catalysts

Supporting Information: Asymmetric Cyanation of Activated Olefins with Ethyl Cyanoformate Catalyzed by Ti(IV)-catalyst: A Theoretical Study

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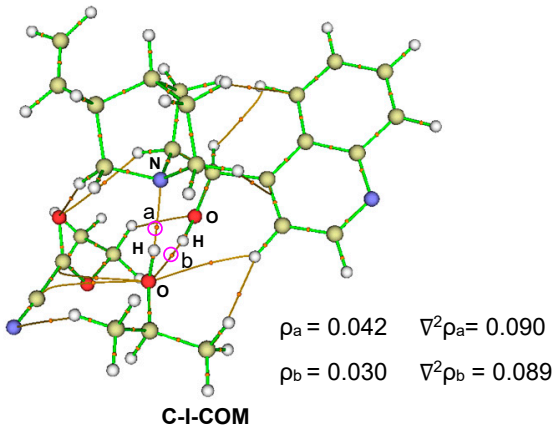


Figure S1. Laplacian ($\nabla^2\varrho$) and electronic density (ϱ, in parentheses) of selected bond critical points (BCP) for molecular complex C-I-COM were obtained by AIM analysis, using Multiwfn software.

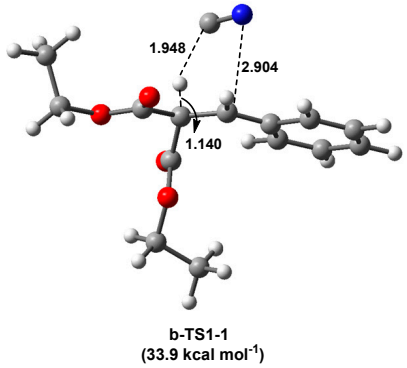
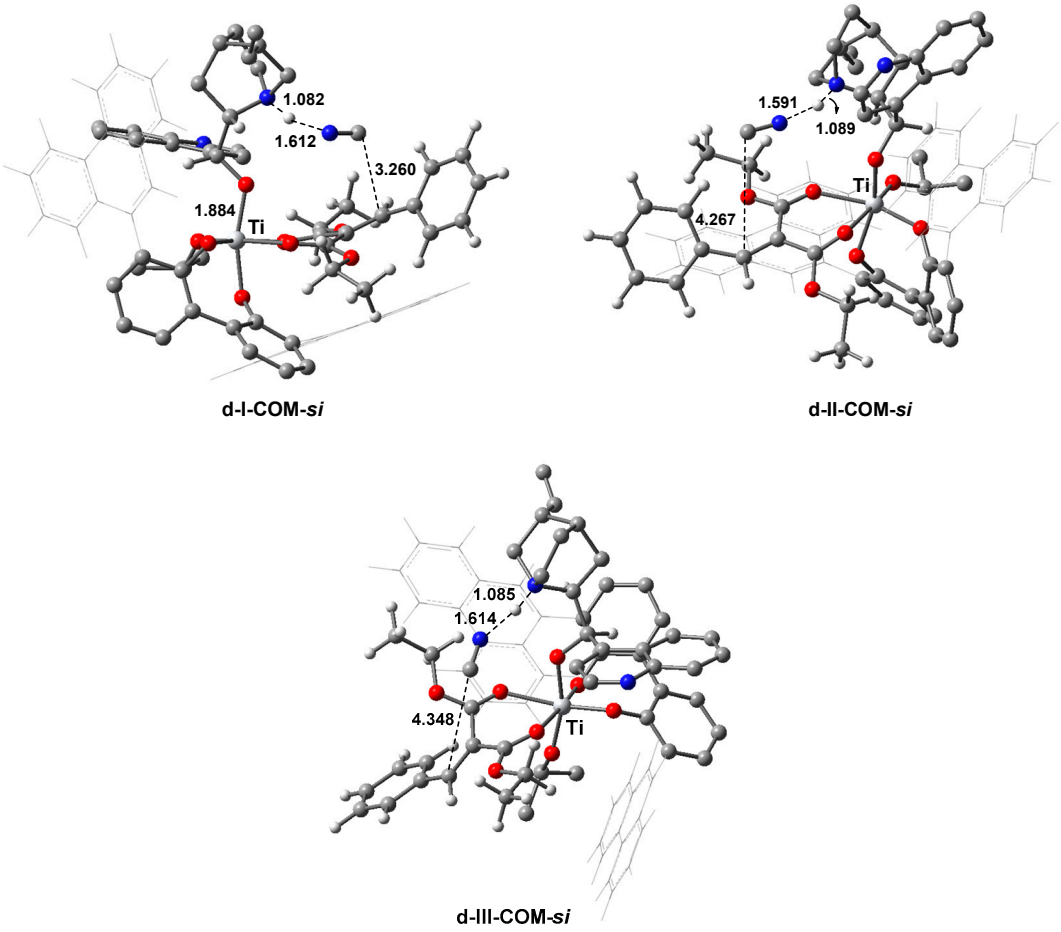
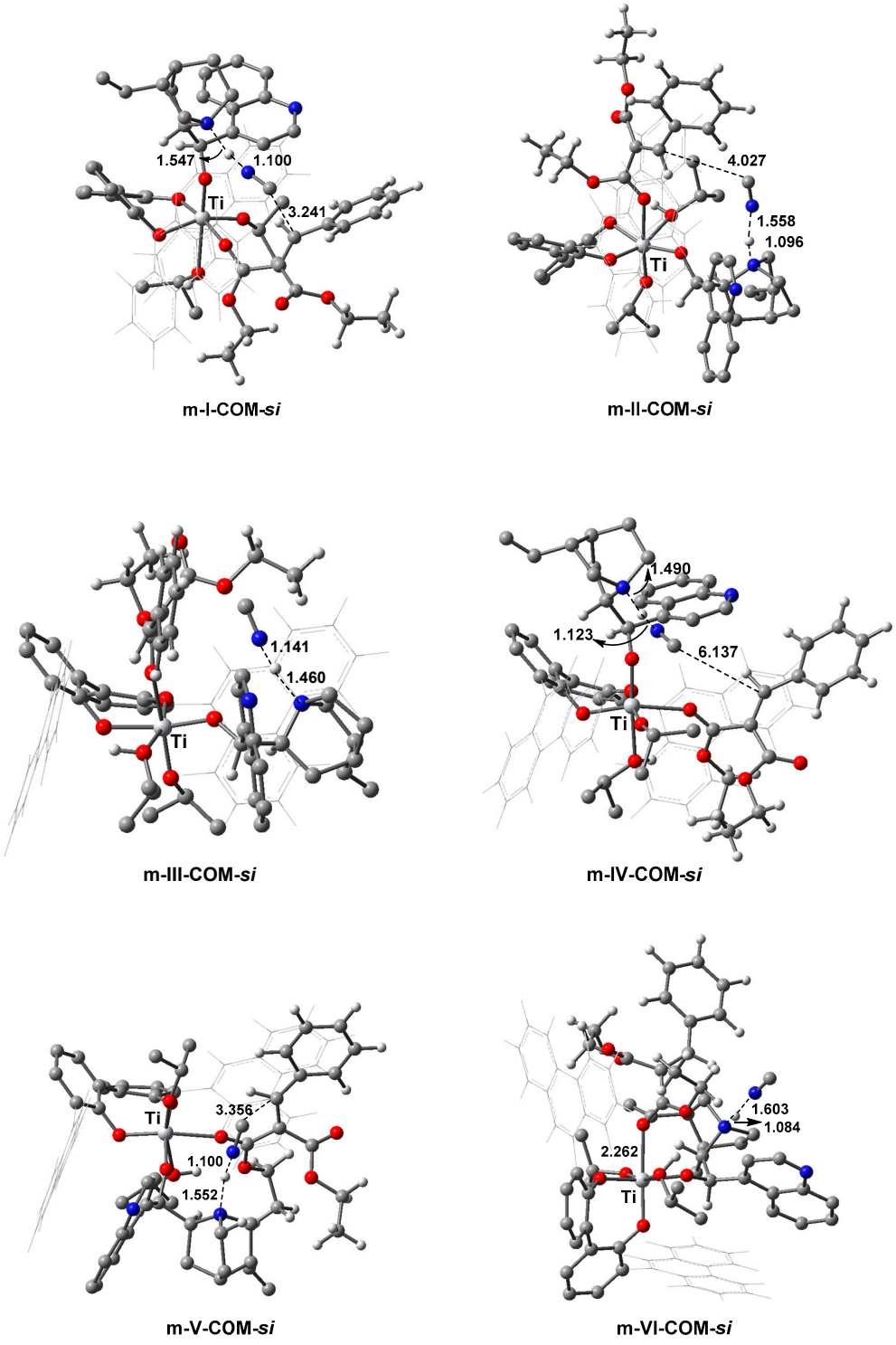


Figure S2. Optimized geometry of transition state b-TS1-1. The intermolecular distance is in Angstroms (Å). The color definitions of atoms are Red=oxygen, blue=nitrogen, gray=carbon, and white=hydrogen.



(a)



(b)

Figure S3. Optimized geometries of low-energy hexacoordinated Ti(IV)-complexes formed by coordinating olefin to metal center in (**a**) bidentate (**b**) monodentate fashion along *si*-face attack pathway. The intermolecular distance is in Angstroms (Å). The color definitions of atoms are Red=oxygen, blue=nitrogen, gray=carbon, and white=hydrogen.

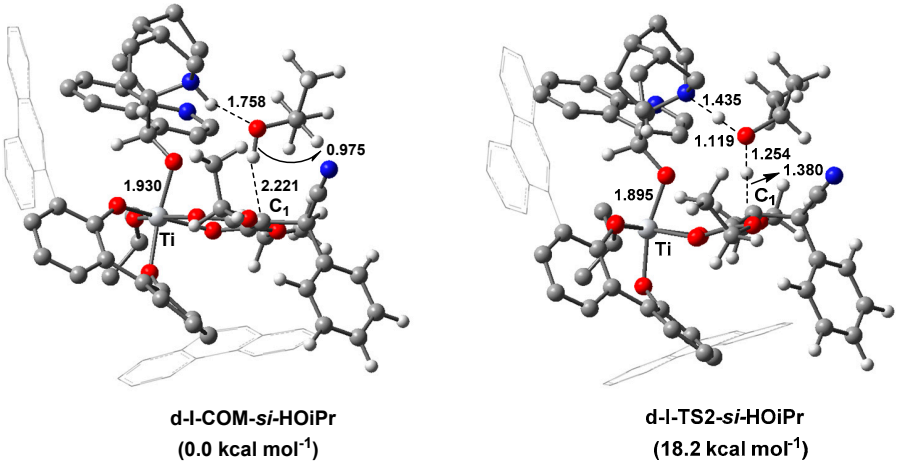


Figure S4. Optimized geometries of hexacoordinated Ti(IV)-complexes and H-shift transition state in the presence of HOiPr along *si*-face attack pathway. The intermolecular distance is in Angstroms (Å). The color definitions of atoms are Red=oxygen, blue=nitrogen, gray=carbon, and white=hydrogen.

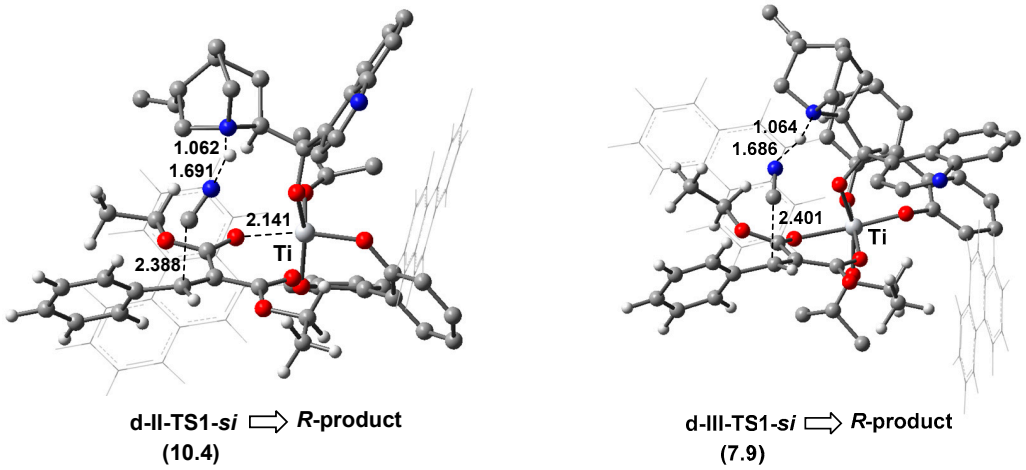


Figure S5. Optimized geometries of two competing transition states in C-C bond formation step in d-II and d-III models as well as their relative Gibbs free energies (in kcal mol^{-1}). The intermolecular distance is in Angstroms (Å). The color definitions of atoms are Red=oxygen, blue=nitrogen, gray=carbon, and white=hydrogen.

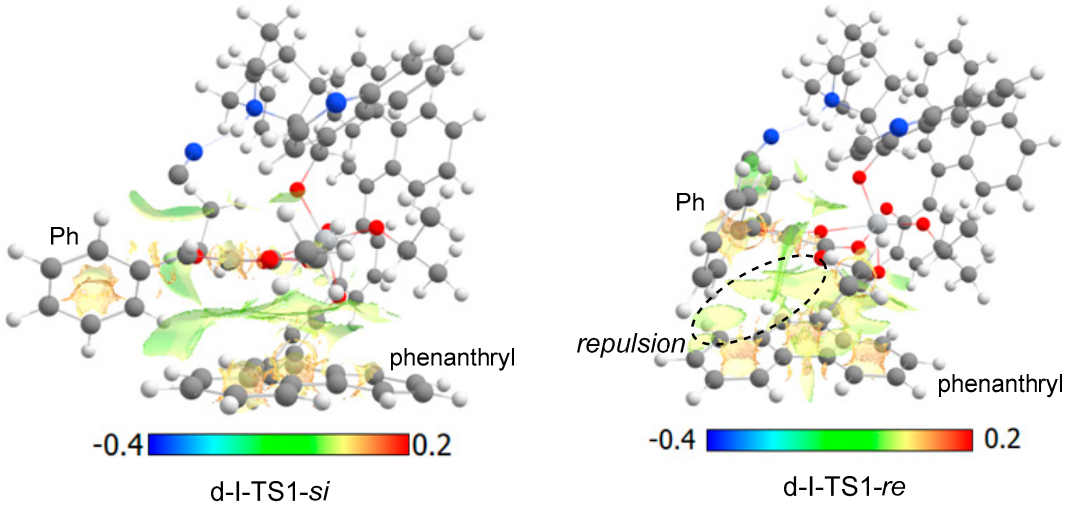


Figure S6. Visualization of the main noncovalent interaction described by contour plots of the reduced density gradient isosurfaces (density cutoff of 0.7 au) for transition states d-I-TS1-*si* and d-I-TS1-*re*. The surface color code is blue for strongly attractive, green for weakly attractive, and red for strongly repulsive interactions.

Cartesian coordinates of all stationary points and the corresponding energies at the B3LYP-D3(BJ)/6-31G(d,p) (SMD, toluene) level

HOiPr

Zero-point correction = 0.10812 (a.u.)

Thermal correction to Gibbs Free Energy = 0.08075 (a.u.)

Sum of electronic and zero-point Energies = -194.26578 (a.u.)

Sum of electronic and thermal Free Energies = -194.29315 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.416207	1.071120	0.428546
2	8	0	1.399076	0.159001	0.749833
3	6	0	1.759211	-0.689250	-0.347663
4	6	0	1.742270	-2.114999	0.187258
5	6	0	3.118932	-0.294811	-0.923356
6	1	0	0.762393	-2.353737	0.611575
7	1	0	1.956444	-2.833120	-0.610615
8	1	0	3.895873	-0.366799	-0.154559
9	1	0	3.104496	0.736527	-1.296787
10	1	0	2.493818	-2.237420	0.974710
11	1	0	3.398487	-0.943234	-1.761144
12	1	0	1.001248	-0.604448	-1.144974

R1

Zero-point correction = 0.08892 (a.u.)

Thermal correction to Gibbs Free Energy = 0.05632 (a.u.)

Sum of electronic and zero-point Energies = -360.53556 (a.u.)

Sum of electronic and thermal Free Energies = -360.56816 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.313953	1.593492	-0.141835
2	7	0	1.321825	2.041182	-0.500162
3	6	0	-0.966396	1.082052	0.377975

4	8	0	-1.399027	0.080643	-0.377690
5	6	0	-2.669491	-0.527934	0.024321
6	6	0	-2.971055	-1.633396	-0.962060
7	1	0	-3.434170	0.253787	0.022664
8	1	0	-3.067302	-1.242356	-1.978898
9	1	0	-2.188650	-2.397523	-0.952905
10	1	0	-3.917484	-2.109224	-0.687270
11	1	0	-2.557842	-0.899132	1.046863
12	8	0	-1.494152	1.552209	1.358189

R2

Zero-point correction = 0.27696 (a.u.)

Thermal correction to Gibbs Free Energy = 0.22893 (a.u.)

Sum of electronic and zero-point Energies = -843.77898 (a.u.)

Sum of electronic and thermal Free Energies = -843.82701 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.962008	-1.403126	-0.806519
2	8	0	-2.078672	-1.973448	-1.869363
3	6	0	-0.710751	-0.607207	-0.477736
4	8	0	-2.948293	-1.500877	0.100763
5	6	0	0.427502	-1.322827	-0.322772
6	6	0	1.800561	-0.949608	0.037069
7	6	0	2.130954	0.140361	0.862423
8	6	0	2.839678	-1.786754	-0.412877
9	6	0	3.457109	0.400431	1.194779
10	6	0	4.167831	-1.514531	-0.095116
11	6	0	4.481074	-0.417819	0.709597
12	1	0	0.306595	-2.395914	-0.472502
13	1	0	1.344963	0.769831	1.261157
14	1	0	2.596499	-2.648966	-1.028042
15	1	0	3.693757	1.240447	1.841320
16	1	0	4.955511	-2.163608	-0.465820
17	1	0	5.514593	-0.209491	0.970187
18	6	0	-2.846659	-0.994234	1.452869
19	6	0	-4.099300	-0.204437	1.775158
20	1	0	-1.951846	-0.381600	1.569506
21	6	0	-0.907717	0.869044	-0.546606

22	8	0	-2.001119	1.388706	-0.388775
23	8	0	0.198190	1.547708	-0.891414
24	6	0	0.050023	2.979616	-1.099431
25	6	0	0.128252	3.758254	0.201512
26	1	0	-0.895836	3.160039	-1.615171
27	1	0	-2.749492	-1.869433	2.105066
28	1	0	0.877033	3.233441	-1.765845
29	1	0	1.075302	3.574407	0.717975
30	1	0	0.065447	4.830095	-0.015527
31	1	0	-0.698921	3.498659	0.866920
32	1	0	-4.170329	0.675002	1.131207
33	1	0	-4.994429	-0.817975	1.636448
34	1	0	-4.068978	0.125366	2.819331

170- **TS1**

Zero-point correction = 0.19644 (a.u.)

Thermal correction to Gibbs Free Energy = 0.15428 (a.u.)

Sum of electronic and zero-point Energies = -554.72573 (a.u.)

Sum of electronic and thermal Free Energies = -554.76790 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.159232	0.571397	0.382563
2	6	0	1.930439	-0.431545	-0.419076
3	6	0	2.244308	-1.589001	0.507686
4	6	0	3.152111	0.299725	-0.947401
5	1	0	1.331915	-2.060268	0.881769
6	1	0	2.809944	-2.345980	-0.044084
7	1	0	3.777709	0.666991	-0.128699
8	1	0	2.871159	1.143336	-1.585988
9	1	0	2.846837	-1.257695	1.358272
10	1	0	3.746772	-0.390711	-1.553339
11	6	0	-0.414684	0.340701	0.799341
12	8	0	-0.856236	-0.545192	-0.074600
13	6	0	-2.289097	-0.850190	0.044049
14	6	0	-2.617673	-1.882260	-1.009131
15	1	0	-2.828643	0.088479	-0.112462
16	1	0	-2.408973	-1.500655	-2.012365
17	1	0	-2.050430	-2.804818	-0.854169
18	1	0	-3.683834	-2.122543	-0.950555

19	1	0	-2.474273	-1.211255	1.059065
20	8	0	-0.665697	0.539344	1.942482
21	1	0	1.275278	-0.743949	-1.234973
22	6	0	-0.792216	2.120853	-0.321098
23	7	0	-1.547458	2.877863	-0.798378
24	1	0	0.935759	1.396079	-0.138605

2-TS1

Zero-point correction = 0.19702 (a.u.)

Thermal correction to Gibbs Free Energy = 0.15599 (a.u.)

Sum of electronic and zero-point Energies = -554.72361 (a.u.)

Sum of electronic and thermal Free Energies = -554.76464 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.233723	2.190310	-0.494276
2	7	0	0.712655	2.729869	-0.938463
3	1	0	1.279482	1.152275	0.143487
4	8	0	1.103689	0.265614	0.574538
5	6	0	1.637687	-0.818324	-0.322102
6	6	0	1.568441	-2.114994	0.458055
7	6	0	3.041163	-0.387355	-0.710644
8	1	0	0.541260	-2.357634	0.740518
9	1	0	1.945468	-2.928323	-0.169460
10	1	0	3.687618	-0.301016	0.167721
11	1	0	3.030668	0.568439	-1.243667
12	1	0	2.182959	-2.062333	1.361486
13	1	0	3.468665	-1.139041	-1.381173
14	1	0	0.980608	-0.838156	-1.193627
15	6	0	-0.509087	0.457469	0.824167
16	8	0	-1.085845	-0.374529	-0.014555
17	6	0	-2.547374	-0.238607	-0.067744
18	6	0	-3.063323	-1.252328	-1.061232
19	1	0	-2.751839	0.791863	-0.373997
20	1	0	-2.652424	-1.072934	-2.058519
21	1	0	-2.816566	-2.272842	-0.753996
22	1	0	-4.152945	-1.167535	-1.119490
23	1	0	-2.936898	-0.401048	0.940677
24	8	0	-0.787513	0.846688	1.909009

IM2

Zero-point correction = 0.18033 (a.u.)

Thermal correction to Gibbs Free Energy = 0.14388 (a.u.)

Sum of electronic and zero-point Energies = -461.40505 (a.u.)

Sum of electronic and thermal Free Energies = -461.44150 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.015508	0.210627	0.543452
2	6	0	1.615951	-0.748026	-0.387055
3	6	0	1.714621	-2.113326	0.280849
4	6	0	2.968156	-0.157255	-0.754537
5	1	0	0.725007	-2.491779	0.549601
6	1	0	2.178030	-2.832930	-0.402157
7	1	0	3.601726	-0.052022	0.131903
8	1	0	2.851690	0.828079	-1.214521
9	1	0	2.327204	-2.056422	1.186480
10	1	0	3.480045	-0.811329	-1.467462
11	1	0	0.977863	-0.806134	-1.272225
12	6	0	-0.308028	0.280846	0.727074
13	8	0	-0.998929	-0.553551	-0.075686
14	6	0	-2.441377	-0.503599	0.071819
15	6	0	-3.033980	-1.484607	-0.917213
16	1	0	-2.777452	0.520188	-0.115924
17	1	0	-2.762812	-1.221745	-1.944193
18	1	0	-2.690827	-2.504176	-0.717457
19	1	0	-4.125618	-1.468902	-0.837256
20	1	0	-2.696806	-0.757007	1.105068
21	8	0	-0.802528	1.036709	1.532592

HCN

Zero-point correction = 0.01648 (a.u.)

Thermal correction to Gibbs Free Energy = -0.00290 (a.u.)

Sum of electronic and zero-point Energies = -93.40975 (a.u.)

Sum of electronic and thermal Free Energies = -93.42912 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	1.668135	2.165078	-0.575128
2	6	0	0.673742	2.396910	-0.901294
3	7	0	-0.399132	2.647039	-1.253203

HNC

Zero-point correction = 0.01432 (a.u.)

Thermal correction to Gibbs Free Energy = -0.00147 (a.u.)

Sum of electronic and zero-point Energies = -93.38716 (a.u.)

Sum of electronic and thermal Free Energies = -93.40294 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.410779	2.648578	-1.255880
2	7	0	0.685508	2.395116	-0.898358
3	1	0	1.629841	2.173637	-0.587330

TS1

Zero-point correction = 0.19477 (a.u.)

Thermal correction to Gibbs Free Energy = 0.15517 (a.u.)

Sum of electronic and zero-point Energies = -554.74288 (a.u.)

Sum of electronic and thermal Free Energies = -554.78248 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.065521	0.420994	0.493587
2	6	0	1.683457	-0.639205	-0.274152
3	6	0	2.133436	-1.747875	0.672319
4	6	0	2.825111	-0.043132	-1.089610
5	1	0	1.289945	-2.159912	1.235544
6	1	0	2.594149	-2.565039	0.108319
7	1	0	3.599314	0.366128	-0.432517
8	1	0	2.461240	0.762751	-1.733480
9	1	0	2.872067	-1.369803	1.387089
10	1	0	3.281795	-0.808547	-1.726254
11	1	0	0.911822	-1.024611	-0.954815
12	1	0	0.480410	0.366296	1.565080

13	6	0	-0.621100	0.811185	0.399052
14	8	0	-1.279587	-0.033766	-0.410442
15	6	0	-1.851185	-1.230925	0.201289
16	6	0	-2.629549	-1.948096	-0.879875
17	1	0	-2.487370	-0.920591	1.032934
18	1	0	-3.425137	-1.311730	-1.277410
19	1	0	-1.979640	-2.249808	-1.706497
20	1	0	-3.088129	-2.848192	-0.458356
21	1	0	-1.043490	-1.851590	0.599978
22	8	0	-0.704148	0.730331	1.699147
23	6	0	-0.576725	2.151397	-0.227600
24	7	0	-0.557419	3.222011	-0.672355

IM1

Zero-point correction = (a.u.)

Thermal correction to Gibbs Free Energy = (a.u.)

Sum of electronic and zero-point Energies = (a.u.)

Sum of electronic and thermal Free Energies = (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.057358	0.118780	0.767193
2	6	0	1.781645	-0.564382	-0.305711
3	6	0	1.783150	-2.060811	-0.021369
4	6	0	3.175007	0.046374	-0.350826
5	1	0	0.762489	-2.446800	0.019404
6	1	0	2.326471	-2.593990	-0.808877
7	1	0	3.686713	-0.087807	0.608115
8	1	0	3.126603	1.116754	-0.570697
9	1	0	2.273036	-2.270413	0.935269
10	1	0	3.774925	-0.436387	-1.128857
11	1	0	1.263239	-0.368660	-1.251346
12	1	0	-0.001169	1.643080	2.075587
13	6	0	-0.225992	0.554526	0.512760
14	8	0	-1.028734	-0.503261	0.131990
15	6	0	-2.424788	-0.213112	-0.110411
16	6	0	-3.090300	-1.503696	-0.542752
17	1	0	-2.507565	0.552772	-0.892608
18	1	0	-2.634687	-1.893535	-1.458017

19	1	0	-3.011156	-2.265757	0.238400
20	1	0	-4.151697	-1.321239	-0.738399
21	1	0	-2.875000	0.179836	0.806511
22	8	0	-0.723185	1.137063	1.671522
23	6	0	-0.203825	1.609008	-0.592562
24	7	0	-0.177870	2.423436	-1.419272

3-TS2

Zero-point correction = 0.19716 (a.u.)

Thermal correction to Gibbs Free Energy = 0.15574 (a.u.)

Sum of electronic and zero-point Energies = -554.74981 (a.u.)

Sum of electronic and thermal Free Energies = -554.79123 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.041804	-0.052119	0.854213
2	6	0	1.741957	-0.560492	-0.371164
3	6	0	2.025030	-2.037290	-0.167210
4	6	0	2.968964	0.318117	-0.512173
5	1	0	1.102115	-2.610377	-0.046200
6	1	0	2.551227	-2.425199	-1.045007
7	1	0	3.632139	0.216043	0.352139
8	1	0	2.675343	1.364500	-0.622392
9	1	0	2.659586	-2.197340	0.709723
10	1	0	3.521711	0.019351	-1.408350
11	1	0	1.054756	-0.394380	-1.202157
12	1	0	-0.680117	1.627285	1.675272
13	6	0	-0.237991	0.078081	0.869012
14	8	0	-0.952068	-0.665854	0.087523
15	6	0	-2.405816	-0.409778	-0.003849
16	6	0	-2.953845	-1.345446	-1.053899
17	1	0	-2.513226	0.642789	-0.276067
18	1	0	-2.495419	-1.157707	-2.028427
19	1	0	-2.797200	-2.392818	-0.780397
20	1	0	-4.030775	-1.173237	-1.144877
21	1	0	-2.832804	-0.584916	0.984801
22	8	0	-0.783948	0.672443	1.915344
23	6	0	-0.348711	2.203639	-0.298286
24	7	0	-0.147309	2.849894	-1.257040

4-TS2

Zero-point correction = 0.19802 (a.u.)

Thermal correction to Gibbs Free Energy = 0.15743 (a.u.)

Sum of electronic and zero-point Energies = -554.74905 (a.u.)

Sum of electronic and thermal Free Energies = -554.78964 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.013726	0.045694	0.758820
2	6	0	1.683443	-0.758965	-0.314301
3	6	0	1.866574	-2.175219	0.198060
4	6	0	2.966536	-0.009632	-0.613398
5	1	0	0.906424	-2.653234	0.408575
6	1	0	2.379366	-2.768172	-0.565795
7	1	0	3.630403	0.004346	0.256595
8	1	0	2.742159	1.017269	-0.910901
9	1	0	2.476206	-2.189141	1.106703
10	1	0	3.488274	-0.506197	-1.437383
11	1	0	1.009863	-0.722521	-1.172563
12	1	0	-0.309457	2.015144	1.269352
13	6	0	-0.259008	0.243100	0.718589
14	8	0	-1.031500	-0.665468	0.220885
15	6	0	-2.443818	-0.313760	-0.051806
16	6	0	-3.044030	-1.464512	-0.822155
17	1	0	-2.412099	0.615530	-0.625476
18	1	0	-2.523328	-1.618611	-1.771039
19	1	0	-3.018301	-2.393214	-0.244938
20	1	0	-4.089859	-1.228284	-1.041930
21	1	0	-2.933224	-0.148108	0.909414
22	8	0	-0.768166	1.170658	1.493347
23	6	0	-0.160447	1.968211	-1.017306
24	7	0	0.183658	3.033255	-0.650161

Cinchona alkaloid (L1)

Zero-point correction = 0.37839 (a.u.)

Thermal correction to Gibbs Free Energy = 0.33194 (a.u.)

Sum of electronic and zero-point Energies = -921.63005 (a.u.)

Sum of electronic and thermal Free Energies = -921.67650 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.130087	-1.984087	-2.097748
2	6	0	0.171919	-0.735531	-1.496602
3	6	0	-1.155035	-0.239384	-0.819446
4	6	0	1.439816	-0.826174	-0.645209
5	7	0	-1.850281	-1.375485	-0.153730
6	6	0	-1.148809	0.998844	0.107899
7	6	0	2.274853	0.309266	-0.379393
8	6	0	1.863109	-2.049672	-0.166730
9	6	0	-1.405903	-1.553998	1.250154
10	6	0	-3.295008	-1.069601	-0.152568
11	6	0	-2.254463	0.793931	1.171314
12	6	0	3.455841	0.099930	0.411076
13	6	0	3.043008	-2.144619	0.604153
14	6	0	2.025493	1.621890	-0.871531
15	6	0	-1.779254	-0.320464	2.121955
16	6	0	-3.590976	0.320108	0.526317
17	7	0	3.818132	-1.121690	0.903000
18	6	0	4.305760	1.200189	0.703181
19	6	0	2.877018	2.665232	-0.581682
20	6	0	4.024371	2.456423	0.219262
21	1	0	0.382793	-0.028071	-2.308511
22	1	0	-1.788039	-0.013691	-1.684627
23	1	0	-1.312423	1.913227	-0.471861
24	1	0	-0.191967	1.120003	0.623527
25	1	0	1.296971	-2.943510	-0.400115
26	1	0	-0.328639	-1.721388	1.249527
27	1	0	-1.872493	-2.468896	1.629126
28	1	0	-3.811576	-1.874023	0.380602
29	1	0	-3.654202	-1.082439	-1.186390
30	1	0	-2.425141	1.724725	1.720825
31	1	0	3.352955	-3.117072	0.985663
32	1	0	1.153670	1.810057	-1.487863
33	1	0	-2.570455	-0.567393	2.839193
34	1	0	-0.913804	0.018212	2.701887
35	1	0	5.183428	1.004115	1.310978
36	1	0	2.667520	3.656538	-0.972857

37	1	0	4.683897	3.289637	0.443572
38	6	0	-4.189163	1.319780	-0.427070
39	1	0	-3.626686	1.521146	-1.340091
40	6	0	-5.346218	1.956215	-0.238205
41	1	0	-5.732408	2.668148	-0.962731
42	1	0	-5.952751	1.788268	0.649523
43	1	0	-4.309005	0.170240	1.341722
44	1	0	-0.864051	-2.329091	-1.545250

C-I-COM

Zero-point correction = 0.57936 (a.u.)

Thermal correction to Gibbs Free Energy = 0.51072 (a.u.)

Sum of electronic and zero-point Energies = -1476.44476 (a.u.)

Sum of electronic and thermal Free Energies = -1476.51340 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.223393	-1.003722	-1.353711
2	6	0	0.833625	-0.127491	-0.982450
3	6	0	0.299243	1.067898	-0.135558
4	6	0	2.029868	-0.918793	-0.445742
5	7	0	-0.215386	0.738786	1.230630
6	6	0	1.232997	2.301297	-0.050805
7	6	0	3.390330	-0.605122	-0.776500
8	6	0	1.811734	-2.033577	0.339661
9	6	0	0.858542	0.788723	2.258441
10	6	0	-1.223458	1.776474	1.567326
11	6	0	0.896686	3.072862	1.245389
12	6	0	4.421032	-1.443355	-0.226750
13	6	0	2.898776	-2.787471	0.831194
14	6	0	3.789318	0.459769	-1.634635
15	6	0	1.415950	2.229665	2.425959
16	6	0	-0.635247	3.224569	1.421385
17	7	0	4.163293	-2.515182	0.578488
18	6	0	5.782420	-1.169238	-0.527037
19	6	0	5.117850	0.693164	-1.913382
20	6	0	6.126772	-0.122777	-1.349610
21	1	0	1.143142	0.335906	-1.925348
22	1	0	-0.592599	1.359362	-0.699314

23	1	0	1.101276	2.922985	-0.940795
24	1	0	2.287057	2.007478	-0.014703
25	1	0	0.802977	-2.342419	0.583989
26	1	0	1.644725	0.094401	1.964042
27	1	0	0.434985	0.414780	3.196479
28	1	0	-1.552808	1.593814	2.594857
29	1	0	-2.088200	1.634896	0.913321
30	1	0	1.379972	4.054909	1.242177
31	1	0	2.703873	-3.654778	1.461221
32	1	0	3.039624	1.097664	-2.087473
33	1	0	1.092344	2.670402	3.376015
34	1	0	2.511146	2.217307	2.433672
35	1	0	6.529396	-1.821831	-0.086547
36	1	0	5.393420	1.508783	-2.575453
37	1	0	7.170275	0.075529	-1.575996
38	6	0	-1.344783	4.037531	0.361568
39	1	0	-2.420748	3.865885	0.302801
40	6	0	-0.807946	4.945452	-0.455735
41	1	0	-1.424325	5.497037	-1.160349
42	1	0	0.251633	5.186360	-0.453504
43	1	0	-0.805033	3.743473	2.376463
44	1	0	-0.744746	-1.273636	-0.571707
45	6	0	-4.815530	-0.599446	-0.059328
46	7	0	-5.521562	-0.790131	0.840909
47	6	0	-3.918401	-0.272668	-1.183650
48	8	0	-3.402765	0.817767	-1.285698
49	8	0	-3.832307	-1.304871	-2.006639
50	6	0	-2.972437	-1.146686	-3.188044
51	6	0	-3.706257	-0.425892	-4.301717
52	1	0	-2.733967	-2.176176	-3.459263
53	1	0	-4.633815	-0.943719	-4.563428
54	1	0	-3.940542	0.605147	-4.024645
55	1	0	-3.067778	-0.401132	-5.191211
56	1	0	-2.058357	-0.641249	-2.874568
57	1	0	-1.276728	-0.756798	1.267936
58	8	0	-1.865734	-1.465973	0.897242
59	6	0	-2.328170	-2.377389	1.906751
60	6	0	-2.803363	-1.624358	3.148523
61	6	0	-1.274331	-3.433886	2.239664
62	1	0	-3.554517	-0.874674	2.886063
63	1	0	-3.251938	-2.313856	3.871661

64	1	0	-0.396126	-2.981417	2.715288
65	1	0	-0.949972	-3.956548	1.334339
66	1	0	-1.965076	-1.122306	3.648168
67	1	0	-1.679301	-4.180691	2.932041
68	1	0	-3.191417	-2.880335	1.454529

C-I-TS1

Zero-point correction = 0.57872 (a.u.)

Thermal correction to Gibbs Free Energy = 0.51497 (a.u.)

Sum of electronic and zero-point Energies = -1476.41256 (a.u.)

Sum of electronic and thermal Free Energies = -1476.47631 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.081760	-0.383147	-2.399747
2	6	0	1.101335	-0.018911	-1.505756
3	6	0	0.787461	1.333278	-0.787306
4	6	0	1.574215	-1.187074	-0.632894
5	7	0	-0.047662	1.326593	0.492201
6	6	0	2.040091	2.191259	-0.499716
7	6	0	2.962318	-1.513357	-0.461787
8	6	0	0.644788	-2.010626	-0.027369
9	6	0	0.798595	1.087796	1.719008
10	6	0	-0.697076	2.686606	0.606074
11	6	0	1.759449	3.148369	0.674765
12	6	0	3.282932	-2.646679	0.362967
13	6	0	1.073589	-3.104308	0.758011
14	6	0	4.043746	-0.809496	-1.065875
15	6	0	1.725793	2.298733	1.959523
16	6	0	0.371605	3.814665	0.514182
17	7	0	2.335156	-3.421979	0.966401
18	6	0	4.642367	-3.003501	0.570333
19	6	0	5.351362	-1.185771	-0.851252
20	6	0	5.657565	-2.288784	-0.020406
21	1	0	1.933269	0.260376	-2.160280
22	1	0	0.156926	1.854928	-1.511326
23	1	0	2.302289	2.731153	-1.412080
24	1	0	2.893658	1.556515	-0.240957
25	1	0	-0.419162	-1.825082	-0.128767

26	1	0	1.354087	0.167401	1.551648
27	1	0	0.108910	0.916122	2.546621
28	1	0	-1.219841	2.698196	1.561887
29	1	0	-1.446882	2.750058	-0.183853
30	1	0	2.542437	3.908070	0.748044
31	1	0	0.328195	-3.738435	1.236112
32	1	0	3.844166	0.032416	-1.718411
33	1	0	1.373085	2.898817	2.804939
34	1	0	2.729849	1.944854	2.210753
35	1	0	4.839153	-3.862661	1.203682
36	1	0	6.154756	-0.634525	-1.330993
37	1	0	6.693414	-2.572602	0.140244
38	6	0	0.188810	4.683299	-0.713445
39	1	0	-0.849771	4.850551	-1.000787
40	6	0	1.146599	5.284361	-1.420352
41	1	0	0.898709	5.921508	-2.264462
42	1	0	2.203664	5.181623	-1.190777
43	1	0	0.216813	4.465958	1.385842
44	1	0	-0.755257	-0.655756	-1.959711
45	6	0	-3.409642	0.821953	-1.143118
46	7	0	-3.529597	1.944366	-1.419241
47	6	0	-3.164123	-0.621218	-0.890891
48	8	0	-2.331706	-1.235398	-1.573164
49	8	0	-4.311178	-1.182985	-0.433393
50	6	0	-4.373994	-2.632591	-0.471838
51	6	0	-4.950990	-3.118984	-1.789808
52	1	0	-5.020802	-2.899539	0.367783
53	1	0	-5.935893	-2.677695	-1.971144
54	1	0	-4.290612	-2.861915	-2.621472
55	1	0	-5.064256	-4.208563	-1.763140
56	1	0	-3.377895	-3.043764	-0.297868
57	1	0	-0.886008	0.614925	0.526457
58	8	0	-2.194243	-0.186980	0.750159
59	6	0	-2.873743	-0.387937	1.972481
60	6	0	-3.052021	0.906568	2.779196
61	6	0	-2.188076	-1.476497	2.810188
62	1	0	-3.524627	1.680952	2.167235
63	1	0	-3.688703	0.735392	3.655523
64	1	0	-1.163668	-1.188790	3.075756
65	1	0	-2.137809	-2.416737	2.252100
66	1	0	-2.092408	1.290568	3.148611

67	1	0	-2.733881	-1.666162	3.742499
68	1	0	-3.885988	-0.749868	1.734427

C-I-IM1

Zero-point correction = 0.58027 (a.u.)

Thermal correction to Gibbs Free Energy = 0.51488 (a.u.)

Sum of electronic and zero-point Energies = -1476.43347 (a.u.)

Sum of electronic and thermal Free Energies = -1476.49885 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.488906	-0.589709	-2.233312
2	6	0	1.440749	0.015629	-1.386237
3	6	0	0.865111	1.311726	-0.737479
4	6	0	2.127505	-0.998701	-0.461311
5	7	0	-0.277777	1.113928	0.248412
6	6	0	1.867300	2.283037	-0.083665
7	6	0	3.540514	-0.983775	-0.211604
8	6	0	1.389775	-2.017599	0.110383
9	6	0	0.191003	0.884402	1.660217
10	6	0	-1.126571	2.354669	0.217075
11	6	0	1.133680	3.105615	1.000354
12	6	0	4.076711	-2.005213	0.646204
13	6	0	2.020052	-2.969446	0.942892
14	6	0	4.452313	-0.040123	-0.766726
15	6	0	0.866363	2.167774	2.193888
16	6	0	-0.239325	3.609735	0.485516
17	7	0	3.308630	-2.977737	1.218451
18	6	0	5.469608	-2.029486	0.924559
19	6	0	5.798937	-0.094819	-0.482208
20	6	0	6.315006	-1.094469	0.375518
21	1	0	2.206265	0.407244	-2.065230
22	1	0	0.388563	1.812042	-1.584675
23	1	0	2.292953	2.924125	-0.858805
24	1	0	2.697090	1.744219	0.383277
25	1	0	0.320614	-2.087230	-0.059241
26	1	0	0.872219	0.036603	1.642974
27	1	0	-0.692339	0.593517	2.231911
28	1	0	-1.900028	2.220547	0.974881

29	1	0	-1.615783	2.390052	-0.758419
30	1	0	1.751054	3.949889	1.318223
31	1	0	1.420431	-3.757094	1.397664
32	1	0	4.090919	0.735653	-1.431656
33	1	0	0.229955	2.665161	2.933227
34	1	0	1.804064	1.910719	2.695030
35	1	0	5.831206	-2.815905	1.579372
36	1	0	6.471969	0.633751	-0.924579
37	1	0	7.378815	-1.123498	0.591716
38	6	0	-0.201787	4.553255	-0.698617
39	1	0	-1.140818	4.629233	-1.248370
40	6	0	0.821344	5.315777	-1.086426
41	1	0	0.723398	5.991104	-1.931501
42	1	0	1.783798	5.314048	-0.582219
43	1	0	-0.713200	4.160206	1.309949
44	1	0	-0.340143	-0.792394	-1.741223
45	6	0	-3.457865	0.142555	-1.559960
46	7	0	-3.754867	1.002558	-2.282992
47	6	0	-2.932272	-0.878404	-0.553685
48	8	0	-1.606128	-0.916987	-0.562232
49	8	0	-3.578133	-2.074917	-0.940850
50	6	0	-3.000109	-3.288610	-0.425670
51	6	0	-2.208352	-4.014358	-1.502719
52	1	0	-3.842847	-3.905248	-0.092725
53	1	0	-2.841341	-4.220879	-2.371761
54	1	0	-1.357692	-3.413706	-1.834127
55	1	0	-1.832996	-4.971130	-1.120412
56	1	0	-2.376975	-3.069570	0.445678
57	1	0	-0.913286	0.252340	-0.058821
58	8	0	-3.350736	-0.453989	0.749953
59	6	0	-4.772767	-0.407201	1.024822
60	6	0	-5.158051	1.031852	1.357355
61	6	0	-5.068229	-1.371620	2.169691
62	1	0	-4.940867	1.698139	0.517671
63	1	0	-6.228668	1.104384	1.577841
64	1	0	-4.495914	-1.095938	3.062618
65	1	0	-4.800525	-2.395896	1.896124
66	1	0	-4.607735	1.385379	2.236805
67	1	0	-6.132775	-1.354023	2.427832
68	1	0	-5.316415	-0.735487	0.132419

C-I-TS2

Zero-point correction = 0.58056 (a.u.)

Thermal correction to Gibbs Free Energy = 0.51497 (a.u.)

Sum of electronic and zero-point Energies = -1476.42210 (a.u.)

Sum of electronic and thermal Free Energies = -1476.42269 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.316776	-1.130792	-1.760201
2	6	0	1.344411	-0.330187	-1.221975
3	6	0	0.796349	1.059398	-0.763041
4	6	0	2.231551	-1.124625	-0.251330
5	7	0	-0.117857	1.062863	0.461114
6	6	0	1.838744	2.179896	-0.550378
7	6	0	3.662553	-1.017952	-0.240939
8	6	0	1.656137	-2.049524	0.599519
9	6	0	0.628834	1.068479	1.771539
10	6	0	-0.996731	2.293866	0.388732
11	6	0	1.358574	3.138219	0.558744
12	6	0	4.384881	-1.837602	0.694210
13	6	0	2.462467	-2.803071	1.481489
14	6	0	4.420998	-0.180521	-1.109396
15	6	0	1.425107	2.386238	1.901193
16	6	0	-0.114904	3.575478	0.327237
17	7	0	3.774780	-2.708398	1.550124
18	6	0	5.802743	-1.762710	0.745638
19	6	0	5.795962	-0.138506	-1.040718
20	6	0	6.496150	-0.929508	-0.099973
21	1	0	1.965059	-0.060124	-2.083644
22	1	0	0.117954	1.327767	-1.576108
23	1	0	1.990361	2.708664	-1.495477
24	1	0	2.807187	1.765901	-0.256526
25	1	0	0.583001	-2.205952	0.607687
26	1	0	1.270340	0.191111	1.786204
27	1	0	-0.125493	0.948707	2.551790
28	1	0	-1.627498	2.271566	1.279200
29	1	0	-1.638906	2.173639	-0.485239
30	1	0	1.999637	4.023131	0.588318
31	1	0	1.988804	-3.513811	2.157555

32	1	0	3.918456	0.430421	-1.850342
33	1	0	1.015204	3.007600	2.703523
34	1	0	2.464361	2.165351	2.161097
35	1	0	6.307596	-2.393761	1.470007
36	1	0	6.348228	0.503716	-1.720343
37	1	0	7.580192	-0.883225	-0.056629
38	6	0	-0.321621	4.355726	-0.947156
39	1	0	-0.247379	3.799699	-1.881518
40	6	0	-0.591716	5.660278	-0.989576
41	1	0	-0.726236	6.182837	-1.932253
42	1	0	-0.695492	6.254053	-0.083485
43	1	0	-0.392932	4.224993	1.164467
44	1	0	-0.412389	-1.240947	-1.113039
45	1	0	-0.751406	0.210945	0.431776
46	6	0	-3.056425	0.155130	-1.525716
47	7	0	-2.959358	1.088743	-2.230302
48	6	0	-2.815845	-1.146850	0.119426
49	8	0	-1.556461	-1.196512	0.238422
50	8	0	-3.517706	-2.215889	-0.318273
51	8	0	-3.479004	-0.436827	1.053965
52	6	0	-4.926730	-0.282445	0.934792
53	1	0	-5.194773	-0.480288	-0.106282
54	6	0	-5.232430	1.168776	1.275110
55	1	0	-4.743803	1.838862	0.562691
56	1	0	-6.311620	1.347806	1.228110
57	1	0	-4.890900	1.414343	2.286887
58	6	0	-5.610809	-1.281282	1.859886
59	1	0	-5.342059	-2.305863	1.592361
60	1	0	-5.323761	-1.105630	2.902477
61	1	0	-6.698938	-1.180900	1.785306
62	6	0	-2.910850	-2.979053	-1.378934
63	6	0	-3.910745	-4.024578	-1.829210
64	1	0	-1.986913	-3.436171	-1.010145
65	1	0	-4.179691	-4.696120	-1.007748
66	1	0	-4.823734	-3.555931	-2.208284
67	1	0	-3.474231	-4.625608	-2.633231
68	1	0	-2.659959	-2.287504	-2.192048

C-I-IM2

Zero-point correction = 0.39872 (a.u.)

Thermal correction to Gibbs Free Energy = 0.34830 (a.u.)
Sum of electronic and zero-point Energies = -1015.03198 (a.u.)
Sum of electronic and thermal Free Energies = -1015.08240 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.089815	1.650366	2.175664
2	6	0	0.196530	0.493098	1.418975
3	6	0	-1.104489	-0.053838	0.756269
4	6	0	1.448498	0.653809	0.546636
5	7	0	-1.727438	0.835349	-0.310532
6	6	0	-1.079962	-1.490988	0.192336
7	6	0	2.418556	-0.394100	0.397945
8	6	0	1.715524	1.862615	-0.066678
9	6	0	-1.156641	0.603434	-1.684993
10	6	0	-3.206748	0.562879	-0.336064
11	6	0	-2.100423	-1.598600	-0.962237
12	6	0	3.571816	-0.122098	-0.416027
13	6	0	2.882808	2.019261	-0.848275
14	6	0	2.334235	-1.673011	1.020338
15	6	0	-1.535805	-0.815858	-2.163088
16	6	0	-3.464161	-0.957922	-0.572368
17	7	0	3.782330	1.075475	-1.036315
18	6	0	4.558624	-1.128668	-0.593945
19	6	0	3.313118	-2.624405	0.834829
20	6	0	4.434074	-2.354892	0.015435
21	1	0	0.422870	-0.273097	2.168297
22	1	0	-1.822796	-0.000888	1.578268
23	1	0	-1.305396	-2.196934	0.996524
24	1	0	-0.088158	-1.747211	-0.191046
25	1	0	1.037690	2.703965	0.031750
26	1	0	-0.080666	0.746798	-1.615434
27	1	0	-1.559069	1.393364	-2.322379
28	1	0	-3.627828	1.179022	-1.132912
29	1	0	-3.616279	0.916057	0.612387
30	1	0	-2.256079	-2.646995	-1.229858
31	1	0	3.068276	2.974935	-1.336522
32	1	0	1.493626	-1.909423	1.662476
33	1	0	-2.275536	-0.771148	-2.968755
34	1	0	-0.651170	-1.319825	-2.562881

35	1	0	5.410764	-0.883575	-1.219766
36	1	0	3.226685	-3.588022	1.328099
37	1	0	5.196948	-3.115335	-0.122343
38	6	0	-4.134728	-1.624977	0.602417
39	1	0	-3.643418	-1.525023	1.570536
40	6	0	-5.272768	-2.314737	0.526671
41	1	0	-5.713641	-2.783291	1.401913
42	1	0	-5.808651	-2.436115	-0.412463
43	1	0	-4.129614	-1.058646	-1.436428
44	1	0	-0.438641	2.365013	1.600813
45	1	0	-1.589186	1.884694	-0.056246
46	6	0	-1.381061	4.579073	0.254497
47	7	0	-1.362631	3.398934	0.306080

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b-IM1

Zero-point correction = 0.29449 (a.u.)

Thermal correction to Gibbs Free Energy = 0.23982 (a.u.)

Sum of electronic and zero-point Energies = -937.17920 (a.u.)

Sum of electronic and thermal Free Energies = -937.23387 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.137174	3.571905	1.605944
2	6	0	1.091666	4.098478	2.038130
3	1	0	-0.684400	3.100773	1.192950
4	6	0	-1.947793	1.292106	-0.183797
5	8	0	-1.976156	2.392439	0.357161
6	6	0	-0.728943	0.403839	-0.085882
7	8	0	-3.018261	0.914582	-0.870609
8	6	0	0.417478	0.910541	-0.600354
9	6	0	1.760366	0.340399	-0.750273
10	6	0	1.997660	-1.016435	-1.032896
11	6	0	2.857246	1.219857	-0.682417
12	6	0	3.296384	-1.481140	-1.217304
13	6	0	4.157289	0.747164	-0.842933
14	6	0	4.379960	-0.604252	-1.113177
15	1	0	0.331751	1.919486	-1.003839
16	1	0	1.161654	-1.699479	-1.132786
17	1	0	2.683278	2.272392	-0.476826

18	1	0	3.465117	-2.528542	-1.449503
19	1	0	4.993647	1.435295	-0.767475
20	1	0	5.392105	-0.971688	-1.254477
21	6	0	-3.044180	-0.234134	-1.763612
22	6	0	-4.374380	-0.935317	-1.592182
23	1	0	-2.211974	-0.902810	-1.549587
24	6	0	-0.931603	-0.832992	0.726945
25	8	0	-2.033031	-1.330542	0.898125
26	8	0	0.189605	-1.266638	1.316753
27	6	0	0.068330	-2.406362	2.214140
28	6	0	0.173319	-3.723551	1.467211
29	1	0	-0.876946	-2.325626	2.754431
30	1	0	-2.925961	0.166291	-2.775863
31	1	0	0.896073	-2.276623	2.913995
32	1	0	1.114549	-3.789382	0.913583
33	1	0	0.144492	-4.548958	2.186520
34	1	0	-0.660694	-3.852252	0.772096
35	1	0	-4.466177	-1.336544	-0.580291
36	1	0	-5.206145	-0.250241	-1.780387
37	1	0	-4.444644	-1.763376	-2.305170

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b-TS1

Zero-point correction = 0.29415 (a.u.)

Thermal correction to Gibbs Free Energy = 0.24436 (a.u.)

Sum of electronic and zero-point Energies = -937.14817 (a.u.)

Sum of electronic and thermal Free Energies = -937.1979 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.899534	-2.626170	1.866376
2	6	0	-0.092047	-2.095014	1.470883
3	1	0	1.821992	-2.614554	1.375827
4	6	0	2.072429	-0.758086	-0.300277
5	8	0	2.388982	-1.959637	-0.217221
6	6	0	0.700875	-0.295748	-0.179379
7	8	0	2.993010	0.206675	-0.442277
8	6	0	-0.319883	-1.279194	-0.103453
9	6	0	-1.765559	-0.937727	-0.351098
10	6	0	-2.084660	-0.264928	-1.540914

11	6	0	-2.802682	-1.329389	0.501486
12	6	0	-3.413073	0.006282	-1.868382
13	6	0	-4.130851	-1.057656	0.172394
14	6	0	-4.442177	-0.390167	-1.013273
15	1	0	-0.017143	-2.200692	-0.610747
16	1	0	-1.289239	0.040545	-2.214391
17	1	0	-2.563797	-1.836211	1.430468
18	1	0	-3.640396	0.528208	-2.793410
19	1	0	-4.923118	-1.364730	0.849140
20	1	0	-5.476768	-0.178312	-1.266907
21	6	0	4.374791	-0.221159	-0.519464
22	6	0	5.225709	1.020980	-0.681566
23	1	0	4.487597	-0.906828	-1.365074
24	6	0	0.419803	1.139947	0.096832
25	8	0	0.881732	2.077700	-0.522317
26	8	0	-0.416469	1.268068	1.153716
27	6	0	-0.801382	2.616149	1.528871
28	6	0	-2.023423	3.089562	0.761178
29	1	0	0.050174	3.281542	1.370058
30	1	0	4.628231	-0.772986	0.391296
31	1	0	-1.007778	2.547398	2.599740
32	1	0	-2.866323	2.407399	0.902785
33	1	0	-2.319380	4.080433	1.123788
34	1	0	-1.810498	3.169423	-0.307885
35	1	0	4.966297	1.560354	-1.597146
36	1	0	5.096768	1.700479	0.165957
37	1	0	6.281384	0.736166	-0.736355

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b-IM2

Zero-point correction = 0.29858 (a.u.)

Thermal correction to Gibbs Free Energy = 0.24802 (a.u.)

Sum of electronic and zero-point Energies = -937.19094 (a.u.)

Sum of electronic and thermal Free Energies = -937.24149 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.204650	0.983388	3.362818
2	6	0	0.923070	1.071690	2.240019
3	1	0	-1.418835	2.767895	1.404546

4	6	0	-1.936463	1.260953	0.335676
5	8	0	-2.045848	2.557124	0.696702
6	6	0	-0.791040	0.520459	0.514876
7	8	0	-3.096462	0.861864	-0.163970
8	6	0	0.529029	1.236504	0.828533
9	6	0	1.668306	0.910638	-0.154173
10	6	0	1.455396	1.165946	-1.514205
11	6	0	2.907644	0.417176	0.260298
12	6	0	2.463995	0.926313	-2.446398
13	6	0	3.918118	0.178536	-0.673865
14	6	0	3.700527	0.429957	-2.028423
15	1	0	0.356563	2.313497	0.706271
16	1	0	0.494629	1.550866	-1.845438
17	1	0	3.087984	0.214800	1.311294
18	1	0	2.284169	1.130481	-3.497991
19	1	0	4.876576	-0.206164	-0.337468
20	1	0	4.487971	0.243717	-2.752747
21	6	0	-3.168185	0.200814	-1.463376
22	6	0	-4.441609	-0.612535	-1.494817
23	1	0	-2.293403	-0.429399	-1.607678
24	6	0	-0.832763	-0.949424	0.525313
25	8	0	-1.792070	-1.655298	0.249409
26	8	0	0.350059	-1.455639	0.951121
27	6	0	0.452132	-2.895922	1.065142
28	6	0	0.856593	-3.532487	-0.253194
29	1	0	-0.501449	-3.289932	1.423624
30	1	0	-3.178783	0.999193	-2.214572
31	1	0	1.214796	-3.049746	1.832072
32	1	0	1.789541	-3.099639	-0.626732
33	1	0	1.010053	-4.607655	-0.109375
34	1	0	0.077794	-3.398193	-1.008464
35	1	0	-4.404829	-1.398959	-0.737802
36	1	0	-5.317678	0.017425	-1.313977
37	1	0	-4.551594	-1.078008	-2.479814

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b-TS2

Zero-point correction = 0.29387 (a.u.)

Thermal correction to Gibbs Free Energy = 0.24370 (a.u.)

Sum of electronic and zero-point Energies = -937.13585 (a.u.)

Sum of electronic and thermal Free Energies = -937.18602 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.073629	-2.674176	2.711158
2	6	0	0.236067	-1.654993	2.180477
3	1	0	-1.391695	0.985998	2.360883
4	6	0	-0.783222	1.819375	1.137353
5	8	0	-1.182859	2.173004	2.301479
6	6	0	-0.809929	0.328716	1.090469
7	8	0	-0.461187	2.742799	0.296311
8	6	0	0.503400	-0.349028	1.552050
9	6	0	1.624483	-0.447843	0.508465
10	6	0	2.689245	0.460044	0.569629
11	6	0	1.603895	-1.403738	-0.516264
12	6	0	3.710365	0.424726	-0.382024
13	6	0	2.625332	-1.438961	-1.465625
14	6	0	3.678964	-0.524039	-1.404490
15	1	0	0.896976	0.269966	2.369126
16	1	0	2.726429	1.194733	1.370737
17	1	0	0.793331	-2.122593	-0.560961
18	1	0	4.531220	1.133241	-0.318035
19	1	0	2.601171	-2.188652	-2.251329
20	1	0	4.474075	-0.557013	-2.143565
21	6	0	0.001771	2.428554	-1.065240
22	6	0	-0.935512	3.085519	-2.052738
23	1	0	0.043893	1.346851	-1.183070
24	6	0	-1.696892	-0.224266	0.075066
25	8	0	-2.484725	0.457526	-0.577937
26	8	0	-1.640066	-1.575477	-0.010812
27	6	0	-2.628258	-2.224809	-0.849949
28	6	0	-2.165099	-2.332016	-2.292411
29	1	0	-3.567385	-1.671968	-0.778718
30	1	0	1.012583	2.838098	-1.114756
31	1	0	-2.756307	-3.211832	-0.399212
32	1	0	-1.220187	-2.879246	-2.367144
33	1	0	-2.916049	-2.874253	-2.877647
34	1	0	-2.038130	-1.341454	-2.736861
35	1	0	-1.937879	2.661282	-1.967122
36	1	0	-0.981751	4.166745	-1.895351
37	1	0	-0.562646	2.903049	-3.066005

P-S

Zero-point correction = 0.29904 (a.u.)

Thermal correction to Gibbs Free Energy = 0.24851 (a.u.)

Sum of electronic and zero-point Energies = -937.23326 (a.u.)

Sum of electronic and thermal Free Energies = -937.28379 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.565143	0.888121	3.304848
2	6	0	-1.071236	0.237694	2.480124
3	6	0	1.916959	-0.752609	0.461936
4	8	0	1.888587	-1.960923	0.576650
5	6	0	0.762146	0.191747	0.797611
6	8	0	2.985634	-0.052913	0.072336
7	6	0	-0.447470	-0.586782	1.436596
8	6	0	-1.481810	-1.112545	0.434449
9	6	0	-1.244562	-2.326654	-0.222808
10	6	0	-2.649579	-0.395708	0.145132
11	6	0	-2.158842	-2.809812	-1.158488
12	6	0	-3.563486	-0.883613	-0.790281
13	6	0	-3.319846	-2.090254	-1.446237
14	1	0	-0.001233	-1.448797	1.944582
15	1	0	-0.339523	-2.883716	-0.005855
16	1	0	-2.855983	0.537127	0.660653
17	1	0	-1.962922	-3.752308	-1.661505
18	1	0	-4.468488	-0.320700	-0.999738
19	1	0	-4.031837	-2.470211	-2.173071
20	6	0	4.158428	-0.821455	-0.318083
21	6	0	5.245481	0.163555	-0.689011
22	1	0	3.882103	-1.466051	-1.157494
23	6	0	0.346485	0.981312	-0.445990
24	8	0	0.575462	0.643808	-1.586002
25	8	0	-0.326875	2.084743	-0.091090
26	6	0	-0.845180	2.899959	-1.180182
27	6	0	-1.582131	4.070062	-0.565366
28	1	0	-1.499362	2.276855	-1.796503
29	1	0	4.450254	-1.461260	0.519755
30	1	0	-0.003606	3.223001	-1.799918

31	1	0	-0.914453	4.679525	0.050768
32	1	0	-1.986530	4.702988	-1.361739
33	1	0	-2.413899	3.730476	0.058631
34	1	0	4.933491	0.801216	-1.521260
35	1	0	5.506760	0.802053	0.160177
36	1	0	6.143029	-0.383729	-0.994117
37	1	0	1.143593	0.909579	1.531121

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d-I-COM-*si*

Zero-point correction = 1.28815 (a.u.)

Thermal correction to Gibbs Free Energy = 1.18829 (a.u.)

Sum of electronic and zero-point Energies = -4590.83903 (a.u.)

Sum of electronic and thermal Free Energies = -4590.93889 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.656244	0.796256	0.090106
2	6	0	1.918617	1.027945	0.654159
3	6	0	2.367990	2.423898	0.170056
4	6	0	1.883392	0.838287	2.166046
5	7	0	1.566125	3.572772	0.745245
6	6	0	3.852586	2.791709	0.308330
7	6	0	2.976233	0.297941	2.907896
8	6	0	0.747291	1.200783	2.859368
9	6	0	2.118816	4.084087	2.050342
10	6	0	1.585646	4.690106	-0.253979
11	6	0	3.977035	4.326359	0.411545
12	6	0	2.824748	0.197883	4.333530
13	6	0	0.710181	1.077779	4.263133
14	6	0	3.492619	4.738948	1.810632
15	6	0	3.058109	5.048426	-0.613995
16	7	0	1.698546	0.597631	4.993593
17	1	0	2.658825	0.340153	0.224533
18	1	0	2.096228	2.410711	-0.887022
19	1	0	4.398256	2.397100	-0.548068
20	1	0	4.288417	2.339341	1.204192
21	6	0	4.188776	-0.167264	2.328119
22	1	0	-0.104637	1.609001	2.332744
23	1	0	2.183468	3.235883	2.723390

24	1	0	1.367440	4.768374	2.446175
25	1	0	1.050606	5.526631	0.197679
26	1	0	1.014668	4.354111	-1.121024
27	1	0	5.012480	4.633842	0.247967
28	6	0	3.881440	-0.341799	5.112488
29	1	0	-0.180297	1.399088	4.801193
30	1	0	3.426321	5.828874	1.885408
31	1	0	4.196321	4.399671	2.575472
32	1	0	3.192102	6.124943	-0.465459
33	6	0	5.043222	-0.771359	4.516959
34	6	0	5.193950	-0.685078	3.113160
35	1	0	5.845587	-1.185971	5.119808
36	1	0	3.728750	-0.401270	6.185094
37	1	0	6.101235	-1.045854	2.643995
38	1	0	4.324879	-0.134826	1.254828
39	6	0	3.380231	4.738021	-2.048940
40	6	0	3.813884	5.636633	-2.931828
41	1	0	3.965922	6.678867	-2.659461
42	1	0	4.029149	5.366768	-3.961849
43	1	0	3.242816	3.706965	-2.366914
44	7	0	-0.999442	3.612994	1.394636
45	6	0	-1.912672	4.051326	1.996152
46	1	0	0.519700	3.359035	0.919476
47	22	0	-0.055048	-0.920812	-0.221178
48	8	0	-1.229851	-2.404680	-0.584737
49	8	0	0.970936	-1.330810	-1.739285
50	6	0	-1.859557	-2.719911	-1.710610
51	6	0	1.309731	-2.516856	-2.266395
52	6	0	-1.122478	-3.135575	-2.847534
53	6	0	-3.276061	-2.656420	-1.766724
54	6	0	0.338859	-3.416357	-2.783916
55	6	0	2.685529	-2.842994	-2.362051
56	6	0	-3.925112	-2.919683	-2.980198
57	6	0	-1.815249	-3.384374	-4.041100
58	6	0	3.072397	-4.069541	-2.917524
59	6	0	0.777746	-4.636527	-3.320995
60	6	0	-3.202820	-3.265665	-4.120161
61	6	0	2.126133	-4.974022	-3.386084
62	1	0	-5.009008	-2.861914	-3.015821
63	1	0	-1.247015	-3.672527	-4.920494
64	1	0	4.130648	-4.300860	-2.988701

65	1	0	0.030241	-5.333761	-3.686457
66	1	0	-3.716314	-3.460433	-5.056383
67	1	0	2.434571	-5.926175	-3.805928
68	8	0	0.757469	-1.797610	1.090875
69	6	0	0.501890	-2.932437	1.913199
70	1	0	-0.257903	-3.534996	1.398601
71	6	0	1.787460	-3.737780	2.048503
72	6	0	-0.056963	-2.463739	3.251438
73	1	0	2.575628	-3.137501	2.513196
74	1	0	-0.968688	-1.885617	3.091894
75	1	0	-0.299673	-3.323919	3.884077
76	1	0	0.669384	-1.839323	3.779200
77	1	0	1.615896	-4.626800	2.665347
78	1	0	2.135615	-4.062944	1.065184
79	6	0	-4.063588	-2.248239	-0.573257
80	6	0	-3.945614	-2.938257	0.697603
81	6	0	-4.935160	-1.198450	-0.678332
82	6	0	-4.669642	-2.467528	1.834221
83	6	0	-5.679649	-0.695359	0.433035
84	6	0	-5.540238	-1.308062	1.708986
85	6	0	-3.143364	-4.094945	0.830096
86	1	0	-5.030832	-0.682547	-1.627450
87	6	0	-4.507316	-3.149817	3.063311
88	6	0	-6.488241	0.455339	0.291170
89	6	0	-6.236459	-0.736972	2.798484
90	6	0	-3.012453	-4.744436	2.040404
91	6	0	-3.690700	-4.258436	3.171624
92	6	0	-7.143348	1.000804	1.376507
93	6	0	-7.017208	0.393780	2.639678
94	1	0	-6.571964	0.916381	-0.688477
95	1	0	-6.158333	-1.178204	3.785093
96	1	0	-7.532698	0.816028	3.496851
97	1	0	-7.749494	1.893503	1.258350
98	1	0	-3.585324	-4.761239	4.128166
99	1	0	-2.387312	-5.628648	2.116869
100	1	0	-5.040756	-2.809125	3.942631
101	1	0	-2.626543	-4.473483	-0.041654
102	6	0	3.736909	-1.863220	-1.972098
103	6	0	4.772074	-2.209083	-1.017310
104	6	0	3.786992	-0.649612	-2.598794
105	6	0	5.857105	-1.309209	-0.781598

106	6	0	4.841225	0.288610	-2.375696
107	6	0	5.886986	-0.023680	-1.459788
108	6	0	4.731624	-3.428928	-0.301054
109	1	0	3.015612	-0.390486	-3.316582
110	6	0	6.880953	-1.710878	0.107812
111	6	0	4.872547	1.518328	-3.075583
112	6	0	6.902244	0.938727	-1.254533
113	6	0	5.735584	-3.783237	0.577011
114	6	0	6.831034	-2.923943	0.767490
115	6	0	5.887991	2.430667	-2.868430
116	6	0	6.904338	2.140369	-1.939083
117	1	0	3.890348	-4.091534	-0.456222
118	1	0	5.678828	-4.723904	1.115578
119	1	0	7.634426	-3.205722	1.441415
120	1	0	7.729250	-1.058519	0.278210
121	1	0	7.698419	0.741941	-0.546152
122	1	0	7.696378	2.861088	-1.761135
123	1	0	5.893530	3.375281	-3.400921
124	1	0	4.077570	1.728984	-3.785571
125	6	0	-2.470533	0.717959	-1.525227
126	8	0	-1.392547	0.124861	-1.596707
127	6	0	-3.025650	1.261240	-0.275197
128	8	0	-3.192494	0.929974	-2.612699
129	6	0	-3.742713	2.410939	-0.144967
130	6	0	-4.292411	3.371048	-1.101260
131	6	0	-5.034940	3.038350	-2.247690
132	6	0	-4.127425	4.731241	-0.767434
133	6	0	-5.569262	4.041231	-3.052363
134	6	0	-4.633051	5.727239	-1.595493
135	6	0	-5.357345	5.385287	-2.739845
136	1	0	-3.850597	2.735510	0.883987
137	1	0	-5.211621	2.000817	-2.489432
138	1	0	-3.575404	4.982501	0.133497
139	1	0	-6.156266	3.771579	-3.925065
140	1	0	-4.477287	6.770523	-1.339207
141	1	0	-5.767748	6.162758	-3.377129
142	6	0	-2.642936	0.431441	-3.872143
143	6	0	-3.729457	0.554822	-4.913703
144	1	0	-2.327583	-0.601132	-3.725374
145	6	0	-2.594963	0.585223	0.974120
146	8	0	-1.696117	-0.256190	1.066432

147	8	0	-3.305586	0.951242	2.022862
148	6	0	-2.911329	0.469857	3.336960
149	6	0	-3.421113	1.478966	4.340308
150	1	0	-1.827442	0.369188	3.357723
151	1	0	-1.763856	1.035152	-4.113608
152	1	0	-3.353529	-0.519951	3.469349
153	1	0	-3.133134	1.168274	5.349783
154	1	0	-2.996559	2.465246	4.132736
155	1	0	-4.511562	1.551834	4.298408
156	1	0	-3.343763	0.197109	-5.873211
157	1	0	-4.595684	-0.058497	-4.649848
158	1	0	-4.051280	1.592821	-5.036445

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Zero-point correction = 1.28837 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19128 (a.u.)

Sum of electronic and zero-point Energies = -4590.83560 (a.u.)

Sum of electronic and thermal Free Energies = -4590.93270 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.571692	-0.743065	-0.209181
2	6	0	-1.659619	-1.225417	0.530839
3	6	0	-2.611931	-1.913986	-0.471739
4	6	0	-1.158085	-2.093536	1.678111
5	7	0	-2.070999	-3.207968	-1.050218
6	6	0	-4.056545	-2.189019	-0.028792
7	6	0	-1.838078	-2.220842	2.926768
8	6	0	0.019427	-2.791958	1.512847
9	6	0	-2.405542	-4.405670	-0.200681
10	6	0	-2.670805	-3.408396	-2.413360
11	6	0	-4.595397	-3.395587	-0.820773
12	6	0	-1.268985	-3.103479	3.906859
13	6	0	0.485879	-3.643345	2.535158
14	6	0	-3.923419	-4.662658	-0.267753
15	6	0	-4.207555	-3.272230	-2.320697
16	7	0	-0.120306	-3.812030	3.695303
17	1	0	-2.250441	-0.398239	0.946588
18	1	0	-2.628256	-1.221544	-1.313190

19	1	0	-4.650043	-1.294255	-0.211802
20	1	0	-4.111073	-2.408237	1.040857
21	6	0	-3.021470	-1.510781	3.265767
22	1	0	0.565823	-2.715256	0.584662
23	1	0	-2.073072	-4.187831	0.809286
24	1	0	-1.802308	-5.229330	-0.584489
25	1	0	-2.360807	-4.399490	-2.745635
26	1	0	-2.210079	-2.678113	-3.074226
27	1	0	-5.682652	-3.456621	-0.725657
28	6	0	-1.914131	-3.258084	5.161797
29	1	0	1.400583	-4.210406	2.371956
30	1	0	-4.148033	-5.523156	-0.905782
31	1	0	-4.297692	-4.890538	0.733890
32	1	0	-4.653201	-4.135338	-2.832653
33	6	0	-3.068541	-2.567925	5.448193
34	6	0	-3.620770	-1.683000	4.492677
35	1	0	-3.554312	-2.691863	6.411342
36	1	0	-1.457885	-3.934614	5.876803
37	1	0	-4.520373	-1.125352	4.731148
38	1	0	-3.448855	-0.806724	2.564723
39	6	0	-4.792833	-2.032441	-2.950437
40	6	0	-4.162822	-1.085598	-3.643236
41	1	0	-3.095485	-1.091669	-3.838214
42	1	0	-4.711908	-0.243778	-4.048362
43	1	0	-5.866587	-1.929605	-2.800457
44	22	0	0.108480	1.009442	0.095884
45	8	0	1.160484	2.606109	0.055842
46	8	0	-1.210453	1.832317	-0.972238
47	6	0	1.687664	3.157788	-1.036869
48	6	0	-1.537447	3.100972	-1.255192
49	6	0	0.848764	3.808022	-1.970808
50	6	0	3.084720	3.079829	-1.258152
51	6	0	-0.593242	4.069476	-1.701639
52	6	0	-2.907204	3.456441	-1.182284
53	6	0	3.615650	3.592658	-2.447224
54	6	0	1.425012	4.301310	-3.151468
55	6	0	-3.314564	4.760932	-1.481156
56	6	0	-1.051725	5.370298	-1.970947
57	6	0	2.791820	4.188578	-3.400069
58	6	0	-2.390160	5.728705	-1.859793
59	1	0	4.686607	3.524172	-2.615051

60	1	0	0.781176	4.774024	-3.886979
61	1	0	-4.369510	5.006332	-1.403944
62	1	0	-0.321320	6.115337	-2.270435
63	1	0	3.212551	4.576902	-4.322400
64	1	0	-2.706656	6.745623	-2.069087
65	8	0	-0.438652	1.263487	1.782449
66	6	0	0.257212	1.706076	2.948692
67	1	0	1.330790	1.584836	2.765603
68	6	0	-0.030333	3.187004	3.168729
69	6	0	-0.150830	0.829932	4.126660
70	1	0	-1.085841	3.353009	3.403162
71	1	0	0.082876	-0.218616	3.926106
72	1	0	0.382700	1.136578	5.033062
73	1	0	-1.226512	0.903681	4.312436
74	1	0	0.570138	3.570070	3.999905
75	1	0	0.224636	3.749767	2.268601
76	6	0	3.961766	2.384446	-0.280890
77	6	0	4.006000	2.771584	1.116274
78	6	0	4.753896	1.356012	-0.709144
79	6	0	4.792423	2.021375	2.040893
80	6	0	5.580143	0.594843	0.176718
81	6	0	5.587533	0.898577	1.567009
82	6	0	3.300034	3.903967	1.582243
83	1	0	4.732323	1.074246	-1.757079
84	6	0	4.782050	2.409428	3.401547
85	6	0	6.352003	-0.487201	-0.305661
86	6	0	6.372783	0.089773	2.420058
87	6	0	3.326012	4.270793	2.912112
88	6	0	4.060242	3.505034	3.834182
89	6	0	7.103894	-1.263815	0.552072
90	6	0	7.113140	-0.969898	1.927926
91	1	0	6.336832	-0.706931	-1.367279
92	1	0	6.400940	0.292003	3.484155
93	1	0	7.705310	-1.574336	2.608382
94	1	0	7.685087	-2.096169	0.167245
95	1	0	4.075002	3.782038	4.884066
96	1	0	2.775787	5.145513	3.243813
97	1	0	5.362683	1.850490	4.125894
98	1	0	2.734108	4.492260	0.871854
99	6	0	-3.976699	2.466461	-0.854752
100	6	0	-4.233839	2.046710	0.507365

101	6	0	-4.835715	2.081529	-1.844425
102	6	0	-5.374711	1.237826	0.802367
103	6	0	-5.970758	1.244667	-1.599518
104	6	0	-6.238614	0.788407	-0.278959
105	6	0	-3.407676	2.484524	1.567129
106	1	0	-4.665683	2.428294	-2.859358
107	6	0	-5.652187	0.937820	2.155696
108	6	0	-6.832305	0.867325	-2.655425
109	6	0	-7.336082	-0.082512	-0.083973
110	6	0	-3.709868	2.177989	2.878604
111	6	0	-4.848735	1.411259	3.175652
112	6	0	-7.905822	0.027891	-2.434190
113	6	0	-8.149172	-0.461529	-1.136650
114	1	0	-2.533155	3.077751	1.334383
115	1	0	-3.073085	2.532371	3.681278
116	1	0	-5.097462	1.187663	4.208132
117	1	0	-6.526214	0.349512	2.408707
118	1	0	-7.550351	-0.470356	0.905141
119	1	0	-8.984310	-1.132000	-0.958049
120	1	0	-8.556675	-0.257295	-3.255045
121	1	0	-6.630386	1.249341	-3.652121
122	1	0	-1.018721	-3.216746	-1.203417
123	7	0	0.486787	-3.821133	-1.665568
124	6	0	1.636368	-3.921722	-1.440537
125	6	0	2.011502	-0.512950	-1.845677
126	8	0	1.281900	0.462323	-1.606429
127	6	0	2.766259	-1.262773	-0.853900
128	8	0	2.110353	-0.969610	-3.087061
129	6	0	3.482533	-2.418953	-1.138761
130	6	0	1.251117	-0.361005	-4.089559
131	6	0	-0.164763	-0.892551	-3.968823
132	1	0	1.715993	-0.652661	-5.032699
133	6	0	2.564096	-0.896275	0.547143
134	8	0	1.852233	0.030326	0.960817
135	8	0	3.254285	-1.636425	1.413521
136	6	0	3.093186	-1.319036	2.823268
137	6	0	3.861499	-2.359630	3.603902
138	1	0	2.028354	-1.327505	3.062182
139	1	0	1.292341	0.724444	-3.981354
140	1	0	3.478138	-0.311156	2.988221
141	1	0	3.793170	-2.131961	4.672264

142	1	0	3.448399	-3.359292	3.443606
143	1	0	4.915381	-2.362075	3.315289
144	1	0	-0.769659	-0.494977	-4.790662
145	1	0	-0.159637	-1.984513	-4.023892
146	1	0	-0.607659	-0.581714	-3.020717
147	1	0	3.769816	-2.987881	-0.263888
148	6	0	4.252945	-2.781564	-2.339399
149	6	0	4.789902	-1.809617	-3.198717
150	6	0	4.612468	-4.125187	-2.538573
151	6	0	5.649324	-2.172798	-4.232780
152	6	0	5.459929	-4.489057	-3.578042
153	6	0	5.983023	-3.512833	-4.430531
154	1	0	4.549522	-0.766732	-3.044384
155	1	0	4.183569	-4.877976	-1.886797
156	1	0	6.060064	-1.405726	-4.881935
157	1	0	5.715073	-5.534061	-3.724473
158	1	0	6.648095	-3.795581	-5.240861

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Zero-point correction = 1.29108 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19269 (a.u.)

Sum of electronic and zero-point Energies = -4590.88316 (a.u.)

Sum of electronic and thermal Free Energies = -4590.98155 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.672372	-0.788624	0.041824
2	6	0	-1.937414	-0.969730	0.601727
3	6	0	-2.713855	-1.745070	-0.499378
4	6	0	-1.825315	-1.642853	1.967428
5	7	0	-1.820550	-2.882900	-0.972288
6	6	0	-4.123529	-2.313758	-0.318324
7	6	0	-2.876831	-1.633161	2.933601
8	6	0	-0.644852	-2.267150	2.314938
9	6	0	-2.019959	-4.153509	-0.185259
10	6	0	-2.096420	-3.145600	-2.422619
11	6	0	-4.236742	-3.588385	-1.182721
12	6	0	-2.647742	-2.312521	4.177797
13	6	0	-0.517060	-2.896190	3.571670

14	6	0	-3.429144	-4.698455	-0.491703
15	6	0	-3.618194	-3.373951	-2.595086
16	7	0	-1.471019	-2.935753	4.480597
17	1	0	-2.470039	-0.017999	0.729409
18	1	0	-2.713506	-1.047490	-1.336937
19	1	0	-4.850746	-1.559070	-0.618737
20	1	0	-4.329215	-2.572909	0.722591
21	6	0	-4.124816	-0.982556	2.740710
22	1	0	0.180053	-2.274675	1.617864
23	1	0	-1.894725	-3.901438	0.863393
24	1	0	-1.220027	-4.829019	-0.484845
25	1	0	-1.502961	-4.014337	-2.706569
26	1	0	-1.725768	-2.284368	-2.971448
27	1	0	-5.284642	-3.882014	-1.284586
28	6	0	-3.678153	-2.347607	5.152581
29	1	0	0.420796	-3.387354	3.827406
30	1	0	-3.369525	-5.582229	-1.133634
31	1	0	-3.913210	-4.999534	0.440899
32	1	0	-3.751462	-4.322198	-3.131728
33	6	0	-4.882441	-1.725543	4.921939
34	6	0	-5.102168	-1.033614	3.708392
35	1	0	-5.665310	-1.755538	5.673645
36	1	0	-3.472399	-2.875196	6.077893
37	1	0	-6.051008	-0.535093	3.542125
38	1	0	-4.306027	-0.431915	1.828176
39	6	0	-4.352506	-2.323698	-3.390705
40	6	0	-3.860457	-1.241589	-3.992476
41	1	0	-2.814514	-0.953311	-3.961152
42	1	0	-4.508753	-0.585972	-4.564758
43	1	0	-5.420409	-2.521952	-3.478577
44	22	0	0.236826	0.936475	-0.024560
45	8	0	1.301253	2.467795	-0.454745
46	8	0	-1.071958	1.556154	-1.243043
47	6	0	1.914233	2.625597	-1.630553
48	6	0	-1.282619	2.620583	-2.020482
49	6	0	1.175494	2.929107	-2.797471
50	6	0	3.317634	2.450185	-1.694300
51	6	0	-0.270567	3.288490	-2.768102
52	6	0	-2.629033	3.049950	-2.140937
53	6	0	3.961931	2.492006	-2.933144
54	6	0	1.863646	2.955281	-4.022377

55	6	0	-2.970765	4.105240	-2.987288
56	6	0	-0.664483	4.365279	-3.584709
57	6	0	3.236586	2.728698	-4.101356
58	6	0	-1.987036	4.772692	-3.712423
59	1	0	5.036660	2.339255	-2.972450
60	1	0	1.299814	3.141589	-4.931331
61	1	0	-4.011079	4.410238	-3.051658
62	1	0	0.109002	4.901758	-4.124779
63	1	0	3.737874	2.748850	-5.064156
64	1	0	-2.243374	5.610661	-4.352896
65	8	0	-0.281686	1.529819	1.579772
66	6	0	0.310518	1.767344	2.850638
67	1	0	1.215835	1.150482	2.910816
68	6	0	0.717179	3.233378	2.941311
69	6	0	-0.661528	1.338794	3.944038
70	1	0	-0.164366	3.881618	2.918800
71	1	0	-0.874533	0.269606	3.875421
72	1	0	-0.237270	1.541455	4.933759
73	1	0	-1.606946	1.881039	3.850783
74	1	0	1.264830	3.423060	3.870342
75	1	0	1.360337	3.492741	2.099372
76	6	0	4.059479	2.138467	-0.444653
77	6	0	4.079077	3.070791	0.664680
78	6	0	4.706812	0.943917	-0.324051
79	6	0	4.696288	2.702177	1.896385
80	6	0	5.349669	0.536007	0.887134
81	6	0	5.333118	1.399427	2.019970
82	6	0	3.509343	4.358982	0.542014
83	1	0	4.691524	0.244348	-1.151476
84	6	0	4.677551	3.633209	2.961022
85	6	0	5.961582	-0.735251	0.984005
86	6	0	5.937215	0.941151	3.213564
87	6	0	3.521606	5.252432	1.593654
88	6	0	4.102835	4.881276	2.818492
89	6	0	6.548270	-1.152309	2.162034
90	6	0	6.534059	-0.304866	3.285750
91	1	0	5.954771	-1.383136	0.113330
92	1	0	5.936330	1.569772	4.096345
93	1	0	6.989429	-0.630330	4.216201
94	1	0	7.014457	-2.131085	2.222789
95	1	0	4.107099	5.576918	3.652302

96	1	0	3.077167	6.235960	1.476307
97	1	0	5.132986	3.374812	3.909830
98	1	0	3.059447	4.640009	-0.402347
99	6	0	-3.698225	2.372217	-1.356271
100	6	0	-3.823775	2.609103	0.067730
101	6	0	-4.617591	1.588812	-1.991326
102	6	0	-4.899909	2.019162	0.796656
103	6	0	-5.688471	0.944283	-1.292893
104	6	0	-5.835340	1.140096	0.109920
105	6	0	-2.916875	3.456462	0.743865
106	1	0	-4.532962	1.428211	-3.060981
107	6	0	-5.021084	2.319186	2.172829
108	6	0	-6.591840	0.098371	-1.977235
109	6	0	-6.882815	0.456565	0.769347
110	6	0	-3.066892	3.733879	2.087011
111	6	0	-4.127651	3.160049	2.807670
112	6	0	-7.599254	-0.564016	-1.303935
113	6	0	-7.740820	-0.384532	0.084448
114	1	0	-2.098471	3.896332	0.188072
115	1	0	-2.365534	4.395003	2.584567
116	1	0	-4.248578	3.377205	3.864545
117	1	0	-5.833540	1.893570	2.748470
118	1	0	-7.026274	0.588944	1.834481
119	1	0	-8.530289	-0.901519	0.621205
120	1	0	-8.281153	-1.215968	-1.841536
121	1	0	-6.469786	-0.028901	-3.047818
122	1	0	-0.865096	-2.505387	-0.843234
123	7	0	0.845515	-4.730744	-1.764092
124	6	0	1.717453	-4.099651	-1.326046
125	6	0	1.782685	-1.120962	-1.665884
126	8	0	1.248953	0.014709	-1.619391
127	6	0	2.272716	-1.852835	-0.564508
128	8	0	1.929890	-1.712582	-2.869888
129	6	0	2.775649	-3.275394	-0.711739
130	6	0	1.654476	-0.891529	-4.036513
131	6	0	0.173117	-0.803312	-4.350993
132	1	0	2.202039	-1.392735	-4.837545
133	6	0	2.275986	-1.223667	0.704188
134	8	0	1.819127	-0.082391	0.975952
135	8	0	2.830528	-1.953802	1.693097
136	6	0	2.901295	-1.352511	3.007975

137	6	0	3.497122	-2.387418	3.936139
138	1	0	1.895798	-1.056993	3.317601
139	1	0	2.078708	0.100988	-3.876987
140	1	0	3.521983	-0.457242	2.949380
141	1	0	3.592185	-1.964542	4.940876
142	1	0	2.865043	-3.279224	3.998493
143	1	0	4.490861	-2.687258	3.594576
144	1	0	0.029330	-0.187565	-5.245169
145	1	0	-0.241989	-1.795346	-4.552569
146	1	0	-0.364424	-0.332754	-3.525223
147	1	0	2.878871	-3.667840	0.305033
148	6	0	4.125767	-3.513905	-1.402492
149	6	0	4.784868	-2.512343	-2.115711
150	6	0	4.729630	-4.769909	-1.277093
151	6	0	6.033529	-2.758639	-2.689212
152	6	0	5.973919	-5.019924	-1.853070
153	6	0	6.632068	-4.011484	-2.559444
154	1	0	4.321955	-1.541675	-2.225545
155	1	0	4.223528	-5.555028	-0.720910
156	1	0	6.535881	-1.967182	-3.237149
157	1	0	6.432433	-5.998134	-1.744007
158	1	0	7.603791	-4.201706	-3.004829

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d-I-TS2-*si*

Zero-point correction = 1.28689 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19315 (a.u.)

Sum of electronic and zero-point Energies = -4590.85560 (a.u.)

Sum of electronic and thermal Free Energies = -4590.94934 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.805621	0.474076	0.857065
2	6	0	2.075121	1.031193	0.788326
3	6	0	2.408382	1.198036	-0.709406
4	6	0	2.145506	2.293678	1.641556
5	7	0	1.423899	2.056660	-1.461560
6	6	0	3.839538	1.628801	-1.080838
7	6	0	3.362935	2.795405	2.200659
8	6	0	0.992169	3.004570	1.898311

9	6	0	1.840387	3.493800	-1.446935
10	6	0	1.455674	1.559701	-2.874284
11	6	0	3.798009	2.320519	-2.452774
12	6	0	3.304715	4.033307	2.926378
13	6	0	1.041392	4.207313	2.632130
14	6	0	3.143634	3.695877	-2.253924
15	6	0	2.911858	1.518156	-3.436451
16	7	0	2.146700	4.729488	3.124260
17	1	0	2.817564	0.316923	1.168881
18	1	0	2.234183	0.189420	-1.087272
19	1	0	4.489916	0.753599	-1.086721
20	1	0	4.251683	2.330660	-0.353777
21	6	0	4.621588	2.143722	2.089349
22	1	0	0.047850	2.643809	1.525770
23	1	0	1.965112	3.784051	-0.406312
24	1	0	1.023562	4.082304	-1.864276
25	1	0	0.828310	2.213255	-3.477607
26	1	0	1.022846	0.559767	-2.872835
27	1	0	4.806589	2.420396	-2.861748
28	6	0	4.495531	4.578702	3.474128
29	1	0	0.120345	4.762304	2.808145
30	1	0	2.930965	4.160274	-3.222524
31	1	0	3.816411	4.364992	-1.709129
32	1	0	2.922489	2.040314	-4.399350
33	6	0	5.698343	3.929326	3.327382
34	6	0	5.757236	2.698170	2.634067
35	1	0	6.604075	4.354618	3.748817
36	1	0	4.412473	5.518715	4.009415
37	1	0	6.707766	2.186208	2.526303
38	1	0	4.690016	1.195596	1.575757
39	6	0	3.393952	0.110303	-3.659437
40	6	0	3.878131	-0.347072	-4.813762
41	1	0	3.957374	0.288379	-5.693441
42	1	0	4.209551	-1.375727	-4.925380
43	1	0	3.332739	-0.569443	-2.811182
44	22	0	-0.243234	-1.038089	0.590638
45	8	0	-1.491008	-2.426748	0.192447
46	8	0	1.064833	-1.933434	-0.423053
47	6	0	-1.954919	-2.841577	-0.980951
48	6	0	1.265436	-3.163845	-0.912365
49	6	0	-1.119619	-3.519735	-1.894783

50	6	0	-3.315281	-2.594019	-1.285519
51	6	0	0.270147	-3.949707	-1.563322
52	6	0	2.594498	-3.654177	-0.832115
53	6	0	-3.822256	-2.958888	-2.533205
54	6	0	-1.668974	-3.862398	-3.143589
55	6	0	2.912036	-4.927913	-1.307524
56	6	0	0.637485	-5.239803	-1.992646
57	6	0	-2.995555	-3.582839	-3.470666
58	6	0	1.928242	-5.738092	-1.867014
59	1	0	-4.865621	-2.759563	-2.760426
60	1	0	-1.031333	-4.346206	-3.876912
61	1	0	3.936052	-5.277964	-1.220063
62	1	0	-0.131137	-5.865327	-2.434747
63	1	0	-3.382891	-3.856711	-4.447036
64	1	0	2.164108	-6.741813	-2.205809
65	8	0	-0.246682	-1.610875	2.294190
66	6	0	-1.128386	-2.463012	3.024166
67	1	0	-2.108778	-2.433227	2.539678
68	6	0	-0.620964	-3.900315	2.977471
69	6	0	-1.254602	-1.918992	4.442282
70	1	0	0.357015	-3.993129	3.460693
71	1	0	-1.615427	-0.886148	4.420771
72	1	0	-1.964636	-2.519105	5.021034
73	1	0	-0.286818	-1.933166	4.955493
74	1	0	-1.320716	-4.564680	3.494435
75	1	0	-0.537531	-4.231728	1.940195
76	6	0	-4.136533	-1.935727	-0.234733
77	6	0	-4.379233	-2.625013	1.018808
78	6	0	-4.600542	-0.664821	-0.401075
79	6	0	-5.007389	-1.943398	2.101362
80	6	0	-5.272678	0.044496	0.647472
81	6	0	-5.453795	-0.571320	1.918987
82	6	0	-3.990757	-3.973448	1.190574
83	1	0	-4.413661	-0.140332	-1.333974
84	6	0	-5.178769	-2.636817	3.322142
85	6	0	-5.715950	1.370475	0.446557
86	6	0	-6.066707	0.184880	2.944075
87	6	0	-4.183554	-4.629088	2.389321
88	6	0	-4.773254	-3.949518	3.469506
89	6	0	-6.323843	2.080286	1.463289
90	6	0	-6.495287	1.482065	2.724681

91	1	0	-5.569122	1.824048	-0.524807
92	1	0	-6.211567	-0.252236	3.924848
93	1	0	-6.966542	2.036852	3.530396
94	1	0	-6.663719	3.095511	1.287119
95	1	0	-4.919536	-4.456978	4.418267
96	1	0	-3.875873	-5.664442	2.497788
97	1	0	-5.643547	-2.138497	4.164668
98	1	0	-3.527300	-4.490691	0.359380
99	6	0	3.692737	-2.777869	-0.333978
100	6	0	3.790497	-2.374551	1.052764
101	6	0	4.652396	-2.373349	-1.218621
102	6	0	4.892296	-1.576587	1.487692
103	6	0	5.752642	-1.542025	-0.835294
104	6	0	5.895179	-1.146540	0.525007
105	6	0	2.807795	-2.760064	1.990430
106	1	0	4.576755	-2.673711	-2.259543
107	6	0	4.949207	-1.199924	2.849635
108	6	0	6.676739	-1.079147	-1.800500
109	6	0	6.991813	-0.321519	0.864317
110	6	0	2.881234	-2.358265	3.308055
111	6	0	3.961957	-1.572713	3.741345
112	6	0	7.724161	-0.254195	-1.441935
113	6	0	7.884674	0.120172	-0.095074
114	1	0	1.977165	-3.366111	1.656234
115	1	0	2.098834	-2.639726	4.003174
116	1	0	4.023208	-1.254127	4.777387
117	1	0	5.771389	-0.593288	3.208418
118	1	0	7.142462	-0.021185	1.894201
119	1	0	8.712493	0.760256	0.194471
120	1	0	8.422300	0.102055	-2.193045
121	1	0	6.535726	-1.372259	-2.836702
122	1	0	-1.549478	3.994206	-0.848276
123	6	0	-1.353810	0.687669	-1.863314
124	8	0	-0.875442	-0.381165	-1.476042
125	6	0	-1.345532	1.892918	-1.014428
126	8	0	-1.786774	0.848758	-3.106042
127	6	0	-1.902047	3.238573	-1.557517
128	6	0	-3.419838	3.432945	-1.679868
129	6	0	-4.052046	4.349248	-0.833855
130	6	0	-4.170124	2.798270	-2.677577
131	6	0	-5.411466	4.626436	-0.975920

132	6	0	-5.530306	3.073639	-2.817608
133	6	0	-6.155469	3.989123	-1.969247
134	6	0	-1.300094	3.614890	-2.843932
135	1	0	-3.475217	4.851495	-0.064740
136	1	0	-3.684873	2.108701	-3.355112
137	1	0	-5.885251	5.346139	-0.315462
138	1	0	-6.099443	2.576339	-3.596816
139	1	0	-7.213043	4.205234	-2.082987
140	6	0	-1.643435	-0.285432	-4.018961
141	6	0	-2.618857	-0.077605	-5.152818
142	1	0	-1.838901	-1.201228	-3.466762
143	6	0	-1.823840	1.561386	0.349442
144	8	0	-1.817421	0.435874	0.869132
145	8	0	-2.296730	2.604964	1.020725
146	6	0	-2.772319	2.350855	2.380837
147	6	0	-3.321472	3.654084	2.910046
148	1	0	-1.927020	1.983919	2.968145
149	1	0	-0.604896	-0.295291	-4.362864
150	1	0	-3.531876	1.570839	2.334270
151	1	0	-3.678185	3.501054	3.932883
152	1	0	-2.553830	4.433833	2.929144
153	1	0	-4.163103	3.997574	2.304333
154	1	0	-2.505908	-0.892258	-5.874422
155	1	0	-3.649991	-0.093641	-4.787497
156	1	0	-2.438275	0.869301	-5.670029
157	7	0	-0.840261	3.960639	-3.852069
158	1	0	0.038689	1.985822	-1.035443

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d-I-IM2-*si*

Zero-point correction = 1.28958 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19295 (a.u.)

Sum of electronic and zero-point Energies = -4590.86305 (a.u.)

Sum of electronic and thermal Free Energies = -4590.95968 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.784818	-0.554052	-0.783317
2	6	0	2.069187	-1.107699	-0.718750
3	6	0	2.453471	-1.232220	0.778919

4	6	0	2.108376	-2.389330	-1.538259
5	7	0	1.573596	-2.141764	1.558286
6	6	0	3.934216	-1.513540	1.112157
7	6	0	3.310551	-2.911327	-2.112904
8	6	0	0.946666	-3.102485	-1.754615
9	6	0	2.095697	-3.530085	1.568049
10	6	0	1.587875	-1.635807	2.947933
11	6	0	3.984115	-2.194468	2.492966
12	6	0	3.235398	-4.173976	-2.792221
13	6	0	0.977883	-4.328676	-2.448921
14	6	0	3.456271	-3.625565	2.310201
15	6	0	3.049451	-1.471427	3.497996
16	7	0	2.071887	-4.873737	-2.941524
17	1	0	2.786838	-0.397829	-1.150756
18	1	0	2.215248	-0.228703	1.137205
19	1	0	4.503363	-0.584162	1.097168
20	1	0	4.399458	-2.185422	0.388320
21	6	0	4.568410	-2.250534	-2.066209
22	1	0	0.006968	-2.721883	-1.386540
23	1	0	2.191600	-3.860003	0.534578
24	1	0	1.344578	-4.163130	2.045581
25	1	0	1.022543	-2.332373	3.570453
26	1	0	1.074023	-0.671522	2.962225
27	1	0	5.007983	-2.195931	2.877877
28	6	0	4.412855	-4.738318	-3.349415
29	1	0	0.051156	-4.884277	-2.591706
30	1	0	3.339668	-4.115614	3.283376
31	1	0	4.168881	-4.220189	1.728776
32	1	0	3.126314	-1.990924	4.460365
33	6	0	5.617333	-4.081231	-3.260753
34	6	0	5.690710	-2.822506	-2.620504
35	1	0	6.512560	-4.521109	-3.689735
36	1	0	4.318132	-5.697758	-3.847050
37	1	0	6.641000	-2.301998	-2.562358
38	1	0	4.645353	-1.279495	-1.599129
39	6	0	3.419223	-0.030747	3.711462
40	6	0	3.857344	0.483237	4.861279
41	1	0	3.984029	-0.130859	5.750773
42	1	0	4.103284	1.537265	4.958377
43	1	0	3.309769	0.630109	2.853037
44	22	0	-0.170530	1.012795	-0.580717

45	8	0	-1.408469	2.407536	-0.151830
46	8	0	1.151275	1.872358	0.425458
47	6	0	-1.839963	2.824498	1.033478
48	6	0	1.385630	3.106041	0.897266
49	6	0	-0.968970	3.469605	1.939220
50	6	0	-3.201789	2.617178	1.362152
51	6	0	0.413579	3.895476	1.574706
52	6	0	2.714123	3.586648	0.774508
53	6	0	-3.669246	2.971219	2.628972
54	6	0	-1.477978	3.798432	3.208257
55	6	0	3.046603	4.862565	1.236684
56	6	0	0.795941	5.183838	1.994070
57	6	0	-2.803132	3.545586	3.561918
58	6	0	2.084085	5.676581	1.826082
59	1	0	-4.714302	2.803643	2.873454
60	1	0	-0.810652	4.254322	3.932941
61	1	0	4.068236	5.209862	1.117251
62	1	0	0.043401	5.811225	2.460575
63	1	0	-3.160377	3.808596	4.552577
64	1	0	2.334978	6.679483	2.156351
65	8	0	-0.164556	1.584088	-2.282028
66	6	0	-1.047487	2.442299	-3.006367
67	1	0	-2.021634	2.424476	-2.508152
68	6	0	-0.523935	3.873846	-2.971114
69	6	0	-1.197145	1.894111	-4.420405
70	1	0	0.450509	3.953280	-3.463356
71	1	0	-1.566874	0.864752	-4.391013
72	1	0	-1.909397	2.498624	-4.991798
73	1	0	-0.236995	1.897076	-4.947348
74	1	0	-1.221540	4.543203	-3.484435
75	1	0	-0.427324	4.209263	-1.936213
76	6	0	-4.077301	2.017600	0.320922
77	6	0	-4.309495	2.732696	-0.920427
78	6	0	-4.622237	0.779183	0.491988
79	6	0	-5.017146	2.104742	-1.986599
80	6	0	-5.375723	0.127331	-0.538218
81	6	0	-5.557441	0.767653	-1.797921
82	6	0	-3.836847	4.053523	-1.096012
83	1	0	-4.448054	0.236912	1.417360
84	6	0	-5.179067	2.818474	-3.196972
85	6	0	-5.904661	-1.166103	-0.331214

86	6	0	-6.261214	0.068089	-2.805269
87	6	0	-4.024313	4.731391	-2.283056
88	6	0	-4.692044	4.102461	-3.348324
89	6	0	-6.596260	-1.820720	-1.331204
90	6	0	-6.772321	-1.197714	-2.579881
91	1	0	-5.760139	-1.638350	0.632320
92	1	0	-6.412616	0.524640	-3.776130
93	1	0	-7.311569	-1.709252	-3.371382
94	1	0	-6.999456	-2.811680	-1.151490
95	1	0	-4.834208	4.626959	-4.288371
96	1	0	-3.652058	5.744966	-2.394084
97	1	0	-5.702686	2.359900	-4.027254
98	1	0	-3.313572	4.532632	-0.277796
99	6	0	3.803550	2.708866	0.258442
100	6	0	3.866182	2.276025	-1.121212
101	6	0	4.797132	2.339897	1.121232
102	6	0	4.961936	1.476725	-1.569326
103	6	0	5.898994	1.518272	0.722490
104	6	0	6.001253	1.085459	-0.629780
105	6	0	2.858678	2.637776	-2.041347
106	1	0	4.748719	2.660543	2.157595
107	6	0	4.982393	1.067897	-2.922829
108	6	0	6.863685	1.099211	1.667446
109	6	0	7.096532	0.265102	-0.983356
110	6	0	2.898094	2.207199	-3.351435
111	6	0	3.969325	1.415133	-3.795769
112	6	0	7.911835	0.281201	1.295880
113	6	0	8.030237	-0.132427	-0.043952
114	1	0	2.036203	3.250227	-1.699414
115	1	0	2.096868	2.472250	-4.031256
116	1	0	4.003880	1.072731	-4.825437
117	1	0	5.798221	0.457652	-3.289954
118	1	0	7.214648	-0.065383	-2.008363
119	1	0	8.856975	-0.769531	-0.343042
120	1	0	8.641761	-0.041767	2.031661
121	1	0	6.751797	1.418940	2.699484
122	1	0	-1.827062	-4.010755	0.603416
123	6	0	-1.434085	-0.749896	1.774990
124	8	0	-0.870670	0.282606	1.434702
125	6	0	-1.525311	-1.932524	0.839758
126	8	0	-1.911009	-0.940251	2.985198

127	6	0	-2.112063	-3.276628	1.363536
128	6	0	-3.622907	-3.422803	1.571191
129	6	0	-4.342412	-4.238991	0.692090
130	6	0	-4.285026	-2.856590	2.667085
131	6	0	-5.700614	-4.479141	0.895559
132	6	0	-5.645779	-3.089556	2.865375
133	6	0	-6.358186	-3.901851	1.982072
134	6	0	-1.408951	-3.693684	2.585041
135	1	0	-3.835057	-4.693415	-0.151683
136	1	0	-3.733288	-2.253157	3.373904
137	1	0	-6.241047	-5.123134	0.208804
138	1	0	-6.145336	-2.643358	3.719539
139	1	0	-7.415319	-4.087905	2.142967
140	6	0	-1.715839	0.134422	3.969156
141	6	0	-2.802271	0.003244	5.008699
142	1	0	-1.752038	1.087506	3.447402
143	6	0	-2.059447	-1.487026	-0.510272
144	8	0	-1.903700	-0.362356	-0.977723
145	8	0	-2.655061	-2.453977	-1.175392
146	6	0	-3.115257	-2.137463	-2.533072
147	6	0	-3.744462	-3.389031	-3.093684
148	1	0	-2.244247	-1.811755	-3.106093
149	1	0	-0.717274	-0.007570	4.389580
150	1	0	-3.823246	-1.312470	-2.459593
151	1	0	-4.096152	-3.182040	-4.108756
152	1	0	-3.023832	-4.210532	-3.143221
153	1	0	-4.603003	-3.698007	-2.493631
154	1	0	-2.660773	0.781262	5.764785
155	1	0	-3.790847	0.144596	4.562895
156	1	0	-2.767090	-0.969539	5.507415
157	7	0	-0.870266	-4.051254	3.548133
158	1	0	-0.434758	-2.107812	0.679170

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d-I-COM-*re*

Zero-point correction = 1.28932 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19187 (a.u.)

Sum of electronic and zero-point Energies = -4590.84747 (a.u.)

Sum of electronic and thermal Free Energies = -4590.94492 (a.u.)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	-1.459464	-1.503731	-2.287075
2	7	0	-0.361485	-1.331721	-3.561339
3	6	0	0.265235	-1.905107	-4.379379
4	8	0	-0.545443	-0.468305	-0.291885
5	6	0	-1.432240	-1.257525	0.445573
6	6	0	-2.649063	-1.521359	-0.473102
7	6	0	-0.692991	-2.459489	1.025672
8	7	0	-2.267610	-2.042147	-1.842145
9	6	0	-3.807456	-2.391276	0.068293
10	6	0	-1.019844	-3.038002	2.290239
11	6	0	0.398334	-2.969609	0.354151
12	6	0	-1.870920	-3.494590	-1.899513
13	6	0	-3.455026	-1.860950	-2.742032
14	6	0	-4.174595	-3.475453	-0.958921
15	6	0	-0.212299	-4.133847	2.749878
16	6	0	1.117479	-4.061885	0.882564
17	6	0	-2.927485	-4.344778	-1.178425
18	6	0	-4.572562	-2.855564	-2.327577
19	7	0	0.839232	-4.636224	2.037939
20	1	0	-1.853219	-0.692620	1.287682
21	1	0	-3.011004	-0.513886	-0.683988
22	1	0	-4.663302	-1.753471	0.294787
23	1	0	-3.517309	-2.881607	0.999254
24	6	0	-2.067180	-2.573527	3.132860
25	1	0	0.702421	-2.521475	-0.581204
26	1	0	-0.881304	-3.595264	-1.471309
27	1	0	-1.791032	-3.725699	-2.961463
28	1	0	-3.105871	-2.015204	-3.763319
29	1	0	-3.774343	-0.821870	-2.642861
30	1	0	-5.003246	-4.079245	-0.580806
31	6	0	-0.498236	-4.728876	4.006586
32	1	0	1.960333	-4.463164	0.325920
33	1	0	-3.163658	-5.229132	-1.776909
34	1	0	-2.543716	-4.690764	-0.213919
35	1	0	-4.605615	-3.673334	-3.055923
36	6	0	-1.528144	-4.261416	4.788509
37	6	0	-2.314034	-3.170362	4.348068
38	1	0	-1.736405	-4.722982	5.748861
39	1	0	0.128773	-5.556996	4.320023

40	1	0	-3.115827	-2.796768	4.977597
41	1	0	-2.671955	-1.730338	2.826485
42	6	0	-5.915807	-2.187268	-2.312186
43	6	0	-6.962672	-2.592121	-3.029036
44	1	0	-6.902344	-3.449813	-3.695715
45	1	0	-7.917180	-2.078239	-2.976746
46	1	0	-6.015907	-1.319563	-1.665216
47	22	0	0.118515	1.208680	0.276471
48	8	0	1.176200	2.790352	0.472328
49	8	0	-1.313698	2.212585	-0.391584
50	6	0	1.523304	3.634831	-0.498983
51	6	0	-1.699420	3.493210	-0.280022
52	6	0	0.552699	4.488741	-1.070864
53	6	0	2.862496	3.658465	-0.960441
54	6	0	-0.837546	4.593875	-0.544260
55	6	0	-3.057997	3.734303	0.036707
56	6	0	3.202657	4.500941	-2.025387
57	6	0	0.938909	5.312894	-2.138739
58	6	0	-3.528511	5.044966	0.164704
59	6	0	-1.353556	5.890833	-0.379118
60	6	0	2.246557	5.320733	-2.621431
61	6	0	-2.675237	6.128304	-0.019249
62	1	0	4.228816	4.507626	-2.380878
63	1	0	0.190191	5.946378	-2.604172
64	1	0	-4.572346	5.200744	0.419681
65	1	0	-0.684507	6.729924	-0.541448
66	1	0	2.518304	5.965891	-3.450947
67	1	0	-3.036474	7.144220	0.104659
68	8	0	-0.168541	1.054568	2.039084
69	6	0	0.679296	1.295344	3.162469
70	1	0	1.714978	1.314105	2.805410
71	6	0	0.349581	2.662689	3.751441
72	6	0	0.518970	0.153003	4.158433
73	1	0	-0.668563	2.686751	4.153276
74	1	0	0.743067	-0.806090	3.684712
75	1	0	1.200436	0.288332	5.005478
76	1	0	-0.504839	0.105007	4.540870
77	1	0	1.042601	2.903298	4.564280
78	1	0	0.440715	3.427846	2.977453
79	6	0	3.866786	2.716518	-0.400627
80	6	0	4.168959	2.663887	1.016334

81	6	0	4.518654	1.865676	-1.250311
82	6	0	5.074455	1.681290	1.517910
83	6	0	5.444632	0.876468	-0.793121
84	6	0	5.720882	0.757994	0.597631
85	6	0	3.592953	3.586546	1.918974
86	1	0	4.299756	1.900461	-2.312320
87	6	0	5.313698	1.638317	2.912064
88	6	0	6.044181	-0.021050	-1.706955
89	6	0	6.606864	-0.261966	1.013677
90	6	0	3.856474	3.528899	3.272177
91	6	0	4.713088	2.534219	3.775564
92	6	0	6.904629	-1.008160	-1.271516
93	6	0	7.188335	-1.125692	0.102824
94	1	0	5.803343	0.075548	-2.761672
95	1	0	6.844789	-0.378747	2.064354
96	1	0	7.867093	-1.898196	0.451497
97	1	0	7.355422	-1.694391	-1.981540
98	1	0	4.918040	2.478703	4.840441
99	1	0	3.401073	4.249162	3.944300
100	1	0	5.990952	0.896804	3.319310
101	1	0	2.934432	4.351882	1.530034
102	6	0	-4.046008	2.622955	0.169805
103	6	0	-4.099345	1.785318	1.349832
104	6	0	-4.994382	2.470671	-0.801175
105	6	0	-5.149903	0.828594	1.501994
106	6	0	-6.064120	1.524703	-0.692370
107	6	0	-6.160547	0.697301	0.463042
108	6	0	-3.143462	1.926950	2.380112
109	1	0	-4.960560	3.104911	-1.682118
110	6	0	-5.183525	0.051510	2.682691
111	6	0	-7.045387	1.425473	-1.706007
112	6	0	-7.252654	-0.196671	0.552642
113	6	0	-3.210910	1.160901	3.526080
114	6	0	-4.239822	0.216648	3.679451
115	6	0	-8.108706	0.553105	-1.583902
116	6	0	-8.210092	-0.264780	-0.443332
117	1	0	-2.345384	2.646529	2.257453
118	1	0	-2.467024	1.284758	4.304430
119	1	0	-4.297529	-0.381743	4.583695
120	1	0	-5.968600	-0.681807	2.823503
121	1	0	-7.356091	-0.840579	1.417989

122	1	0	-9.039424	-0.958107	-0.345077
123	1	0	-8.861014	0.495749	-2.364318
124	1	0	-6.953002	2.060992	-2.582087
125	6	0	1.888772	0.374810	-2.167231
126	8	0	1.065182	1.134576	-1.652671
127	6	0	2.537974	-0.775552	-1.488290
128	8	0	2.267956	0.527684	-3.419687
129	6	0	2.790798	-1.859713	-2.273168
130	6	0	1.484002	1.456461	-4.234554
131	6	0	1.897961	1.227216	-5.668402
132	1	0	1.692820	2.470313	-3.884554
133	6	0	2.624802	-0.694426	-0.018664
134	8	0	2.008408	0.128973	0.663426
135	8	0	3.411580	-1.589479	0.549366
136	6	0	3.416975	-1.628717	2.007203
137	6	0	4.277693	-2.796776	2.427363
138	1	0	2.385053	-1.738828	2.344009
139	1	0	0.430966	1.225372	-4.070443
140	1	0	3.801180	-0.673583	2.368110
141	1	0	4.321514	-2.826414	3.520655
142	1	0	3.858241	-3.743500	2.079378
143	1	0	5.295619	-2.693138	2.043373
144	1	0	1.339051	1.908536	-6.317575
145	1	0	2.966279	1.416168	-5.811619
146	1	0	1.671953	0.199230	-5.964571
147	1	0	2.462919	-1.731715	-3.301016
148	6	0	3.239864	-3.221160	-1.993523
149	6	0	2.528368	-4.235273	-2.669378
150	6	0	4.313804	-3.579612	-1.160832
151	6	0	2.830685	-5.574919	-2.448956
152	6	0	4.634656	-4.921571	-0.976902
153	6	0	3.884124	-5.921795	-1.599649
154	1	0	1.728343	-3.948420	-3.346510
155	1	0	4.903958	-2.809736	-0.687781
156	1	0	2.256496	-6.347141	-2.951035
157	1	0	5.473186	-5.187560	-0.340754
158	1	0	4.130079	-6.966677	-1.436597

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d-I-TS1-*re*

Zero-point correction = 1.28855 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19431 (a.u.)
Sum of electronic and zero-point Energies = -4590.83575 (a.u.)
Sum of electronic and thermal Free Energies = -4590.92999 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.608583	-0.533034	-0.628574
2	6	0	-1.708717	-1.232046	-0.114479
3	6	0	-2.614654	-1.555210	-1.322317
4	6	0	-1.216332	-2.413482	0.711985
5	7	0	-2.004116	-2.554651	-2.282883
6	6	0	-4.065063	-1.994736	-1.077340
7	6	0	-1.942439	-2.951260	1.817678
8	6	0	0.005308	-2.978488	0.405171
9	6	0	-2.329587	-3.977812	-1.919648
10	6	0	-2.530980	-2.275234	-3.660820
11	6	0	-4.524466	-2.855485	-2.270392
12	6	0	-1.372463	-4.079182	2.500287
13	6	0	0.481403	-4.077011	1.151305
14	6	0	-3.832095	-4.224240	-2.157869
15	6	0	-4.073552	-2.209908	-3.612955
16	7	0	-0.170829	-4.629118	2.156992
17	1	0	-2.322328	-0.587363	0.528528
18	1	0	-2.623459	-0.615140	-1.872994
19	1	0	-4.685269	-1.106499	-0.966637
20	1	0	-4.159157	-2.577895	-0.157301
21	6	0	-3.170792	-2.422666	2.300725
22	1	0	0.586205	-2.584573	-0.417497
23	1	0	-2.051385	-4.115138	-0.878627
24	1	0	-1.679485	-4.605693	-2.530546
25	1	0	-2.169181	-3.079324	-4.301947
26	1	0	-2.064779	-1.350762	-3.996423
27	1	0	-5.611710	-2.966074	-2.260438
28	6	0	-2.067971	-4.655876	3.594944
29	1	0	1.445487	-4.513343	0.898337
30	1	0	-3.994457	-4.810722	-3.067664
31	1	0	-4.243969	-4.794703	-1.321167
32	1	0	-4.462227	-2.851782	-4.414089
33	6	0	-3.268498	-4.135234	4.016260
34	6	0	-3.816399	-3.003341	3.368696

35	1	0	-3.791819	-4.581398	4.856525
36	1	0	-1.610286	-5.510619	4.081965
37	1	0	-4.747403	-2.576447	3.724275
38	1	0	-3.596436	-1.538464	1.844220
39	6	0	-4.676036	-0.842388	-3.814606
40	6	0	-4.050780	0.313148	-4.035149
41	1	0	-2.971409	0.413886	-4.093829
42	1	0	-4.614419	1.230604	-4.168288
43	1	0	-5.763059	-0.837232	-3.760895
44	22	0	0.021722	1.038260	0.223842
45	8	0	1.060014	2.593819	0.601183
46	8	0	-1.361062	2.111542	-0.491916
47	6	0	1.429731	3.559272	-0.238228
48	6	0	-1.783721	3.337202	-0.142579
49	6	0	0.458526	4.474203	-0.713403
50	6	0	2.782775	3.680705	-0.643281
51	6	0	-0.939762	4.481105	-0.203086
52	6	0	-3.137513	3.501516	0.232612
53	6	0	3.128938	4.702835	-1.541036
54	6	0	0.851815	5.465589	-1.621978
55	6	0	-3.617966	4.762942	0.602398
56	6	0	-1.463961	5.723000	0.189032
57	6	0	2.175687	5.584937	-2.039476
58	6	0	-2.784741	5.876288	0.596684
59	1	0	4.168211	4.800232	-1.839480
60	1	0	0.099834	6.150490	-2.001523
61	1	0	-4.658609	4.855521	0.899114
62	1	0	-0.802219	6.583391	0.175538
63	1	0	2.462463	6.364962	-2.737805
64	1	0	-3.158013	6.849135	0.900408
65	8	0	-0.537803	0.763777	1.904250
66	6	0	0.134871	0.772195	3.162754
67	1	0	1.207900	0.666776	2.969389
68	6	0	-0.096117	2.114885	3.848161
69	6	0	-0.338809	-0.420262	3.984585
70	1	0	-1.146440	2.245700	4.122264
71	1	0	-0.130696	-1.354947	3.458059
72	1	0	0.176796	-0.446573	4.951259
73	1	0	-1.416280	-0.366682	4.164739
74	1	0	0.504466	2.182679	4.761716
75	1	0	0.193364	2.927007	3.177176

76	6	0	3.839724	2.714876	-0.235710
77	6	0	4.118663	2.367907	1.146658
78	6	0	4.625796	2.175563	-1.219550
79	6	0	5.167505	1.446132	1.453146
80	6	0	5.741939	1.325911	-0.948917
81	6	0	6.027205	0.944437	0.391415
82	6	0	3.393268	2.948246	2.212729
83	1	0	4.413784	2.412051	-2.257332
84	6	0	5.371834	1.084114	2.805665
85	6	0	6.584771	0.889668	-1.997858
86	6	0	7.168356	0.143551	0.625254
87	6	0	3.630321	2.590899	3.524498
88	6	0	4.614596	1.632604	3.822725
89	6	0	7.706591	0.127708	-1.736169
90	6	0	7.998356	-0.245910	-0.410498
91	1	0	6.343906	1.186751	-3.014739
92	1	0	7.423832	-0.155249	1.634928
93	1	0	8.879086	-0.844265	-0.198210
94	1	0	8.357432	-0.186365	-2.546360
95	1	0	4.793471	1.334824	4.851620
96	1	0	3.055727	3.050785	4.322153
97	1	0	6.140218	0.363032	3.057612
98	1	0	2.633554	3.682190	1.988015
99	6	0	-4.123966	2.377283	0.233831
100	6	0	-4.380487	1.629935	1.447199
101	6	0	-4.920844	2.175796	-0.855728
102	6	0	-5.467556	0.705352	1.506116
103	6	0	-6.007831	1.243209	-0.849194
104	6	0	-6.285168	0.484902	0.324099
105	6	0	-3.593205	1.843156	2.601335
106	1	0	-4.753911	2.760739	-1.755060
107	6	0	-5.730138	0.058759	2.736350
108	6	0	-6.824590	1.078986	-1.991322
109	6	0	-7.345948	-0.449203	0.280197
110	6	0	-3.875642	1.196086	3.787268
111	6	0	-4.958747	0.303433	3.856707
112	6	0	-7.864538	0.171308	-2.000675
113	6	0	-8.116585	-0.609114	-0.856505
114	1	0	-2.760770	2.531202	2.535953
115	1	0	-3.266292	1.379200	4.666200
116	1	0	-5.189864	-0.197073	4.791833

117	1	0	-6.563353	-0.629535	2.815816
118	1	0	-7.564866	-1.059817	1.148221
119	1	0	-8.924878	-1.334098	-0.862010
120	1	0	-8.482864	0.056249	-2.885804
121	1	0	-6.613380	1.682700	-2.868691
122	1	0	-0.947269	-2.487958	-2.380692
123	7	0	0.552507	-2.830685	-3.026666
124	6	0	1.726935	-2.853843	-3.022912
125	6	0	2.120051	0.267732	-1.982605
126	8	0	1.246278	1.028728	-1.546953
127	6	0	2.795616	-0.783863	-1.224472
128	8	0	2.495008	0.352995	-3.257007
129	6	0	3.495432	-1.747058	-1.929966
130	6	0	1.702024	1.224490	-4.113881
131	6	0	0.371737	0.577848	-4.458098
132	1	0	2.330461	1.354915	-4.996259
133	6	0	2.580465	-0.802564	0.219511
134	8	0	1.772950	-0.086831	0.829927
135	8	0	3.371728	-1.627649	0.888251
136	6	0	3.195782	-1.707824	2.327268
137	6	0	4.257502	-2.654623	2.838568
138	1	0	2.183618	-2.066428	2.531796
139	1	0	1.571667	2.186083	-3.614422
140	1	0	3.304245	-0.705931	2.744931
141	1	0	4.182406	-2.730889	3.927761
142	1	0	4.137662	-3.652350	2.409081
143	1	0	5.255889	-2.289889	2.582209
144	1	0	-0.159010	1.207708	-5.179895
145	1	0	0.526809	-0.411799	-4.895398
146	1	0	-0.244056	0.475887	-3.562238
147	1	0	3.755943	-1.491013	-2.947237
148	6	0	4.243830	-2.887779	-1.344235
149	6	0	3.635996	-4.083654	-0.948109
150	6	0	5.622233	-2.727575	-1.165844
151	6	0	4.393713	-5.093613	-0.359278
152	6	0	6.375219	-3.734680	-0.564105
153	6	0	5.764522	-4.919715	-0.154789
154	1	0	2.576242	-4.217631	-1.124118
155	1	0	6.098792	-1.805348	-1.472668
156	1	0	3.911605	-6.020582	-0.062976
157	1	0	7.441069	-3.587042	-0.418280

158	1	0	6.351606	-5.706395	0.309465

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d-I-IM1-*re*

Zero-point correction = 1.29137 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19690 (a.u.)

Sum of electronic and zero-point Energies = -4590.88160 (a.u.)

Sum of electronic and thermal Free Energies = -4590.97607 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.562055	-0.498827	-0.333502
2	6	0	-1.790381	-1.067691	-0.002931
3	6	0	-2.410843	-1.388890	-1.394235
4	6	0	-1.593956	-2.238266	0.957339
5	7	0	-1.307759	-2.006054	-2.243662
6	6	0	-3.675757	-2.222803	-1.608109
7	6	0	-2.653417	-2.824966	1.713947
8	6	0	-0.324887	-2.749562	1.134125
9	6	0	-1.253002	-3.506453	-2.124588
10	6	0	-1.524914	-1.630197	-3.678499
11	6	0	-3.536748	-2.948568	-2.964207
12	6	0	-2.329264	-3.934681	2.566071
13	6	0	-0.109232	-3.836085	2.008549
14	6	0	-2.520615	-4.089141	-2.782787
15	6	0	-2.979934	-1.993355	-4.059695
16	7	0	-1.062613	-4.427210	2.701534
17	1	0	-2.465644	-0.339845	0.465971
18	1	0	-2.555414	-0.400830	-1.831500
19	1	0	-4.542297	-1.560661	-1.593000
20	1	0	-3.814827	-2.966815	-0.820790
21	6	0	-4.000927	-2.377782	1.673855
22	1	0	0.500483	-2.311108	0.595065
23	1	0	-1.192378	-3.740472	-1.065030
24	1	0	-0.333204	-3.824894	-2.613716
25	1	0	-0.785938	-2.176340	-4.264116
26	1	0	-1.308799	-0.568897	-3.764500
27	1	0	-4.504695	-3.344302	-3.281864
28	6	0	-3.359654	-4.565898	3.310069
29	1	0	0.898259	-4.230680	2.124854

30	1	0	-2.279218	-4.543510	-3.748319
31	1	0	-2.934557	-4.872928	-2.143418
32	1	0	-2.943747	-2.577217	-4.988185
33	6	0	-4.658064	-4.121351	3.226589
34	6	0	-4.977148	-3.015540	2.404935
35	1	0	-5.441253	-4.612294	3.796157
36	1	0	-3.078780	-5.404125	3.939118
37	1	0	-6.002278	-2.666726	2.348444
38	1	0	-4.265367	-1.523231	1.066352
39	6	0	-3.898329	-0.823719	-4.318777
40	6	0	-3.613487	0.477702	-4.283756
41	1	0	-2.635355	0.876267	-4.032794
42	1	0	-4.372035	1.216295	-4.522527
43	1	0	-4.913705	-1.122283	-4.579664
44	22	0	0.189824	1.164749	0.312929
45	8	0	1.171120	2.787121	0.543372
46	8	0	-1.187700	2.139583	-0.561353
47	6	0	1.601749	3.581665	-0.436218
48	6	0	-1.595143	3.411420	-0.462392
49	6	0	0.684481	4.418452	-1.115861
50	6	0	2.970630	3.576916	-0.804226
51	6	0	-0.741797	4.524704	-0.704423
52	6	0	-2.958484	3.642647	-0.164587
53	6	0	3.397954	4.406925	-1.849199
54	6	0	1.156781	5.221189	-2.164144
55	6	0	-3.457469	4.945497	-0.082695
56	6	0	-1.285194	5.815608	-0.599835
57	6	0	2.500868	5.224405	-2.532559
58	6	0	-2.623712	6.039388	-0.294089
59	1	0	4.448834	4.399222	-2.123346
60	1	0	0.448909	5.845562	-2.701047
61	1	0	-4.506891	5.089360	0.157938
62	1	0	-0.623421	6.661884	-0.756157
63	1	0	2.844429	5.858456	-3.344003
64	1	0	-3.008297	7.051441	-0.217095
65	8	0	-0.385996	1.059371	2.002410
66	6	0	0.198074	0.917194	3.289157
67	1	0	1.235634	0.588841	3.149630
68	6	0	0.203742	2.278465	3.976244
69	6	0	-0.565754	-0.150619	4.064758
70	1	0	-0.818525	2.622300	4.157232

71	1	0	-0.535340	-1.104336	3.531260
72	1	0	-0.126157	-0.295279	5.058106
73	1	0	-1.614208	0.138195	4.185397
74	1	0	0.728498	2.223806	4.936300
75	1	0	0.710840	3.007875	3.341401
76	6	0	3.922853	2.604270	-0.206434
77	6	0	4.144623	2.495122	1.221439
78	6	0	4.614643	1.778045	-1.048387
79	6	0	5.010368	1.482575	1.734189
80	6	0	5.520044	0.777215	-0.581366
81	6	0	5.712950	0.598685	0.816875
82	6	0	3.536993	3.396001	2.125059
83	1	0	4.452700	1.851657	-2.118501
84	6	0	5.173188	1.385221	3.136420
85	6	0	6.215565	-0.047056	-1.496813
86	6	0	6.598460	-0.419030	1.239373
87	6	0	3.725731	3.284227	3.487425
88	6	0	4.538724	2.257853	3.999219
89	6	0	7.087747	-1.021656	-1.053897
90	6	0	7.273348	-1.211238	0.328605
91	1	0	6.056487	0.110721	-2.560079
92	1	0	6.769562	-0.583714	2.296560
93	1	0	7.951997	-1.980795	0.683477
94	1	0	7.628278	-1.638184	-1.766090
95	1	0	4.682725	2.159376	5.071035
96	1	0	3.245058	3.986338	4.161281
97	1	0	5.815465	0.616953	3.550807
98	1	0	2.909180	4.183584	1.730057
99	6	0	-3.898856	2.508383	0.074023
100	6	0	-4.145813	2.047481	1.424092
101	6	0	-4.604287	1.968185	-0.961708
102	6	0	-5.140485	1.053729	1.670550
103	6	0	-5.610962	0.969021	-0.761593
104	6	0	-5.898538	0.508248	0.555311
105	6	0	-3.421646	2.585015	2.513367
106	1	0	-4.422439	2.317377	-1.973469
107	6	0	-5.353634	0.635419	3.003965
108	6	0	-6.342042	0.449449	-1.855832
109	6	0	-6.916662	-0.461247	0.712617
110	6	0	-3.666296	2.166594	3.805738
111	6	0	-4.636939	1.179826	4.051563

112	6	0	-7.317159	-0.510732	-1.672380
113	6	0	-7.604507	-0.969913	-0.373460
114	1	0	-2.664477	3.333074	2.313583
115	1	0	-3.106873	2.594478	4.631302
116	1	0	-4.824349	0.842007	5.066211
117	1	0	-6.091299	-0.127572	3.218799
118	1	0	-7.179405	-0.809955	1.703908
119	1	0	-8.377858	-1.716326	-0.220314
120	1	0	-7.867487	-0.902000	-2.522723
121	1	0	-6.117763	0.821547	-2.849339
122	1	0	-0.453145	-1.557460	-1.857297
123	7	0	1.618734	-2.866075	-3.882803
124	6	0	2.347416	-2.532023	-3.041743
125	6	0	2.040627	0.099239	-1.889719
126	8	0	1.289547	1.019183	-1.484619
127	6	0	2.494179	-1.017766	-1.142836
128	8	0	2.504766	0.162004	-3.156454
129	6	0	3.202524	-2.150225	-1.897140
130	6	0	2.126603	1.320038	-3.945249
131	6	0	0.725121	1.196090	-4.511372
132	1	0	2.874430	1.341570	-4.740975
133	6	0	2.480817	-0.872257	0.265285
134	8	0	1.850354	0.016029	0.904237
135	8	0	3.229207	-1.739250	0.961153
136	6	0	3.161317	-1.676758	2.402926
137	6	0	4.076319	-2.761439	2.928356
138	1	0	2.124430	-1.829572	2.717465
139	1	0	2.226356	2.216641	-3.331660
140	1	0	3.472529	-0.683877	2.732678
141	1	0	4.052699	-2.762661	4.022901
142	1	0	3.765478	-3.746479	2.570137
143	1	0	5.105334	-2.590084	2.601706
144	1	0	0.530402	2.032760	-5.190453
145	1	0	0.614933	0.263329	-5.072289
146	1	0	-0.012998	1.235687	-3.707552
147	1	0	4.156104	-1.797582	-2.310045
148	6	0	3.475419	-3.435907	-1.111418
149	6	0	2.423207	-4.248342	-0.679095
150	6	0	4.788050	-3.816830	-0.836923
151	6	0	2.679285	-5.413300	0.040049
152	6	0	5.048399	-4.982338	-0.115847

153	6	0	3.995861	-5.782961	0.327553
154	1	0	1.399827	-3.962997	-0.895132
155	1	0	5.604576	-3.183528	-1.163441
156	1	0	1.852969	-6.033786	0.373586
157	1	0	6.075091	-5.262228	0.100366
158	1	0	4.196994	-6.690997	0.887806

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d-I-TS2-*re*

Zero-point correction = 1.28581 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19015 (a.u.)

Sum of electronic and zero-point Energies = -4590.85652 (a.u.)

Sum of electronic and thermal Free Energies = -4590.95218 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.779308	-0.512908	-0.783009
2	6	0	2.048333	-1.063677	-0.653217
3	6	0	2.350109	-1.137285	0.858784
4	6	0	2.131465	-2.378600	-1.422073
5	7	0	1.370069	-1.985623	1.629125
6	6	0	3.783477	-1.500213	1.285910
7	6	0	3.357536	-2.905217	-1.938959
8	6	0	0.985370	-3.112183	-1.641000
9	6	0	1.809790	-3.413920	1.709937
10	6	0	1.353009	-1.433664	3.016569
11	6	0	3.728690	-2.143134	2.680614
12	6	0	3.311573	-4.180656	-2.596714
13	6	0	1.048161	-4.359212	-2.298383
14	6	0	3.128690	-3.544985	2.509054
15	6	0	2.792792	-1.338462	3.616145
16	7	0	2.159603	-4.895810	-2.759623
17	1	0	2.796524	-0.371772	-1.062610
18	1	0	2.137050	-0.114939	1.175754
19	1	0	4.400867	-0.601402	1.273712
20	1	0	4.240364	-2.213563	0.598285
21	6	0	4.613136	-2.245205	-1.848297
22	1	0	0.034669	-2.744175	-1.291345
23	1	0	1.910527	-3.788445	0.695213
24	1	0	1.004108	-3.975714	2.181421

25	1	0	0.715048	-2.079154	3.625211
26	1	0	0.902706	-0.443459	2.971878
27	1	0	4.728727	-2.194836	3.118559
28	6	0	4.508490	-4.745482	-3.109978
29	1	0	0.135098	-4.937352	-2.427603
30	1	0	2.947642	-4.004864	3.486382
31	1	0	3.825740	-4.192282	1.968949
32	1	0	2.793173	-1.828468	4.596061
33	6	0	5.708074	-4.084922	-2.986501
34	6	0	5.756585	-2.822049	-2.352646
35	1	0	6.618686	-4.526808	-3.379541
36	1	0	4.433221	-5.711967	-3.597187
37	1	0	6.703820	-2.301454	-2.258604
38	1	0	4.674596	-1.271567	-1.384469
39	6	0	3.229846	0.089402	3.803871
40	6	0	3.663872	0.601461	4.955135
41	1	0	3.729734	0.001697	5.860698
42	1	0	3.970626	1.640513	5.035287
43	1	0	3.182658	0.733610	2.927390
44	22	0	-0.249791	1.025696	-0.630658
45	8	0	-1.462906	2.467762	-0.313526
46	8	0	1.079890	1.943662	0.346215
47	6	0	-1.911820	2.961414	0.834736
48	6	0	1.312913	3.201609	0.742218
49	6	0	-1.057397	3.677161	1.701087
50	6	0	-3.272899	2.754907	1.166519
51	6	0	0.338212	4.055720	1.335673
52	6	0	2.651847	3.655671	0.625605
53	6	0	-3.761756	3.204242	2.394111
54	6	0	-1.588597	4.104689	2.931144
55	6	0	2.996859	4.954720	1.006057
56	6	0	0.732728	5.365154	1.670634
57	6	0	-2.916985	3.870171	3.285149
58	6	0	2.033098	5.825496	1.505558
59	1	0	-4.805841	3.035492	2.641861
60	1	0	-0.935272	4.620783	3.627835
61	1	0	4.027905	5.275306	0.891879
62	1	0	-0.021237	6.036206	2.069411
63	1	0	-3.291716	4.211527	4.245095
64	1	0	2.291981	6.845735	1.770182
65	8	0	-0.230409	1.498318	-2.364054

66	6	0	-1.103232	2.309921	-3.149075
67	1	0	-2.073545	2.351483	-2.646379
68	6	0	-0.549170	3.727561	-3.231794
69	6	0	-1.275155	1.652761	-4.513193
70	1	0	0.425549	3.743165	-3.730431
71	1	0	-1.672179	0.639605	-4.398374
72	1	0	-1.975184	2.227653	-5.128628
73	1	0	-0.317904	1.587324	-5.042034
74	1	0	-1.231754	4.369684	-3.797739
75	1	0	-0.440692	4.142827	-2.227305
76	6	0	-4.115062	2.031002	0.177834
77	6	0	-4.355104	2.615688	-1.128183
78	6	0	-4.605544	0.789734	0.456684
79	6	0	-5.008919	1.857290	-2.142535
80	6	0	-5.307646	0.010137	-0.518885
81	6	0	-5.488795	0.518341	-1.837075
82	6	0	-3.938925	3.934964	-1.420247
83	1	0	-4.418794	0.341006	1.428403
84	6	0	-5.174152	2.444838	-3.418415
85	6	0	-5.780840	-1.281242	-0.197588
86	6	0	-6.134025	-0.307537	-2.785818
87	6	0	-4.128467	4.488118	-2.670100
88	6	0	-4.741091	3.729936	-3.683040
89	6	0	-6.418231	-2.060572	-1.142694
90	6	0	-6.591228	-1.569467	-2.449197
91	1	0	-5.633398	-1.653237	0.808886
92	1	0	-6.280529	0.045193	-3.799895
93	1	0	-7.085098	-2.180846	-3.198427
94	1	0	-6.779004	-3.048379	-0.876546
95	1	0	-4.883245	4.155274	-4.671861
96	1	0	-3.799146	5.502778	-2.870642
97	1	0	-5.657081	1.885126	-4.210546
98	1	0	-3.455865	4.512238	-0.641437
99	6	0	3.738865	2.731480	0.192748
100	6	0	3.840123	2.233679	-1.162768
101	6	0	4.698920	2.391673	1.104270
102	6	0	4.957873	1.430943	-1.545905
103	6	0	5.814371	1.557329	0.774996
104	6	0	5.972460	1.089491	-0.560321
105	6	0	2.845746	2.529299	-2.120752
106	1	0	4.620254	2.761509	2.122447

107	6	0	5.018952	0.961600	-2.878456
108	6	0	6.749003	1.177874	1.766059
109	6	0	7.098589	0.286371	-0.852873
110	6	0	2.921164	2.032845	-3.405640
111	6	0	4.018947	1.244685	-3.788490
112	6	0	7.824902	0.370555	1.454895
113	6	0	8.003704	-0.069585	0.130350
114	1	0	2.003218	3.139410	-1.827414
115	1	0	2.126211	2.242047	-4.111945
116	1	0	4.082210	0.851742	-4.798489
117	1	0	5.851629	0.346852	-3.196272
118	1	0	7.265859	-0.061021	-1.865322
119	1	0	8.856202	-0.692345	-0.122994
120	1	0	8.532791	0.080501	2.225173
121	1	0	6.596068	1.526401	2.783516
122	1	0	-1.473522	-3.080723	2.796929
123	6	0	-1.370254	-0.552321	1.903482
124	8	0	-0.916378	0.502713	1.455066
125	6	0	-1.382545	-1.792648	1.109144
126	8	0	-1.761520	-0.651015	3.170995
127	6	0	-1.907681	-3.086959	1.790976
128	6	0	-3.421795	-3.285901	1.961670
129	6	0	-4.139649	-4.166925	1.145739
130	6	0	-4.092550	-2.637701	3.006743
131	6	0	-5.496286	-4.398471	1.371169
132	6	0	-5.453024	-2.857519	3.221660
133	6	0	-6.160692	-3.742588	2.407150
134	6	0	-1.323915	-4.255055	1.112994
135	1	0	-3.635177	-4.688639	0.341750
136	1	0	-3.545233	-1.970416	3.658161
137	1	0	-6.031129	-5.097315	0.735451
138	1	0	-5.955353	-2.345414	4.036688
139	1	0	-7.217019	-3.921617	2.581141
140	6	0	-1.647871	0.556232	3.991744
141	6	0	-2.604111	0.408484	5.151434
142	1	0	-1.883384	1.417899	3.372364
143	6	0	-1.882586	-1.520551	-0.259252
144	8	0	-1.842769	-0.428164	-0.846640
145	8	0	-2.415922	-2.579273	-0.847734
146	6	0	-2.892342	-2.410889	-2.219155
147	6	0	-3.454585	-3.741908	-2.657780

148	1	0	-2.043476	-2.093520	-2.829987
149	1	0	-0.606661	0.634303	4.319627
150	1	0	-3.643372	-1.620994	-2.222903
151	1	0	-3.805805	-3.658090	-3.690613
152	1	0	-2.695306	-4.528060	-2.613892
153	1	0	-4.302345	-4.032654	-2.033105
154	1	0	-2.516467	1.285869	5.798902
155	1	0	-3.638019	0.352802	4.798418
156	1	0	-2.383028	-0.480898	5.749338
157	7	0	-0.860718	-5.175405	0.579808
158	1	0	0.005629	-1.911027	1.151570

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d-I-IM2-*re*

Zero-point correction = 1.28926 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19231 (a.u.)

Sum of electronic and zero-point Energies = -4590.86298 (a.u.)

Sum of electronic and thermal Free Energies = -4590.95992 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.752213	-0.557340	-0.700148
2	6	0	2.037169	-1.110012	-0.634922
3	6	0	2.422989	-1.214647	0.863283
4	6	0	2.076481	-2.402543	-1.438489
5	7	0	1.517822	-2.086322	1.659636
6	6	0	3.894579	-1.534969	1.201768
7	6	0	3.279105	-2.925622	-2.012936
8	6	0	0.918934	-3.125648	-1.634350
9	6	0	1.988354	-3.492013	1.690351
10	6	0	1.548965	-1.561066	3.038462
11	6	0	3.923792	-2.204154	2.589418
12	6	0	3.203952	-4.192582	-2.683312
13	6	0	0.951050	-4.361984	-2.312822
14	6	0	3.351849	-3.620707	2.422016
15	6	0	3.014480	-1.441935	3.589700
16	7	0	2.043321	-4.900390	-2.816052
17	1	0	2.753741	-0.404494	-1.075546
18	1	0	2.210782	-0.198598	1.203856
19	1	0	4.492138	-0.623083	1.176085

20	1	0	4.338014	-2.228368	0.484844
21	6	0	4.536698	-2.264590	-1.971899
22	1	0	-0.019533	-2.757046	-1.252608
23	1	0	2.054158	-3.849263	0.664824
24	1	0	1.216349	-4.091709	2.180942
25	1	0	0.951902	-2.223837	3.673423
26	1	0	1.074298	-0.577513	3.038915
27	1	0	4.946917	-2.235221	2.974458
28	6	0	4.379665	-4.756511	-3.244430
29	1	0	0.029824	-4.931520	-2.420523
30	1	0	3.232907	-4.100757	3.400189
31	1	0	4.040975	-4.239815	1.838553
32	1	0	3.075994	-1.953649	4.557393
33	6	0	5.584035	-4.097987	-3.163589
34	6	0	5.658383	-2.837838	-2.526843
35	1	0	6.478166	-4.538683	-3.594179
36	1	0	4.283772	-5.718920	-3.736157
37	1	0	6.608684	-2.317183	-2.471399
38	1	0	4.614778	-1.292583	-1.507103
39	6	0	3.429183	-0.010766	3.786611
40	6	0	3.904182	0.497146	4.924200
41	1	0	4.029727	-0.114351	5.815602
42	1	0	4.186402	1.543164	5.007425
43	1	0	3.324318	0.646439	2.924452
44	22	0	-0.197155	1.023332	-0.597219
45	8	0	-1.419887	2.454112	-0.248454
46	8	0	1.133293	1.914645	0.375945
47	6	0	-1.850583	2.935473	0.912768
48	6	0	1.380243	3.167606	0.785285
49	6	0	-0.975862	3.619706	1.786038
50	6	0	-3.212257	2.749764	1.253863
51	6	0	0.414319	4.007413	1.408602
52	6	0	2.716932	3.621099	0.652819
53	6	0	-3.676604	3.171189	2.501282
54	6	0	-1.481762	4.016126	3.036154
55	6	0	3.065800	4.914144	1.050620
56	6	0	0.812449	5.310764	1.762092
57	6	0	-2.808048	3.789916	3.402894
58	6	0	2.109997	5.774074	1.583224
59	1	0	-4.721816	3.018729	2.754867
60	1	0	-0.811272	4.504813	3.736255

61	1	0	4.094210	5.238391	0.924397
62	1	0	0.064907	5.973452	2.186011
63	1	0	-3.164419	4.108552	4.377538
64	1	0	2.373241	6.789231	1.862634
65	8	0	-0.169361	1.503583	-2.325081
66	6	0	-1.040469	2.325708	-3.104189
67	1	0	-2.020854	2.336675	-2.618086
68	6	0	-0.510727	3.754760	-3.135304
69	6	0	-1.174403	1.706166	-4.489896
70	1	0	0.469092	3.804370	-3.620579
71	1	0	-1.550494	0.681518	-4.413400
72	1	0	-1.875628	2.284644	-5.100729
73	1	0	-0.207284	1.677167	-5.003119
74	1	0	-1.198893	4.400386	-3.690161
75	1	0	-0.423192	4.141118	-2.117586
76	6	0	-4.093635	2.081092	0.261251
77	6	0	-4.331959	2.700358	-1.029299
78	6	0	-4.645766	0.863432	0.531600
79	6	0	-5.060255	2.000689	-2.035417
80	6	0	-5.416227	0.141618	-0.436866
81	6	0	-5.613060	0.688502	-1.737562
82	6	0	-3.847264	3.997994	-1.312186
83	1	0	-4.468539	0.393043	1.495138
84	6	0	-5.228015	2.620172	-3.295991
85	6	0	-5.945822	-1.130889	-0.127229
86	6	0	-6.340577	-0.077228	-2.677772
87	6	0	-4.041838	4.584376	-2.545876
88	6	0	-4.728173	3.882404	-3.552043
89	6	0	-6.658612	-1.852111	-1.064217
90	6	0	-6.855186	-1.319433	-2.351116
91	1	0	-5.780574	-1.535574	0.863627
92	1	0	-6.505079	0.307225	-3.677243
93	1	0	-7.410974	-1.883718	-3.093790
94	1	0	-7.060235	-2.826482	-0.806960
95	1	0	-4.874648	4.334012	-4.528489
96	1	0	-3.660207	5.581954	-2.738928
97	1	0	-5.765924	2.104669	-4.082725
98	1	0	-3.309234	4.532850	-0.539427
99	6	0	3.796648	2.705751	0.184164
100	6	0	3.871217	2.231714	-1.181150
101	6	0	4.775107	2.352578	1.070294

102	6	0	4.973399	1.423648	-1.596171
103	6	0	5.879559	1.517789	0.706982
104	6	0	6.002815	1.058970	-0.635024
105	6	0	2.869490	2.562098	-2.119542
106	1	0	4.717521	2.706556	2.095440
107	6	0	5.008465	0.978655	-2.937850
108	6	0	6.833571	1.123034	1.673087
109	6	0	7.110778	0.243006	-0.958538
110	6	0	2.921711	2.093410	-3.415946
111	6	0	4.001346	1.295581	-3.828737
112	6	0	7.892940	0.306383	1.331418
113	6	0	8.034424	-0.129308	0.000889
114	1	0	2.042144	3.181365	-1.802486
115	1	0	2.124640	2.333825	-4.109769
116	1	0	4.046038	0.923545	-4.847622
117	1	0	5.828806	0.360092	-3.279619
118	1	0	7.248088	-0.102581	-1.976153
119	1	0	8.871669	-0.762902	-0.275390
120	1	0	8.615087	0.003066	2.083082
121	1	0	6.706350	1.463031	2.696873
122	1	0	-1.586133	-3.131661	2.669832
123	6	0	-1.391333	-0.603582	1.883942
124	8	0	-0.908139	0.439617	1.466162
125	6	0	-1.514893	-1.821334	1.004078
126	8	0	-1.729157	-0.764601	3.148494
127	6	0	-2.053604	-3.117310	1.679660
128	6	0	-3.564097	-3.278159	1.885890
129	6	0	-4.320812	-4.138965	1.083864
130	6	0	-4.193057	-2.618825	2.949502
131	6	0	-5.676562	-4.339263	1.340738
132	6	0	-5.552247	-2.810306	3.198257
133	6	0	-6.299217	-3.674811	2.397278
134	6	0	-1.488862	-4.270618	0.965301
135	1	0	-3.847682	-4.668873	0.265895
136	1	0	-3.615317	-1.967340	3.591190
137	1	0	-6.243189	-5.021612	0.714888
138	1	0	-6.022781	-2.291814	4.027894
139	1	0	-7.354452	-3.831342	2.597283
140	6	0	-1.522204	0.393337	4.030548
141	6	0	-1.940383	-0.023598	5.419193
142	1	0	-2.115878	1.219735	3.639400

143	6	0	-2.093439	-1.450487	-0.346994
144	8	0	-1.925029	-0.365422	-0.900301
145	8	0	-2.739455	-2.443502	-0.913346
146	6	0	-3.215648	-2.242355	-2.285959
147	6	0	-3.822416	-3.548427	-2.737366
148	1	0	-2.355702	-1.946417	-2.891040
149	1	0	-0.467525	0.669642	3.978493
150	1	0	-3.938291	-1.427196	-2.270453
151	1	0	-4.187489	-3.434437	-3.762408
152	1	0	-3.083731	-4.354694	-2.721791
153	1	0	-4.668050	-3.825660	-2.104015
154	1	0	-1.769488	0.812621	6.103629
155	1	0	-3.003184	-0.280096	5.457674
156	1	0	-1.356337	-0.878947	5.770870
157	7	0	-1.022596	-5.171183	0.402496
158	1	0	-0.424928	-1.995068	0.820351

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d-II-COM-*si*

Zero-point correction = 1.28727 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19149 (a.u.)

Sum of electronic and zero-point Energies = -4590.83348 (a.u.)

Sum of electronic and thermal Free Energies = -4590.9292 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.968769	-2.074811	1.861468
2	8	0	0.072375	-1.743502	1.291747
3	6	0	-2.036947	-1.122002	2.265158
4	8	0	-1.199606	-3.325639	2.232185
5	6	0	-2.852759	-1.502512	3.289477
6	6	0	-3.863956	-0.817613	4.085595
7	6	0	-4.961541	-1.590553	4.514601
8	6	0	-3.752444	0.515215	4.520764
9	6	0	-5.972016	-1.022938	5.283225
10	6	0	-4.749192	1.064345	5.320735
11	6	0	-5.868303	0.311239	5.684566
12	1	0	-2.722115	-2.540879	3.582238
13	1	0	-5.024322	-2.634644	4.220533
14	1	0	-2.870121	1.097713	4.273550

15	1	0	-6.825916	-1.621786	5.584163
16	1	0	-4.648583	2.088951	5.664680
17	1	0	-6.646269	0.754790	6.298801
18	6	0	-0.181666	-4.319884	1.909289
19	6	0	-0.818698	-5.680319	2.067254
20	1	0	0.656232	-4.171069	2.596623
21	6	0	-2.126435	0.137664	1.492257
22	8	0	-1.393890	0.433080	0.538955
23	8	0	-3.126258	0.909966	1.843849
24	6	0	-3.271330	2.182411	1.155448
25	6	0	-4.263197	3.008986	1.938970
26	1	0	-3.602831	1.977150	0.135603
27	1	0	0.159895	-4.139830	0.893626
28	1	0	-2.288995	2.646569	1.140976
29	1	0	-4.455374	3.940504	1.396382
30	1	0	-5.210389	2.481678	2.060468
31	1	0	-3.858037	3.258961	2.922709
32	1	0	-0.072560	-6.450435	1.852762
33	1	0	-1.192248	-5.834068	3.084239
34	1	0	-1.646695	-5.803882	1.363730
35	8	0	1.325009	0.484965	0.187331
36	6	0	2.260397	1.422346	-0.246712
37	6	0	1.492700	2.718008	-0.627852
38	6	0	3.327770	1.608121	0.821513
39	7	0	0.867754	3.426227	0.551599
40	6	0	2.212680	3.782771	-1.476770
41	6	0	4.636410	2.108009	0.536652
42	6	0	3.009935	1.335526	2.134572
43	6	0	1.793035	4.392440	1.241554
44	6	0	-0.323539	4.182471	0.045080
45	6	0	1.653118	5.175471	-1.125977
46	6	0	5.482644	2.415316	1.653015
47	6	0	3.933457	1.647089	3.156722
48	6	0	2.157962	5.539677	0.279026
49	6	0	0.102309	5.168619	-1.079342
50	7	0	5.113017	2.198565	2.949144
51	1	0	2.733957	1.086484	-1.180978
52	1	0	0.643766	2.334692	-1.194042
53	1	0	2.074812	3.545057	-2.535029
54	1	0	3.287000	3.787775	-1.286127
55	6	0	5.158149	2.295111	-0.772215

56	1	0	2.035615	0.934053	2.380929
57	1	0	2.663681	3.833238	1.566789
58	1	0	1.260761	4.724267	2.134079
59	1	0	-0.765455	4.689645	0.903857
60	1	0	-1.033602	3.440659	-0.319771
61	1	0	1.990262	5.912987	-1.858451
62	6	0	6.777493	2.947438	1.419115
63	1	0	3.663965	1.447980	4.192003
64	1	0	1.711269	6.482493	0.609261
65	1	0	3.242617	5.676854	0.266146
66	1	0	-0.220526	6.177330	-0.801449
67	6	0	-0.534415	4.810445	-2.392582
68	7	0	-0.240131	2.358602	2.687792
69	6	0	-0.860891	2.250576	3.682461
70	1	0	0.484628	2.772552	1.333764
71	6	0	7.238590	3.142670	0.137442
72	6	0	6.424424	2.800304	-0.967305
73	1	0	8.233769	3.543269	-0.030055
74	1	0	7.385970	3.175261	2.288033
75	1	0	6.806901	2.918427	-1.976430
76	1	0	4.568827	1.996853	-1.630207
77	6	0	-1.244652	5.647654	-3.146564
78	1	0	-1.417763	6.680074	-2.850269
79	1	0	-1.683833	5.328046	-4.087160
80	1	0	-0.401222	3.783804	-2.723685
81	22	0	0.054494	-0.584440	-0.642471
82	8	0	1.157494	-1.895628	-1.341273
83	8	0	-1.476150	-1.822964	-0.846141
84	6	0	1.165810	-3.234261	-1.291113
85	6	0	-1.810313	-2.360004	-2.019377
86	6	0	0.122391	-3.999244	-1.862097
87	6	0	2.269387	-3.866012	-0.676288
88	6	0	-1.022531	-3.393532	-2.591920
89	6	0	-2.986329	-1.928217	-2.689035
90	6	0	2.298832	-5.260877	-0.587037
91	6	0	0.196049	-5.397387	-1.753131
92	6	0	-3.317439	-2.492088	-3.928223
93	6	0	-1.386490	-3.919456	-3.838596
94	6	0	1.262906	-6.028996	-1.117743
95	6	0	-2.517030	-3.468813	-4.515992
96	1	0	3.147173	-5.734950	-0.102908

97	1	0	-0.614717	-5.989332	-2.166594
98	1	0	-4.223940	-2.162397	-4.426693
99	1	0	-0.764266	-4.694473	-4.276714
100	1	0	1.288919	-7.111556	-1.042294
101	1	0	-2.782895	-3.888172	-5.481097
102	8	0	-0.133831	0.376888	-2.147970
103	6	0	-0.033625	0.223580	-3.564608
104	1	0	-0.739441	-0.563456	-3.857736
105	6	0	-0.433486	1.533198	-4.233682
106	6	0	1.378072	-0.200978	-3.954438
107	1	0	0.331514	2.298804	-4.065518
108	1	0	1.656613	-1.124625	-3.450098
109	1	0	1.439419	-0.352703	-5.037289
110	1	0	2.101902	0.572726	-3.674544
111	1	0	-0.529916	1.392876	-5.315789
112	1	0	-1.388708	1.894791	-3.848975
113	6	0	3.368514	-3.047642	-0.096972
114	6	0	4.249671	-2.279373	-0.951431
115	6	0	3.567843	-3.042542	1.252231
116	6	0	5.306315	-1.512409	-0.376011
117	6	0	4.604130	-2.275753	1.872591
118	6	0	5.484152	-1.498758	1.067698
119	6	0	4.094400	-2.288084	-2.356726
120	1	0	2.904518	-3.616302	1.892049
121	6	0	6.153163	-0.785157	-1.242844
122	6	0	4.754269	-2.272232	3.277751
123	6	0	6.485643	-0.743132	1.716174
124	6	0	4.930685	-1.557060	-3.176792
125	6	0	5.970064	-0.797397	-2.612457
126	6	0	5.742372	-1.522345	3.883580
127	6	0	6.612559	-0.750943	3.092549
128	1	0	4.068168	-2.866759	3.874878
129	1	0	7.159435	-0.124186	1.136983
130	1	0	7.375014	-0.139748	3.564210
131	1	0	5.842842	-1.518702	4.964600
132	1	0	6.634740	-0.222006	-3.250141
133	1	0	4.787710	-1.575371	-4.253020
134	1	0	6.960690	-0.194061	-0.831091
135	1	0	3.302795	-2.887315	-2.789819
136	6	0	-3.909215	-0.955324	-2.042243
137	6	0	-4.341736	0.253769	-2.717972

138	6	0	-4.403079	-1.229405	-0.797312
139	6	0	-5.316706	1.105632	-2.108890
140	6	0	-5.385859	-0.413633	-0.158498
141	6	0	-5.880197	0.748172	-0.816398
142	6	0	-3.795911	0.634574	-3.966918
143	1	0	-4.063559	-2.118385	-0.277116
144	6	0	-5.689714	2.290754	-2.784778
145	6	0	-5.889638	-0.761851	1.116010
146	6	0	-6.889645	1.499470	-0.171027
147	6	0	-4.184244	1.797202	-4.602898
148	6	0	-5.141940	2.633793	-4.005601
149	6	0	-6.863982	-0.003041	1.728846
150	6	0	-7.374727	1.132133	1.071158
151	1	0	-3.047069	-0.001283	-4.420568
152	1	0	-3.740579	2.066799	-5.556459
153	1	0	-5.448071	3.552084	-4.497323
154	1	0	-6.416269	2.957265	-2.335448
155	1	0	-7.302868	2.378829	-0.650916
156	1	0	-8.149314	1.728452	1.543865
157	1	0	-7.225458	-0.274141	2.714883
158	1	0	-5.488236	-1.641366	1.608457

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d-II-TS1-*si*

Zero-point correction = 1.28813 (a.u.)

Thermal correction to Gibbs Free Energy = 1.19092 (a.u.)

Sum of electronic and zero-point Energies = -4590.82503 (a.u.)

Sum of electronic and thermal Free Energies = -4590.92225 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.993496	-0.534288	-0.239633
2	6	0	-1.585461	-0.945041	-1.434383
3	6	0	-0.572655	-1.873960	-2.151942
4	6	0	-2.940718	-1.570842	-1.159704
5	7	0	-0.377855	-3.209608	-1.465570
6	6	0	-0.751326	-2.169701	-3.649705
7	6	0	-3.980357	-1.613848	-2.138565
8	6	0	-3.177242	-2.152275	0.067414
9	6	0	-1.336072	-4.268072	-1.946195

10	6	0	1.025500	-3.669599	-1.738842
11	6	0	-0.088487	-3.525242	-3.971892
12	6	0	-5.168847	-2.343799	-1.807289
13	6	0	-4.393842	-2.829794	0.296490
14	6	0	-0.996198	-4.629532	-3.404469
15	6	0	1.292752	-3.641342	-3.272837
16	7	0	-5.355551	-2.951557	-0.598823
17	1	0	-1.714963	-0.096493	-2.118034
18	1	0	0.370172	-1.349171	-2.000609
19	1	0	-0.308513	-1.353794	-4.224755
20	1	0	-1.807576	-2.222274	-3.921297
21	6	0	-3.923997	-0.957982	-3.398785
22	1	0	-2.419924	-2.110917	0.839584
23	1	0	-2.339002	-3.865274	-1.844100
24	1	0	-1.234330	-5.101338	-1.250418
25	1	0	1.115859	-4.672538	-1.321581
26	1	0	1.688557	-3.016729	-1.175435
27	1	0	0.036415	-3.642665	-5.050863
28	6	0	-6.218285	-2.434303	-2.759033
29	1	0	-4.570181	-3.291816	1.265051
30	1	0	-0.495565	-5.601061	-3.461585
31	1	0	-1.919086	-4.701175	-3.986040
32	1	0	1.730456	-4.605249	-3.551013
33	6	0	2.256606	-2.559615	-3.684445
34	6	0	-6.116873	-1.810015	-3.980576
35	6	0	-4.962822	-1.055287	-4.296903
36	1	0	-6.927137	-1.881200	-4.699831
37	1	0	-7.098586	-3.003019	-2.477851
38	1	0	-4.903339	-0.536770	-5.248827
39	1	0	-3.063482	-0.349228	-3.648566
40	6	0	3.453005	-2.784398	-4.226846
41	1	0	3.817660	-3.792044	-4.413396
42	1	0	4.112111	-1.964714	-4.497544
43	1	0	1.946146	-1.529405	-3.517351
44	22	0	-0.036383	1.092244	-0.004870
45	8	0	-1.461958	2.245361	0.225961
46	8	0	1.151315	2.419607	0.800701
47	6	0	-1.714859	3.346282	0.946327
48	6	0	1.369558	3.551445	0.127222
49	6	0	-0.859975	4.475178	0.913815
50	6	0	-2.903433	3.372767	1.710776

51	6	0	0.372756	4.560438	0.084489
52	6	0	2.608510	3.761662	-0.536238
53	6	0	-3.207470	4.505367	2.472647
54	6	0	-1.211173	5.591180	1.690414
55	6	0	2.800302	4.939567	-1.271111
56	6	0	0.603100	5.713399	-0.678201
57	6	0	-2.363930	5.613694	2.469638
58	6	0	1.799816	5.904104	-1.365508
59	1	0	-4.122729	4.509321	3.056710
60	1	0	-0.545096	6.448328	1.687093
61	1	0	3.753251	5.097792	-1.767077
62	1	0	-0.175685	6.468792	-0.726211
63	1	0	-2.603662	6.488452	3.065963
64	1	0	1.960571	6.805239	-1.948837
65	8	0	0.277179	1.387159	-1.745830
66	6	0	0.191388	2.315958	-2.816130
67	1	0	0.879538	3.139751	-2.590823
68	6	0	0.645146	1.624698	-4.098282
69	6	0	-1.220637	2.882357	-2.927443
70	1	0	-0.068398	0.845692	-4.388683
71	1	0	-1.511893	3.370769	-1.997824
72	1	0	-1.267557	3.616862	-3.738405
73	1	0	-1.944670	2.087305	-3.136815
74	1	0	0.713147	2.343749	-4.921733
75	1	0	1.628126	1.166447	-3.960291
76	6	0	-3.836506	2.212643	1.718563
77	6	0	-4.580134	1.843644	0.530649
78	6	0	-4.060939	1.540512	2.885174
79	6	0	-5.522593	0.773476	0.584908
80	6	0	-4.973077	0.441320	2.976283
81	6	0	-5.712049	0.041312	1.827622
82	6	0	-4.416036	2.551509	-0.682310
83	1	0	-3.519514	1.833091	3.780036
84	6	0	-6.263990	0.473148	-0.580462
85	6	0	-5.146265	-0.252771	4.196075
86	6	0	-6.590558	-1.058989	1.952335
87	6	0	-5.148195	2.226901	-1.806548
88	6	0	-6.084438	1.180418	-1.752586
89	6	0	-6.011769	-1.324164	4.288486
90	6	0	-6.737534	-1.729193	3.153152
91	1	0	-4.583704	0.076431	5.064603

92	1	0	-7.140376	-1.414041	1.089997
93	1	0	-7.413792	-2.576299	3.215453
94	1	0	-6.132247	-1.852038	5.229656
95	1	0	-6.661020	0.916510	-2.632415
96	1	0	-5.005285	2.784881	-2.727138
97	1	0	-6.990868	-0.328461	-0.563459
98	1	0	-3.709920	3.371309	-0.715030
99	6	0	3.726944	2.793717	-0.378656
100	6	0	4.445655	2.259828	-1.520593
101	6	0	4.122268	2.430019	0.878581
102	6	0	5.616647	1.462317	-1.321859
103	6	0	5.272562	1.620712	1.122751
104	6	0	6.063533	1.162437	0.029957
105	6	0	3.981133	2.463095	-2.842181
106	1	0	3.561209	2.789879	1.733614
107	6	0	6.269592	0.930948	-2.458850
108	6	0	5.654761	1.296250	2.446882
109	6	0	7.217658	0.398134	0.317317
110	6	0	4.632393	1.917722	-3.930833
111	6	0	5.794147	1.150344	-3.737565
112	6	0	6.787951	0.548506	2.696398
113	6	0	7.576033	0.098998	1.619347
114	1	0	3.083523	3.047896	-2.990888
115	1	0	4.245417	2.081378	-4.931997
116	1	0	6.315812	0.724344	-4.589374
117	1	0	7.158672	0.324620	-2.332590
118	1	0	7.845911	0.038775	-0.489147
119	1	0	8.472417	-0.483263	1.810036
120	1	0	7.073019	0.311035	3.716638
121	1	0	5.039244	1.656778	3.266225
122	1	0	-0.473738	-3.182536	-0.407902
123	7	0	-0.334268	-3.880366	1.126505
124	6	0	0.457410	-3.937784	1.994156
125	6	0	0.392118	-0.511955	2.669239
126	8	0	-0.137639	0.422082	2.053632
127	6	0	1.578936	-1.263837	2.255441
128	8	0	-0.098926	-0.889531	3.847647
129	6	0	1.939605	-2.368722	3.015155
130	6	0	3.235521	-3.071726	3.060101
131	6	0	4.428965	-2.331797	3.013251
132	6	0	3.300687	-4.449954	3.312677

133	6	0	5.655961	-2.960774	3.204060
134	6	0	4.530295	-5.077566	3.487783
135	6	0	5.712743	-4.336210	3.434122
136	1	0	1.311704	-2.547913	3.877123
137	1	0	4.395470	-1.262892	2.839693
138	1	0	2.376364	-5.015177	3.324331
139	1	0	6.566029	-2.371369	3.162900
140	1	0	4.565901	-6.148362	3.664273
141	1	0	6.671369	-4.827846	3.570923
142	6	0	-1.303942	-0.216708	4.305281
143	6	0	-1.645851	-0.808720	5.654025
144	1	0	-2.090695	-0.378459	3.566047
145	6	0	2.126829	-0.992508	0.934481
146	8	0	1.710658	-0.137989	0.137260
147	8	0	3.134847	-1.780213	0.572706
148	6	0	3.840383	-1.421830	-0.647430
149	6	0	4.972425	-2.404638	-0.820809
150	1	0	4.193563	-0.400559	-0.536527
151	1	0	-1.099414	0.855582	4.360375
152	1	0	3.146196	-1.446258	-1.486624
153	1	0	5.519596	-2.157089	-1.735085
154	1	0	5.664763	-2.359365	0.023131
155	1	0	4.598798	-3.428994	-0.911079
156	1	0	-2.522771	-0.301916	6.066680
157	1	0	-1.874222	-1.874789	5.568767
158	1	0	-0.818101	-0.681716	6.358085

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d-III-COM-*si*

Zero-point correction = 1.28736 (a.u.)

Thermal correction to Gibbs Free Energy = 1.18799 (a.u.)

Sum of electronic and zero-point Energies = -4590.83511 (a.u.)

Sum of electronic and thermal Free Energies = -4590.93448 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.490608	-1.104404	-0.502616
2	6	0	-0.182864	-2.460239	-0.419151
3	6	0	-1.448171	-3.225145	-0.841305
4	6	0	1.105335	-2.787122	-1.159822

5	7	0	-1.969426	-2.843732	-2.208426
6	6	0	-1.424074	-4.759224	-0.763885
7	6	0	2.052619	-3.724714	-0.647029
8	6	0	1.418009	-2.117560	-2.324455
9	6	0	-1.363249	-3.657038	-3.318279
10	6	0	-3.449752	-3.061825	-2.200500
11	6	0	-2.428819	-5.317439	-1.794137
12	6	0	3.254236	-3.935917	-1.401936
13	6	0	2.618956	-2.417644	-3.000260
14	6	0	1.903196	-4.419136	0.585616
15	6	0	-1.824911	-5.121360	-3.194269
16	6	0	-3.762051	-4.522886	-1.745858
17	7	0	3.513808	-3.291233	-2.577440
18	6	0	4.243259	-4.825633	-0.906211
19	6	0	2.885814	-5.266148	1.044510
20	6	0	4.065506	-5.475794	0.292629
21	1	0	-0.045824	-2.758527	0.624176
22	1	0	-2.203032	-2.833569	-0.157995
23	1	0	-1.663975	-5.069344	0.255669
24	1	0	-0.425320	-5.145802	-0.988184
25	1	0	0.749185	-1.359244	-2.713677
26	1	0	-0.285517	-3.559764	-3.230952
27	1	0	-1.668838	-3.175794	-4.248030
28	1	0	-3.808758	-2.863437	-3.211468
29	1	0	-3.881314	-2.314747	-1.534848
30	1	0	-2.627394	-6.374847	-1.603517
31	1	0	2.849608	-1.900089	-3.930185
32	1	0	1.015771	-4.265495	1.186407
33	1	0	-2.564057	-5.367572	-3.963227
34	1	0	-0.970074	-5.787773	-3.337869
35	1	0	5.140074	-4.959133	-1.502430
36	1	0	2.759037	-5.770316	1.997603
37	1	0	4.832736	-6.144777	0.670214
38	6	0	-4.434420	-4.585752	-0.400809
39	1	0	-3.837618	-4.296525	0.462642
40	6	0	-5.696557	-4.969790	-0.208995
41	1	0	-6.138738	-4.996179	0.782617
42	1	0	-6.333495	-5.274212	-1.036705
43	1	0	-4.442347	-4.962003	-2.482759
44	22	0	0.303131	0.302300	0.497019
45	8	0	-0.660338	-0.013942	2.081306

46	8	0	1.676115	-0.813406	1.041638
47	6	0	-1.035010	-1.215108	2.532573
48	6	0	2.167922	-1.113518	2.251911
49	6	0	-0.064228	-2.118722	3.042106
50	6	0	-2.408328	-1.565972	2.523080
51	6	0	1.366307	-1.743984	3.237674
52	6	0	3.524954	-0.821113	2.513126
53	6	0	-2.779102	-2.852910	2.943801
54	6	0	-0.488353	-3.395371	3.440111
55	6	0	4.082470	-1.180767	3.743426
56	6	0	1.969288	-2.075464	4.461298
57	6	0	4.325333	-0.105797	1.479584
58	6	0	-3.456499	-0.640995	2.010087
59	6	0	-1.829122	-3.772925	3.379313
60	6	0	3.311596	-1.810468	4.717784
61	6	0	4.745024	1.262869	1.704739
62	6	0	4.631840	-0.719852	0.300490
63	6	0	-3.590198	0.733055	2.459339
64	6	0	-4.353460	-1.123411	1.096613
65	6	0	5.463951	1.964303	0.689249
66	6	0	5.367454	-0.061350	-0.734418
67	6	0	-4.583696	1.579387	1.877448
68	6	0	-5.402002	-0.330968	0.537013
69	6	0	5.789190	1.288074	-0.556535
70	6	0	-5.524606	1.036014	0.910117
71	1	0	-3.832132	-3.117138	2.941838
72	1	0	0.255002	-4.099019	3.801699
73	1	0	5.127054	-0.952633	3.932814
74	1	0	1.357049	-2.539071	5.228641
75	1	0	-2.132793	-4.765106	3.697908
76	1	0	3.748172	-2.080517	5.674061
77	6	0	4.438864	1.935138	2.911830
78	1	0	4.306958	-1.740305	0.128187
79	6	0	-2.772446	1.256616	3.486806
80	1	0	-4.274676	-2.150759	0.763043
81	6	0	5.835277	3.306348	0.935760
82	6	0	5.673641	-0.737633	-1.939509
83	6	0	-4.632873	2.935117	2.279421
84	6	0	-6.304525	-0.888621	-0.399589
85	6	0	6.503709	1.906952	-1.609303
86	6	0	-6.561277	1.794278	0.319144

87	6	0	-2.860418	2.577405	3.876167
88	6	0	-3.782299	3.432257	3.247827
89	6	0	-7.304455	-0.121605	-0.963001
90	6	0	-7.430965	1.232199	-0.597993
91	6	0	4.819763	3.245134	3.123986
92	6	0	5.524161	3.938139	2.124435
93	6	0	6.377135	-0.107089	-2.946117
94	6	0	6.795479	1.226471	-2.777109
95	1	0	3.886471	1.403348	3.675977
96	1	0	4.568097	3.739231	4.057380
97	1	0	5.823186	4.969878	2.282853
98	1	0	6.377587	3.861328	0.179554
99	1	0	6.838305	2.932756	-1.508701
100	1	0	7.347827	1.726326	-3.567174
101	1	0	6.605026	-0.637933	-3.865642
102	1	0	5.333578	-1.760085	-2.067109
103	1	0	-6.201293	-1.938292	-0.659469
104	1	0	-6.690270	2.836785	0.584874
105	1	0	-8.217462	1.839449	-1.035317
106	1	0	-7.992816	-0.558434	-1.679943
107	1	0	-3.842970	4.477083	3.537707
108	1	0	-2.213300	2.953570	4.661604
109	1	0	-5.357541	3.603355	1.829396
110	1	0	-2.060868	0.603717	3.972429
111	8	0	0.816079	1.945889	1.095207
112	6	0	0.473626	3.022167	1.939869
113	6	0	0.723369	2.630766	3.395362
114	6	0	1.269762	4.260772	1.535524
115	1	0	-0.601232	3.227716	1.815384
116	1	0	0.412856	3.434195	4.072875
117	1	0	1.788658	2.440183	3.549786
118	1	0	0.170975	1.722675	3.638339
119	1	0	0.982730	5.124751	2.145475
120	1	0	1.092043	4.509448	0.486751
121	1	0	2.340776	4.080167	1.669376
122	6	0	1.068834	1.932474	-2.036280
123	6	0	-0.091557	2.826269	-1.822305
124	8	0	1.902119	2.352427	-2.964374
125	6	0	0.022375	4.160490	-1.995186
126	6	0	-0.942047	5.194711	-1.621674
127	6	0	-1.833535	5.041981	-0.543131

128	6	0	-0.940558	6.408423	-2.329857
129	6	0	-2.721587	6.058661	-0.212928
130	6	0	-1.840746	7.419743	-2.005932
131	6	0	-2.735671	7.246548	-0.948807
132	1	0	0.959465	4.516816	-2.414626
133	1	0	-1.807922	4.143610	0.062383
134	1	0	-0.239296	6.544724	-3.147889
135	1	0	-3.394663	5.927323	0.628277
136	1	0	-1.838242	8.345796	-2.572127
137	1	0	-3.429357	8.040081	-0.688607
138	6	0	3.063721	1.510647	-3.247006
139	6	0	3.736699	2.093972	-4.466575
140	1	0	3.042430	2.133968	-5.310709
141	1	0	4.110758	3.102416	-4.267326
142	1	0	4.585898	1.464039	-4.741607
143	1	0	2.703835	0.495071	-3.415621
144	1	0	3.710090	1.511801	-2.368646
145	6	0	-1.339967	2.152675	-1.374720
146	8	0	-1.393339	1.331931	-0.457674
147	8	0	-2.387666	2.518617	-2.075433
148	6	0	-3.651316	1.845421	-1.799644
149	6	0	-4.479114	1.917089	-3.060557
150	1	0	-4.114851	2.365760	-0.959891
151	1	0	-3.433075	0.819638	-1.507351
152	1	0	-3.965998	1.395383	-3.872142
153	1	0	-5.443298	1.432768	-2.881165
154	1	0	-4.661487	2.953485	-3.360031
155	8	0	1.262650	0.901435	-1.384228
156	7	0	-1.627612	-0.474365	-3.368613
157	6	0	-0.908714	0.333315	-3.837750
158	1	0	-1.796563	-1.805092	-2.470346

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d-III-TS1-*si*

Zero-point correction = 1.28792 (a.u.)

Thermal correction to Gibbs Free Energy = 1.18860 (a.u.)

Sum of electronic and zero-point Energies = -4590.82825 (a.u.)

Sum of electronic and thermal Free Energies = -4590.92758 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.493205	-0.332037	-0.646552
2	6	0	-0.146833	-1.497625	-1.334577
3	6	0	-1.417627	-2.089002	-1.972378
4	6	0	1.035621	-1.254435	-2.262188
5	7	0	-2.081389	-1.238545	-3.034379
6	6	0	-1.301617	-3.513527	-2.543011
7	6	0	2.097421	-2.199094	-2.403930
8	6	0	1.133150	-0.064943	-2.954903
9	6	0	-1.516180	-1.456330	-4.414338
10	6	0	-3.540745	-1.581814	-3.044461
11	6	0	-2.335627	-3.690475	-3.675256
12	6	0	3.166378	-1.868405	-3.302296
13	6	0	2.227362	0.159175	-3.817026
14	6	0	2.185225	-3.418102	-1.675299
15	6	0	-1.843339	-2.884759	-4.887464
16	6	0	-3.715834	-3.117593	-3.259386
17	7	0	3.213441	-0.698279	-4.004503
18	6	0	4.250580	-2.772566	-3.458604
19	6	0	3.262312	-4.260288	-1.829841
20	6	0	4.301492	-3.941259	-2.735409
21	1	0	0.143758	-2.287613	-0.637676
22	1	0	-2.130446	-2.080872	-1.146091
23	1	0	-1.447227	-4.230762	-1.732435
24	1	0	-0.300086	-3.687837	-2.947801
25	1	0	0.363389	0.690454	-2.855827
26	1	0	-0.447518	-1.278574	-4.349133
27	1	0	-1.948143	-0.674651	-5.039719
28	1	0	-3.998184	-1.000250	-3.846046
29	1	0	-3.958148	-1.241554	-2.096138
30	1	0	-2.442717	-4.746932	-3.933051
31	1	0	2.281208	1.093115	-4.374348
32	1	0	1.408912	-3.680388	-0.968443
33	1	0	-2.606634	-2.872825	-5.671653
34	1	0	-0.945894	-3.343942	-5.310788
35	1	0	5.034993	-2.497083	-4.156099
36	1	0	3.319488	-5.171413	-1.242861
37	1	0	5.142962	-4.617583	-2.849164
38	6	0	-4.292524	-3.813639	-2.057519
39	1	0	-3.640503	-3.910847	-1.191880
40	6	0	-5.526748	-4.313198	-1.994082

41	1	0	-5.893752	-4.805056	-1.097774
42	1	0	-6.215483	-4.250903	-2.833913
43	1	0	-4.407613	-3.257466	-4.096232
44	22	0	0.347636	0.079273	1.062300
45	8	0	-0.599753	-1.166339	2.089831
46	8	0	1.725767	-1.133671	0.760883
47	6	0	-0.935521	-2.426989	1.812790
48	6	0	2.268130	-2.087123	1.532040
49	6	0	0.068359	-3.421935	1.661824
50	6	0	-2.306634	-2.775427	1.714056
51	6	0	1.503721	-3.189647	1.992102
52	6	0	3.643151	-2.000303	1.840479
53	6	0	-2.646690	-4.091028	1.360697
54	6	0	-0.326849	-4.713904	1.282369
55	6	0	4.242150	-2.994121	2.620301
56	6	0	2.147617	-4.157720	2.780444
57	6	0	4.461346	-0.864745	1.329547
58	6	0	-3.398555	-1.783708	1.915951
59	6	0	-1.668867	-5.050861	1.115714
60	6	0	3.500036	-4.071803	3.095640
61	6	0	4.977237	0.131824	2.244800
62	6	0	4.762337	-0.784108	0.001338
63	6	0	-3.481675	-0.922260	3.082554
64	6	0	-4.403203	-1.733329	0.987705
65	6	0	5.815603	1.180552	1.757170
66	6	0	5.615235	0.236591	-0.525350
67	6	0	-4.549249	0.021682	3.193961
68	6	0	-5.531714	-0.866048	1.104009
69	6	0	6.161121	1.224623	0.344515
70	6	0	-5.610140	0.041150	2.196947
71	1	0	-3.697372	-4.356790	1.299236
72	1	0	0.441231	-5.465107	1.127590
73	1	0	5.299276	-2.909560	2.853600
74	1	0	1.559535	-4.986160	3.162461
75	1	0	-1.949497	-6.060417	0.832823
76	1	0	3.967749	-4.834615	3.709937
77	6	0	4.658177	0.093625	3.622807
78	1	0	4.371164	-1.529651	-0.682030
79	6	0	-2.549745	-1.019743	4.141742
80	1	0	-4.363078	-2.381442	0.121281
81	6	0	6.290462	2.141387	2.679880

82	6	0	5.942848	0.258672	-1.901690
83	6	0	-4.563666	0.892382	4.308851
84	6	0	-6.568333	-0.906454	0.142476
85	6	0	7.025218	2.195929	-0.212319
86	6	0	-6.737368	0.891702	2.269371
87	6	0	-2.606583	-0.174388	5.230276
88	6	0	-3.608818	0.807884	5.302897
89	6	0	-7.664186	-0.073636	0.248780
90	6	0	-7.744153	0.834021	1.321985
91	6	0	5.151198	1.038446	4.500078
92	6	0	5.972196	2.074251	4.022930
93	6	0	6.799911	1.212121	-2.412783
94	6	0	7.345715	2.188129	-1.557624
95	1	0	4.003504	-0.690338	3.983204
96	1	0	4.890970	0.989366	5.553029
97	1	0	6.354468	2.826105	4.706766
98	1	0	6.920244	2.953169	2.335325
99	1	0	7.462517	2.959452	0.420341
100	1	0	8.019813	2.941525	-1.954083
101	1	0	7.045661	1.213542	-3.470298
102	1	0	5.503687	-0.488470	-2.552216
103	1	0	-6.485946	-1.614693	-0.677745
104	1	0	-6.834354	1.595716	3.087269
105	1	0	-8.601128	1.494933	1.408573
106	1	0	-8.458286	-0.114091	-0.490420
107	1	0	-3.643614	1.490505	6.146609
108	1	0	-1.872264	-0.266126	6.024220
109	1	0	-5.344156	1.638621	4.397551
110	1	0	-1.775295	-1.771853	4.093489
111	8	0	0.895310	1.074508	2.474221
112	6	0	0.882325	2.422401	2.891782
113	6	0	-0.183743	2.597828	3.971160
114	6	0	2.275366	2.825776	3.362598
115	1	0	0.610245	3.050695	2.030128
116	1	0	-0.248363	3.645228	4.288041
117	1	0	0.058283	1.986350	4.846616
118	1	0	-1.159494	2.282189	3.594356
119	1	0	2.298131	3.888466	3.630167
120	1	0	3.013580	2.648562	2.576543
121	1	0	2.569578	2.242077	4.238463
122	6	0	1.014922	2.519229	-0.793638

123	6	0	-0.343797	3.056532	-0.839631
124	8	0	1.873242	3.173503	-1.573348
125	6	0	-0.653239	3.985544	-1.822348
126	6	0	-1.720489	5.000415	-1.789284
127	6	0	-2.089847	5.584228	-0.566334
128	6	0	-2.268992	5.510775	-2.975462
129	6	0	-2.998457	6.638196	-0.530929
130	6	0	-3.182787	6.558456	-2.937564
131	6	0	-3.552709	7.125445	-1.715345
132	1	0	0.142518	4.197529	-2.524955
133	1	0	-1.644240	5.222588	0.353709
134	1	0	-1.999734	5.041263	-3.914475
135	1	0	-3.270288	7.080780	0.422466
136	1	0	-3.611012	6.932127	-3.862615
137	1	0	-4.266109	7.943624	-1.687290
138	6	0	3.256341	2.716178	-1.584893
139	6	0	3.962271	3.521147	-2.650851
140	1	0	3.518375	3.341886	-3.634733
141	1	0	3.905996	4.592367	-2.434623
142	1	0	5.013118	3.228806	-2.686554
143	1	0	3.273495	1.645221	-1.786354
144	1	0	3.679278	2.881921	-0.591435
145	6	0	-1.374560	2.412759	-0.026617
146	8	0	-1.177637	1.587024	0.881345
147	8	0	-2.600053	2.762770	-0.362876
148	6	0	-3.721627	2.027864	0.191737
149	6	0	-4.889118	2.322877	-0.722947
150	1	0	-3.889361	2.368640	1.216602
151	1	0	-3.461262	0.969541	0.220383
152	1	0	-4.655105	1.995993	-1.740163
153	1	0	-5.781187	1.801942	-0.372437
154	1	0	-5.096579	3.396885	-0.748779
155	8	0	1.407895	1.574273	-0.095950
156	7	0	-2.104707	1.431914	-3.316506
157	6	0	-1.584951	2.478994	-3.443730
158	1	0	-2.014155	-0.189949	-2.865815

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m-I-COM-*si*

Zero-point correction = 1.39461 (a.u.)

Thermal correction to Gibbs Free Energy = 1.28691 (a.u.)

Sum of electronic and zero-point Energies = -4785.11811 (a.u.)
Sum of electronic and thermal Free Energies = -4785.22581 (a.u.)

Standard orientation:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.569807	1.202024	2.250047
2	7	0	-2.718953	1.893994	1.833225
3	22	0	0.323042	-0.187627	-0.653990
4	8	0	-0.028317	1.367731	0.232442
5	8	0	0.754591	-1.317649	0.708163
6	8	0	-0.168020	0.351277	-2.452268
7	8	0	2.083732	0.236921	-1.092715
8	6	0	0.887607	2.310651	0.732988
9	6	0	1.549908	-2.444609	1.015733
10	6	0	-0.179337	1.650759	-2.752992
11	6	0	2.818086	0.682871	-2.120967
12	6	0	0.225619	3.703342	0.626694
13	6	0	1.376735	1.867143	2.102972
14	6	0	1.031978	2.347053	-2.985118
15	6	0	-1.424349	2.321803	-2.853773
16	6	0	2.353348	1.659127	-3.046087
17	6	0	4.130389	0.158392	-2.247743
18	6	0	0.692830	-3.709768	0.979064
19	6	0	2.199615	-2.230229	2.378970
20	7	0	-1.023690	3.859852	1.423205
21	6	0	1.149768	4.918425	0.873715
22	6	0	2.694031	2.146736	2.579788
23	6	0	0.540597	1.132952	2.918726
24	6	0	-1.442044	3.686337	-3.156705
25	6	0	0.964596	3.721380	-3.272221
26	6	0	4.951504	0.576769	-3.298603
27	6	0	3.215330	2.029274	-4.093960
28	6	0	4.640769	-0.819322	-1.245464
29	6	0	-2.694003	1.595193	-2.581749
30	6	0	-0.765474	4.251890	2.836104
31	6	0	-1.815094	4.936671	0.783007
32	6	0	0.312756	6.055290	1.494610
33	6	0	3.024356	1.719403	3.910197

34	6	0	0.970588	0.746729	4.205037
35	6	0	3.702502	2.799994	1.816166
36	6	0	-0.253788	4.389354	-3.362473
37	6	0	4.495804	1.504877	-4.229685
38	6	0	4.976458	-2.176293	-1.629636
39	6	0	4.798176	-0.433866	0.054182
40	6	0	-3.085079	0.420749	-3.337873
41	6	0	-3.522155	2.058294	-1.599173
42	6	0	-0.059856	5.628131	2.921678
43	6	0	-1.008375	6.277944	0.712481
44	7	0	2.157144	1.031290	4.707722
45	6	0	4.310955	2.010372	4.436751
46	6	0	4.945900	3.053674	2.350890
47	6	0	5.425712	-3.106579	-0.640903
48	6	0	5.281094	-1.319727	1.064880
49	6	0	-4.300202	-0.258308	-3.021984
50	6	0	-4.761977	1.428697	-1.271260
51	6	0	5.250316	2.669700	3.678722
52	6	0	5.578483	-2.672497	0.738613
53	6	0	-5.161185	0.254219	-1.967412
54	1	0	1.749658	2.354377	0.056706
55	1	0	2.344420	-2.523630	0.259134
56	1	0	-0.106278	3.722012	-0.414250
57	1	0	0.176785	-3.786136	0.020272
58	1	0	-0.057735	-3.687648	1.776732
59	1	0	1.312351	-4.602228	1.120980
60	1	0	2.917506	-3.026467	2.599129
61	1	0	1.441189	-2.220665	3.168592
62	1	0	2.726659	-1.277015	2.404620
63	1	0	1.618991	5.222927	-0.066101
64	1	0	1.956554	4.672119	1.568775
65	1	0	-0.451834	0.870320	2.577112
66	1	0	-2.398626	4.193817	-3.238227
67	1	0	1.889153	4.268617	-3.428791
68	1	0	5.952504	0.163962	-3.377772
69	1	0	2.851585	2.740061	-4.828505
70	1	0	-0.167440	3.471559	3.298220
71	1	0	-1.734860	4.255898	3.342662
72	1	0	-2.735763	5.062286	1.359937
73	1	0	-2.092473	4.599075	-0.218404
74	1	0	0.888823	6.984787	1.507277

75	1	0	0.291663	0.184857	4.844038
76	1	0	3.495910	3.095388	0.794572
77	1	0	-0.279657	5.446233	-3.606735
78	1	0	5.129846	1.816746	-5.053569
79	6	0	4.847455	-2.615490	-2.969729
80	1	0	4.544979	0.578665	0.348569
81	6	0	-2.293770	-0.059982	-4.407484
82	1	0	-3.226268	2.924467	-1.017627
83	1	0	-0.711882	6.377659	3.382632
84	1	0	0.840333	5.554709	3.540107
85	1	0	4.518795	1.683568	5.450286
86	1	0	5.701224	3.546117	1.746624
87	6	0	5.443844	-0.863394	2.393231
88	6	0	-4.638882	-1.411783	-3.768355
89	6	0	-5.587676	1.954899	-0.251872
90	1	0	6.232923	2.881993	4.088323
91	6	0	6.010188	-3.525704	1.780847
92	6	0	-6.385836	-0.348775	-1.604229
93	6	0	-0.777238	6.728965	-0.699531
94	1	0	-0.268427	6.020166	-1.349180
95	6	0	-1.156018	7.907348	-1.193412
96	1	0	-0.959367	8.183750	-2.225770
97	1	0	-1.678713	8.641923	-0.584021
98	1	0	-1.571563	7.059837	1.234427
99	6	0	-6.782006	1.347314	0.075737
100	6	0	-7.181215	0.185195	-0.608687
101	6	0	-2.653086	-1.185335	-5.121753
102	6	0	-3.835234	-1.873685	-4.792628
103	1	0	-5.254982	2.840034	0.280350
104	1	0	-7.405712	1.756571	0.864519
105	1	0	-8.114987	-0.303760	-0.348164
106	1	0	-6.714668	-1.251904	-2.102858
107	1	0	-5.555363	-1.945202	-3.544805
108	1	0	-4.127244	-2.755863	-5.355028
109	1	0	-2.031553	-1.527908	-5.943915
110	1	0	-1.391893	0.476826	-4.670471
111	6	0	5.869904	-1.717989	3.387885
112	6	0	6.150147	-3.062226	3.076338
113	6	0	5.146064	-3.912778	-3.335891
114	6	0	5.579754	-4.830589	-2.363652
115	1	0	4.502115	-1.911817	-3.716447

116	1	0	5.041659	-4.221660	-4.371693
117	1	0	5.812098	-5.853521	-2.643777
118	1	0	6.240688	-4.563931	1.572829
119	1	0	6.481817	-3.741023	3.856351
120	1	0	5.979938	-1.358192	4.406234
121	1	0	5.212321	0.171222	2.618172
122	6	0	5.712846	-4.430449	-1.048276
123	1	0	6.050847	-5.155386	-0.317333
124	8	0	0.275308	-2.151291	-1.913591
125	6	0	1.407365	-2.575781	-2.722678
126	6	0	1.435852	-4.095250	-2.802644
127	6	0	1.370804	-1.914986	-4.092143
128	1	0	-0.494630	-2.008402	-2.487130
129	1	0	2.278346	-2.227021	-2.167349
130	1	0	2.342980	-4.424817	-3.316606
131	1	0	0.572012	-4.473858	-3.359754
132	1	0	1.434590	-4.539806	-1.804377
133	1	0	2.247714	-2.210392	-4.675573
134	1	0	1.353292	-0.829831	-3.998966
135	1	0	0.478414	-2.230635	-4.647060
136	6	0	-2.412454	-1.801678	-0.299092
137	8	0	-1.700077	-0.798700	-0.403156
138	6	0	-2.993226	-2.166963	1.010705
139	8	0	-2.570461	-2.533221	-1.392710
140	6	0	-2.275792	-1.764952	2.093547
141	6	0	-2.614491	-1.865303	3.507942
142	6	0	-1.574753	-2.073335	4.430518
143	6	0	-3.925042	-1.689191	3.986617
144	6	0	-1.844225	-2.166688	5.793713
145	6	0	-4.187645	-1.761164	5.349588
146	6	0	-3.152315	-2.012976	6.255306
147	1	0	-1.308497	-1.318910	1.873849
148	1	0	-0.557659	-2.179273	4.067838
149	1	0	-4.717478	-1.434161	3.293723
150	1	0	-1.033987	-2.345466	6.493466
151	1	0	-5.199282	-1.603477	5.710228
152	1	0	-3.363468	-2.068444	7.318869
153	6	0	-3.169128	-3.855882	-1.426548
154	6	0	-2.490432	-4.620208	-2.540647
155	1	0	-2.582494	-4.078782	-3.485612
156	1	0	-1.432254	-4.774708	-2.319771

157	1	0	-2.968289	-5.598530	-2.652923
158	1	0	-4.236807	-3.727623	-1.604238
159	1	0	-3.018696	-4.350532	-0.463424
160	6	0	-4.305533	-2.870803	1.071301
161	8	0	-4.317935	-3.830321	2.011269
162	8	0	-5.245264	-2.625952	0.339707
163	6	0	-5.594993	-4.464057	2.268146
164	6	0	-5.427064	-5.318615	3.505303
165	1	0	-5.877019	-5.054141	1.390372
166	1	0	-6.351954	-3.686459	2.404432
167	1	0	-5.140531	-4.703882	4.363022
168	1	0	-6.371280	-5.821206	3.737079
169	1	0	-4.658766	-6.082872	3.355201
170	1	0	-1.952729	2.629701	1.549296

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m-II-COM-*si*

Zero-point correction = 1.39765 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29455 (a.u.)

Sum of electronic and zero-point Energies = -4785.11868 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22179 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.888984	2.458945	0.431102
2	8	0	0.540463	1.343751	0.042528
3	6	0	1.669478	3.362657	-0.471334
4	8	0	0.580669	2.830472	1.656131
5	6	0	2.634487	2.777503	-1.222841
6	6	0	3.613120	3.343228	-2.155889
7	6	0	4.394720	4.467100	-1.840057
8	6	0	3.858968	2.648451	-3.353624
9	6	0	5.391579	4.896627	-2.711560
10	6	0	4.836967	3.103495	-4.234299
11	6	0	5.610078	4.221364	-3.914916
12	1	0	2.692452	1.695628	-1.123278
13	1	0	4.232779	4.984503	-0.903432
14	1	0	3.250937	1.780946	-3.604922
15	1	0	5.999989	5.757275	-2.450240
16	1	0	5.003203	2.573228	-5.167048

17	1	0	6.385181	4.561685	-4.595356
18	6	0	1.129101	3.984466	2.339736
19	6	0	-0.009429	4.846734	2.837643
20	1	0	1.812892	4.531570	1.687395
21	6	0	1.069216	4.709291	-0.649959
22	8	0	-0.110951	4.916163	-0.411608
23	8	0	1.900390	5.637754	-1.133213
24	6	0	1.302747	6.909912	-1.494351
25	6	0	2.404749	7.775191	-2.064229
26	1	0	0.849319	7.348993	-0.600893
27	1	0	1.702522	3.568338	3.170428
28	1	0	0.505832	6.724428	-2.219923
29	1	0	2.857190	7.304698	-2.941332
30	1	0	1.991174	8.742986	-2.364353
31	1	0	3.189299	7.953505	-1.322795
32	1	0	-0.578166	5.257891	2.001309
33	1	0	-0.676274	4.257180	3.471411
34	1	0	0.394253	5.671294	3.434498
35	8	0	-1.972143	0.454519	-0.856787
36	6	0	-1.759948	0.680000	-2.279072
37	1	0	-1.031730	-0.080755	-2.554197
38	6	0	-3.076538	0.480341	-3.018326
39	6	0	-1.152202	2.048007	-2.543077
40	1	0	-3.756486	1.316647	-2.840259
41	1	0	-0.151748	2.113677	-2.122267
42	1	0	-1.074858	2.208600	-3.622491
43	1	0	-1.778308	2.843823	-2.124569
44	1	0	-2.891134	0.426118	-4.096078
45	1	0	-3.582058	-0.437029	-2.703990
46	8	0	0.249238	-1.287410	-0.436104
47	6	0	0.322173	-2.683726	-0.507398
48	6	0	-0.735172	-3.168431	-1.534758
49	6	0	1.749967	-3.117074	-0.794907
50	7	0	-0.382532	-2.926281	-2.985545
51	6	0	-1.220680	-4.625294	-1.428230
52	6	0	2.267452	-4.389682	-0.398540
53	6	0	2.579291	-2.268594	-1.494697
54	6	0	0.413322	-4.051155	-3.584767
55	6	0	-1.662928	-2.784644	-3.754616
56	6	0	-1.717647	-5.091005	-2.809697
57	6	0	3.588306	-4.731783	-0.840604

58	6	0	3.870000	-2.700587	-1.867634
59	6	0	-0.480369	-5.302081	-3.700765
60	6	0	-2.596147	-3.994659	-3.468583
61	7	0	4.368823	-3.887564	-1.578344
62	1	0	-0.002962	-3.124340	0.443693
63	1	0	-1.573573	-2.500858	-1.338894
64	1	0	-2.010908	-4.677622	-0.677693
65	1	0	-0.417069	-5.288967	-1.103169
66	6	0	1.577442	-5.317308	0.428372
67	1	0	2.226175	-1.291037	-1.791559
68	1	0	1.272234	-4.218805	-2.941827
69	1	0	0.779393	-3.687999	-4.546263
70	1	0	-1.390536	-2.711311	-4.808343
71	1	0	-2.113873	-1.841643	-3.458086
72	1	0	-2.291799	-6.016062	-2.717584
73	6	0	4.136378	-5.992565	-0.487912
74	1	0	4.506103	-2.027547	-2.437782
75	1	0	-0.784172	-5.473742	-4.738231
76	1	0	0.079618	-6.182474	-3.373728
77	1	0	-2.954716	-4.383388	-4.427280
78	6	0	-3.796363	-3.604925	-2.644964
79	7	0	0.857233	-0.773720	-3.855436
80	6	0	1.565168	0.141232	-4.072705
81	1	0	0.168754	-2.000745	-3.186218
82	6	0	3.425777	-6.878291	0.289129
83	6	0	2.139135	-6.529545	0.761714
84	1	0	3.855964	-7.838806	0.556003
85	1	0	5.135061	-6.219055	-0.846861
86	1	0	1.596851	-7.216683	1.403989
87	1	0	0.605979	-5.056689	0.829285
88	6	0	-5.060313	-3.798822	-3.018559
89	1	0	-5.311978	-4.269044	-3.966900
90	1	0	-5.887575	-3.485363	-2.389177
91	1	0	-3.605538	-3.119417	-1.688918
92	22	0	-0.752238	-0.290966	0.794403
93	8	0	0.273776	-0.343225	2.326563
94	8	0	-1.791584	1.195145	1.567884
95	6	0	0.514741	0.435048	3.387496
96	6	0	-2.553472	0.981607	2.640482
97	6	0	-0.525731	0.969463	4.185137
98	6	0	1.866877	0.697216	3.705839

99	6	0	-1.977929	0.771627	3.921598
100	6	0	-3.967370	0.968265	2.496882
101	6	0	2.178012	1.478760	4.821394
102	6	0	-0.163216	1.751639	5.295284
103	6	0	-4.772891	0.684827	3.605430
104	6	0	-2.824974	0.469351	4.998165
105	6	0	1.165743	2.003244	5.624048
106	6	0	-4.208804	0.412831	4.850271
107	1	0	3.221984	1.670919	5.050206
108	1	0	-0.955609	2.186019	5.896536
109	1	0	-5.851945	0.681418	3.484204
110	1	0	-2.379070	0.274415	5.968934
111	1	0	1.408629	2.612552	6.488915
112	1	0	-4.841451	0.177762	5.700222
113	8	0	-1.873565	-1.627841	1.225424
114	6	0	-2.492780	-2.333213	2.292951
115	1	0	-3.170162	-1.635245	2.798054
116	6	0	-3.310729	-3.484258	1.715572
117	6	0	-1.454055	-2.817540	3.300477
118	1	0	-2.655043	-4.261987	1.310652
119	1	0	-0.917160	-1.979336	3.742837
120	1	0	-1.946343	-3.378039	4.102397
121	1	0	-0.722653	-3.474737	2.817691
122	1	0	-3.930902	-3.940695	2.494687
123	1	0	-3.967799	-3.129545	0.917755
124	6	0	2.945798	0.223845	2.796384
125	6	0	3.265954	-1.181070	2.664724
126	6	0	3.661801	1.145897	2.088717
127	6	0	4.311702	-1.591528	1.785181
128	6	0	4.682909	0.775211	1.157695
129	6	0	5.006932	-0.599242	0.979863
130	6	0	2.582351	-2.156953	3.425262
131	1	0	3.436858	2.201687	2.204649
132	6	0	4.642106	-2.964439	1.734338
133	6	0	5.346540	1.757292	0.387897
134	6	0	5.983197	-0.931091	0.013169
135	6	0	2.920386	-3.492689	3.342573
136	6	0	3.966492	-3.897193	2.496158
137	6	0	6.290181	1.404152	-0.555503
138	6	0	6.607130	0.046321	-0.742146
139	1	0	5.084574	2.800349	0.536805

140	1	0	6.234323	-1.968887	-0.167863
141	1	0	7.341029	-0.240313	-1.489216
142	1	0	6.771713	2.167044	-1.158622
143	1	0	4.234475	-4.945416	2.423006
144	1	0	2.382719	-4.227675	3.934068
145	1	0	5.436467	-3.302730	1.081607
146	1	0	1.788456	-1.837588	4.089565
147	6	0	-4.569038	1.299937	1.177295
148	6	0	-5.489997	0.402804	0.505831
149	6	0	-4.241478	2.486192	0.577477
150	6	0	-6.098953	0.796097	-0.726977
151	6	0	-4.800165	2.901369	-0.669929
152	6	0	-5.761991	2.079419	-1.322859
153	6	0	-5.775358	-0.881857	1.026908
154	1	0	-3.532489	3.147845	1.063659
155	6	0	-6.988925	-0.107164	-1.352943
156	6	0	-4.394700	4.119811	-1.264684
157	6	0	-6.301692	2.535958	-2.547682
158	6	0	-6.641423	-1.745006	0.385421
159	6	0	-7.262508	-1.348563	-0.811613
160	6	0	-4.927709	4.529878	-2.469438
161	6	0	-5.894945	3.732013	-3.109788
162	1	0	-5.293855	-1.187579	1.946062
163	1	0	-6.840309	-2.725832	0.806269
164	1	0	-7.954403	-2.016946	-1.315229
165	1	0	-7.466645	0.169169	-2.285053
166	1	0	-7.040122	1.940839	-3.071623
167	1	0	-6.320809	4.053954	-4.055161
168	1	0	-4.604118	5.461962	-2.922001
169	1	0	-3.645463	4.720189	-0.756493
170	1	0	-2.511670	1.156535	-0.450822

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m-III-COM-*si*

Zero-point correction = 1.39467 (a.u.)

Thermal correction to Gibbs Free Energy = 1.28959 (a.u.)

Sum of electronic and zero-point Energies = -4785.12334 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22842 (a.u.)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	8	0	1.621714	-0.839053	-1.672895
2	6	0	1.766857	-0.542532	-3.085715
3	1	0	0.915493	0.098851	-3.314061
4	6	0	3.058503	0.231720	-3.298793
5	6	0	1.672887	-1.817179	-3.908325
6	1	0	3.927029	-0.393055	-3.071851
7	1	0	0.746679	-2.346100	-3.676394
8	1	0	1.685422	-1.576865	-4.976757
9	1	0	2.520263	-2.476768	-3.704475
10	1	0	3.135699	0.565481	-4.338293
11	1	0	3.088094	1.113920	-2.655342
12	1	0	2.116961	-1.646200	-1.444657
13	6	0	1.290146	-0.196425	2.237526
14	8	0	1.191808	-0.415731	1.030309
15	6	0	2.191128	0.915082	2.674398
16	8	0	0.568479	-0.913283	3.071709
17	6	0	3.266671	1.163344	1.894914
18	6	0	4.249591	2.236458	2.016381
19	6	0	4.560102	2.878448	3.229164
20	6	0	4.900549	2.656009	0.841591
21	6	0	5.468167	3.932013	3.254150
22	6	0	5.794905	3.721143	0.867814
23	6	0	6.079359	4.363662	2.073871
24	1	0	3.402776	0.498476	1.047441
25	1	0	4.112269	2.536443	4.155183
26	1	0	4.676053	2.158865	-0.095189
27	1	0	5.703658	4.415144	4.197326
28	1	0	6.266372	4.049083	-0.052826
29	1	0	6.782347	5.190742	2.097434
30	6	0	0.928447	-1.165606	4.462950
31	6	0	-0.306207	-0.970497	5.311554
32	1	0	1.737448	-0.504134	4.766648
33	6	0	1.747358	1.875872	3.746165
34	8	0	1.744846	1.679455	4.945662
35	8	0	1.359961	3.020980	3.172699
36	6	0	0.827022	4.038953	4.059361
37	6	0	0.280889	5.145404	3.185932
38	1	0	1.633361	4.383172	4.714433
39	1	0	1.274032	-2.201520	4.473656
40	1	0	0.048884	3.578305	4.671513

41	1	0	-0.511725	4.760172	2.539447
42	1	0	-0.139232	5.935255	3.816526
43	1	0	1.063904	5.584204	2.560845
44	1	0	-0.664397	0.058107	5.239183
45	1	0	-1.105152	-1.644525	4.987893
46	1	0	-0.067086	-1.194010	6.356416
47	22	0	-0.221185	-1.241777	-0.468130
48	8	0	0.896188	-2.846467	-0.234786
49	8	0	-1.428374	-1.851174	0.777908
50	6	0	1.287236	-3.417574	0.901460
51	6	0	-1.934664	-3.045421	1.131834
52	6	0	0.356616	-4.007413	1.793247
53	6	0	2.672233	-3.472251	1.209614
54	6	0	-1.100380	-4.125838	1.515692
55	6	0	-3.342874	-3.196883	1.152701
56	6	0	3.099241	-4.035798	2.416788
57	6	0	0.830183	-4.563781	2.992187
58	6	0	-3.894775	-4.454933	1.425947
59	6	0	-1.703850	-5.369811	1.763407
60	6	0	2.184073	-4.575077	3.317211
61	6	0	-3.081805	-5.548870	1.701049
62	1	0	4.163308	-4.060897	2.632597
63	1	0	0.108299	-4.983241	3.685898
64	1	0	-4.974841	-4.560590	1.435973
65	1	0	-1.063102	-6.209292	2.013263
66	1	0	2.520707	-5.008304	4.253763
67	1	0	-3.517795	-6.523715	1.894820
68	8	0	-1.040927	-1.731730	-1.991639
69	6	0	-2.349567	-2.138630	-2.365579
70	1	0	-3.021545	-1.944951	-1.522937
71	6	0	-2.817454	-1.311400	-3.558443
72	6	0	-2.333350	-3.635588	-2.657444
73	1	0	-2.179488	-1.488948	-4.431094
74	1	0	-2.028756	-4.193524	-1.768209
75	1	0	-3.323617	-3.983908	-2.967163
76	1	0	-1.623405	-3.857415	-3.461411
77	1	0	-3.848398	-1.569299	-3.822108
78	1	0	-2.784532	-0.244051	-3.321615
79	6	0	3.688761	-2.916334	0.278299
80	6	0	3.865437	-3.451740	-1.060531
81	6	0	4.535501	-1.938231	0.717978

82	6	0	4.876703	-2.916658	-1.916501
83	6	0	5.550906	-1.363986	-0.109618
84	6	0	5.714446	-1.822506	-1.447515
85	6	0	3.082188	-4.537280	-1.520630
86	1	0	4.425823	-1.558155	1.728816
87	6	0	5.047850	-3.495813	-3.195980
88	6	0	6.375955	-0.325881	0.380319
89	6	0	6.686116	-1.186776	-2.253462
90	6	0	3.275528	-5.080906	-2.773872
91	6	0	4.267641	-4.554589	-3.619513
92	6	0	7.322451	0.270833	-0.428058
93	6	0	7.471135	-0.160832	-1.758567
94	1	0	6.241977	0.006587	1.404573
95	1	0	6.821596	-1.494193	-3.283584
96	1	0	8.205625	0.312480	-2.402910
97	1	0	7.938961	1.076339	-0.042020
98	1	0	4.425469	-4.981504	-4.605196
99	1	0	2.664815	-5.916011	-3.102057
100	1	0	5.816330	-3.117628	-3.859451
101	1	0	2.329071	-4.951611	-0.863425
102	6	0	-4.250739	-2.024938	1.010778
103	6	0	-5.308500	-1.996825	0.019110
104	6	0	-4.136096	-0.990361	1.896836
105	6	0	-6.233400	-0.908029	-0.006562
106	6	0	-5.059573	0.098967	1.925304
107	6	0	-6.125527	0.151672	0.981996
108	6	0	-5.426184	-3.013259	-0.960266
109	1	0	-3.333180	-0.995678	2.626319
110	6	0	-7.229819	-0.896578	-1.010566
111	6	0	-4.928341	1.122194	2.894243
112	6	0	-7.014983	1.249625	1.042709
113	6	0	-6.406216	-2.969485	-1.931580
114	6	0	-7.318373	-1.899847	-1.955763
115	6	0	-5.818429	2.175159	2.934746
116	6	0	-6.868188	2.238515	1.997912
117	1	0	-4.718703	-3.831939	-0.944809
118	1	0	-6.469675	-3.758743	-2.674696
119	1	0	-8.093222	-1.860178	-2.715520
120	1	0	-7.938358	-0.079078	-1.049591
121	1	0	-7.826415	1.329539	0.330263
122	1	0	-7.568025	3.068508	2.023677

123	1	0	-5.707249	2.954953	3.682045
124	1	0	-4.099960	1.070613	3.592186
125	8	0	-0.694302	0.547786	-0.540069
126	6	0	-0.797431	1.472991	-1.577694
127	6	0	-2.221724	2.075006	-1.546101
128	6	0	0.357678	2.459774	-1.495821
129	7	0	-2.554277	2.845452	-0.313007
130	6	0	-2.645894	2.893069	-2.785166
131	6	0	0.966232	3.047166	-2.647145
132	6	0	0.872995	2.783131	-0.257446
133	6	0	-2.163023	4.278619	-0.411888
134	6	0	-4.030812	2.779044	-0.147943
135	6	0	-3.699726	3.927101	-2.344384
136	6	0	2.051956	3.961864	-2.430188
137	6	0	1.925621	3.715607	-0.154206
138	6	0	-2.981571	4.999217	-1.510988
139	6	0	-4.768971	3.264376	-1.434399
140	7	0	2.507591	4.296394	-1.187927
141	1	0	-0.751824	0.952720	-2.545028
142	1	0	-2.846841	1.180734	-1.483367
143	1	0	-3.036815	2.224274	-3.557866
144	1	0	-1.795176	3.425162	-3.218953
145	6	0	0.594725	2.755229	-3.989706
146	1	0	0.469504	2.325671	0.634539
147	1	0	-1.096676	4.326647	-0.615824
148	1	0	-2.326381	4.721502	0.574770
149	1	0	-4.294519	3.390242	0.716580
150	1	0	-4.288403	1.749747	0.093618
151	1	0	-4.186516	4.372164	-3.216445
152	6	0	2.700222	4.550689	-3.548057
153	1	0	2.300984	3.976677	0.830867
154	1	0	-3.713799	5.685298	-1.072309
155	1	0	-2.317437	5.593723	-2.146061
156	1	0	-5.490458	4.040923	-1.157414
157	6	0	-5.518252	2.160902	-2.130343
158	7	0	-1.720466	2.024633	1.999722
159	6	0	-1.480070	1.787184	3.122109
160	1	0	-2.025206	2.308881	0.937019
161	6	0	2.310330	4.246814	-4.830877
162	6	0	1.250257	3.336082	-5.051505
163	1	0	2.816482	4.699215	-5.678108

164	1	0	3.513960	5.238911	-3.344374
165	1	0	0.954119	3.091054	-6.066856
166	1	0	-0.208044	2.054311	-4.184562
167	6	0	-6.758603	2.273665	-2.604730
168	1	0	-7.329614	3.193473	-2.495639
169	1	0	-7.246998	1.451892	-3.119339
170	1	0	-4.994784	1.213577	-2.253825

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m-IV-COM-*si*

Zero-point correction = 1.39582 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29118 (a.u.)

Sum of electronic and zero-point Energies = -4785.11725 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22189 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.263881	-1.605581	1.275180
2	6	0	-1.594548	-2.163044	2.526202
3	1	0	-2.521865	-1.681053	2.856244
4	6	0	-1.839952	-3.660028	2.358581
5	6	0	-0.495583	-1.854087	3.538204
6	1	0	-0.919908	-4.161424	2.041664
7	1	0	-0.343475	-0.775886	3.615682
8	1	0	-0.780527	-2.225708	4.528500
9	1	0	0.444648	-2.323762	3.241330
10	1	0	-2.176196	-4.100299	3.303264
11	1	0	-2.607810	-3.839646	1.603582
12	22	0	-0.722888	-0.702935	-0.149468
13	8	0	-1.377864	0.933965	0.386790
14	6	0	-1.249745	2.180371	-0.254100
15	6	0	-2.550764	2.991029	-0.054992
16	6	0	0.040532	2.839158	0.190641
17	7	0	-2.909227	3.325036	1.356183
18	6	0	-2.658872	4.264899	-0.924303
19	6	0	0.886631	3.548780	-0.713594
20	6	0	0.448836	2.716721	1.503354
21	6	0	-2.251875	4.568557	1.849460
22	6	0	-4.376532	3.548272	1.392524
23	6	0	-3.511481	5.305729	-0.172209

24	6	0	2.086751	4.129270	-0.182236
25	6	0	1.630042	3.352294	1.930143
26	6	0	-2.690642	5.804218	1.025745
27	6	0	-4.811027	4.668489	0.388599
28	7	0	2.435980	4.034392	1.135050
29	1	0	-1.203055	2.028387	-1.333969
30	1	0	-3.321021	2.286110	-0.375104
31	1	0	-3.090822	4.007621	-1.894270
32	1	0	-1.671906	4.696760	-1.117471
33	6	0	0.648219	3.658250	-2.112730
34	1	0	-0.138950	2.137965	2.205151
35	1	0	-1.176945	4.426691	1.800697
36	1	0	-2.517907	4.664496	2.905899
37	1	0	-4.645348	3.813440	2.418746
38	1	0	-4.870540	2.602424	1.157600
39	1	0	-3.771368	6.135304	-0.835839
40	6	0	2.984121	4.798337	-1.055485
41	1	0	1.927583	3.279455	2.973875
42	1	0	-3.287330	6.492367	1.633749
43	1	0	-1.812113	6.356195	0.676895
44	1	0	-5.349097	5.448375	0.939021
45	6	0	-5.716254	4.140465	-0.685377
46	7	0	-2.501826	1.635524	3.299846
47	6	0	-2.368890	1.027453	4.294755
48	1	0	-2.635597	2.277895	2.393045
49	6	0	2.723277	4.877656	-2.402944
50	6	0	1.547124	4.297827	-2.934611
51	1	0	3.424030	5.376141	-3.065351
52	1	0	3.883227	5.222034	-0.620397
53	1	0	1.358194	4.344422	-4.002219
54	1	0	-0.234885	3.207894	-2.546703
55	6	0	-6.938118	4.603195	-0.947505
56	1	0	-7.374672	5.421195	-0.377979
57	1	0	-7.550006	4.180089	-1.739522
58	1	0	-5.322200	3.315819	-1.274147
59	8	0	-2.038167	-1.181024	-1.404429
60	8	0	0.273310	0.139733	-1.610312
61	6	0	-2.821013	-0.261782	-1.987977
62	6	0	0.223461	0.196266	-2.932974
63	6	0	-2.342154	0.550804	-3.039439
64	6	0	-4.151829	-0.142568	-1.527156

65	6	0	-0.996744	0.380831	-3.658873
66	6	0	1.445441	0.124098	-3.664651
67	6	0	-5.002241	0.799436	-2.105602
68	6	0	-3.226187	1.507708	-3.574424
69	6	0	1.438124	0.255813	-5.058906
70	6	0	-0.943883	0.467004	-5.060020
71	6	0	-4.537376	1.634626	-3.124835
72	6	0	0.252657	0.419660	-5.765064
73	1	0	-6.024781	0.878159	-1.749169
74	1	0	-2.866032	2.165345	-4.359100
75	1	0	2.384815	0.227973	-5.589180
76	1	0	-1.877540	0.568429	-5.603688
77	1	0	-5.193464	2.377936	-3.566766
78	1	0	0.259234	0.502355	-6.847152
79	8	0	0.288960	-2.590706	-0.883868
80	6	0	-0.252235	-3.431580	-1.941795
81	1	0	1.206792	-2.346527	-1.081993
82	1	0	-0.642603	-2.768345	-2.719999
83	6	0	0.857268	-4.304538	-2.506033
84	6	0	-1.389257	-4.235881	-1.338996
85	6	0	2.328658	-1.103834	1.068406
86	8	0	1.252870	-0.535089	0.900652
87	6	0	3.159278	-0.847313	2.286791
88	8	0	2.751047	-1.953377	0.134570
89	6	0	3.452806	0.451757	2.547901
90	6	0	4.160126	1.132166	3.628068
91	6	0	4.572245	2.456519	3.364784
92	6	0	4.403919	0.596701	4.907141
93	6	0	5.240424	3.203276	4.329127
94	6	0	5.056814	1.354420	5.872876
95	6	0	5.487409	2.652545	5.587187
96	1	0	3.086607	1.139861	1.792264
97	1	0	4.350701	2.904754	2.402308
98	1	0	4.080510	-0.405234	5.144898
99	1	0	5.552554	4.217718	4.102387
100	1	0	5.230188	0.929037	6.856318
101	1	0	6.001392	3.234511	6.346197
102	6	0	4.080754	-2.553711	0.115941
103	6	0	3.947762	-4.020534	-0.220143
104	1	0	4.587541	-2.392078	1.065126
105	6	0	3.548429	-2.040462	3.085374

106	8	0	4.492836	-2.136606	3.844366
107	8	0	2.699239	-3.058185	2.829339
108	6	0	2.965322	-4.312805	3.507887
109	6	0	1.830280	-5.257006	3.179483
110	1	0	3.040557	-4.117299	4.580569
111	1	0	4.633525	-2.018173	-0.650563
112	1	0	3.933541	-4.690860	3.165267
113	1	0	1.736866	-5.406353	2.099889
114	1	0	2.020120	-6.228937	3.645445
115	1	0	0.879684	-4.874351	3.558518
116	1	0	1.252919	-4.977063	-1.737970
117	1	0	-2.128487	-3.575738	-0.888086
118	1	0	-1.886025	-4.819113	-2.119784
119	1	0	-1.011154	-4.925370	-0.577205
120	1	0	0.470482	-4.914989	-3.328059
121	1	0	1.678312	-3.700085	-2.904395
122	1	0	3.330996	-4.543452	0.514486
123	1	0	3.510251	-4.156231	-1.211539
124	1	0	4.944320	-4.473143	-0.227839
125	6	0	-4.599761	-1.035534	-0.422849
126	6	0	-4.855792	-2.436288	-0.680214
127	6	0	-4.722327	-0.548930	0.843560
128	6	0	-5.196786	-3.307705	0.397031
129	6	0	-5.084186	-1.380956	1.950093
130	6	0	-5.308798	-2.771574	1.745625
131	6	0	-4.764327	-2.961510	-1.989410
132	1	0	-4.481785	0.488441	1.045398
133	6	0	-5.404959	-4.676287	0.107328
134	6	0	-5.172007	-0.839256	3.252678
135	6	0	-5.609938	-3.567534	2.874117
136	6	0	-4.982997	-4.300891	-2.241347
137	6	0	-5.300399	-5.166873	-1.180477
138	6	0	-5.462058	-1.643004	4.336298
139	6	0	-5.682666	-3.018843	4.141578
140	1	0	-4.971335	0.217295	3.391128
141	1	0	-5.780028	-4.631319	2.756712
142	1	0	-5.908383	-3.656315	4.991193
143	1	0	-5.507157	-1.217664	5.333806
144	1	0	-5.467939	-6.222672	-1.370946
145	1	0	-4.906734	-4.683766	-3.254513
146	1	0	-5.657601	-5.362153	0.907317

147	1	0	-4.513079	-2.289066	-2.801550
148	6	0	2.759817	-0.034143	-2.984863
149	6	0	3.691644	-1.061211	-3.424316
150	6	0	3.140506	0.821467	-1.988845
151	6	0	5.025435	-1.087116	-2.911642
152	6	0	4.452151	0.801729	-1.419846
153	6	0	5.426681	-0.117737	-1.904040
154	6	0	3.297182	-2.079593	-4.327693
155	1	0	2.437331	1.563351	-1.633287
156	6	0	5.901243	-2.104778	-3.358655
157	6	0	4.805229	1.709700	-0.392921
158	6	0	6.721233	-0.082723	-1.335309
159	6	0	4.171650	-3.068627	-4.733705
160	6	0	5.491683	-3.074724	-4.252613
161	6	0	6.073015	1.711337	0.152136
162	6	0	7.039121	0.807582	-0.326730
163	1	0	2.280060	-2.081152	-4.697863
164	1	0	3.835197	-3.840136	-5.419442
165	1	0	6.186965	-3.844741	-4.572638
166	1	0	6.917396	-2.139519	-2.984372
167	1	0	7.486470	-0.765302	-1.685881
168	1	0	8.038968	0.808466	0.096268
169	1	0	6.324446	2.404042	0.948473
170	1	0	4.058926	2.412624	-0.043553

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m-V-COM-*si*

Zero-point correction = 1.39604 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29015 (a.u.)

Sum of electronic and zero-point Energies = -4785.11406 (a.u.)

Sum of electronic and thermal Free Energies = -4785.21995 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.496995	-1.378301	1.772880
2	6	0	0.004700	-1.747954	3.043103
3	1	0	-0.298322	-0.816146	3.541566
4	6	0	-1.203331	-2.670039	2.906514
5	6	0	1.139030	-2.382057	3.842537
6	1	0	-0.917784	-3.609010	2.423493

7	1	0	1.990164	-1.698179	3.898266
8	1	0	0.808943	-2.608531	4.862198
9	1	0	1.465592	-3.312032	3.366705
10	1	0	-1.622732	-2.897875	3.892740
11	1	0	-1.973692	-2.199746	2.293180
12	8	0	1.475421	0.405982	-0.019759
13	6	0	2.330629	1.267359	-0.690481
14	6	0	1.493797	2.511496	-1.107146
15	6	0	3.531590	1.565248	0.197426
16	7	0	0.949831	3.278638	0.051162
17	6	0	2.119265	3.494736	-2.123706
18	6	0	4.767853	2.081891	-0.301719
19	6	0	3.413140	1.388321	1.559901
20	6	0	1.902843	4.297234	0.570912
21	6	0	-0.261794	3.986558	-0.423996
22	6	0	1.596021	4.912302	-1.825342
23	6	0	5.731456	2.532919	0.659215
24	6	0	4.441447	1.835873	2.417865
25	6	0	2.216801	5.372174	-0.498876
26	6	0	0.055467	4.904922	-1.651119
27	7	0	5.544434	2.430279	2.007672
28	1	0	2.673207	0.803266	-1.626700
29	1	0	0.619157	2.044842	-1.565339
30	1	0	1.874375	3.180833	-3.143394
31	1	0	3.206605	3.516488	-2.050079
32	6	0	5.111978	2.154409	-1.679207
33	1	0	2.512989	0.947184	1.966492
34	1	0	2.804310	3.786440	0.895125
35	1	0	1.441957	4.731263	1.463054
36	1	0	-0.654827	4.568188	0.412738
37	1	0	-1.014305	3.240485	-0.680613
38	1	0	1.866231	5.593498	-2.637086
39	6	0	6.952794	3.098500	0.207899
40	1	0	4.325547	1.716802	3.493245
41	1	0	1.810141	6.347582	-0.210400
42	1	0	3.299003	5.490496	-0.610596
43	1	0	-0.256991	5.930923	-1.427263
44	6	0	-0.650222	4.462081	-2.900637
45	7	0	0.122688	2.136720	2.280812
46	6	0	-0.284164	1.778761	3.319224
47	1	0	0.493222	2.490640	1.307630

48	6	0	7.235074	3.187579	-1.135544
49	6	0	6.310109	2.696403	-2.086448
50	1	0	8.175468	3.615628	-1.469662
51	1	0	7.652388	3.436771	0.965229
52	1	0	6.556208	2.727286	-3.143445
53	1	0	4.438645	1.739177	-2.418622
54	6	0	-1.320390	5.268202	-3.724888
55	1	0	-1.409736	6.334663	-3.529443
56	1	0	-1.798058	4.897301	-4.627217
57	1	0	-0.585552	3.399948	-3.134943
58	22	0	0.372000	-1.044135	0.040226
59	8	0	1.599312	-2.225942	-0.744594
60	8	0	-1.055998	-2.320421	-0.286986
61	6	0	1.816558	-3.484443	-0.317488
62	6	0	-1.307185	-3.314679	-1.126917
63	6	0	0.886162	-4.510277	-0.586630
64	6	0	3.012884	-3.773565	0.376553
65	6	0	-0.339407	-4.320514	-1.406256
66	6	0	-2.599234	-3.432396	-1.715245
67	6	0	3.224382	-5.067890	0.866401
68	6	0	1.139744	-5.795296	-0.078347
69	6	0	-2.835835	-4.420347	-2.681127
70	6	0	-0.614224	-5.271856	-2.398473
71	6	0	2.287419	-6.076667	0.655753
72	6	0	-1.838097	-5.311492	-3.061896
73	1	0	4.143967	-5.274639	1.405214
74	1	0	0.405781	-6.574767	-0.257782
75	1	0	-3.828432	-4.502723	-3.112643
76	1	0	0.152026	-6.004364	-2.633884
77	1	0	2.457137	-7.074984	1.046719
78	1	0	-2.027340	-6.059593	-3.825066
79	8	0	-0.180702	-0.289855	-2.086446
80	6	0	-0.038937	-1.010697	-3.338846
81	1	0	-1.087468	0.051015	-2.000884
82	1	0	-0.345086	-2.047815	-3.169451
83	6	0	-0.944112	-0.374760	-4.384060
84	6	0	1.430847	-0.968881	-3.716035
85	6	0	-2.363399	0.926865	0.035157
86	8	0	-1.345626	0.335960	0.385792
87	6	0	-3.363288	1.391148	1.023336
88	8	0	-2.506011	1.145441	-1.284785

89	6	0	-3.293162	0.766215	2.232169
90	6	0	-3.992401	0.908503	3.497478
91	6	0	-3.388034	0.258185	4.594948
92	6	0	-5.207938	1.590102	3.705937
93	6	0	-3.962244	0.302131	5.859164
94	6	0	-5.780586	1.625499	4.972134
95	6	0	-5.163060	0.987695	6.051516
96	1	0	-2.502336	0.024959	2.272560
97	1	0	-2.451382	-0.267080	4.443074
98	1	0	-5.716187	2.047563	2.870703
99	1	0	-3.476537	-0.197021	6.691390
100	1	0	-6.722726	2.145202	5.116943
101	1	0	-5.620419	1.018374	7.035866
102	6	0	-3.782743	1.365703	-1.967998
103	6	0	-3.668228	2.551739	-2.893603
104	1	0	-4.585084	1.466305	-1.241576
105	6	0	-4.253653	2.550029	0.721014
106	8	0	-5.457792	2.592841	0.890549
107	8	0	-3.546785	3.588972	0.240246
108	6	0	-4.319069	4.790678	-0.040988
109	6	0	-3.354821	5.879101	-0.452420
110	1	0	-4.877693	5.055388	0.859962
111	1	0	-3.959110	0.452292	-2.528897
112	1	0	-5.043041	4.561038	-0.828049
113	1	0	-2.806557	5.606558	-1.357024
114	1	0	-3.917063	6.795868	-0.656727
115	1	0	-2.639332	6.091072	0.346820
116	1	0	-0.658249	0.668070	-4.561360
117	1	0	2.038290	-1.360359	-2.899330
118	1	0	1.607302	-1.581097	-4.606254
119	1	0	1.744327	0.057873	-3.935654
120	1	0	-0.866730	-0.915660	-5.332202
121	1	0	-1.993887	-0.405280	-4.073010
122	1	0	-3.412905	3.466095	-2.360088
123	1	0	-2.908365	2.374024	-3.659055
124	1	0	-4.628802	2.690321	-3.400009
125	6	0	4.067199	-2.747173	0.596000
126	6	0	4.795085	-2.171487	-0.517361
127	6	0	4.433755	-2.427665	1.871831
128	6	0	5.901690	-1.304027	-0.270045
129	6	0	5.533786	-1.562407	2.164263

130	6	0	6.298472	-1.010826	1.098481
131	6	0	4.453374	-2.478473	-1.855048
132	1	0	3.884189	-2.854631	2.704233
133	6	0	6.588273	-0.760121	-1.379081
134	6	0	5.887771	-1.274553	3.502523
135	6	0	7.414678	-0.210799	1.426749
136	6	0	5.143514	-1.929976	-2.917676
137	6	0	6.218204	-1.057161	-2.676186
138	6	0	6.977245	-0.477547	3.791725
139	6	0	7.747956	0.052415	2.741788
140	1	0	5.285525	-1.698801	4.301384
141	1	0	8.019547	0.223312	0.640697
142	1	0	8.603833	0.682211	2.963232
143	1	0	7.239282	-0.260012	4.822675
144	1	0	6.759164	-0.612938	-3.506388
145	1	0	4.856270	-2.176632	-3.935511
146	1	0	7.409777	-0.074230	-1.216529
147	1	0	3.633092	-3.159054	-2.041483
148	6	0	-3.734535	-2.628144	-1.193198
149	6	0	-4.653588	-1.920159	-2.061369
150	6	0	-3.969712	-2.630578	0.154583
151	6	0	-5.799671	-1.265456	-1.507672
152	6	0	-5.096355	-1.990149	0.748694
153	6	0	-6.035527	-1.305585	-0.073612
154	6	0	-4.419505	-1.817478	-3.455881
155	1	0	-3.288150	-3.165689	0.804746
156	6	0	-6.658056	-0.562369	-2.385581
157	6	0	-5.299082	-2.048266	2.147987
158	6	0	-7.140912	-0.687426	0.554215
159	6	0	-5.274497	-1.116406	-4.284256
160	6	0	-6.408695	-0.486070	-3.742713
161	6	0	-6.394048	-1.445717	2.729884
162	6	0	-7.318739	-0.756545	1.923447
163	1	0	-3.540934	-2.294070	-3.871158
164	1	0	-5.066674	-1.049958	-5.347782
165	1	0	-7.087925	0.063433	-4.387265
166	1	0	-7.532707	-0.060315	-1.989410
167	1	0	-7.869323	-0.145303	-0.036975
168	1	0	-8.174764	-0.269002	2.379351
169	1	0	-6.533210	-1.484826	3.805147
170	1	0	-4.569470	-2.573849	2.756938

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m-VI-COM-*si*

Zero-point correction = 1.39931 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29514 (a.u.)

Sum of electronic and zero-point Energies = -4785.11280 (a.u.)

Sum of electronic and thermal Free Energies = -4785.21697 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.618312	-1.876140	1.892295
2	6	0	0.011830	-2.821488	2.802636
3	1	0	0.013353	-3.754976	2.236894
4	6	0	1.439209	-2.413576	3.132821
5	6	0	-0.860994	-2.965999	4.040080
6	1	0	1.464287	-1.473445	3.692282
7	1	0	-1.882156	-3.240577	3.770491
8	1	0	-0.456757	-3.737850	4.702406
9	1	0	-0.893497	-2.026917	4.607037
10	1	0	1.905222	-3.186420	3.753384
11	1	0	2.027367	-2.293195	2.224892
12	1	0	-0.749780	-1.020377	2.334580
13	22	0	0.111360	-1.367330	-0.178590
14	8	0	1.349263	-2.760454	-0.083081
15	8	0	-1.252543	-2.591974	-0.722388
16	6	0	1.523544	-3.782223	-0.942590
17	6	0	-1.600812	-3.780724	-0.222903
18	6	0	0.563335	-4.811195	-1.068648
19	6	0	2.716276	-3.825565	-1.699978
20	6	0	-0.692474	-4.869728	-0.274227
21	6	0	-2.898023	-3.973581	0.315309
22	6	0	2.918073	-4.868214	-2.610183
23	6	0	0.810526	-5.842222	-1.989784
24	6	0	-3.217841	-5.210515	0.892721
25	6	0	-1.051974	-6.082290	0.330104
26	6	0	-3.952438	-2.937133	0.151205
27	6	0	3.742507	-2.757143	-1.565147
28	6	0	1.967907	-5.875116	-2.761853
29	6	0	-2.295468	-6.252202	0.933443
30	6	0	-4.781755	-2.496323	1.255735

31	6	0	-4.203655	-2.448735	-1.101234
32	6	0	4.474779	-2.566450	-0.329909
33	6	0	4.029311	-1.971020	-2.643681
34	6	0	-5.882810	-1.616025	1.015142
35	6	0	-5.290921	-1.569278	-1.384102
36	6	0	5.476541	-1.552874	-0.246145
37	6	0	4.992024	-0.915755	-2.591488
38	6	0	-6.166771	-1.168346	-0.337525
39	6	0	5.735119	-0.700025	-1.396874
40	6	0	-4.519545	-2.904744	2.585707
41	6	0	4.233043	-3.385624	0.796800
42	6	0	-5.529041	-1.125406	-2.706017
43	6	0	6.177421	-1.401436	0.972871
44	6	0	5.186500	-0.062541	-3.702479
45	6	0	-7.266818	-0.347456	-0.669754
46	6	0	6.674081	0.357365	-1.383573
47	6	0	6.088457	0.981441	-3.648577
48	6	0	6.842417	1.187317	-2.477692
49	6	0	4.929035	-3.206773	1.975128
50	6	0	5.905784	-2.200588	2.065723
51	6	0	-6.606828	-0.315398	-2.998583
52	6	0	-7.484161	0.072549	-1.968165
53	6	0	-5.305555	-2.488018	3.641701
54	6	0	-6.390371	-1.626004	3.405127
55	6	0	-6.663054	-1.200358	2.119514
56	1	0	3.836278	-4.884086	-3.189501
57	1	0	0.060850	-6.618538	-2.106424
58	1	0	-4.215429	-5.356334	1.294496
59	1	0	-0.338603	-6.900812	0.314195
60	1	0	2.128913	-6.679992	-3.471975
61	1	0	-2.556498	-7.198314	1.396892
62	1	0	-3.576042	-2.764553	-1.927347
63	1	0	3.490294	-2.125880	-3.572362
64	1	0	-3.680997	-3.563244	2.767626
65	1	0	3.484706	-4.164512	0.724272
66	1	0	-4.848433	-1.445592	-3.489856
67	1	0	6.936875	-0.636788	1.066689
68	1	0	4.601706	-0.239760	-4.600804
69	1	0	-7.960177	-0.032550	0.101218
70	1	0	7.278738	0.527810	-0.502102
71	1	0	6.223177	1.634413	-4.505401

72	1	0	7.567118	1.994757	-2.434107
73	1	0	4.720414	-3.842088	2.830094
74	1	0	6.451806	-2.051158	2.991889
75	1	0	-6.784579	0.014284	-4.018072
76	1	0	-8.340238	0.701436	-2.194075
77	1	0	-5.077917	-2.817341	4.651101
78	1	0	-7.009866	-1.287844	4.230263
79	1	0	-7.494189	-0.523221	1.961695
80	8	0	0.317757	-0.727534	-1.857140
81	6	0	-0.316318	-1.117138	-3.079279
82	1	0	-0.505823	-2.196030	-3.022843
83	6	0	-1.654187	-0.394516	-3.211448
84	6	0	0.628042	-0.837772	-4.241901
85	1	0	-1.510317	0.689234	-3.233285
86	1	0	1.574179	-1.362536	-4.096019
87	1	0	0.184645	-1.185661	-5.181323
88	1	0	0.838619	0.231446	-4.337603
89	1	0	-2.155290	-0.698709	-4.137260
90	1	0	-2.298260	-0.635560	-2.365236
91	8	0	1.146067	-0.137164	0.751375
92	6	0	2.270771	0.683453	0.635345
93	6	0	1.929029	1.782977	-0.428754
94	6	0	2.689187	1.168396	2.021056
95	7	0	1.709534	3.206222	0.047686
96	6	0	2.874489	1.837318	-1.639402
97	6	0	4.015927	1.596594	2.336554
98	6	0	1.760490	1.174386	3.033546
99	6	0	2.970776	4.017292	0.138155
100	6	0	0.787915	3.865237	-0.941485
101	6	0	2.844603	3.251994	-2.238922
102	6	0	4.279000	2.012943	3.683386
103	6	0	2.123772	1.598447	4.330869
104	6	0	3.581532	4.187734	-1.267211
105	6	0	1.380243	3.752868	-2.375214
106	7	0	3.331256	1.998596	4.666550
107	1	0	3.101195	0.099081	0.217843
108	1	0	0.946168	1.476580	-0.780254
109	1	0	2.555242	1.073152	-2.350239
110	1	0	3.901458	1.593470	-1.358869
111	6	0	5.076127	1.668839	1.395245
112	1	0	0.747371	0.866134	2.825978

113	1	0	3.639149	3.500745	0.818835
114	1	0	2.686572	4.961572	0.604669
115	1	0	0.670424	4.901390	-0.622205
116	1	0	-0.182294	3.373894	-0.860675
117	1	0	3.323843	3.259109	-3.220699
118	6	0	5.572373	2.482984	4.028427
119	1	0	1.368236	1.617092	5.113993
120	1	0	3.501402	5.226325	-1.602860
121	1	0	4.644732	3.932952	-1.237580
122	1	0	1.408972	4.753416	-2.818643
123	6	0	0.556964	2.858488	-3.260675
124	6	0	6.567886	2.566468	3.082778
125	6	0	6.313212	2.157108	1.754200
126	1	0	7.549707	2.942756	3.353154
127	1	0	5.732310	2.786783	5.057609
128	1	0	7.101600	2.222285	1.011138
129	1	0	4.912089	1.336864	0.379057
130	6	0	0.168998	3.168617	-4.497456
131	1	0	0.407995	4.129179	-4.948775
132	1	0	-0.394897	2.469540	-5.107817
133	1	0	0.293271	1.886572	-2.849438
134	6	0	-1.873016	0.996693	0.926599
135	8	0	-1.543000	0.150668	0.093976
136	6	0	-2.586762	2.208796	0.483875
137	8	0	-1.528403	0.801494	2.202864
138	6	0	-2.291658	3.433014	0.974922
139	6	0	-2.830141	4.727081	0.564574
140	6	0	-4.076134	4.893767	-0.069778
141	6	0	-2.054201	5.867753	0.848107
142	6	0	-4.506607	6.159953	-0.450308
143	6	0	-2.485339	7.131447	0.453988
144	6	0	-3.707684	7.280210	-0.202860
145	1	0	-1.506738	3.495856	1.721607
146	1	0	-4.727230	4.042374	-0.226643
147	1	0	-1.118377	5.743642	1.383660
148	1	0	-5.473317	6.276580	-0.930293
149	1	0	-1.873877	8.001579	0.671544
150	1	0	-4.047601	8.266204	-0.504653
151	6	0	-2.285215	1.369058	3.331599
152	6	0	-3.707603	0.854517	3.326822
153	1	0	-2.207881	2.453754	3.315277

154	6	0	-3.555218	1.973505	-0.636520
155	8	0	-4.629153	1.433988	-0.474086
156	8	0	-3.102353	2.468624	-1.793799
157	6	0	-4.009788	2.434824	-2.929004
158	6	0	-3.661122	3.612322	-3.812813
159	1	0	-5.035918	2.473598	-2.559219
160	1	0	-1.724242	1.010671	4.195827
161	1	0	-3.871280	1.476767	-3.435785
162	1	0	-4.294783	3.605601	-4.705476
163	1	0	-3.820279	4.554759	-3.280861
164	1	0	-2.614958	3.569294	-4.128062
165	1	0	-4.227807	1.233964	4.211949
166	1	0	-4.255431	1.186509	2.441242
167	1	0	-3.727815	-0.236800	3.355974
168	1	0	1.233461	3.307293	1.016823
169	7	0	0.571548	3.903909	2.349024
170	6	0	0.112403	4.231939	3.384340

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Zero-point correction = 1.20992 (a.u.)

Thermal correction to Gibbs Free Energy = 1.11262 (a.u.)

Sum of electronic and zero-point Energies = -4133.53904 (a.u.)

Sum of electronic and thermal Free Energies = -4133.63633 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.381669	0.405226	-0.884904
2	8	0	-1.337446	-0.244570	-0.789092
3	6	0	-3.002014	1.127066	0.246651
4	8	0	-3.029616	0.511368	-2.023396
5	6	0	-3.824713	2.207474	0.134227
6	6	0	-2.404447	0.026124	-3.248199
7	6	0	-2.443893	1.149246	-4.262393
8	1	0	-2.983368	-0.847442	-3.553688
9	6	0	-2.543439	0.738915	1.598549
10	8	0	-1.640908	-0.063172	1.856453
11	8	0	-3.229294	1.312909	2.577417
12	6	0	-2.850808	0.966078	3.939930
13	6	0	-3.843665	1.639788	4.858024

14	1	0	-1.826523	1.308961	4.108439
15	1	0	-1.392005	-0.297798	-3.015366
16	1	0	-2.875944	-0.120611	4.028879
17	1	0	-3.597383	1.399062	5.896640
18	1	0	-3.816652	2.727018	4.742341
19	1	0	-4.859984	1.291270	4.654504
20	1	0	-1.950921	0.821774	-5.184242
21	1	0	-3.472775	1.430708	-4.502566
22	1	0	-1.930207	2.027860	-3.866119
23	1	0	-3.957142	2.759579	1.060709
24	6	0	-4.548574	2.792427	-0.990793
25	6	0	-5.328574	2.038236	-1.884484
26	6	0	-4.553553	4.195337	-1.100955
27	6	0	-6.076139	2.672018	-2.871534
28	6	0	-5.268955	4.821887	-2.115245
29	6	0	-6.036186	4.062235	-3.000256
30	1	0	-5.363030	0.962525	-1.786994
31	1	0	-3.956140	4.783502	-0.413328
32	1	0	-6.689309	2.079722	-3.543720
33	1	0	-5.234427	5.902308	-2.209770
34	1	0	-6.609280	4.552232	-3.781516
35	6	0	3.858630	-2.522752	-0.215091
36	6	0	3.653310	-2.039695	1.082262
37	6	0	5.087470	-2.265080	-0.842860
38	6	0	4.655716	-1.340841	1.763110
39	6	0	6.099616	-1.552644	-0.193313
40	6	0	5.872428	-1.103412	1.113836
41	1	0	5.247484	-2.615098	-1.858474
42	6	0	4.414497	-0.872720	3.177420
43	1	0	4.521168	-1.701817	3.887857
44	8	0	0.787679	0.687613	0.612380
45	6	0	2.092695	1.155693	0.432729
46	6	0	2.425933	1.047264	-1.072242
47	6	0	2.220952	2.535916	1.061243
48	7	0	1.571179	1.936323	-1.948018
49	6	0	3.882635	1.218799	-1.528628
50	6	0	3.452043	3.034492	1.589397
51	6	0	1.108235	3.347869	1.138013
52	6	0	2.158397	3.308431	-2.143703
53	6	0	1.435286	1.260535	-3.280818
54	6	0	3.878724	1.719193	-2.986208

55	6	0	3.452476	4.364070	2.129917
56	6	0	1.221512	4.644286	1.685065
57	6	0	3.448738	3.193995	-2.975924
58	6	0	2.844218	0.932172	-3.835661
59	7	0	2.339862	5.154970	2.163274
60	1	0	2.808073	0.476776	0.913938
61	1	0	2.108244	0.034420	-1.315195
62	1	0	4.388142	0.256477	-1.430575
63	1	0	4.422179	1.940619	-0.910620
64	6	0	4.664681	2.292960	1.625827
65	1	0	0.159089	3.006975	0.745975
66	1	0	2.341545	3.717359	-1.154295
67	1	0	1.378416	3.909389	-2.611202
68	1	0	0.882484	1.943437	-3.926475
69	1	0	0.823190	0.375618	-3.117403
70	1	0	4.872472	1.609731	-3.429530
71	6	0	4.656194	4.899008	2.659816
72	1	0	0.341455	5.284683	1.713615
73	1	0	3.289103	3.551661	-3.998205
74	1	0	4.227667	3.817564	-2.528936
75	1	0	2.905437	1.340679	-4.853321
76	6	0	5.813664	4.156277	2.668318
77	6	0	5.814006	2.839844	2.150528
78	1	0	6.728070	4.574902	3.077644
79	1	0	4.620398	5.908535	3.055911
80	1	0	6.727848	2.253628	2.169956
81	1	0	4.688645	1.280494	1.245871
82	6	0	3.194620	-0.534017	-3.931483
83	6	0	2.399810	-1.588767	-3.759199
84	1	0	1.351945	-1.508519	-3.491635
85	1	0	2.778331	-2.599012	-3.871126
86	1	0	4.236647	-0.710173	-4.200447
87	22	0	-0.011943	-0.986746	0.744811
88	8	0	-1.072318	-2.585614	0.541827
89	8	0	1.171791	-1.709869	-0.522274
90	6	0	-1.691353	-2.975817	-0.574285
91	6	0	1.472991	-2.943834	-0.954399
92	6	0	-0.944577	-3.470092	-1.672454
93	6	0	-3.102997	-2.865468	-0.660325
94	6	0	0.506293	-3.787225	-1.561415
95	6	0	2.830027	-3.353134	-0.889776

96	6	0	-3.739534	-3.185379	-1.865284
97	6	0	-1.627021	-3.766219	-2.862234
98	6	0	3.213690	-4.564792	-1.474885
99	6	0	0.943450	-5.002909	-2.115447
100	6	0	-3.009181	-3.620561	-2.969444
101	6	0	2.279080	-5.389400	-2.093971
102	1	0	-4.820566	-3.100407	-1.926026
103	1	0	-1.055387	-4.114899	-3.716977
104	1	0	4.254614	-4.867190	-1.412257
105	1	0	0.202270	-5.662504	-2.555095
106	1	0	-3.513376	-3.860806	-3.900366
107	1	0	2.581576	-6.338393	-2.525383
108	8	0	0.649977	-1.547904	2.324855
109	6	0	0.126854	-2.442542	3.302016
110	1	0	-0.961686	-2.492660	3.168370
111	6	0	0.709605	-3.834012	3.076985
112	6	0	0.437321	-1.884358	4.686184
113	1	0	1.796366	-3.825261	3.212501
114	1	0	0.022405	-0.878090	4.796504
115	1	0	0.011513	-2.523554	5.467711
116	1	0	1.519679	-1.826469	4.842149
117	1	0	0.281509	-4.550338	3.787201
118	1	0	0.485453	-4.171792	2.062884
119	6	0	-3.879865	-2.365994	0.500615
120	6	0	-3.611558	-2.812421	1.801092
121	6	0	-4.897031	-1.416068	0.317701
122	6	0	-4.327796	-2.327535	2.898385
123	6	0	-5.618418	-0.900807	1.398171
124	6	0	-5.323572	-1.368845	2.683675
125	1	0	-5.103670	-1.051256	-0.683415
126	6	0	-4.023766	-2.835766	4.286342
127	6	0	-6.637203	0.190352	1.197714
128	1	0	-7.019935	0.206450	0.173813
129	1	0	-4.506779	-2.224239	5.053927
130	1	0	0.573328	2.087141	-1.585475
131	1	0	-2.824515	-3.540203	1.956270
132	1	0	-7.487267	0.076722	1.877841
133	1	0	-6.194513	1.174934	1.395704
134	1	0	-2.945929	-2.839204	4.482010
135	1	0	-4.373504	-3.866625	4.418761
136	1	0	-5.878372	-0.976333	3.532959

137	1	0	5.120135	-0.091875	3.472390
138	1	0	3.400047	-0.479433	3.293341
139	1	0	2.705107	-2.215403	1.574097
140	6	0	7.395252	-1.234238	-0.897542
141	1	0	6.658515	-0.559692	1.633645
142	1	0	7.409074	-0.195754	-1.252364
143	1	0	7.547910	-1.880231	-1.766804
144	1	0	8.255158	-1.356068	-0.230834
145	7	0	-0.909080	2.815046	-1.570699
146	6	0	-1.284214	3.932862	-1.641341

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Zero-point correction = 1.21041 (a.u.)

Thermal correction to Gibbs Free Energy = 1.11618 (a.u.)

Sum of electronic and zero-point Energies = -4133.53266 (a.u.)

Sum of electronic and thermal Free Energies = -4133.62689 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.821534	-2.502989	2.684273
2	6	0	-1.805298	-2.965627	2.236848
3	6	0	-2.475966	0.093727	1.134342
4	8	0	-1.531236	0.824936	0.800978
5	6	0	-2.938538	-1.053627	0.368848
6	8	0	-3.101454	0.303922	2.281985
7	6	0	-3.601183	-2.133112	0.945897
8	6	0	-2.620025	1.387126	3.127797
9	6	0	-1.316881	1.021488	3.808796
10	1	0	-3.430876	1.518050	3.846151
11	6	0	-2.414229	-1.191752	-0.982929
12	8	0	-1.634465	-0.412266	-1.554514
13	8	0	-2.897082	-2.245420	-1.644440
14	6	0	-2.408035	-2.448443	-2.996428
15	6	0	-3.141951	-3.646187	-3.554830
16	1	0	-1.327585	-2.609270	-2.952606
17	1	0	-2.523399	2.288356	2.521340
18	1	0	-2.601333	-1.539842	-3.570226
19	1	0	-2.802423	-3.838536	-4.577101
20	1	0	-2.948918	-4.541035	-2.955922

21	1	0	-4.220954	-3.467324	-3.577594
22	1	0	-1.065634	1.788434	4.548903
23	1	0	-1.400194	0.054424	4.311589
24	1	0	-0.515639	0.973439	3.071248
25	1	0	-3.587503	-3.033256	0.342997
26	6	0	-4.642149	-2.149503	1.990101
27	6	0	-5.538509	-1.078672	2.127052
28	6	0	-4.871848	-3.319080	2.733870
29	6	0	-6.624626	-1.168487	2.994824
30	6	0	-5.948898	-3.403582	3.607671
31	6	0	-6.831818	-2.327834	3.741249
32	1	0	-5.390926	-0.184829	1.538126
33	1	0	-4.166968	-4.137593	2.643510
34	1	0	-7.310445	-0.331409	3.083066
35	1	0	-6.102614	-4.309162	4.186494
36	1	0	-7.674147	-2.395172	4.423157
37	6	0	3.812142	2.570399	-0.150959
38	6	0	3.655903	1.824770	-1.325892
39	6	0	5.005803	2.442362	0.573690
40	6	0	4.680679	1.002279	-1.804548
41	6	0	6.031396	1.596499	0.139853
42	6	0	5.858845	0.889826	-1.057353
43	1	0	5.131551	3.007414	1.492224
44	6	0	4.511045	0.289079	-3.123477
45	1	0	4.507468	1.004910	-3.953918
46	8	0	0.538804	-0.722616	0.123814
47	6	0	1.855782	-1.187912	0.039080
48	6	0	2.476605	-0.911854	1.427012
49	6	0	1.851192	-2.627440	-0.462097
50	7	0	1.758907	-1.656885	2.532440
51	6	0	3.983034	-1.089923	1.665644
52	6	0	2.983372	-3.240902	-1.082900
53	6	0	0.698797	-3.376831	-0.342680
54	6	0	2.344706	-3.020720	2.777569
55	6	0	1.860148	-0.844381	3.790831
56	6	0	4.206868	-1.410271	3.156760
57	6	0	2.859979	-4.612858	-1.486633
58	6	0	0.683137	-4.719442	-0.779075
59	6	0	3.744167	-2.857587	3.399615
60	6	0	3.340101	-0.477758	4.047699
61	7	0	1.713596	-5.337290	-1.323033

62	1	0	2.452985	-0.581009	-0.656436
63	1	0	2.222299	0.135479	1.586034
64	1	0	4.486848	-0.170316	1.366870
65	1	0	4.396718	-1.904663	1.068396
66	6	0	4.211005	-2.572763	-1.340425
67	1	0	-0.179948	-2.942747	0.112744
68	1	0	2.374656	-3.529256	1.817253
69	1	0	1.635372	-3.547500	3.416296
70	1	0	1.439193	-1.453306	4.591586
71	1	0	1.220140	0.023354	3.659098
72	1	0	5.262082	-1.293782	3.418289
73	6	0	3.968015	-5.263021	-2.090533
74	1	0	-0.228333	-5.303371	-0.658382
75	1	0	3.723949	-3.077088	4.471751
76	1	0	4.435446	-3.564035	2.932557
77	1	0	3.571836	-0.731785	5.090288
78	6	0	5.147950	-4.589831	-2.305727
79	6	0	5.265083	-3.230495	-1.933530
80	1	0	5.988692	-5.095618	-2.770594
81	1	0	3.840917	-6.302030	-2.376012
82	1	0	6.192449	-2.698938	-2.123375
83	1	0	4.317441	-1.528070	-1.081518
84	6	0	3.703372	0.975999	3.856815
85	6	0	2.926080	1.983950	3.462826
86	1	0	1.877316	1.873003	3.208212
87	1	0	3.322886	2.989037	3.367464
88	1	0	4.750158	1.188483	4.076807
89	22	0	-0.057516	0.840073	-0.752033
90	8	0	-0.968458	2.441790	-1.286701
91	8	0	1.103541	1.914461	0.266385
92	6	0	-1.692145	3.203180	-0.461395
93	6	0	1.406470	3.221798	0.302156
94	6	0	-1.047122	4.028343	0.491253
95	6	0	-3.106879	3.125529	-0.516653
96	6	0	0.429191	4.239648	0.485061
97	6	0	2.781135	3.569579	0.232362
98	6	0	-3.863285	3.861199	0.401803
99	6	0	-1.850898	4.740174	1.396300
100	6	0	3.175973	4.893542	0.449701
101	6	0	0.882353	5.558767	0.667708
102	6	0	-3.242484	4.662333	1.359331

103	6	0	2.232247	5.889901	0.681216
104	1	0	-4.947172	3.802102	0.358764
105	1	0	-1.369692	5.356488	2.149483
106	1	0	4.231686	5.140596	0.388609
107	1	0	0.141751	6.344054	0.778365
108	1	0	-3.837876	5.224187	2.072335
109	1	0	2.541350	6.920574	0.824537
110	8	0	0.782168	0.649215	-2.338273
111	6	0	0.262402	0.808846	-3.658010
112	1	0	-0.831796	0.799032	-3.593890
113	6	0	0.710055	2.159909	-4.204468
114	6	0	0.715157	-0.367174	-4.514737
115	1	0	1.800114	2.196386	-4.303825
116	1	0	0.409957	-1.312399	-4.056857
117	1	0	0.274821	-0.307340	-5.516377
118	1	0	1.804602	-0.374502	-4.621779
119	1	0	0.270561	2.343782	-5.191151
120	1	0	0.394231	2.955234	-3.525090
121	6	0	-3.745048	2.189177	-1.475751
122	6	0	-3.327874	2.118309	-2.813723
123	6	0	-4.745696	1.310536	-1.042365
124	6	0	-3.870317	1.182830	-3.693926
125	6	0	-5.296426	0.348671	-1.898603
126	6	0	-4.846704	0.296748	-3.220144
127	1	0	-5.076956	1.358626	-0.009583
128	6	0	-3.383790	1.091698	-5.119034
129	6	0	-6.292681	-0.661270	-1.389646
130	1	0	-6.904462	-0.258991	-0.577533
131	1	0	-4.211707	0.933752	-5.818209
132	1	0	0.727873	-1.803442	2.349126
133	1	0	-2.554364	2.792249	-3.161328
134	1	0	-6.963687	-0.998258	-2.185719
135	1	0	-5.777679	-1.547833	-0.999295
136	1	0	-2.689655	0.251380	-5.248964
137	1	0	-2.854561	2.000041	-5.419533
138	1	0	-5.267077	-0.445896	-3.895350
139	1	0	5.316962	-0.425832	-3.307343
140	1	0	3.561180	-0.251272	-3.159953
141	1	0	2.734965	1.906817	-1.889718
142	6	0	7.279960	1.418064	0.967340
143	1	0	6.661164	0.249487	-1.417510

144	1	0	7.171689	0.583805	1.672914
145	1	0	7.501316	2.312889	1.556776
146	1	0	8.150840	1.199506	0.341761

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d-I-TS1-*re*-L2a

Zero-point correction = 1.21106 (a.u.)

Thermal correction to Gibbs Free Energy = 1.11794 (a.u.)

Sum of electronic and zero-point Energies = -4133.53561 (a.u.)

Sum of electronic and thermal Free Energies = -4133.62873 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.722917	1.927454	-3.286371
2	6	0	-1.843530	2.166228	-3.027560
3	6	0	-2.219098	-0.611115	-1.655221
4	8	0	-1.254380	-1.219385	-1.166187
5	6	0	-2.918866	0.501065	-1.033191
6	8	0	-2.681810	-0.951878	-2.855562
7	6	0	-3.571451	1.396325	-1.894098
8	6	0	-2.005794	-2.032852	-3.560647
9	6	0	-0.666890	-1.594328	-4.117338
10	1	0	-2.710334	-2.289165	-4.353833
11	6	0	-2.791591	0.613697	0.403401
12	8	0	-1.976234	-0.012387	1.107506
13	8	0	-3.699374	1.392481	0.987644
14	6	0	-3.594114	1.583690	2.419679
15	6	0	-4.823435	2.353270	2.848743
16	1	0	-2.671801	2.136148	2.624629
17	1	0	-1.901941	-2.880351	-2.883204
18	1	0	-3.527788	0.606408	2.899484
19	1	0	-4.778361	2.546624	3.925005
20	1	0	-4.890337	3.310203	2.324359
21	1	0	-5.731841	1.781840	2.638351
22	1	0	-0.276687	-2.374941	-4.778714
23	1	0	-0.763334	-0.663002	-4.681111
24	1	0	0.041257	-1.446664	-3.302194
25	1	0	-3.881678	0.975367	-2.840602
26	6	0	-4.298589	2.625783	-1.519155
27	6	0	-3.729799	3.631847	-0.725583

28	6	0	-5.602615	2.794739	-1.999435
29	6	0	-4.458395	4.769296	-0.401525
30	6	0	-6.343631	3.926888	-1.656210
31	6	0	-5.773324	4.916297	-0.858184
32	1	0	-2.713341	3.515971	-0.371217
33	1	0	-6.041309	2.029994	-2.633661
34	1	0	-4.003285	5.545987	0.205647
35	1	0	-7.359142	4.037816	-2.023493
36	1	0	-6.342133	5.804816	-0.601607
37	6	0	4.069848	-1.903586	0.969194
38	6	0	3.522192	-1.127063	1.996709
39	6	0	5.361104	-1.599797	0.511931
40	6	0	4.251719	-0.093397	2.593291
41	6	0	6.099847	-0.550500	1.066992
42	6	0	5.535718	0.189399	2.114403
43	1	0	5.788590	-2.184393	-0.296931
44	6	0	3.654970	0.666973	3.751961
45	1	0	3.635044	0.046227	4.655893
46	8	0	0.394277	0.666591	-0.209209
47	6	0	1.605258	1.336178	-0.003397
48	6	0	2.498304	0.981357	-1.215237
49	6	0	1.332814	2.815672	0.236213
50	7	0	1.895789	1.449800	-2.526296
51	6	0	3.981851	1.375438	-1.235878
52	6	0	2.241525	3.674123	0.928790
53	6	0	0.157552	3.366251	-0.232219
54	6	0	2.315225	2.850059	-2.893031
55	6	0	2.338550	0.507062	-3.608719
56	6	0	4.425690	1.541359	-2.702861
57	6	0	1.889822	5.060815	1.046479
58	6	0	-0.087207	4.747172	-0.069333
59	6	0	3.817368	2.850037	-3.232761
60	6	0	3.879346	0.378118	-3.575552
61	7	0	0.735050	5.581802	0.536395
62	1	0	2.144388	0.932993	0.865205
63	1	0	2.424666	-0.105410	-1.246932
64	1	0	4.548642	0.595220	-0.727546
65	1	0	4.161548	2.314526	-0.709009
66	6	0	3.460783	3.236698	1.513361
67	1	0	-0.554335	2.741083	-0.753589
68	1	0	2.085269	3.483056	-2.041040

69	1	0	1.673907	3.152088	-3.720892
70	1	0	1.975985	0.919046	-4.550765
71	1	0	1.829776	-0.437343	-3.435981
72	1	0	5.516687	1.569075	-2.768829
73	6	0	2.772462	5.947268	1.717848
74	1	0	-1.003358	5.174078	-0.474671
75	1	0	3.974568	2.935560	-4.312519
76	1	0	4.295846	3.712987	-2.762009
77	1	0	4.249653	0.550904	-4.594195
78	6	0	3.950934	5.490399	2.260192
79	6	0	4.293619	4.121700	2.159916
80	1	0	4.618365	6.176780	2.772264
81	1	0	2.477181	6.989195	1.784893
82	1	0	5.219677	3.764362	2.599846
83	1	0	3.738708	2.193042	1.458388
84	6	0	4.420475	-0.961025	-3.134547
85	6	0	3.747679	-2.039786	-2.736774
86	1	0	2.666312	-2.080162	-2.664095
87	1	0	4.267054	-2.946601	-2.447074
88	1	0	5.509446	-1.011325	-3.160889
89	22	0	-0.104046	-0.956819	0.628100
90	8	0	-0.807650	-2.694770	1.024596
91	8	0	1.430707	-1.813263	-0.068481
92	6	0	-1.156009	-3.607487	0.112667
93	6	0	1.980559	-3.030349	0.069715
94	6	0	-0.160984	-4.308470	-0.610952
95	6	0	-2.530516	-3.827793	-0.152860
96	6	0	1.283311	-4.226904	-0.253481
97	6	0	3.342463	-3.097192	0.467830
98	6	0	-2.895571	-4.727911	-1.159065
99	6	0	-0.577311	-5.190192	-1.621813
100	6	0	4.013910	-4.324602	0.445878
101	6	0	2.001955	-5.435622	-0.233770
102	6	0	-1.926037	-5.404378	-1.899055
103	6	0	3.353925	-5.494400	0.083250
104	1	0	-3.950384	-4.889282	-1.362464
105	1	0	0.177694	-5.710783	-2.202975
106	1	0	5.053227	-4.355072	0.758977
107	1	0	1.466305	-6.353407	-0.452831
108	1	0	-2.218408	-6.092932	-2.685804
109	1	0	3.873864	-6.447228	0.090616

110	8	0	0.355480	-0.623996	2.342738
111	6	0	-0.369995	-0.940048	3.531187
112	1	0	-1.400337	-1.183490	3.243877
113	6	0	0.259058	-2.167203	4.182230
114	6	0	-0.387665	0.281622	4.442130
115	1	0	1.285883	-1.956581	4.499529
116	1	0	-0.800948	1.144713	3.913045
117	1	0	-1.002111	0.092321	5.329601
118	1	0	0.624176	0.535139	4.774572
119	1	0	-0.314981	-2.474749	5.063545
120	1	0	0.275771	-2.995201	3.469783
121	6	0	-3.551672	-3.025815	0.567066
122	6	0	-3.539604	-2.905112	1.961155
123	6	0	-4.519414	-2.317678	-0.160780
124	6	0	-4.469264	-2.099346	2.625441
125	6	0	-5.441754	-1.482861	0.473995
126	6	0	-5.409301	-1.391675	1.870295
127	1	0	-4.515130	-2.379692	-1.244768
128	6	0	-4.443973	-1.989361	4.130453
129	6	0	-6.387928	-0.625314	-0.326002
130	1	0	-6.416199	-0.932217	-1.375449
131	1	0	-4.840649	-2.895125	4.605303
132	1	0	0.847797	1.444998	-2.520128
133	1	0	-2.781651	-3.430615	2.531169
134	1	0	-7.409414	-0.667922	0.067539
135	1	0	-6.069828	0.423074	-0.293431
136	1	0	-5.045736	-1.145902	4.481827
137	1	0	-3.422905	-1.856563	4.503696
138	1	0	-6.120351	-0.742939	2.376997
139	1	0	4.224196	1.570168	3.985498
140	1	0	2.622524	0.958617	3.539054
141	1	0	2.522810	-1.342390	2.352684
142	6	0	7.457636	-0.191889	0.516629
143	1	0	6.110628	0.994317	2.567470
144	1	0	7.384922	0.616174	-0.223157
145	1	0	7.926595	-1.045886	0.019134
146	1	0	8.133636	0.155265	1.304329

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d-II-COM-*re*

Zero-point correction = (a.u.)

Thermal correction to Gibbs Free Energy = (a.u.)
Sum of electronic and zero-point Energies = (a.u.)
Sum of electronic and thermal Free Energies = (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.048745	1.728167	-1.754191
2	8	0	-0.089045	1.464768	-1.028372
3	6	0	-2.304606	0.949131	-1.803541
4	8	0	-1.028093	2.734783	-2.605403
5	6	0	-3.532391	1.496120	-1.933518
6	6	0	-3.863851	2.905559	-1.733604
7	6	0	-4.901058	3.503374	-2.466587
8	6	0	-3.208136	3.651260	-0.735390
9	6	0	-5.231567	4.839351	-2.252414
10	6	0	-3.551893	4.981068	-0.515967
11	6	0	-4.554924	5.581746	-1.281365
12	1	0	-4.366809	0.820013	-2.090762
13	1	0	-5.430337	2.920250	-3.213861
14	1	0	-2.467530	3.165833	-0.107522
15	1	0	-6.021150	5.300814	-2.837423
16	1	0	-3.045099	5.542135	0.263230
17	1	0	-4.822281	6.619883	-1.108948
18	6	0	0.124741	3.620170	-2.535779
19	6	0	-0.122237	4.741095	-3.518610
20	1	0	1.018703	3.038449	-2.771188
21	6	0	-2.171359	-0.508200	-1.592236
22	8	0	-1.389278	-1.012138	-0.776592
23	8	0	-3.007770	-1.215626	-2.319859
24	6	0	-2.885415	-2.663251	-2.276242
25	6	0	-3.993676	-3.225874	-3.134582
26	1	0	-2.955922	-2.990511	-1.238522
27	1	0	0.205795	3.981090	-1.507573
28	1	0	-1.897205	-2.895386	-2.675873
29	1	0	-3.965827	-4.319264	-3.093234
30	1	0	-4.970797	-2.889396	-2.780929
31	1	0	-3.874364	-2.916168	-4.176584
32	1	0	0.715321	5.445124	-3.487429
33	1	0	-0.210219	4.356144	-4.538286
34	1	0	-1.037669	5.284766	-3.267548

35	8	0	1.345275	-0.666895	-0.295656
36	6	0	2.361457	-1.565144	0.012913
37	6	0	1.759699	-2.984861	-0.120352
38	6	0	3.580031	-1.259492	-0.846070
39	7	0	1.240715	-3.286623	-1.506815
40	6	0	2.590405	-4.197790	0.333335
41	6	0	4.909732	-1.612136	-0.460213
42	6	0	3.402933	-0.603366	-2.046144
43	6	0	2.292212	-3.862401	-2.414771
44	6	0	0.121553	-4.272864	-1.357639
45	6	0	2.160285	-5.432929	-0.483309
46	6	0	5.965045	-1.319539	-1.386705
47	6	0	4.515502	-0.361635	-2.881208
48	6	0	2.702185	-5.259112	-1.911162
49	6	0	0.614082	-5.527172	-0.577713
50	7	0	5.752974	-0.713259	-2.590652
51	1	0	2.648421	-1.478843	1.071576
52	1	0	0.860894	-2.915862	0.494242
53	1	0	2.443376	-4.350810	1.405717
54	1	0	3.657471	-4.031284	0.174158
55	6	0	5.256528	-2.199777	0.786936
56	1	0	2.409774	-0.301520	-2.353893
57	1	0	3.123675	-3.163457	-2.419846
58	1	0	1.856124	-3.866634	-3.414539
59	1	0	-0.215793	-4.525512	-2.363892
60	1	0	-0.685131	-3.755564	-0.839360
61	1	0	2.554131	-6.344796	-0.028222
62	6	0	7.303047	-1.649908	-1.045170
63	1	0	4.364532	0.147504	-3.830938
64	1	0	2.304527	-6.042806	-2.563263
65	1	0	3.791902	-5.347510	-1.919573
66	1	0	0.373773	-6.417042	-1.168971
67	6	0	-0.049557	-5.662372	0.764424
68	7	0	0.263695	-1.541368	-3.248062
69	6	0	-0.110382	-0.573021	-3.805379
70	1	0	0.837411	-2.430983	-2.048420
71	6	0	7.597683	-2.239408	0.162596
72	6	0	6.563251	-2.511375	1.087943
73	1	0	8.624489	-2.486730	0.414307
74	1	0	8.074025	-1.415519	-1.771919
75	1	0	6.804659	-2.951127	2.050769

76	1	0	4.486670	-2.374403	1.528068
77	6	0	-0.728535	-6.736320	1.165261
78	1	0	-0.857166	-7.604540	0.522550
79	1	0	-1.175799	-6.791841	2.153626
80	1	0	0.045928	-4.814486	1.438576
81	22	0	-0.083750	0.046019	0.644568
82	8	0	0.829074	1.318954	1.617385
83	8	0	-1.774029	1.030204	0.987456
84	6	0	0.599534	2.566392	2.043697
85	6	0	-2.223251	1.081322	2.243057
86	6	0	-0.546657	2.892625	2.806505
87	6	0	1.572109	3.550920	1.752797
88	6	0	-1.578023	1.897859	3.207090
89	6	0	-3.370854	0.341717	2.615976
90	6	0	1.361007	4.867877	2.171647
91	6	0	-0.710622	4.226130	3.214794
92	6	0	-3.759126	0.299456	3.959230
93	6	0	-2.000303	1.834688	4.541590
94	6	0	0.220979	5.210937	2.896864
95	6	0	-3.060488	1.016905	4.930483
96	1	0	2.110424	5.616977	1.934478
97	1	0	-1.600445	4.484284	3.780811
98	1	0	-4.629493	-0.289228	4.235313
99	1	0	-1.480544	2.437831	5.280674
100	1	0	0.063719	6.235717	3.218617
101	1	0	-3.363180	0.969630	5.971757
102	8	0	-0.201139	-1.210864	1.924153
103	6	0	-0.137586	-1.456631	3.323778
104	1	0	-1.080329	-1.102443	3.761305
105	6	0	-0.012536	-2.960091	3.551542
106	6	0	1.013307	-0.694043	3.971496
107	1	0	0.948272	-3.325289	3.171304
108	1	0	0.891424	0.380101	3.846349
109	1	0	1.048240	-0.919190	5.042774
110	1	0	1.969183	-0.983441	3.522972
111	1	0	-0.063898	-3.193724	4.620008
112	1	0	-0.815034	-3.498595	3.043473
113	6	0	2.800139	3.190743	0.992799
114	6	0	3.786102	2.288180	1.552893
115	6	0	3.023416	3.750394	-0.231159
116	6	0	4.961746	1.968324	0.809322

117	6	0	4.175446	3.440475	-1.020922
118	6	0	5.156519	2.542351	-0.513623
119	6	0	3.624169	1.744089	2.847320
120	1	0	2.293476	4.440382	-0.642486
121	6	0	5.912120	1.103929	1.398111
122	6	0	4.343552	4.008146	-2.304284
123	6	0	6.275059	2.252018	-1.325374
124	6	0	4.573422	0.906259	3.397942
125	6	0	5.726974	0.582664	2.663839
126	6	0	5.446117	3.701538	-3.077213
127	6	0	6.418397	2.815671	-2.579747
128	1	0	3.584641	4.692201	-2.674577
129	1	0	7.030056	1.557331	-0.980051
130	1	0	7.280479	2.558733	-3.187092
131	1	0	5.561705	4.138927	-4.064308
132	1	0	6.474537	-0.081566	3.085110
133	1	0	4.429561	0.505376	4.396945
134	1	0	6.804639	0.829894	0.849631
135	1	0	2.741035	2.005385	3.416358
136	6	0	-4.239012	-0.271151	1.565716
137	6	0	-4.272184	-1.694971	1.319330
138	6	0	-5.068215	0.548214	0.855072
139	6	0	-5.193619	-2.239851	0.373019
140	6	0	-5.997796	0.049785	-0.111091
141	6	0	-6.082717	-1.350225	-0.356154
142	6	0	-3.389532	-2.563879	1.999331
143	1	0	-5.037356	1.618940	1.031032
144	6	0	-5.190572	-3.639627	0.167686
145	6	0	-6.834759	0.938383	-0.826606
146	6	0	-7.022852	-1.801855	-1.311718
147	6	0	-3.399013	-3.923775	1.763304
148	6	0	-4.310445	-4.466524	0.840048
149	6	0	-7.730290	0.468486	-1.766067
150	6	0	-7.825455	-0.915328	-2.005961
151	1	0	-2.696386	-2.131565	2.707484
152	1	0	-2.707212	-4.575661	2.285963
153	1	0	-4.321140	-5.535952	0.652697
154	1	0	-5.882128	-4.080317	-0.540316
155	1	0	-7.126540	-2.862180	-1.510767
156	1	0	-8.534159	-1.290687	-2.737659
157	1	0	-8.362836	1.160854	-2.313129

158	1	0	-6.749828	2.002413	-0.629103

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d-III-COM-*re*

Zero-point correction = 1.28757 (a.u.)

Thermal correction to Gibbs Free Energy = 1.18661 (a.u.)

Sum of electronic and zero-point Energies = -4590.83712 (a.u.)

Sum of electronic and thermal Free Energies = -4590.93767 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.001074	-0.652880	-0.600847
2	6	0	-1.176038	-2.026233	-0.758827
3	6	0	-2.559003	-2.216778	-1.405015
4	6	0	0.011803	-2.666641	-1.461916
5	7	0	-2.739864	-1.443349	-2.691903
6	6	0	-3.059820	-3.648115	-1.649860
7	6	0	0.497205	-3.957610	-1.091122
8	6	0	0.692777	-1.972135	-2.440081
9	6	0	-2.295275	-2.208561	-3.907742
10	6	0	-4.195380	-1.123466	-2.825758
11	6	0	-4.045389	-3.627710	-2.838123
12	6	0	1.648595	-4.459370	-1.784158
13	6	0	1.802866	-2.568844	-3.074270
14	6	0	-0.059537	-4.752284	-0.050495
15	6	0	-3.225731	-3.418152	-4.122115
16	6	0	-5.032642	-2.436474	-2.713939
17	7	0	2.277955	-3.763798	-2.776202
18	6	0	2.187229	-5.721895	-1.421499
19	6	0	0.491531	-5.968271	0.283143
20	6	0	1.623148	-6.461023	-0.408233
21	1	0	-1.280786	-2.516481	0.213382
22	1	0	-3.220918	-1.709615	-0.702167
23	1	0	-3.524863	-4.026385	-0.736620
24	1	0	-2.226775	-4.317457	-1.884678
25	1	0	0.382919	-0.970193	-2.712868
26	1	0	-1.266822	-2.510146	-3.735314
27	1	0	-2.301608	-1.496113	-4.733320
28	1	0	-4.328275	-0.635091	-3.792278
29	1	0	-4.439115	-0.401427	-2.046926

30	1	0	-4.606720	-4.563956	-2.886625
31	1	0	2.323862	-2.024305	-3.860338
32	1	0	-0.917890	-4.391683	0.501836
33	1	0	-3.892371	-3.254809	-4.974658
34	1	0	-2.627191	-4.306606	-4.340821
35	1	0	3.057979	-6.069446	-1.967881
36	1	0	0.059971	-6.550496	1.091423
37	1	0	2.047773	-7.420880	-0.130678
38	6	0	-5.868470	-2.493262	-1.463821
39	1	0	-5.337210	-2.609766	-0.520676
40	6	0	-7.198786	-2.408182	-1.445281
41	1	0	-7.758071	-2.448279	-0.515125
42	1	0	-7.776993	-2.296237	-2.359936
43	1	0	-5.711526	-2.471212	-3.572094
44	22	0	0.099772	0.191879	0.702414
45	8	0	-1.105054	-0.023222	2.139149
46	8	0	0.954263	-1.409252	1.078549
47	6	0	-1.889042	-1.090433	2.325954
48	6	0	1.188075	-2.022670	2.248788
49	6	0	-1.318407	-2.334026	2.707686
50	6	0	-3.293068	-0.968703	2.171893
51	6	0	0.121563	-2.481527	3.062216
52	6	0	2.526492	-2.238219	2.638654
53	6	0	-4.091675	-2.115383	2.303150
54	6	0	-2.160066	-3.449908	2.823691
55	6	0	2.795330	-2.916660	3.831804
56	6	0	0.440262	-3.152701	4.252479
57	6	0	3.638993	-1.736250	1.784166
58	6	0	-3.942355	0.324537	1.823031
59	6	0	-3.533778	-3.355220	2.604570
60	6	0	1.758819	-3.376653	4.639835
61	6	0	4.469347	-0.641593	2.242784
62	6	0	3.882778	-2.305338	0.568296
63	6	0	-3.724241	1.540630	2.584930
64	6	0	-4.820915	0.352488	0.775115
65	6	0	5.557923	-0.187436	1.437694
66	6	0	4.970006	-1.890159	-0.264077
67	6	0	-4.360003	2.755980	2.183721
68	6	0	-5.515614	1.533398	0.369468
69	6	0	5.832529	-0.841085	0.167655
70	6	0	-5.280163	2.756984	1.056187

71	1	0	-5.166466	-2.015128	2.185500
72	1	0	-1.718046	-4.405759	3.087416
73	1	0	3.829482	-3.073897	4.123285
74	1	0	-0.372517	-3.489595	4.888662
75	1	0	-4.165646	-4.232413	2.701435
76	1	0	1.974575	-3.898251	5.566918
77	6	0	4.209687	0.008599	3.472909
78	1	0	3.248680	-3.112651	0.217868
79	6	0	-2.918835	1.547614	3.746892
80	1	0	-5.007050	-0.553421	0.211845
81	6	0	6.331873	0.898810	1.907517
82	6	0	5.205933	-2.523671	-1.507645
83	6	0	-4.086412	3.932712	2.919558
84	6	0	-6.421882	1.497996	-0.716893
85	6	0	6.917193	-0.484559	-0.667288
86	6	0	-5.968375	3.908922	0.610791
87	6	0	-2.687965	2.708349	4.456475
88	6	0	-3.259725	3.917374	4.025654
89	6	0	-7.082823	2.639165	-1.125231
90	6	0	-6.849274	3.854629	-0.454481
91	6	0	4.988271	1.063541	3.906229
92	6	0	6.059664	1.513003	3.114628
93	6	0	6.274736	-2.153056	-2.299275
94	6	0	7.139954	-1.128516	-1.870452
95	1	0	3.373973	-0.329158	4.073072
96	1	0	4.767168	1.550154	4.851269
97	1	0	6.671819	2.345978	3.446920
98	1	0	7.156264	1.269608	1.310058
99	1	0	7.599460	0.301296	-0.364860
100	1	0	7.984924	-0.837873	-2.487623
101	1	0	6.447022	-2.650247	-3.249188
102	1	0	4.523369	-3.300254	-1.837008
103	1	0	-6.597640	0.548965	-1.215506
104	1	0	-5.815701	4.858970	1.108862
105	1	0	-7.365196	4.755686	-0.771730
106	1	0	-7.779843	2.601549	-1.956805
107	1	0	-3.069436	4.836494	4.571674
108	1	0	-2.061913	2.685330	5.342578
109	1	0	-4.540652	4.870409	2.622242
110	1	0	-2.476855	0.619761	4.082604
111	8	0	1.058017	1.433719	1.613210

112	6	0	1.070419	2.620665	2.365511
113	6	0	0.917352	2.269724	3.844228
114	6	0	2.355461	3.396162	2.080501
115	1	0	0.205207	3.230561	2.056914
116	1	0	0.818874	3.174256	4.454845
117	1	0	1.792754	1.709816	4.187347
118	1	0	0.031313	1.648267	3.983139
119	1	0	2.371528	4.341145	2.635891
120	1	0	2.444056	3.621610	1.014695
121	1	0	3.226996	2.804423	2.376136
122	6	0	1.666531	1.763477	-1.523134
123	6	0	0.827206	2.978426	-1.395940
124	8	0	2.739258	1.914329	-2.267617
125	6	0	1.239850	4.265130	-1.496399
126	6	0	2.533260	4.865898	-1.846163
127	6	0	3.234221	4.559300	-3.023354
128	6	0	3.031459	5.871796	-0.998730
129	6	0	4.422505	5.221623	-3.321807
130	6	0	4.235792	6.507339	-1.284457
131	6	0	4.934826	6.183177	-2.448889
132	1	0	0.488071	4.998418	-1.212085
133	1	0	2.831583	3.822287	-3.704310
134	1	0	2.477092	6.135158	-0.102742
135	1	0	4.949761	4.985690	-4.241038
136	1	0	4.621333	7.262893	-0.607153
137	1	0	5.867154	6.688694	-2.681452
138	6	0	3.655789	0.779786	-2.359187
139	6	0	4.667812	1.120403	-3.427104
140	1	0	4.176276	1.291948	-4.389358
141	1	0	5.240512	2.012427	-3.158541
142	1	0	5.361973	0.284287	-3.535001
143	1	0	3.074783	-0.110647	-2.599023
144	1	0	4.112289	0.637866	-1.378362
145	6	0	-0.581709	2.754744	-0.967110
146	8	0	-0.947208	1.894291	-0.166509
147	8	0	-1.423053	3.615140	-1.503914
148	6	0	-2.847816	3.387249	-1.271413
149	6	0	-3.584615	3.884764	-2.492339
150	1	0	-3.119987	3.922199	-0.359453
151	1	0	-2.995379	2.320703	-1.110947
152	1	0	-3.257804	3.326945	-3.373642

153	1	0	-4.656888	3.725993	-2.349145
154	1	0	-3.410249	4.951648	-2.661439
155	8	0	1.419119	0.693429	-0.960896
156	7	0	-1.519699	0.832302	-3.330793
157	6	0	-0.525640	1.351011	-3.694809
158	1	0	-2.203814	-0.503214	-2.714476

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m-I-COM-*re*

Zero-point correction = 1.39505 (a.u.)

Thermal correction to Gibbs Free Energy = 1.28858 (a.u.)

Sum of electronic and zero-point Energies = -4785.12641 (a.u.)

Sum of electronic and thermal Free Energies = -4785.23287 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.221614	3.261311	3.768071
2	7	0	-1.627410	3.216057	2.754489
3	22	0	0.357794	-0.574146	-0.377579
4	8	0	0.122770	1.185501	0.114597
5	8	0	1.058819	-1.336480	1.135018
6	8	0	-0.584918	-0.505702	-2.063178
7	8	0	1.945040	-0.288338	-1.282205
8	6	0	1.029549	2.248035	-0.090062
9	6	0	2.246398	-2.022569	1.508457
10	6	0	-0.602132	0.598096	-2.808110
11	6	0	2.414284	-0.430107	-2.533919
12	6	0	0.239609	3.536516	-0.434620
13	6	0	1.965838	2.360576	1.098552
14	6	0	0.528512	0.977008	-3.573686
15	6	0	-1.788044	1.365520	-2.865015
16	6	0	1.753153	0.134877	-3.656216
17	6	0	3.635741	-1.124491	-2.704851
18	6	0	1.970314	-3.502241	1.763467
19	6	0	2.849568	-1.346437	2.735242
20	7	0	-0.432309	4.225473	0.710229
21	6	0	1.025489	4.584880	-1.258459
22	6	0	3.327028	2.777382	0.976220
23	6	0	1.485089	2.083945	2.360624
24	6	0	-1.843349	2.491692	-3.687471

25	6	0	0.440962	2.136562	-4.362457
26	6	0	4.158166	-1.304512	-3.989028
27	6	0	2.317629	-0.078110	-4.925384
28	6	0	4.384208	-1.610469	-1.513205
29	6	0	-2.976264	0.949395	-2.063180
30	6	0	0.470681	5.165426	1.440700
31	6	0	-1.553899	5.018301	0.139963
32	6	0	0.504984	5.992640	-0.907530
33	6	0	4.066143	2.988739	2.188605
34	6	0	2.303514	2.309622	3.486620
35	6	0	3.997393	2.982277	-0.262354
36	6	0	-0.728077	2.890205	-4.428684
37	6	0	3.498982	-0.791139	-5.102443
38	6	0	4.560478	-3.024220	-1.259870
39	6	0	4.899017	-0.701187	-0.635660
40	6	0	-3.973568	0.076583	-2.643873
41	6	0	-3.129002	1.384012	-0.780811
42	6	0	0.963261	6.308250	0.522456
43	6	0	-1.045532	6.045833	-0.923845
44	7	0	3.540638	2.765015	3.428160
45	6	0	5.406955	3.450803	2.115981
46	6	0	5.305383	3.412198	-0.298922
47	6	0	5.263464	-3.455889	-0.092364
48	6	0	5.595504	-1.088650	0.549197
49	6	0	-5.140669	-0.271031	-1.898781
50	6	0	-4.291499	1.076860	-0.004724
51	6	0	6.013204	3.665628	0.900065
52	6	0	5.783641	-2.469061	0.840692
53	6	0	-5.326960	0.276588	-0.564542
54	1	0	1.614586	2.027912	-0.988795
55	1	0	2.952187	-1.938118	0.678810
56	1	0	-0.574325	3.159577	-1.056347
57	1	0	1.603322	-3.996596	0.861156
58	1	0	1.235162	-3.623883	2.566523
59	1	0	2.892456	-4.009367	2.064457
60	1	0	3.806394	-1.807315	2.996401
61	1	0	2.177124	-1.442749	3.594974
62	1	0	3.021136	-0.286657	2.543182
63	1	0	0.919245	4.358229	-2.322194
64	1	0	2.093648	4.550753	-1.027778
65	1	0	0.473788	1.724422	2.489782

66	1	0	-2.767014	3.061095	-3.734311
67	1	0	1.311513	2.443910	-4.933909
68	1	0	5.093186	-1.844787	-4.102059
69	1	0	1.798892	0.321753	-5.790671
70	1	0	1.300772	4.592585	1.841922
71	1	0	-0.101201	5.540873	2.293343
72	1	0	-2.054234	5.523508	0.970313
73	1	0	-2.268592	4.316984	-0.297756
74	1	0	0.900859	6.728709	-1.612790
75	1	0	1.901176	2.122160	4.480211
76	1	0	3.480261	2.780211	-1.192413
77	1	0	-0.770978	3.779781	-5.048899
78	1	0	3.903110	-0.939896	-6.098762
79	6	0	4.026881	-3.997985	-2.136854
80	1	0	4.759166	0.358689	-0.817400
81	6	0	-3.796151	-0.467751	-3.937230
82	1	0	-2.343552	1.964172	-0.311298
83	1	0	0.561783	7.274223	0.846283
84	1	0	2.054768	6.377992	0.561624
85	1	0	5.928860	3.613589	3.053300
86	1	0	5.799970	3.550909	-1.255146
87	6	0	6.064899	-0.107697	1.452012
88	6	0	-6.072117	-1.154540	-2.488910
89	6	0	-4.427774	1.584625	1.306393
90	1	0	7.041310	4.011131	0.855317
91	6	0	6.445826	-2.807815	2.043663
92	6	0	-6.489841	0.060183	0.210066
93	6	0	-1.618773	5.783343	-2.284783
94	1	0	-1.413710	4.801600	-2.703255
95	6	0	-2.339121	6.654487	-2.990390
96	1	0	-2.725524	6.407120	-3.975435
97	1	0	-2.573034	7.646657	-2.609635
98	1	0	-1.344300	7.053037	-0.612097
99	6	0	-5.569215	1.343523	2.044741
100	6	0	-6.613047	0.584457	1.484157
101	6	0	-4.723919	-1.331756	-4.484460
102	6	0	-5.872629	-1.677994	-3.752077
103	1	0	-3.617816	2.167169	1.728822
104	1	0	-5.659894	1.747626	3.048442
105	1	0	-7.522444	0.410302	2.051620
106	1	0	-7.313654	-0.512545	-0.199637

107	1	0	-6.962312	-1.440559	-1.940680
108	1	0	-6.603232	-2.360682	-4.175503
109	1	0	-4.564208	-1.745322	-5.475699
110	1	0	-2.905439	-0.200567	-4.494399
111	6	0	6.700900	-0.468562	2.621182
112	6	0	6.892510	-1.831849	2.916196
113	6	0	4.183569	-5.348193	-1.893335
114	6	0	4.883783	-5.775139	-0.751790
115	1	0	3.481854	-3.663830	-3.011308
116	1	0	3.765229	-6.076568	-2.581333
117	1	0	5.012511	-6.835424	-0.556190
118	1	0	6.603568	-3.848409	2.302202
119	1	0	7.391734	-2.121586	3.835931
120	1	0	7.044279	0.294279	3.312996
121	1	0	5.902854	0.936979	1.213130
122	6	0	5.407510	-4.845700	0.125944
123	1	0	5.942207	-5.198324	0.999983
124	6	0	-2.054910	-2.057029	1.138745
125	8	0	-1.611191	-1.122425	0.481767
126	6	0	-3.354667	-1.951396	1.863213
127	8	0	-1.361301	-3.191720	1.197612
128	6	0	-3.531522	-1.258639	3.010885
129	6	0	-2.566069	-0.602161	3.879805
130	6	0	-3.082277	0.034405	5.025529
131	6	0	-1.169415	-0.600063	3.682337
132	6	0	-2.243706	0.648848	5.947709
133	6	0	-0.335926	0.008635	4.613071
134	6	0	-0.864457	0.632895	5.745519
135	1	0	-4.557078	-1.224344	3.364596
136	1	0	-4.156654	0.044738	5.181734
137	1	0	-0.703591	-1.056679	2.818306
138	1	0	-2.664969	1.144725	6.815699
139	1	0	0.734336	-0.000114	4.444864
140	1	0	-0.203755	1.110408	6.462354
141	6	0	-1.741206	-4.317332	2.046229
142	6	0	-2.100318	-5.507570	1.184812
143	1	0	-2.978982	-5.294081	0.573492
144	1	0	-1.266696	-5.783521	0.532611
145	1	0	-2.318692	-6.362782	1.832665
146	1	0	-2.558553	-4.012421	2.700659
147	1	0	-0.857553	-4.508487	2.657688

148	6	0	-4.450683	-2.665764	1.176248
149	8	0	-5.603856	-2.665503	1.860398
150	8	0	-4.294070	-3.238016	0.107704
151	6	0	-6.723346	-3.308484	1.204677
152	6	0	-7.946529	-3.070822	2.060678
153	1	0	-6.498461	-4.374026	1.095720
154	1	0	-6.829914	-2.885891	0.203048
155	1	0	-8.145181	-2.001112	2.167752
156	1	0	-8.817879	-3.540405	1.593739
157	1	0	-7.819839	-3.500275	3.058853
158	8	0	0.295937	-2.763795	-1.024140
159	6	0	-0.244408	-3.339058	-2.246827
160	6	0	0.321635	-4.741849	-2.417547
161	6	0	-1.765683	-3.309627	-2.242771
162	1	0	-0.087493	-3.221731	-0.258448
163	1	0	0.135162	-2.680033	-3.028689
164	1	0	0.015186	-5.159690	-3.382191
165	1	0	-0.049613	-5.412853	-1.632879
166	1	0	1.412001	-4.731288	-2.369661
167	1	0	-2.148257	-3.662333	-3.206198
168	1	0	-2.127979	-2.296239	-2.082416
169	1	0	-2.176500	-3.958666	-1.464319
170	1	0	-1.068272	3.487935	1.801932

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m-II-COM-*re*

Zero-point correction = 1.39680 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29067 (a.u.)

Sum of electronic and zero-point Energies = -4785.12341 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22954 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.088816	-0.564578	-0.525247
2	6	0	-2.210220	-0.765643	-1.959487
3	1	0	-1.215838	-1.095201	-2.256944
4	6	0	-3.260360	-1.834753	-2.227982
5	6	0	-2.516111	0.536806	-2.677551
6	1	0	-4.259439	-1.462197	-1.991811
7	1	0	-1.717117	1.253522	-2.509710

8	1	0	-2.580256	0.353823	-3.753695
9	1	0	-3.471118	0.956430	-2.340424
10	1	0	-3.251714	-2.109488	-3.288122
11	1	0	-3.085905	-2.734399	-1.633215
12	1	0	-2.824307	-0.037833	-0.166239
13	8	0	0.738060	-0.930957	-0.430941
14	6	0	1.444792	-2.131676	-0.289049
15	6	0	0.695511	-3.246264	-1.067702
16	6	0	2.896378	-1.935357	-0.689266
17	7	0	0.817802	-3.183755	-2.571361
18	6	0	0.986650	-4.700461	-0.648123
19	6	0	3.957893	-2.720738	-0.140913
20	6	0	3.208149	-0.999529	-1.652263
21	6	0	2.037181	-3.893912	-3.084950
22	6	0	-0.391883	-3.843409	-3.164730
23	6	0	0.738380	-5.631608	-1.849716
24	6	0	5.266010	-2.547115	-0.701896
25	6	0	4.540453	-0.885512	-2.104890
26	6	0	1.883998	-5.411628	-2.852806
27	6	0	-0.591318	-5.259449	-2.553767
28	7	0	5.541139	-1.631995	-1.676921
29	1	0	1.403678	-2.465879	0.754973
30	1	0	-0.351845	-3.018413	-0.865991
31	1	0	0.351820	-4.958923	0.201667
32	1	0	2.022959	-4.817796	-0.326154
33	6	0	3.808055	-3.647441	0.927164
34	1	0	2.428633	-0.384234	-2.083166
35	1	0	2.897795	-3.486799	-2.563781
36	1	0	2.126016	-3.624088	-4.138729
37	1	0	-0.231534	-3.879202	-4.243165
38	1	0	-1.241602	-3.192531	-2.978541
39	1	0	0.703520	-6.673887	-1.522820
40	6	0	6.338773	-3.350140	-0.233242
41	1	0	4.776357	-0.154342	-2.873904
42	1	0	1.671503	-5.933805	-3.790973
43	1	0	2.819358	-5.817027	-2.457183
44	1	0	-0.750210	-5.966216	-3.374852
45	6	0	-1.787933	-5.328069	-1.641476
46	6	0	6.144329	-4.271383	0.769341
47	6	0	4.869170	-4.406593	1.366639
48	1	0	6.971172	-4.882081	1.119002

49	1	0	7.309524	-3.201399	-0.694745
50	1	0	4.729971	-5.104189	2.186739
51	1	0	2.848804	-3.743618	1.420049
52	6	0	-2.830222	-6.137669	-1.822135
53	1	0	-2.883577	-6.825223	-2.663512
54	1	0	-3.671817	-6.134221	-1.135784
55	1	0	-1.795977	-4.655306	-0.785346
56	22	0	-0.412638	-0.179996	0.841061
57	8	0	0.744714	0.622197	2.044294
58	8	0	-1.891349	0.897586	1.572158
59	6	0	0.727182	1.608049	2.948705
60	6	0	-2.325841	0.596641	2.797261
61	6	0	-0.348802	1.798417	3.854412
62	6	0	1.857066	2.460012	3.007206
63	6	0	-1.558485	0.934381	3.939506
64	6	0	-3.568934	-0.070105	2.956220
65	6	0	1.879835	3.523504	3.914361
66	6	0	-0.271761	2.875125	4.754880
67	6	0	-3.990552	-0.448009	4.235835
68	6	0	-2.012441	0.522509	5.201592
69	6	0	0.817642	3.738953	4.788789
70	6	0	-3.209553	-0.172850	5.357303
71	1	0	2.752618	4.168866	3.938126
72	1	0	-1.108068	3.039595	5.426827
73	1	0	-4.943189	-0.957373	4.346844
74	1	0	-1.406069	0.753365	6.072395
75	1	0	0.840359	4.565908	5.491498
76	1	0	-3.538549	-0.482466	6.344168
77	8	0	-0.696506	-1.690090	1.758159
78	6	0	-0.730893	-2.354240	3.011441
79	1	0	-1.603618	-1.978396	3.558672
80	6	0	-0.904975	-3.850334	2.767237
81	6	0	0.522994	-2.043521	3.823172
82	1	0	-0.004702	-4.274964	2.310584
83	1	0	0.593475	-0.977295	4.035258
84	1	0	0.495962	-2.585235	4.774654
85	1	0	1.422842	-2.344179	3.276705
86	1	0	-1.083772	-4.375637	3.711540
87	1	0	-1.752926	-4.035105	2.102704
88	6	0	3.021123	2.267470	2.101183
89	6	0	3.851024	1.081991	2.185833

90	6	0	3.383187	3.277037	1.254680
91	6	0	4.999072	0.957265	1.348197
92	6	0	4.519651	3.188324	0.389436
93	6	0	5.307911	2.002718	0.385986
94	6	0	3.586283	0.073123	3.140175
95	1	0	2.784175	4.181929	1.215673
96	6	0	5.835503	-0.168943	1.518597
97	6	0	4.850034	4.249359	-0.484130
98	6	0	6.361591	1.905083	-0.551955
99	6	0	4.422051	-1.015838	3.281437
100	6	0	5.561186	-1.132869	2.467751
101	6	0	5.907359	4.141415	-1.364922
102	6	0	6.656108	2.950854	-1.409299
103	1	0	4.239945	5.148138	-0.464415
104	1	0	6.936262	0.989573	-0.625497
105	1	0	7.467099	2.847684	-2.123714
106	1	0	6.145080	4.959588	-2.037535
107	1	0	6.221909	-1.985382	2.573620
108	1	0	4.204130	-1.775560	4.025854
109	1	0	6.720810	-0.278161	0.905306
110	1	0	2.721788	0.177388	3.782360
111	6	0	-4.430459	-0.303604	1.766545
112	6	0	-4.892929	-1.628425	1.401125
113	6	0	-4.791340	0.765887	0.991344
114	6	0	-5.786284	-1.793132	0.297644
115	6	0	-5.666228	0.641234	-0.131006
116	6	0	-6.203856	-0.631637	-0.472468
117	6	0	-4.434115	-2.779387	2.084927
118	1	0	-4.410166	1.752016	1.231928
119	6	0	-6.191113	-3.103312	-0.047837
120	6	0	-6.005481	1.780494	-0.899825
121	6	0	-7.087710	-0.703709	-1.574164
122	6	0	-4.840172	-4.046524	1.716163
123	6	0	-5.735297	-4.208624	0.644275
124	6	0	-6.864135	1.674971	-1.975008
125	6	0	-7.411494	0.421402	-2.309584
126	1	0	-3.739048	-2.652557	2.904282
127	1	0	-4.468274	-4.913505	2.253652
128	1	0	-6.064203	-5.201790	0.353367
129	1	0	-6.862440	-3.254951	-0.884565
130	1	0	-7.523951	-1.653833	-1.858600

131	1	0	-8.091503	0.335188	-3.151526
132	1	0	-7.121200	2.552699	-2.560538
133	1	0	-5.560160	2.732318	-0.628572
134	6	0	-0.470522	2.788026	-0.421101
135	8	0	-0.327296	1.572455	-0.513710
136	6	0	-0.959745	3.562281	-1.609771
137	8	0	-0.178009	3.388749	0.713240
138	6	0	-0.282401	3.656843	-2.779636
139	6	0	1.046261	3.199340	-3.146985
140	6	0	2.034606	2.781702	-2.235483
141	6	0	1.334793	3.148321	-4.525003
142	6	0	3.257921	2.316383	-2.697404
143	6	0	2.557585	2.674526	-4.983613
144	6	0	3.522752	2.257961	-4.067822
145	1	0	-0.840079	4.113818	-3.592019
146	1	0	1.869833	2.824120	-1.166785
147	1	0	0.573667	3.458609	-5.233844
148	1	0	4.006850	1.997621	-1.986102
149	1	0	2.752890	2.623815	-6.049627
150	1	0	4.483923	1.892188	-4.416422
151	6	0	-0.298568	4.822623	0.909901
152	6	0	-1.419501	5.114395	1.883842
153	1	0	-0.440403	5.314272	-0.055428
154	6	0	-2.381736	3.957138	-1.510974
155	8	0	-3.083663	3.688869	-0.546257
156	8	0	-2.830276	4.610580	-2.594822
157	6	0	-4.251350	4.892131	-2.630714
158	6	0	-4.520113	5.689680	-3.887367
159	1	0	-4.526192	5.441082	-1.725734
160	1	0	0.668668	5.125455	1.316356
161	1	0	-4.789556	3.939884	-2.628737
162	1	0	-4.236083	5.123672	-4.779255
163	1	0	-5.588001	5.920565	-3.952424
164	1	0	-3.964802	6.632175	-3.881007
165	1	0	-2.379155	4.796034	1.473733
166	1	0	-1.244427	4.595955	2.828775
167	1	0	-1.452716	6.191742	2.079075
168	7	0	0.657166	-0.971879	-3.913986
169	6	0	0.326606	-0.232475	-4.770469
170	1	0	0.813260	-2.150443	-3.007369

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m-III-COM-*re*

Zero-point correction = 1.39498 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29187 (a.u.)

Sum of electronic and zero-point Energies = -4785.11780 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22091 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.593791	0.491328	-1.843307
2	6	0	1.424762	1.135999	-3.140497
3	1	0	0.435808	1.594971	-3.078943
4	6	0	2.490656	2.206604	-3.317029
5	6	0	1.422782	0.108087	-4.260361
6	1	0	3.493560	1.771792	-3.268513
7	1	0	0.724318	-0.697263	-4.036547
8	1	0	1.120878	0.584336	-5.199122
9	1	0	2.418463	-0.314859	-4.407645
10	1	0	2.376200	2.691766	-4.292643
11	1	0	2.406099	2.978575	-2.548995
12	1	0	2.182505	-0.277489	-1.946715
13	22	0	-0.131410	-0.599785	-0.782286
14	8	0	0.964654	-2.039876	-1.511384
15	8	0	-1.309515	-1.780506	-0.000776
16	6	0	1.476593	-3.052554	-0.802429
17	6	0	-1.735529	-3.032044	-0.252369
18	6	0	0.643317	-4.035979	-0.223995
19	6	0	2.881140	-3.135877	-0.632486
20	6	0	-0.826017	-4.107763	-0.444794
21	6	0	-3.130574	-3.278616	-0.296098
22	6	0	3.426124	-4.145055	0.164338
23	6	0	1.234389	-5.039082	0.562730
24	6	0	-3.596292	-4.560484	-0.619922
25	6	0	-1.348021	-5.366858	-0.783267
26	6	0	2.606987	-5.094324	0.771240
27	6	0	-2.714674	-5.600244	-0.886057
28	1	0	4.502082	-4.177179	0.305402
29	1	0	0.588800	-5.772898	1.035493
30	1	0	-4.667568	-4.731155	-0.650879
31	1	0	-0.648319	-6.174786	-0.970043

32	1	0	3.034686	-5.861704	1.407500
33	1	0	-3.085838	-6.584933	-1.151716
34	8	0	-1.086084	-0.203343	-2.252202
35	6	0	-2.272158	-0.595625	-2.925564
36	1	0	-3.050991	-0.755510	-2.169843
37	6	0	-2.706762	0.534914	-3.853116
38	6	0	-2.033876	-1.899900	-3.680820
39	1	0	-1.975118	0.679668	-4.655408
40	1	0	-1.724844	-2.693533	-2.997853
41	1	0	-2.946467	-2.216423	-4.195217
42	1	0	-1.248419	-1.769596	-4.431741
43	1	0	-3.677501	0.309106	-4.306254
44	1	0	-2.796462	1.475575	-3.301795
45	6	0	3.781277	-2.131916	-1.262669
46	6	0	3.944912	-2.081580	-2.703583
47	6	0	4.513628	-1.286358	-0.477975
48	6	0	4.832632	-1.128405	-3.289406
49	6	0	5.414502	-0.316660	-1.023062
50	6	0	5.562604	-0.203915	-2.434621
51	6	0	3.252153	-2.984330	-3.544060
52	1	0	4.397746	-1.330504	0.599550
53	6	0	4.981465	-1.130320	-4.696510
54	6	0	6.137170	0.551653	-0.173609
55	6	0	6.410956	0.810136	-2.936687
56	6	0	3.417016	-2.958415	-4.913655
57	6	0	4.290639	-2.022034	-5.494681
58	6	0	6.965752	1.525281	-0.691533
59	6	0	7.095537	1.658853	-2.086015
60	1	0	6.008510	0.455225	0.899005
61	1	0	6.529883	0.937474	-4.006275
62	1	0	7.736419	2.431944	-2.499065
63	1	0	7.501435	2.194986	-0.026318
64	1	0	4.427603	-2.000195	-6.571572
65	1	0	2.876208	-3.661577	-5.539319
66	1	0	5.658691	-0.427018	-5.166218
67	1	0	2.588849	-3.709766	-3.089399
68	6	0	-4.143172	-2.253470	0.083281
69	6	0	-5.226267	-1.904860	-0.816859
70	6	0	-4.131306	-1.731337	1.345727
71	6	0	-6.291694	-1.068400	-0.362585
72	6	0	-5.176459	-0.891982	1.840029

73	6	0	-6.274191	-0.555288	0.997347
74	6	0	-5.243122	-2.362021	-2.157397
75	1	0	-3.319594	-1.982822	2.016018
76	6	0	-7.329291	-0.751861	-1.270191
77	6	0	-5.122173	-0.384164	3.159498
78	6	0	-7.272370	0.301012	1.515821
79	6	0	-6.265383	-2.025368	-3.021501
80	6	0	-7.323812	-1.217795	-2.570059
81	6	0	-6.117301	0.442580	3.640476
82	6	0	-7.198642	0.789663	2.807644
83	1	0	-4.429612	-2.986256	-2.502914
84	1	0	-6.251137	-2.386042	-4.045603
85	1	0	-8.134780	-0.954131	-3.242199
86	1	0	-8.148254	-0.121381	-0.947412
87	1	0	-8.111805	0.592673	0.896024
88	1	0	-7.979250	1.446534	3.179485
89	1	0	-6.062892	0.831162	4.652770
90	1	0	-4.266610	-0.634297	3.777495
91	8	0	-0.404654	0.985111	0.137257
92	6	0	-0.643878	2.284621	-0.322776
93	6	0	-2.172949	2.522200	-0.333674
94	6	0	0.182042	3.276575	0.479466
95	7	0	-2.825508	2.425615	1.003868
96	6	0	-2.674036	3.791879	-1.058835
97	6	0	0.693670	4.487517	-0.079014
98	6	0	0.490044	2.995788	1.793438
99	6	0	-2.809134	3.711725	1.755511
100	6	0	-4.239411	2.049959	0.758154
101	6	0	-3.974182	4.263830	-0.381411
102	6	0	1.422117	5.365197	0.791969
103	6	0	1.210617	3.931303	2.564896
104	6	0	-3.603608	4.809140	1.005843
105	6	0	-4.954937	3.080555	-0.171685
106	7	0	1.654757	5.085530	2.107331
107	1	0	-0.351231	2.366912	-1.376600
108	1	0	-2.536540	1.646558	-0.876601
109	1	0	-2.830059	3.575764	-2.120132
110	1	0	-1.942876	4.601833	-1.001561
111	6	0	0.571616	4.854766	-1.448742
112	1	0	0.170079	2.060848	2.232297
113	1	0	-1.773333	4.002997	1.904386

114	1	0	-3.231661	3.500597	2.741749
115	1	0	-4.740505	1.975833	1.723490
116	1	0	-4.235391	1.057206	0.311786
117	1	0	-4.457364	5.037541	-0.984726
118	6	0	1.959570	6.572936	0.274118
119	1	0	1.429175	3.703954	3.606455
120	1	0	-4.509578	5.084346	1.555897
121	1	0	-2.995110	5.713396	0.904748
122	1	0	-5.836563	3.473438	0.346957
123	6	0	-5.413681	2.456864	-1.458257
124	6	0	1.814678	6.897794	-1.054285
125	6	0	1.121226	6.024178	-1.924408
126	1	0	2.238148	7.819424	-1.441621
127	1	0	2.497174	7.213812	0.965247
128	1	0	1.025079	6.275945	-2.976065
129	1	0	0.051037	4.198942	-2.135767
130	6	0	-6.649780	2.547334	-1.947035
131	1	0	-7.431291	3.093735	-1.422693
132	1	0	-6.928959	2.072586	-2.882407
133	1	0	-4.669850	1.884621	-2.010861
134	6	0	1.514655	-1.313563	1.966838
135	8	0	1.475011	-0.765728	0.859553
136	6	0	2.594874	-1.031133	2.944991
137	8	0	0.530749	-2.147122	2.254565
138	6	0	3.366192	0.093048	3.034187
139	6	0	3.606675	1.313074	2.279366
140	6	0	3.192067	1.588793	0.961301
141	6	0	4.436960	2.259525	2.928526
142	6	0	3.609454	2.753596	0.328410
143	6	0	4.823413	3.434156	2.299796
144	6	0	4.413850	3.680342	0.987291
145	1	0	4.011956	0.055824	3.908160
146	1	0	2.573622	0.884543	0.433199
147	1	0	4.771743	2.058730	3.942327
148	1	0	3.302091	2.933513	-0.693016
149	1	0	5.445072	4.152117	2.824828
150	1	0	4.718108	4.591241	0.482205
151	6	0	0.236214	-2.746561	3.543277
152	6	0	-1.222926	-3.138606	3.520666
153	1	0	0.437537	-2.017175	4.332385
154	6	0	3.006456	-2.139058	3.864151

155	8	0	3.141116	-3.293024	3.504982
156	8	0	3.268100	-1.716857	5.115324
157	6	0	3.790497	-2.718616	6.024553
158	6	0	4.021694	-2.040258	7.356427
159	1	0	4.713072	-3.129547	5.603982
160	1	0	0.879231	-3.617515	3.662585
161	1	0	3.064385	-3.533380	6.098439
162	1	0	3.089612	-1.627853	7.753165
163	1	0	4.409894	-2.768085	8.075712
164	1	0	4.749430	-1.228510	7.264067
165	1	0	-1.848605	-2.249251	3.450200
166	1	0	-1.433282	-3.801798	2.677765
167	1	0	-1.467533	-3.665769	4.448711
168	7	0	-1.891529	0.777038	2.791472
169	6	0	-1.386610	0.245021	3.705913
170	1	0	-2.266512	1.423349	1.938425

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m-IV-COM-*re*

Zero-point correction = 1.39586 (a.u.)

Thermal correction to Gibbs Free Energy = 1.28848 (a.u.)

Sum of electronic and zero-point Energies = -4785.11548 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22286 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.318051	-1.659470	1.140185
2	6	0	-2.060013	-2.223106	2.197809
3	1	0	-2.893205	-1.542552	2.399805
4	6	0	-2.611088	-3.577477	1.763379
5	6	0	-1.199134	-2.317960	3.451248
6	1	0	-1.792762	-4.287104	1.600073
7	1	0	-0.766715	-1.346719	3.696879
8	1	0	-1.807456	-2.644058	4.301031
9	1	0	-0.396022	-3.042481	3.303681
10	1	0	-3.277108	-3.982949	2.531617
11	1	0	-3.176014	-3.482933	0.834679
12	22	0	-0.547306	-0.648736	-0.091524
13	8	0	-1.200455	0.971323	0.480913
14	6	0	-1.024901	2.233454	-0.124874

15	6	0	-2.329171	3.051847	0.018742
16	6	0	0.241962	2.883363	0.387118
17	7	0	-2.780817	3.332670	1.414243
18	6	0	-2.369332	4.361062	-0.802564
19	6	0	1.112221	3.620282	-0.472338
20	6	0	0.594032	2.754245	1.713909
21	6	0	-2.153342	4.550811	2.001205
22	6	0	-4.247086	3.561778	1.359176
23	6	0	-3.271065	5.374228	-0.069823
24	6	0	2.259130	4.243099	0.123013
25	6	0	1.729763	3.429624	2.202991
26	6	0	-2.535501	5.821006	1.201797
27	6	0	-4.607989	4.719876	0.370285
28	7	0	2.540867	4.157180	1.456538
29	1	0	-0.925430	2.101064	-1.202424
30	1	0	-3.082625	2.370245	-0.380657
31	1	0	-2.731194	4.147192	-1.810641
32	1	0	-1.369918	4.794170	-0.905261
33	6	0	0.945492	3.723510	-1.881916
34	1	0	-0.009620	2.151830	2.382251
35	1	0	-1.078133	4.403844	2.015522
36	1	0	-2.487207	4.604177	3.041346
37	1	0	-4.584111	3.790246	2.373842
38	1	0	-4.725855	2.627734	1.056715
39	1	0	-3.481999	6.231203	-0.715743
40	6	0	3.172515	4.952840	-0.700717
41	1	0	1.974538	3.357960	3.258807
42	1	0	-3.174543	6.483293	1.795277
43	1	0	-1.635535	6.385929	0.938985
44	1	0	-5.185582	5.478432	0.910537
45	6	0	-5.430672	4.238144	-0.788869
46	6	0	2.982405	5.024904	-2.060720
47	6	0	1.862060	4.398047	-2.655211
48	1	0	3.696957	5.553671	-2.683927
49	1	0	4.027559	5.413951	-0.217313
50	1	0	1.730070	4.436419	-3.731725
51	1	0	0.106288	3.239191	-2.363340
52	6	0	-6.630394	4.713297	-1.121421
53	1	0	-7.110000	5.506683	-0.551799
54	1	0	-7.180339	4.325632	-1.974591
55	1	0	-4.993005	3.439679	-1.383266

56	8	0	-1.736408	-0.980055	-1.508167
57	8	0	0.646573	0.231922	-1.383876
58	6	0	-2.399874	-0.010329	-2.152322
59	6	0	0.762686	0.328328	-2.703186
60	6	0	-1.753696	0.805050	-3.107984
61	6	0	-3.771759	0.160523	-1.868411
62	6	0	-0.355007	0.574471	-3.564307
63	6	0	2.055633	0.232922	-3.295302
64	6	0	-4.493332	1.160278	-2.524043
65	6	0	-2.510021	1.823150	-3.718324
66	6	0	2.211154	0.370415	-4.680740
67	6	0	-0.142672	0.665117	-4.949675
68	6	0	-3.860948	2.006140	-3.436848
69	6	0	1.121555	0.572650	-5.517806
70	1	0	-5.550508	1.274685	-2.304985
71	1	0	-2.017895	2.481615	-4.426911
72	1	0	3.211946	0.316892	-5.097221
73	1	0	-1.006425	0.806573	-5.591084
74	1	0	-4.417551	2.798520	-3.927090
75	1	0	1.253518	0.657406	-6.591570
76	6	0	-4.444924	-0.740396	-0.888821
77	6	0	-4.941774	-2.030088	-1.315601
78	6	0	-4.607487	-0.349781	0.406184
79	6	0	-5.638746	-2.867073	-0.392698
80	6	0	-5.304005	-1.153359	1.364591
81	6	0	-5.840330	-2.413112	0.975392
82	6	0	-4.730041	-2.486304	-2.637293
83	1	0	-4.171006	0.583305	0.742964
84	6	0	-6.088223	-4.128984	-0.845580
85	6	0	-5.443160	-0.713135	2.701283
86	6	0	-6.517166	-3.177156	1.953439
87	6	0	-5.177519	-3.726320	-3.046972
88	6	0	-5.863875	-4.554057	-2.141289
89	6	0	-6.097870	-1.487923	3.636897
90	6	0	-6.643732	-2.727496	3.254971
91	1	0	-4.997421	0.233487	2.987434
92	1	0	-6.944363	-4.137594	1.690324
93	1	0	-7.163568	-3.338786	3.986590
94	1	0	-6.185611	-1.145844	4.663326
95	1	0	-6.217415	-5.530942	-2.457306
96	1	0	-4.999104	-4.060066	-4.064715

97	1	0	-6.614468	-4.788131	-0.165272
98	1	0	-4.200410	-1.841934	-3.329374
99	6	0	3.294704	0.059911	-2.488185
100	6	0	4.234748	-1.001570	-2.809145
101	6	0	3.621667	0.967153	-1.520439
102	6	0	5.514331	-1.043729	-2.175000
103	6	0	4.895629	0.966346	-0.871522
104	6	0	5.866416	-0.021760	-1.203931
105	6	0	3.906373	-2.027037	-3.730159
106	1	0	2.917382	1.750692	-1.268865
107	6	0	6.399879	-2.095662	-2.507338
108	6	0	5.226218	1.977494	0.061308
109	6	0	7.128644	0.038245	-0.568982
110	6	0	4.790141	-3.046049	-4.028727
111	6	0	6.053436	-3.077566	-3.414767
112	6	0	6.471271	2.016193	0.656285
113	6	0	7.427377	1.033730	0.342558
114	1	0	2.934705	-2.005607	-4.206667
115	1	0	4.504138	-3.821077	-4.733160
116	1	0	6.754243	-3.873767	-3.646139
117	1	0	7.373972	-2.144645	-2.035500
118	1	0	7.889234	-0.697410	-0.802420
119	1	0	8.406541	1.060272	0.810723
120	1	0	6.714069	2.801233	1.365077
121	1	0	4.480676	2.728258	0.295996
122	6	0	2.218718	-1.388206	1.596861
123	8	0	1.228563	-0.706268	1.352365
124	6	0	2.482657	-1.901608	2.982754
125	8	0	3.028355	-1.717589	0.597198
126	6	0	2.909142	-1.197667	4.054205
127	6	0	3.428177	0.148937	4.217938
128	6	0	3.551837	0.613889	5.543689
129	6	0	3.862404	0.976634	3.167615
130	6	0	4.070968	1.873222	5.815913
131	6	0	4.397606	2.230010	3.446908
132	6	0	4.498225	2.684281	4.763377
133	1	0	2.876088	-1.775955	4.975100
134	1	0	3.228683	-0.028438	6.357389
135	1	0	3.803870	0.645614	2.136848
136	1	0	4.149096	2.217577	6.842178
137	1	0	4.705138	2.873023	2.634310

138	1	0	4.909124	3.668799	4.964324
139	6	0	4.260319	-2.472953	0.802399
140	6	0	4.244043	-3.686387	-0.098247
141	1	0	4.351793	-2.740238	1.855856
142	6	0	2.119786	-3.323988	3.259058
143	8	0	2.177947	-3.848611	4.354474
144	8	0	1.730447	-3.972124	2.146211
145	6	0	1.314514	-5.349444	2.350216
146	6	0	0.897663	-5.912377	1.012820
147	1	0	0.490315	-5.353201	3.068467
148	1	0	5.066092	-1.784908	0.546424
149	1	0	2.147937	-5.900706	2.794242
150	1	0	1.740869	-5.964458	0.318649
151	1	0	0.507713	-6.925652	1.150978
152	1	0	0.115569	-5.296384	0.566846
153	1	0	3.421330	-4.351094	0.170192
154	1	0	4.146346	-3.394654	-1.144955
155	1	0	5.187816	-4.228905	0.014266
156	7	0	-2.523092	1.542726	3.280559
157	6	0	-2.455814	0.869561	4.239501
158	1	0	-2.587393	2.245215	2.404158
159	8	0	0.569899	-2.495305	-0.849518
160	6	0	0.145254	-3.192202	-2.063034
161	1	0	1.475998	-2.171079	-0.981037
162	1	0	-0.027715	-2.430170	-2.829273
163	6	0	1.247279	-4.141699	-2.505497
164	6	0	-1.158081	-3.914145	-1.768261
165	1	0	1.413193	-4.921529	-1.757101
166	1	0	-1.903587	-3.230254	-1.368765
167	1	0	-1.549517	-4.336897	-2.699039
168	1	0	-1.003644	-4.735371	-1.063718
169	1	0	0.964585	-4.623603	-3.447073
170	1	0	2.189921	-3.615824	-2.675595

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m-V-COM-*re*

Zero-point correction = 1.39831 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29589 (a.u.)

Sum of electronic and zero-point Energies = -4785.10659 (a.u.)

Sum of electronic and thermal Free Energies = -4785.20901 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.523574	-1.356046	2.140101
2	6	0	0.142198	-2.001007	3.348853
3	1	0	0.419634	-1.312256	4.153929
4	6	0	-1.365607	-2.221613	3.399946
5	6	0	0.915574	-3.300750	3.535614
6	1	0	-1.664870	-2.972007	2.665205
7	1	0	1.992804	-3.128710	3.501201
8	1	0	0.670712	-3.733512	4.511919
9	1	0	0.659036	-4.025025	2.761332
10	1	0	-1.658077	-2.568432	4.396432
11	1	0	-1.891265	-1.288705	3.189516
12	8	0	1.388043	0.429840	0.206187
13	6	0	2.344517	1.057740	-0.584065
14	6	0	1.614409	1.951227	-1.627009
15	6	0	3.329043	1.812181	0.300619
16	7	0	0.967974	3.190497	-1.053453
17	6	0	2.387155	2.387674	-2.886725
18	6	0	4.637410	2.189175	-0.135170
19	6	0	2.914787	2.236927	1.544359
20	6	0	1.891057	4.377362	-0.999692
21	6	0	-0.208832	3.537137	-1.920541
22	6	0	1.798202	3.715477	-3.401595
23	6	0	5.377811	3.089324	0.701062
24	6	0	3.747142	3.080406	2.311455
25	6	0	2.233701	4.826139	-2.432414
26	6	0	0.247725	3.669061	-3.400374
27	7	0	4.922451	3.525456	1.912071
28	1	0	2.882670	0.302883	-1.175752
29	1	0	0.778898	1.320987	-1.924659
30	1	0	2.323001	1.593277	-3.635235
31	1	0	3.444780	2.545239	-2.675394
32	6	0	5.246301	1.740244	-1.337865
33	1	0	1.931646	1.967974	1.904663
34	1	0	2.772832	4.079333	-0.441495
35	1	0	1.366703	5.133879	-0.415310
36	1	0	-0.629783	4.460620	-1.525218
37	1	0	-0.954043	2.756600	-1.782996
38	1	0	2.154815	3.922851	-4.413488

39	6	0	6.641604	3.565711	0.263521
40	1	0	3.399500	3.425203	3.283693
41	1	0	1.727136	5.764114	-2.680191
42	1	0	3.309737	5.002615	-2.514011
43	1	0	-0.114620	4.625977	-3.789863
44	6	0	-0.292706	2.571178	-4.274711
45	6	0	7.173912	3.152974	-0.935238
46	6	0	6.477279	2.214839	-1.731572
47	1	0	8.140543	3.524607	-1.261742
48	1	0	7.164543	4.257596	0.915347
49	1	0	6.921797	1.852526	-2.653333
50	1	0	4.754213	0.987119	-1.939486
51	6	0	-0.940972	2.766641	-5.422120
52	1	0	-1.141863	3.766426	-5.800536
53	1	0	-1.295225	1.936761	-6.027099
54	1	0	-0.126380	1.553100	-3.928865
55	22	0	0.253368	-1.009753	0.417849
56	8	0	1.354646	-2.264697	-0.434224
57	8	0	-1.255546	-2.203719	0.236038
58	6	0	1.608440	-3.480611	0.090609
59	6	0	-1.618347	-3.325629	-0.371027
60	6	0	0.636797	-4.506358	0.081287
61	6	0	2.887685	-3.712668	0.637825
62	6	0	-0.706442	-4.409023	-0.558013
63	6	0	-2.968280	-3.479121	-0.814545
64	6	0	3.180943	-4.948549	1.218173
65	6	0	0.972365	-5.731046	0.689319
66	6	0	-3.345496	-4.652491	-1.484913
67	6	0	-1.127847	-5.527256	-1.293886
68	6	0	2.220804	-5.957178	1.258849
69	6	0	-2.429941	-5.658771	-1.762779
70	1	0	4.167571	-5.107016	1.642569
71	1	0	0.217300	-6.509122	0.730119
72	1	0	-4.381891	-4.774377	-1.780021
73	1	0	-0.409726	-6.319232	-1.480170
74	1	0	2.441878	-6.909471	1.730360
75	1	0	-2.732352	-6.546110	-2.309405
76	6	0	3.940958	-2.658751	0.596926
77	6	0	4.716974	-2.460161	-0.608766
78	6	0	4.230460	-1.926870	1.709544
79	6	0	5.835891	-1.574730	-0.596759

80	6	0	5.319409	-0.999484	1.753760
81	6	0	6.170275	-0.855999	0.622335
82	6	0	4.385023	-3.136247	-1.806381
83	1	0	3.626306	-2.046750	2.602338
84	6	0	6.565989	-1.405687	-1.796162
85	6	0	5.575299	-0.245670	2.921573
86	6	0	7.286107	0.002609	0.733944
87	6	0	5.110187	-2.939056	-2.964907
88	6	0	6.212285	-2.065616	-2.957989
89	6	0	6.654644	0.610971	2.989824
90	6	0	7.524350	0.721310	1.889609
91	1	0	4.900184	-0.351844	3.765920
92	1	0	7.966060	0.118917	-0.100168
93	1	0	8.378648	1.388260	1.940906
94	1	0	6.833424	1.198136	3.884834
95	1	0	6.787846	-1.908518	-3.865452
96	1	0	4.832685	-3.460726	-3.875873
97	1	0	7.413109	-0.731383	-1.814916
98	1	0	3.540597	-3.815686	-1.802145
99	6	0	-4.018596	-2.474108	-0.498885
100	6	0	-5.009107	-2.069035	-1.486967
101	6	0	-4.110580	-1.959890	0.766428
102	6	0	-6.102829	-1.227895	-1.103030
103	6	0	-5.176740	-1.107987	1.183933
104	6	0	-6.204909	-0.751907	0.266940
105	6	0	-4.874422	-2.407629	-2.857232
106	1	0	-3.364796	-2.230772	1.500926
107	6	0	-7.020220	-0.816931	-2.097952
108	6	0	-5.236234	-0.642279	2.519081
109	6	0	-7.257762	0.070738	0.731530
110	6	0	-5.777757	-1.973873	-3.807507
111	6	0	-6.871616	-1.181761	-3.421940
112	6	0	-6.276574	0.158040	2.943072
113	6	0	-7.294583	0.517220	2.039423
114	1	0	-4.027253	-3.004787	-3.166194
115	1	0	-5.636656	-2.242107	-4.850012
116	1	0	-7.590115	-0.842449	-4.161638
117	1	0	-7.854413	-0.181844	-1.825335
118	1	0	-8.062450	0.354421	0.063475
119	1	0	-8.116932	1.143002	2.372023
120	1	0	-6.318410	0.504116	3.971255

121	1	0	-4.444137	-0.928350	3.203522
122	6	0	-2.218152	1.187263	0.322062
123	8	0	-1.294968	0.540881	0.811154
124	6	0	-3.070561	2.102949	1.089112
125	8	0	-2.445060	1.016193	-0.999682
126	6	0	-3.199827	2.104505	2.445239
127	6	0	-2.442711	1.504770	3.536119
128	6	0	-3.142701	1.197274	4.721321
129	6	0	-1.039254	1.406452	3.528644
130	6	0	-2.468617	0.742796	5.847364
131	6	0	-0.366847	1.014136	4.682365
132	6	0	-1.073004	0.660822	5.832770
133	1	0	-4.014594	2.732904	2.795342
134	1	0	-4.220812	1.318657	4.744834
135	1	0	-0.493036	1.704548	2.647915
136	1	0	-3.022568	0.485824	6.744783
137	1	0	0.717955	0.985664	4.678522
138	1	0	-0.539032	0.340077	6.722263
139	6	0	-3.763466	1.046583	-1.641039
140	6	0	-3.724080	1.872257	-2.903576
141	1	0	-4.513158	1.386619	-0.928627
142	6	0	-3.776465	3.193386	0.350878
143	8	0	-3.286957	3.801405	-0.582026
144	8	0	-4.994569	3.455317	0.853532
145	6	0	-5.700396	4.578588	0.268989
146	6	0	-7.063621	4.635134	0.921601
147	1	0	-5.767890	4.422342	-0.811429
148	1	0	-3.972124	0.005481	-1.867218
149	1	0	-5.118140	5.488063	0.443689
150	1	0	-6.976757	4.794443	2.000292
151	1	0	-7.640186	5.462841	0.497340
152	1	0	-7.614438	3.705528	0.751322
153	1	0	-3.549076	2.926676	-2.691458
154	1	0	-2.949579	1.512463	-3.584023
155	1	0	-4.689892	1.762597	-3.408316
156	7	0	-0.150952	3.594911	1.258576
157	6	0	-0.598478	4.495539	1.875780
158	1	0	0.560742	3.095164	-0.043848
159	8	0	-0.336023	-0.516792	-1.795952
160	6	0	-0.281937	-1.507256	-2.859488
161	1	0	-1.241956	-0.173057	-1.690372

162	1	0	-0.381173	-2.490767	-2.398017
163	6	0	-1.433159	-1.286249	-3.828046
164	6	0	1.085644	-1.399383	-3.510965
165	1	0	-1.349975	-0.321228	-4.338562
166	1	0	1.868243	-1.504968	-2.757469
167	1	0	1.212897	-2.198291	-4.248615
168	1	0	1.202665	-0.439111	-4.025514
169	1	0	-1.436319	-2.072506	-4.589148
170	1	0	-2.396779	-1.327239	-3.312091

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m-VI-COM-*re*

Zero-point correction = 1.39949 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29667 (a.u.)

Sum of electronic and zero-point Energies = -4785.12406 (a.u.)

Sum of electronic and thermal Free Energies = -4785.22688 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.434529	-0.993668	-1.931005
2	6	0	0.242340	-2.024672	-2.922084
3	1	0	0.175067	-2.951791	-2.348706
4	6	0	-1.065500	-1.795011	-3.668559
5	6	0	1.460347	-2.070834	-3.833974
6	1	0	-1.028415	-0.857447	-4.233002
7	1	0	2.362905	-2.259366	-3.248341
8	1	0	1.355701	-2.870797	-4.575094
9	1	0	1.580462	-1.122069	-4.367256
10	1	0	-1.249518	-2.611916	-4.374866
11	1	0	-1.896563	-1.753238	-2.963308
12	1	0	0.373150	-0.081004	-2.342968
13	6	0	2.374163	0.983249	-0.049051
14	8	0	1.221882	0.675984	0.262640
15	6	0	3.099350	2.011711	0.766783
16	8	0	2.927457	0.417552	-1.097743
17	6	0	3.611350	3.193483	0.333927
18	6	0	3.660592	3.843540	-0.969287
19	6	0	2.948252	3.425767	-2.111021
20	6	0	4.459082	5.002503	-1.065524
21	6	0	3.032866	4.141544	-3.299217

22	6	0	4.561578	5.703193	-2.262041
23	6	0	3.844654	5.276030	-3.381957
24	1	0	4.046965	3.795084	1.124185
25	1	0	2.292093	2.565657	-2.088346
26	1	0	5.003436	5.342131	-0.188902
27	1	0	2.437418	3.813019	-4.144750
28	1	0	5.188587	6.587320	-2.318877
29	1	0	3.910744	5.830211	-4.313143
30	6	0	4.320445	0.604163	-1.489537
31	6	0	4.416442	0.274660	-2.959370
32	1	0	4.911115	-0.068240	-0.877358
33	6	0	3.073454	1.745957	2.240325
34	8	0	2.416503	0.877952	2.780663
35	8	0	3.865461	2.594945	2.923868
36	6	0	3.850315	2.456617	4.362662
37	6	0	4.843966	3.452379	4.918468
38	1	0	4.111661	1.428365	4.622518
39	1	0	4.633984	1.625050	-1.294911
40	1	0	2.833436	2.641212	4.723204
41	1	0	4.866545	3.380596	6.010154
42	1	0	5.849941	3.252564	4.538403
43	1	0	4.570953	4.476918	4.648153
44	1	0	5.456300	0.388354	-3.279334
45	1	0	4.110884	-0.753555	-3.151402
46	1	0	3.790849	0.947569	-3.551424
47	22	0	-0.266809	-1.023170	0.095283
48	8	0	-1.361712	-2.485797	-0.323422
49	8	0	1.212015	-2.214816	0.479801
50	6	0	-1.651791	-3.457466	0.562914
51	6	0	1.571756	-3.448831	0.146730
52	6	0	-0.682804	-4.435693	0.873774
53	6	0	-2.930288	-3.506011	1.165795
54	6	0	0.642299	-4.529074	0.205345
55	6	0	2.924384	-3.739455	-0.203635
56	6	0	-3.190706	-4.503536	2.119082
57	6	0	-0.987449	-5.406222	1.840976
58	6	0	3.268015	-5.043596	-0.596957
59	6	0	1.029871	-5.799482	-0.241727
60	6	0	4.031738	-2.768995	-0.000077
61	6	0	-4.035361	-2.550326	0.875497
62	6	0	-2.226665	-5.441536	2.471049

63	6	0	2.327906	-6.062845	-0.663686
64	6	0	5.136323	-2.676926	-0.943368
65	6	0	4.101185	-2.051787	1.164827
66	6	0	-4.609973	-2.395000	-0.448476
67	6	0	-4.628490	-1.918606	1.935041
68	6	0	6.329328	-1.973562	-0.586547
69	6	0	5.259988	-1.306163	1.541730
70	6	0	-5.807307	-1.632763	-0.616308
71	6	0	-5.854447	-1.192739	1.818253
72	6	0	6.407163	-1.292072	0.696511
73	6	0	-6.479699	-1.073237	0.545845
74	6	0	5.043217	-3.223565	-2.247401
75	6	0	-4.030413	-3.008405	-1.582391
76	6	0	5.299372	-0.621122	2.780262
77	6	0	-6.321063	-1.463761	-1.921473
78	6	0	-6.484347	-0.653095	2.963234
79	6	0	7.545757	-0.573182	1.127222
80	6	0	-7.744330	-0.448622	0.484084
81	6	0	-7.720244	-0.044449	2.870877
82	6	0	-8.356692	0.047302	1.619921
83	6	0	-4.567462	-2.838366	-2.843293
84	6	0	-5.713431	-2.045555	-3.016570
85	6	0	6.424109	0.075501	3.171123
86	6	0	7.556809	0.099045	2.335277
87	6	0	6.083152	-3.129589	-3.150471
88	6	0	7.271265	-2.476389	-2.782682
89	6	0	7.381073	-1.904785	-1.530116
90	1	0	-4.175500	-4.538026	2.573751
91	1	0	-0.224235	-6.132564	2.100837
92	1	0	4.304736	-5.261020	-0.827927
93	1	0	0.291794	-6.595579	-0.230517
94	1	0	-2.443245	-6.199849	3.216895
95	1	0	2.613238	-7.056785	-0.993020
96	1	0	3.267143	-2.082022	1.855660
97	1	0	-4.194220	-2.023833	2.924907
98	1	0	4.123342	-3.710978	-2.542713
99	1	0	-3.139491	-3.607041	-1.457696
100	1	0	4.418095	-0.651797	3.411434
101	1	0	-7.196808	-0.846991	-2.079199
102	1	0	-5.986611	-0.750356	3.924531
103	1	0	8.434696	-0.545839	0.508018

104	1	0	-8.256861	-0.357888	-0.465391
105	1	0	-8.203255	0.353119	3.758550
106	1	0	-9.330834	0.519993	1.541272
107	1	0	-4.094970	-3.309140	-3.699676
108	1	0	-6.123792	-1.886502	-4.009015
109	1	0	6.441708	0.595917	4.123968
110	1	0	8.445519	0.642984	2.640651
111	1	0	5.975578	-3.549965	-4.145549
112	1	0	8.095263	-2.403303	-3.485861
113	1	0	8.293574	-1.378058	-1.276979
114	8	0	-0.768207	-0.770535	1.785804
115	6	0	-0.846991	-1.159411	3.143472
116	1	0	-1.683437	-1.867607	3.224200
117	6	0	0.437384	-1.857560	3.578251
118	6	0	-1.153525	0.077300	3.983041
119	1	0	1.284749	-1.176727	3.469192
120	1	0	-2.067933	0.564417	3.628975
121	1	0	-1.295175	-0.192382	5.035170
122	1	0	-0.323944	0.788676	3.916031
123	1	0	0.358789	-2.169484	4.625737
124	1	0	0.615197	-2.741235	2.963968
125	8	0	-1.437370	0.293213	-0.596721
126	6	0	-2.410041	1.084192	0.004580
127	6	0	-1.680563	2.407589	0.367110
128	6	0	-3.602217	1.238584	-0.931230
129	7	0	-1.045968	3.000971	-0.874151
130	6	0	-2.373286	3.558104	1.114126
131	6	0	-4.856969	1.772993	-0.507274
132	6	0	-3.453268	0.916605	-2.263476
133	6	0	-1.960890	3.930970	-1.627115
134	6	0	0.174989	3.765235	-0.462153
135	6	0	-1.734861	4.892391	0.675577
136	6	0	-5.826195	2.068409	-1.521517
137	6	0	-4.498801	1.190053	-3.171142
138	6	0	-2.206388	5.183663	-0.761606
139	6	0	-0.188977	4.791056	0.645743
140	7	0	-5.634529	1.774620	-2.841511
141	1	0	-2.740838	0.650025	0.958824
142	1	0	-0.830322	2.055503	0.951392
143	1	0	-2.273335	3.393915	2.189948
144	1	0	-3.439083	3.601861	0.892897

145	6	0	-5.198789	2.037813	0.846887
146	1	0	-2.519860	0.495198	-2.609730
147	1	0	-2.875987	3.387518	-1.836849
148	1	0	-1.462855	4.136863	-2.575600
149	1	0	0.566759	4.242604	-1.357405
150	1	0	0.890041	3.033488	-0.108559
151	1	0	-2.040276	5.696181	1.349557
152	6	0	-7.044082	2.699836	-1.154519
153	1	0	-4.369823	0.933337	-4.220957
154	1	0	-1.671290	6.047591	-1.167129
155	1	0	-3.272613	5.424187	-0.768774
156	1	0	0.206115	5.766216	0.343491
157	6	0	0.433825	4.428037	1.967929
158	6	0	-7.311136	3.001553	0.159708
159	6	0	-6.388151	2.647808	1.171235
160	1	0	-8.245731	3.483527	0.429916
161	1	0	-7.747476	2.926562	-1.949112
162	1	0	-6.633150	2.831798	2.211488
163	1	0	-4.520488	1.736415	1.635546
164	6	0	1.344931	5.171378	2.594239
165	1	0	1.690546	6.117440	2.183091
166	1	0	1.775944	4.864936	3.542387
167	1	0	0.131483	3.481853	2.413269
168	1	0	-0.735561	2.230909	-1.508864
169	7	0	0.250396	1.481958	-3.001860
170	6	0	0.165732	2.316677	-3.832322

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b-TS1-1

Zero-point correction = 0.29326 (a.u.)

Thermal correction to Gibbs Free Energy = 0.24109 (a.u.)

Sum of electronic and zero-point Energies = -937.11355 (a.u.)

Sum of electronic and thermal Free Energies = -937.16573 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.654704	-0.941384	1.143490
2	6	0	-0.106958	-2.746724	1.630137
3	7	0	0.596884	-3.385722	0.928900
4	6	0	-0.625535	-0.282189	0.213325

5	6	0	-0.507882	1.193643	0.613628
6	6	0	-1.949164	-0.555528	-0.509737
7	8	0	-2.061376	-1.240500	-1.502635
8	8	0	-2.948887	0.047501	0.139670
9	8	0	-0.366710	1.605563	1.742209
10	8	0	-0.595603	1.960952	-0.486024
11	6	0	-0.578076	3.406862	-0.294201
12	6	0	0.839916	3.945616	-0.274106
13	6	0	-4.298421	-0.150367	-0.376799
14	6	0	-4.920754	-1.410978	0.192828
15	1	0	-5.953863	-1.495712	-0.161059
16	1	0	-4.374499	-2.301176	-0.129234
17	1	0	-4.253352	-0.176310	-1.467589
18	1	0	-4.835796	0.745327	-0.058612
19	1	0	-1.140935	3.791866	-1.146890
20	1	0	-1.113985	3.641509	0.627683
21	1	0	0.810736	5.039143	-0.221134
22	1	0	1.390609	3.579745	0.596306
23	6	0	0.505033	-0.871049	-0.520221
24	1	0	0.208283	-1.551427	-1.315218
25	6	0	1.881704	-0.686996	-0.325537
26	6	0	2.440843	0.068829	0.747070
27	6	0	3.812689	0.186009	0.862392
28	6	0	4.653084	-0.436435	-0.074680
29	6	0	2.756891	-1.333601	-1.247201
30	6	0	4.127714	-1.196114	-1.127565
31	1	0	4.791642	-1.683715	-1.832968
32	1	0	2.327777	-1.933376	-2.043227
33	1	0	5.729817	-0.337369	0.027495
34	1	0	4.242645	0.748002	1.684445
35	1	0	1.793616	0.520606	1.488783
36	1	0	-4.932832	-1.383146	1.286214
37	1	0	1.380753	3.663465	-1.182547

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d-I-COM-*si*-HOiPr

Zero-point correction = 1.40243 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29866 (a.u.)

Sum of electronic and zero-point Energies = -4785.17866 (a.u.)

Sum of electronic and thermal Free Energies = -4785.28243 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.946192	-0.846818	0.105906
2	6	0	-2.197632	-0.753513	0.719415
3	6	0	-3.122737	-1.652058	-0.131701
4	6	0	-2.089429	-1.101994	2.200373
5	7	0	-2.605366	-3.082489	-0.161334
6	6	0	-4.634248	-1.720419	0.111779
7	6	0	-3.044534	-0.697000	3.180488
8	6	0	-1.000050	-1.831261	2.629725
9	6	0	-3.174359	-3.921125	0.953110
10	6	0	-2.981563	-3.693514	-1.481131
11	6	0	-5.135867	-3.104635	-0.342325
12	6	0	-2.843794	-1.142969	4.530832
13	6	0	-0.891753	-2.211872	3.983383
14	6	0	-4.679830	-4.133152	0.703733
15	6	0	-4.501268	-3.504006	-1.706435
16	7	0	-1.775741	-1.903388	4.913145
17	1	0	-2.623460	0.255665	0.626753
18	1	0	-2.949402	-1.286123	-1.142644
19	1	0	-5.114159	-0.919437	-0.448167
20	1	0	-4.884906	-1.580279	1.165481
21	6	0	-4.154158	0.147324	2.907160
22	1	0	-0.237230	-2.102336	1.915382
23	1	0	-2.978347	-3.391301	1.880210
24	1	0	-2.610531	-4.853803	0.965933
25	1	0	-2.702917	-4.746795	-1.434851
26	1	0	-2.363828	-3.217170	-2.240070
27	1	0	-6.224878	-3.100962	-0.431168
28	6	0	-3.778502	-0.772682	5.532405
29	1	0	-0.035234	-2.802870	4.305395
30	1	0	-4.877782	-5.150639	0.352673
31	1	0	-5.224968	-3.995543	1.640915
32	1	0	-4.921869	-4.482811	-1.970388
33	6	0	-4.856906	0.023259	5.225232
34	6	0	-5.035919	0.496445	3.904438
35	1	0	-5.563605	0.307260	5.999026
36	1	0	-3.598974	-1.131684	6.540314
37	1	0	-5.867658	1.155021	3.678641

38	1	0	-4.290805	0.549488	1.912356
39	6	0	-4.894665	-2.548339	-2.805345
40	6	0	-4.107279	-1.819165	-3.594232
41	1	0	-3.023960	-1.823709	-3.534918
42	1	0	-4.532429	-1.173391	-4.355673
43	1	0	-5.972879	-2.468732	-2.936185
44	22	0	0.096709	0.759815	-0.133588
45	8	0	1.307822	2.187571	-0.622338
46	8	0	-1.132586	1.443989	-1.382561
47	6	0	2.002151	2.209557	-1.756556
48	6	0	-1.186087	2.354485	-2.354397
49	6	0	1.350075	2.362303	-3.004726
50	6	0	3.409927	2.057236	-1.698313
51	6	0	-0.073377	2.796706	-3.132047
52	6	0	-2.480285	2.859575	-2.648347
53	6	0	4.135041	1.899190	-2.883011
54	6	0	2.118308	2.183584	-4.167938
55	6	0	-2.677428	3.773506	-3.683504
56	6	0	-0.327384	3.746197	-4.142215
57	6	0	3.487991	1.927865	-4.117946
58	6	0	-1.597350	4.226247	-4.435598
59	1	0	5.210250	1.759605	-2.824389
60	1	0	1.622449	2.234596	-5.132416
61	1	0	-3.681279	4.141799	-3.873203
62	1	0	0.519961	4.127079	-4.702510
63	1	0	4.048992	1.783634	-5.036126
64	1	0	-1.737292	4.959687	-5.223334
65	8	0	-0.330847	1.519695	1.432532
66	6	0	0.394533	2.022410	2.549116
67	1	0	1.368766	1.515864	2.565895
68	6	0	0.620061	3.517633	2.363152
69	6	0	-0.362490	1.696699	3.831763
70	1	0	-0.329791	4.056858	2.432392
71	1	0	-0.462550	0.617945	3.966226
72	1	0	0.170541	2.101825	4.699222
73	1	0	-1.364897	2.135578	3.805630
74	1	0	1.296740	3.903569	3.132028
75	1	0	1.063332	3.704235	1.385339
76	6	0	4.088975	2.040237	-0.376014
77	6	0	4.002755	3.183505	0.513836
78	6	0	4.832492	0.959268	-0.000975

79	6	0	4.581856	3.119257	1.816491
80	6	0	5.459282	0.867476	1.281633
81	6	0	5.295837	1.919386	2.226848
82	6	0	3.386918	4.386682	0.098977
83	1	0	4.924340	0.114690	-0.672067
84	6	0	4.477299	4.253469	2.655151
85	6	0	6.201074	-0.283211	1.635600
86	6	0	5.853495	1.748265	3.515100
87	6	0	3.317130	5.483861	0.933347
88	6	0	3.857838	5.412422	2.228683
89	6	0	6.750192	-0.413163	2.895603
90	6	0	6.562474	0.607500	3.846589
91	1	0	6.322364	-1.066434	0.896005
92	1	0	5.728265	2.520161	4.265604
93	1	0	6.979819	0.503781	4.843700
94	1	0	7.319523	-1.300894	3.154940
95	1	0	3.800324	6.270209	2.892024
96	1	0	2.842260	6.397699	0.589666
97	1	0	4.909659	4.228853	3.648744
98	1	0	2.971404	4.440375	-0.899770
99	6	0	-3.658568	2.416987	-1.851619
100	6	0	-3.843531	2.876179	-0.488898
101	6	0	-4.630494	1.662165	-2.442799
102	6	0	-5.036452	2.540808	0.219814
103	6	0	-5.811806	1.249682	-1.746593
104	6	0	-6.016391	1.661270	-0.398636
105	6	0	-2.882831	3.703262	0.136714
106	1	0	-4.503284	1.341562	-3.472176
107	6	0	-5.228947	3.089582	1.508348
108	6	0	-6.764867	0.411601	-2.370258
109	6	0	-7.153543	1.171111	0.282873
110	6	0	-3.093995	4.208938	1.403566
111	6	0	-4.279658	3.904882	2.093170
112	6	0	-7.872130	-0.044523	-1.682381
113	6	0	-8.059275	0.330742	-0.338945
114	1	0	-1.972762	3.944930	-0.397431
115	1	0	-2.347858	4.849873	1.860525
116	1	0	-4.453470	4.312345	3.084306
117	1	0	-6.144756	2.882471	2.049184
118	1	0	-7.320593	1.442227	1.318501
119	1	0	-8.920234	-0.035605	0.211766

120	1	0	-8.593449	-0.691463	-2.172587
121	1	0	-6.603416	0.123685	-3.404442
122	1	0	-1.562624	-3.093641	-0.094598
123	8	0	0.067278	-3.739017	-0.229788
124	6	0	0.714627	-4.896464	0.338315
125	1	0	1.730903	-4.948417	-0.060643
126	6	0	0.787633	-4.792966	1.856908
127	6	0	-0.033451	-6.124438	-0.153246
128	1	0	1.305482	-5.662315	2.275832
129	1	0	0.452064	-7.035884	0.207927
130	1	0	-1.067875	-6.133375	0.208073
131	1	0	-0.039310	-6.147988	-1.246040
132	1	0	1.343866	-3.897865	2.150754
133	1	0	-0.211567	-4.742289	2.300212
134	1	0	0.697878	-2.997246	-0.274269
135	7	0	2.619676	-4.843682	-2.611441
136	6	0	3.002379	-3.982485	-1.933031
137	6	0	1.785338	-1.235117	-1.842468
138	8	0	0.912556	-0.343058	-1.741133
139	6	0	2.513929	-1.822828	-0.778566
140	8	0	2.062768	-1.736154	-3.059554
141	6	0	3.515221	-2.948713	-1.013657
142	6	0	1.177903	-1.375269	-4.148763
143	6	0	-0.121699	-2.154033	-4.063404
144	1	0	1.747519	-1.636831	-5.042341
145	6	0	2.406789	-1.232225	0.508577
146	8	0	1.689238	-0.249503	0.825973
147	8	0	3.141170	-1.831129	1.467579
148	6	0	3.052120	-1.290268	2.810978
149	6	0	3.702731	-2.292844	3.737720
150	1	0	2.001405	-1.123290	3.057289
151	1	0	1.011342	-0.298342	-4.128908
152	1	0	3.568117	-0.328590	2.831317
153	1	0	3.694942	-1.900978	4.759374
154	1	0	3.166820	-3.247412	3.731219
155	1	0	4.741543	-2.471345	3.449944
156	1	0	-0.732836	-1.948744	-4.948611
157	1	0	0.076040	-3.228934	-4.013332
158	1	0	-0.681999	-1.849575	-3.175989
159	1	0	3.629375	-3.462329	-0.054122
160	6	0	4.926655	-2.534069	-1.446752

161	6	0	5.145360	-1.618211	-2.481702
162	6	0	6.025169	-3.090611	-0.785178
163	6	0	6.445371	-1.256792	-2.833147
164	6	0	7.326349	-2.730551	-1.139258
165	6	0	7.538933	-1.808476	-2.163860
166	1	0	4.304204	-1.178626	-3.001421
167	1	0	5.860123	-3.801406	0.020032
168	1	0	6.601161	-0.537785	-3.631523
169	1	0	8.169457	-3.163853	-0.609759
170	1	0	8.549111	-1.519952	-2.437424

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b-I-TS2-*si*-HOiPr

Zero-point correction = 1.39339 (a.u.)

Thermal correction to Gibbs Free Energy = 1.29336 (a.u.)

Sum of electronic and zero-point Energies = -4785.15538 (a.u.)

Sum of electronic and thermal Free Energies = -4785.25541 (a.u.)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.762370	0.784716	0.098921
2	6	0	1.988964	0.809747	0.782260
3	6	0	2.945052	1.664291	-0.076389
4	6	0	1.773689	1.251251	2.223585
5	7	0	2.555910	3.113398	-0.179617
6	6	0	4.452690	1.558274	0.222270
7	6	0	2.606224	0.837186	3.307451
8	6	0	0.704970	2.072179	2.519175
9	6	0	3.170575	3.916903	0.917984
10	6	0	3.093350	3.604721	-1.481219
11	6	0	5.124300	2.871583	-0.212772
12	6	0	2.314115	1.360423	4.612802
13	6	0	0.499706	2.523215	3.838443
14	6	0	4.711686	3.957240	0.789216
15	6	0	4.610666	3.299102	-1.615061
16	7	0	1.269148	2.203134	4.861478
17	1	0	2.447228	-0.189041	0.793319
18	1	0	2.773769	1.259687	-1.074559
19	1	0	4.863457	0.704015	-0.315711

20	1	0	4.646915	1.396672	1.285828
21	6	0	3.675744	-0.089701	3.180455
22	1	0	0.043405	2.384469	1.726097
23	1	0	2.860919	3.472586	1.860780
24	1	0	2.740820	4.919246	0.873242
25	1	0	2.913158	4.679980	-1.526360
26	1	0	2.500860	3.145699	-2.273350
27	1	0	6.211377	2.753221	-0.237191
28	6	0	3.124386	0.981529	5.714791
29	1	0	-0.336201	3.188368	4.052075
30	1	0	5.051828	4.940888	0.447303
31	1	0	5.173014	3.772626	1.764174
32	1	0	5.126519	4.236875	-1.862898
33	6	0	4.168810	0.103499	5.547910
34	6	0	4.436223	-0.443859	4.271505
35	1	0	4.780730	-0.185693	6.397023
36	1	0	2.876457	1.401611	6.683992
37	1	0	5.239058	-1.162684	4.151804
38	1	0	3.880643	-0.548053	2.222174
39	6	0	5.011273	2.297902	-2.668813
40	6	0	4.231031	1.593155	-3.486387
41	1	0	3.149815	1.666617	-3.487899
42	1	0	4.658744	0.900157	-4.203777
43	1	0	6.088553	2.146443	-2.730233
44	22	0	-0.151856	-0.868860	-0.049397
45	8	0	-1.404752	-2.255377	-0.502000
46	8	0	1.102796	-1.618652	-1.212174
47	6	0	-2.032494	-2.368060	-1.670632
48	6	0	1.193913	-2.609722	-2.103545
49	6	0	-1.314174	-2.654910	-2.856427
50	6	0	-3.435155	-2.178132	-1.707526
51	6	0	0.105160	-3.122747	-2.869611
52	6	0	2.499652	-3.119966	-2.318657
53	6	0	-4.090851	-2.121555	-2.940243
54	6	0	-2.013547	-2.575475	-4.073427
55	6	0	2.724439	-4.134400	-3.250525
56	6	0	0.386918	-4.170630	-3.769144
57	6	0	-3.377030	-2.287402	-4.127046
58	6	0	1.664977	-4.674578	-3.972957
59	1	0	-5.163835	-1.955663	-2.956711
60	1	0	-1.466957	-2.733377	-4.998023

61	1	0	3.735248	-4.508118	-3.382336
62	1	0	-0.443185	-4.606336	-4.314920
63	1	0	-3.882427	-2.225858	-5.085902
64	1	0	1.828496	-5.485565	-4.675480
65	8	0	0.183531	-1.515304	1.584136
66	6	0	-0.622958	-1.969062	2.669636
67	1	0	-1.614636	-1.509679	2.563876
68	6	0	-0.773079	-3.482076	2.576314
69	6	0	-0.000877	-1.507181	3.982286
70	1	0	0.190091	-3.973942	2.744993
71	1	0	0.039663	-0.417161	4.033689
72	1	0	-0.594403	-1.868596	4.829400
73	1	0	1.018046	-1.893073	4.083658
74	1	0	-1.485589	-3.844909	3.323901
75	1	0	-1.142645	-3.754453	1.587030
76	6	0	-4.180912	-2.034802	-0.429293
77	6	0	-4.185220	-3.114909	0.540452
78	6	0	-4.892551	-0.900313	-0.168729
79	6	0	-4.835201	-2.941812	1.798757
80	6	0	-5.585935	-0.698994	1.066915
81	6	0	-5.523470	-1.692198	2.085280
82	6	0	-3.577739	-4.358504	0.251061
83	1	0	-4.910454	-0.099588	-0.898695
84	6	0	-4.817657	-4.016806	2.717599
85	6	0	-6.296144	0.500781	1.303506
86	6	0	-6.150495	-1.416505	3.322249
87	6	0	-3.586802	-5.393587	1.163692
88	6	0	-4.205460	-5.217376	2.413355
89	6	0	-6.914726	0.733405	2.515868
90	6	0	-6.828850	-0.230242	3.537628
91	1	0	-6.338229	1.239296	0.511208
92	1	0	-6.104765	-2.142042	4.125951
93	1	0	-7.302146	-0.047449	4.497694
94	1	0	-7.459510	1.657709	2.684002
95	1	0	-4.213414	-6.026664	3.137387
96	1	0	-3.114279	-6.339228	0.916489
97	1	0	-5.308317	-3.911147	3.677921
98	1	0	-3.103984	-4.494212	-0.713217
99	6	0	3.670563	-2.573109	-1.575309
100	6	0	3.860272	-2.850802	-0.165211
101	6	0	4.647909	-1.915152	-2.265738

102	6	0	5.072169	-2.456341	0.479655
103	6	0	5.849403	-1.447829	-1.643444
104	6	0	6.068137	-1.695220	-0.259088
105	6	0	2.888487	-3.561765	0.575977
106	1	0	4.515257	-1.728943	-3.327058
107	6	0	5.273704	-2.845435	1.823705
108	6	0	6.817145	-0.731909	-2.384681
109	6	0	7.236892	-1.167564	0.336024
110	6	0	3.108000	-3.907416	1.894000
111	6	0	4.315518	-3.556860	2.519738
112	6	0	7.956717	-0.239630	-1.780351
113	6	0	8.159684	-0.450723	-0.403767
114	1	0	1.963488	-3.845202	0.090696
115	1	0	2.351940	-4.459543	2.441615
116	1	0	4.496712	-3.842500	3.551126
117	1	0	6.203712	-2.595276	2.320178
118	1	0	7.415400	-1.308822	1.395610
119	1	0	9.046003	-0.052418	0.080659
120	1	0	8.690061	0.311782	-2.360998
121	1	0	6.642935	-0.569784	-3.444188
122	1	0	1.145577	3.371279	-0.227102
123	8	0	0.071335	3.659408	-0.349556
124	6	0	-0.331044	5.004657	-0.017200
125	1	0	-1.371731	5.082977	-0.338197
126	6	0	-0.285612	5.245749	1.487491
127	6	0	0.463783	6.023340	-0.823193
128	1	0	-0.619783	6.263349	1.714937
129	1	0	0.034677	7.021627	-0.690593
130	1	0	1.508774	6.068503	-0.502193
131	1	0	0.425443	5.775864	-1.886802
132	1	0	-0.948388	4.548810	2.007085
133	1	0	0.723871	5.122820	1.887851
134	1	0	-0.851131	2.843567	-0.587619
135	6	0	-1.443681	1.236887	-1.969523
136	8	0	-0.939275	0.122697	-1.808168
137	8	0	-1.482837	1.783847	-3.182408
138	6	0	-0.895252	1.019194	-4.278923
139	6	0	0.618012	1.088839	-4.246758
140	1	0	-1.306580	1.500697	-5.167139
141	6	0	-2.257585	1.409712	0.360275
142	8	0	-1.824578	0.304855	0.713411

143	8	0	-2.997543	2.136471	1.196991
144	6	0	-3.200112	1.603031	2.540482
145	6	0	-3.950283	2.655601	3.322174
146	1	0	-2.220357	1.383682	2.970668
147	1	0	-1.256232	-0.008378	-4.217036
148	1	0	-3.763375	0.673622	2.458590
149	1	0	-4.148535	2.280500	4.330478
150	1	0	-3.371424	3.580831	3.405425
151	1	0	-4.909289	2.880902	2.849549
152	1	0	1.022831	0.584253	-5.130085
153	1	0	0.953016	2.130236	-4.263026
154	1	0	1.008575	0.589077	-3.358448
155	6	0	-1.969609	2.101616	-0.909390
156	7	0	-2.138966	4.922960	-3.069801
157	6	0	-2.502422	4.117008	-2.317914
158	6	0	-3.015354	3.172810	-1.310953
159	1	0	-3.170267	3.779922	-0.415017
160	6	0	-4.403261	2.675974	-1.731095
161	6	0	-4.594972	1.707847	-2.723786
162	6	0	-5.523167	3.245222	-1.115906
163	6	0	-5.883474	1.311346	-3.080899
164	6	0	-6.812391	2.855247	-1.479815
165	6	0	-6.995945	1.882459	-2.462550
166	1	0	-3.748547	1.258691	-3.224344
167	1	0	-5.383860	3.996420	-0.343599
168	1	0	-6.011977	0.552434	-3.845888
169	1	0	-7.670066	3.305381	-0.989446
170	1	0	-7.997282	1.571189	-2.742736
