Supporting Information

Computational Exploration on the Mechanism of Copper-Catalyzed Aromatic C-H Bond Amination of Benzene via a Nitrene Insertion Approach

Kaipeng Hou,[a] David A. Hrovat,[b] and Xiaoguang Bao[a]*

[a] College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China.

[b] Department of Chemistry and the Center for Advanced Scientific Computing and Modeling, University of North Texas, 1155 Union Circle, #305070, Denton, Texas 76203-5017, United States

E-mail: xgbao@suda.edu.cn

List of Contents

Computational Methods

The M06 functional[1] was employed in this work to carry out all the calculations. This functional has shown excellent performance to describe similar intermediate in literature.[2] The LANL2DZ basis set, in conjunction with the LANL2DZ pseudo potential,[3] was used for the Cu and Br atoms and the 6-31G(d) basis set[4] was used for other atoms in all geometry optimizations. Vibrational frequency analyses at the same level of theory were performed on all optimized structures to characterize stationary points as local minima or transition states. Further, intrinsic reaction coordinates (IRC) calculations were carried out to confirm that transition states connect appropriate reactants and products. The gas-phase Gibbs free energies for all species were obtained at 298.15K and 1 atm at optimized structures.

To consider solvation effects, single-point energy calculations using the SMD solvent model[5] with benzene as solvent were performed based on the optimized gas-phase geometries of all the species. Larger basis sets (LANL2DZ for Cu and 6-311++G(d,p) for other atoms) were utilized in such single-point energy calculations. The solution-phase Gibbs free energy was determined by adding the solvation single-point energy and the gas-phase thermal correction to the Gibbs free energy obtained from vibrational frequency calculation. Unless otherwise specified, the solution-phase Gibbs free energy was used in the discussion. Such single-point energy calculations with the SMD solvent model were also executed using ωB97XD functional[6], which supported the reliability of M06 functional in describing the copper-nitrene complex.

The broken-symmetry method was used in optimizing the structure of open-shell singlet state.[7] The real energy of open-shell singlet state (E_{os}) was evaluated by the following formula[8]:

$$E_{os} = (S_1^2 E_0 - S_0^2 E_1)/(S_1^2 - S_0^2)$$

where E_0 is the energy of optimized broken-symmetry solution and E_1 is the energy of triplet state at the same geometry, respectively. S_0 and S_1 refer to spin contaminations of the open-shell singlet state and triplet state, respectively. The Gaussian 09 suite of programs[9] was used for all of the calculations.

The single-point CASSCF energy calculations were carried out at the geometries optimized at the B3LYP[10]/6-31G(d)-LANL2DZ(Cu) level of theory. The 14-electron/14-orbital active space consisted of the two electrons occupying the in-phase and out-of-phase combinations of a p-orbital on the nitrene nitrogen and a d-orbital on copper along with the twelve electrons in the six highest energy occupied π MOs and corresponding antibonding MOs of the Tp ligand. The CASSCF calculations were performed using the MOLCAS program (Version 8.0).[11]

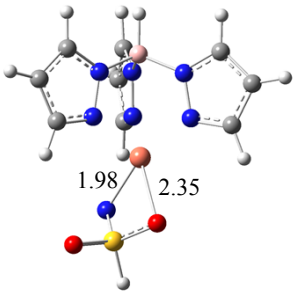
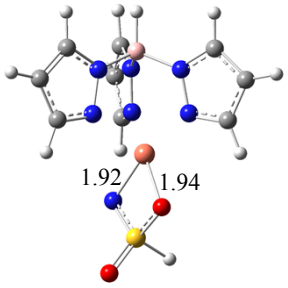
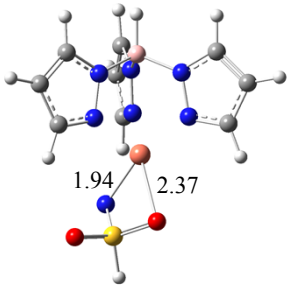
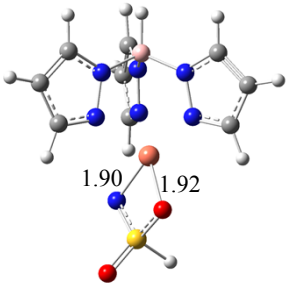
B3LYP		
M06		
	κ²N,O-**INT1-a** (triplet)	κ²N,O-**INT1-a** (singlet)

Figure S1. The optimized triplet and singlet structures of κ²N,O-**INT1-a**, a truncated simpler model of κ²N,O-**INT1**, at the B3LYP/6-31G(d)-LANL2DZ(Cu) and the M06/6-31G(d)-LANL2DZ(Cu) levels of theory. Bond lengths are shown in Å.

Table S1. Calculated singlet triplet splitting of κ²N,O-**INT1-a** at various levels of theory.

Method	ΔE [a]	ΔG [a]
B3LYP/6-31G(d)-LANL2DZ(Cu)	-5.1	-7.8
B3LYP/6-311++G(d,p)-LANL2DZ(Cu)//B3LYP/6-31G(d)-LANL2DZ(Cu)	-4.9	-7.5
M06/6-31G(d)-LANL2DZ(Cu)	-4.4	-6.2
M06/6-311++G(d,p)-LANL2DZ(Cu)//M06/6-31G(d)-LANL2DZ(Cu)	-4.3	-6.1
(14/14)CASSCF/6-31G(d)-LANL2DZ(Cu)//B3LYP/6-31G(d)-LANL2DZ(Cu)	-7.3	-10.0[b]

[a] Electronic energies and Gibbs free energies are in kcal/mol (ΔE = E(triplet) – E(singlet)). Negative number means that triplet is the ground state. [b] Thermal and entropic corrections are calculated at the B3LYP/6-31G(d)-LANL2DZ(Cu) level of theory.

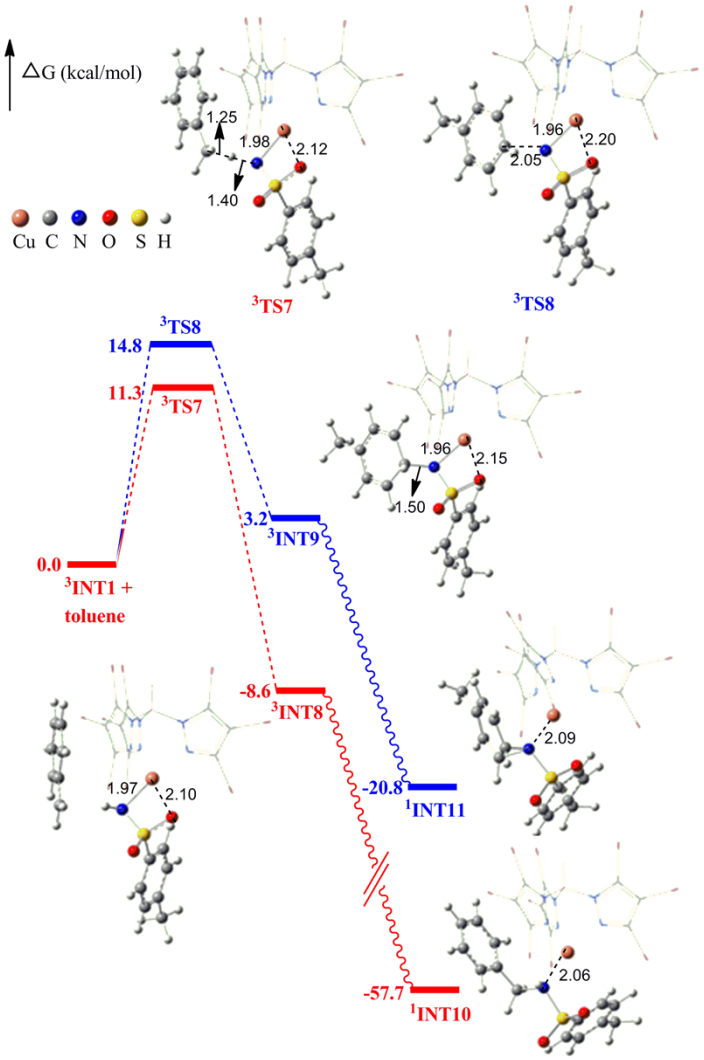


Figure S2. Free energy profiles for the benzylic C-H bond amination of toluene via the HAA/RR path (shown in red) and the formation of the aziridine intermediate via the nitrene addition path (shown in blue). The Tp^{Br3} ligand is shown in line style for clarity. Bond lengths are shown in Å.

References:

(1) Y. Zhao and D. G. Truhlar, *J. Chem. Phys*., 2006, **125**, 194101.

(2) L. Maestre, W. M. C. Sameera, M. M. Díaz-Requejo, F. Maseras and P. J. Peŕez, *J. Am. Chem. Soc*., 2013, **135**, 1338.

(3) P. J. Hay and W. R. Wadt, *J. Chem. Phys*., 1985, **82**, 299.

(4) W. J. Hehre, R. Ditchfield and J. A. Pople, J. *Chem. Phys*., 1972, **56**, 2257.

(5) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.,* 2009, **113***,* 6378

(6) J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615.

(7) L. Noodleman, *Chem. Phys.*, 1981, **74**, 5737.

(8) K. S. Chan, X. Z. Li, W. I. Dzik and B. de Bruin, *J. Am. Chem. Soc.,* 2008, **130**, 2051.

(9) M. J. T. Frisch, G. W. H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision C.01*; Gaussian, Inc.: Wallingford CT, 2010.

(10) (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648. (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785.

(11) F. Aquilante, L. De Vico, N. Ferré, G. Ghigo, P. Malmqvist, P. Neogrády, T. B. Pedersen, M. Pitoňák, M. Reiher, B. O. Roos, L. Serrano-Andrés, M. Urban, V. Veryazov, R. Lindh, *J. Comput. Chem.* 2010, **31**, 224.

Cartesian Coordinates and Energies

κ^2N,O-**INT1** (triplet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.670230	-0.026643	-0.818924
2	1	0	-2.647922	-0.079380	-1.489611
3	7	0	-0.518860	-0.824466	-1.496749
4	6	0	-0.534087	-1.632447	-2.577094
5	6	0	0.731718	-2.155787	-2.771193
6	6	0	1.481301	-1.602092	-1.729501
7	7	0	-1.945021	-0.617586	0.582394
8	6	0	-3.031987	-1.224489	1.102277
9	6	0	-1.435563	-1.181128	2.596625
10	6	0	-2.754834	-1.606594	2.402418
11	7	0	-1.221923	1.453023	-0.655086
12	6	0	-1.829962	2.585823	-1.061022
13	6	0	-1.055029	3.672382	-0.698744
14	6	0	0.039861	3.096461	-0.050060
15	7	0	-0.062539	1.775465	-0.016693
16	7	0	-0.959201	-0.590762	1.515813
17	7	0	0.736358	-0.813645	-0.972555
18	29	0	0.963480	0.203387	0.861601
19	7	0	2.113825	-1.171458	1.735246
20	16	0	2.974697	-0.019046	2.567164
21	8	0	2.160093	1.217998	2.303165
22	8	0	3.287320	-0.368692	3.940644
23	6	0	4.444733	0.086875	1.602911
24	6	0	4.587314	1.092491	0.649615
25	6	0	5.406701	-0.909256	1.767544
26	6	0	5.728325	1.103238	-0.139548
27	1	0	3.816565	1.854777	0.538673
28	6	0	6.531363	-0.887120	0.958323
29	1	0	5.267212	-1.682876	2.521016
30	6	0	6.709470	0.116147	-0.002386
31	1	0	5.859710	1.886237	-0.885847
32	1	0	7.292309	-1.659062	1.071177
33	6	0	7.944280	0.143230	-0.848899
34	1	0	8.750322	0.695724	-0.345731
35	1	0	8.320883	-0.867865	-1.044932
36	1	0	7.764833	0.635206	-1.812046
37	35	0	-2.084210	-1.969777	-3.628558
38	35	0	1.315642	-3.335001	-4.143114
39	35	0	3.338692	-1.848145	-1.383908
40	35	0	1.533802	4.014925	0.689770
41	35	0	-1.403034	5.516063	-1.001581
42	35	0	-3.506079	2.622927	-1.961491
43	35	0	-4.656197	-1.474079	0.139307
44	35	0	-3.894676	-2.497328	3.635172
45	35	0	-0.357320	-1.363811	4.153725

Zero-point correction= 0.240562 (Hartree/Particle)
Thermal correction to Energy= 0.280543
Thermal correction to Enthalpy= 0.281487
Thermal correction to Gibbs Free Energy= 0.156336
Sum of electronic and zero-point Energies= -1884.539766
Sum of electronic and thermal Energies= -1884.499786
Sum of electronic and thermal Enthalpies= -1884.498842
Sum of electronic and thermal Free Energies= -1884.623992

κ^2N,O-**INT1** (singlet)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	5	0	-1.775293	0.187329	-0.672652
2	1	0	-2.817023	0.305475	-1.229644
3	7	0	-1.039320	-1.085334	-1.201430
4	6	0	-1.511388	-2.075688	-1.983554
5	6	0	-0.512752	-3.009438	-2.192736
6	6	0	0.576189	-2.505082	-1.478013
7	7	0	-1.979458	0.055664	0.841983
8	6	0	-3.099243	0.048409	1.594845
9	6	0	-1.345564	-0.224718	2.873375
10	6	0	-2.744098	-0.130363	2.916696
11	7	0	-0.875000	1.420233	-0.966522
12	6	0	-1.156154	2.583961	-1.584770
13	6	0	-0.016368	3.368882	-1.616746
14	6	0	0.945270	2.586721	-0.973112
15	7	0	0.426662	1.432189	-0.579097
16	7	0	-0.890868	-0.113066	1.638178
17	7	0	0.257069	-1.361417	-0.883492
18	29	0	1.128522	-0.155136	0.493247
19	7	0	2.121175	-1.501433	1.356706
20	16	0	3.069443	-0.512131	2.161347
21	8	0	2.306241	0.755540	1.696631
22	8	0	3.254756	-0.678692	3.590808
23	6	0	4.680274	-0.375427	1.439509
24	6	0	4.809028	-0.362897	0.050153
25	6	0	5.794944	-0.272702	2.266273
26	6	0	6.069715	-0.224868	-0.507043
27	1	0	3.931426	-0.475768	-0.585637
28	6	0	7.050984	-0.143344	1.688776
29	1	0	5.669270	-0.299356	3.346129
30	6	0	7.207228	-0.110596	0.301247
31	1	0	6.181265	-0.215101	-1.591123
32	1	0	7.931142	-0.068576	2.326927
33	6	0	8.562108	0.057325	-0.314624
34	1	0	8.759427	1.113596	-0.545845
35	1	0	9.357193	-0.282222	0.359448
36	1	0	8.649266	-0.499781	-1.255363
37	35	0	-3.285655	-2.134574	-2.666403
38	35	0	-0.599925	-4.597577	-3.232310
39	35	0	2.316862	-3.266207	-1.411007
40	35	0	2.783211	3.003679	-0.711446
41	35	0	0.190486	5.102753	-2.365413
42	35	0	-2.874418	3.028983	-2.265878
43	35	0	-4.851920	0.262674	0.875341
44	35	0	-3.887832	-0.227614	4.432715
45	35	0	-0.165511	-0.475704	4.345177

Zero-point correction= 0.241445 (Hartree/Particle)
Thermal correction to Energy= 0.281064
Thermal correction to Enthalpy= 0.282008
Thermal correction to Gibbs Free Energy= 0.157727
Sum of electronic and zero-point Energies= -1884.520627
Sum of electronic and thermal Energies= -1884.481008
Sum of electronic and thermal Enthalpies= -1884.480064
Sum of electronic and thermal Free Energies= -1884.604345

κ^2N,O-**INT1** (open-shell singlet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.679732	-0.010704	-0.812444
2	1	0	-2.661227	-0.042306	-1.478859
3	7	0	-0.543433	-0.821847	-1.497119
4	6	0	-0.569999	-1.630524	-2.576239
5	6	0	0.690351	-2.165609	-2.773744
6	6	0	1.449802	-1.618272	-1.735654

7	7	0	-1.955805	-0.596276	0.588309
8	6	0	-3.042787	-1.199622	1.112068
9	6	0	-1.442275	-1.154169	2.602803
10	6	0	-2.763096	-1.577877	2.412491
11	7	0	-1.201387	1.461030	-0.647505
12	6	0	-1.793137	2.602262	-1.051911
13	6	0	-0.995742	3.676911	-0.703217
14	6	0	0.096565	3.087503	-0.063270
15	7	0	-0.029510	1.766881	-0.022664
16	7	0	-0.967362	-0.568045	1.518864
17	7	0	0.713329	-0.822011	-0.977696
18	29	0	0.976748	0.205283	0.846222
19	7	0	2.093294	-1.165494	1.732299
20	16	0	2.945071	-0.030863	2.565245
21	8	0	2.155133	1.228801	2.287916
22	8	0	3.253290	-0.343256	3.949869
23	6	0	4.423240	0.041560	1.607408
24	6	0	4.590609	1.032556	0.642850
25	6	0	5.368553	-0.967868	1.791367
26	6	0	5.737220	1.015339	-0.137806
27	1	0	3.833221	1.806236	0.519580
28	6	0	6.499223	-0.974239	0.990704
29	1	0	5.209708	-1.730023	2.552485
30	6	0	6.700964	0.013780	0.018696
31	1	0	5.887015	1.787438	-0.892057
32	1	0	7.246938	-1.756784	1.118492
33	6	0	7.941705	0.010507	-0.819528
34	1	0	8.756899	0.546033	-0.312690
35	1	0	8.296798	-1.009354	-1.010607
36	1	0	7.779505	0.503602	-1.785185
37	35	0	-2.126482	-1.951648	-3.622417
38	35	0	1.257819	-3.350725	-4.147199
39	35	0	3.306233	-1.879514	-1.402037
40	35	0	1.607964	3.994419	0.650339
41	35	0	-1.312260	5.523815	-1.018187
42	35	0	-3.477984	2.664951	-1.933150
43	35	0	-4.668019	-1.449510	0.151047
44	35	0	-3.901848	-2.462506	3.650517
45	35	0	-0.364722	-1.332945	4.159684

Zero-point correction= 0.240600 (Hartree/Particle)
Thermal correction to Energy= 0.279619
Thermal correction to Enthalpy= 0.280563
Thermal correction to Gibbs Free Energy= 0.159906
Sum of electronic and zero-point Energies= -1884.528697
Sum of electronic and thermal Energies= -1884.489678
Sum of electronic and thermal Enthalpies= -1884.488734
Sum of electronic and thermal Free Energies= -1884.609391

κ^1N-**INT1** (triplet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.912917	0.365219	-0.647980
2	7	0	-0.485073	-0.832085	-1.576426
3	7	0	-1.657890	-1.041519	-0.923230
4	7	0	0.488404	-0.709378	1.155745
5	7	0	-0.830248	-0.864127	1.448240
6	7	0	-0.613630	1.708889	-0.169208
7	7	0	-1.778023	1.169681	0.280192
8	6	0	-0.538593	-1.522341	-2.703988
9	6	0	-1.751616	-2.205917	-2.819016
10	6	0	-2.427785	-1.867553	-1.659202
11	6	0	1.168267	-1.248318	2.151953
12	6	0	0.314582	-1.768503	3.129559
13	6	0	-0.948290	-1.499622	2.632369
14	6	0	-0.789496	3.018557	-0.237631

15	6	0	-2.080078	3.372767	0.169239
16	6	0	-2.668601	2.161604	0.487145
17	5	0	-1.911186	-0.364001	0.454136
18	1	0	-2.994899	-0.637317	0.851087
19	35	0	-2.336497	-3.332618	-4.233461
20	35	0	-4.161878	-2.441919	-1.125975
21	35	0	0.920883	-1.499496	-3.926947
22	35	0	-2.621873	-1.931332	3.431012
23	35	0	0.773550	-2.639551	4.755478
24	35	0	3.073896	-1.278687	2.121471
25	35	0	-4.444739	1.866046	1.107834
26	35	0	-2.849262	5.108464	0.246423
27	35	0	0.609955	4.152178	-0.844195
28	7	0	2.593354	1.010584	-0.912355
29	16	0	3.779657	2.089202	-0.428811
30	6	0	5.179851	1.021786	-0.496163
31	8	0	3.517530	2.461168	0.952861
32	8	0	3.863378	3.088941	-1.483354
33	6	0	5.766665	0.579403	0.686027
34	6	0	5.645299	0.604531	-1.744390
35	6	0	6.840030	-0.297548	0.609630
36	1	0	5.382638	0.932987	1.641357
37	6	0	6.712025	-0.276925	-1.797416
38	1	0	5.173971	0.974048	-2.653657
39	6	0	7.323231	-0.739841	-0.625532
40	1	0	7.316530	-0.648731	1.524592
41	1	0	7.085494	-0.617533	-2.763060
42	6	0	8.490653	-1.674249	-0.702438
43	1	0	9.407641	-1.132968	-0.974401
44	1	0	8.674746	-2.171928	0.256531
45	1	0	8.337049	-2.447262	-1.465812

Zero-point correction= 0.241094 (Hartree/Particle)
Thermal correction to Energy= 0.281256
Thermal correction to Enthalpy= 0.282200
Thermal correction to Gibbs Free Energy= 0.156217
Sum of electronic and zero-point Energies= -1884.533609
Sum of electronic and thermal Energies= -1884.493447
Sum of electronic and thermal Enthalpies= -1884.492503
Sum of electronic and thermal Free Energies= -1884.618486

κ^1N-**INT1** (singlet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.956624	0.679216	0.112272
2	7	0	0.538910	-0.293988	1.613102
3	7	0	1.688584	-0.734840	1.032017
4	7	0	-0.483297	-0.859014	-1.106022
5	7	0	0.825577	-1.171039	-1.289732
6	7	0	0.648021	1.724363	-0.511221
7	7	0	1.828180	1.081106	-0.700814
8	6	0	0.604763	-0.648942	2.882356
9	6	0	1.792489	-1.333894	3.169648
10	6	0	2.447874	-1.363941	1.954031
11	6	0	-1.201178	-1.728646	-1.801591
12	6	0	-0.374087	-2.637347	-2.464794
13	6	0	0.903468	-2.244308	-2.101885
14	6	0	0.860026	3.015654	-0.715288
15	6	0	2.198905	3.251571	-1.039322
16	6	0	2.773217	1.992173	-1.008579
17	5	0	1.936136	-0.447739	-0.466165
18	1	0	3.004436	-0.831746	-0.813525
19	35	0	2.370311	-2.049852	4.834169
20	35	0	4.136006	-2.158297	1.563643
21	35	0	-0.800967	-0.222060	4.099062
22	35	0	2.541813	-3.064776	-2.611215

23	35	0	-0.879796	-4.074107	-3.600824
24	35	0	-3.102303	-1.666667	-1.789995
25	35	0	4.602856	1.550057	-1.289688
26	35	0	3.034807	4.911470	-1.434630
27	35	0	-0.563513	4.261121	-0.546156
28	7	0	-2.607215	0.878356	0.824448
29	16	0	-3.724237	1.767037	0.044776
30	6	0	-5.288371	1.032117	0.380475
31	8	0	-3.587671	1.925568	-1.393578
32	8	0	-3.488624	2.915425	0.952539
33	6	0	-6.131588	0.697014	-0.673979
34	6	0	-5.644017	0.786334	1.707659
35	6	0	-7.353778	0.101624	-0.387901
36	1	0	-5.824009	0.905317	-1.696817
37	6	0	-6.867594	0.194939	1.970044
38	1	0	-4.960877	1.052553	2.511950
39	6	0	-7.737978	-0.156710	0.929751
40	1	0	-8.024524	-0.169937	-1.202477
41	1	0	-7.158874	-0.008125	3.000521
42	6	0	-9.061194	-0.786854	1.237081
43	1	0	-9.765610	-0.045747	1.639757
44	1	0	-9.518674	-1.225629	0.343059
45	1	0	-8.961813	-1.576254	1.992908

Zero-point correction= 0.240665 (Hartree/Particle)
Thermal correction to Energy= 0.280798
Thermal correction to Enthalpy= 0.281742
Thermal correction to Gibbs Free Energy= 0.156337
Sum of electronic and zero-point Energies= -1884.513326
Sum of electronic and thermal Energies= -1884.473193
Sum of electronic and thermal Enthalpies= -1884.472249
Sum of electronic and thermal Free Energies= -1884.597654

κ^1N-**INT1** (open-shell singlet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.942855	0.394143	-0.551207
2	7	0	-0.451413	-0.794857	-1.584549
3	7	0	-1.636982	-1.022727	-0.960762
4	7	0	0.465158	-0.722020	1.160046
5	7	0	-0.857142	-0.887633	1.427305
6	7	0	-0.617717	1.712666	-0.118150
7	7	0	-1.792828	1.161131	0.285508
8	6	0	-0.476919	-1.470338	-2.721184
9	6	0	-1.682865	-2.161356	-2.872644
10	6	0	-2.385629	-1.844417	-1.723614
11	6	0	1.134100	-1.282762	2.153603
12	6	0	0.265937	-1.827630	3.103958
13	6	0	-0.990429	-1.549843	2.594116
14	6	0	-0.797397	3.023071	-0.172024
15	6	0	-2.102374	3.363711	0.199698
16	6	0	-2.694495	2.145046	0.479824
17	5	0	-1.923410	-0.375615	0.420972
18	1	0	-3.012472	-0.664698	0.790641
19	35	0	-2.229942	-3.276105	-4.311878
20	35	0	-4.124835	-2.440422	-1.229282
21	35	0	1.008497	-1.424859	-3.912843
22	35	0	-2.674077	-1.997138	3.360433
23	35	0	0.701592	-2.734098	4.716758
24	35	0	3.038485	-1.307009	2.155648
25	35	0	-4.485393	1.832009	1.046494
26	35	0	-2.882943	5.094020	0.282806
27	35	0	0.609645	4.177753	-0.714861
28	7	0	2.595752	1.022112	-0.901365
29	16	0	3.752483	2.090531	-0.394835
30	6	0	5.167551	1.041976	-0.462130

31	8	0	3.483950	2.440293	0.995084
32	8	0	3.853432	3.123128	-1.418892
33	6	0	5.742214	0.578884	0.719247
34	6	0	5.657720	0.656262	-1.712422
35	6	0	6.827811	-0.281541	0.640528
36	1	0	5.341061	0.908846	1.675877
37	6	0	6.736984	-0.208549	-1.768308
38	1	0	5.194672	1.039648	-2.620053
39	6	0	7.335785	-0.690439	-0.597067
40	1	0	7.295409	-0.646551	1.554687
41	1	0	7.130207	-0.522398	-2.735133
42	6	0	8.514707	-1.609367	-0.676526
43	1	0	9.425560	-1.054883	-0.942743
44	1	0	8.702343	-2.111426	0.279420
45	1	0	8.372744	-2.378728	-1.445941

Zero-point correction= 0.240852 (Hartree/Particle)
Thermal correction to Energy= 0.281067
Thermal correction to Enthalpy= 0.282011
Thermal correction to Gibbs Free Energy= 0.156587
Sum of electronic and zero-point Energies= -1884.514886
Sum of electronic and thermal Energies= -1884.474672
Sum of electronic and thermal Enthalpies= -1884.473727
Sum of electronic and thermal Free Energies= -1884.599151

Benzene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.240939	0.629721	-0.000001
2	6	0	1.165891	-0.759793	-0.000009
3	6	0	-0.075125	-1.389292	0.000012
4	6	0	-1.240951	-0.629697	-0.000002
5	6	0	-1.165905	0.759771	-0.000013
6	6	0	0.075152	1.389291	0.000007
7	1	0	2.211888	1.122775	0.000010
8	1	0	2.078218	-1.354273	-0.000008
9	1	0	-0.133690	-2.476629	0.000028
10	1	0	-2.211864	-1.122821	-0.000001
11	1	0	-2.078190	1.354315	-0.000009
12	1	0	0.133639	2.476632	0.000007

Zero-point correction= 0.100123 (Hartree/Particle)
Thermal correction to Energy= 0.104555
Thermal correction to Enthalpy= 0.105499
Thermal correction to Gibbs Free Energy= 0.072649
Sum of electronic and zero-point Energies= -231.955296
Sum of electronic and thermal Energies= -231.950864
Sum of electronic and thermal Enthalpies= -231.949920
Sum of electronic and thermal Free Energies= -231.982770

^{3}TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.792091	0.892265	-0.018750
2	1	0	2.893519	1.316629	0.115333
3	7	0	1.104542	0.776947	1.371178
4	6	0	1.556941	1.059912	2.607520
5	6	0	0.537872	0.849634	3.519649
6	6	0	-0.538756	0.435194	2.728089
7	7	0	1.830387	-0.498130	-0.692718
8	6	0	2.851596	-1.370332	-0.816082
9	6	0	1.112749	-2.130442	-1.896189

10	6	0	2.442360	-2.439499	-1.588481
11	7	0	0.941527	1.874071	-0.877176
12	6	0	1.268381	3.069647	-1.410886
13	6	0	0.142236	3.641266	-1.975878
14	6	0	-0.864246	2.703313	-1.731747
15	7	0	-0.387055	1.655294	-1.080740
16	7	0	0.740098	-0.985370	-1.347449
17	7	0	-0.193675	0.382665	1.448383
18	29	0	-1.130255	-0.115068	-0.403545
19	7	0	-2.163998	-1.582349	0.394229
20	16	0	-3.144035	-1.786451	-0.907618
21	8	0	-2.665821	-0.665361	-1.794981
22	8	0	-3.218481	-3.134277	-1.454211
23	6	0	-4.741641	-1.317550	-0.317616
24	6	0	-4.946542	-0.010861	0.128538
25	6	0	-5.757935	-2.264027	-0.280716
26	6	0	-6.194814	0.341421	0.611707
27	1	0	-4.135718	0.716743	0.094862
28	6	0	-7.005877	-1.888079	0.202532
29	1	0	-5.566622	-3.274029	-0.636703
30	6	0	-7.241844	-0.589166	0.654029
31	1	0	-6.370141	1.357896	0.964678
32	1	0	-7.814244	-2.618238	0.231500
33	6	0	-8.587705	-0.181160	1.169683
34	1	0	-9.056324	0.560008	0.507910
35	1	0	-9.268538	-1.036487	1.246652
36	1	0	-8.510336	0.281280	2.162441
37	35	0	3.324883	1.669206	2.962552
38	35	0	0.591728	1.091910	5.404219
39	35	0	-2.297896	0.027526	3.328584
40	35	0	-2.705147	2.827583	-2.193072
41	35	0	-0.002377	5.313175	-2.866907
42	35	0	3.017581	3.814743	-1.354630
43	35	0	4.542228	-1.125568	0.029452
44	35	0	3.464644	-3.952176	-2.121285
45	35	0	-0.070743	-3.114583	-3.014234
46	1	0	-1.397574	-2.558210	0.526359
47	6	0	0.612620	-5.538982	0.297488
48	6	0	1.692106	-5.145163	1.084548
49	6	0	1.712827	-3.888381	1.683522
50	6	0	0.645741	-3.007736	1.493457
51	6	0	-0.398396	-3.433786	0.696179
52	6	0	-0.461675	-4.671665	0.090110
53	1	0	0.607000	-6.522526	-0.170539
54	1	0	2.530055	-5.825002	1.228893
55	1	0	2.557750	-3.588966	2.302803
56	1	0	0.644314	-2.018330	1.953236
57	1	0	-1.307551	-4.951552	-0.535861

Zero-point correction= 0.335963 (Hartree/Particle)
Thermal correction to Energy= 0.381187
Thermal correction to Enthalpy= 0.382131
Thermal correction to Gibbs Free Energy= 0.247600
Sum of electronic and zero-point Energies= -2116.472610
Sum of electronic and thermal Energies= -2116.427386
Sum of electronic and thermal Enthalpies= -2116.426441
Sum of electronic and thermal Free Energies= -2116.560973

^{3}INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.544177	0.818147	0.747138
2	1	0	2.532353	1.123541	1.331653
3	7	0	0.647258	-0.056668	1.664278
4	6	0	0.948462	-0.707236	2.804432
5	6	0	-0.172279	-1.388329	3.245067

6	6	0	-1.139776	-1.096652	2.277702
7	7	0	1.887830	0.029909	-0.539284
8	6	0	3.061449	-0.409263	-1.036096
9	6	0	1.459125	-0.859564	-2.452789
10	6	0	2.840173	-0.986296	-2.273259
11	7	0	0.744635	2.094332	0.352556
12	6	0	1.050523	3.393686	0.545550
13	6	0	0.017904	4.181567	0.072515
14	6	0	-0.911081	3.258198	-0.414710
15	7	0	-0.474593	2.017376	-0.253410
16	7	0	0.894866	-0.257980	-1.420038
17	7	0	-0.646279	-0.310798	1.332999
18	29	0	-1.130724	0.144755	-0.720266
19	7	0	-1.962546	-1.594113	-1.131648
20	16	0	-3.026026	-0.971313	-2.198516
21	8	0	-2.627278	0.484952	-2.178728
22	8	0	-3.104325	-1.658684	-3.478629
23	6	0	-4.603599	-1.043024	-1.404946
24	6	0	-4.960720	-0.054472	-0.489679
25	6	0	-5.441583	-2.119340	-1.671141
26	6	0	-6.179596	-0.155468	0.162740
27	1	0	-4.290990	0.784049	-0.302086
28	6	0	-6.659258	-2.202408	-1.007379
29	1	0	-5.145124	-2.871532	-2.399281
30	6	0	-7.044095	-1.227711	-0.084642
31	1	0	-6.474606	0.613103	0.877577
32	1	0	-7.328357	-3.037949	-1.211359
33	6	0	-8.360679	-1.310742	0.626090
34	1	0	-9.000385	-0.453904	0.374864
35	1	0	-8.907054	-2.223803	0.363419
36	1	0	-8.227207	-1.299269	1.716001
37	35	0	2.677890	-0.692547	3.598753
38	35	0	-0.337342	-2.495286	4.781130
39	35	0	-2.945934	-1.692361	2.244873
40	35	0	-2.600717	3.640275	-1.194832
41	35	0	-0.105712	6.077348	0.083242
42	35	0	2.676138	3.996601	1.329175
43	35	0	4.719951	-0.247099	-0.115780
44	35	0	4.118256	-1.768843	-3.442889
45	35	0	0.406764	-1.431003	-3.935687
46	1	0	-1.326956	-2.232587	-1.632016
47	6	0	2.927851	-4.422812	-0.908206
48	6	0	2.905998	-4.088813	0.444457
49	6	0	1.758157	-3.553498	1.025711
50	6	0	0.616551	-3.330660	0.248569
51	6	0	0.701464	-3.662684	-1.082039
52	6	0	1.797211	-4.210286	-1.704347
53	1	0	3.827815	-4.848146	-1.351817
54	1	0	3.791778	-4.254321	1.055447
55	1	0	1.742157	-3.313414	2.090159
56	1	0	-0.295038	-2.917794	0.681709
57	1	0	1.804243	-4.453275	-2.766473

Zero-point correction= 0.342554 (Hartree/Particle)
Thermal correction to Energy= 0.388173
Thermal correction to Enthalpy= 0.389117
Thermal correction to Gibbs Free Energy= 0.253002
Sum of electronic and zero-point Energies= -2116.483634
Sum of electronic and thermal Energies= -2116.438015
Sum of electronic and thermal Enthalpies= -2116.437071
Sum of electronic and thermal Free Energies= -2116.573186

[1]TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.128450	0.110757	0.589143

2	1	0	-3.172358	0.222887	1.142310
3	7	0	-1.004023	-0.119526	1.641651
4	6	0	-1.072647	-0.166663	2.988308
5	6	0	0.177186	-0.475144	3.493875
6	6	0	0.969591	-0.606164	2.348787
7	7	0	-1.831316	1.391981	-0.223755
8	6	0	-2.541797	2.533042	-0.351119
9	6	0	-0.724741	2.663460	-1.556784
10	6	0	-1.868450	3.388502	-1.202616
11	7	0	-2.164802	-1.113683	-0.363620
12	6	0	-3.150407	-2.007345	-0.590162
13	6	0	-2.700025	-2.962325	-1.482308
14	6	0	-1.387418	-2.564824	-1.754663
15	7	0	-1.070279	-1.464616	-1.093383
16	7	0	-0.702777	1.478673	-0.974946
17	7	0	0.268934	-0.389923	1.249183
18	29	0	0.639798	-0.264721	-0.871165
19	7	0	2.377860	0.806695	-0.725274
20	16	0	3.129494	0.039662	-1.973937
21	8	0	1.958109	-0.820653	-2.350020
22	8	0	3.742112	0.903706	-2.973245
23	6	0	4.367234	-1.077826	-1.378118
24	6	0	3.978696	-2.307584	-0.848807
25	6	0	5.704120	-0.694482	-1.405378
26	6	0	4.951391	-3.157865	-0.345996
27	1	0	2.928557	-2.596948	-0.845189
28	6	0	6.662604	-1.559189	-0.892926
29	1	0	5.988906	0.263348	-1.835711
30	6	0	6.303581	-2.798265	-0.358803
31	1	0	4.658704	-4.124270	0.064992
32	1	0	7.713161	-1.270011	-0.911697
33	6	0	7.341459	-3.742357	0.166667
34	1	0	8.295622	-3.234787	0.349997
35	1	0	7.018733	-4.212024	1.104381
36	1	0	7.532488	-4.553852	-0.549234
37	35	0	-2.668161	0.153579	3.978987
38	35	0	0.688699	-0.687120	5.313939
39	35	0	2.812811	-1.098051	2.270349
40	35	0	-0.128974	-3.434966	-2.889013
41	35	0	-3.644440	-4.461004	-2.173069
42	35	0	-4.869883	-1.922233	0.225368
43	35	0	-4.196673	2.852919	0.540337
44	35	0	-2.380458	5.132458	-1.764545
45	35	0	0.670603	3.208218	-2.740504
46	6	0	5.892064	3.447321	-0.163984
47	6	0	5.862568	3.553637	1.225253
48	6	0	4.795384	3.038521	1.959844
49	6	0	3.745136	2.403863	1.304079
50	6	0	3.791988	2.347495	-0.078481
51	6	0	4.851223	2.814102	-0.840703
52	1	0	6.727587	3.860548	-0.726542
53	1	0	6.687415	4.039365	1.743820
54	1	0	4.786173	3.121439	3.044933
55	1	0	2.903880	1.971791	1.842706
56	1	0	2.769902	2.047013	-0.662304
57	1	0	4.844774	2.709950	-1.924819

Zero-point correction= 0.336697 (Hartree/Particle)
Thermal correction to Energy= 0.382551
Thermal correction to Enthalpy= 0.383495
Thermal correction to Gibbs Free Energy= 0.244552
Sum of electronic and zero-point Energies= -2116.468630
Sum of electronic and thermal Energies= -2116.422776
Sum of electronic and thermal Enthalpies= -2116.421832
Sum of electronic and thermal Free Energies= -2116.560774

[1]INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.764441	-0.567210	0.577386
2	1	0	-2.775265	-0.979171	1.041456
3	7	0	-0.597981	-0.932866	1.525555
4	6	0	-0.657427	-1.558000	2.720058
5	6	0	0.615860	-1.642709	3.247373
6	6	0	1.409678	-1.026352	2.276373
7	7	0	-1.867628	0.969120	0.422206
8	6	0	-2.901328	1.791263	0.704288
9	6	0	-1.284232	2.934980	-0.206565
10	6	0	-2.572665	3.076245	0.318191
11	7	0	-1.549293	-1.216021	-0.812409
12	6	0	-2.370632	-2.036427	-1.501014
13	6	0	-1.827717	-2.276638	-2.748079
14	6	0	-0.643391	-1.535859	-2.738050
15	7	0	-0.468700	-0.906564	-1.584448
16	7	0	-0.857413	1.686130	-0.141311
17	7	0	0.694280	-0.600085	1.245398
18	29	0	0.898818	0.439825	-0.726980
19	7	0	2.406405	1.742995	-1.385228
20	16	0	3.741783	1.003599	-2.296231
21	8	0	3.091419	0.615483	-3.535154
22	8	0	4.871068	1.917646	-2.288037
23	6	0	4.173629	-0.424063	-1.353753
24	6	0	3.370389	-1.561636	-1.427673
25	6	0	5.372094	-0.422326	-0.647892
26	6	0	3.773589	-2.707100	-0.760245
27	1	0	2.457101	-1.554469	-2.022222
28	6	0	5.759932	-1.584828	0.006829
29	1	0	5.993193	0.470416	-0.633677
30	6	0	4.968581	-2.734891	-0.032829
31	1	0	3.155011	-3.603004	-0.808965
32	1	0	6.699082	-1.602137	0.559753
33	6	0	5.365886	-3.964907	0.721331
34	1	0	6.446158	-3.999324	0.904354
35	1	0	4.865367	-3.992024	1.700396
36	1	0	5.078178	-4.878137	0.186395
37	35	0	-2.264005	-2.213902	3.509626
38	35	0	1.147732	-2.411874	4.903624
39	35	0	3.301600	-0.785574	2.373822
40	35	0	0.601528	-1.364248	-4.166661
41	35	0	-2.525051	-3.357363	-4.148586
42	35	0	-4.011133	-2.726940	-0.820409
43	35	0	-4.528492	1.222363	1.517365
44	35	0	-3.625688	4.652601	0.465734
45	35	0	-0.212521	4.321305	-0.968491
46	6	0	3.693902	4.919656	0.108247
47	6	0	3.485258	4.675084	1.464007
48	6	0	2.945647	3.462278	1.876400
49	6	0	2.609384	2.494635	0.935136
50	6	0	2.819201	2.742535	-0.414324
51	6	0	3.366085	3.954722	-0.834404
52	1	0	4.112572	5.869361	-0.218859
53	1	0	3.738624	5.436736	2.199076
54	1	0	2.771717	3.265548	2.932686
55	1	0	2.147891	1.557846	1.239922
56	1	0	1.883516	2.200777	-2.144495
57	1	0	3.527977	4.140289	-1.894677

Zero-point correction= 0.346044 (Hartree/Particle)
Thermal correction to Energy= 0.391211
Thermal correction to Enthalpy= 0.392155
Thermal correction to Gibbs Free Energy= 0.258015
Sum of electronic and zero-point Energies= -2116.601882
Sum of electronic and thermal Energies= -2116.556716
Sum of electronic and thermal Enthalpies= -2116.555771
Sum of electronic and thermal Free Energies= -2116.689912

^{3}TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.782963	-0.117756	-0.971521
2	1	0	-2.743342	-0.361001	-1.628645
3	7	0	-0.527989	-0.784508	-1.596231
4	6	0	-0.437293	-1.854925	-2.410827
5	6	0	0.893814	-2.085575	-2.704942
6	6	0	1.567232	-1.088925	-1.991460
7	7	0	-1.992759	-0.658601	0.472328
8	6	0	-3.051926	-1.263270	1.047704
9	6	0	-1.530199	-0.862418	2.565916
10	6	0	-2.799551	-1.425684	2.398877
11	7	0	-1.566362	1.417399	-0.878925
12	6	0	-2.319079	2.426404	-1.367356
13	6	0	-1.773299	3.633625	-0.973185
14	6	0	-0.657765	3.261856	-0.217539
15	7	0	-0.538301	1.946145	-0.155555
16	7	0	-1.047621	-0.414637	1.418108
17	7	0	0.722213	-0.316484	-1.329954
18	29	0	0.743789	0.576633	0.710855
19	7	0	2.283072	-0.527753	1.215152
20	16	0	2.890606	0.541762	2.312849
21	8	0	1.857522	1.631012	2.293880
22	8	0	3.300609	-0.005691	3.601816
23	6	0	4.313501	1.161999	1.465773
24	6	0	4.145303	2.128564	0.475752
25	6	0	5.555043	0.583261	1.708554
26	6	0	5.245925	2.526248	-0.266526
27	1	0	3.160002	2.559639	0.300160
28	6	0	6.644662	0.991175	0.950795
29	1	0	5.661654	-0.165806	2.491151
30	6	0	6.507732	1.964333	-0.043069
31	1	0	5.127978	3.284457	-1.040834
32	1	0	7.624646	0.549629	1.131767
33	6	0	7.690592	2.419058	-0.842092
34	1	0	8.506746	1.687845	-0.809529
35	1	0	7.425109	2.588661	-1.893094
36	1	0	8.085740	3.368609	-0.454218
37	35	0	-1.938672	-2.890289	-2.960678
38	35	0	1.628249	-3.456800	-3.801077
39	35	0	3.448816	-0.791041	-1.941717
40	35	0	0.588612	4.415166	0.640278
41	35	0	-2.395359	5.386303	-1.363576
42	35	0	-3.888935	2.173361	-2.412715
43	35	0	-4.627076	-1.759232	0.098568
44	35	0	-3.919783	-2.213251	3.717213
45	35	0	-0.542791	-0.679843	4.184003
46	6	0	3.812025	-3.635977	1.005725
47	6	0	2.929426	-4.091787	0.013826
48	6	0	1.569263	-3.761463	0.075620
49	6	0	1.098741	-2.934135	1.073619
50	6	0	2.006262	-2.348192	2.010258
51	6	0	3.358121	-2.818037	2.015743
52	1	0	4.855058	-3.946800	0.982450
53	1	0	3.293474	-4.726850	-0.792870
54	1	0	0.877971	-4.180643	-0.655717
55	1	0	0.040687	-2.677801	1.123874
56	1	0	1.595577	-1.958671	2.943966
57	1	0	4.024787	-2.466394	2.801251

Zero-point correction= 0.341260 (Hartree/Particle)
Thermal correction to Energy= 0.386571
Thermal correction to Enthalpy= 0.387515
Thermal correction to Gibbs Free Energy= 0.251436

Sum of electronic and zero-point Energies= -2116.486960
Sum of electronic and thermal Energies= -2116.441649
Sum of electronic and thermal Enthalpies= -2116.440705
Sum of electronic and thermal Free Energies= -2116.576785

^{3}INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.953209	-0.052559	-0.809229
2	1	0	-2.975177	-0.227443	-1.391502
3	7	0	-0.812913	-0.841736	-1.508064
4	6	0	-0.886624	-1.920393	-2.312125
5	6	0	0.382867	-2.239119	-2.758657
6	6	0	1.198125	-1.285087	-2.142664
7	7	0	-2.074094	-0.521557	0.662933
8	6	0	-3.126748	-0.954243	1.384079
9	6	0	-1.371927	-0.802756	2.680452
10	6	0	-2.724320	-1.159288	2.691713
11	7	0	-1.586295	1.456480	-0.796783
12	6	0	-2.254311	2.516464	-1.295139
13	6	0	-1.535567	3.669160	-1.039228
14	6	0	-0.405992	3.213855	-0.352486
15	7	0	-0.443548	1.898524	-0.199128
16	7	0	-0.986025	-0.423592	1.471615
17	7	0	0.488497	-0.458318	-1.392174
18	29	0	0.792183	0.466185	0.576243
19	7	0	2.304466	-0.665858	1.097053
20	16	0	2.991037	0.419231	2.109086
21	8	0	2.052809	1.576159	1.920435
22	8	0	3.269394	-0.055086	3.459552
23	6	0	4.522733	0.897929	1.364101
24	6	0	4.505449	1.478730	0.095458
25	6	0	5.715836	0.687125	2.044726
26	6	0	5.705122	1.849017	-0.488581
27	1	0	3.561501	1.634714	-0.426450
28	6	0	6.909584	1.068010	1.443012
29	1	0	5.697528	0.240513	3.037082
30	6	0	6.922549	1.653471	0.175976
31	1	0	5.704586	2.302012	-1.480229
32	1	0	7.851872	0.911439	1.967857
33	6	0	8.208211	2.089124	-0.457837
34	1	0	8.233424	1.843458	-1.526947
35	1	0	8.337827	3.177387	-0.375833
36	1	0	9.074938	1.618745	0.020982
37	35	0	-2.516088	-2.836992	-2.673222
38	35	0	0.895420	-3.663872	-3.908820
39	35	0	3.081489	-1.087830	-2.335085
40	35	0	1.045231	4.259671	0.286443
41	35	0	-1.980489	5.454063	-1.515479
42	35	0	-3.938428	2.391886	-2.170570
43	35	0	-4.870894	-1.193890	0.659168
44	35	0	-3.768904	-1.779487	4.152771
45	35	0	-0.149125	-0.809550	4.137380
46	6	0	3.927182	-3.679362	0.476038
47	6	0	2.887330	-4.287757	-0.270327
48	6	0	1.555758	-3.867180	-0.072839
49	6	0	1.251460	-2.841550	0.776044
50	6	0	2.298823	-2.093726	1.538339
51	6	0	3.674141	-2.668522	1.350707
52	1	0	4.947629	-4.043138	0.358111
53	1	0	3.109679	-5.086632	-0.975114
54	1	0	0.751773	-4.375514	-0.606863
55	1	0	0.217467	-2.526853	0.917232
56	1	0	2.042694	-2.118133	2.617920
57	1	0	4.476691	-2.224444	1.940325

Zero-point correction= 0.343056 (Hartree/Particle)
Thermal correction to Energy= 0.387965
Thermal correction to Enthalpy= 0.388909
Thermal correction to Gibbs Free Energy= 0.254530
Sum of electronic and zero-point Energies= -2116.507618
Sum of electronic and thermal Energies= -2116.462709
Sum of electronic and thermal Enthalpies= -2116.461765
Sum of electronic and thermal Free Energies= -2116.596144

^{1}TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.899651	0.304716	0.660058
2	1	0	2.936139	0.270909	1.244061
3	7	0	0.741353	-0.109867	1.628305
4	6	0	0.769312	-0.713543	2.832030
5	6	0	-0.520886	-0.804287	3.325403
6	6	0	-1.299759	-0.223460	2.322461
7	7	0	1.931127	-0.659934	-0.549383
8	6	0	2.795834	-1.637301	-0.893722
9	6	0	1.228621	-1.473102	-2.410442
10	6	0	2.386443	-2.192579	-2.090678
11	7	0	1.609450	1.747917	0.151920
12	6	0	2.356030	2.869438	0.255988
13	6	0	1.671558	3.929276	-0.309223
14	6	0	0.477347	3.351680	-0.750757
15	7	0	0.443480	2.059499	-0.483148
16	7	0	0.955443	-0.568886	-1.489698
17	7	0	-0.546365	0.184411	1.314614
18	29	0	-0.905427	0.507284	-0.725131
19	7	0	-2.046877	-1.037534	-0.837577
20	16	0	-3.034280	-0.471693	-1.979074
21	8	0	-2.268040	0.829730	-2.186472
22	8	0	-3.301803	-1.340334	-3.116951
23	6	0	-4.610241	0.035849	-1.343044
24	6	0	-4.724499	1.243021	-0.656964
25	6	0	-5.698357	-0.821979	-1.474083
26	6	0	-5.950560	1.590979	-0.108615
27	1	0	-3.863518	1.905148	-0.571670
28	6	0	-6.914829	-0.461061	-0.909673
29	1	0	-5.593868	-1.748968	-2.035111
30	6	0	-7.060502	0.747873	-0.225040
31	1	0	-6.053878	2.539377	0.419001
32	1	0	-7.773495	-1.124971	-1.009922
33	6	0	-8.388049	1.150878	0.341069
34	1	0	-8.273923	1.780400	1.231810
35	1	0	-8.967576	1.729740	-0.391850
36	1	0	-8.992622	0.277775	0.614713
37	35	0	2.351197	-1.383605	3.650657
38	35	0	-1.094381	-1.591656	4.959163
39	35	0	-3.185193	0.052168	2.328707
40	35	0	-0.992656	4.205148	-1.609299
41	35	0	2.222475	5.742363	-0.455732
42	35	0	4.085100	2.925621	1.049825
43	35	0	4.312504	-2.134672	0.149183
44	35	0	3.179580	-3.632919	-3.049302
45	35	0	0.137027	-1.662969	-3.959374
46	1	0	-2.088886	-3.653945	-2.326872
47	6	0	-1.689595	-3.621855	-1.315113
48	6	0	-2.525117	-3.236598	-0.250040
49	6	0	-0.352568	-3.914573	-1.075089
50	6	0	-2.019242	-3.219203	1.062190
51	1	0	-3.590092	-3.075574	-0.420481
52	6	0	0.155738	-3.825985	0.216964
53	1	0	0.300188	-4.197995	-1.900235
54	6	0	-0.683661	-3.495707	1.289113
55	1	0	-2.679177	-2.965910	1.891143

56	1	0	1.212817	-4.029359	0.397941
57	1	0	-0.284985	-3.467111	2.302921

Zero-point correction= 0.342230 (Hartree/Particle)
Thermal correction to Energy= 0.386923
Thermal correction to Enthalpy= 0.387867
Thermal correction to Gibbs Free Energy= 0.255434
Sum of electronic and zero-point Energies= -2116.488623
Sum of electronic and thermal Energies= -2116.443930
Sum of electronic and thermal Enthalpies= -2116.442986
Sum of electronic and thermal Free Energies= -2116.575419

[1]INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.803637	0.785724	-0.048380
2	1	0	-2.847327	1.347030	0.003053
3	7	0	-0.863914	1.585486	-0.991379
4	6	0	-1.035406	2.825013	-1.500855
5	6	0	0.178787	3.295253	-1.963424
6	6	0	1.063174	2.251172	-1.670640
7	7	0	-2.038862	-0.669353	-0.529260
8	6	0	-3.198638	-1.277730	-0.861477
9	6	0	-1.653104	-2.782461	-0.524474
10	6	0	-2.999393	-2.644812	-0.883848
11	7	0	-1.161507	0.746254	1.365879
12	6	0	-1.694655	1.138743	2.543392
13	6	0	-0.772613	0.930276	3.548753
14	6	0	0.325746	0.384879	2.873502
15	7	0	0.100258	0.267862	1.576798
16	7	0	-1.076926	-1.610876	-0.328819
17	7	0	0.444050	1.229523	-1.107632
18	29	0	0.900384	-0.674314	-0.289547
19	7	0	2.246607	-2.005013	-1.150828
20	16	0	3.134472	-2.768126	0.144764
21	8	0	2.228939	-2.727780	1.277750
22	8	0	3.692378	-4.028100	-0.332974
23	6	0	4.455273	-1.605496	0.349140
24	6	0	4.175911	-0.288563	0.714902
25	6	0	5.762416	-2.041673	0.157919
26	6	0	5.229567	0.595415	0.885579
27	1	0	3.149596	0.044563	0.876124
28	6	0	6.803968	-1.140625	0.342274
29	1	0	5.953070	-3.075070	-0.124062
30	6	0	6.555594	0.183497	0.708837
31	1	0	5.019624	1.627411	1.167731
32	1	0	7.832416	-1.471773	0.200377
33	6	0	7.680385	1.147361	0.930813
34	1	0	7.476766	2.117492	0.460100
35	1	0	7.827509	1.337491	2.002959
36	1	0	8.626716	0.765309	0.530965
37	35	0	-2.709953	3.733260	-1.542867
38	35	0	0.558386	4.966742	-2.788757
39	35	0	2.960241	2.267880	-1.898065
40	35	0	1.990890	-0.119191	3.659181
41	35	0	-0.950816	1.309862	5.404916
42	35	0	-3.458633	1.841111	2.732031
43	35	0	-4.820706	-0.340935	-1.217964
44	35	0	-4.263240	-4.010663	-1.279411
45	35	0	-0.709644	-4.421124	-0.242629
46	1	0	2.048866	-3.984353	-2.025011
47	6	0	1.830977	-2.939281	-2.246538
48	6	0	2.993305	-2.019946	-2.447643
49	6	0	0.592581	-2.620194	-2.966084
50	6	0	2.825670	-0.878444	-3.349245
51	1	0	3.989820	-2.457907	-2.362294

52	6	0	0.486032	-1.482300	-3.678512
53	1	0	-0.212430	-3.351893	-2.950635
54	6	0	1.617431	-0.598357	-3.872603
55	1	0	3.703077	-0.287322	-3.601607
56	1	0	-0.442956	-1.256820	-4.199984
57	1	0	1.495888	0.268832	-4.520502

Zero-point correction= 0.345360 (Hartree/Particle)
Thermal correction to Energy= 0.390404
Thermal correction to Enthalpy= 0.391348
Thermal correction to Gibbs Free Energy= 0.256591
Sum of electronic and zero-point Energies= -2116.543274
Sum of electronic and thermal Energies= -2116.498230
Sum of electronic and thermal Enthalpies= -2116.497286
Sum of electronic and thermal Free Energies= -2116.632043

^{1}TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.064411	-0.125147	-0.708888
2	1	0	-3.142311	-0.280792	-1.190378
3	7	0	-1.025555	-1.050806	-1.414819
4	6	0	-1.212386	-2.258052	-1.985044
5	6	0	-0.015577	-2.683695	-2.535515
6	6	0	0.866572	-1.641400	-2.227796
7	7	0	-2.097538	-0.479071	0.798813
8	6	0	-3.132589	-0.525803	1.661480
9	6	0	-1.257502	-0.721097	2.760724
10	6	0	-2.643587	-0.691191	2.944317
11	7	0	-1.626816	1.350273	-0.873497
12	6	0	-2.229121	2.363756	-1.532185
13	6	0	-1.445322	3.496640	-1.436519
14	6	0	-0.347005	3.075947	-0.678452
15	7	0	-0.458111	1.803495	-0.335732
16	7	0	-0.927820	-0.596033	1.484722
17	7	0	0.272113	-0.676669	-1.552835
18	29	0	0.824141	0.438648	0.453844
19	7	0	2.459363	-0.502982	1.109801
20	16	0	3.197139	0.551924	2.129534
21	8	0	2.327027	1.734356	2.121764
22	8	0	3.572845	-0.087313	3.397068
23	6	0	4.715141	1.027807	1.323798
24	6	0	4.676754	1.420599	-0.014175
25	6	0	5.910077	1.007266	2.031121
26	6	0	5.856476	1.789548	-0.640365
27	1	0	3.730142	1.420226	-0.555278
28	6	0	7.085128	1.383212	1.385909
29	1	0	5.910033	0.696399	3.074358
30	6	0	7.076061	1.779121	0.049094
31	1	0	5.839538	2.093265	-1.687665
32	1	0	8.028505	1.370469	1.932364
33	6	0	8.338425	2.200011	-0.641108
34	1	0	8.435863	1.727534	-1.627345
35	1	0	8.357246	3.286328	-0.805206
36	1	0	9.226375	1.940977	-0.052286
37	35	0	-2.883536	-3.174752	-1.961216
38	35	0	0.341669	-4.316519	-3.454701
39	35	0	2.710358	-1.483134	-2.711734
40	35	0	1.174476	4.103566	-0.179152
41	35	0	-1.790038	5.223438	-2.155167
42	35	0	-3.907921	2.209226	-2.421333
43	35	0	-4.954605	-0.366509	1.127951
44	35	0	-3.625894	-0.848325	4.566023
45	35	0	0.088036	-0.906393	4.104670
46	1	0	2.534910	-2.018641	2.609829
47	6	0	2.626234	-1.924358	1.503326

48	6	0	3.990815	-2.306245	1.098536
49	6	0	1.551981	-2.738855	0.902360
50	6	0	4.235575	-3.279547	0.161911
51	1	0	4.807608	-1.742686	1.548413
52	6	0	1.817749	-3.758673	0.041385
53	1	0	0.529072	-2.466386	1.165903
54	6	0	3.153491	-3.996240	-0.358109
55	1	0	5.244375	-3.488354	-0.185458
56	1	0	1.015314	-4.347941	-0.397413
57	1	0	3.339217	-4.763484	-1.110357

Zero-point correction= 0.344235 (Hartree/Particle)
Thermal correction to Energy= 0.388655
Thermal correction to Enthalpy= 0.389599
Thermal correction to Gibbs Free Energy= 0.257999
Sum of electronic and zero-point Energies= -2116.510635
Sum of electronic and thermal Energies= -2116.466215
Sum of electronic and thermal Enthalpies= -2116.465271
Sum of electronic and thermal Free Energies= -2116.596871

[1]INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.908419	-0.102936	-1.049363
2	1	0	-2.877790	-0.252862	-1.726727
3	7	0	-0.681693	-0.825970	-1.681589
4	6	0	-0.635994	-2.035400	-2.278975
5	6	0	0.680572	-2.340171	-2.575536
6	6	0	1.380962	-1.228833	-2.091288
7	7	0	-2.144034	-0.710816	0.362248
8	6	0	-3.281516	-0.998823	1.025889
9	6	0	-1.575997	-1.230842	2.365939
10	6	0	-2.968574	-1.348498	2.328296
11	7	0	-1.606527	1.408408	-0.884413
12	6	0	-2.255765	2.477126	-1.394942
13	6	0	-1.687160	3.635278	-0.901015
14	6	0	-0.667345	3.171839	-0.064180
15	7	0	-0.622396	1.849422	-0.047843
16	7	0	-1.082355	-0.852230	1.198965
17	7	0	0.576227	-0.331299	-1.556187
18	29	0	0.699897	0.545633	0.706057
19	7	0	2.335955	-0.292702	1.356651
20	16	0	3.229644	0.627437	2.378904
21	8	0	2.387724	1.738692	2.799760
22	8	0	3.880386	-0.235466	3.375367
23	6	0	4.521655	1.295037	1.346245
24	6	0	4.166549	1.994080	0.195343
25	6	0	5.858749	1.112095	1.686129
26	6	0	5.165663	2.497424	-0.626261
27	1	0	3.114911	2.130857	-0.058868
28	6	0	6.846207	1.627007	0.855024
29	1	0	6.110368	0.575336	2.599813
30	6	0	6.516127	2.322382	-0.311341
31	1	0	4.894158	3.040363	-1.531596
32	1	0	7.896645	1.492125	1.116263
33	6	0	7.595034	2.863897	-1.200258
34	1	0	7.179716	3.443994	-2.032371
35	1	0	8.279248	3.517664	-0.643297
36	1	0	8.203946	2.055892	-1.628450
37	35	0	-2.178633	-3.111666	-2.589616
38	35	0	1.367747	-3.906387	-3.416327
39	35	0	3.275749	-0.933569	-2.126934
40	35	0	0.565176	4.203919	0.951076
41	35	0	-2.189270	5.434130	-1.259328
42	35	0	-3.732551	2.358088	-2.592773
43	35	0	-5.008553	-0.928178	0.225688

44	35	0	-4.152722	-1.877488	3.720278
45	35	0	-0.411855	-1.556080	3.848619
46	1	0	2.611548	-2.111563	2.341809
47	6	0	2.674533	-1.655265	1.274578
48	6	0	4.056186	-2.139194	1.124657
49	6	0	1.644057	-2.564135	0.778601
50	6	0	4.317243	-3.433190	0.738586
51	1	0	4.861490	-1.480886	1.441117
52	6	0	1.943353	-3.846261	0.375478
53	1	0	0.615087	-2.202084	0.823372
54	6	0	3.271678	-4.276095	0.343998
55	1	0	5.344654	-3.787572	0.700905
56	1	0	1.142946	-4.512009	0.059230
57	1	0	3.497309	-5.290121	0.017945

Zero-point correction= 0.341642 (Hartree/Particle)
Thermal correction to Energy= 0.387187
Thermal correction to Enthalpy= 0.388131
Thermal correction to Gibbs Free Energy= 0.251883
Sum of electronic and zero-point Energies= -2116.522340
Sum of electronic and thermal Energies= -2116.476795
Sum of electronic and thermal Enthalpies= -2116.475850
Sum of electronic and thermal Free Energies= -2116.612099

^{1}TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.743311	-0.022815	-1.113891
2	1	0	-2.635454	-0.139940	-1.895352
3	7	0	-0.435106	-0.640287	-1.681569
4	6	0	-0.296939	-1.767602	-2.409982
5	6	0	1.048182	-1.997395	-2.630536
6	6	0	1.667222	-0.935003	-1.962587
7	7	0	-2.100560	-0.778160	0.197087
8	6	0	-3.276521	-1.233296	0.669901
9	6	0	-1.707495	-1.604323	2.137669
10	6	0	-3.076979	-1.785444	1.924343
11	7	0	-1.522754	1.471479	-0.774907
12	6	0	-2.149274	2.563016	-1.262996
13	6	0	-1.715941	3.680917	-0.577113
14	6	0	-0.798843	3.168366	0.344477
15	7	0	-0.681903	1.853536	0.230830
16	7	0	-1.124925	-1.004322	1.113545
17	7	0	0.791095	-0.129643	-1.387451
18	29	0	0.582072	0.465509	0.981160
19	7	0	2.187841	-0.360697	1.764663
20	16	0	3.144064	0.683872	2.662109
21	8	0	2.230485	1.714235	3.125547
22	8	0	3.960691	-0.071203	3.611418
23	6	0	4.205047	1.391081	1.430157
24	6	0	3.651183	2.282930	0.510497
25	6	0	5.547710	1.038753	1.371135
26	6	0	4.457073	2.804777	-0.486735
27	1	0	2.600059	2.561625	0.583637
28	6	0	6.340997	1.572248	0.360019
29	1	0	5.967512	0.378226	2.127617
30	6	0	5.808733	2.451602	-0.583398
31	1	0	4.033444	3.498497	-1.213016
32	1	0	7.397062	1.307624	0.307776
33	6	0	6.653348	3.005550	-1.689658
34	1	0	6.574076	4.099043	-1.744688
35	1	0	7.711041	2.748543	-1.560672
36	1	0	6.329949	2.613423	-2.663935
37	35	0	-1.768877	-2.851048	-2.953372
38	35	0	1.855599	-3.441053	-3.574852
39	35	0	3.549141	-0.608483	-1.823204

40	35	0	0.196497	4.150456	1.633176
41	35	0	-2.251136	5.488857	-0.822927
42	35	0	-3.417579	2.521884	-2.682555
43	35	0	-4.917544	-1.076779	-0.284256
44	35	0	-4.358841	-2.606311	3.064422
45	35	0	-0.679642	-2.122433	3.668312
46	1	0	2.123188	-1.690741	2.509799
47	6	0	2.668383	-1.720107	1.452166
48	6	0	4.011279	-2.194832	1.626722
49	6	0	1.764385	-2.542734	0.701644
50	6	0	4.372589	-3.432386	1.135627
51	1	0	4.711753	-1.605138	2.207442
52	6	0	2.156735	-3.777846	0.230754
53	1	0	0.746737	-2.183466	0.557299
54	6	0	3.464771	-4.219483	0.424102
55	1	0	5.387140	-3.789752	1.298815
56	1	0	1.443067	-4.388549	-0.318929
57	1	0	3.776146	-5.185463	0.031877

Zero-point correction= 0.340389 (Hartree/Particle)
Thermal correction to Energy= 0.385404
Thermal correction to Enthalpy= 0.386348
Thermal correction to Gibbs Free Energy= 0.253210
Sum of electronic and zero-point Energies= -2116.507298
Sum of electronic and thermal Energies= -2116.462283
Sum of electronic and thermal Enthalpies= -2116.461339
Sum of electronic and thermal Free Energies= -2116.594477

[1]INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.181473	0.047620	0.473958
2	1	0	-3.303637	0.118392	0.852775
3	7	0	-1.279638	-0.407446	1.649487
4	6	0	-1.632005	-0.668447	2.926805
5	6	0	-0.516782	-1.084574	3.626044
6	6	0	0.498661	-1.046397	2.665174
7	7	0	-1.722841	1.437867	-0.037928
8	6	0	-2.427908	2.582946	-0.156559
9	6	0	-0.420639	2.874715	-0.955101
10	6	0	-1.628356	3.545620	-0.742564
11	7	0	-2.106795	-0.980172	-0.682425
12	6	0	-3.087756	-1.686442	-1.283378
13	6	0	-2.539748	-2.446731	-2.299836
14	6	0	-1.178299	-2.133040	-2.247548
15	7	0	-0.921614	-1.261379	-1.286984
16	7	0	-0.468424	1.623103	-0.534266
17	7	0	0.053802	-0.640280	1.486963
18	29	0	0.730052	-0.243802	-0.602434
19	7	0	2.660428	0.148892	-1.273019
20	16	0	3.478888	-1.437790	-1.381406
21	8	0	2.824732	-2.277023	-0.396979
22	8	0	3.457903	-1.736561	-2.804948
23	6	0	5.137408	-1.131436	-0.866168
24	6	0	5.417856	-1.054095	0.496403
25	6	0	6.117549	-0.908646	-1.827552
26	6	0	6.704318	-0.727141	0.893193
27	1	0	4.633370	-1.249845	1.225872
28	6	0	7.404276	-0.597159	-1.407666
29	1	0	5.868699	-0.992299	-2.883990
30	6	0	7.711640	-0.488706	-0.049035
31	1	0	6.939737	-0.659680	1.955113
32	1	0	8.187999	-0.435134	-2.147300
33	6	0	9.090116	-0.111837	0.399160
34	1	0	9.831371	-0.265611	-0.393473
35	1	0	9.130827	0.947857	0.687586

36	1	0	9.400759	-0.694202	1.275393
37	35	0	-3.399914	-0.465632	3.612208
38	35	0	-0.392652	-1.587457	5.456375
39	35	0	2.325575	-1.525236	2.967269
40	35	0	0.224410	-2.784579	-3.354365
41	35	0	-3.430688	-3.632385	-3.490385
42	35	0	-4.923225	-1.594914	-0.777713
43	35	0	-4.236295	2.788159	0.409972
44	35	0	-2.078652	5.343397	-1.173750
45	35	0	1.152392	3.597983	-1.768916
46	1	0	2.573824	0.428615	-2.256104
47	6	0	3.349858	1.184173	-0.534139
48	6	0	4.354779	1.926624	-1.152686
49	6	0	3.003877	1.432560	0.788583
50	6	0	5.015198	2.919745	-0.442406
51	1	0	4.614729	1.722807	-2.192655
52	6	0	3.678048	2.419262	1.500629
53	1	0	2.194304	0.865573	1.246754
54	6	0	4.682120	3.161951	0.888630
55	1	0	5.793549	3.504726	-0.928618
56	1	0	3.404551	2.614257	2.535685
57	1	0	5.199551	3.941475	1.444663

Zero-point correction= 0.345571 (Hartree/Particle)
Thermal correction to Energy= 0.390909
Thermal correction to Enthalpy= 0.391853
Thermal correction to Gibbs Free Energy= 0.256285
Sum of electronic and zero-point Energies= -2116.598999
Sum of electronic and thermal Energies= -2116.553661
Sum of electronic and thermal Enthalpies= -2116.552717
Sum of electronic and thermal Free Energies= -2116.688285

^{3}TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.779701	0.358172	-0.656593
2	1	0	-2.871924	0.434515	-1.115671
3	7	0	-1.067369	-0.897149	-1.221413
4	6	0	-1.518449	-1.830200	-2.083159
5	6	0	-0.475119	-2.663995	-2.435053
6	6	0	0.613076	-2.161043	-1.714456
7	7	0	-1.864959	0.293735	0.883946
8	6	0	-2.939580	0.357875	1.696987
9	6	0	-1.110397	0.407380	2.892998
10	6	0	-2.506355	0.427740	3.007835
11	7	0	-0.947230	1.614992	-1.048668
12	6	0	-1.317574	2.735938	-1.700806
13	6	0	-0.228352	3.580823	-1.810080
14	6	0	0.799179	2.879101	-1.174019
15	7	0	0.368755	1.714173	-0.715338
16	7	0	-0.728979	0.317090	1.630080
17	7	0	0.255213	-1.113729	-0.987486
18	29	0	1.175478	0.165357	0.402215
19	7	0	2.439782	-1.183730	1.106021
20	16	0	3.263967	-0.099582	2.013901
21	8	0	2.532576	1.177802	1.671682
22	8	0	3.441032	-0.430814	3.421642
23	6	0	4.859247	-0.003269	1.254644
24	6	0	4.965482	0.369018	-0.084828
25	6	0	5.984645	-0.322519	2.007552
26	6	0	6.222690	0.424363	-0.666759
27	1	0	4.077803	0.621415	-0.664566
28	6	0	7.234691	-0.255621	1.407758
29	1	0	5.868115	-0.604851	3.051843
30	6	0	7.372222	0.111789	0.066468
31	1	0	6.319320	0.718545	-1.711716

32	1	0	8.124882	-0.493455	1.990335
33	6	0	8.725383	0.148193	-0.575463
34	1	0	9.040696	-0.857934	-0.885899
35	1	0	8.732804	0.782520	-1.469621
36	1	0	9.488363	0.524758	0.117041
37	35	0	-3.334946	-1.972113	-2.636936
38	35	0	-0.519569	-4.159387	-3.609044
39	35	0	2.405190	-2.799119	-1.780669
40	35	0	2.611665	3.422221	-0.975872
41	35	0	-0.152782	5.292360	-2.632014
42	35	0	-3.083562	3.055778	-2.333461
43	35	0	-4.739407	0.344088	1.066999
44	35	0	-3.556607	0.534192	4.588941
45	35	0	0.164846	0.488331	4.303413
46	1	0	1.711756	-2.016338	1.967296
47	6	0	1.123377	-2.868975	2.671048
48	1	0	0.765557	-2.288278	3.528022
49	1	0	1.962804	-3.521514	2.935649
50	6	0	0.100333	-3.469457	1.824437
51	6	0	-1.204162	-2.946232	1.790071
52	6	0	0.414885	-4.534979	0.962311
53	6	0	-2.153560	-3.456701	0.918065
54	1	0	-1.462186	-2.132582	2.468518
55	6	0	-0.538247	-5.056052	0.100701
56	1	0	1.426516	-4.942010	0.975571
57	6	0	-1.822391	-4.510245	0.065489
58	1	0	-2.563072	-4.900839	-0.631954
59	1	0	-3.156106	-3.028222	0.897326
60	1	0	-0.279613	-5.882007	-0.560334

Zero-point correction= 0.365222 (Hartree/Particle)
Thermal correction to Energy= 0.411483
Thermal correction to Enthalpy= 0.412427
Thermal correction to Gibbs Free Energy= 0.276071
Sum of electronic and zero-point Energies= -2155.750252
Sum of electronic and thermal Energies= -2155.703991
Sum of electronic and thermal Enthalpies= -2155.703047
Sum of electronic and thermal Free Energies= -2155.839404

^{3}INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.785578	0.819848	0.237646
2	1	0	2.856165	1.203232	0.577180
3	7	0	1.002623	0.287301	1.468389
4	6	0	1.365838	0.203812	2.762379
5	6	0	0.275651	-0.193426	3.512648
6	6	0	-0.745311	-0.337699	2.567786
7	7	0	1.930417	-0.291726	-0.819214
8	6	0	3.025057	-0.934901	-1.274132
9	6	0	1.252679	-1.684883	-2.309520
10	6	0	2.641021	-1.843725	-2.240583
11	7	0	0.965088	1.999325	-0.363527
12	6	0	1.301093	3.296416	-0.513071
13	6	0	0.216334	3.994172	-1.012402
14	6	0	-0.777518	3.019883	-1.139070
15	7	0	-0.328427	1.832661	-0.756695
16	7	0	0.829815	-0.766536	-1.459094
17	7	0	-0.307131	-0.055724	1.351127
18	29	0	-1.112260	-0.049876	-0.614077
19	7	0	-2.198007	-1.677885	-0.422054
20	16	0	-3.175797	-1.330190	-1.668293
21	8	0	-2.593567	-0.003594	-2.102632
22	8	0	-3.354396	-2.376912	-2.664991
23	6	0	-4.753433	-0.949517	-0.965355
24	6	0	-4.874547	0.139014	-0.104332

25	6	0	-5.846706	-1.752546	-1.270344
26	6	0	-6.109990	0.413385	0.462369
27	1	0	-4.012201	0.768224	0.114979
28	6	0	-7.077488	-1.457537	-0.698955
29	1	0	-5.726550	-2.585845	-1.959293
30	6	0	-7.226205	-0.379681	0.177111
31	1	0	-6.216749	1.263642	1.135763
32	1	0	-7.944268	-2.073502	-0.939252
33	6	0	-8.553833	-0.091670	0.809597
34	1	0	-8.734798	-0.755541	1.666558
35	1	0	-8.611719	0.939596	1.177139
36	1	0	-9.377888	-0.248414	0.102506
37	35	0	3.131249	0.554915	3.382613
38	35	0	0.208934	-0.538988	5.381481
39	35	0	-2.556846	-0.816357	2.906484
40	35	0	-2.566699	3.279481	-1.725296
41	35	0	0.098533	5.845758	-1.421435
42	35	0	3.013098	4.000870	-0.073761
43	35	0	4.786760	-0.621534	-0.620347
44	35	0	3.731104	-3.081857	-3.186271
45	35	0	0.033129	-2.595292	-3.451503
46	1	0	-1.693842	-2.557664	-0.604824
47	6	0	-0.957736	-4.739261	-0.525484
48	1	0	-0.628359	-5.009521	-1.526544
49	1	0	-1.993317	-4.950552	-0.260410
50	6	0	-0.066715	-4.198564	0.413739
51	6	0	1.292052	-3.939203	0.082327
52	6	0	-0.493367	-3.879710	1.733198
53	6	0	2.164414	-3.407246	1.014175
54	1	0	1.641894	-4.182809	-0.922410
55	6	0	0.390387	-3.362168	2.659675
56	1	0	-1.535431	-4.056875	2.002605
57	6	0	1.724907	-3.120453	2.311590
58	1	0	2.415370	-2.711308	3.049311
59	1	0	3.204973	-3.231406	0.738557
60	1	0	0.046435	-3.140746	3.670493

Zero-point correction= 0.369216 (Hartree/Particle)
Thermal correction to Energy= 0.416246
Thermal correction to Enthalpy= 0.417190
Thermal correction to Gibbs Free Energy= 0.278630
Sum of electronic and zero-point Energies= -2155.777813
Sum of electronic and thermal Energies= -2155.730783
Sum of electronic and thermal Enthalpies= -2155.729839
Sum of electronic and thermal Free Energies= -2155.868399

[1]INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.317416	1.198421	0.547378
2	1	0	2.147976	1.876028	1.061726
3	7	0	0.393938	0.597914	1.647454
4	6	0	0.488989	0.663669	2.991745
5	6	0	-0.632338	0.078717	3.552371
6	6	0	-1.376478	-0.320991	2.439216
7	7	0	2.014518	0.075060	-0.269234
8	6	0	3.299520	-0.340747	-0.267652
9	6	0	2.209396	-1.352735	-1.858523
10	6	0	3.480242	-1.259158	-1.284870
11	7	0	0.447606	2.072925	-0.399190
12	6	0	0.546177	3.396591	-0.655449
13	6	0	-0.410803	3.752995	-1.585319
14	6	0	-1.071506	2.549798	-1.849908
15	7	0	-0.573288	1.551298	-1.142610
16	7	0	1.337285	-0.572979	-1.251011
17	7	0	-0.765211	-0.024491	1.305129

18	29	0	-0.868856	-0.492915	-0.855278
19	7	0	-1.372514	-2.436827	-1.328443
20	16	0	-2.834895	-2.561872	-2.276086
21	8	0	-2.590283	-1.669077	-3.394320
22	8	0	-3.127272	-3.973735	-2.478632
23	6	0	-4.051259	-1.884160	-1.188711
24	6	0	-4.190752	-0.500250	-1.101271
25	6	0	-4.878023	-2.745926	-0.475883
26	6	0	-5.166711	0.021349	-0.267455
27	1	0	-3.556983	0.157040	-1.695899
28	6	0	-5.847836	-2.202255	0.357826
29	1	0	-4.767248	-3.822629	-0.589376
30	6	0	-5.998568	-0.818058	0.481527
31	1	0	-5.283916	1.102331	-0.189821
32	1	0	-6.503755	-2.863269	0.924103
33	6	0	-7.000432	-0.239675	1.431743
34	1	0	-6.514408	0.027285	2.381655
35	1	0	-7.454163	0.676401	1.034602
36	1	0	-7.802642	-0.950726	1.660703
37	35	0	1.954548	1.446408	3.923834
38	35	0	-1.063472	-0.111567	5.395194
39	35	0	-3.053050	-1.237224	2.444955
40	35	0	-2.495952	2.277456	-3.088360
41	35	0	-0.755541	5.472595	-2.319396
42	35	0	1.807276	4.555756	0.179807
43	35	0	4.594815	0.219807	1.011795
44	35	0	5.067069	-2.200099	-1.749516
45	35	0	1.678161	-2.410675	-3.365909
46	1	0	-0.636273	-2.625904	-2.027660
47	6	0	-1.272139	-3.456239	-0.233838
48	1	0	-1.666296	-4.412091	-0.608431
49	1	0	-1.912843	-3.109378	0.586475
50	6	0	0.152299	-3.611129	0.215931
51	6	0	1.031997	-4.402101	-0.526745
52	6	0	0.629020	-2.957897	1.352667
53	6	0	2.369955	-4.504547	-0.163085
54	1	0	0.664056	-4.934379	-1.406127
55	6	0	1.967473	-3.054771	1.718444
56	1	0	-0.056293	-2.369161	1.959814
57	6	0	2.842028	-3.823697	0.956422
58	1	0	3.893953	-3.888893	1.231736
59	1	0	3.048550	-5.109439	-0.762628
60	1	0	2.326060	-2.527333	2.602395

Zero-point correction= 0.376197 (Hartree/Particle)
Thermal correction to Energy= 0.422133
Thermal correction to Enthalpy= 0.423077
Thermal correction to Gibbs Free Energy= 0.287919
Sum of electronic and zero-point Energies= -2155.861016
Sum of electronic and thermal Energies= -2155.815080
Sum of electronic and thermal Enthalpies= -2155.814136
Sum of electronic and thermal Free Energies= -2155.949293

^{3}TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.022637	-0.126575	-0.685016
2	1	0	-3.077137	-0.359582	-1.180718
3	7	0	-0.906436	-0.952892	-1.381517
4	6	0	-0.999750	-2.049835	-2.158809
5	6	0	0.257940	-2.372458	-2.634124
6	6	0	1.085504	-1.396456	-2.068763
7	7	0	-2.069658	-0.480475	0.820698
8	6	0	-3.115024	-0.813048	1.604721
9	6	0	-1.319480	-0.606846	2.833362
10	6	0	-2.682159	-0.913315	2.913513

11	7	0	-1.684631	1.382932	-0.828965
12	6	0	-2.343842	2.367766	-1.473176
13	6	0	-1.639656	3.549871	-1.338590
14	6	0	-0.525914	3.187170	-0.575644
15	7	0	-0.557460	1.900499	-0.266916
16	7	0	-0.952082	-0.351789	1.586987
17	7	0	0.394055	-0.557190	-1.317421
18	29	0	0.773405	0.559598	0.559974
19	7	0	2.433312	-0.385412	0.978841
20	16	0	2.986013	0.711774	2.071806
21	8	0	1.924326	1.771452	1.989933
22	8	0	3.343228	0.208487	3.396322
23	6	0	4.453449	1.348791	1.314840
24	6	0	4.369579	1.954434	0.059980
25	6	0	5.672945	1.201269	1.965723
26	6	0	5.528887	2.424930	-0.534189
27	1	0	3.408221	2.046855	-0.445718
28	6	0	6.824274	1.680872	1.353115
29	1	0	5.706686	0.725204	2.943679
30	6	0	6.770125	2.298103	0.102319
31	1	0	5.477696	2.899211	-1.514395
32	1	0	7.786415	1.574870	1.854242
33	6	0	8.010320	2.833190	-0.545709
34	1	0	8.916166	2.406108	-0.099672
35	1	0	8.026265	2.619012	-1.621774
36	1	0	8.073247	3.924822	-0.435267
37	35	0	-2.635371	-2.970431	-2.483129
38	35	0	0.738656	-3.815591	-3.779025
39	35	0	2.959929	-1.180695	-2.340191
40	35	0	0.909776	4.308777	-0.027844
41	35	0	-2.086006	5.264505	-2.025791
42	35	0	-3.984514	2.113242	-2.403718
43	35	0	-4.884068	-1.077722	0.948201
44	35	0	-3.700123	-1.355267	4.457281
45	35	0	-0.072435	-0.528910	4.269693
46	6	0	4.037805	-3.554045	0.723694
47	6	0	3.049820	-4.152183	-0.083617
48	6	0	1.702441	-3.820254	0.144908
49	6	0	1.348047	-2.901440	1.109375
50	6	0	2.350588	-2.227835	1.863333
51	6	0	3.704981	-2.640581	1.695809
52	1	0	5.079718	-3.840119	0.576771
53	1	0	0.930669	-4.321101	-0.442292
54	1	0	0.300294	-2.656017	1.281840
55	1	0	2.071373	-1.762996	2.806169
56	1	0	4.467530	-2.188198	2.328905
57	6	0	3.427784	-5.106604	-1.169268
58	1	0	4.358875	-5.638312	-0.936298
59	1	0	2.639625	-5.848224	-1.351081
60	1	0	3.585940	-4.570387	-2.117971

Zero-point correction= 0.369046 (Hartree/Particle)
Thermal correction to Energy= 0.415893
Thermal correction to Enthalpy= 0.416837
Thermal correction to Gibbs Free Energy= 0.278128
Sum of electronic and zero-point Energies= -2155.747077
Sum of electronic and thermal Energies= -2155.700229
Sum of electronic and thermal Enthalpies= -2155.699285
Sum of electronic and thermal Free Energies= -2155.837994

^{3}INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.972628	-0.200426	-0.809920
2	1	0	-2.971134	-0.504227	-1.378573
3	7	0	-0.762468	-0.928939	-1.455419

4	6	0	-0.735017	-2.058171	-2.190405
5	6	0	0.564696	-2.301102	-2.595678
6	6	0	1.289731	-1.249340	-2.027417
7	7	0	-2.061230	-0.579626	0.691059
8	6	0	-3.059795	-1.108652	1.425024
9	6	0	-1.368809	-0.639870	2.730957
10	6	0	-2.661133	-1.174638	2.747886
11	7	0	-1.749391	1.334038	-0.901055
12	6	0	-2.530467	2.291247	-1.442568
13	6	0	-1.929763	3.523602	-1.264610
14	6	0	-0.750512	3.224299	-0.575994
15	7	0	-0.650349	1.922724	-0.351206
16	7	0	-1.011644	-0.287695	1.505176
17	7	0	0.502023	-0.436952	-1.342733
18	29	0	0.693397	0.672043	0.547704
19	7	0	2.281593	-0.285033	1.171756
20	16	0	2.862422	0.931225	2.101363
21	8	0	1.832827	1.986558	1.819471
22	8	0	3.166058	0.588127	3.485845
23	6	0	4.357214	1.473283	1.326285
24	6	0	4.300591	1.979903	0.027465
25	6	0	5.560549	1.380937	2.014354
26	6	0	5.472746	2.396709	-0.579790
27	1	0	3.345791	2.051555	-0.492926
28	6	0	6.726601	1.807393	1.388771
29	1	0	5.570239	0.995550	3.032132
30	6	0	6.701044	2.315878	0.089731
31	1	0	5.442237	2.799185	-1.592597
32	1	0	7.675968	1.750054	1.920874
33	6	0	7.958071	2.766074	-0.589681
34	1	0	8.806560	2.791370	0.103604
35	1	0	8.224323	2.093853	-1.417014
36	1	0	7.841629	3.769332	-1.020030
37	35	0	-2.276748	-3.125724	-2.518801
38	35	0	1.212546	-3.746328	-3.647949
39	35	0	3.159845	-0.927201	-2.189355
40	35	0	0.598497	4.443845	-0.025442
41	35	0	-2.561948	5.228196	-1.817693
42	35	0	-4.203148	1.940585	-2.280191
43	35	0	-4.739382	-1.631453	0.698299
44	35	0	-3.644007	-1.833710	4.234524
45	35	0	-0.194697	-0.394264	4.207103
46	6	0	4.157835	-3.166486	0.859361
47	6	0	3.224059	-3.912488	0.086514
48	6	0	1.851674	-3.597330	0.229434
49	6	0	1.418020	-2.563035	1.006547
50	6	0	2.358069	-1.666251	1.746560
51	6	0	3.779582	-2.142321	1.666688
52	1	0	5.211073	-3.449945	0.811817
53	1	0	1.118442	-4.206150	-0.305528
54	1	0	0.351945	-2.353476	1.097749
55	1	0	2.046414	-1.610939	2.808767
56	1	0	4.510662	-1.608280	2.273883
57	6	0	3.686707	-4.967300	-0.862482
58	1	0	4.591661	-5.472686	-0.499506
59	1	0	2.913427	-5.726953	-1.036231
60	1	0	3.932111	-4.534184	-1.846628

Zero-point correction= 0.371305 (Hartree/Particle)
Thermal correction to Energy= 0.417660
Thermal correction to Enthalpy= 0.418604
Thermal correction to Gibbs Free Energy= 0.281524
Sum of electronic and zero-point Energies= -2155.766641
Sum of electronic and thermal Energies= -2155.720286
Sum of electronic and thermal Enthalpies= -2155.719341
Sum of electronic and thermal Free Energies= -2155.856421

[1]INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.579222	-1.068396	0.052431
2	1	0	-2.523887	-1.769908	0.228212
3	7	0	-0.566709	-1.280290	1.214969
4	6	0	-0.559433	-2.211105	2.193682
5	6	0	0.690615	-2.234485	2.780720
6	6	0	1.404376	-1.267177	2.064072
7	7	0	-2.049393	0.413600	-0.023137
8	6	0	-3.161503	0.992904	0.471220
9	6	0	-2.111640	2.410133	-0.814654
10	6	0	-3.254040	2.283874	-0.016724
11	7	0	-0.879625	-1.438665	-1.280583
12	6	0	-1.258398	-2.348382	-2.206465
13	6	0	-0.390431	-2.292965	-3.277048
14	6	0	0.512967	-1.289525	-2.908465
15	7	0	0.235716	-0.781537	-1.722069
16	7	0	-1.387564	1.306641	-0.806490
17	7	0	0.656296	-0.688151	1.142365
18	29	0	0.735738	0.906427	-0.346024
19	7	0	1.617471	2.673755	0.331976
20	16	0	2.790570	3.164068	-0.868487
21	8	0	2.134550	2.918135	-2.140151
22	8	0	3.304669	4.482376	-0.516964
23	6	0	4.050424	1.958989	-0.580856
24	6	0	3.901169	0.689991	-1.134354
25	6	0	5.153460	2.285128	0.201853
26	6	0	4.867916	-0.270203	-0.884101
27	1	0	3.046876	0.464164	-1.769549
28	6	0	6.107105	1.304551	0.449418
29	1	0	5.270379	3.295461	0.589029
30	6	0	5.973311	0.016587	-0.076583
31	1	0	4.754469	-1.266805	-1.312125
32	1	0	6.977433	1.543344	1.060362
33	6	0	6.968782	-1.055967	0.240513
34	1	0	7.888568	-0.646134	0.673333
35	1	0	6.547164	-1.767961	0.965090
36	1	0	7.237811	-1.633077	-0.653025
37	35	0	-2.073092	-3.268408	2.665317
38	35	0	1.287148	-3.296581	4.241552
39	35	0	3.248458	-0.818945	2.297632
40	35	0	1.973909	-0.657302	-3.964452
41	35	0	-0.411787	-3.335306	-4.868356
42	35	0	-2.747027	-3.523434	-2.010859
43	35	0	-4.316644	0.124934	1.713701
44	35	0	-4.570686	3.597099	0.387669
45	35	0	-1.554220	3.915390	-1.849459
46	6	0	1.583283	2.199120	2.826220
47	6	0	0.280372	1.962896	3.090944
48	6	0	-0.743939	2.720526	2.388138
49	6	0	-0.449161	3.642918	1.454105
50	6	0	0.929762	3.829022	0.995007
51	6	0	1.993332	3.073540	1.727073
52	1	0	2.361134	1.759363	3.447375
53	1	0	-1.779044	2.596221	2.715265
54	1	0	-1.214291	4.313763	1.067824
55	1	0	1.200911	4.792319	0.562317
56	1	0	2.976288	3.542694	1.789004
57	6	0	-0.169175	1.013343	4.154292
58	1	0	0.675566	0.537326	4.668037
59	1	0	-0.791890	1.518867	4.905682
60	1	0	-0.791004	0.216345	3.715095

Zero-point correction= 0.373593 (Hartree/Particle)
Thermal correction to Energy= 0.419616
Thermal correction to Enthalpy= 0.420560
Thermal correction to Gibbs Free Energy= 0.285976

Sum of electronic and zero-point Energies= -2155.806608
Sum of electronic and thermal Energies= -2155.760586
Sum of electronic and thermal Enthalpies= -2155.759641
Sum of electronic and thermal Free Energies= -2155.894225

κ^2N,O-^{1}**INT1-a** (B3LYP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.317458	-0.066517	0.012398
2	1	0	-3.516110	-0.127193	-0.014724
3	7	0	-1.712562	-1.230195	-0.830566
4	6	0	-2.312589	-2.313006	-1.367514
5	6	0	-1.338797	-3.143658	-1.910235
6	6	0	-0.127886	-2.487445	-1.654469
7	7	0	-1.789136	-0.161006	1.452061
8	6	0	-2.468907	-0.319459	2.614680
9	6	0	-0.302289	-0.229294	3.013351
10	6	0	-1.550499	-0.367636	3.650110
11	7	0	-1.832696	1.266713	-0.620566
12	6	0	-2.523105	2.367138	-0.985547
13	6	0	-1.621651	3.342401	-1.395596
14	6	0	-0.362843	2.745271	-1.243750
15	7	0	-0.508291	1.499199	-0.778908
16	7	0	-0.450291	-0.104394	1.694134
17	7	0	-0.373724	-1.341379	-1.012219
18	29	0	0.803666	0.063068	-0.301407
19	7	0	2.291036	-1.142119	-0.154347
20	16	0	3.345893	0.021065	-0.065966
21	8	0	2.340803	1.210147	-0.016281
22	8	0	4.403118	-0.028288	0.937860
23	1	0	-3.601734	2.379026	-0.924119
24	1	0	-1.844113	4.336947	-1.752257
25	1	0	0.625163	3.139245	-1.436709
26	1	0	-3.386989	-2.416608	-1.319270
27	1	0	-1.484874	-4.085955	-2.416696
28	1	0	0.890559	-2.768970	-1.878168
29	1	0	-3.547836	-0.385735	2.617026
30	1	0	-1.751952	-0.485128	4.704772
31	1	0	0.689594	-0.216278	3.445842
32	1	0	4.004661	0.268738	-1.237366

Zero-point correction= 0.225655 (Hartree/Particle)
Thermal correction to Energy= 0.243984
Thermal correction to Enthalpy= 0.244928
Thermal correction to Gibbs Free Energy= 0.178001
Sum of electronic and zero-point Energies= -1502.173166
Sum of electronic and thermal Energies= -1502.154837
Sum of electronic and thermal Enthalpies= -1502.153893
Sum of electronic and thermal Free Energies= -1502.220821

κ^2N,O-^{3}**INT1-a** (B3LYP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.190573	-0.041562	0.607164
2	1	0	-3.313313	-0.067237	1.031565
3	7	0	-2.041615	-1.049335	-0.563689
4	6	0	-2.917924	-1.965405	-1.032764
5	6	0	-2.307412	-2.679497	-2.054697
6	6	0	-1.021082	-2.125770	-2.150049
7	7	0	-1.185493	-0.390702	1.732978
8	6	0	-1.422788	-0.762459	3.012323
9	6	0	0.753538	-0.730558	2.646334
10	6	0	-0.206386	-0.990852	3.638480

11	7	0	-1.856229	1.377071	0.067348
12	6	0	-2.587125	2.511149	0.067915
13	6	0	-1.826762	3.531067	-0.491506
14	6	0	-0.606215	2.923356	-0.816091
15	7	0	-0.639391	1.629514	-0.476422
16	7	0	0.157240	-0.370071	1.507186
17	7	0	-0.874231	-1.147217	-1.253322
18	29	0	0.655985	0.103448	-0.535215
19	7	0	2.180867	-1.040470	-1.054789
20	16	0	3.341489	-0.032968	-0.510113
21	8	0	2.673862	1.310654	-0.605734
22	8	0	3.954069	-0.446777	0.754951
23	1	0	-3.591342	2.512277	0.466464
24	1	0	-2.114071	4.561221	-0.639767
25	1	0	0.283912	3.343036	-1.263812
26	1	0	-3.907383	-2.043859	-0.605494
27	1	0	-2.730775	-3.480180	-2.642763
28	1	0	-0.201294	-2.382105	-2.806851
29	1	0	-2.435912	-0.837105	3.381180
30	1	0	-0.039523	-1.298115	4.660242
31	1	0	1.833257	-0.782918	2.691706
32	1	0	4.323361	-0.028441	-1.453678

Zero-point correction= 0.224355 (Hartree/Particle)
Thermal correction to Energy= 0.243434
Thermal correction to Enthalpy= 0.244378
Thermal correction to Gibbs Free Energy= 0.173786
Sum of electronic and zero-point Energies= -1502.182632
Sum of electronic and thermal Energies= -1502.163553
Sum of electronic and thermal Enthalpies= -1502.162608
Sum of electronic and thermal Free Energies= -1502.233201

κ^2N,O-^{1}**INT1-a** (M06)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.301290	-0.067957	0.064964
2	1	0	-3.502705	-0.133133	0.082109
3	7	0	-1.720342	-1.199824	-0.833073
4	6	0	-2.326182	-2.280228	-1.356050
5	6	0	-1.368926	-3.094813	-1.938513
6	6	0	-0.160185	-2.431122	-1.717487
7	7	0	-1.712299	-0.204179	1.473732
8	6	0	-2.336293	-0.416675	2.653322
9	6	0	-0.163655	-0.330066	2.954746
10	6	0	-1.376403	-0.503390	3.640839
11	7	0	-1.839436	1.281312	-0.544491
12	6	0	-2.535761	2.395655	-0.828998
13	6	0	-1.650745	3.384020	-1.226600
14	6	0	-0.394300	2.777576	-1.149863
15	7	0	-0.527567	1.515892	-0.741786
16	7	0	-0.370602	-0.149725	1.655651
17	7	0	-0.394422	-1.296803	-1.060971
18	29	0	0.779673	0.081296	-0.351302
19	7	0	2.235200	-1.127192	-0.234282
20	16	0	3.291757	0.028727	-0.100927
21	8	0	2.298584	1.208131	-0.027962
22	8	0	4.329228	-0.052016	0.907001
23	1	0	-3.614033	2.402913	-0.722969
24	1	0	-1.882049	4.396832	-1.527379
25	1	0	0.590323	3.178853	-1.361231
26	1	0	-3.400537	-2.390691	-1.267830
27	1	0	-1.523457	-4.036268	-2.447952
28	1	0	0.855980	-2.701452	-1.977957
29	1	0	-3.417147	-0.489560	2.696492
30	1	0	-1.529343	-0.667181	4.699385
31	1	0	0.850789	-0.329701	3.339422

32	1	0	3.958500	0.300944	-1.258471

Zero-point correction= 0.225451 (Hartree/Particle)
Thermal correction to Energy= 0.243749
Thermal correction to Enthalpy= 0.244693
Thermal correction to Gibbs Free Energy= 0.177577
Sum of electronic and zero-point Energies= -1501.604803
Sum of electronic and thermal Energies= -1501.586505
Sum of electronic and thermal Enthalpies= -1501.585561
Sum of electronic and thermal Free Energies= -1501.652677

κ^2N,O-^{3}**INT1-a** (M06)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.151192	-0.023707	0.665603
2	1	0	-3.253802	-0.044763	1.147542
3	7	0	-2.053590	-1.045615	-0.494565
4	6	0	-2.934196	-1.984516	-0.893363
5	6	0	-2.363957	-2.719440	-1.916837
6	6	0	-1.094838	-2.152956	-2.083867
7	7	0	-1.087574	-0.356208	1.740787
8	6	0	-1.256443	-0.736200	3.023142
9	6	0	0.889936	-0.693844	2.549734
10	6	0	-0.014009	-0.962673	3.584988
11	7	0	-1.837898	1.385046	0.095588
12	6	0	-2.552657	2.523547	0.130880
13	6	0	-1.807440	3.534668	-0.452251
14	6	0	-0.611561	2.914586	-0.825263
15	7	0	-0.647278	1.624898	-0.492510
16	7	0	0.236152	-0.328635	1.450084
17	7	0	-0.922371	-1.148964	-1.229425
18	29	0	0.617433	0.102888	-0.576122
19	7	0	2.094287	-1.071705	-1.044024
20	16	0	3.271017	-0.057423	-0.550409
21	8	0	2.667600	1.287454	-0.743659
22	8	0	3.825023	-0.419100	0.745637
23	1	0	-3.542297	2.529736	0.572024
24	1	0	-2.088494	4.570454	-0.585633
25	1	0	0.269086	3.325368	-1.306295
26	1	0	-3.903591	-2.060366	-0.414478
27	1	0	-2.803682	-3.543974	-2.461718
28	1	0	-0.297577	-2.418939	-2.769016
29	1	0	-2.253925	-0.817488	3.439638
30	1	0	0.206753	-1.274091	4.597137
31	1	0	1.973897	-0.742028	2.535694
32	1	0	4.265676	-0.167925	-1.469191

Zero-point correction= 0.224226 (Hartree/Particle)
Thermal correction to Energy= 0.243116
Thermal correction to Enthalpy= 0.244060
Thermal correction to Gibbs Free Energy= 0.174771
Sum of electronic and zero-point Energies= -1501.613098
Sum of electronic and thermal Energies= -1501.594208
Sum of electronic and thermal Enthalpies= -1501.593264
Sum of electronic and thermal Free Energies= -1501.662553