|---|---|---|
| H | 1.61762700 | 5.28670200 | -2.34066600 |
| H | -1.26917100 | 6.89512300 | 0.41628200 |
| C | -5.39057100 | -1.06527600 | -1.10589800 |
| C | -5.41857300 | 1.39074800 | -1.97752700 |
| H | -5.31079600 | 3.45663100 | -2.56940400 |
| H | 1.74537200 | -1.50637200 | 4.40261700 |
| C | -0.36291100 | -1.94039600 | 4.56094700 |
| H | -2.47381600 | -2.34609400 | 4.39752200 |
| C | -4.32663600 | -3.35029600 | -1.75849800 |
| H | -3.31340200 | -5.20055100 | -2.18381100 |
| H | 3.55264200 | -3.50742500 | -2.64956400 |
| C | 2.93240500 | -4.94271300 | -1.16424600 |
| H | 2.11018000 | -6.15701100 | 0.41972700 |
| H | -1.93570000 | 1.65917700 | 5.55218000 |
| H | 0.56215600 | 7.24099600 | -1.22650100 |
| C | -5.97028700 | -1.13025900 | 0.33330100 |
| C | -6.50844300 | -1.37051500 | -2.10989200 |
| H | -6.38920600 | 1.24427100 | -2.43835400 |
| H | -0.36166500 | -1.95737400 | 5.64734800 |
| H | -5.25827400 | -3.68577200 | -2.20052900 |
| H | 3.70097400 | -5.66509400 | -1.42486600 |
| H | -5.19937700 | -0.90951500 | 1.07734400 |
| H | -6.36925600 | -2.13045300 | 0.53513500 |
| H | -6.77811900 | -0.39911900 | 0.44823900 |
| H | -7.32570400 | -0.65074800 | -2.00662200 |
| H | -6.93467800 | -2.36047800 | -1.92302400 |
| H | -6.14415100 | -1.33767800 | -3.14175700 |
| O | 1.95050100 | 0.57982000 | -1.72999700 |
| C | 2.72192000 | 0.52649600 | -0.71423200 |
| C | 4.19385000 | 0.54474300 | -0.97783200 |
| C | 5.12493500 | 0.46185000 | -0.01457200 |
| H | 4.70361500 | 0.39332300 | 0.98316600 |
| O | 2.32020000 | 0.43432100 | 0.47513000 |
| C | 6.58025500 | 0.44947400 | -0.12006800 |
| C | 7.32705000 | 0.34299300 | 1.06917700 |
| C | 7.28363200 | 0.53612800 | -1.33891300 |
| C | 8.71869800 | 0.32283900 | 1.04937600 |
| H | 6.79834000 | 0.27586800 | 2.01666900 |
| C | 8.67533500 | 0.51580600 | -1.35479500 |
| H | 6.73327000 | 0.61981600 | -2.26639900 |
| C | 9.40093700 | 0.40923500 | -0.16548300 |
| H | 9.27083300 | 0.24006700 | 1.98158500 |
| H | 9.19881500 | 0.58423700 | -2.30469500 |
| H | 10.48705900 | 0.39421300 | -0.18602500 |

| | | | |
|---|---|---|---|
| F | 4.52374700 | 0.63630400 | -2.28660100 |

**I**

Total electronic energy =-3061.052874

Thermal corrections to Gibbs free energy = 0.708891

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.21535400 | 0.49078600 | -0.50688300 |
| P | -1.47396800 | 1.87257900 | -0.10330100 |
| P | -0.02980600 | -1.68393500 | 0.07138200 |
| C | -1.95644700 | 1.77575900 | 1.66093200 |
| C | -1.17770000 | 3.65378300 | -0.39587900 |
| C | -3.04351100 | 1.52412400 | -0.98794700 |
| C | -0.29968900 | -1.77956300 | 1.88341900 |
| C | -1.42940300 | -2.62321600 | -0.66140100 |
| C | 1.41838200 | -2.77789100 | -0.16884400 |
| C | -3.28747000 | 1.82604300 | 2.09335900 |
| C | -0.92564300 | 1.62423800 | 2.60040000 |
| C | -0.07746400 | 4.00502100 | -1.19108200 |
| C | -1.98386700 | 4.65930200 | 0.15820200 |
| C | -3.50484600 | 0.20189600 | -0.98305900 |
| C | -3.77341300 | 2.45982500 | -1.73101800 |
| C | 0.75599400 | -1.35973600 | 2.71063900 |
| C | -1.50308500 | -2.19806700 | 2.46011900 |
| C | -1.31466600 | -3.90781300 | -1.20959100 |
| C | -2.66187900 | -1.97305000 | -0.80222500 |
| C | 2.39347800 | -2.38904200 | -1.09627000 |
| C | 1.60081100 | -3.95520400 | 0.57506500 |
| H | -4.08927900 | 1.92784600 | 1.36821000 |
| C | -3.58587600 | 1.73054400 | 3.45297500 |
| C | -1.22954400 | 1.54014200 | 3.95768600 |
| H | 0.10523900 | 1.55208800 | 2.26391600 |
| C | 0.19652800 | 5.35005200 | -1.44703400 |
| H | 0.57133700 | 3.22510500 | -1.58280200 |
| C | -1.70614300 | 6.00024400 | -0.09994800 |
| H | -2.81869800 | 4.38946200 | 0.79878800 |
| O | -2.76887300 | -0.70997500 | -0.25196100 |
| C | -4.63757600 | -0.22671600 | -1.67729600 |
| H | -3.44351600 | 3.49235200 | -1.76235300 |
| C | -4.90641700 | 2.06316000 | -2.44281000 |
| H | 1.67159600 | -0.98494300 | 2.26346600 |
| C | 0.61040000 | -1.39309000 | 4.09505200 |

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|---|---|---|---|
| H | -2.32530900 | -2.52136600 | 1.83065000 |
| C | -1.64988300 | -2.20697900 | 3.84841500 |
| H | -0.37389200 | -4.44049000 | -1.12819900 |
| C | -2.39052400 | -4.48745000 | -1.88120600 |
| C | -3.75688400 | -2.52151400 | -1.47492000 |
| H | 2.28269500 | -1.45638700 | -1.64006300 |
| C | 3.53218000 | -3.17506800 | -1.28644100 |
| H | 0.86057100 | -4.24451200 | 1.31540100 |
| C | 2.73405800 | -4.74058100 | 0.37684000 |
| H | -4.62107300 | 1.76399500 | 3.78207800 |
| C | -2.55739500 | 1.58981100 | 4.38587200 |
| H | -0.42844200 | 1.41002900 | 4.67776500 |
| C | -0.61770400 | 6.34586600 | -0.90652800 |
| H | 1.05249400 | 5.61770500 | -2.05989200 |
| H | -2.33237200 | 6.77600700 | 0.33204800 |
| C | -5.04581000 | -1.69439500 | -1.51672600 |
| C | -5.33309800 | 0.73373600 | -2.41863000 |
| H | -5.46103100 | 2.79503900 | -3.02242700 |
| H | 1.43402800 | -1.07382900 | 4.72804400 |
| C | -0.59239000 | -1.81462300 | 4.66813200 |
| H | -2.59091000 | -2.52744900 | 4.28693500 |
| C | -3.59764900 | -3.79884800 | -2.01949000 |
| H | -2.28648600 | -5.48069600 | -2.30770100 |
| H | 4.29112900 | -2.84485400 | -1.98779400 |
| C | 3.70079900 | -4.35102100 | -0.55644600 |
| H | 2.86937900 | -5.65094800 | 0.95451800 |
| H | -2.79064500 | 1.50975000 | 5.44407500 |
| H | -0.39988200 | 7.39214500 | -1.10265600 |
| C | -5.76482800 | -1.84690900 | -0.14879100 |
| C | -5.99076300 | -2.15586000 | -2.63251100 |
| H | -6.21565300 | 0.44900000 | -2.98075700 |
| H | -0.70670300 | -1.82875900 | 5.74861400 |
| H | -4.41699100 | -4.26517500 | -2.55536600 |
| H | 4.58853400 | -4.96080400 | -0.70254100 |
| H | -5.12039900 | -1.51879100 | 0.67195200 |
| H | -6.03467700 | -2.89503700 | 0.02144400 |
| H | -6.67759900 | -1.24106800 | -0.13231000 |
| H | -6.90992400 | -1.56268700 | -2.62850500 |
| H | -6.28712700 | -3.19780800 | -2.48029300 |
| H | -5.52389000 | -2.06750800 | -3.61880400 |
| O | 1.99862100 | 0.97388000 | -1.44987000 |
| C | 2.70066100 | 0.91746300 | -0.37917800 |
| O | 2.18058300 | 0.80058700 | 0.76716700 |
| C | 6.48721900 | 1.36716900 | -0.38959600 |

| | | | |
|---|---|---|---|
| C | 6.29983200 | -0.14905200 | -0.75194100 |
| B | 4.27832800 | 0.85084700 | -0.49962500 |
| O | 4.89828400 | -0.19796100 | -1.13464900 |
| O | 5.15338400 | 1.74459100 | 0.05584400 |
| C | 6.45360000 | -1.08330900 | 0.45297200 |
| H | 6.08267000 | -2.07552300 | 0.17996300 |
| H | 7.49932700 | -1.17166800 | 0.76524400 |
| H | 5.86262400 | -0.72767000 | 1.30241500 |
| C | 7.47138300 | 1.64263300 | 0.74085400 |
| H | 8.47707100 | 1.30168600 | 0.46948400 |
| H | 7.51691100 | 2.71870400 | 0.93498200 |
| H | 7.16925400 | 1.14486600 | 1.66445100 |
| C | 6.80898900 | 2.24123700 | -1.60542800 |
| H | 6.71321300 | 3.29292400 | -1.31977300 |
| H | 7.82867400 | 2.07069800 | -1.96603700 |
| H | 6.11041900 | 2.04680700 | -2.42490100 |
| C | 7.14197500 | -0.64397300 | -1.92147200 |
| H | 8.21047200 | -0.54464400 | -1.69908900 |
| H | 6.93135700 | -1.70264500 | -2.10456300 |
| H | 6.92088900 | -0.09106200 | -2.83670100 |

**J**

Total electronic energy = -1008.361596

Thermal corrections to Gibbs free energy = 0.263306

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -6.00241700 | -1.22566000 | 0.36208000 |
| C | -4.63301200 | -1.01862100 | 0.23022000 |
| C | -4.13216700 | 0.26635200 | -0.06336700 |
| C | -5.05000500 | 1.32349100 | -0.21762500 |
| C | -6.41872300 | 1.11138800 | -0.08464800 |
| C | -6.90047900 | -0.16625200 | 0.20616700 |
| H | -6.37266800 | -2.22152500 | 0.58831300 |
| H | -3.94702500 | -1.84598800 | 0.35294800 |
| H | -4.67524600 | 2.31820900 | -0.44403300 |
| H | -7.10870000 | 1.94115000 | -0.20763900 |
| H | -7.96819200 | -0.33627300 | 0.31072400 |
| C | -2.71639300 | 0.56959800 | -0.21798100 |
| H | -2.45662800 | 1.59924200 | -0.44483200 |
| C | -1.64919500 | -0.24104400 | -0.12071000 |
| C | -0.26700000 | 0.25601400 | -0.30597500 |
| O | 0.64989700 | -0.73306700 | -0.20926200 |

| | | | |
|---|---|---|---|
| O | 0.00890800 | 1.41367600 | -0.54587300 |
| F | -1.75149200 | -1.55771400 | 0.15551200 |
| C | 4.22870200 | -0.53348100 | -0.39187300 |
| C | 3.87124200 | 0.64973400 | 0.58527700 |
| B | 1.99744400 | -0.39939800 | -0.08616600 |
| C | 4.70326500 | 0.70395600 | 1.85981000 |
| H | 5.76124100 | 0.86047000 | 1.62176400 |
| H | 4.36720800 | 1.53886400 | 2.48204500 |
| H | 4.60718400 | -0.21424500 | 2.44286700 |
| C | 3.84911300 | 2.01738900 | -0.10299700 |
| H | 3.39987100 | 2.74628100 | 0.57723500 |
| H | 4.85859300 | 2.35381300 | -0.35965200 |
| H | 3.24149500 | 1.99249500 | -1.01224500 |
| C | 4.72095000 | -1.78822400 | 0.33329700 |
| H | 4.74436100 | -2.62121200 | -0.37528100 |
| H | 5.72824400 | -1.64779200 | 0.73777900 |
| H | 4.05036700 | -2.05867900 | 1.15475200 |
| C | 5.17498200 | -0.16425500 | -1.52689700 |
| H | 6.14089300 | 0.16668200 | -1.12949200 |
| H | 5.34886900 | -1.03875800 | -2.16130200 |
| H | 4.76109000 | 0.63092600 | -2.15006200 |
| O | 2.49085800 | 0.34655300 | 0.94202900 |
| O | 2.92809700 | -0.86585800 | -0.96456100 |

**K**

Total electronic energy = -3569.314320

Thermal corrections to Gibbs free energy = 0.825809

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -2.06218500 | 1.48049100 | 0.03079600 |
| P | -0.45718000 | -2.14342300 | -0.61288100 |
| O | -3.24252900 | -1.15999000 | -0.71014700 |
| C | -3.63488200 | 0.74917700 | 0.64492400 |
| C | -4.44823300 | 1.39782000 | 1.58628800 |
| H | -4.12485400 | 2.34478100 | 2.00593700 |
| C | -5.64905700 | 0.82531000 | 1.99826700 |
| H | -6.26577000 | 1.33289900 | 2.73358000 |
| C | -6.06968300 | -0.39686900 | 1.46495900 |
| H | -7.01575700 | -0.81742100 | 1.78722800 |
| C | -5.28938600 | -1.07489700 | 0.52693200 |
| C | -4.07143200 | -0.48806800 | 0.16113700 |
| C | -3.22219100 | -2.53599400 | -0.58582100 |

| | | | |
|---|---|---|---|
| C | -1.97919300 | -3.17584400 | -0.66975100 |
| C | -1.97233100 | -4.57674800 | -0.63395100 |
| H | -1.03385100 | -5.10947600 | -0.73279900 |
| C | -3.15864800 | -5.28481000 | -0.45331900 |
| H | -3.13992100 | -6.36996800 | -0.42424000 |
| C | -4.36760800 | -4.60774500 | -0.27722700 |
| H | -5.27255200 | -5.17623000 | -0.09389600 |
| C | -4.42122700 | -3.21340000 | -0.34327600 |
| C | -5.68973900 | -2.36935900 | -0.19076700 |
| C | -6.79454700 | -3.12476100 | 0.55813600 |
| H | -7.08224600 | -4.02778200 | 0.01234600 |
| H | -7.69413600 | -2.50796600 | 0.64057600 |
| H | -6.47653900 | -3.41370500 | 1.56517000 |
| C | -6.20477500 | -1.99531600 | -1.60705200 |
| H | -5.44070500 | -1.45750100 | -2.17524600 |
| H | -7.09127900 | -1.35647900 | -1.53005500 |
| H | -6.47095800 | -2.90162800 | -2.16164300 |
| C | -1.40248800 | 2.30180600 | 1.52533000 |
| C | -1.70607200 | 3.62802100 | 1.85605900 |
| H | -2.33633500 | 4.21873400 | 1.19886000 |
| C | -1.17085600 | 4.19734500 | 3.01199400 |
| H | -1.40323600 | 5.22871700 | 3.26189700 |
| C | -0.32581400 | 3.45065900 | 3.83644800 |
| H | 0.10017900 | 3.90164000 | 4.72796500 |
| C | -0.01811400 | 2.12832400 | 3.50635700 |
| H | 0.64716700 | 1.54271500 | 4.13305600 |
| C | -0.55323100 | 1.55499700 | 2.35417600 |
| H | -0.30047200 | 0.53264900 | 2.09575000 |
| C | -2.60333700 | 2.84708300 | -1.06005000 |
| C | -3.93695300 | 3.25809200 | -1.18968000 |
| H | -4.71943300 | 2.75835400 | -0.62927000 |
| C | -4.26318700 | 4.31106400 | -2.04565100 |
| H | -5.29945500 | 4.62240100 | -2.14385300 |
| C | -3.26362000 | 4.96037800 | -2.77180600 |
| H | -3.52065900 | 5.78011800 | -3.43681800 |
| C | -1.93420100 | 4.55198500 | -2.64597700 |
| H | -1.14779500 | 5.05080600 | -3.20221700 |
| C | -1.60162600 | 3.49517800 | -1.80122800 |
| H | -0.56674000 | 3.17943300 | -1.71627200 |
| C | -0.06238500 | -2.08101800 | 1.17980400 |
| C | 1.21737100 | -1.61535200 | 1.52520000 |
| H | 1.97353400 | -1.42409900 | 0.77161800 |
| C | 1.54487500 | -1.38335000 | 2.85981600 |
| H | 2.53970200 | -1.01317000 | 3.08495300 |

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|---|---|---|---|
| C | 0.59578500 | -1.60798900 | 3.86154600 |
| H | 0.84595500 | -1.42461400 | 4.90287700 |
| C | -0.67954100 | -2.06515800 | 3.52108400 |
| H | -1.42091700 | -2.23874200 | 4.29615400 |
| C | -1.01248800 | -2.30156200 | 2.18495200 |
| H | -2.00738600 | -2.65349700 | 1.93016800 |
| C | 0.87740100 | -3.15779700 | -1.32513900 |
| C | 1.45042700 | -2.73580300 | -2.53186000 |
| H | 1.12382600 | -1.80599100 | -2.98523400 |
| C | 2.47578300 | -3.48150500 | -3.11507900 |
| H | 2.92918000 | -3.13972100 | -4.04038200 |
| C | 2.93430800 | -4.64443200 | -2.49664700 |
| H | 3.73842500 | -5.21839600 | -2.94809200 |
| C | 2.38367000 | -5.05587000 | -1.27964900 |
| H | 2.76277200 | -5.94347900 | -0.78166900 |
| C | 1.36715100 | -4.30996700 | -0.68877800 |
| H | 0.97227100 | -4.60297000 | 0.27948100 |
| Cu | -0.60903200 | 0.09672400 | -0.95725300 |
| C | 2.43825300 | 1.86759100 | -0.18938100 |
| H | 2.00083600 | 1.54166000 | 0.76395900 |
| C | 1.91544900 | 3.22748800 | -0.55283300 |
| C | 1.04172800 | 5.82332600 | -1.18027700 |
| C | 1.33960800 | 4.04214400 | 0.42640400 |
| C | 2.06109400 | 3.73348700 | -1.85276800 |
| C | 1.62839400 | 5.02129600 | -2.16336300 |
| C | 0.89870300 | 5.32900000 | 0.11560400 |
| H | 1.23669500 | 3.66541600 | 1.43820300 |
| H | 2.51890400 | 3.11611200 | -2.61779200 |
| H | 1.75402000 | 5.40142900 | -3.17383100 |
| H | 0.44326300 | 5.94066000 | 0.88905100 |
| H | 0.69932200 | 6.82510700 | -1.42494800 |
| C | 3.96341000 | 1.74557900 | -0.01445400 |
| B | 4.28004700 | 0.15966700 | -0.21999200 |
| O | 4.11575000 | -0.59975300 | 0.99782100 |
| C | 5.12769300 | -1.61927900 | 1.00353400 |
| C | 6.25169300 | -0.96421500 | 0.12678500 |
| O | 5.49682300 | -0.23298200 | -0.84276300 |
| C | 7.15416000 | -1.95661800 | -0.60196700 |
| H | 6.57724500 | -2.58413000 | -1.28537800 |
| H | 7.68684800 | -2.60173000 | 0.10732800 |
| H | 7.89862100 | -1.41141500 | -1.19161000 |
| C | 7.10107100 | 0.03906300 | 0.92380500 |
| H | 6.46001800 | 0.74587600 | 1.45883200 |
| H | 7.71575400 | 0.60914600 | 0.22014700 |

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|---|---|---|---|
| H | 7.76399700 | -0.45646400 | 1.64241800 |
| C | 5.52549300 | -1.90227300 | 2.45024700 |
| H | 4.68909900 | -2.37047300 | 2.98207600 |
| H | 5.78823000 | -0.97973300 | 2.97294700 |
| H | 6.37927300 | -2.58883800 | 2.49676000 |
| C | 4.54871000 | -2.88547100 | 0.36018100 |
| H | 5.25890500 | -3.72005800 | 0.38339500 |
| H | 4.26145100 | -2.69767000 | -0.67694700 |
| H | 3.65243500 | -3.18948800 | 0.90908400 |
| C | 2.14482900 | 0.74351300 | -1.18696600 |
| O | 3.05996700 | -0.15818400 | -1.22604900 |
| O | 1.09833200 | 0.69096500 | -1.87683500 |
| F | 4.57550800 | 2.51499500 | -0.99037300 |
| F | 4.35307100 | 2.28220900 | 1.19528600 |

**L-CuF**

Total electronic energy = -2560.953447

Thermal corrections to Gibbs free energy = 0.528516

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 1.85648700 | -0.70520000 | -0.31036100 |
| P | -1.92674400 | -0.45632200 | -0.26413100 |
| C | 1.87967500 | -0.95851000 | 1.50390900 |
| C | 3.30909800 | -1.61582800 | -0.94138800 |
| C | 2.31418900 | 1.06234100 | -0.49113400 |
| C | -2.06452200 | -0.86394300 | 1.52007600 |
| C | -2.12445600 | 1.37137700 | -0.34814500 |
| C | -3.46628200 | -1.12434700 | -0.98538400 |
| C | 2.51653400 | -0.08186700 | 2.39118700 |
| C | 1.19582200 | -2.07253800 | 2.01186500 |
| C | 3.15657000 | -2.27214200 | -2.17314500 |
| C | 4.53087200 | -1.68611300 | -0.25626500 |
| C | 1.33251300 | 2.01036300 | -0.18000500 |
| C | 3.52572000 | 1.53372800 | -1.01072900 |
| C | -2.43298800 | -2.17162100 | 1.87612000 |
| C | -1.71092900 | 0.04073900 | 2.52897200 |
| C | -3.28812700 | 2.01870800 | -0.78491400 |
| C | -1.00126000 | 2.17030600 | -0.10116400 |
| C | -3.35781700 | -1.76941500 | -2.22820600 |
| C | -4.71525700 | -1.02755300 | -0.35082400 |
| H | 3.03488200 | 0.79191800 | 2.00800600 |
| C | 2.47462000 | -0.32058700 | 3.76573000 |

| | | | |
|---|---|---|---|
| C | 1.16482600 | -2.31523200 | 3.38269900 |
| H | 0.67163700 | -2.73713700 | 1.33101100 |
| C | 4.23377600 | -2.97307100 | -2.71947600 |
| H | 2.19348700 | -2.24682100 | -2.68209100 |
| C | 5.60008400 | -2.39019400 | -0.80722000 |
| H | 4.63818800 | -1.19819900 | 0.70856700 |
| O | 0.14314300 | 1.52470100 | 0.32808100 |
| C | 1.48683700 | 3.38301900 | -0.37620200 |
| H | 4.30716200 | 0.82771100 | -1.26996500 |
| C | 3.71552500 | 2.90111900 | -1.21642100 |
| H | -2.70839500 | -2.88322900 | 1.10282100 |
| C | -2.46451900 | -2.55711700 | 3.21482700 |
| H | -1.41197100 | 1.05049900 | 2.27390100 |
| C | -1.73485700 | -0.35129400 | 3.86706300 |
| H | -4.17450800 | 1.43471500 | -1.00482500 |
| C | -3.29911600 | 3.40066400 | -0.96971500 |
| C | -0.97431000 | 3.55507300 | -0.28513000 |
| H | -2.37891700 | -1.88262900 | -2.69752100 |
| C | -4.50461500 | -2.29104500 | -2.83309800 |
| H | -4.79103100 | -0.55163300 | 0.62293600 |
| C | -5.85190200 | -1.55197800 | -0.96219300 |
| H | 2.96738900 | 0.36722700 | 4.44765000 |
| C | 1.80213400 | -1.43782200 | 4.26241200 |
| H | 0.62003600 | -3.17232300 | 3.76476500 |
| C | 5.45236400 | -3.03008700 | -2.04153000 |
| H | 4.11515200 | -3.48241800 | -3.67151700 |
| H | 6.54550200 | -2.44477000 | -0.27440600 |
| C | 0.32832000 | 4.28897000 | 0.05396100 |
| C | 2.70573500 | 3.81582900 | -0.90852800 |
| H | 4.65562400 | 3.25767100 | -1.62657700 |
| H | -2.76272600 | -3.56886600 | 3.47603200 |
| C | -2.11529700 | -1.64726100 | 4.21533400 |
| H | -1.45275300 | 0.35973900 | 4.63828200 |
| C | -2.15231100 | 4.16126600 | -0.72974600 |
| H | -4.20539100 | 3.88959300 | -1.31432800 |
| H | -4.42124600 | -2.79326500 | -3.79271500 |
| C | -5.74641000 | -2.18051000 | -2.20716500 |
| H | -6.81729400 | -1.47539500 | -0.46936300 |
| H | 1.76566800 | -1.61959300 | 5.33292400 |
| H | 6.28620400 | -3.58097400 | -2.46814900 |
| C | 0.40016300 | 4.46474400 | 1.59493700 |
| C | 0.39992700 | 5.66898300 | -0.61059500 |
| H | 2.87437500 | 4.87216100 | -1.08662100 |
| H | -2.13568600 | -1.94870800 | 5.25883400 |

| | | | |
|---|---|---|---|
| H | -2.18178900 | 5.23270000 | -0.89418400 |
| H | -6.63340000 | -2.59147000 | -2.68187800 |
| H | 0.36260300 | 3.49647000 | 2.10262200 |
| H | -0.44132200 | 5.07195700 | 1.94629200 |
| H | 1.33505300 | 4.96268000 | 1.87501500 |
| H | 1.32884800 | 6.17910600 | -0.33937900 |
| H | -0.42115100 | 6.30535600 | -0.26776900 |
| H | 0.34995300 | 5.59385100 | -1.70158000 |
| Cu | -0.07278200 | -1.19099400 | -1.31931800 |
| F | -0.24630800 | -2.07720100 | -2.93538600 |

**L-CuTc**

Total electronic energy = -3202.152752

Thermal corrections to Gibbs free energy =0.588867

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -1.24265300 | 1.78122100 | -0.08462200 |
| P | 0.69631600 | -1.54258800 | 0.07415000 |
| C | -1.67204700 | 1.59840200 | 1.68609200 |
| C | -1.21013600 | 3.58776100 | -0.36606600 |
| C | -2.75747300 | 1.21194200 | -0.94891300 |
| C | 0.47928100 | -1.70179900 | 1.88823800 |
| C | -0.56542600 | -2.66632600 | -0.64751500 |
| C | 2.28550500 | -2.40000200 | -0.22291700 |
| C | -2.98949000 | 1.46581100 | 2.14210100 |
| C | -0.61166500 | 1.56969000 | 2.60416600 |
| C | -0.18358600 | 4.09967500 | -1.17233200 |
| C | -2.14502600 | 4.46262400 | 0.20714000 |
| C | -3.02467600 | -0.16279900 | -0.94174400 |
| C | -3.62284000 | 2.03488800 | -1.67977800 |
| C | 1.48061200 | -1.15479500 | 2.70863800 |
| C | -0.64747600 | -2.28849600 | 2.47351700 |
| C | -0.27624800 | -3.92361100 | -1.19439200 |
| C | -1.87839500 | -2.19613000 | -0.77495400 |
| C | 3.13542700 | -1.88911800 | -1.21416400 |
| C | 2.69324600 | -3.51108300 | 0.53162900 |
| H | -3.81172400 | 1.47107600 | 1.43277500 |
| C | -3.24573600 | 1.31043800 | 3.50471400 |
| C | -0.87511100 | 1.42458600 | 3.96481300 |
| H | 0.41305200 | 1.63915700 | 2.24861700 |
| C | -0.10902900 | 5.47175900 | -1.41987600 |
| H | 0.56385600 | 3.42405200 | -1.58142600 |

| | | | |
|---|---|---|---|
| C | -2.06657300 | 5.83132500 | -0.04250300 |
| H | -2.92339400 | 4.07096900 | 0.85577900 |
| O | -2.15665600 | -0.96042200 | -0.22221000 |
| C | -4.09292300 | -0.74813800 | -1.62354600 |
| H | -3.44426000 | 3.10400200 | -1.71218800 |
| C | -4.69625800 | 1.48096900 | -2.37875700 |
| H | 2.33039400 | -0.65288900 | 2.25637600 |
| C | 1.36154600 | -1.22849900 | 4.09411600 |
| H | -1.42767900 | -2.71121900 | 1.84955500 |
| C | -0.77115200 | -2.33755100 | 3.86313700 |
| H | 0.73113100 | -4.31801600 | -1.12118000 |
| C | -1.26665000 | -4.65048700 | -1.85400600 |
| C | -2.89214800 | -2.89488200 | -1.43559000 |
| H | 2.84275300 | -1.00496100 | -1.77126900 |
| C | 4.37719600 | -2.48241900 | -1.44681100 |
| H | 2.04809600 | -3.89623500 | 1.31573600 |
| C | 3.92958500 | -4.10677400 | 0.28915500 |
| H | -4.26952400 | 1.20149700 | 3.85250800 |
| C | -2.18927300 | 1.29162600 | 4.41666600 |
| H | -0.04993500 | 1.38885300 | 4.66826300 |
| C | -1.05043000 | 6.33586200 | -0.85961500 |
| H | 0.69058700 | 5.86402800 | -2.04156700 |
| H | -2.79186300 | 6.50573700 | 0.40427700 |
| C | -4.28588000 | -2.25922500 | -1.46247200 |
| C | -4.92765000 | 0.10407000 | -2.35353500 |
| H | -5.35715800 | 2.12658300 | -2.94928700 |
| H | 2.14421900 | -0.81100500 | 4.72187200 |
| C | 0.23561500 | -1.81759400 | 4.67564100 |
| H | -1.65327500 | -2.78953000 | 4.30813300 |
| C | -2.55987400 | -4.13831500 | -1.98064000 |
| H | -1.02870500 | -5.62049800 | -2.28018500 |
| H | 5.03795800 | -2.06040600 | -2.19812100 |
| C | 4.77352200 | -3.59131600 | -0.69918900 |
| H | 4.24007900 | -4.96608300 | 0.87727400 |
| H | -2.38906100 | 1.16410700 | 5.47702400 |
| H | -0.98814600 | 7.40392500 | -1.04893800 |
| C | -4.96125300 | -2.51373500 | -0.08745000 |
| C | -5.16726800 | -2.84944100 | -2.56960900 |
| H | -5.76716500 | -0.30329600 | -2.90602500 |
| H | 0.14086200 | -1.86354100 | 5.75710600 |
| H | -3.31084600 | -4.71661400 | -2.50745200 |
| H | 5.74323600 | -4.04851800 | -0.87591100 |
| H | -4.36118000 | -2.09825700 | 0.72737900 |
| H | -5.07760700 | -3.58973800 | 0.08286600 |

| | | | |
|---|---|---|---|
| H | -5.95061700 | -2.04381700 | -0.05986000 |
| H | -6.16139800 | -2.39321500 | -2.55462200 |
| H | -5.31078000 | -3.92305800 | -2.41685800 |
| H | -4.72819700 | -2.69462800 | -3.56046000 |
| Cu | 0.60564600 | 0.64348600 | -0.52156700 |
| O | 2.33851000 | 1.29177800 | -1.42244800 |
| O | 2.56779200 | 1.19959800 | 0.80464300 |
| C | 3.04783900 | 1.30682500 | -0.35325300 |
| C | 4.51712900 | 1.38406900 | -0.52244400 |
| C | 5.47888000 | 1.37830000 | 0.45773300 |
| S | 5.23572800 | 1.40907600 | -2.11172100 |
| C | 6.80432600 | 1.39933400 | -0.06187700 |
| H | 5.21835800 | 1.35404500 | 1.50887300 |
| C | 6.82953900 | 1.41542600 | -1.43383400 |
| H | 7.69785700 | 1.40058400 | 0.55304200 |
| H | 7.69725600 | 1.43640100 | -2.08018800 |

**LiF**

Total electronic energy = -107.491140

Thermal corrections to Gibbs free energy = -0.017016

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | -1.16431400 |
| F | 0.00000000 | 0.00000000 | 0.38810500 |

**LiO$^t$Bu**

Total electronic energy = -240.692760

Thermal corrections to Gibbs free energy = 0.095877

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | 1.26998100 | -0.00007100 | 0.00014200 |
| C | -0.11575300 | -0.00001000 | -0.00001200 |
| C | -0.63039700 | -1.36083300 | -0.51119200 |
| H | -0.25758700 | -1.54046000 | -1.52646700 |
| H | -0.25784100 | -2.16441300 | 0.13495000 |
| H | -1.72661400 | -1.41099700 | -0.53018600 |
| C | -0.63054100 | 0.23777600 | 1.43401500 |
| H | -1.72676300 | 0.24642100 | 1.48678100 |
| H | -0.25784300 | -0.55164000 | 2.09731500 |
| H | -0.25799800 | 1.19914500 | 1.80687300 |

| | | | |
|---|---|---|---|
| C | -0.63025000 | 1.12312300 | -0.92297600 |
| H | -0.25768700 | 2.09218900 | -0.57063200 |
| H | -0.25732900 | 0.96555700 | -1.94186900 |
| H | -1.72646000 | 1.16451200 | -0.95727200 |
| Li | 2.86930700 | -0.00002500 | 0.00012000 |

**LiTc**

Total electronic energy = -748.684657

Thermal corrections to Gibbs free energy = 0.039493

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | -2.01441900 | -1.09185600 | -0.00004000 |
| O | -2.21899500 | 1.13192200 | 0.00005400 |
| C | -1.49594700 | 0.07777300 | 0.00000900 |
| C | -0.03046600 | 0.21316800 | -0.00000100 |
| C | 0.70839200 | 1.37312200 | -0.00002600 |
| S | 0.99525400 | -1.19599600 | 0.00002800 |
| C | 2.10996700 | 1.13449200 | -0.00000300 |
| H | 0.23964900 | 2.34956100 | -0.00004300 |
| C | 2.41215100 | -0.20539100 | -0.00002200 |
| H | 2.86023600 | 1.91735800 | -0.00002900 |
| H | 3.39335800 | -0.66173600 | -0.00004100 |
| Li | -3.59152600 | -0.11625200 | -0.00006100 |

**S-1**

Total electronic energy =-3442.900024

Thermal corrections to Gibbs free energy = 0.707751

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| O | -0.71147600 | 1.22493100 | -2.39049700 |
| C | -0.16332900 | 0.65513100 | -3.55349100 |
| Li | -1.85069600 | 2.36842100 | -1.76596800 |
| P | -0.91789300 | -1.36105400 | 0.33045700 |
| P | 1.55257500 | 1.53554100 | 0.44620600 |
| C | -0.73116000 | -1.79650500 | 2.10553000 |
| C | -2.62320100 | -1.88841200 | -0.07674800 |
| C | 0.13065300 | -2.60143800 | -0.53504100 |
| C | 1.73519300 | 1.32673500 | 2.25082100 |
| C | 3.06553400 | 0.75744900 | -0.24650900 |
| C | 1.83413900 | 3.31390200 | 0.11932200 |

| | | | |
|---|---|---|---|
| C | 0.31680000 | -2.59764200 | 2.57609200 |
| C | -1.64514300 | -1.25627900 | 3.02451900 |
| C | -3.24532300 | -1.25463900 | -1.16262900 |
| C | -3.32015300 | -2.87259200 | 0.63737500 |
| C | 1.51402900 | -2.38578800 | -0.56893200 |
| C | -0.37152100 | -3.68333100 | -1.26796000 |
| C | 0.56843300 | 1.35621500 | 3.02933500 |
| C | 2.97806100 | 1.10885600 | 2.86234500 |
| C | 4.14792200 | 1.46143400 | -0.78705000 |
| C | 3.06603000 | -0.63503500 | -0.38909600 |
| C | 1.40407800 | 3.80366500 | -1.12536100 |
| C | 2.43377500 | 4.18660500 | 1.03462300 |
| H | 1.02597200 | -3.03408900 | 1.88273200 |
| C | 0.45612800 | -2.84700900 | 3.94187600 |
| C | -1.51349200 | -1.52772000 | 4.38443600 |
| H | -2.43220000 | -0.59463400 | 2.68166000 |
| C | -4.54000700 | -1.60927600 | -1.53683700 |
| H | -2.71019600 | -0.48237100 | -1.70534900 |
| C | -4.62146600 | -3.21505400 | 0.26904500 |
| H | -2.84913600 | -3.35855500 | 1.48577700 |
| O | 1.99098300 | -1.31052100 | 0.15539700 |
| C | 2.40721200 | -3.18120100 | -1.29011700 |
| H | -1.43880600 | -3.87625600 | -1.26997800 |
| C | 0.49029100 | -4.48849400 | -2.01310600 |
| H | -0.40524400 | 1.49780400 | 2.56485100 |
| C | 0.65643900 | 1.17781200 | 4.40984700 |
| H | 3.87945400 | 1.07409500 | 2.25736400 |
| C | 3.05529400 | 0.92230400 | 4.24222600 |
| H | 4.17942700 | 2.54211300 | -0.69860100 |
| C | 5.15924700 | 0.78218300 | -1.46774600 |
| C | 4.04791300 | -1.34429800 | -1.08173700 |
| H | 0.91877200 | 3.12453300 | -1.82293500 |
| C | 1.59230400 | 5.14541200 | -1.45326900 |
| H | 2.75647900 | 3.81396400 | 2.00193800 |
| C | 2.60823000 | 5.53277100 | 0.70706900 |
| H | 1.27950200 | -3.46321200 | 4.29258900 |
| C | -0.46000800 | -2.31706000 | 4.84970900 |
| H | -2.22871300 | -1.10320400 | 5.08379000 |
| C | -5.23167300 | -2.58530500 | -0.81819500 |
| H | -5.01654300 | -1.10279100 | -2.37001900 |
| H | -5.15883100 | -3.97392500 | 0.83130900 |
| C | 3.90187900 | -2.86729900 | -1.15842400 |
| C | 1.86448300 | -4.23872000 | -2.02679100 |
| H | 0.08964700 | -5.31807000 | -2.58799700 |

| | | | |
|---|---|---|---|
| H | -0.25117000 | 1.18788400 | 5.00471200 |
| C | 1.89347400 | 0.95696400 | 5.01670600 |
| H | 4.01988900 | 0.74665000 | 4.71108300 |
| C | 5.10313800 | -0.60420200 | -1.62534800 |
| H | 5.99168600 | 1.33737200 | -1.88987300 |
| H | 1.26467000 | 5.51695600 | -2.42071900 |
| C | 2.19238200 | 6.01271700 | -0.53600300 |
| H | 3.06963900 | 6.20650100 | 1.42387600 |
| H | -0.35200300 | -2.51491100 | 5.91265300 |
| H | -6.24738200 | -2.84988600 | -1.09911900 |
| C | 4.40207500 | -3.47049800 | 0.18191000 |
| C | 4.71714200 | -3.46467700 | -2.31180100 |
| H | 2.51398300 | -4.87903800 | -2.61328000 |
| H | 1.95309800 | 0.80390000 | 6.09097700 |
| H | 5.88931700 | -1.10745500 | -2.17714300 |
| H | 2.33009500 | 7.06059100 | -0.78781800 |
| H | 3.84424500 | -3.05989800 | 1.02871100 |
| H | 5.46341100 | -3.24053200 | 0.32709900 |
| H | 4.27407200 | -4.55865200 | 0.17875900 |
| H | 4.61572600 | -4.55366300 | -2.33241000 |
| H | 5.78196600 | -3.24993200 | -2.18320700 |
| H | 4.39602400 | -3.06631500 | -3.27964600 |
| Cu | -0.31700400 | 0.65889100 | -0.46694300 |
| O | -2.00820900 | 2.25389700 | 0.01725000 |
| O | -2.62301600 | 1.44683700 | 2.03251800 |
| C | -2.86084100 | 1.77805400 | 0.86498600 |
| C | -4.24840400 | 1.58340400 | 0.34025300 |
| C | -5.29046400 | 0.90814500 | 0.91931000 |
| S | -4.69158700 | 2.15621000 | -1.24883200 |
| C | -6.44722400 | 0.83821500 | 0.08794800 |
| H | -5.20390400 | 0.46546800 | 1.90376000 |
| C | -6.27617900 | 1.46343700 | -1.11956800 |
| H | -7.36797500 | 0.34116800 | 0.37316700 |
| H | -6.99116500 | 1.57625400 | -1.92333900 |
| C | -0.90933100 | -0.64429900 | -3.90270500 |
| H | -1.97677800 | -0.44163000 | -4.04959700 |
| H | -0.51728200 | -1.10433400 | -4.81835400 |
| H | -0.80742000 | -1.36833700 | -3.08803700 |
| C | -0.31801900 | 1.66863100 | -4.70114100 |
| H | 0.08337900 | 1.28855700 | -5.64849400 |
| H | -1.37954300 | 1.90438600 | -4.85230200 |
| H | 0.20927100 | 2.59798200 | -4.45315400 |
| C | 1.32559300 | 0.33718900 | -3.34349600 |
| H | 1.87818600 | 1.23566700 | -3.05051800 |

| | | | |
|---|---|---|---|
| H | 1.43983100 | -0.40274700 | -2.54662000 |
| H | 1.78504100 | -0.07105100 | -4.25212500 |

**S-2**

Total electronic energy = -3516.897950

Thermal corrections to Gibbs free energy = 0.996361

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.18031700 | -0.15720000 | -0.59859800 |
| O | 2.08176600 | -0.56470900 | -1.22743000 |
| C | 2.42052900 | -0.90403300 | -2.59025600 |
| C | 1.13780400 | -1.42683900 | -3.23992600 |
| H | 0.76650600 | -2.31158800 | -2.71344200 |
| H | 0.36381000 | -0.65279500 | -3.22384400 |
| H | 1.31688600 | -1.69779700 | -4.28681500 |
| C | 3.47968400 | -2.00929900 | -2.63574800 |
| H | 3.63969200 | -2.32723600 | -3.67361900 |
| H | 4.42594100 | -1.66085000 | -2.22910800 |
| H | 3.15503600 | -2.86948100 | -2.04455000 |
| C | 2.89060500 | 0.35718100 | -3.32803600 |
| H | 2.11721900 | 1.13185000 | -3.27067800 |
| H | 3.79017800 | 0.75528500 | -2.85966000 |
| H | 3.08677900 | 0.13823800 | -4.38514900 |
| C | 1.80816300 | 1.45518100 | 3.25076500 |
| C | 0.93702000 | 0.15952200 | 3.21610600 |
| O | 0.98864700 | -0.19771700 | 1.79962400 |
| O | 2.71955600 | 1.24545700 | 2.14828300 |
| B | 2.17580000 | 0.32644500 | 1.26629100 |
| C | 5.37388600 | 0.35288700 | -0.05454100 |
| C | 5.14607900 | -1.06578400 | 0.65721700 |
| B | 3.06594200 | -0.23381100 | -0.12832500 |
| O | 3.81624700 | -1.42907500 | 0.31277500 |
| O | 4.09636300 | 0.71172800 | -0.56356300 |
| C | 5.84043200 | 1.46250900 | 0.90225300 |
| H | 6.80957300 | 1.23089400 | 1.36022600 |
| H | 5.95182400 | 2.39278100 | 0.33286100 |
| H | 5.10179200 | 1.63849300 | 1.68513200 |
| C | 6.35373200 | 0.30712400 | -1.23794800 |
| H | 6.35921900 | 1.28907700 | -1.72361300 |
| H | 7.37678900 | 0.08086400 | -0.91592700 |
| H | 6.05705700 | -0.42906800 | -1.98807400 |
| C | 6.08237600 | -2.17856200 | 0.16588700 |

| | | | |
|---|---|---|---|
| H | 7.12958800 | -1.96123100 | 0.40674100 |
| H | 5.80865500 | -3.11638000 | 0.66228400 |
| H | 5.99978800 | -2.33857400 | -0.91048500 |
| C | 5.25774800 | -1.01009400 | 2.19286000 |
| H | 4.96579900 | -1.98707600 | 2.59455200 |
| H | 6.27999400 | -0.79676500 | 2.52578800 |
| H | 4.59175700 | -0.25518300 | 2.61186700 |
| C | 1.55836600 | -1.02238200 | 3.96721000 |
| H | 1.52144000 | -0.87515300 | 5.05193700 |
| H | 0.99302500 | -1.92619700 | 3.71987600 |
| H | 2.59749500 | -1.18152400 | 3.66699400 |
| C | -0.50320100 | 0.35727200 | 3.65642600 |
| H | -1.03936300 | -0.59225400 | 3.62175200 |
| H | -0.53419500 | 0.72575100 | 4.68904800 |
| H | -1.02372000 | 1.07391200 | 3.02172900 |
| C | 1.01171400 | 2.72340100 | 2.92737500 |
| H | 0.33999100 | 3.00792000 | 3.74409400 |
| H | 1.71361100 | 3.54358000 | 2.74889200 |
| H | 0.41441400 | 2.58930700 | 2.02323700 |
| C | 2.62005300 | 1.64598700 | 4.52716600 |
| H | 3.21550000 | 2.56124400 | 4.44960000 |
| H | 1.96154600 | 1.74005800 | 5.39864200 |
| H | 3.30400800 | 0.81099400 | 4.69401700 |
| P | -1.14075100 | -1.97041500 | -0.26372800 |
| P | -0.74517300 | 1.84264900 | -0.98120900 |
| C | -2.48137300 | -2.33492500 | -1.46952900 |
| C | -0.18026300 | -3.51852300 | -0.08517100 |
| C | -2.13484700 | -1.86005100 | 1.27391700 |
| C | -1.80848600 | 1.77091200 | -2.47635000 |
| C | -1.85836700 | 2.48119300 | 0.33586800 |
| C | 0.40377700 | 3.21538800 | -1.34514400 |
| C | -3.58232000 | -3.13656600 | -1.12632800 |
| C | -2.42730800 | -1.77022300 | -2.74942300 |
| C | 1.15028500 | -3.37649200 | 0.34279300 |
| C | -0.66909900 | -4.79373000 | -0.40436800 |
| C | -2.87710500 | -0.69236600 | 1.47571600 |
| C | -2.19625600 | -2.84836700 | 2.26183800 |
| C | -1.17528600 | 1.65424800 | -3.72498500 |
| C | -3.20554100 | 1.71786700 | -2.41387300 |
| C | -1.80306700 | 3.79379900 | 0.82461400 |
| C | -2.72622800 | 1.58950900 | 0.98092200 |
| C | 1.75218200 | 3.04205300 | -1.00435300 |
| C | -0.00282400 | 4.39795400 | -1.98572700 |
| H | -3.65755000 | -3.55104700 | -0.12569100 |

| | | | |
|---|---|---|---|
| C | -4.59125600 | -3.38748500 | -2.05457200 |
| C | -3.43810700 | -2.02083900 | -3.67801700 |
| H | -1.60778900 | -1.11686800 | -3.01657700 |
| C | 1.97552100 | -4.49399400 | 0.45536700 |
| H | 1.55912600 | -2.40011400 | 0.56454300 |
| C | 0.15986200 | -5.90987300 | -0.28524000 |
| H | -1.68642800 | -4.91399800 | -0.76252100 |
| O | -2.77331000 | 0.29271100 | 0.50706800 |
| C | -3.66931000 | -0.46488300 | 2.60110200 |
| H | -1.62260800 | -3.76101800 | 2.13681600 |
| C | -2.97692400 | -2.65190200 | 3.40290400 |
| H | -0.09229800 | 1.70167400 | -3.78745800 |
| C | -1.92800300 | 1.48638100 | -4.88531800 |
| H | -3.71118500 | 1.80624600 | -1.45926700 |
| C | -3.95667100 | 1.54802500 | -3.57749700 |
| H | -1.13030500 | 4.50690500 | 0.36219800 |
| C | -2.57207600 | 4.17192400 | 1.92362000 |
| C | -3.51358900 | 1.93906300 | 2.08289300 |
| H | 2.09746500 | 2.12388400 | -0.54675300 |
| C | 2.68199800 | 4.04365500 | -1.28588600 |
| H | -1.04147400 | 4.52555000 | -2.27791100 |
| C | 0.92765600 | 5.39783300 | -2.25996400 |
| H | -5.43684000 | -4.01079600 | -1.77681800 |
| C | -4.51867400 | -2.83269100 | -3.33483100 |
| H | -3.38329700 | -1.56340200 | -4.66052200 |
| C | 1.48175800 | -5.76190200 | 0.14374900 |
| H | 3.00720600 | -4.34906600 | 0.76039400 |
| H | -0.22410000 | -6.89449400 | -0.53818200 |
| C | -4.43462700 | 0.86009200 | 2.66352300 |
| C | -3.70701100 | -1.47269200 | 3.57026300 |
| H | -3.01539500 | -3.42074100 | 4.16878400 |
| H | -1.42502100 | 1.40083600 | -5.84441500 |
| C | -3.32269700 | 1.43096000 | -4.81437100 |
| H | -5.04021100 | 1.50465700 | -3.51407900 |
| C | -3.41513800 | 3.25182600 | 2.55082600 |
| H | -2.50906200 | 5.18827600 | 2.30025800 |
| H | 3.72295900 | 3.87514200 | -1.02875500 |
| C | 2.27100000 | 5.22168400 | -1.90814500 |
| H | 0.60947600 | 6.31112500 | -2.75526000 |
| H | -5.30782800 | -3.02513700 | -4.05647000 |
| H | 2.12667200 | -6.63314100 | 0.22091500 |
| C | -5.68461200 | 0.74443500 | 1.75009100 |
| C | -4.88552600 | 1.19668200 | 4.08953800 |
| H | -4.30050800 | -1.33922200 | 4.46781100 |

| | | | |
|---|---|---|---|
| H | -3.91005400 | 1.29945400 | -5.71874900 |
| H | -3.99673300 | 3.56482900 | 3.41067000 |
| H | 2.99437500 | 6.00077400 | -2.13298800 |
| H | -5.39954200 | 0.49441800 | 0.72414600 |
| H | -6.23236500 | 1.69318000 | 1.73650000 |
| H | -6.35120300 | -0.04166500 | 2.12127600 |
| H | -5.55252400 | 0.42009600 | 4.47488900 |
| H | -5.44974200 | 2.13373800 | 4.10531200 |
| H | -4.03268600 | 1.29151500 | 4.76952500 |

**S-3**

Total electronic energy = -3516.912093

Thermal corrections to Gibbs free energy = 0.993179

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | -0.26308600 | 0.20436000 | -0.20072200 |
| O | -2.27144100 | 1.69928400 | -0.64396300 |
| C | -2.28878900 | 2.66988500 | -1.72854500 |
| C | -0.99325600 | 3.45930000 | -1.56407700 |
| H | -0.95721200 | 3.93158400 | -0.57784800 |
| H | -0.13256800 | 2.79476300 | -1.65133600 |
| H | -0.91446300 | 4.23697200 | -2.33121300 |
| C | -3.50018800 | 3.59034700 | -1.54476300 |
| H | -3.48893500 | 4.38526500 | -2.29850900 |
| H | -4.43452000 | 3.03214200 | -1.64788100 |
| H | -3.47010000 | 4.05409600 | -0.55274500 |
| C | -2.32638600 | 1.94725900 | -3.07752500 |
| H | -1.51110200 | 1.22221000 | -3.14081700 |
| H | -3.26675500 | 1.40797200 | -3.20667700 |
| H | -2.21735700 | 2.66934500 | -3.89508700 |
| C | -1.27258900 | -3.83712400 | 0.74928100 |
| C | -0.41005100 | -3.40898400 | 1.97887100 |
| O | 0.08924800 | -2.11957900 | 1.55884100 |
| O | -1.69615200 | -2.55202200 | 0.21845100 |
| B | -0.74755200 | -1.57795400 | 0.57884600 |
| C | -5.15899900 | -0.44688500 | -0.59224900 |
| C | -4.83401300 | -0.21855700 | 0.93174000 |
| B | -3.33026400 | 0.88862100 | -0.35402100 |
| O | -3.50056800 | 0.34070400 | 0.89107400 |
| O | -4.34876400 | 0.57638700 | -1.23258700 |
| C | -4.67078600 | -1.79878700 | -1.12059800 |
| H | -5.30017900 | -2.61708600 | -0.75331600 |

| | | | |
|---|---|---|---|
| H | -4.72792900 | -1.78530200 | -2.21420600 |
| H | -3.63794600 | -1.99689200 | -0.82396900 |
| C | -6.61534300 | -0.21750800 | -0.97951800 |
| H | -6.73805600 | -0.37647600 | -2.05565300 |
| H | -7.26952200 | -0.92313600 | -0.45528800 |
| H | -6.94014100 | 0.79911000 | -0.74706900 |
| C | -5.72988400 | 0.83763000 | 1.58758900 |
| H | -6.75122200 | 0.47062500 | 1.73339100 |
| H | -5.30599900 | 1.09960100 | 2.56093000 |
| H | -5.76879800 | 1.75022300 | 0.98425600 |
| C | -4.79282600 | -1.48878000 | 1.77097600 |
| H | -4.56316000 | -1.23246000 | 2.81077500 |
| H | -5.75954500 | -2.00481500 | 1.75240600 |
| H | -4.01603800 | -2.15913000 | 1.40391600 |
| C | -1.23351400 | -3.16990900 | 3.25006400 |
| H | -1.59082500 | -4.10612900 | 3.69369400 |
| H | -0.59933700 | -2.65721300 | 3.98036100 |
| H | -2.09474300 | -2.52865500 | 3.03943700 |
| C | 0.77981100 | -4.31299900 | 2.28460400 |
| H | 1.33541900 | -3.90178300 | 3.13378200 |
| H | 0.45038000 | -5.32586700 | 2.54608700 |
| H | 1.46094500 | -4.37092600 | 1.43324600 |
| C | -0.44897500 | -4.51542600 | -0.35188100 |
| H | -0.14451500 | -5.52914300 | -0.06846300 |
| H | -1.05626800 | -4.57724200 | -1.26079200 |
| H | 0.44590500 | -3.93400200 | -0.58546800 |
| C | -2.50081100 | -4.67816200 | 1.07712600 |
| H | -3.07237500 | -4.86889900 | 0.16255800 |
| H | -2.20510200 | -5.64579600 | 1.49977900 |
| H | -3.15927300 | -4.17871500 | 1.79043500 |
| P | 0.57194000 | 1.63156800 | 1.38127000 |
| P | 1.01602500 | -0.18196100 | -2.05296300 |
| C | 1.70402700 | 3.07585100 | 1.18854500 |
| C | -0.75600200 | 2.21137600 | 2.49759100 |
| C | 1.60847900 | 0.55267500 | 2.45931700 |
| C | 2.15053500 | 0.99086000 | -2.90700700 |
| C | 2.15466000 | -1.51868300 | -1.49208900 |
| C | 0.09881500 | -0.99154100 | -3.42312700 |
| C | 2.11920200 | 3.86646800 | 2.27153500 |
| C | 2.23160500 | 3.33154700 | -0.08214900 |
| C | -1.54562600 | 1.24171300 | 3.13740100 |
| C | -1.12217800 | 3.56051100 | 2.59797600 |
| C | 2.50099100 | -0.31496100 | 1.82337600 |
| C | 1.51768200 | 0.47524200 | 3.85273500 |

| | | | |
|---|---|---|---|
| C | 1.59989000 | 2.01468400 | -3.69950100 |
| C | 3.52604900 | 1.02159600 | -2.63489700 |
| C | 2.36049300 | -2.70360800 | -2.20947500 |
| C | 2.77350600 | -1.40229700 | -0.24118400 |
| C | -1.06380800 | -1.70401800 | -3.08181600 |
| C | 0.49171700 | -0.92534000 | -4.76710500 |
| H | 1.73126400 | 3.66542800 | 3.26588000 |
| C | 3.02568600 | 4.90675000 | 2.07764500 |
| C | 3.14799300 | 4.36699600 | -0.27607100 |
| H | 1.93663800 | 2.70979800 | -0.91801800 |
| C | -2.64984000 | 1.62149100 | 3.89542400 |
| H | -1.30208300 | 0.19154900 | 3.01603000 |
| C | -2.24254400 | 3.93526300 | 3.34183100 |
| H | -0.53130500 | 4.32061700 | 2.09723400 |
| O | 2.58200500 | -0.22366900 | 0.44497200 |
| C | 3.27207600 | -1.26349300 | 2.49570900 |
| H | 0.83154000 | 1.12783400 | 4.38148600 |
| C | 2.26721000 | -0.46657900 | 4.55755700 |
| H | 0.53730600 | 2.01200400 | -3.92110700 |
| C | 2.40237800 | 3.03501400 | -4.20428400 |
| H | 3.97238800 | 0.24365000 | -2.02528200 |
| C | 4.32699300 | 2.05013900 | -3.13282500 |
| H | 1.88862100 | -2.82889900 | -3.17777400 |
| C | 3.13258500 | -3.73139100 | -1.66926800 |
| C | 3.56121900 | -2.40911100 | 0.32430200 |
| H | -1.36538900 | -1.77046300 | -2.04150100 |
| C | -1.81787000 | -2.33106200 | -4.07216900 |
| H | 1.39010600 | -0.38230400 | -5.04197300 |
| C | -0.27166900 | -1.54892300 | -5.75552900 |
| H | 3.33729200 | 5.51679700 | 2.92139900 |
| C | 3.54080800 | 5.15938300 | 0.80203500 |
| H | 3.54994800 | 4.54323400 | -1.26932500 |
| C | -3.00405700 | 2.96851800 | 3.99980900 |
| H | -3.24660900 | 0.86016600 | 4.39062100 |
| H | -2.51466800 | 4.98512200 | 3.41151000 |
| C | 4.23925200 | -2.11018200 | 1.66441700 |
| C | 3.13128000 | -1.33298400 | 3.88424300 |
| H | 2.17912700 | -0.52718400 | 5.63854100 |
| H | 1.95882500 | 3.81396600 | -4.81850100 |
| C | 3.77041300 | 3.06082200 | -3.91770200 |
| H | 5.38978600 | 2.05872600 | -2.90681700 |
| C | 3.72098300 | -3.58711500 | -0.41063600 |
| H | 3.27277000 | -4.65221400 | -2.22756300 |
| H | -2.71573400 | -2.87619700 | -3.79412300 |

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|---|---|---|---|
| C | -1.42807300 | -2.25111700 | -5.41106600 |
| H | 0.03973700 | -1.48710200 | -6.79484500 |
| H | 4.25078200 | 5.96884500 | 0.65452900 |
| H | -3.87141100 | 3.26200600 | 4.58493800 |
| C | 5.50348800 | -1.25448800 | 1.37803600 |
| C | 4.66232900 | -3.39060800 | 2.39498400 |
| H | 3.70107300 | -2.06096700 | 4.45131000 |
| H | 4.39544700 | 3.85997600 | -4.30614400 |
| H | 4.31439000 | -4.39974500 | -0.00630600 |
| H | -2.02164700 | -2.73375400 | -6.18276600 |
| H | 5.23928000 | -0.32801800 | 0.85972100 |
| H | 6.20639200 | -1.81406500 | 0.75042100 |
| H | 6.00163700 | -0.99062500 | 2.31753300 |
| H | 5.16574800 | -3.14804200 | 3.33534100 |
| H | 5.37714400 | -3.96028700 | 1.79377100 |
| H | 3.80294000 | -4.03099500 | 2.61497300 |

**S-4**

Total electronic energy =-3513.937452

Thermal corrections to Gibbs free energy = 0.933764

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 0.25110200 | -1.37296800 | 1.57886600 |
| P | 0.99632100 | 2.00524500 | -0.11727000 |
| C | 1.48368800 | -0.90207700 | 2.86007300 |
| C | -0.84704300 | -2.53227700 | 2.47618600 |
| C | 1.23126700 | -2.48863000 | 0.49670100 |
| C | 2.09385100 | 2.48861300 | 1.28405300 |
| C | 2.16715900 | 1.44750000 | -1.42214400 |
| C | 0.40742300 | 3.63907100 | -0.69600400 |
| C | 2.71919300 | -1.54539400 | 3.00512700 |
| C | 1.14897000 | 0.13545500 | 3.74088800 |
| C | -2.18460100 | -2.63149000 | 2.06806700 |
| C | -0.38164200 | -3.32207800 | 3.53936400 |
| C | 2.21879600 | -1.89794100 | -0.29670800 |
| C | 1.05764800 | -3.87255400 | 0.38718700 |
| C | 1.60050500 | 3.40698300 | 2.22507900 |
| C | 3.36951400 | 1.94462000 | 1.47769100 |
| C | 2.49794100 | 2.17332400 | -2.57313400 |
| C | 2.70997200 | 0.16452500 | -1.29819200 |
| C | -0.95040800 | 3.79431400 | -1.00554300 |
| C | 1.27252500 | 4.74108300 | -0.80328700 |

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|---|---|---|---|
| H | 2.99376200 | -2.34883700 | 2.32968100 |
| C | 3.60020700 | -1.15985800 | 4.01667700 |
| C | 2.02426900 | 0.51285600 | 4.75572000 |
| H | 0.20162000 | 0.65206900 | 3.62790400 |
| C | -3.04269600 | -3.52086100 | 2.71924500 |
| H | -2.56912600 | -2.01596600 | 1.25780300 |
| C | -1.24499200 | -4.20615600 | 4.18363100 |
| H | 0.65076100 | -3.23887700 | 3.86470400 |
| O | 2.36852000 | -0.53530300 | -0.15877200 |
| C | 3.03959100 | -2.59977100 | -1.17759500 |
| H | 0.30262000 | -4.36747800 | 0.98835600 |
| C | 1.85092600 | -4.60710600 | -0.49745100 |
| H | 0.61920900 | 3.84734100 | 2.08651500 |
| C | 2.37094500 | 3.78090500 | 3.32391300 |
| H | 3.77366300 | 1.23396400 | 0.76845800 |
| C | 4.13640400 | 2.31697500 | 2.58137300 |
| H | 2.08376900 | 3.16413600 | -2.72067100 |
| C | 3.33788400 | 1.61449300 | -3.53645600 |
| C | 3.55950200 | -0.42344000 | -2.23542300 |
| H | -1.62647100 | 2.95584600 | -0.90125400 |
| C | -1.43163300 | 5.03432000 | -1.43231300 |
| H | 2.32061000 | 4.63192400 | -0.54031200 |
| C | 0.78794200 | 5.97446900 | -1.23228200 |
| H | 4.55674800 | -1.66547000 | 4.11795400 |
| C | 3.25340500 | -0.13391400 | 4.89545000 |
| H | 1.75589900 | 1.32644500 | 5.42205500 |
| C | -2.57769800 | -4.30693900 | 3.77349000 |
| H | -4.08013400 | -3.58378500 | 2.40365600 |
| H | -0.88009400 | -4.81299400 | 5.00783200 |
| C | 4.13225200 | -1.80569700 | -1.90077600 |
| C | 2.83175600 | -3.97892200 | -1.26922500 |
| H | 1.70685400 | -5.68001400 | -0.58316400 |
| H | 1.97657600 | 4.50122000 | 4.03552500 |
| C | 3.64357500 | 3.23720200 | 3.50561700 |
| H | 5.12196200 | 1.88140900 | 2.71764600 |
| C | 3.86301900 | 0.33050900 | -3.37095400 |
| H | 3.58239300 | 2.18265100 | -4.42901500 |
| H | -2.48600200 | 5.14376800 | -1.66904100 |
| C | -0.56638200 | 6.12149800 | -1.54904800 |
| H | 1.46299800 | 6.82178400 | -1.31517000 |
| H | 3.94139100 | 0.16844900 | 5.67988500 |
| H | -3.25068800 | -4.99255200 | 4.28134500 |
| C | 5.30613400 | -1.60586200 | -0.90243300 |
| C | 4.65390700 | -2.53319600 | -3.14470500 |

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|---|---|---|---|
| H | 3.43414000 | -4.57196700 | -1.94829200 |
| H | 4.24478000 | 3.52639000 | 4.36300300 |
| H | 4.50703900 | -0.08336700 | -4.13861600 |
| H | -0.94375100 | 7.08518300 | -1.87999800 |
| H | 4.96761800 | -1.10389200 | 0.00922900 |
| H | 6.09294000 | -0.99650000 | -1.36050700 |
| H | 5.73099400 | -2.57583600 | -0.62095000 |
| H | 5.07705400 | -3.50478900 | -2.87217500 |
| H | 5.45863000 | -1.95996000 | -3.61494900 |
| H | 3.85668700 | -2.68658500 | -3.87588400 |
| Cu | -0.55096100 | 0.39714900 | 0.40899400 |
| O | -2.48889000 | 1.18934600 | 0.46709400 |
| C | -3.10543900 | 1.80807600 | 1.61314200 |
| C | -3.75256500 | 0.75005500 | 2.51357800 |
| H | -4.17818000 | 1.21846700 | 3.40910600 |
| H | -4.53908300 | 0.21169600 | 1.98469500 |
| H | -3.00621100 | 0.01248800 | 2.82636400 |
| C | -4.11311000 | 2.87065000 | 1.15579100 |
| H | -3.60439000 | 3.62568500 | 0.54730800 |
| H | -4.90225500 | 2.43376300 | 0.54937000 |
| H | -4.55634800 | 3.37007500 | 2.02577400 |
| C | -1.97103300 | 2.50639800 | 2.36876700 |
| H | -1.19217600 | 1.78774700 | 2.64416400 |
| H | -1.51900900 | 3.27762300 | 1.73856700 |
| H | -2.34426700 | 2.97919300 | 3.28410500 |
| C | 1.13085400 | -0.83683100 | -4.87565700 |
| C | 0.30222700 | -0.41178200 | -3.84176900 |
| C | -0.21289600 | -1.33602000 | -2.91056700 |
| C | 0.16028900 | -2.68599300 | -3.04573600 |
| C | 0.98677200 | -3.10796700 | -4.08255800 |
| C | 1.47053600 | -2.18502500 | -5.01176100 |
| H | 1.51508700 | -0.10618900 | -5.58156600 |
| H | 0.04458300 | 0.63333000 | -3.75282900 |
| H | -0.20848600 | -3.40772700 | -2.32306900 |
| H | 1.25244200 | -4.15853500 | -4.16394500 |
| H | 2.10585100 | -2.51122800 | -5.83108400 |
| C | -1.16635500 | -0.99440100 | -1.85235700 |
| H | -1.46892500 | -1.81795800 | -1.21268100 |
| C | -1.88164900 | 0.13600000 | -1.64559800 |
| F | -1.61704100 | 1.21179900 | -2.46733200 |
| C | -5.37386500 | 0.07225600 | -1.34811700 |
| C | -4.77241800 | -1.31396700 | -0.86654600 |
| B | -3.14444700 | 0.35910300 | -0.60397800 |
| O | -4.27074800 | 0.97359600 | -1.27908700 |

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|---|---|---|---|
| O | -3.63744200 | -0.92252000 | -0.09728400 |
| C | -5.69916100 | -2.13428600 | 0.03527600 |
| H | -6.63094800 | -2.39449700 | -0.47982100 |
| H | -5.19874000 | -3.06855400 | 0.31418400 |
| H | -5.94610900 | -1.59661200 | 0.95342400 |
| C | -4.31916900 | -2.21188200 | -2.03123100 |
| H | -3.76437400 | -3.06335200 | -1.62172600 |
| H | -5.17348500 | -2.60057200 | -2.59604100 |
| H | -3.65791200 | -1.68433000 | -2.71995400 |
| C | -6.49449200 | 0.58785200 | -0.43048300 |
| H | -6.74395200 | 1.61348500 | -0.72155700 |
| H | -7.40197100 | -0.02043500 | -0.51595700 |
| H | -6.18778800 | 0.60047800 | 0.61788800 |
| C | -5.89915400 | 0.06295100 | -2.78774800 |
| H | -6.71939100 | -0.65410400 | -2.91377300 |
| H | -6.27677900 | 1.05959900 | -3.03956400 |
| H | -5.10569100 | -0.18118900 | -3.49714000 |

**S-5**

Total electronic energy = -3692.114198

Thermal corrections to Gibbs free energy = 0.984940

No. of imaginary frequency: 0

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 0.39943300 | -0.19093300 | 1.98198500 |
| P | 0.43923300 | 1.58552100 | -1.44424700 |
| C | 0.64015800 | 1.44413700 | 2.77620200 |
| C | -0.48697700 | -1.17011600 | 3.25270500 |
| C | 2.09136700 | -0.90210600 | 2.01593500 |
| C | 0.59724800 | 3.22368100 | -0.61998700 |
| C | 2.14982700 | 1.15153400 | -1.96564800 |
| C | -0.40762400 | 2.04968100 | -2.99905000 |
| C | 1.77399300 | 1.77879200 | 3.52596700 |
| C | -0.37558600 | 2.39410300 | 2.60606800 |
| C | -1.39041000 | -2.15619400 | 2.83157100 |
| C | -0.29448100 | -0.94892800 | 4.62375300 |
| C | 3.01116500 | -0.39885500 | 1.09076200 |
| C | 2.51463400 | -1.95204700 | 2.83899700 |
| C | -0.54278000 | 4.04262400 | -0.58650000 |
| C | 1.76421400 | 3.65979200 | 0.01771000 |
| C | 2.59200200 | 1.14694300 | -3.29476500 |
| C | 3.03858700 | 0.67804900 | -0.99385500 |
| C | -1.49720800 | 1.29184800 | -3.44538500 |

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|---|---|---|---|
| C | -0.00158500 | 3.17947800 | -3.73120200 |
| H | 2.57327300 | 1.05465900 | 3.65036400 |
| C | 1.88023300 | 3.04269500 | 4.10983400 |
| C | -0.27450900 | 3.64871600 | 3.19981100 |
| H | -1.23797400 | 2.13392800 | 2.00493500 |
| C | -2.07845300 | -2.91865000 | 3.77613700 |
| H | -1.59845300 | -2.30911300 | 1.77815000 |
| C | -0.98919000 | -1.71030900 | 5.56378700 |
| H | 0.38875100 | -0.17289900 | 4.95555400 |
| O | 2.57368700 | 0.64936800 | 0.30612000 |
| C | 4.30547400 | -0.89097400 | 0.92990200 |
| H | 1.82952800 | -2.36803900 | 3.56969600 |
| C | 3.80364700 | -2.47043600 | 2.70552800 |
| H | -1.45048400 | 3.71940500 | -1.08505300 |
| C | -0.51077400 | 5.27606900 | 0.06004100 |
| H | 2.65331700 | 3.04251400 | 0.01206900 |
| C | 1.79207600 | 4.89402900 | 0.66726100 |
| H | 1.92471000 | 1.47714600 | -4.08214500 |
| C | 3.87435100 | 0.69591600 | -3.60802700 |
| C | 4.33405500 | 0.23598100 | -1.26909000 |
| H | -1.84454700 | 0.42536000 | -2.89780500 |
| C | -2.16200000 | 1.65712700 | -4.61892800 |
| H | 0.82806700 | 3.78361200 | -3.37551800 |
| C | -0.66573900 | 3.53469900 | -4.90198600 |
| H | 2.76445400 | 3.29612900 | 4.68857500 |
| C | 0.85476400 | 3.97576100 | 3.95353800 |
| H | -1.06361700 | 4.37933400 | 3.05238900 |
| C | -1.88139300 | -2.69836400 | 5.14051300 |
| H | -2.78305000 | -3.67350500 | 3.43801500 |
| H | -0.83759300 | -1.52875400 | 6.62437000 |
| C | 5.20849400 | -0.17866100 | -0.08110100 |
| C | 4.68694700 | -1.95119600 | 1.75691100 |
| H | 4.12095700 | -3.29234200 | 3.34048500 |
| H | -1.39992800 | 5.90069200 | 0.06906000 |
| C | 0.65936100 | 5.70695000 | 0.68831100 |
| H | 2.70369700 | 5.21659600 | 1.16181000 |
| C | 4.73908800 | 0.25118500 | -2.60546500 |
| H | 4.20344400 | 0.69146600 | -4.64286200 |
| H | -3.00706600 | 1.06188300 | -4.95223400 |
| C | -1.74942700 | 2.77073200 | -5.34816300 |
| H | -0.34422700 | 4.40798700 | -5.46294200 |
| H | 0.94032500 | 4.95956800 | 4.40651800 |
| H | -2.42631300 | -3.28793300 | 5.87295800 |
| C | 5.74668800 | 1.11439000 | 0.59081500 |

| | | | |
|---|---|---|---|
| C | 6.39516600 | -1.04907400 | -0.50965400 |
| H | 5.67799900 | -2.38024400 | 1.66249500 |
| H | 0.68611100 | 6.66772600 | 1.19469600 |
| H | 5.73104800 | -0.09461100 | -2.87358600 |
| H | -2.27086500 | 3.05074500 | -6.25961900 |
| H | 4.92571600 | 1.75609500 | 0.92490200 |
| H | 6.36211900 | 1.68105600 | -0.11664700 |
| H | 6.35775500 | 0.85923100 | 1.46372500 |
| H | 7.01700200 | -1.30051400 | 0.35478200 |
| H | 7.03649700 | -0.50761900 | -1.21163400 |
| H | 6.05656200 | -1.97575300 | -0.97972000 |
| Cu | -0.48266800 | -0.02573900 | -0.13483000 |
| C | 3.79316000 | -3.08583500 | -2.44947400 |
| C | 2.53688900 | -2.55556500 | -2.17050600 |
| C | 1.82859400 | -2.96264900 | -1.02193100 |
| C | 2.44148800 | -3.89567700 | -0.16348200 |
| C | 3.69819400 | -4.42090100 | -0.44427800 |
| C | 4.37956400 | -4.02455900 | -1.59686800 |
| H | 4.31973600 | -2.75573200 | -3.34042200 |
| H | 2.10231100 | -1.82384400 | -2.83612400 |
| H | 1.91726600 | -4.20234400 | 0.73690000 |
| H | 4.14630100 | -5.13947500 | 0.23653800 |
| H | 5.35680200 | -4.44074200 | -1.82712500 |
| C | 0.48671200 | -2.49834700 | -0.67528900 |
| H | 0.10454300 | -2.85227700 | 0.27764700 |
| C | -0.41801400 | -1.79547400 | -1.39863500 |
| F | -0.03740900 | -1.39141600 | -2.66479300 |
| C | -3.75981800 | -2.43985400 | -2.23478000 |
| C | -3.31341300 | -3.39692000 | -1.06015400 |
| B | -1.98409400 | -1.49267700 | -1.02141000 |
| O | -2.73828100 | -1.44146400 | -2.25846400 |
| O | -2.60145800 | -2.51346000 | -0.18073800 |
| C | -4.46304900 | -4.02433000 | -0.27413400 |
| H | -5.08398700 | -4.65594200 | -0.91996200 |
| H | -4.05837600 | -4.65263000 | 0.52709000 |
| H | -5.09776900 | -3.26298300 | 0.18357800 |
| C | -2.35814000 | -4.50795000 | -1.52573600 |
| H | -1.93076900 | -4.99450400 | -0.64270400 |
| H | -2.88078500 | -5.26630600 | -2.11890600 |
| H | -1.53297800 | -4.11083900 | -2.11988300 |
| C | -5.10895800 | -1.75819400 | -1.97369400 |
| H | -5.24717300 | -0.96370100 | -2.71312300 |
| H | -5.94492400 | -2.46246900 | -2.05310700 |
| H | -5.12748300 | -1.29211200 | -0.98983100 |

| | | | |
|---|---|---|---|
| C | -3.79840000 | -3.11150300 | -3.60940900 |
| H | -4.51450600 | -3.94199000 | -3.62789900 |
| H | -4.10907800 | -2.37880800 | -4.36193800 |
| H | -2.81361200 | -3.48712000 | -3.89459500 |
| C | -4.39572300 | 1.49350600 | 0.42559400 |
| C | -4.07715500 | 0.69053900 | 1.73581700 |
| B | -2.62816800 | 0.04951900 | 0.04854000 |
| O | -3.61633700 | 0.78655000 | -0.57724200 |
| O | -2.77291100 | 0.13363000 | 1.43191500 |
| C | -5.86178700 | 1.48333700 | 0.00561100 |
| H | -6.48173700 | 1.98305100 | 0.75908500 |
| H | -5.97573900 | 2.01978800 | -0.94161600 |
| H | -6.23602200 | 0.46844100 | -0.13566900 |
| C | -3.87465100 | 2.93372300 | 0.45503300 |
| H | -3.95869200 | 3.35794100 | -0.55052100 |
| H | -4.45151700 | 3.55920300 | 1.14463700 |
| H | -2.82211000 | 2.97047300 | 0.74615200 |
| C | -3.97620000 | 1.52392000 | 3.00924400 |
| H | -4.95157100 | 1.95249600 | 3.26706600 |
| H | -3.65359500 | 0.88185100 | 3.83480600 |
| H | -3.25498500 | 2.33710800 | 2.91841900 |
| C | -5.00621700 | -0.50306300 | 1.97885100 |
| H | -4.59548900 | -1.09926700 | 2.79908800 |
| H | -6.01897500 | -0.18390700 | 2.24649900 |
| H | -5.05538800 | -1.14723800 | 1.09872000 |

**S-ts1**

Total electronic energy = -3516.891070

Thermal corrections to Gibbs free energy = 0.998603

No. of imaginary frequency: 1 (142.20*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| Cu | 0.45995100 | 0.19041500 | -0.39486400 |
| O | 2.10871500 | -0.23116400 | -1.78196000 |
| C | 2.38763500 | 0.39834900 | -3.05368700 |
| C | 1.57677700 | -0.39455900 | -4.08162800 |
| H | 1.89569300 | -1.44056000 | -4.09279200 |
| H | 0.51258900 | -0.37519500 | -3.83935400 |
| H | 1.70800400 | 0.02888900 | -5.08408800 |
| C | 3.87392100 | 0.30789800 | -3.40302800 |
| H | 4.04283100 | 0.67000100 | -4.42377400 |
| H | 4.46835600 | 0.91589000 | -2.72079400 |
| H | 4.21068600 | -0.73120900 | -3.34497900 |

| | | | |
|---|---|---|---|
| C | 1.92889600 | 1.85944500 | -3.00079000 |
| H | 0.86252900 | 1.90689100 | -2.75366000 |
| H | 2.48434300 | 2.40319500 | -2.23317500 |
| H | 2.07780900 | 2.35245400 | -3.96898500 |
| C | 1.57444000 | -1.35469600 | 3.34687800 |
| C | 1.33365500 | -2.64771700 | 2.49521500 |
| O | 1.03518100 | -2.09648500 | 1.18768600 |
| O | 1.98752500 | -0.38601200 | 2.34682400 |
| B | 1.54578700 | -0.79944100 | 1.09316700 |
| C | 4.74567900 | 0.95927600 | 0.37293000 |
| C | 5.02903900 | -0.60022300 | 0.24621100 |
| B | 2.87166100 | -0.11525800 | -0.56801200 |
| O | 3.77520900 | -1.15659100 | -0.19191800 |
| O | 3.51654700 | 1.13473200 | -0.34617000 |
| C | 4.54108300 | 1.44497100 | 1.81536700 |
| H | 5.45283000 | 1.32452400 | 2.41047200 |
| H | 4.29529900 | 2.51165700 | 1.79776900 |
| H | 3.71880600 | 0.91756400 | 2.29799000 |
| C | 5.80609900 | 1.84767900 | -0.28512000 |
| H | 5.47955500 | 2.89177400 | -0.23230900 |
| H | 6.76573100 | 1.76603000 | 0.23784400 |
| H | 5.96494600 | 1.59958100 | -1.33599500 |
| C | 6.08169200 | -0.96802700 | -0.80928100 |
| H | 7.08126600 | -0.62601900 | -0.51830400 |
| H | 6.10704500 | -2.05810600 | -0.90660800 |
| H | 5.84308600 | -0.55296200 | -1.78806600 |
| C | 5.43771600 | -1.25209300 | 1.56733700 |
| H | 5.56310800 | -2.32968200 | 1.42031000 |
| H | 6.39190000 | -0.84753200 | 1.92374200 |
| H | 4.68261100 | -1.09037700 | 2.33450200 |
| C | 2.57412800 | -3.52866700 | 2.32534900 |
| H | 2.87681400 | -3.99445700 | 3.26957600 |
| H | 2.34051700 | -4.32314100 | 1.60921100 |
| H | 3.40684600 | -2.95324100 | 1.92112600 |
| C | 0.15274100 | -3.49625400 | 2.95187600 |
| H | 0.03100900 | -4.34912900 | 2.27825200 |
| H | 0.32231300 | -3.88158200 | 3.96466300 |
| H | -0.77964800 | -2.93218300 | 2.94111900 |
| C | 0.29300300 | -0.80206400 | 3.97662800 |
| H | -0.06695200 | -1.43582600 | 4.79467600 |
| H | 0.49080800 | 0.19817600 | 4.37165600 |
| H | -0.49783000 | -0.71234900 | 3.23126500 |
| C | 2.66083800 | -1.47603200 | 4.40991100 |
| H | 2.80145800 | -0.50887700 | 4.90353700 |

| | | | |
|---|---|---|---|
| H | 2.37099400 | -2.20810800 | 5.17286600 |
| H | 3.61739600 | -1.78472300 | 3.98557800 |
| P | -1.02391600 | -1.38426600 | -1.30565500 |
| P | -0.64522600 | 2.09608900 | 0.19072200 |
| C | -2.36000000 | -0.77109600 | -2.41294400 |
| C | -0.26488900 | -2.75287400 | -2.26148900 |
| C | -2.00538400 | -2.25562900 | -0.02352100 |
| C | -1.94904000 | 2.78910300 | -0.91716300 |
| C | -1.53555800 | 1.79617600 | 1.78111200 |
| C | 0.32016100 | 3.61338900 | 0.55010300 |
| C | -3.62224700 | -1.37755000 | -2.48475800 |
| C | -2.09731600 | 0.34318900 | -3.22034700 |
| C | 0.96525300 | -3.25798600 | -1.80893700 |
| C | -0.81875800 | -3.24932700 | -3.44902700 |
| C | -2.62491700 | -1.45271000 | 0.93628400 |
| C | -2.13757500 | -3.64043800 | 0.10795000 |
| C | -1.52619300 | 3.56267500 | -2.01167100 |
| C | -3.31720500 | 2.54270600 | -0.75543700 |
| C | -1.35149900 | 2.56338400 | 2.93818800 |
| C | -2.36538900 | 0.67443400 | 1.88568500 |
| C | 1.71541600 | 3.52374900 | 0.59908800 |
| C | -0.30371600 | 4.85504500 | 0.76049200 |
| H | -3.84314500 | -2.23627600 | -1.85853800 |
| C | -4.59491100 | -0.88466000 | -3.35501400 |
| C | -3.06192700 | 0.82451100 | -4.10318800 |
| H | -1.14068300 | 0.84646300 | -3.14257900 |
| C | 1.62086900 | -4.24990200 | -2.53628900 |
| H | 1.40230400 | -2.87083700 | -0.89694200 |
| C | -0.15214800 | -4.23555600 | -4.17764500 |
| H | -1.76236100 | -2.85731900 | -3.81358800 |
| O | -2.51048100 | -0.08945200 | 0.74749700 |
| C | -3.31743300 | -1.94759400 | 2.04007900 |
| H | -1.66431100 | -4.29216200 | -0.61886600 |
| C | -2.85037800 | -4.17471800 | 1.18338200 |
| H | -0.46959200 | 3.77455100 | -2.14529600 |
| C | -2.45124200 | 4.08592800 | -2.91168900 |
| H | -3.66981900 | 1.94859600 | 0.07788900 |
| C | -4.24166900 | 3.06009700 | -1.66369900 |
| H | -0.70036600 | 3.42886000 | 2.90951000 |
| C | -1.98020800 | 2.20425400 | 4.13055200 |
| C | -3.02107300 | 0.29064300 | 3.05863200 |
| H | 2.20913700 | 2.57519600 | 0.41448600 |
| C | 2.47766700 | 4.66647700 | 0.85745900 |
| H | -1.38567000 | 4.93142200 | 0.70884200 |

| | | | |
|---|---|---|---|
| C | 0.46083500 | 5.98843700 | 1.02543600 |
| H | -5.57039100 | -1.36173100 | -3.39903900 |
| C | -4.31413900 | 0.21303400 | -4.17063000 |
| H | -2.84310200 | 1.69314000 | -4.71496600 |
| C | 1.06890800 | -4.73667000 | -3.72373600 |
| H | 2.57503900 | -4.62893300 | -2.18085000 |
| H | -0.58651000 | -4.60858300 | -5.10131000 |
| C | -3.94754100 | -0.93046900 | 2.99701400 |
| C | -3.42347500 | -3.33977900 | 2.14551200 |
| H | -2.94751600 | -5.25173300 | 1.28319700 |
| H | -2.10672600 | 4.69223600 | -3.74513700 |
| C | -3.81489300 | 3.83530300 | -2.74075100 |
| H | -5.29935900 | 2.85467500 | -1.52514800 |
| C | -2.80766600 | 1.08143700 | 4.19116300 |
| H | -1.82153200 | 2.80333200 | 5.02222200 |
| H | 3.56122800 | 4.59079600 | 0.88116200 |
| C | 1.85574800 | 5.89518800 | 1.07331500 |
| H | -0.02828900 | 6.94490000 | 1.18868100 |
| H | -5.07161100 | 0.59580000 | -4.84907400 |
| H | 1.59005800 | -5.50019200 | -4.29515300 |
| C | -5.30385900 | -0.47702000 | 2.39386400 |
| C | -4.18920300 | -1.53229500 | 4.38726900 |
| H | -3.95411800 | -3.78112100 | 2.98197700 |
| H | -4.53744100 | 4.23958100 | -3.44405500 |
| H | -3.28273700 | 0.82251900 | 5.13073700 |
| H | 2.45183100 | 6.78181700 | 1.27202400 |
| H | -5.16484300 | -0.05564400 | 1.39361100 |
| H | -5.76678500 | 0.28610000 | 3.02933000 |
| H | -5.98613400 | -1.33047700 | 2.31296400 |
| H | -4.86492800 | -2.38998500 | 4.32441700 |
| H | -4.66679300 | -0.80300900 | 5.04803100 |
| H | -3.25232300 | -1.86049400 | 4.84894600 |

**S-ts2**

Total electronic energy = -3513.921230

Thermal corrections to Gibbs free energy = 0.929308

No. of imaginary frequency: 1 (159.90*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.88448500 | -0.20955000 | 2.03436200 |
| P | -1.29288600 | -0.92293700 | -1.69253400 |
| C | -2.61404300 | -0.75224900 | 2.30041300 |
| C | -0.05171100 | -0.57712200 | 3.62416800 |

| | | | |
|---|---|---|---|
| C | -0.99874300 | 1.62253300 | 2.06400100 |
| C | -3.00020300 | -1.55614100 | -1.46101500 |
| C | -1.48436500 | 0.79431500 | -2.32071500 |
| C | -0.69298200 | -1.85771800 | -3.14968400 |
| C | -3.61424200 | 0.10242900 | 2.78060600 |
| C | -2.93619300 | -2.08309200 | 2.00053100 |
| C | 1.34958900 | -0.65312700 | 3.61132800 |
| C | -0.74417900 | -0.76663000 | 4.82784200 |
| C | -1.45486600 | 2.25776100 | 0.90338900 |
| C | -0.51674700 | 2.42991400 | 3.10003100 |
| C | -3.20553300 | -2.94609800 | -1.44255000 |
| C | -4.08377400 | -0.70949200 | -1.19460500 |
| C | -1.23547500 | 1.16426800 | -3.64725300 |
| C | -1.69593600 | 1.82169400 | -1.39359400 |
| C | 0.68110700 | -2.13022300 | -3.23448000 |
| C | -1.54787800 | -2.30232700 | -4.17018300 |
| H | -3.37440800 | 1.13688200 | 3.00612900 |
| C | -4.91446900 | -0.37059500 | 2.96411200 |
| C | -4.22997600 | -2.55789200 | 2.19837800 |
| H | -2.17153200 | -2.74004600 | 1.59672900 |
| C | 2.04578500 | -0.90350800 | 4.79330600 |
| H | 1.89744600 | -0.54310100 | 2.68053400 |
| C | -0.04239000 | -1.02519600 | 6.00586800 |
| H | -1.82847900 | -0.71463600 | 4.84162700 |
| O | -1.94606600 | 1.43593500 | -0.08932000 |
| C | -1.40778600 | 3.63736000 | 0.70719000 |
| H | -0.15294500 | 1.97052200 | 4.01264500 |
| C | -0.47021300 | 3.81589100 | 2.94267500 |
| H | -2.37505700 | -3.61585700 | -1.64485800 |
| C | -4.47061800 | -3.47254800 | -1.19158600 |
| H | -3.94405500 | 0.36497200 | -1.19215800 |
| C | -5.34587300 | -1.24018100 | -0.92823500 |
| H | -1.04435000 | 0.39706900 | -4.38895700 |
| C | -1.18665000 | 2.51114500 | -4.00422100 |
| C | -1.65223000 | 3.17943100 | -1.71527100 |
| H | 1.35318600 | -1.77939600 | -2.46347700 |
| C | 1.18614100 | -2.84166700 | -4.32358100 |
| H | -2.61235400 | -2.09807200 | -4.10987700 |
| C | -1.03777900 | -3.01405800 | -5.25531800 |
| H | -5.68549100 | 0.30088500 | 3.33223100 |
| C | -5.22255200 | -1.70108100 | 2.67828300 |
| H | -4.46985900 | -3.58689800 | 1.95105600 |
| C | 1.35287200 | -1.09088900 | 5.99109800 |
| H | 3.13032500 | -0.96664300 | 4.77068300 |

| | | | |
|---|---|---|---|
| H | -0.58523300 | -1.17504100 | 6.93519000 |
| C | -1.96103000 | 4.19291500 | -0.60781100 |
| C | -0.89754200 | 4.41055700 | 1.75443000 |
| H | -0.08401400 | 4.43676300 | 3.74568400 |
| H | -4.61564600 | -4.54963900 | -1.19678100 |
| C | -5.54628500 | -2.62028200 | -0.93286700 |
| H | -6.17437000 | -0.57004100 | -0.71735100 |
| C | -1.38360600 | 3.50782400 | -3.04672700 |
| H | -0.98012900 | 2.78799600 | -5.03381200 |
| H | 2.25171600 | -3.04640600 | -4.37615400 |
| C | 0.33051000 | -3.28718700 | -5.33202300 |
| H | -1.70746200 | -3.35489700 | -6.04027100 |
| H | -6.23576900 | -2.06749800 | 2.81773500 |
| H | 1.89644000 | -1.29467400 | 6.90966200 |
| C | -3.50433400 | 4.29408500 | -0.47122100 |
| C | -1.38900600 | 5.58055300 | -0.92469100 |
| H | -0.82132200 | 5.48580600 | 1.64278900 |
| H | -6.53184000 | -3.03008300 | -0.73050700 |
| H | -1.32028300 | 4.54848500 | -3.34307200 |
| H | 0.72611300 | -3.84499500 | -6.17657500 |
| H | -3.94234100 | 3.31864800 | -0.23740400 |
| H | -3.94466300 | 4.65367700 | -1.40787900 |
| H | -3.76860300 | 4.99036500 | 0.33263400 |
| H | -1.65253300 | 6.29278900 | -0.13694700 |
| H | -1.81813000 | 5.97029600 | -1.85265700 |
| H | -0.30092900 | 5.55195100 | -1.02422400 |
| Cu | 0.10245400 | -0.77683300 | 0.09697500 |
| O | 1.57150800 | -2.35038200 | 0.00879100 |
| C | 1.58281300 | -3.73234200 | 0.44113400 |
| C | 1.62141500 | -3.77576300 | 1.97024400 |
| H | 1.59920500 | -4.81172800 | 2.32803000 |
| H | 2.52667900 | -3.29105700 | 2.34379900 |
| H | 0.76038400 | -3.24459300 | 2.38696700 |
| C | 2.78411400 | -4.45790500 | -0.17156100 |
| H | 2.79058900 | -4.33393200 | -1.25804800 |
| H | 3.72500800 | -4.06366500 | 0.22326600 |
| H | 2.73822900 | -5.52698300 | 0.06417300 |
| C | 0.27475800 | -4.31639100 | -0.09376700 |
| H | -0.57504000 | -3.73967700 | 0.28705500 |
| H | 0.25658300 | -4.26730700 | -1.18705400 |
| H | 0.15700500 | -5.35949300 | 0.21898200 |
| C | 2.15225300 | 4.71115500 | -2.15610300 |
| C | 1.92862900 | 3.39006100 | -1.77513000 |
| C | 2.00419400 | 3.00948200 | -0.41812200 |

| | | | |
|---|---|---|---|
| C | 2.30346200 | 4.01323200 | 0.52610500 |
| C | 2.52648900 | 5.33192100 | 0.14200700 |
| C | 2.45578100 | 5.69075300 | -1.20678900 |
| H | 2.08359800 | 4.97834000 | -3.20781500 |
| H | 1.68159900 | 2.64663600 | -2.51855000 |
| H | 2.34383800 | 3.74318300 | 1.57787800 |
| H | 2.75523100 | 6.08194300 | 0.89511600 |
| H | 2.63129300 | 6.71864700 | -1.51254300 |
| C | 1.76212200 | 1.65239700 | 0.07133700 |
| H | 1.74879700 | 1.56158600 | 1.15483700 |
| C | 1.54521200 | 0.48181000 | -0.57541700 |
| F | 1.61688400 | 0.57630100 | -1.97767200 |
| C | 4.77374500 | -0.88196000 | -0.81677500 |
| C | 4.73054800 | -0.75946800 | 0.77786700 |
| B | 2.69980000 | -1.51104800 | -0.03131400 |
| O | 3.52558500 | -1.52536000 | -1.14302900 |
| O | 3.37939500 | -1.13417700 | 1.12323000 |
| C | 5.64547500 | -1.74838300 | 1.50842100 |
| H | 6.70379200 | -1.53828900 | 1.32243100 |
| H | 5.46324700 | -1.66626100 | 2.58493900 |
| H | 5.43772900 | -2.78038700 | 1.21368500 |
| C | 4.98708800 | 0.65181900 | 1.30818500 |
| H | 4.86444400 | 0.65270100 | 2.39676800 |
| H | 6.00775900 | 0.97855700 | 1.08122500 |
| H | 4.28455100 | 1.37099100 | 0.88677800 |
| C | 5.89117400 | -1.78408600 | -1.34661800 |
| H | 5.80121600 | -1.85749300 | -2.43487400 |
| H | 6.87914500 | -1.37215300 | -1.11386600 |
| H | 5.82635000 | -2.79441800 | -0.93659700 |
| C | 4.83160500 | 0.46029000 | -1.55400400 |
| H | 5.78836700 | 0.96406800 | -1.37925600 |
| H | 4.73298600 | 0.27116400 | -2.62715400 |
| H | 4.02305100 | 1.12633700 | -1.26017700 |

**S-ts3**

Total electronic energy = -3692.099349

Thermal corrections to Gibbs free energy = 0.981726

No. of imaginary frequency: 1 (72.25*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 0.17565500 | 0.77970600 | -1.92280400 |
| P | 0.02463400 | 1.19935700 | 1.85614600 |
| C | 0.61752100 | 2.55611300 | -1.98336300 |

| | | | |
|---|---|---|---|
| C | 1.00288200 | 0.09679300 | -3.41018000 |
| C | -1.59520800 | 0.75738500 | -2.39231900 |
| C | 0.50790900 | 2.96969200 | 1.74309300 |
| C | -1.80629300 | 1.20892100 | 2.07380100 |
| C | 0.64398400 | 0.73585900 | 3.51634800 |
| C | -0.18329400 | 3.52416600 | -2.59996100 |
| C | 1.83371200 | 2.93950200 | -1.40216500 |
| C | 1.23655400 | -1.28496900 | -3.45487800 |
| C | 1.42731000 | 0.90313100 | -4.47406600 |
| C | -2.51504300 | 1.11441900 | -1.40013200 |
| C | -2.09849600 | 0.23484200 | -3.58833700 |
| C | 1.79938400 | 3.34099100 | 2.15054800 |
| C | -0.33811300 | 3.94698300 | 1.20391400 |
| C | -2.43630200 | 0.89959600 | 3.28477300 |
| C | -2.61857000 | 1.33275900 | 0.94019900 |
| C | 1.15093600 | -0.55586900 | 3.70693700 |
| C | 0.60461400 | 1.63024100 | 4.59943600 |
| H | -1.13039000 | 3.23562500 | -3.04529000 |
| C | 0.23575500 | 4.85525500 | -2.64621400 |
| C | 2.25691800 | 4.26380700 | -1.46116500 |
| H | 2.43730800 | 2.18722500 | -0.90885400 |
| C | 1.88128100 | -1.84916000 | -4.55486100 |
| H | 0.95542300 | -1.91521200 | -2.61830100 |
| C | 2.07987500 | 0.33495300 | -5.56946100 |
| H | 1.25834200 | 1.97466900 | -4.44239800 |
| O | -1.97973000 | 1.64553500 | -0.24526800 |
| C | -3.89119900 | 0.92961900 | -1.51621600 |
| H | -1.41204300 | -0.05612600 | -4.37611000 |
| C | -3.47357900 | 0.05348300 | -3.74636700 |
| H | 2.46331000 | 2.59685300 | 2.57754200 |
| C | 2.22555300 | 4.66317000 | 2.04166000 |
| H | -1.33120300 | 3.67945300 | 0.86573400 |
| C | 0.09347600 | 5.26821000 | 1.09091800 |
| H | -1.84053000 | 0.76797500 | 4.18011000 |
| C | -3.81695600 | 0.71383000 | 3.33361200 |
| C | -4.00277200 | 1.14970200 | 0.95151300 |
| H | 1.18577600 | -1.26439800 | 2.88893100 |
| C | 1.61209500 | -0.94382300 | 4.96687400 |
| H | 0.21816700 | 2.63470300 | 4.45669600 |
| C | 1.06610500 | 1.23712800 | 5.85362800 |
| H | -0.39236900 | 5.60175000 | -3.12496000 |
| C | 1.45795200 | 5.22505900 | -2.08433300 |
| H | 3.19593300 | 4.55124300 | -0.99844600 |
| C | 2.30783900 | -1.04186000 | -5.61202400 |

| | | | |
|---|---|---|---|
| H | 2.06571800 | -2.91990300 | -4.57455800 |
| H | 2.41083700 | 0.96879700 | -6.38779600 |
| C | -4.77780500 | 1.37679200 | -0.35149500 |
| C | -4.35677400 | 0.38349000 | -2.71675100 |
| H | -3.85985300 | -0.36160000 | -4.67265600 |
| H | 3.22388200 | 4.93503200 | 2.37407400 |
| C | 1.37151500 | 5.63290500 | 1.51372300 |
| H | -0.57294500 | 6.01301200 | 0.66583900 |
| C | -4.59022700 | 0.82765000 | 2.17770400 |
| H | -4.29270700 | 0.46221100 | 4.27682000 |
| H | 2.00574000 | -1.94733000 | 5.10172900 |
| C | 1.57251200 | -0.05300400 | 6.03870000 |
| H | 1.03163100 | 1.93544200 | 6.68545100 |
| H | 1.78182200 | 6.26150600 | -2.11926100 |
| H | 2.81997900 | -1.48239000 | -6.46330800 |
| C | -5.02532200 | 2.90222800 | -0.49871900 |
| C | -6.12489000 | 0.64175300 | -0.34974500 |
| H | -5.41685700 | 0.20229600 | -2.85046600 |
| H | 1.70234800 | 6.66403100 | 1.42653200 |
| H | -5.65872600 | 0.65572200 | 2.23489400 |
| H | 1.93513600 | -0.35827200 | 7.01664800 |
| H | -4.07966400 | 3.45344700 | -0.51069500 |
| H | -5.62782800 | 3.27112700 | 0.33880000 |
| H | -5.55608100 | 3.11173200 | -1.43428500 |
| H | -6.67266800 | 0.84326100 | -1.27517900 |
| H | -6.75686600 | 0.99881400 | 0.46881800 |
| H | -5.99247200 | -0.43814900 | -0.24693100 |
| Cu | 0.41601100 | -0.27271900 | 0.13623800 |
| C | -5.31982500 | -2.85164500 | 1.18097100 |
| C | -3.99137500 | -2.44854200 | 1.06664100 |
| C | -3.35865400 | -2.40246500 | -0.19338700 |
| C | -4.12064900 | -2.76983000 | -1.32092900 |
| C | -5.44718200 | -3.17473000 | -1.20311700 |
| C | -6.05748300 | -3.22071000 | 0.05293200 |
| H | -5.78513300 | -2.87257900 | 2.16345800 |
| H | -3.44004200 | -2.14943800 | 1.94619900 |
| H | -3.65699000 | -2.71857900 | -2.30219600 |
| H | -6.00719800 | -3.45235700 | -2.09268200 |
| H | -7.09301300 | -3.53521200 | 0.15044600 |
| C | -1.98404800 | -1.94879700 | -0.40748400 |
| H | -1.69654800 | -1.84765600 | -1.45033100 |
| C | -1.01503400 | -1.60858100 | 0.46785300 |
| F | -1.31686300 | -1.79436100 | 1.81268100 |
| C | 1.62502700 | -4.26638100 | 1.21235100 |

| | | | |
|---|---|---|---|
| C | 1.25913400 | -4.42899500 | -0.31292500 |
| B | 1.26293300 | -2.18906400 | 0.27120900 |
| O | 1.30092100 | -2.88910800 | 1.48087900 |
| O | 1.38224200 | -3.07404300 | -0.81052500 |
| C | 2.22461100 | -5.30173900 | -1.11145500 |
| H | 2.23356100 | -6.32839800 | -0.72818100 |
| H | 1.90573700 | -5.33360300 | -2.15855400 |
| H | 3.24244800 | -4.90670900 | -1.08031700 |
| C | -0.17857000 | -4.89951600 | -0.55150600 |
| H | -0.40898800 | -4.80159300 | -1.61737800 |
| H | -0.30232300 | -5.95015200 | -0.26801700 |
| H | -0.89870100 | -4.29425300 | -0.00115600 |
| C | 3.12310600 | -4.42962500 | 1.49920800 |
| H | 3.31541700 | -4.12738000 | 2.53297000 |
| H | 3.45446000 | -5.46540500 | 1.36958900 |
| H | 3.71945600 | -3.78109700 | 0.85219000 |
| C | 0.80977400 | -5.14277200 | 2.15899000 |
| H | 0.97078300 | -6.20658900 | 1.94964600 |
| H | 1.11827600 | -4.94772900 | 3.19121400 |
| H | -0.25608700 | -4.92144700 | 2.07857700 |
| C | 4.48832500 | -0.32638100 | -0.96181700 |
| C | 4.69226600 | -0.24926600 | 0.59148300 |
| C | 5.90889200 | -1.00091400 | 1.11861800 |
| H | 6.83329600 | -0.57992200 | 0.70686900 |
| H | 5.95008800 | -0.91595200 | 2.20896200 |
| H | 5.86365400 | -2.06176200 | 0.86397000 |
| C | 4.67176800 | 1.18073700 | 1.13737900 |
| H | 3.80132900 | 1.73216500 | 0.77293200 |
| H | 4.60904100 | 1.13919600 | 2.22920200 |
| H | 5.57727600 | 1.73132100 | 0.86140600 |
| C | 5.01917400 | 0.85963200 | -1.75781400 |
| H | 6.11226400 | 0.90814800 | -1.69571600 |
| H | 4.73723800 | 0.74297300 | -2.80882600 |
| H | 4.60923500 | 1.80763900 | -1.40581900 |
| C | 4.98114600 | -1.63844900 | -1.58226900 |
| H | 4.60899500 | -1.69691000 | -2.60924000 |
| H | 6.07440100 | -1.69659300 | -1.59700700 |
| H | 4.58756500 | -2.50178900 | -1.03777600 |
| B | 2.53624200 | -0.88096300 | 0.10356100 |
| O | 3.04093800 | -0.35334100 | -1.07099300 |
| O | 3.49539700 | -0.90719600 | 1.09307200 |

**TS1**

Total electronic energy = -3380.605555

Thermal corrections to Gibbs free energy =0.811890

No. of imaginary frequency: 1 (174.88*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.95825800 | -0.05611100 | -2.87976600 |
| C | -1.82659100 | 0.95887300 | -2.32140000 |
| B | 0.78066200 | -0.88921000 | -2.13659300 |
| O | 0.81054800 | -2.26441900 | -2.09113200 |
| O | 1.99902400 | -0.35688200 | -2.49716800 |
| C | 2.07879500 | -2.70513000 | -2.66164500 |
| C | 2.98062500 | -1.43576000 | -2.47029800 |
| C | 1.79940200 | -3.03293700 | -4.13050600 |
| C | 2.53731000 | -3.94452000 | -1.90361300 |
| C | 3.99439600 | -1.18742700 | -3.57962800 |
| C | 3.65836200 | -1.38217000 | -1.10000400 |
| H | 2.69055500 | -3.42435000 | -4.63248700 |
| H | 1.44941100 | -2.14689600 | -4.66804900 |
| H | 1.01175700 | -3.79055400 | -4.18087300 |
| H | 3.53031900 | -4.26109200 | -2.24297500 |
| H | 1.83804100 | -4.76639200 | -2.08833500 |
| H | 2.57051200 | -3.76712800 | -0.82678300 |
| H | 4.70952000 | -2.01569400 | -3.64382700 |
| H | 4.55296900 | -0.27093500 | -3.36474600 |
| H | 3.50613000 | -1.06853700 | -4.54892100 |
| H | 4.47153900 | -2.11231700 | -1.02487600 |
| H | 2.94093900 | -1.58122200 | -0.30171300 |
| H | 4.07098600 | -0.38242900 | -0.94235300 |
| Cu | -0.44359100 | 0.23070800 | -0.89670600 |
| P | -1.12185300 | -1.25399800 | 0.68511400 |
| P | 0.73827800 | 1.96732500 | -0.09104600 |
| C | -1.95667100 | -0.42494700 | 2.08568600 |
| C | -2.28421800 | -2.59561800 | 0.22209600 |
| C | 0.25522500 | -2.18742400 | 1.46986800 |
| C | -0.26010700 | 2.84495300 | 1.17232400 |
| C | 2.35518900 | 1.64956500 | 0.71905200 |
| C | 1.13877600 | 3.29401300 | -1.28825400 |
| C | -1.68573300 | -0.71952400 | 3.42729600 |
| C | -2.93195800 | 0.53208700 | 1.76779700 |
| C | -2.00131200 | -3.36370100 | -0.91931000 |
| C | -3.45757400 | -2.84135700 | 0.94493300 |
| C | 1.34522400 | -1.46518700 | 1.96453300 |
| C | 0.33175000 | -3.58415500 | 1.52712300 |
| C | -1.44786900 | 3.45047300 | 0.73378000 |

| | | | |
|---|---|---|---|
| C | 0.06331400 | 2.87876700 | 2.53202200 |
| C | 3.54327700 | 2.31993100 | 0.40015500 |
| C | 2.44421800 | 0.56309500 | 1.59292300 |
| C | 1.35107800 | 2.94706100 | -2.63012900 |
| C | 1.25194700 | 4.63648900 | -0.89545700 |
| H | -0.93495800 | -1.46197100 | 3.67894400 |
| C | -2.38267300 | -0.06241600 | 4.44173600 |
| C | -3.64009100 | 1.16792300 | 2.78444900 |
| H | -3.14100800 | 0.77607400 | 0.73232400 |
| C | -2.88668400 | -4.36078900 | -1.32501500 |
| H | -1.10150800 | -3.16798400 | -1.49184200 |
| C | -4.34352300 | -3.83588900 | 0.52840900 |
| H | -3.68980900 | -2.24585000 | 1.82045600 |
| O | 1.26156000 | -0.08861600 | 1.88659500 |
| C | 2.49408000 | -2.05474300 | 2.49784700 |
| H | -0.49166300 | -4.17936300 | 1.15021600 |
| C | 1.47204500 | -4.20788000 | 2.03466700 |
| H | -1.71828000 | 3.39934300 | -0.31480700 |
| C | -2.28236700 | 4.10194700 | 1.63608300 |
| H | 0.97482100 | 2.41103100 | 2.88738600 |
| C | -0.78591700 | 3.51646000 | 3.43837100 |
| H | 3.51534700 | 3.16250900 | -0.28144900 |
| C | 4.75857000 | 1.88565300 | 0.92969500 |
| C | 3.64383200 | 0.09218700 | 2.12977500 |
| H | 1.26410000 | 1.91434400 | -2.94447200 |
| C | 1.67180900 | 3.93385800 | -3.56376500 |
| H | 1.08009300 | 4.91118800 | 0.14054200 |
| C | 1.57373700 | 5.61768300 | -1.83190400 |
| H | -2.16330200 | -0.29038000 | 5.48144200 |
| C | -3.36414300 | 0.87719600 | 4.12168600 |
| H | -4.39595700 | 1.90137100 | 2.52297300 |
| C | -4.06225000 | -4.59565100 | -0.60737300 |
| H | -2.66468100 | -4.94484100 | -2.21388900 |
| H | -5.25638100 | -4.01148000 | 1.09090300 |
| C | 3.56967400 | -1.12039100 | 3.06142600 |
| C | 2.54459700 | -3.45194200 | 2.51329700 |
| H | 1.52466800 | -5.29218700 | 2.06083300 |
| H | -3.19895000 | 4.56495500 | 1.28173600 |
| C | -1.95341500 | 4.13516800 | 2.99336700 |
| H | -0.53095500 | 3.52893900 | 4.49428900 |
| C | 4.81048000 | 0.77750300 | 1.77918500 |
| H | 5.67507900 | 2.40795600 | 0.67182800 |
| H | 1.82604900 | 3.65706100 | -4.60276600 |
| C | 1.78324100 | 5.26734400 | -3.16825000 |

| | | | |
|---|---|---|---|
| H | 1.65729700 | 6.65510100 | -1.51993900 |
| H | -3.90893400 | 1.38484500 | 4.91305700 |
| H | -4.75661900 | -5.36453900 | -0.93470400 |
| C | 3.10162800 | -0.63514500 | 4.45987400 |
| C | 4.92605300 | -1.82106900 | 3.20052700 |
| H | 3.41979800 | -3.95839200 | 2.90493300 |
| H | -2.61104000 | 4.63067600 | 3.70197700 |
| H | 5.76906700 | 0.44740000 | 2.16382800 |
| H | 2.02738700 | 6.03379300 | -3.89866400 |
| H | 2.13065800 | -0.13531100 | 4.39605100 |
| H | 3.82722300 | 0.07159600 | 4.87741800 |
| H | 3.00579700 | -1.48643600 | 5.14280900 |
| H | 4.85161100 | -2.67326800 | 3.88227100 |
| H | 5.66976400 | -1.14051800 | 3.62526000 |
| H | 5.29448600 | -2.17942200 | 2.23372600 |
| F | -1.55440400 | -1.24250200 | -3.23071900 |
| F | -0.24752500 | 0.37897200 | -3.99836500 |
| H | -1.50721100 | 1.96431100 | -2.58177100 |
| C | -3.20835200 | 0.83002100 | -1.87275500 |
| C | -3.90681600 | -0.38775000 | -1.69775800 |
| C | -3.90345300 | 2.01138000 | -1.51438500 |
| C | -5.17944500 | -0.41617300 | -1.13504500 |
| H | -3.43774700 | -1.31848200 | -1.98054200 |
| C | -5.17753300 | 1.97684900 | -0.95627300 |
| H | -3.41717700 | 2.97079500 | -1.67536300 |
| C | -5.82786000 | 0.75814300 | -0.74305900 |
| H | -5.66464100 | -1.37881400 | -0.99613600 |
| H | -5.66655100 | 2.91101100 | -0.68803200 |
| H | -6.81870300 | 0.72629600 | -0.29942400 |

**TS1-1** R1= -(CH=CH2), R2= -H

Total electronic energy = -3073.240311

Thermal corrections to Gibbs free energy = 0.721111

No. of imaginary frequency: 1 (160.80*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.18362300 | 2.54011200 | 1.56353700 |
| C | -2.33111900 | 1.65611700 | 1.60802100 |
| B | 0.69747100 | 2.29635500 | 0.70063500 |
| O | 0.99254100 | 2.94637700 | -0.48000400 |
| O | 1.75600400 | 2.29908100 | 1.57761000 |
| C | 2.28424000 | 3.60320700 | -0.31380800 |
| C | 2.92876900 | 2.76960100 | 0.85009800 |

| | | | |
|---|---|---|---|
| C | 1.98699100 | 5.05440700 | 0.07179500 |
| C | 3.02915700 | 3.53673700 | -1.64134000 |
| C | 3.80119700 | 3.56827300 | 1.80991000 |
| C | 3.67022300 | 1.52376600 | 0.35953800 |
| H | 2.90597100 | 5.64236900 | 0.16772000 |
| H | 1.43376800 | 5.10400700 | 1.01379600 |
| H | 1.36533900 | 5.50650100 | -0.70671000 |
| H | 4.04156200 | 3.94421200 | -1.53863100 |
| H | 2.49859100 | 4.13430200 | -2.38985900 |
| H | 3.09630700 | 2.51260100 | -2.01362300 |
| H | 4.65685500 | 4.00606500 | 1.28281600 |
| H | 4.18565400 | 2.90612200 | 2.59214400 |
| H | 3.23665800 | 4.36965800 | 2.29054700 |
| H | 4.61495200 | 1.78358700 | -0.13028600 |
| H | 3.05925800 | 0.95857800 | -0.34667500 |
| H | 3.88544900 | 0.87544800 | 1.21333800 |
| Cu | -0.68309500 | 0.77598700 | 0.62796000 |
| P | -0.73756300 | 0.32969200 | -1.57307500 |
| P | 0.02724500 | -0.86377800 | 1.99254300 |
| C | -1.87876900 | -1.02466900 | -2.03056000 |
| C | 0.87831500 | -0.12268900 | -2.32772800 |
| C | -1.00409500 | -2.36621900 | 1.83063900 |
| C | 1.73871200 | -1.48600500 | 1.80700000 |
| C | -1.42918700 | -2.27118600 | -2.48213300 |
| C | -3.24933600 | -0.83242600 | -1.78791800 |
| C | 1.73395500 | -1.00697000 | -1.66252600 |
| C | 1.35141700 | 0.46304300 | -3.50959200 |
| C | -2.28326300 | -2.22420700 | 1.27469400 |
| C | -0.55485000 | -3.63589800 | 2.21854200 |
| C | 2.66123100 | -1.62185800 | 2.85102100 |
| C | 2.18938900 | -1.73611900 | 0.50835700 |
| H | -0.37278800 | -2.43475200 | -2.66686500 |
| C | -2.33679400 | -3.31050800 | -2.69079400 |
| C | -4.15261000 | -1.86770800 | -2.01562100 |
| H | -3.61006300 | 0.11913100 | -1.41843700 |
| O | 1.25966100 | -1.58818200 | -0.50431600 |
| C | 3.03069800 | -1.30403700 | -2.09554600 |
| H | 0.71032500 | 1.14631500 | -4.05495900 |
| C | 2.64078700 | 0.19414100 | -3.96662800 |
| H | -2.62459600 | -1.24359600 | 0.96000400 |
| C | -3.10310900 | -3.33953400 | 1.10961500 |
| H | 0.43929900 | -3.75121600 | 2.64063900 |
| C | -1.37663000 | -4.75000400 | 2.04972300 |
| H | 2.34090000 | -1.44355000 | 3.87234700 |

| | | | |
|---|---|---|---|
| C | 3.98654000 | -1.96286900 | 2.57577900 |
| C | 3.50586000 | -2.07400200 | 0.19563000 |
| H | -1.97704800 | -4.27618900 | -3.03509400 |
| C | -3.69905100 | -3.11114900 | -2.46301100 |
| H | -5.20838100 | -1.69547600 | -1.82771900 |
| C | 3.83678000 | -2.31969200 | -1.27866600 |
| C | 3.47596700 | -0.67503200 | -3.26111600 |
| H | 2.99977200 | 0.66576700 | -4.87646300 |
| H | -4.08355800 | -3.21877100 | 0.66104600 |
| C | -2.65040900 | -4.60240400 | 1.49457500 |
| H | -1.02216600 | -5.73317900 | 2.34723700 |
| C | 4.40629500 | -2.17942600 | 1.26097800 |
| H | 4.69929400 | -2.05841100 | 3.38951300 |
| H | -4.40294300 | -3.92195000 | -2.62966200 |
| C | 3.34931700 | -3.74400900 | -1.65757700 |
| C | 5.34142800 | -2.21419800 | -1.55397800 |
| H | 4.47797100 | -0.86473600 | -3.62939200 |
| H | -3.28586800 | -5.47310200 | 1.35730300 |
| H | 5.44342400 | -2.43202600 | 1.07029500 |
| H | 2.27791600 | -3.85500800 | -1.46758300 |
| H | 3.88268100 | -4.49561000 | -1.06528700 |
| H | 3.53403600 | -3.93674500 | -2.72014500 |
| H | 5.55702700 | -2.41587600 | -2.60725000 |
| H | 5.89202100 | -2.95845200 | -0.97137600 |
| H | 5.72746100 | -1.22083300 | -1.30287000 |
| F | -1.35683300 | 3.75795600 | 0.93552200 |
| F | -0.66887300 | 2.79735900 | 2.81801100 |
| H | -2.43882400 | 1.15663500 | 2.56636400 |
| C | -3.52234600 | 1.69421500 | 0.77374000 |
| C | -3.70120300 | 2.52599800 | -0.35656100 |
| C | -4.58151100 | 0.80336600 | 1.08023800 |
| C | -4.84980900 | 2.44198400 | -1.13861900 |
| H | -2.92344100 | 3.22687300 | -0.62849900 |
| C | -5.72843600 | 0.72901400 | 0.29770100 |
| H | -4.48013700 | 0.15596700 | 1.94849200 |
| C | -5.87510200 | 1.54256300 | -0.83084500 |
| H | -4.94187600 | 3.08980700 | -2.00748100 |
| H | -6.51467500 | 0.02840700 | 0.57030500 |
| H | -6.76835500 | 1.48546700 | -1.44589600 |
| C | -0.05133600 | -0.40283200 | 3.74832200 |
| H | 0.49679000 | 0.50790300 | 3.98568500 |
| C | -0.81421500 | -0.99889500 | 4.66841800 |
| H | -1.39559100 | -1.88886200 | 4.44291000 |
| H | -0.88983600 | -0.60617900 | 5.67965800 |

| | | | |
|---|---|---|---|
| C | -1.22084900 | 1.76280200 | -2.58502400 |
| H | -0.68198600 | 2.66472700 | -2.30052600 |
| C | -2.17024300 | 1.78909200 | -3.52164700 |
| H | -2.43244900 | 2.71523500 | -4.02796900 |
| H | -2.73803600 | 0.90532600 | -3.79686100 |

**TS1-2** R1= -Ph, R2= -OMe

Total electronic energy = -3495.147721

Thermal corrections to Gibbs free energy = 0.842372

No. of imaginary frequency: 1 (195.50*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.67734100 | -0.02470400 | -2.89247800 |
| C | -1.50679900 | 1.02370900 | -2.32955600 |
| B | 0.86111700 | -1.09529800 | -2.08418900 |
| O | 0.68197900 | -2.44507900 | -1.87496700 |
| O | 2.13687900 | -0.81001600 | -2.51877300 |
| C | 1.85012700 | -3.14520900 | -2.39446400 |
| C | 2.94193100 | -2.01823400 | -2.37144500 |
| C | 1.48506200 | -3.60798900 | -3.80714300 |
| C | 2.13174700 | -4.33720900 | -1.48803700 |
| C | 3.94588400 | -2.06460700 | -3.51594200 |
| C | 3.66242500 | -1.90853400 | -1.02713800 |
| H | 2.29251900 | -4.19244300 | -4.26076900 |
| H | 1.25926800 | -2.75465200 | -4.45297600 |
| H | 0.59053800 | -4.23562900 | -3.75388800 |
| H | 3.05162600 | -4.84871700 | -1.79411000 |
| H | 1.30593000 | -5.05241600 | -1.55805200 |
| H | 2.22512400 | -4.03460500 | -0.44321000 |
| H | 4.52135300 | -2.99707900 | -3.48882200 |
| H | 4.64720200 | -1.22947400 | -3.42096300 |
| H | 3.45132000 | -1.98471100 | -4.48604800 |
| H | 4.35780900 | -2.74114800 | -0.87510900 |
| H | 2.94858700 | -1.89991900 | -0.20165800 |
| H | 4.22577800 | -0.97258700 | -0.99584700 |
| Cu | -0.19837100 | 0.23882300 | -0.87953300 |
| P | -1.02085800 | -1.03080900 | 0.81281900 |
| P | 1.22511600 | 1.86549900 | -0.25528400 |
| C | -1.83310700 | 0.01838400 | 2.07865700 |
| C | -2.30324000 | -2.30357400 | 0.46980000 |
| C | 0.24867500 | -2.01084600 | 1.71926000 |
| C | 0.46187100 | 2.92618900 | 1.02652400 |
| C | 2.83226100 | 1.39361000 | 0.49259100 |

| | | | |
|---|---|---|---|
| C | 1.71429800 | 3.03709400 | -1.57520400 |
| C | -1.27797000 | 0.30256400 | 3.33043900 |
| C | -3.05914500 | 0.60234400 | 1.72041100 |
| C | -2.22317500 | -3.03813900 | -0.72217700 |
| C | -3.35364100 | -2.55894000 | 1.36239500 |
| C | 1.44807500 | -1.39848300 | 2.09807000 |
| C | 0.13651400 | -3.39015100 | 1.93906800 |
| C | -0.92411300 | 3.12528600 | 0.96339400 |
| C | 1.20459900 | 3.55119500 | 2.03630400 |
| C | 4.08450100 | 1.85976900 | 0.07575800 |
| C | 2.80635300 | 0.40155500 | 1.47613500 |
| C | 2.20520800 | 2.50629800 | -2.77983400 |
| C | 1.59022300 | 4.42540700 | -1.43182100 |
| H | -0.33056300 | -0.13611100 | 3.62163700 |
| C | -1.94557000 | 1.15209200 | 4.21466800 |
| C | -3.73323900 | 1.42873600 | 2.61429600 |
| H | -3.49363800 | 0.39916600 | 0.75006700 |
| C | -3.19197400 | -3.99592100 | -1.02160000 |
| H | -1.41280500 | -2.85186000 | -1.41635900 |
| C | -4.32501400 | -3.51155800 | 1.05475200 |
| H | -3.42459800 | -2.00214300 | 2.28979500 |
| O | 1.55617400 | -0.04150500 | 1.86504300 |
| C | 2.52587400 | -2.08307100 | 2.66839100 |
| H | -0.77308300 | -3.90344900 | 1.65060500 |
| C | 1.19714500 | -4.10726800 | 2.49154000 |
| H | -1.50539000 | 2.61545800 | 0.20245400 |
| C | -1.55466600 | 3.95518500 | 1.88773200 |
| H | 2.27808400 | 3.39794300 | 2.09146500 |
| C | 0.56695100 | 4.36802800 | 2.97045900 |
| H | 4.14132200 | 2.62690900 | -0.68868200 |
| C | 5.25029100 | 1.31598100 | 0.61779200 |
| C | 3.94981000 | -0.17491000 | 2.02894900 |
| H | 2.29344200 | 1.43204900 | -2.90100700 |
| C | 2.57358300 | 3.36063000 | -3.81782700 |
| H | 1.20894600 | 4.84204500 | -0.50560600 |
| C | 1.95181800 | 5.27389800 | -2.47932500 |
| H | -1.50305100 | 1.37276400 | 5.18207100 |
| C | -3.17604000 | 1.70860100 | 3.86456000 |
| H | -4.68790200 | 1.85566000 | 2.32006000 |
| C | -4.25002300 | -4.22853800 | -0.14091800 |
| H | -3.12629200 | -4.54962200 | -1.95409000 |
| H | -5.13954300 | -3.69278000 | 1.75084500 |
| C | 3.74811000 | -1.25957400 | 3.08986400 |
| C | 2.38251700 | -3.46150300 | 2.84969600 |

| | | | |
|---|---|---|---|
| H | 1.10045800 | -5.17800700 | 2.64423500 |
| H | -2.62925800 | 4.09365600 | 1.83388100 |
| C | -0.81178900 | 4.57462600 | 2.89402700 |
| H | 1.14754300 | 4.84512100 | 3.75546300 |
| C | 5.18449800 | 0.30296400 | 1.57768600 |
| H | 6.21858600 | 1.67843100 | 0.28548200 |
| H | 2.94883500 | 2.94235800 | -4.74760600 |
| C | 2.44513400 | 4.74391700 | -3.67225100 |
| H | 1.84726900 | 6.34895900 | -2.36133800 |
| H | -3.69459400 | 2.36269800 | 4.56018400 |
| H | -5.01040200 | -4.96600200 | -0.38315000 |
| C | 3.42225100 | -0.56618400 | 4.43997000 |
| C | 4.99705400 | -2.13216500 | 3.26225800 |
| H | 3.19464600 | -4.03912000 | 3.27687300 |
| H | -1.30713100 | 5.21050900 | 3.62264200 |
| H | 6.10404200 | -0.11560800 | 1.97146700 |
| H | 2.72343200 | 5.40573600 | -4.48780000 |
| H | 2.53985900 | 0.07386200 | 4.34841800 |
| H | 4.26577400 | 0.05646400 | 4.75792800 |
| H | 3.22636800 | -1.31652300 | 5.21382800 |
| H | 4.83841000 | -2.88491600 | 4.03990100 |
| H | 5.84985100 | -1.52526100 | 3.57986600 |
| H | 5.26176600 | -2.64335600 | 2.33086700 |
| F | -1.33768100 | -1.14952000 | -3.35556200 |
| F | 0.11935200 | 0.42554000 | -3.93224200 |
| H | -1.15025500 | 2.01596300 | -2.59182700 |
| C | -2.90435300 | 0.93761200 | -1.91030100 |
| C | -3.66963100 | -0.24312000 | -1.84055200 |
| C | -3.55030700 | 2.12103600 | -1.47168000 |
| C | -4.95078200 | -0.26674600 | -1.28559900 |
| H | -3.25154300 | -1.17182300 | -2.19687700 |
| C | -4.82902500 | 2.11136600 | -0.93278600 |
| H | -3.01545500 | 3.06545100 | -1.54334500 |
| C | -5.53461100 | 0.90786900 | -0.80400700 |
| H | -5.46632700 | -1.21826400 | -1.22274800 |
| H | -5.29619200 | 3.02896900 | -0.58690800 |
| O | -6.76637100 | 0.98336700 | -0.19352200 |
| C | -7.43908800 | -0.23703900 | 0.03802800 |
| H | -6.83081300 | -0.92434000 | 0.64377000 |
| H | -8.35285900 | 0.01507800 | 0.58076500 |
| H | -7.70588100 | -0.74109400 | -0.90173500 |

**TS1-3** R1= -Ph, R2= -CN

Total electronic energy = -3472.879755

Thermal corrections to Gibbs free energy = 0.809168

No. of imaginary frequency: 1 (145.03*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.65360000 | -0.16157800 | -2.90463900 |
| C | -1.57441000 | 0.85105000 | -2.43024700 |
| B | 0.99177900 | -1.08244400 | -1.97652900 |
| O | 0.92431800 | -2.44493200 | -1.81114300 |
| O | 2.24221100 | -0.66728500 | -2.37063600 |
| C | 2.15586000 | -3.02334100 | -2.33765700 |
| C | 3.14684700 | -1.80869100 | -2.26025400 |
| C | 1.84598900 | -3.46391200 | -3.77030000 |
| C | 2.52823800 | -4.21779000 | -1.46837500 |
| C | 4.15862900 | -1.72409700 | -3.39569100 |
| C | 3.84659300 | -1.68720000 | -0.90662300 |
| H | 2.70507900 | -3.96036600 | -4.23341000 |
| H | 1.55429700 | -2.61008700 | -4.38863400 |
| H | 1.00831800 | -4.16726000 | -3.75092400 |
| H | 3.49411700 | -4.63502900 | -1.77529400 |
| H | 1.77020700 | -4.99979200 | -1.57788800 |
| H | 2.57901300 | -3.94485900 | -0.41228300 |
| H | 4.81311900 | -2.60319500 | -3.39766300 |
| H | 4.78358800 | -0.83539300 | -3.26222000 |
| H | 3.66569900 | -1.65079600 | -4.36711200 |
| H | 4.60764700 | -2.46438000 | -0.77790400 |
| H | 3.13052200 | -1.76600400 | -0.08648600 |
| H | 4.33071600 | -0.70983600 | -0.83997800 |
| Cu | -0.24975600 | 0.15034800 | -0.90321700 |
| P | -1.02596900 | -1.13559300 | 0.81196500 |
| P | 0.98321000 | 1.94080400 | -0.25346900 |
| C | -1.93503100 | -0.15208500 | 2.06370000 |
| C | -2.18398800 | -2.51067600 | 0.43725400 |
| C | 0.31369600 | -1.99878900 | 1.73363100 |
| C | 0.12340800 | 2.93906700 | 1.01450600 |
| C | 2.61684700 | 1.60428100 | 0.50532400 |
| C | 1.37501600 | 3.13559000 | -1.58390300 |
| C | -1.41171200 | 0.17758900 | 3.31828200 |
| C | -3.20248100 | 0.33063200 | 1.69863400 |
| C | -1.98459500 | -3.25197700 | -0.73735800 |
| C | -3.25401800 | -2.83719500 | 1.28157200 |
| C | 1.45306000 | -1.28422700 | 2.11734400 |
| C | 0.31269200 | -3.37982600 | 1.96843400 |
| C | -1.27471800 | 3.00894100 | 0.94959700 |

| | | | |
|---|---|---|---|
| C | 0.80517400 | 3.64437000 | 2.01459500 |
| C | 3.82866800 | 2.17801200 | 0.10486700 |
| C | 2.66156400 | 0.62033400 | 1.49596200 |
| C | 1.94160300 | 2.63868400 | -2.76998900 |
| C | 1.09636900 | 4.50415700 | -1.47155600 |
| H | -0.43446800 | -0.18408300 | 3.61619500 |
| C | -2.15038000 | 0.97140400 | 4.19741200 |
| C | -3.94727600 | 1.09894100 | 2.58852100 |
| H | -3.61549600 | 0.08877700 | 0.72778900 |
| C | -2.85704700 | -4.28857500 | -1.06708800 |
| H | -1.15675600 | -3.01243900 | -1.39355600 |
| C | -4.12986600 | -3.86843600 | 0.94170200 |
| H | -3.41790500 | -2.27570300 | 2.19412000 |
| O | 1.44845200 | 0.07397400 | 1.86740900 |
| C | 2.57689100 | -1.86883800 | 2.70902900 |
| H | -0.54829900 | -3.96962800 | 1.67681700 |
| C | 1.42314700 | -3.99928500 | 2.54092300 |
| H | -1.80862100 | 2.43864200 | 0.19716900 |
| C | -1.97993400 | 3.79085900 | 1.86178300 |
| H | 1.88812200 | 3.59126900 | 2.07133000 |
| C | 0.09432100 | 4.41236300 | 2.93701000 |
| H | 3.83026600 | 2.94175900 | -0.66507100 |
| C | 5.02815100 | 1.74519400 | 0.67280800 |
| C | 3.84146800 | 0.15195000 | 2.07348600 |
| H | 2.14968900 | 1.57848900 | -2.86688800 |
| C | 2.23184200 | 3.50802200 | -3.82007700 |
| H | 0.65625800 | 4.89429000 | -0.56006700 |
| C | 1.38050800 | 5.36669600 | -2.53150800 |
| H | -1.73292700 | 1.22702200 | 5.16725200 |
| C | -3.42045900 | 1.42482700 | 3.84067800 |
| H | -4.93576500 | 1.44128600 | 2.29578200 |
| C | -3.93692400 | -4.59294300 | -0.23563000 |
| H | -2.70004000 | -4.84853100 | -1.98479900 |
| H | -4.96511100 | -4.10075500 | 1.59610200 |
| C | 3.71944900 | -0.94104900 | 3.13831400 |
| C | 2.54601200 | -3.25251100 | 2.90485600 |
| H | 1.41420400 | -5.07234500 | 2.70644500 |
| H | -3.06255100 | 3.82981500 | 1.80684500 |
| C | -1.29761100 | 4.49034700 | 2.85832400 |
| H | 0.62783200 | 4.95215900 | 3.71460700 |
| C | 5.03566100 | 0.73727000 | 1.64049300 |
| H | 5.96595600 | 2.19091400 | 0.35493000 |
| H | 2.66741400 | 3.11613400 | -4.73486500 |
| C | 1.94937900 | 4.87133300 | -3.70544000 |

| | | | |
|---|---|---|---|
| H | 1.15680800 | 6.42573300 | -2.43779000 |
| H | -3.99612500 | 2.03202800 | 4.53355900 |
| H | -4.62452800 | -5.39034700 | -0.50321300 |
| C | 3.31911000 | -0.27084900 | 4.48013500 |
| C | 5.03630700 | -1.70285900 | 3.32989100 |
| H | 3.39760500 | -3.75582300 | 3.34879100 |
| H | -1.84983000 | 5.08864800 | 3.57760900 |
| H | 5.98182300 | 0.40645500 | 2.05411800 |
| H | 2.16724800 | 5.54385600 | -4.53041400 |
| H | 2.38654700 | 0.29126300 | 4.37445100 |
| H | 4.10248200 | 0.42307000 | 4.80420000 |
| H | 3.17835600 | -1.03105200 | 5.25623700 |
| H | 4.93342800 | -2.46271900 | 4.10987700 |
| H | 5.83034100 | -1.02409500 | 3.65418700 |
| H | 5.35479100 | -2.19373600 | 2.40444300 |
| F | -1.20924400 | -1.34893600 | -3.32422300 |
| F | 0.15410100 | 0.28709100 | -3.92991200 |
| H | -1.24431300 | 1.86159700 | -2.65116300 |
| C | -2.94116800 | 0.69539700 | -2.00059700 |
| C | -3.64138100 | -0.53811700 | -1.90841800 |
| C | -3.65712500 | 1.85908900 | -1.60035700 |
| C | -4.91559800 | -0.60969500 | -1.37510600 |
| H | -3.16269400 | -1.44761500 | -2.23693500 |
| C | -4.93279800 | 1.79230000 | -1.07400900 |
| H | -3.17120100 | 2.82656300 | -1.69801100 |
| C | -5.58282700 | 0.54907500 | -0.92667500 |
| H | -5.40253000 | -1.57554900 | -1.28322600 |
| H | -5.44088700 | 2.69928200 | -0.76015800 |
| C | -6.86498700 | 0.46838900 | -0.31226400 |
| N | -7.90499400 | 0.40701600 | 0.21170500 |

**TS2**

Total electronic energy = -3380.589864

Thermal corrections to Gibbs free energy = 0.813329

No. of imaginary frequency: 1 (186.11*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 1.58177000 | 0.87881200 | 0.70305900 |
| O | 2.27354100 | -0.13582000 | 1.33812600 |
| O | 1.49507000 | 2.00020200 | 1.50946400 |
| C | 2.78446500 | 0.35496700 | 2.60994900 |
| C | 1.88700500 | 1.62216200 | 2.85788600 |
| C | 4.26578900 | 0.67448000 | 2.40714900 |

| | | | |
|---|---|---|---|
| C | 2.61697300 | -0.75731500 | 3.64008300 |
| C | 2.60680300 | 2.80607800 | 3.49165800 |
| C | 0.59295300 | 1.30936800 | 3.61490600 |
| H | 4.73779600 | 0.99028500 | 3.34394700 |
| H | 4.40930300 | 1.45307600 | 1.65674300 |
| H | 4.77607000 | -0.22466500 | 2.04942100 |
| H | 2.92076900 | -0.41302000 | 4.63550800 |
| H | 3.25263500 | -1.60553100 | 3.36657400 |
| H | 1.58755900 | -1.11544000 | 3.68685600 |
| H | 2.98314700 | 2.54611900 | 4.48749600 |
| H | 1.91007100 | 3.64376300 | 3.59980500 |
| H | 3.44548800 | 3.13625500 | 2.87506700 |
| H | 0.78504600 | 1.09111500 | 4.67086800 |
| H | 0.07683800 | 0.45497900 | 3.17256600 |
| H | -0.07839400 | 2.17054600 | 3.55179600 |
| Cu | 0.41090100 | 0.34479100 | -0.86377100 |
| P | 0.24230300 | -1.87907200 | -0.62771500 |
| P | -1.52364900 | 1.49545800 | -0.54161200 |
| C | -1.14360900 | -2.57777300 | -1.60180700 |
| C | 1.68144200 | -2.90722600 | -1.12040600 |
| C | -0.11721200 | -2.47527600 | 1.07425600 |
| C | -2.79371400 | 0.96835400 | -1.75042100 |
| C | -2.34694600 | 1.38850500 | 1.10045500 |
| C | -1.42126800 | 3.31370000 | -0.78246600 |
| C | -1.94448600 | -3.62909700 | -1.13714400 |
| C | -1.38812900 | -2.03087900 | -2.86838400 |
| C | 2.92127300 | -2.66768500 | -0.50415500 |
| C | 1.58876600 | -3.89046800 | -2.11388400 |
| C | -1.17333400 | -1.86146000 | 1.75477800 |
| C | 0.62343000 | -3.43767100 | 1.76804300 |
| C | -2.47969700 | 1.10718500 | -3.11381500 |
| C | -4.01684600 | 0.40276000 | -1.37897700 |
| C | -2.82948900 | 2.49884400 | 1.80637600 |
| C | -2.36264500 | 0.15424200 | 1.75784400 |
| C | -0.41668000 | 4.01026000 | -0.08983300 |
| C | -2.29917500 | 4.02439400 | -1.61036800 |
| H | -1.75849800 | -4.05874900 | -0.15788200 |
| C | -2.98200200 | -4.12202100 | -1.92809600 |
| C | -2.41467600 | -2.53805500 | -3.66324800 |
| H | -0.77954900 | -1.20043300 | -3.21334600 |
| C | 4.04212800 | -3.41008600 | -0.87263200 |
| H | 2.99979000 | -1.89306300 | 0.25083900 |
| C | 2.71810400 | -4.62111700 | -2.48771200 |
| H | 0.63830700 | -4.08332000 | -2.59892600 |

| | | | |
|---|---|---|---|
| O | -1.90309900 | -0.93139400 | 1.04168300 |
| C | -1.50655300 | -2.13388900 | 3.08282800 |
| H | 1.44805900 | -3.93745800 | 1.27321200 |
| C | 0.32414700 | -3.73083300 | 3.09933500 |
| H | -1.51487700 | 1.51334200 | -3.40353700 |
| C | -3.40236500 | 0.72255200 | -4.08296400 |
| H | -4.26458200 | 0.28810000 | -0.32868800 |
| C | -4.92273000 | -0.01467500 | -2.35644000 |
| H | -2.83470900 | 3.47259600 | 1.33043600 |
| C | -3.26427400 | 2.36255800 | 3.12418900 |
| C | -2.77795000 | -0.01671600 | 3.08115800 |
| H | 0.25720900 | 3.47315900 | 0.56964100 |
| C | -0.29208000 | 5.39091300 | -0.23691500 |
| H | -3.08377300 | 3.50157000 | -2.14535900 |
| C | -2.16533600 | 5.40596100 | -1.75836000 |
| H | -3.60482000 | -4.93189400 | -1.55779700 |
| C | -3.21662500 | -3.57880000 | -3.19276400 |
| H | -2.60186000 | -2.10269000 | -4.63915400 |
| C | 3.94541600 | -4.38565000 | -1.86767000 |
| H | 4.99556700 | -3.21336900 | -0.38976100 |
| H | 2.63524600 | -5.37635800 | -3.26436000 |
| C | -2.73898100 | -1.43298100 | 3.66254600 |
| C | -0.72459100 | -3.08113700 | 3.75322100 |
| H | 0.91432200 | -4.46978200 | 3.63305500 |
| H | -3.15958800 | 0.84894600 | -5.13463100 |
| C | -4.62368600 | 0.15535000 | -3.70745900 |
| H | -5.86600200 | -0.46402100 | -2.05853200 |
| C | -3.22764600 | 1.11936100 | 3.75972500 |
| H | -3.62760400 | 3.23195700 | 3.66405400 |
| H | 0.49060800 | 5.91836400 | 0.30179400 |
| C | -1.16109200 | 6.09234900 | -1.07546100 |
| H | -2.84960100 | 5.94442700 | -2.40830700 |
| H | -4.02592500 | -3.96256700 | -3.80788300 |
| H | 4.82263400 | -4.95588700 | -2.16053300 |
| C | -3.99906800 | -2.19488600 | 3.17047700 |
| C | -2.72369400 | -1.42205100 | 5.19605300 |
| H | -0.93729300 | -3.32440000 | 4.78833400 |
| H | -5.33470100 | -0.15939500 | -4.46637800 |
| H | -3.55477200 | 1.04040100 | 4.79048300 |
| H | -1.05655600 | 7.16716300 | -1.19511800 |
| H | -4.03542000 | -2.22443000 | 2.07748800 |
| H | -4.90661200 | -1.69949200 | 3.53296800 |
| H | -3.98739000 | -3.22548100 | 3.54218500 |
| H | -2.71437400 | -2.44263300 | 5.58930800 |

| | | | |
|---|---|---|---|
| H | -3.62470300 | -0.94190300 | 5.58851100 |
| H | -1.84865200 | -0.89084500 | 5.58461100 |
| C | 4.22173200 | 2.56561400 | -0.70653000 |
| C | 3.47604000 | 1.46333200 | -1.15512500 |
| C | 4.15758800 | 0.27287600 | -1.45019000 |
| C | 5.53854700 | 0.18994200 | -1.29574500 |
| C | 6.27249600 | 1.29287600 | -0.85098000 |
| C | 5.60678300 | 2.48525700 | -0.56234600 |
| H | 3.70301500 | 3.48982800 | -0.46505900 |
| H | 3.60053900 | -0.58583100 | -1.79713900 |
| H | 6.04320000 | -0.74486800 | -1.52635400 |
| H | 7.35029600 | 1.22407400 | -0.73248500 |
| H | 6.16377900 | 3.35290800 | -0.21828500 |
| C | 2.00520200 | 1.61285500 | -1.29811100 |
| H | 1.67460200 | 2.62422900 | -1.07344600 |
| C | 1.25556500 | 1.08250500 | -2.47117800 |
| F | 0.69282100 | 2.11017200 | -3.23304500 |
| F | 2.01418800 | 0.33166100 | -3.34904300 |

**TS2-1** R1= -(CH=CH2), R2= -H

Total electronic energy = -3073.225819

Thermal corrections to Gibbs free energy = 0.721068

No. of imaginary frequency: 1 (168.77*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 1.85597400 | 0.43381800 | -0.52669700 |
| O | 2.27544900 | 1.15680600 | 0.57171900 |
| O | 2.10578200 | 1.10081900 | -1.71059100 |
| C | 2.96245600 | 2.35450200 | 0.11077400 |
| C | 2.46725000 | 2.47234500 | -1.38015400 |
| C | 4.46264700 | 2.09290900 | 0.24682400 |
| C | 2.54272000 | 3.50923100 | 1.01528100 |
| C | 3.52698200 | 2.93496400 | -2.37273100 |
| C | 1.19217100 | 3.30703500 | -1.52937200 |
| H | 5.04883700 | 2.98027800 | -0.01627100 |
| H | 4.78257700 | 1.25800100 | -0.37805500 |
| H | 4.68137200 | 1.82773800 | 1.28518400 |
| H | 2.97877600 | 4.45346000 | 0.66881900 |
| H | 2.90245900 | 3.32236300 | 2.03205600 |
| H | 1.45765900 | 3.61502700 | 1.06144500 |
| H | 3.87903400 | 3.94315000 | -2.12639100 |
| H | 3.09909100 | 2.96071100 | -3.38021000 |
| H | 4.38343300 | 2.25755300 | -2.38284300 |

| | | | |
|---|---|---|---|
| H | 1.38739700 | 4.37372800 | -1.37568900 |
| H | 0.42779900 | 2.98824000 | -0.81781400 |
| H | 0.78627000 | 3.16747400 | -2.53521500 |
| Cu | 0.56006800 | -1.07171000 | -0.18773000 |
| P | -0.09531500 | -0.57659100 | 1.89008100 |
| P | -0.91467400 | -0.75514500 | -1.86118100 |
| C | -1.54680400 | -1.53047100 | 2.46936100 |
| C | -0.58737500 | 1.16289100 | 2.21689000 |
| C | -2.32111300 | -1.92668000 | -1.86421800 |
| C | -1.67711300 | 0.90039600 | -2.08386300 |
| C | -2.31158200 | -1.13977000 | 3.57788400 |
| C | -1.91905700 | -2.66463600 | 1.73711400 |
| C | -1.43893200 | 1.78841000 | 1.30265900 |
| C | -0.10730600 | 1.93223500 | 3.28257400 |
| C | -2.03002400 | -3.29228200 | -1.70003600 |
| C | -3.65530400 | -1.50951100 | -1.92874500 |
| C | -1.81094700 | 1.52384900 | -3.33184700 |
| C | -2.02979300 | 1.64108500 | -0.95165900 |
| H | -2.03344200 | -0.25369600 | 4.14124300 |
| C | -3.43505900 | -1.87812000 | 3.94652200 |
| C | -3.04834600 | -3.39713300 | 2.10266400 |
| H | -1.32649200 | -2.95296200 | 0.87505100 |
| O | -1.91585000 | 1.00782700 | 0.26782300 |
| C | -1.80238600 | 3.13479600 | 1.37637600 |
| H | 0.54755000 | 1.47616900 | 4.01730500 |
| C | -0.44751000 | 3.28131900 | 3.38808200 |
| H | -0.99621100 | -3.61648800 | -1.62602300 |
| C | -3.06628400 | -4.22056800 | -1.61873000 |
| H | -3.88756500 | -0.45662800 | -2.05312700 |
| C | -4.68922100 | -2.44199500 | -1.82346300 |
| H | -1.55464700 | 0.97180700 | -4.22988100 |
| C | -2.23810000 | 2.84825500 | -3.41725400 |
| C | -2.44496800 | 2.97524000 | -0.99923900 |
| H | -4.02630300 | -1.57119200 | 4.80502900 |
| C | -3.80624300 | -3.00485700 | 3.20668700 |
| H | -3.34041200 | -4.26042300 | 1.51245300 |
| C | -2.78712100 | 3.66030700 | 0.32716800 |
| C | -1.27954400 | 3.87926000 | 2.43945100 |
| H | -0.05888700 | 3.87320600 | 4.21140300 |
| H | -2.83294300 | -5.27526300 | -1.50062800 |
| C | -4.39772500 | -3.79748500 | -1.67132300 |
| H | -5.72210600 | -2.10711700 | -1.86332600 |
| C | -2.53912500 | 3.57061000 | -2.26022900 |
| H | -2.32880000 | 3.32560100 | -4.38843400 |

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|---|---|---|---|
| H | -4.68958300 | -3.57109400 | 3.48944800 |
| C | -4.21738000 | 3.22590700 | 0.74615200 |
| C | -2.73998900 | 5.18880700 | 0.21131100 |
| H | -1.52671200 | 4.93050600 | 2.53760900 |
| H | -5.20336100 | -4.52225200 | -1.59247400 |
| H | -2.85099900 | 4.60541500 | -2.34772000 |
| H | -4.28457800 | 2.13827500 | 0.83973100 |
| H | -4.94669100 | 3.55407700 | -0.00278100 |
| H | -4.47971500 | 3.67115800 | 1.71216100 |
| H | -3.00344100 | 5.65592800 | 1.16458600 |
| H | -3.46766800 | 5.54341100 | -0.52436800 |
| H | -1.74587900 | 5.53901100 | -0.08527600 |
| C | 4.84279500 | -1.24304100 | -1.18208200 |
| C | 3.77532100 | -1.51927300 | -0.31252500 |
| C | 4.04757300 | -1.63611300 | 1.06003000 |
| C | 5.34572500 | -1.48371800 | 1.53960100 |
| C | 6.40152300 | -1.21217100 | 0.66518600 |
| C | 6.14386500 | -1.09654400 | -0.70123700 |
| H | 4.64306800 | -1.13963800 | -2.24556300 |
| H | 3.23728100 | -1.84935800 | 1.74446300 |
| H | 5.53564400 | -1.57793200 | 2.60583100 |
| H | 7.41230400 | -1.09324800 | 1.04523300 |
| H | 6.95403200 | -0.88727600 | -1.39491000 |
| C | 2.41670100 | -1.67947300 | -0.88741400 |
| H | 2.40712900 | -1.55931800 | -1.96861800 |
| C | 1.49849200 | -2.77075500 | -0.47531400 |
| F | 1.21663400 | -3.64705300 | -1.52603800 |
| F | 1.96292500 | -3.55611800 | 0.56043000 |
| C | -0.08107100 | -0.97614200 | -3.46291400 |
| H | 0.77853600 | -0.31572300 | -3.57683300 |
| C | -0.37207900 | -1.89258500 | -4.38810300 |
| H | -1.21025500 | -2.57493900 | -4.27824400 |
| H | 0.23684500 | -2.00493100 | -5.28209500 |
| C | 1.19546300 | -0.82533500 | 3.14427100 |
| H | 2.08943900 | -0.23249100 | 2.95807200 |
| C | 1.15121800 | -1.71539800 | 4.13833700 |
| H | 0.27442100 | -2.33124900 | 4.31851200 |
| H | 2.00224700 | -1.86939400 | 4.79769700 |

**TS2-2** R1= -Ph, R2= -OMe

Total electronic energy = -3495.134913

Thermal corrections to Gibbs free energy = 0.842802

No. of imaginary frequency: 1 (187.95*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 1.39508900 | 0.64781300 | 0.75249000 |
| O | 1.92506500 | -0.45467900 | 1.39793400 |
| O | 1.44271200 | 1.76691300 | 1.56666700 |
| C | 2.46521100 | -0.04443700 | 2.68534700 |
| C | 1.74281200 | 1.33203200 | 2.92100200 |
| C | 3.98122000 | 0.07137200 | 2.52184600 |
| C | 2.12233700 | -1.12797600 | 3.70258000 |
| C | 2.59982600 | 2.40305300 | 3.58431500 |
| C | 0.39799500 | 1.19500200 | 3.64128900 |
| H | 4.46807300 | 0.31398100 | 3.47285500 |
| H | 4.24738600 | 0.82815000 | 1.78275300 |
| H | 4.37330500 | -0.88664800 | 2.16778400 |
| H | 2.44598200 | -0.83297400 | 4.70757700 |
| H | 2.64233400 | -2.05403600 | 3.43739800 |
| H | 1.05287100 | -1.34209700 | 3.72255800 |
| H | 2.91010500 | 2.08865500 | 4.58722300 |
| H | 2.02123400 | 3.32748700 | 3.68181300 |
| H | 3.49209300 | 2.61893000 | 2.99274600 |
| H | 0.52928200 | 0.94826400 | 4.70029800 |
| H | -0.21747900 | 0.42101000 | 3.17844400 |
| H | -0.14792400 | 2.13993400 | 3.56731200 |
| Cu | 0.20167400 | 0.27849300 | -0.84523900 |
| P | -0.25512200 | -1.90808300 | -0.63138600 |
| P | -1.57661000 | 1.66441900 | -0.55996100 |
| C | -1.69440100 | -2.42207500 | -1.64276000 |
| C | 1.05334100 | -3.10921300 | -1.09761500 |
| C | -0.73107800 | -2.46212800 | 1.05664500 |
| C | -2.87240400 | 1.31476300 | -1.80540800 |
| C | -2.45060500 | 1.65557100 | 1.05929400 |
| C | -1.23349900 | 3.45567000 | -0.78065000 |
| C | -2.62714800 | -3.37285900 | -1.20826100 |
| C | -1.84358000 | -1.83565000 | -2.90642400 |
| C | 2.29495500 | -3.03974200 | -0.44333000 |
| C | 0.86498500 | -4.05908600 | -2.10990000 |
| C | -1.71699900 | -1.72119900 | 1.71567600 |
| C | -0.13913600 | -3.51579200 | 1.76053600 |
| C | -2.50707000 | 1.41977000 | -3.15904700 |
| C | -4.16760700 | 0.90950800 | -1.47059200 |
| C | -2.80627900 | 2.81463200 | 1.76221100 |
| C | -2.63959200 | 0.42989000 | 1.70579000 |
| C | -0.16570700 | 4.01138100 | -0.05610300 |
| C | -1.98910300 | 4.27948400 | -1.62418600 |

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|---|---|---|---|
| H | -2.51572400 | -3.83260200 | -0.23132700 |
| C | -3.69987600 | -3.72692000 | -2.02607500 |
| C | -2.90715900 | -2.20509000 | -3.72820500 |
| H | -1.13128200 | -1.08182500 | -3.22785200 |
| C | 3.32177500 | -3.91542300 | -0.79281900 |
| H | 2.45044400 | -2.29064300 | 0.32532800 |
| C | 1.90180500 | -4.92414100 | -2.46441500 |
| H | -0.08734600 | -4.12120900 | -2.62470300 |
| O | -2.30283600 | -0.70147700 | 0.99237800 |
| C | -2.11730000 | -1.95585100 | 3.03235800 |
| H | 0.62679900 | -4.11518400 | 1.28230800 |
| C | -0.50849700 | -3.77538500 | 3.08118100 |
| H | -1.49049900 | 1.69970800 | -3.41999000 |
| C | -3.44557100 | 1.16278100 | -4.15492800 |
| H | -4.45585100 | 0.82181900 | -0.42806200 |
| C | -5.09339200 | 0.61768600 | -2.47464000 |
| H | -2.67559100 | 3.78353200 | 1.29427800 |
| C | -3.28843200 | 2.72805600 | 3.06769000 |
| C | -3.10757300 | 0.30643900 | 3.01679200 |
| H | 0.41559400 | 3.38683400 | 0.61437600 |
| C | 0.14083400 | 5.36502600 | -0.18666300 |
| H | -2.81991700 | 3.86618800 | -2.18466900 |
| C | -1.67321900 | 5.63282400 | -1.75552900 |
| H | -4.42436700 | -4.45881400 | -1.67909100 |
| C | -3.83964400 | -3.14532200 | -3.28776000 |
| H | -3.01909700 | -1.73946300 | -4.70165000 |
| C | 3.13018700 | -4.85713700 | -1.80653200 |
| H | 4.27811600 | -3.84866200 | -0.28118800 |
| H | 1.74584500 | -5.65189100 | -3.25594700 |
| C | -3.26503000 | -1.10627000 | 3.58647900 |
| C | -1.48167700 | -2.99961200 | 3.71404400 |
| H | -0.03260700 | -4.58728500 | 3.62301600 |
| H | -3.16072200 | 1.26279000 | -5.19886600 |
| C | -4.73929200 | 0.75550600 | -3.81596800 |
| H | -6.09420200 | 0.29188400 | -2.20504300 |
| C | -3.42643800 | 1.48703800 | 3.69347700 |
| H | -3.55207500 | 3.63383000 | 3.60566100 |
| H | 0.97076400 | 5.78293900 | 0.37693800 |
| C | -0.60714400 | 6.17872600 | -1.04037000 |
| H | -2.26403200 | 6.25956400 | -2.41792200 |
| H | -4.67633300 | -3.42083800 | -3.92391800 |
| H | 3.93542900 | -5.53140900 | -2.08466800 |
| C | -4.59851500 | -1.69817900 | 3.05546600 |
| C | -3.28948600 | -1.10585200 | 5.11995100 |

| | | | |
|---|---|---|---|
| H | -1.75130600 | -3.21916500 | 4.74116100 |
| H | -5.46447000 | 0.53920600 | -4.59566100 |
| H | -3.78752400 | 1.44506800 | 4.71503700 |
| H | -0.36090900 | 7.23158800 | -1.14698400 |
| H | -4.60924200 | -1.71683900 | 1.96168500 |
| H | -5.44477600 | -1.09293100 | 3.39896400 |
| H | -4.72823200 | -2.72389800 | 3.41811600 |
| H | -3.42094700 | -2.12138700 | 5.50436200 |
| H | -4.13203500 | -0.51665600 | 5.49329500 |
| H | -2.36452900 | -0.69298500 | 5.53571000 |
| C | 4.27631000 | 1.95140200 | -0.56982500 |
| C | 3.39471400 | 0.97846100 | -1.05425400 |
| C | 3.91921100 | -0.29348900 | -1.34522600 |
| C | 5.26151900 | -0.57546000 | -1.14865700 |
| C | 6.13256800 | 0.41043100 | -0.66188800 |
| C | 5.63530700 | 1.68588100 | -0.37837000 |
| H | 3.89255000 | 2.93926100 | -0.32831000 |
| H | 3.26443000 | -1.06590900 | -1.72279800 |
| H | 5.66165800 | -1.56052000 | -1.36789400 |
| H | 6.28281000 | 2.47131300 | -0.00634900 |
| C | 1.96312100 | 1.32972800 | -1.23250900 |
| H | 1.76716300 | 2.37447800 | -1.00279700 |
| C | 1.17505300 | 0.91290400 | -2.42383300 |
| F | 0.76553900 | 2.01221700 | -3.18510700 |
| F | 1.84996800 | 0.07896800 | -3.29602900 |
| O | 7.43551100 | 0.02858200 | -0.49766100 |
| C | 8.34339500 | 0.99043700 | 0.00469000 |
| H | 8.05136700 | 1.33726700 | 1.00559100 |
| H | 9.31213900 | 0.49070800 | 0.06429100 |
| H | 8.42386100 | 1.85869300 | -0.66335400 |

**TS2-3** R1= -Ph, R2= -CN

Total electronic energy = -3472.857334

Thermal corrections to Gibbs free energy = 0.808706

No. of imaginary frequency: 1 (185.91*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | 1.38272600 | 0.78291100 | 0.78755400 |
| O | 2.00773800 | -0.27133700 | 1.42443600 |
| O | 1.31684900 | 1.89358300 | 1.60832100 |
| C | 2.48381600 | 0.17163500 | 2.72881300 |
| C | 1.63164300 | 1.47165900 | 2.96577500 |
| C | 3.98462100 | 0.43069800 | 2.59624200 |

| | | | |
|---|---|---|---|
| C | 2.22473700 | -0.95259000 | 3.72610200 |
| C | 2.37147500 | 2.60998000 | 3.65690100 |
| C | 0.29302300 | 1.20063800 | 3.65800700 |
| H | 4.43000500 | 0.70203400 | 3.55919000 |
| H | 4.19188700 | 1.22341400 | 1.87601700 |
| H | 4.47215900 | -0.48004500 | 2.23622600 |
| H | 2.49530800 | -0.63982100 | 4.74113700 |
| H | 2.83855300 | -1.82057100 | 3.46514600 |
| H | 1.18074600 | -1.26902100 | 3.71815200 |
| H | 2.69073400 | 2.31296400 | 4.66209800 |
| H | 1.70652500 | 3.47435700 | 3.75336700 |
| H | 3.25108500 | 2.91728900 | 3.08732600 |
| H | 0.42863900 | 0.95620800 | 4.71685300 |
| H | -0.23762500 | 0.37641300 | 3.17758900 |
| H | -0.33843300 | 2.09040600 | 3.58241300 |
| Cu | 0.24767700 | 0.33203500 | -0.83172800 |
| P | -0.01915900 | -1.88881700 | -0.63687100 |
| P | -1.63595000 | 1.57824900 | -0.56069600 |
| C | -1.39168200 | -2.50605500 | -1.68134600 |
| C | 1.39496700 | -2.96836900 | -1.09110700 |
| C | -0.47946500 | -2.49320900 | 1.03732300 |
| C | -2.88028800 | 1.12919800 | -1.82594300 |
| C | -2.52395400 | 1.47981100 | 1.04615300 |
| C | -1.43483700 | 3.39192800 | -0.76576700 |
| C | -2.24215000 | -3.54315400 | -1.27635200 |
| C | -1.57269200 | -1.91431000 | -2.93829000 |
| C | 2.60005500 | -2.84273000 | -0.37892600 |
| C | 1.32105600 | -3.87582900 | -2.15584500 |
| C | -1.53137700 | -1.83651900 | 1.68412200 |
| C | 0.17475600 | -3.51017100 | 1.74027000 |
| C | -2.51041900 | 1.27546200 | -3.17444500 |
| C | -4.14048600 | 0.61402500 | -1.50870000 |
| C | -2.98635600 | 2.59849700 | 1.75214700 |
| C | -2.62225700 | 0.23562700 | 1.67726400 |
| C | -0.42697000 | 4.02789100 | -0.02160200 |
| C | -2.24224100 | 4.15668400 | -1.61691700 |
| H | -2.10517000 | -4.00689800 | -0.30461700 |
| C | -3.26608900 | -3.97769300 | -2.11733700 |
| C | -2.58653600 | -2.36332700 | -3.78312500 |
| H | -0.92499200 | -1.09582900 | -3.23724600 |
| C | 3.70257400 | -3.62405300 | -0.72162300 |
| H | 2.66853200 | -2.12078800 | 0.42724400 |
| C | 2.43378100 | -4.64364400 | -2.50435100 |
| H | 0.39851600 | -3.98097400 | -2.71583600 |

| | | | |
|---|---|---|---|
| O | -2.17872400 | -0.85585900 | 0.95974700 |
| C | -1.93856200 | -2.11785000 | 2.98962500 |
| H | 0.99037500 | -4.04739900 | 1.27063200 |
| C | -0.19925200 | -3.81303700 | 3.05023500 |
| H | -1.51909100 | 1.64313300 | -3.42253200 |
| C | -3.41272000 | 0.94765300 | -4.18289400 |
| H | -4.43230400 | 0.49465800 | -0.47038800 |
| C | -5.02732200 | 0.25347200 | -2.52540900 |
| H | -2.92765500 | 3.57964100 | 1.29528600 |
| C | -3.48412200 | 2.45838200 | 3.04701100 |
| C | -3.10450100 | 0.05990600 | 2.97694900 |
| H | 0.19151300 | 3.44858700 | 0.65603900 |
| C | -0.22931200 | 5.40268900 | -0.14065700 |
| H | -3.02851900 | 3.68107300 | -2.19194900 |
| C | -2.03513300 | 5.53193200 | -1.73656500 |
| H | -3.92739900 | -4.77692300 | -1.79385100 |
| C | -3.43779100 | -3.38996900 | -3.37231600 |
| H | -2.72444800 | -1.89394400 | -4.75136400 |
| C | 3.62459400 | -4.52339900 | -1.78777500 |
| H | 4.62773700 | -3.51958500 | -0.16117700 |
| H | 2.36590600 | -5.33852700 | -3.33664100 |
| C | -3.15926200 | -1.36694100 | 3.53012300 |
| C | -1.23921600 | -3.11942600 | 3.67206300 |
| H | 0.32455600 | -4.59493600 | 3.59179800 |
| H | -3.12602900 | 1.07974400 | -5.22268700 |
| C | -4.67107500 | 0.43041000 | -3.86157800 |
| H | -6.00029200 | -0.15664700 | -2.26965300 |
| C | -3.53215100 | 1.20317700 | 3.65776800 |
| H | -3.83154300 | 3.33337300 | 3.58817400 |
| H | 0.55446000 | 5.88350600 | 0.43854800 |
| C | -1.02777100 | 6.15801200 | -1.00227200 |
| H | -2.66484100 | 6.11280800 | -2.40475600 |
| H | -4.23640700 | -3.72864400 | -4.02653600 |
| H | 4.48817200 | -5.12372500 | -2.05968600 |
| C | -4.43202600 | -2.05629000 | 2.96835400 |
| C | -3.21113400 | -1.38503500 | 5.06283300 |
| H | -1.51132100 | -3.37178700 | 4.69089200 |
| H | -5.36694500 | 0.16024800 | -4.65101200 |
| H | -3.90884400 | 1.12051800 | 4.67111700 |
| H | -0.86635000 | 7.22794200 | -1.09973700 |
| H | -4.42157800 | -2.06400800 | 1.87439100 |
| H | -5.32937800 | -1.52325200 | 3.30147200 |
| H | -4.48703400 | -3.09278700 | 3.31899600 |
| H | -3.26872500 | -2.41173500 | 5.43529900 |

| | | | |
|---|---|---|---|
| H | -4.10444900 | -0.86872600 | 5.42569100 |
| H | -2.32960000 | -0.90464400 | 5.49986000 |
| C | 4.18299800 | 2.30460600 | -0.53491400 |
| C | 3.36240500 | 1.26537600 | -1.00776000 |
| C | 3.95383100 | 0.02156800 | -1.28573600 |
| C | 5.30987000 | -0.18286500 | -1.08408400 |
| C | 6.12083300 | 0.86098900 | -0.60341100 |
| C | 5.54532900 | 2.11459200 | -0.33836900 |
| H | 3.73705200 | 3.26955100 | -0.31156200 |
| H | 3.34033700 | -0.78947300 | -1.64974500 |
| H | 5.74957600 | -1.15304500 | -1.29162900 |
| H | 6.16815000 | 2.92402800 | 0.02839000 |
| C | 1.91581600 | 1.52228300 | -1.18521700 |
| H | 1.64763600 | 2.55025200 | -0.95299700 |
| C | 1.17462900 | 1.05674000 | -2.39837300 |
| F | 0.69931400 | 2.13338400 | -3.14830700 |
| F | 1.92770000 | 0.29132700 | -3.26848400 |
| C | 7.51559300 | 0.64371100 | -0.37375200 |
| N | 8.64880800 | 0.46235300 | -0.17925100 |

**TS3**

Total electronic energy = -3380.647925

Thermal corrections to Gibbs free energy = 0.809971

No. of imaginary frequency: 1 (150.59*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.64638900 | 2.02933500 | -1.86888200 |
| C | -1.30944500 | 2.87480700 | -0.91479200 |
| B | -2.78558600 | 2.53124600 | -0.50459800 |
| O | -3.25405700 | 1.23764000 | -0.57011000 |
| O | -3.66911800 | 3.40045100 | 0.06445900 |
| C | -4.38847400 | 1.16854500 | 0.33754300 |
| C | -4.89305700 | 2.65629600 | 0.32904500 |
| C | -3.82559100 | 0.72118500 | 1.69146200 |
| C | -5.37906900 | 0.14059500 | -0.19397800 |
| C | -5.47398000 | 3.14201900 | 1.65103100 |
| C | -5.85097800 | 2.95895100 | -0.82608400 |
| H | -4.61936300 | 0.59816100 | 2.43559800 |
| H | -3.09259100 | 1.44104200 | 2.06680200 |
| H | -3.32003700 | -0.23931600 | 1.56268000 |
| H | -6.28234400 | 0.11955500 | 0.42606600 |
| H | -4.92264200 | -0.85315200 | -0.16439200 |
| H | -5.66863300 | 0.35495500 | -1.22527400 |

| | | | |
|---|---|---|---|
| H | -6.35530500 | 2.55133600 | 1.92591600 |
| H | -5.77969100 | 4.18855000 | 1.55704600 |
| H | -4.73949800 | 3.07397800 | 2.45594700 |
| H | -6.82957800 | 2.49321700 | -0.67054800 |
| H | -5.44230300 | 2.60512100 | -1.77766100 |
| H | -5.98865900 | 4.04174100 | -0.89767900 |
| H | -1.33748300 | 1.43450000 | -2.46216700 |
| Cu | 0.17621600 | 0.54343000 | -0.63680000 |
| P | 1.90274000 | 0.73794200 | 0.83401300 |
| P | -0.47638400 | -1.55969900 | -1.15824800 |
| C | 3.28596100 | -0.35134100 | 0.33044300 |
| C | 2.76315300 | 2.33226600 | 1.15516000 |
| C | 1.43350300 | 0.21580300 | 2.53763600 |
| C | 0.88449000 | -2.75992600 | -1.39018600 |
| C | -1.47473000 | -2.27879000 | 0.20041200 |
| C | -1.52560700 | -1.82327500 | -2.63861500 |
| C | 3.66814400 | -1.49865100 | 1.03125100 |
| C | 3.96591700 | -0.00118000 | -0.84871200 |
| C | 2.00043400 | 3.50841400 | 1.21388900 |
| C | 4.14774800 | 2.40029000 | 1.36515000 |
| C | 0.59117400 | -0.88920300 | 2.71054700 |
| C | 1.74473800 | 0.96743300 | 3.67897000 |
| C | 1.96231600 | -2.36355600 | -2.19516500 |
| C | 0.87792200 | -4.04211900 | -0.82795500 |
| C | -2.75419700 | -2.82942100 | 0.06494200 |
| C | -0.94445100 | -2.17852800 | 1.49153900 |
| C | -2.63711900 | -0.98170400 | -2.81415800 |
| C | -1.24208000 | -2.79771500 | -3.60503000 |
| H | 3.14440100 | -1.77939900 | 1.93918300 |
| C | 4.72972700 | -2.27984600 | 0.56994800 |
| C | 5.04079600 | -0.76825500 | -1.28856300 |
| H | 3.66282700 | 0.87653600 | -1.41293800 |
| C | 2.62048700 | 4.73152200 | 1.46832900 |
| H | 0.92941900 | 3.46003900 | 1.05221300 |
| C | 4.76322600 | 3.62770800 | 1.61251200 |
| H | 4.74796600 | 1.49792300 | 1.32791000 |
| O | 0.32188000 | -1.64489100 | 1.58674500 |
| C | 0.01338400 | -1.24401300 | 3.93247900 |
| H | 2.39114100 | 1.83229400 | 3.58719500 |
| C | 1.20019400 | 0.63165500 | 4.91741500 |
| H | 1.98517300 | -1.36003800 | -2.61137500 |
| C | 3.00537300 | -3.25020000 | -2.45212500 |
| H | 0.04533800 | -4.35511100 | -0.20576000 |
| C | 1.93632800 | -4.91858100 | -1.06896100 |

| | | | |
|---|---|---|---|
| H | -3.19407600 | -2.92282400 | -0.92186000 |
| C | -3.46701700 | -3.22964800 | 1.19626800 |
| C | -1.62271500 | -2.58165000 | 2.64306300 |
| H | -2.86207400 | -0.22419000 | -2.07107300 |
| C | -3.45425200 | -1.12612400 | -3.93447600 |
| H | -0.38583000 | -3.45160100 | -3.48074800 |
| C | -2.05709300 | -2.92789800 | -4.73073300 |
| H | 5.01608100 | -3.17394400 | 1.11661100 |
| C | 5.42596900 | -1.90995500 | -0.58029300 |
| H | 5.56897100 | -0.47880500 | -2.19303900 |
| C | 4.00165200 | 4.79645100 | 1.66156200 |
| H | 2.02066700 | 5.63671000 | 1.50288600 |
| H | 5.83804100 | 3.66865800 | 1.76711400 |
| C | -0.86963900 | -2.49589800 | 3.97361800 |
| C | 0.33231300 | -0.45464600 | 5.04105800 |
| H | 1.44391100 | 1.22784500 | 5.79161100 |
| H | 3.83684400 | -2.93379300 | -3.07316300 |
| C | 2.99716600 | -4.52659700 | -1.88651100 |
| H | 1.92743200 | -5.91001300 | -0.62416200 |
| C | -2.90948700 | -3.10283000 | 2.47144000 |
| H | -4.46350900 | -3.64665700 | 1.08516500 |
| H | -4.31316400 | -0.47205600 | -4.05863300 |
| C | -3.16444000 | -2.09516200 | -4.89783700 |
| H | -1.82611300 | -3.68398700 | -5.47609800 |
| H | 6.25867300 | -2.51400200 | -0.92999500 |
| H | 4.48261700 | 5.75249100 | 1.84986700 |
| C | 0.05814500 | -3.73705800 | 4.07413200 |
| C | -1.82636500 | -2.48460800 | 5.17263300 |
| H | -0.09278300 | -0.68641400 | 6.01128400 |
| H | 3.81971200 | -5.21053600 | -2.07627300 |
| H | -3.48313400 | -3.42248500 | 3.33428400 |
| H | -3.79642200 | -2.19870600 | -5.77549100 |
| H | 0.75025900 | -3.77664100 | 3.22755400 |
| H | -0.53704000 | -4.65702600 | 4.07521700 |
| H | 0.64581600 | -3.69572100 | 4.99779200 |
| H | -1.26854000 | -2.45696900 | 6.11289100 |
| H | -2.43040100 | -3.39634100 | 5.19294600 |
| H | -2.49876600 | -1.62125300 | 5.14121000 |
| C | 0.66288200 | 2.24848700 | -2.48845400 |
| C | 1.09046100 | 1.34943200 | -3.50173400 |
| C | 1.59141900 | 3.23646200 | -2.08262400 |
| C | 2.37017600 | 1.41454900 | -4.04487500 |
| H | 0.39301900 | 0.58977800 | -3.84971400 |
| C | 2.87256000 | 3.28941000 | -2.62432000 |

| | | | |
|---|---|---|---|
| H | 1.30041800 | 3.95452800 | -1.32867600 |
| C | 3.28241000 | 2.37994900 | -3.60526100 |
| H | 2.65689200 | 0.70623300 | -4.81931200 |
| H | 3.56045800 | 4.05344800 | -2.26989900 |
| H | 4.28263900 | 2.43075200 | -4.02613300 |
| F | -0.82434700 | 2.57451300 | 0.59089500 |
| F | -1.01676800 | 4.21854500 | -0.94810400 |

**TS4**

Total electronic energy = -3621.434338

Thermal corrections to Gibbs free energy = 0.932505

No. of imaginary frequency: 1 (172.65*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -0.98697900 | -0.61020800 | 1.97761000 |
| P | -1.36403200 | -0.61528200 | -1.84590500 |
| C | -2.73279400 | -1.16743400 | 2.05757500 |
| C | -0.20639800 | -1.43917000 | 3.41692600 |
| C | -1.09743200 | 1.17465000 | 2.37804000 |
| C | -3.08789700 | -1.24881300 | -1.82752000 |
| C | -1.54311600 | 1.19571800 | -2.11363700 |
| C | -0.72447000 | -1.25215300 | -3.44027800 |
| C | -3.69001600 | -0.49544300 | 2.82848000 |
| C | -3.10818400 | -2.31514000 | 1.34708500 |
| C | 1.02937800 | -0.98489400 | 3.91006800 |
| C | -0.74457100 | -2.63583600 | 3.91605400 |
| C | -1.54429200 | 2.01214800 | 1.34465700 |
| C | -0.64114500 | 1.78038700 | 3.55271400 |
| C | -3.31097800 | -2.60638700 | -2.11121900 |
| C | -4.17574600 | -0.44549400 | -1.46448900 |
| C | -1.31105300 | 1.81969000 | -3.34433800 |
| C | -1.76703000 | 2.01827300 | -1.00110100 |
| C | 0.63049000 | -1.60616700 | -3.50763100 |
| C | -1.53229500 | -1.40109900 | -4.57877700 |
| H | -3.40716400 | 0.39778400 | 3.37671100 |
| C | -5.00108500 | -0.96709700 | 2.88824100 |
| C | -4.41291500 | -2.79898300 | 1.42631800 |
| H | -2.38000000 | -2.82001400 | 0.72148700 |
| C | 1.70132400 | -1.72129100 | 4.88674400 |
| H | 1.48752800 | -0.05329400 | 3.57424100 |
| C | -0.05657800 | -3.37182600 | 4.88189700 |
| H | -1.70067100 | -2.99625500 | 3.55155000 |
| O | -2.00952500 | 1.38529400 | 0.20313700 |

| | | | |
|---|---|---|---|
| C | -1.51310100 | 3.40324300 | 1.41040700 |
| H | -0.28088400 | 1.17077900 | 4.37179200 |
| C | -0.59948400 | 3.17157100 | 3.65089200 |
| H | -2.47682200 | -3.24186700 | -2.39594400 |
| C | -4.59698300 | -3.13924900 | -2.05858700 |
| H | -4.02236200 | 0.60207900 | -1.23340200 |
| C | -5.46044100 | -0.98501400 | -1.39797300 |
| H | -1.11011900 | 1.21453000 | -4.22097900 |
| C | -1.29630500 | 3.21053900 | -3.43622100 |
| C | -1.75292100 | 3.41368100 | -1.05799800 |
| H | 1.26988100 | -1.48386100 | -2.64433800 |
| C | 1.16847300 | -2.09830100 | -4.69738200 |
| H | -2.58487800 | -1.13909300 | -4.53200500 |
| C | -0.99085100 | -1.89400800 | -5.76519200 |
| H | -5.73878000 | -0.43526600 | 3.48298400 |
| C | -5.36256000 | -2.12269600 | 2.19291400 |
| H | -4.69244300 | -3.68436500 | 0.86559500 |
| C | 1.16968100 | -2.91869200 | 5.36997300 |
| H | 2.64856100 | -1.34446900 | 5.26250700 |
| H | -0.48594900 | -4.29749600 | 5.25584800 |
| C | -2.06871900 | 4.19342200 | 0.22255000 |
| C | -1.01768900 | 3.97223200 | 2.58864600 |
| H | -0.21553000 | 3.63225200 | 4.55545300 |
| H | -4.75570000 | -4.18760000 | -2.29696000 |
| C | -5.67740100 | -2.32872200 | -1.70142300 |
| H | -6.29343600 | -0.34987300 | -1.11050400 |
| C | -1.50691400 | 3.99771900 | -2.30325900 |
| H | -1.10535200 | 3.68549300 | -4.39397300 |
| H | 2.22053000 | -2.36676300 | -4.73275800 |
| C | 0.36101600 | -2.24435600 | -5.82586300 |
| H | -1.62315100 | -2.00554500 | -6.64178600 |
| H | -6.38372800 | -2.49049900 | 2.24195600 |
| H | 1.70322500 | -3.49192200 | 6.12324000 |
| C | -3.61268000 | 4.25708700 | 0.37256400 |
| C | -1.50515400 | 5.61992700 | 0.17558900 |
| H | -0.94810800 | 5.04994600 | 2.67871200 |
| H | -6.68004600 | -2.74435600 | -1.65576500 |
| H | -1.46830500 | 5.07700500 | -2.39313100 |
| H | 0.78005100 | -2.63092100 | -6.75096000 |
| H | -4.04405400 | 3.25197800 | 0.41574600 |
| H | -4.05544400 | 4.78631500 | -0.47872400 |
| H | -3.88164600 | 4.78483600 | 1.29438700 |
| H | -1.77170000 | 6.16689400 | 1.08474400 |
| H | -1.93782500 | 6.17760900 | -0.66036900 |

| | | | |
|---|---|---|---|
| H | -0.41705800 | 5.61813000 | 0.07220700 |
| Cu | 0.01360600 | -0.77001000 | -0.04669200 |
| O | 1.63545000 | -2.24157100 | -0.03606400 |
| C | 1.72184800 | -3.66722800 | 0.24075400 |
| C | 2.43091400 | -3.88076100 | 1.58031700 |
| H | 2.42321300 | -4.94397600 | 1.84635600 |
| H | 3.46938500 | -3.54463900 | 1.53821800 |
| H | 1.92354200 | -3.32021200 | 2.36975600 |
| C | 2.44115900 | -4.36602900 | -0.91591400 |
| H | 1.93685700 | -4.14622700 | -1.86220400 |
| H | 3.47770700 | -4.02945900 | -1.00239700 |
| H | 2.44294700 | -5.45048600 | -0.75970200 |
| C | 0.26979400 | -4.13510600 | 0.32989600 |
| H | -0.23125600 | -3.64919500 | 1.17160200 |
| H | -0.26709300 | -3.88630900 | -0.59187600 |
| H | 0.22534300 | -5.21878500 | 0.48186300 |
| C | 2.00482400 | 5.05898700 | -1.43855700 |
| C | 1.75297900 | 3.69700900 | -1.28300000 |
| C | 1.82513400 | 3.10286800 | -0.00875300 |
| C | 2.15980400 | 3.91258100 | 1.09775000 |
| C | 2.41514800 | 5.27101400 | 0.93187000 |
| C | 2.33701600 | 5.85283100 | -0.33755300 |
| H | 1.93535500 | 5.50451200 | -2.42788900 |
| H | 1.48177500 | 3.09174700 | -2.13643600 |
| H | 2.23503400 | 3.44135900 | 2.07510800 |
| H | 2.67662100 | 5.87819600 | 1.79471200 |
| H | 2.53358400 | 6.91389600 | -0.46715900 |
| C | 1.55635800 | 1.68842100 | 0.26239500 |
| H | 1.40923800 | 1.49160400 | 1.32190600 |
| C | 1.44424100 | 0.60156900 | -0.54198200 |
| F | 1.57445700 | 0.88537600 | -1.91120500 |
| C | 4.63399100 | -0.74285100 | -1.42768400 |
| C | 4.94208500 | -0.81667400 | 0.12122100 |
| B | 2.70874800 | -1.39111600 | -0.30756500 |
| O | 3.35208400 | -1.40314800 | -1.53271600 |
| O | 3.61403100 | -0.97368100 | 0.70978500 |
| C | 5.74658000 | -2.04994800 | 0.53641200 |
| H | 6.77951000 | -1.99177300 | 0.17944300 |
| H | 5.76133700 | -2.11373400 | 1.62874300 |
| H | 5.29761600 | -2.96841300 | 0.14945800 |
| C | 5.58245800 | 0.43953500 | 0.70952700 |
| H | 5.70845700 | 0.32424600 | 1.79226200 |
| H | 6.57326500 | 0.60758600 | 0.27519300 |
| H | 4.98299900 | 1.33587700 | 0.52548400 |

| | | | |
|---|---|---|---|
| C | 5.61915700 | -1.52129700 | -2.29840400 |
| H | 5.31670100 | -1.43372000 | -3.34642600 |
| H | 6.63222500 | -1.11558100 | -2.20278800 |
| H | 5.63941300 | -2.58219200 | -2.04010400 |
| C | 4.51457800 | 0.68767800 | -1.96162100 |
| H | 5.50010700 | 1.16351100 | -2.00319400 |
| H | 4.10170500 | 0.65107300 | -2.97261100 |
| H | 3.85137000 | 1.30635500 | -1.35985700 |
| Li | 3.06172400 | 0.46260300 | 1.80955800 |
| F | 2.76825300 | 1.32241100 | 3.16417900 |

**TS5**

Total electronic energy = -3058.021210

Thermal corrections to Gibbs free energy = 0.643090

No. of imaginary frequency: 1 (180.94*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.40802700 | 0.51229400 | -1.62497000 |
| C | -3.19976700 | -0.43834200 | -1.05888400 |
| Cu | -0.50158200 | 0.12153900 | -1.17352500 |
| P | 0.29072500 | -1.88313200 | -0.43114700 |
| P | 0.41305800 | 1.96741000 | -0.15761200 |
| C | -0.00356600 | -1.97592700 | 1.38013700 |
| C | -0.48787400 | -3.42913500 | -1.03075000 |
| C | 2.08566200 | -2.22451300 | -0.57880800 |
| C | -0.23446700 | 1.81276100 | 1.55166900 |
| C | 2.22985800 | 2.20170700 | 0.00834400 |
| C | -0.17131900 | 3.62197100 | -0.66662000 |
| C | 0.94809600 | -2.45688300 | 2.28782700 |
| C | -1.26729700 | -1.59108600 | 1.84862300 |
| C | -1.11794100 | -3.42176100 | -2.28222200 |
| C | -0.47802600 | -4.60565400 | -0.26507500 |
| C | 2.96373200 | -1.23712100 | -0.12127100 |
| C | 2.64266600 | -3.36982700 | -1.15935800 |
| C | -1.63098800 | 1.85869600 | 1.70424600 |
| C | 0.57496800 | 1.59121300 | 2.66997500 |
| C | 2.87922300 | 3.42532500 | -0.20869500 |
| C | 3.03642100 | 1.07704200 | 0.21538000 |
| C | -0.55785300 | 3.81633100 | -1.99794300 |
| C | -0.24162200 | 4.68987500 | 0.24138500 |
| H | 1.93076000 | -2.75668600 | 1.93824000 |
| C | 0.63430400 | -2.55720600 | 3.64413500 |
| C | -1.58318900 | -1.70971100 | 3.19945600 |

| | | | |
|---|---|---|---|
| H | -2.00333700 | -1.19259000 | 1.16130300 |
| C | -1.72433100 | -4.58395000 | -2.76481300 |
| H | -1.15476900 | -2.50959500 | -2.86828900 |
| C | -1.08314600 | -5.76225400 | -0.75236900 |
| H | -0.00666200 | -4.61009300 | 0.71299100 |
| O | 2.38372500 | -0.11812100 | 0.44165200 |
| C | 4.35325000 | -1.33410900 | -0.20291100 |
| H | 1.99123700 | -4.15624100 | -1.52431200 |
| C | 4.02807600 | -3.48961900 | -1.27852400 |
| H | -2.26418200 | 2.00895900 | 0.83707400 |
| C | -2.20324400 | 1.70589300 | 2.96365500 |
| H | 1.65343200 | 1.54419800 | 2.56162200 |
| C | -0.00484000 | 1.43226600 | 3.92982200 |
| H | 2.29155600 | 4.31948300 | -0.38043500 |
| C | 4.27166200 | 3.48982600 | -0.23478100 |
| C | 4.43303800 | 1.10262200 | 0.17936700 |
| H | -0.55642800 | 2.98523100 | -2.69385600 |
| C | -0.99402700 | 5.07288100 | -2.42048900 |
| H | 0.03671700 | 4.53445200 | 1.27963500 |
| C | -0.67814200 | 5.94256400 | -0.18493900 |
| H | 1.37991400 | -2.92841800 | 4.34215500 |
| C | -0.63267000 | -2.19147800 | 4.10089800 |
| H | -2.56867100 | -1.40936900 | 3.54067700 |
| C | -1.70689100 | -5.75264400 | -2.00370400 |
| H | -2.21694800 | -4.56696100 | -3.73261300 |
| H | -1.07418100 | -6.66943200 | -0.15448600 |
| C | 5.17428500 | -0.21245900 | 0.44010100 |
| C | 4.87431200 | -2.48407400 | -0.80499800 |
| H | 4.45334300 | -4.37598400 | -1.73942300 |
| H | -3.28476100 | 1.72970900 | 3.06218300 |
| C | -1.39016200 | 1.49543500 | 4.08010000 |
| H | 0.62954100 | 1.25478900 | 4.79362900 |
| C | 5.04155100 | 2.33900900 | -0.05315500 |
| H | 4.76212900 | 4.44268200 | -0.40947100 |
| H | -1.30491000 | 5.21133200 | -3.45170700 |
| C | -1.05219500 | 6.13518700 | -1.51820200 |
| H | -0.73255300 | 6.76594300 | 0.52190400 |
| H | -0.87533200 | -2.27470000 | 5.15667100 |
| H | -2.18416100 | -6.65393800 | -2.37840200 |
| C | 5.20001000 | -0.45909100 | 1.97322800 |
| C | 6.61402000 | -0.17705100 | -0.08628300 |
| H | 5.94760500 | -2.60475000 | -0.90222300 |
| H | -1.83596000 | 1.36700400 | 5.06255900 |
| H | 6.12272200 | 2.41119000 | -0.09397000 |

| | | | |
|---|---|---|---|
| H | -1.39927500 | 7.11065500 | -1.84781800 |
| H | 4.18562600 | -0.49779900 | 2.38146000 |
| H | 5.74390400 | 0.34753000 | 2.47696100 |
| H | 5.69625700 | -1.41046800 | 2.19463500 |
| H | 7.12510500 | -1.12028900 | 0.12744100 |
| H | 7.18734500 | 0.61135400 | 0.40989700 |
| H | 6.64407300 | -0.00189300 | -1.16649200 |
| H | -2.91465800 | -1.45693700 | -1.31387400 |
| F | -2.80047700 | 1.83033800 | -1.39674200 |
| C | -4.26717600 | -0.32545300 | -0.06265800 |
| C | -4.64227900 | -1.49412600 | 0.63200100 |
| C | -4.88281100 | 0.88812000 | 0.30980300 |
| C | -5.56339800 | -1.45354500 | 1.67520400 |
| H | -4.18188800 | -2.43932500 | 0.35438800 |
| C | -5.80947800 | 0.92315200 | 1.34945400 |
| H | -4.63013000 | 1.79446700 | -0.22235800 |
| C | -6.14954700 | -0.24071500 | 2.04439500 |
| H | -5.82626200 | -2.36933400 | 2.19803600 |
| H | -6.27327600 | 1.86918800 | 1.61686600 |
| H | -6.86996500 | -0.20420600 | 2.85678000 |
| C | -1.78494000 | 0.39590400 | -3.77312900 |
| O | -1.67335700 | -0.76731500 | -4.01461300 |
| O | -1.78950200 | 1.55105600 | -4.05641400 |

**TS6**

Total electronic energy = -3061.012019

Thermal corrections to Gibbs free energy = 0.705254

No. of imaginary frequency: 1 (96.93*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| B | -0.90832900 | -1.82127800 | -1.13279200 |
| O | -2.23362300 | -1.92320300 | -0.73044000 |
| O | -0.28656900 | -3.06207100 | -1.06517500 |
| C | -2.56748700 | -3.32626200 | -0.55962000 |
| C | -1.15780800 | -3.97024400 | -0.33644500 |
| C | -3.24342400 | -3.78133300 | -1.85641400 |
| C | -3.52753400 | -3.44926200 | 0.61889000 |
| C | -0.98642700 | -5.37328500 | -0.90535500 |
| C | -0.70297600 | -3.92459700 | 1.12684500 |
| H | -3.57466700 | -4.82391400 | -1.79770500 |
| H | -2.56889000 | -3.66675900 | -2.70891100 |
| H | -4.11963100 | -3.15051700 | -2.03652000 |
| H | -3.74328400 | -4.50123400 | 0.84093400 |

| | | | |
|---|---|---|---|
| H | -4.47183200 | -2.95210700 | 0.37429500 |
| H | -3.12343600 | -2.97202800 | 1.51391300 |
| H | -1.67883200 | -6.07618400 | -0.42716600 |
| H | 0.03460400 | -5.72254500 | -0.71947400 |
| H | -1.15985100 | -5.38960500 | -1.98347400 |
| H | -1.24832300 | -4.64595200 | 1.74587000 |
| H | -0.84428200 | -2.92542100 | 1.54631600 |
| H | 0.36474900 | -4.15654800 | 1.17639100 |
| Cu | 0.01219200 | -0.04769100 | -1.26449900 |
| P | -1.32695700 | 1.59052300 | -0.37282000 |
| P | 2.14010000 | -0.05131400 | -0.45991400 |
| C | -0.68903400 | 3.20728400 | 0.20866800 |
| C | -2.83341200 | 1.99740500 | -1.32997000 |
| C | -1.99797700 | 0.84028800 | 1.16466400 |
| C | 3.02117600 | 1.52520500 | -0.14935200 |
| C | 2.11460300 | -0.91285000 | 1.16557400 |
| C | 3.33608800 | -1.05912100 | -1.41486200 |
| C | -1.15697500 | 3.84215500 | 1.36754700 |
| C | 0.33313800 | 3.80824800 | -0.53808900 |
| C | -3.50514400 | 0.93666100 | -1.96447500 |
| C | -3.30003200 | 3.30760100 | -1.49525500 |
| C | -1.07915200 | 0.28168300 | 2.05820700 |
| C | -3.35704800 | 0.68516100 | 1.45357100 |
| C | 3.40923500 | 2.29242200 | -1.26127300 |
| C | 3.21940600 | 2.04270100 | 1.13569000 |
| C | 2.97979900 | -1.96453100 | 1.49275300 |
| C | 1.08602600 | -0.61792000 | 2.06761200 |
| C | 2.83648100 | -2.20386300 | -2.05824700 |
| C | 4.70181000 | -0.75714600 | -1.50449100 |
| H | -1.94409900 | 3.37845000 | 1.95439100 |
| C | -0.60974400 | 5.06019200 | 1.77046100 |
| C | 0.87146500 | 5.03094200 | -0.14037800 |
| H | 0.71802600 | 3.30432600 | -1.41939700 |
| C | -4.63233000 | 1.19392400 | -2.74289000 |
| H | -3.15366600 | -0.08219700 | -1.83143700 |
| C | -4.42382600 | 3.55753400 | -2.28491500 |
| H | -2.78557600 | 4.13061000 | -1.01000500 |
| O | 0.25852700 | 0.43745800 | 1.74353700 |
| C | -1.44208400 | -0.42522100 | 3.20540000 |
| H | -4.09693100 | 1.09160800 | 0.77304900 |
| C | -3.75784600 | -0.02380900 | 2.58638800 |
| H | 3.24445500 | 1.90731800 | -2.26452100 |
| C | 4.01103800 | 3.53601100 | -1.08626100 |
| H | 2.91880200 | 1.46494500 | 2.00322300 |

| | | | |
|---|---|---|---|
| C | 3.80151200 | 3.29953400 | 1.30769500 |
| H | 3.78331300 | -2.22543300 | 0.81334000 |
| C | 2.78732700 | -2.69704900 | 2.66318700 |
| C | 0.85142700 | -1.34579400 | 3.23740100 |
| H | 1.78403300 | -2.45662600 | -1.97009100 |
| C | 3.69802800 | -3.02820400 | -2.78134500 |
| H | 5.09636700 | 0.12166700 | -1.00518100 |
| C | 5.55615100 | -1.58133600 | -2.23806600 |
| H | -0.97442600 | 5.54417400 | 2.67253200 |
| C | 0.40332000 | 5.65656300 | 1.01616700 |
| H | 1.67091100 | 5.48003400 | -0.72029600 |
| C | -5.09176200 | 2.50310500 | -2.90872700 |
| H | -5.14638600 | 0.36912100 | -3.22858600 |
| H | -4.77690700 | 4.57753100 | -2.41042200 |
| C | -0.31835800 | -0.91185900 | 4.12607900 |
| C | -2.81129100 | -0.57741900 | 3.45101000 |
| H | -4.81568400 | -0.15099200 | 2.79611100 |
| H | 4.32026400 | 4.11194500 | -1.95427400 |
| C | 4.20604900 | 4.04511500 | 0.20096400 |
| H | 3.94329100 | 3.69251800 | 2.31052800 |
| C | 1.72585500 | -2.39877200 | 3.52002000 |
| H | 3.45981200 | -3.51496500 | 2.90392000 |
| H | 3.30432300 | -3.91269400 | -3.27430000 |
| C | 5.05599600 | -2.71676400 | -2.87817300 |
| H | 6.61278300 | -1.33717500 | -2.30624000 |
| H | 0.83111700 | 6.60364900 | 1.33343300 |
| H | -5.96533800 | 2.70021700 | -3.52405200 |
| C | 0.14849400 | 0.28983900 | 4.99080500 |
| C | -0.78487700 | -2.04493700 | 5.04869100 |
| H | -3.14707900 | -1.12614300 | 4.32396300 |
| H | 4.66586200 | 5.01977400 | 0.33788500 |
| H | 1.58133900 | -2.99693400 | 4.41270600 |
| H | 5.72269700 | -3.35673100 | -3.44964100 |
| H | 0.48418000 | 1.11791600 | 4.35947600 |
| H | 0.97983900 | -0.00968200 | 5.63870800 |
| H | -0.67566700 | 0.64824500 | 5.61746800 |
| H | -1.60874900 | -1.70942400 | 5.68507500 |
| H | 0.02222900 | -2.35677300 | 5.71783500 |
| H | -1.11895800 | -2.91623000 | 4.47604000 |
| C | -0.71202100 | -0.56336500 | -3.52400700 |
| O | 0.03560300 | 0.37091000 | -3.60174500 |
| O | -1.47452400 | -1.37756300 | -3.92296400 |

**TS7**

Total electronic energy = -3380.645440

Thermal corrections to Gibbs free energy = 0.810968

No. of imaginary frequency: 1 (296.46*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.86054800 | 1.63082300 | 0.57367900 |
| C | -2.47917700 | 1.65740400 | -0.69778700 |
| B | -3.93016900 | 1.13745000 | -1.05214400 |
| O | -4.98127700 | 1.99988100 | -0.91034800 |
| O | -4.29266900 | -0.10282800 | -1.49885400 |
| C | -6.14309700 | 1.36249700 | -1.50857400 |
| C | -5.75015900 | -0.15877300 | -1.46253000 |
| C | -6.25663100 | 1.91655900 | -2.93200700 |
| C | -7.37415200 | 1.73378600 | -0.69102500 |
| C | -6.23654200 | -0.97481300 | -2.65459000 |
| C | -6.13814300 | -0.84892900 | -0.15165100 |
| H | -7.14723100 | 1.53667300 | -3.44278500 |
| H | -5.37467200 | 1.65915200 | -3.52629100 |
| H | -6.32372600 | 3.00714800 | -2.88131800 |
| H | -8.26121600 | 1.21393200 | -1.07021400 |
| H | -7.55241200 | 2.81089100 | -0.76523600 |
| H | -7.24397000 | 1.48334900 | 0.36359000 |
| H | -7.32950300 | -0.93802900 | -2.72395800 |
| H | -5.94414000 | -2.02209500 | -2.53380100 |
| H | -5.81257000 | -0.60844500 | -3.59158700 |
| H | -7.22145600 | -0.99305900 | -0.08610600 |
| H | -5.80409300 | -0.27565100 | 0.71681400 |
| H | -5.65328600 | -1.82877600 | -0.11072300 |
| H | -1.35883100 | 2.56344500 | 0.82396700 |
| Cu | -0.10201500 | 0.50754600 | -0.21236200 |
| P | 0.24800100 | -1.71694400 | 0.15043700 |
| P | 1.76226200 | 1.79048900 | 0.01262500 |
| C | 0.88502300 | -2.07597500 | 1.83177000 |
| C | -1.22939800 | -2.78832800 | -0.00442700 |
| C | 1.42998700 | -2.57007800 | -0.97930300 |
| C | 2.55019000 | 1.39356600 | 1.62068100 |
| C | 3.12726700 | 1.54389000 | -1.18713900 |
| C | 1.59599200 | 3.61512100 | 0.05729500 |
| C | 2.19584500 | -2.49801900 | 2.07920400 |
| C | 0.01958200 | -1.84906100 | 2.91346600 |
| C | -2.15756900 | -2.44904100 | -0.99926400 |
| C | -1.44845400 | -3.91954900 | 0.79354700 |
| C | 2.62895100 | -1.93331000 | -1.31514400 |

| | | | |
|---|---|---|---|
| C | 1.15508600 | -3.79120300 | -1.61056600 |
| C | 1.70684100 | 1.13544800 | 2.71041700 |
| C | 3.93842900 | 1.34155400 | 1.79957300 |
| C | 3.73925700 | 2.55216900 | -1.94111600 |
| C | 3.52000700 | 0.22486400 | -1.43251600 |
| C | 0.56105400 | 4.19762200 | -0.68771900 |
| C | 2.46332400 | 4.43570300 | 0.79345700 |
| H | 2.87795000 | -2.67142700 | 1.25436200 |
| C | 2.63141300 | -2.70037000 | 3.38968200 |
| C | 0.45174800 | -2.07393700 | 4.21747500 |
| H | -0.99246300 | -1.50607900 | 2.73721100 |
| C | -3.28334100 | -3.24767800 | -1.19982200 |
| H | -2.02272800 | -1.54155700 | -1.58081000 |
| C | -2.58618900 | -4.70281100 | 0.60038800 |
| H | -0.73675700 | -4.17969600 | 1.57016000 |
| O | 2.90113900 | -0.74489400 | -0.66949800 |
| C | 3.53677400 | -2.42545500 | -2.25753300 |
| H | 0.23607400 | -4.31714700 | -1.37972200 |
| C | 2.04127300 | -4.31547400 | -2.55034400 |
| H | 0.62968000 | 1.13558400 | 2.57612000 |
| C | 2.24490200 | 0.85206900 | 3.96342600 |
| H | 4.59916600 | 1.52969000 | 0.95880000 |
| C | 4.47440900 | 1.04175700 | 3.05258600 |
| H | 3.46084000 | 3.58750300 | -1.77710300 |
| C | 4.68771300 | 2.22173500 | -2.91062200 |
| C | 4.46637700 | -0.14178800 | -2.38891100 |
| H | -0.13460100 | 3.56794300 | -1.23102400 |
| C | 0.40456000 | 5.58457500 | -0.70483800 |
| H | 3.25759600 | 3.98939200 | 1.38374100 |
| C | 2.30202400 | 5.82035700 | 0.77543800 |
| H | 3.65362100 | -3.02056300 | 3.57106700 |
| C | 1.76009400 | -2.49897400 | 4.46029800 |
| H | -0.23748600 | -1.90185400 | 5.03928000 |
| C | -3.50262900 | -4.37137200 | -0.40115600 |
| H | -3.99436400 | -2.97313600 | -1.97147900 |
| H | -2.75491600 | -5.57340400 | 1.22836900 |
| C | 4.82497800 | -1.62738000 | -2.48768100 |
| C | 3.21628400 | -3.63541600 | -2.87832000 |
| H | 1.81207200 | -5.25841600 | -3.03773800 |
| H | 1.57983300 | 0.64199600 | 4.79425900 |
| C | 3.62883400 | 0.80112400 | 4.13658000 |
| H | 5.55263700 | 0.99712600 | 3.18092200 |
| C | 5.04478800 | 0.88998800 | -3.13595400 |
| H | 5.15277800 | 3.00817400 | -3.49756000 |

| | | | |
|---|---|---|---|
| H | -0.40509000 | 6.02570800 | -1.27899500 |
| C | 1.27375300 | 6.39660600 | 0.02469200 |
| H | 2.97602900 | 6.44986900 | 1.35001600 |
| H | 2.10140400 | -2.66426500 | 5.47860700 |
| H | -4.38645800 | -4.98519600 | -0.55348800 |
| C | 5.81200400 | -1.96024200 | -1.33600100 |
| C | 5.48428500 | -1.97227700 | -3.82845800 |
| H | 3.88470800 | -4.05710600 | -3.62084800 |
| H | 4.04693000 | 0.56372300 | 5.11087000 |
| H | 5.78175400 | 0.65975500 | -3.89752700 |
| H | 1.14673900 | 7.47566900 | 0.01657600 |
| H | 5.37490700 | -1.71688500 | -0.36300700 |
| H | 6.73598400 | -1.38276200 | -1.45130700 |
| H | 6.05968100 | -3.02746300 | -1.34622400 |
| H | 5.75749600 | -3.03094100 | -3.86382900 |
| H | 6.40933400 | -1.40332700 | -3.96003500 |
| H | 4.81980800 | -1.75582000 | -4.67109700 |
| C | -2.33085300 | 0.84391700 | 1.71215400 |
| C | -2.01302100 | 1.26112700 | 3.02529200 |
| C | -3.07502400 | -0.35152600 | 1.58867400 |
| C | -2.42020600 | 0.53584500 | 4.14212600 |
| H | -1.44782700 | 2.18097300 | 3.15834100 |
| C | -3.49743200 | -1.06408800 | 2.70809900 |
| H | -3.29811900 | -0.74192800 | 0.60549000 |
| C | -3.17361600 | -0.63345200 | 3.99854600 |
| H | -2.15494300 | 0.89340800 | 5.13441200 |
| H | -4.06113500 | -1.98244300 | 2.56304900 |
| H | -3.49529700 | -1.19705300 | 4.86944900 |
| F | -2.26118400 | 2.83647400 | -1.36733400 |
| F | -1.56116200 | 0.65043600 | -1.79600500 |

**TS8**

Total electronic energy = -3569.258320

Thermal corrections to Gibbs free energy = 0.819639

No. of imaginary frequency: 1 (146.00*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | -1.27066300 | 1.91508100 | 0.32529800 |
| P | -0.39973600 | -1.89182700 | 0.55110900 |
| O | -2.57573300 | -0.49731700 | -0.78316600 |
| C | -3.06407300 | 1.68003400 | -0.03198900 |
| C | -4.01624400 | 2.68378000 | 0.20202900 |
| H | -3.68994600 | 3.64680400 | 0.58101500 |

| | | | |
|---|---|---|---|
| C | -5.36631200 | 2.44323600 | -0.03582200 |
| H | -6.09775200 | 3.22164000 | 0.15899500 |
| C | -5.78857300 | 1.20303900 | -0.52761300 |
| H | -6.84547000 | 1.03949100 | -0.70725400 |
| C | -4.87101700 | 0.18775600 | -0.80194600 |
| C | -3.52236300 | 0.46373600 | -0.54138600 |
| C | -2.94253300 | -1.80573800 | -0.58899300 |
| C | -1.96454900 | -2.65032100 | -0.05646200 |
| C | -2.30506500 | -3.99832200 | 0.12144800 |
| H | -1.57012800 | -4.68488600 | 0.52707100 |
| C | -3.58631700 | -4.44831400 | -0.19453600 |
| H | -3.84247800 | -5.49340300 | -0.04888800 |
| C | -4.55289400 | -3.55904300 | -0.67230100 |
| H | -5.55064400 | -3.92721900 | -0.88427900 |
| C | -4.24803800 | -2.21121100 | -0.88045300 |
| C | -5.21752600 | -1.16375500 | -1.43923800 |
| C | -6.68076100 | -1.55360100 | -1.18912200 |
| H | -6.91587000 | -2.50384500 | -1.67683200 |
| H | -7.35753200 | -0.80812600 | -1.61618700 |
| H | -6.89635300 | -1.64819400 | -0.11985900 |
| C | -4.97572400 | -1.04623000 | -2.96693300 |
| H | -3.94071300 | -0.76562500 | -3.17554500 |
| H | -5.63523300 | -0.28362800 | -3.39626600 |
| H | -5.17960600 | -2.00525800 | -3.45644600 |
| C | -1.24149000 | 2.13972800 | 2.15282800 |
| C | -0.04201000 | 2.52543300 | 2.77794900 |
| H | 0.85175000 | 2.68589500 | 2.18583500 |
| C | 0.00683800 | 2.69867300 | 4.16005200 |
| H | 0.93697700 | 3.01492800 | 4.62420900 |
| C | -1.12081700 | 2.45051400 | 4.94355400 |
| H | -1.07711000 | 2.57704200 | 6.02173900 |
| C | -2.29775200 | 2.01607200 | 4.33549600 |
| H | -3.17387900 | 1.79304600 | 4.93772100 |
| C | -2.36165400 | 1.86658300 | 2.95007300 |
| H | -3.28691300 | 1.53528700 | 2.49361400 |
| C | -1.05163300 | 3.60259700 | -0.38296600 |
| C | -1.55960100 | 3.83530500 | -1.67204200 |
| H | -2.10554500 | 3.05121700 | -2.18489700 |
| C | -1.37423100 | 5.06592000 | -2.29706200 |
| H | -1.77435500 | 5.22783100 | -3.29422300 |
| C | -0.67953600 | 6.08612500 | -1.64343800 |
| H | -0.53259600 | 7.04620600 | -2.12993200 |
| C | -0.18033600 | 5.86481200 | -0.36068600 |
| H | 0.35679000 | 6.65297400 | 0.15935800 |

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|---|---|---|---|
| C | -0.36267900 | 4.63145400 | 0.26684700 |
| H | 0.03227100 | 4.48140200 | 1.26285200 |
| C | -0.75058900 | -1.67808000 | 2.34444600 |
| C | 0.16192400 | -0.91370700 | 3.09086600 |
| H | 1.01643700 | -0.45946100 | 2.59896300 |
| C | -0.03057400 | -0.73466700 | 4.45914200 |
| H | 0.68111500 | -0.14253800 | 5.02483000 |
| C | -1.14892900 | -1.28042300 | 5.09047600 |
| H | -1.30503500 | -1.12288500 | 6.15405500 |
| C | -2.07316700 | -2.01554900 | 4.34839200 |
| H | -2.95092400 | -2.43622400 | 4.83168200 |
| C | -1.87331000 | -2.22111900 | 2.98273100 |
| H | -2.59330000 | -2.80272600 | 2.41827800 |
| C | 0.76576000 | -3.30624700 | 0.48642600 |
| C | 0.81151800 | -4.11546400 | -0.65919300 |
| H | 0.09857500 | -3.95835700 | -1.46253200 |
| C | 1.76773300 | -5.12098300 | -0.77630700 |
| H | 1.79149500 | -5.73855600 | -1.66975900 |
| C | 2.69695100 | -5.32665000 | 0.24505500 |
| H | 3.44793800 | -6.10572200 | 0.15048300 |
| C | 2.65898300 | -4.52333100 | 1.38434300 |
| H | 3.38049800 | -4.67375100 | 2.18234100 |
| C | 1.69929600 | -3.51885900 | 1.50690700 |
| H | 1.68480400 | -2.89750000 | 2.39516300 |
| Cu | 0.11349300 | 0.17885100 | -0.35037500 |
| C | 1.90075000 | 0.46151700 | -1.68402800 |
| H | 2.30095000 | 1.44018600 | -1.93629000 |
| C | 0.72106200 | 0.16362600 | -2.54461300 |
| C | -1.54022800 | -0.28591300 | -4.19936800 |
| C | -0.02009400 | 1.23864700 | -3.09208900 |
| C | 0.28315500 | -1.14890200 | -2.85303100 |
| C | -0.82845700 | -1.36167000 | -3.66512400 |
| C | -1.12927700 | 1.01669300 | -3.90144400 |
| H | 0.30326200 | 2.25266000 | -2.87800600 |
| H | 0.85021100 | -1.98955800 | -2.47830200 |
| H | -1.13273200 | -2.38047600 | -3.89213100 |
| H | -1.66461700 | 1.86558800 | -4.31987800 |
| H | -2.38927900 | -0.45804000 | -4.85424700 |
| C | 3.01031900 | -0.54994600 | -1.67363600 |
| B | 4.36718200 | -0.08894300 | -0.98599400 |
| O | 4.80796100 | 1.20081100 | -1.07454000 |
| C | 5.97487000 | 1.30679600 | -0.20772300 |
| C | 6.44876200 | -0.19214900 | -0.10504700 |
| O | 5.21840800 | -0.93423600 | -0.34149000 |

| | | | |
|---|---|---|---|
| C | 6.99852100 | -0.59759600 | 1.25718300 |
| H | 6.25517900 | -0.45422800 | 2.04365600 |
| H | 7.89177800 | -0.01261800 | 1.50405100 |
| H | 7.27700600 | -1.65591400 | 1.23988000 |
| C | 7.41895600 | -0.59965900 | -1.21758600 |
| H | 7.02748400 | -0.32371500 | -2.20136000 |
| H | 7.54399900 | -1.68627700 | -1.19649400 |
| H | 8.40095100 | -0.13332200 | -1.08740000 |
| C | 6.97290400 | 2.25439000 | -0.86264600 |
| H | 6.54173200 | 3.25891700 | -0.91282800 |
| H | 7.22061800 | 1.94040000 | -1.87875200 |
| H | 7.89680100 | 2.30837100 | -0.27567000 |
| C | 5.48393900 | 1.88570600 | 1.12206400 |
| H | 6.31815400 | 2.06833000 | 1.80765400 |
| H | 4.76272700 | 1.21978200 | 1.60145700 |
| H | 4.97660700 | 2.83436400 | 0.92422800 |
| C | 2.09597100 | 1.24567300 | 0.37597600 |
| O | 1.97069700 | 2.44400500 | 0.28255300 |
| O | 2.50449800 | 0.35900000 | 1.10023900 |
| F | 2.59064900 | -1.74710800 | -1.10380100 |
| F | 3.35655800 | -0.89973100 | -2.99571900 |

**TS9**

Total electronic energy = -1008.285592

Thermal corrections to Gibbs free energy = 0.262184

No. of imaginary frequency: 1 (412.29*i*)

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 4.70958400 | 0.34506200 | 1.27228300 |
| C | 3.39160000 | -0.03199800 | 1.04668300 |
| C | 2.77586900 | 0.25176900 | -0.19459900 |
| C | 3.52694400 | 0.92227500 | -1.18639400 |
| C | 4.84266600 | 1.29910800 | -0.95153700 |
| C | 5.43729300 | 1.01011300 | 0.28019900 |
| H | 5.17539700 | 0.12035500 | 2.22698100 |
| H | 2.83025100 | -0.54626400 | 1.81363300 |
| H | 3.05975700 | 1.14153600 | -2.14257300 |
| H | 5.40662500 | 1.81403400 | -1.72322300 |
| H | 6.46681300 | 1.30179000 | 0.46661500 |
| C | 1.41883500 | -0.11248000 | -0.51185400 |
| H | 1.07384400 | 0.15294800 | -1.50932800 |
| C | 0.45752500 | -0.75071300 | 0.23731400 |
| F | 0.75392700 | -1.08188100 | 1.52797500 |

| | | | |
|---|---|---|---|
| C | -2.49854600 | 1.25351000 | -0.37890000 |
| C | -3.16566600 | 0.18603000 | 0.56173900 |
| B | -1.16400500 | -0.58521900 | -0.19259900 |
| O | -1.49368500 | 0.47059600 | -1.06193400 |
| O | -2.04561600 | -0.67139200 | 0.88641000 |
| C | -3.73812400 | 0.74317500 | 1.86026400 |
| H | -4.52907800 | 1.47359500 | 1.65447200 |
| H | -4.17139000 | -0.06987200 | 2.45135800 |
| H | -2.96409000 | 1.22310900 | 2.46294000 |
| C | -4.21604800 | -0.66676800 | -0.16028200 |
| H | -4.46862400 | -1.52257400 | 0.47284700 |
| H | -5.13177000 | -0.09907400 | -0.35722300 |
| H | -3.82924800 | -1.04903900 | -1.10916500 |
| C | -1.77802700 | 2.36089800 | 0.40122000 |
| H | -1.15147300 | 2.93034100 | -0.29248400 |
| H | -2.48410600 | 3.05083600 | 0.87500500 |
| H | -1.13263900 | 1.93797100 | 1.17725300 |
| C | -3.43062600 | 1.86191200 | -1.42087700 |
| H | -4.26009300 | 2.39141700 | -0.93819300 |
| H | -2.87976000 | 2.58168800 | -2.03511400 |
| H | -3.83988800 | 1.09568100 | -2.08243100 |
| C | 0.03661300 | -2.32523600 | -0.68620800 |
| O | 0.79518600 | -3.23140300 | -0.62853600 |
| O | -1.10028400 | -1.98597500 | -1.09774800 |

**Xantphos**

Total electronic energy = -2263.609459

Thermal corrections to Gibbs free energy = 0.527129

Imaginary frequency

Cartesian coordinates

| ATOM | X | Y | Z |
|---|---|---|---|
| P | 2.09813000 | -0.77662800 | -1.01363400 |
| P | -1.98159600 | -0.59652100 | -0.80216900 |
| C | 1.67838000 | -1.48298000 | 0.63684000 |
| C | 3.81789400 | -1.41186000 | -1.25904500 |
| C | 2.46361100 | 0.97888800 | -0.56903800 |
| C | -2.22964100 | -1.30847900 | 0.88589100 |
| C | -2.10364600 | 1.21954200 | -0.45541900 |
| C | -3.64108500 | -0.90897600 | -1.55240800 |
| C | 2.01096600 | -0.87606400 | 1.85667400 |
| C | 0.98651300 | -2.70117400 | 0.65502400 |
| C | 4.30361900 | -1.44870700 | -2.57502800 |

| | | | |
|---|---|---|---|
| C | 4.65212700 | -1.84939600 | -0.22023600 |
| C | 1.41154300 | 1.77594200 | -0.09681000 |
| C | 3.70445300 | 1.59946500 | -0.75934800 |
| C | -2.64265000 | -2.64813600 | 0.98412200 |
| C | -1.96056200 | -0.60405600 | 2.06522600 |
| C | -3.26855700 | 1.98030800 | -0.61973000 |
| C | -0.94672500 | 1.89818800 | -0.04718900 |
| C | -3.69700900 | -1.01164100 | -2.94995400 |
| C | -4.83195700 | -1.03395500 | -0.81912600 |
| H | 2.54024100 | 0.07183400 | 1.85884800 |
| C | 1.66305500 | -1.47853400 | 3.06498400 |
| C | 0.64907100 | -3.30988300 | 1.86299200 |
| H | 0.69690400 | -3.16458000 | -0.28436200 |
| C | 5.59843400 | -1.89255000 | -2.84684800 |
| H | 3.65960000 | -1.12701900 | -3.38990800 |
| C | 5.94220300 | -2.30506500 | -0.49211300 |
| H | 4.28853900 | -1.83586500 | 0.80207700 |
| O | 0.19829900 | 1.13995100 | 0.08578200 |
| C | 1.54899500 | 3.13321800 | 0.20451600 |
| H | 4.54322100 | 1.01383400 | -1.11863300 |
| C | 3.86543500 | 2.96097600 | -0.50155300 |
| H | -2.84987900 | -3.21448200 | 0.07987400 |
| C | -2.81512300 | -3.25316600 | 2.22679800 |
| H | -1.63779100 | 0.42978100 | 2.01836600 |
| C | -2.11602000 | -1.21673200 | 3.30970000 |
| H | -4.18100300 | 1.49464400 | -0.94527900 |
| C | -3.26261200 | 3.35391700 | -0.38319100 |
| C | -0.91936700 | 3.26676500 | 0.24527600 |
| H | -2.77894600 | -0.92910500 | -3.52622500 |
| C | -4.91242100 | -1.22266200 | -3.60306000 |
| H | -4.80420200 | -0.96263300 | 0.26340200 |
| C | -6.04571600 | -1.25293600 | -1.46988000 |
| H | 1.92066700 | -0.99415300 | 4.00334700 |
| C | 0.98317200 | -2.69778100 | 3.07047400 |
| H | 0.09976400 | -4.24577900 | 1.86150500 |
| C | 6.42009300 | -2.32401200 | -1.80433500 |
| H | 5.96106200 | -1.91046400 | -3.87103500 |
| H | 6.57681700 | -2.64421800 | 0.32241500 |
| C | 0.36056400 | 3.84442400 | 0.85060900 |
| C | 2.79828100 | 3.72008100 | -0.02219400 |
| H | 4.83158100 | 3.43029800 | -0.66294300 |
| H | -3.15228900 | -4.28502800 | 2.28125500 |
| C | -2.55179000 | -2.53805900 | 3.39730300 |
| H | -1.89991400 | -0.65334500 | 4.21340400 |

| | | | |
|---|---|---|---|
| C | -2.09999500 | 3.98917500 | 0.05369700 |
| H | -4.17195600 | 3.93056600 | -0.52541900 |
| H | -4.93857500 | -1.29937000 | -4.68657800 |
| C | -6.08911700 | -1.34554500 | -2.86333600 |
| H | -6.95958100 | -1.34866200 | -0.88954300 |
| H | 0.70016800 | -3.16081900 | 4.01112000 |
| H | 7.42563900 | -2.67864300 | -2.01345300 |
| C | 0.36760700 | 3.49338600 | 2.36422000 |
| C | 0.43998700 | 5.36826800 | 0.69280000 |
| H | 2.94655500 | 4.77362200 | 0.18676500 |
| H | -2.68113100 | -3.00936800 | 4.36767200 |
| H | -2.12019200 | 5.05442500 | 0.25490200 |
| H | -7.03557700 | -1.51719100 | -3.36860400 |
| H | 0.32506800 | 2.40985300 | 2.51305100 |
| H | -0.49725600 | 3.94483900 | 2.86323900 |
| H | 1.28362800 | 3.86743900 | 2.83524000 |
| H | 1.34897500 | 5.75805500 | 1.15959000 |
| H | -0.40238400 | 5.85358900 | 1.19401300 |
| H | 0.43576400 | 5.66441000 | -0.36116100 |