

Supporting information

DFT Study on the Mechanism of Amides to Aldehydes Using $\text{Cp}_2\text{Zr}(\text{H})\text{Cl}$

Juping Wang^{a,b}, Huiying Xu^a, Hui Gao^a, Cheng-Yong Su^a, Cunyuan Zhao^{a*} and David Lee Phillips^{*c}

^a MOE Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, P. R. China; ^b School of Pharmacy, Guangdong Pharmaceutical University, P. R. China; ^c Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, P. R. China.

Complete List of Authors for References with more than 10 Authors

(20) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision D.01; Gaussian, Inc.: Wallingford CT, 2004.

Table S1. Thermodynamic Properties (the Relative Electronic Energies Corrected With ZPE and Free Energies in the Gas Phase and the Relative Energies in Solution) of the Structures in Figure 3^a.

Species	$\Delta E_{\text{gas}}^{\text{rel}}$	$\Delta G_{\text{gas}}^{\text{rel}}$	$\Delta E_{\text{sol}}^{\text{rel}}$
Cp ₂ Zr(H)Cl + Nicotinamide	0.0	0.0	0.0
1A	-5.2	4.0	-1.8
TS _{1A-3A}	14.3	28.7	15.5
3A	-28.9	-16.3	-26.8
TS _{3A-4A}	4.7	16.4	1.4
5...4	-1.3	9.7	-2.7
1B	-4.5	4.3	-1.3
TS _{1B-2B}	0.1	12.6	3.9
2B	-2.5	9.5	-1.4
TS _{2B-3B}	7.4	22.2	7.7
3B	-28.9	-16.6	-26.8
TS _{3B-4B}	5.2	16.6	-0.1

^a These values, in kcal/mol, were calculated at the B3LYP/6-31G(d, p) (LANL2DZ for Zr) level of theory, using single-point PCM calculations to model the effect of the solvent (THF).

Table S2. Thermodynamic Properties (the Relative Electronic Energies Corrected With ZPE and Free Energies in the Gas Phase and the Relative Energies in Solution) of the Structures in Figure 5^a.

Species	$\Delta E_{\text{gas}}^{\text{rel}}$	$\Delta G_{\text{gas}}^{\text{rel}}$	$\Delta E_{\text{sol}}^{\text{rel}}$
3B + 2H ₂ O	0.0	0.0	0.0
6C	-17.2	-0.1	-11.9
TS _{6C-9}	58.5	78.2	61.5
6D	-17.5	1.3	-12.7
6D'	-12.1	6.6	-6.9

TS _{6D'-7D}	2.3	22.2	9.1
7D	-0.3	17.8	4.9
TS _{7D'-8D}	1.4	20.9	9.6
8D	-9.2	9.1	-5.0
8D'	-17.7	0.3	-13.9
TS _{8D'-9}	-4.8	14.4	1.8
9	-18.7	-4.4	-12.1

^a These values, in kcal/mol, were calculated at the B3LYP/6-31G(d, p) (LANL2DZ for Zr) level of theory, using single-point PCM calculations to model the effect of the solvent (THF).

Structures for the reaction converting Amides to Aldehydes Using Cp₂Zr(H)Cl

Coordinates of the Transition States and Ground States involved

Cp₂Zr(H)Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	0.000004	0.122471	-0.217973
2	1	0	0.000096	0.027638	-2.044028
3	6	0	1.684102	-1.169193	1.176782
4	6	0	1.660412	-1.801576	-0.099507
5	6	0	2.245781	0.123824	1.010483
6	1	0	1.368421	-1.609888	2.112859
7	6	0	2.199657	-0.896553	-1.050312
8	1	0	1.315148	-2.805718	-0.305141
9	6	0	2.549328	0.297978	-0.363299
10	1	0	2.385054	0.863446	1.787718
11	1	0	2.328772	-1.083426	-2.106234
12	1	0	2.955510	1.194118	-0.812076
13	6	0	-2.549336	0.298084	-0.362922
14	6	0	-2.199751	-0.896209	-1.050381
15	6	0	-2.245594	0.123472	1.010767
16	1	0	-2.955552	1.194384	-0.811344
17	6	0	-1.660452	-1.801583	-0.099933
18	1	0	-2.328975	-1.082720	-2.106354
19	6	0	-1.683979	-1.169633	1.176569
20	1	0	-2.384752	0.862840	1.788265
21	1	0	-1.315253	-2.805669	-0.305954
22	1	0	-1.368184	-1.610647	2.112456
23	17	0	-0.000085	2.547361	0.077604

Sum of electronic and zero-point Energies= -894.402423
 Zero-point correction= 0.176460 (Hartree/Particle)
 No imaginary frequency

N-methoxy-N-methylnicotinamide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.650481	-0.991973	-0.219071
2	8	0	-0.767829	-2.193741	-0.434171
3	7	0	-1.783716	-0.186412	-0.133846
4	6	0	0.705868	-0.367250	-0.094997
5	6	0	1.743162	-1.193157	0.355011
6	6	0	1.037057	0.939022	-0.480989
7	6	0	3.031670	-0.676453	0.439133
8	1	0	1.519090	-2.220076	0.623891
9	1	0	0.278580	1.602829	-0.882552
10	6	0	3.243214	0.645841	0.045321
11	1	0	3.858146	-1.283308	0.795121
12	1	0	4.238101	1.084645	0.099375
13	7	0	2.273365	1.443060	-0.421310
14	6	0	-3.069557	-0.848423	0.067891
15	1	0	-3.105866	-1.717635	-0.586184
16	1	0	-3.189374	-1.172639	1.108264
17	1	0	-3.875214	-0.159977	-0.195180
18	8	0	-1.636556	0.955871	0.692831
19	6	0	-2.194461	2.110692	0.066487
20	1	0	-3.282319	2.027991	-0.045501
21	1	0	-1.966808	2.937872	0.742250
22	1	0	-1.745614	2.296923	-0.915394

Sum of electronic and zero-point Energies= -570.586452
Zero-point correction= 0.175817 (Hartree/Particle)
No imaginary frequency

1A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.032139	-1.426158	-0.410909
2	6	0	-1.036551	-1.620158	-0.765138
3	6	0	-1.594887	-1.150790	-1.983486
4	6	0	-2.033564	-2.387520	-0.097719
5	6	0	-2.935211	-1.618284	-2.063718
6	1	0	-1.088613	-0.550775	-2.725383
7	6	0	-3.201208	-2.392152	-0.905672
8	1	0	-1.911896	-2.905677	0.844016
9	1	0	-3.639151	-1.404914	-2.856456
10	1	0	-4.141407	-2.871996	-0.667732
11	40	0	-2.868931	0.008136	-0.090520
12	1	0	-2.161571	1.261422	-1.227238
13	17	0	-5.254069	0.354357	-0.522237
14	6	0	-2.094753	-0.109856	2.326671
15	6	0	-1.138094	0.693388	1.643666
16	6	0	-3.325702	0.597318	2.355293
17	1	0	-1.908224	-1.077925	2.771834
18	6	0	-1.783778	1.897046	1.253133
19	1	0	-0.105731	0.433186	1.446639
20	6	0	-3.136658	1.832085	1.683109
21	1	0	-4.254350	0.247887	2.787129
22	1	0	-1.326809	2.721661	0.726023
23	1	0	-3.898211	2.579942	1.509800

24	7	0	2.893103	1.420042	-0.827469
25	6	0	2.907248	0.254658	-0.111270
26	8	0	1.854167	-0.213540	0.335213
27	6	0	4.211993	-0.435452	0.167396
28	6	0	5.295490	-0.527503	-0.721807
29	6	0	4.297355	-1.145398	1.372888
30	1	0	5.262824	-0.022398	-1.680851
31	7	0	6.403983	-1.231913	-0.465682
32	6	0	5.453355	-1.863101	1.656850
33	1	0	3.455359	-1.126911	2.056766
34	6	0	6.477439	-1.871563	0.707658
35	1	0	5.559278	-2.413281	2.586396
36	1	0	7.396649	-2.424353	0.894306
37	6	0	1.687271	2.059143	-1.323564
38	1	0	0.831813	1.470627	-0.996397
39	1	0	1.594801	3.077645	-0.931677
40	1	0	1.717907	2.099392	-2.416732
41	8	0	4.078879	1.961832	-1.330293
42	6	0	4.603898	2.960877	-0.442056
43	1	0	5.488136	3.353661	-0.947632
44	1	0	3.882241	3.769425	-0.282560
45	1	0	4.889690	2.520385	0.518767

Sum of electronic and zero-point Energies= -1464.997114
Zero-point correction= 0.353073 (Hartree/Particle)
No imaginary frequency

***TS*_{1A-3A}**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.569691	-2.404803	-1.193134
2	6	0	0.220665	-2.400894	-0.456945
3	6	0	0.055202	-2.247030	0.947849
4	6	0	1.602353	-2.532860	-0.726167
5	6	0	1.337301	-2.293532	1.544550
6	1	0	-0.881350	-2.124659	1.470594
7	6	0	2.298609	-2.450129	0.514948
8	1	0	2.048144	-2.679217	-1.699929
9	1	0	1.552042	-2.162954	2.594358
10	1	0	3.369121	-2.516146	0.654129
11	40	0	1.343457	-0.138471	0.102762
12	1	0	-0.185127	0.385803	1.108065
13	17	0	2.190769	0.660654	2.369643
14	6	0	3.607096	-0.121807	-1.354060
15	6	0	2.544906	0.263632	-2.217760
16	6	0	3.746840	0.866918	-0.363230
17	1	0	4.178695	-1.037990	-1.419438
18	6	0	2.095893	1.545523	-1.801644
19	1	0	2.191744	-0.278198	-3.085399
20	6	0	2.803501	1.906844	-0.636795
21	1	0	4.432924	0.846927	0.470645
22	1	0	1.306810	2.107445	-2.278453
23	1	0	2.687260	2.814206	-0.060349
24	7	0	-1.719536	2.079557	-0.107910
25	6	0	-1.440246	0.790206	-0.451623
26	8	0	-0.448075	0.543920	-1.212658
27	6	0	-2.533955	-0.226008	-0.304617
28	6	0	-3.163685	-0.544616	0.908694

29	6	0	-2.917016	-0.931940	-1.450724
30	1	0	-2.866373	-0.039981	1.822021
31	7	0	-4.116664	-1.475145	1.019532
32	6	0	-3.921617	-1.891000	-1.346499
33	1	0	-2.429752	-0.723215	-2.398153
34	6	0	-4.489180	-2.122445	-0.093069
35	1	0	-4.254484	-2.451154	-2.214417
36	1	0	-5.275422	-2.865613	0.026725
37	6	0	-0.677211	3.089275	0.014037
38	1	0	-0.086635	3.109464	-0.899302
39	1	0	-1.159185	4.057140	0.155619
40	1	0	-0.033644	2.858811	0.872743
41	8	0	-2.734580	2.258334	0.846977
42	6	0	-3.869459	2.897775	0.249130
43	1	0	-4.580173	3.031885	1.066712
44	1	0	-3.601031	3.874808	-0.168951
45	1	0	-4.310557	2.268768	-0.530857

Sum of electronic and zero-point Energies= -1464.966148
Zero-point correction= 0.353025 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

3A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.474594	-2.667399	0.177966
2	6	0	-0.578088	-2.548287	-0.039395
3	6	0	-1.147369	-2.359531	-1.324849
4	6	0	-1.625161	-2.498144	0.915223
5	6	0	-2.551387	-2.222972	-1.167991
6	1	0	-0.607453	-2.316318	-2.261048
7	6	0	-2.850689	-2.297491	0.213245
8	1	0	-1.517010	-2.624913	1.983998
9	1	0	-3.261586	-2.045889	-1.962683
10	1	0	-3.837045	-2.234875	0.652931
11	40	0	-1.481497	-0.128599	-0.045611
12	1	0	1.655783	0.308933	-2.111971
13	17	0	-2.626273	0.889308	-2.002299
14	6	0	-1.356403	0.504651	2.426594
15	6	0	-0.969559	1.687118	1.739015
16	6	0	-2.746381	0.287934	2.180442
17	1	0	-0.728498	-0.087545	3.080126
18	6	0	-2.088817	2.154971	1.019166
19	1	0	0.031513	2.093966	1.684161
20	6	0	-3.192941	1.291646	1.296425
21	1	0	-3.345239	-0.513576	2.590613
22	1	0	-2.111186	3.007955	0.355321
23	1	0	-4.188665	1.388574	0.885386
24	7	0	2.154106	1.877462	-0.925546
25	6	0	1.664346	0.502915	-1.028915
26	8	0	0.365946	0.330035	-0.538999
27	6	0	2.640692	-0.462625	-0.376201
28	6	0	3.580927	-1.140846	-1.159058
29	6	0	2.649850	-0.709005	1.000234
30	1	0	3.602486	-0.979321	-2.236852
31	7	0	4.485994	-2.001582	-0.678237
32	6	0	3.586667	-1.600477	1.519090
33	1	0	1.939304	-0.202110	1.643491
34	6	0	4.481080	-2.218396	0.642050
35	1	0	3.627820	-1.814308	2.582955

36	1	0	5.223650	-2.921102	1.016611
37	6	0	1.299908	2.852271	-1.606836
38	1	0	0.279839	2.880974	-1.207381
39	1	0	1.757234	3.840177	-1.513488
40	1	0	1.258569	2.591652	-2.668566
41	8	0	2.172226	2.241233	0.472072
42	6	0	3.457282	2.761825	0.792731
43	1	0	3.689188	3.655291	0.199303
44	1	0	3.410092	3.036113	1.850698
45	1	0	4.243321	2.014816	0.638039

Sum of electronic and zero-point Energies= -1465.034914
Zero-point correction= 0.357816 (Hartree/Particle)
No imaginary frequency

TS_{3A-4A}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.833762	-2.751664	-1.354925
2	6	0	-3.126698	-1.709503	-1.330142
3	6	0	-2.755883	-0.715595	-2.273764
4	6	0	-4.039955	-1.115371	-0.405410
5	6	0	-3.359872	0.498225	-1.886631
6	1	0	-2.055092	-0.845492	-3.086297
7	6	0	-4.167191	0.245863	-0.733561
8	1	0	-4.517803	-1.620091	0.423301
9	1	0	-3.236768	1.457866	-2.369583
10	1	0	-4.747414	0.984986	-0.197387
11	40	0	-1.625390	-0.069253	0.002231
12	1	0	1.516959	0.478770	-1.818875
13	17	0	-1.723117	2.471472	0.340114
14	6	0	-2.359548	-0.889897	2.433579
15	6	0	-1.695007	-1.973669	1.791813
16	6	0	-1.410583	0.130925	2.652826
17	1	0	-3.411310	-0.843775	2.682678
18	6	0	-0.323697	-1.628173	1.657438
19	1	0	-2.143363	-2.916436	1.506321
20	6	0	-0.150980	-0.320441	2.167754
21	1	0	-1.610289	1.102808	3.081564
22	1	0	0.443704	-2.243805	1.208648
23	1	0	0.771963	0.244174	2.179515
24	7	0	2.343057	1.806065	-0.556628
25	6	0	2.263015	0.597993	-1.039730
26	8	0	-0.088203	-0.174584	-1.050108
27	6	0	3.029549	-0.575161	-0.652417
28	6	0	4.291017	-0.557168	-0.024787
29	6	0	2.493074	-1.825895	-1.017112
30	1	0	4.755216	0.381162	0.257023
31	7	0	4.997210	-1.656604	0.237776
32	6	0	3.221932	-2.973079	-0.733289
33	1	0	1.502449	-1.851348	-1.461912
34	6	0	4.462311	-2.837259	-0.104601
35	1	0	2.838742	-3.956262	-0.985711
36	1	0	5.056070	-3.716404	0.138183
37	6	0	1.445176	2.895014	-0.956335
38	1	0	0.764669	3.111106	-0.129528
39	1	0	2.027718	3.772828	-1.243598
40	1	0	0.849036	2.546693	-1.797400
41	8	0	3.020662	1.995106	0.647085
42	6	0	3.983694	3.062522	0.581868

43	1	0	3.499091	4.038386	0.487837
44	1	0	4.503277	3.008687	1.539058
45	1	0	4.691815	2.906502	-0.238938

Sum of electronic and zero-point Energies= -1464.981449
Zero-point correction= 0.355238 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

5...4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.970845	-2.182342	2.283601
2	6	0	1.756599	-1.440400	2.237985
3	6	0	1.647719	-0.087000	2.630452
4	6	0	3.063733	-1.641207	1.716721
5	6	0	2.898470	0.545440	2.380348
6	1	0	0.765509	0.391019	3.034578
7	6	0	3.775886	-0.414210	1.832199
8	1	0	3.462332	-2.576815	1.346109
9	1	0	3.124297	1.588315	2.553474
10	1	0	4.798103	-0.238051	1.525060
11	40	0	1.849751	-0.071752	0.013285
12	1	0	-1.382137	0.226195	-0.310565
13	17	0	1.652781	2.484348	-0.016878
14	6	0	3.923536	-0.925292	-1.429940
15	6	0	2.802933	-1.769669	-1.698746
16	6	0	3.630882	0.356746	-1.926014
17	1	0	4.821289	-1.215615	-0.901340
18	6	0	1.854474	-1.011350	-2.435241
19	1	0	2.725976	-2.822189	-1.456622
20	6	0	2.340639	0.307350	-2.541361
21	1	0	4.254597	1.236688	-1.841392
22	1	0	0.889023	-1.362443	-2.771299
23	1	0	1.833711	1.142862	-3.004424
24	7	0	-2.783914	1.753063	-0.310457
25	6	0	-2.493861	0.489083	-0.289143
26	8	0	0.029197	-0.454727	-0.113605
27	6	0	-3.392338	-0.644365	-0.188776
28	6	0	-4.800934	-0.641851	-0.318555
29	6	0	-2.748999	-1.883938	0.025348
30	1	0	-5.331417	0.279545	-0.529496
31	7	0	-5.544365	-1.742560	-0.223409
32	6	0	-3.528017	-3.029347	0.130815
33	1	0	-1.661776	-1.895388	0.098265
34	6	0	-4.912893	-2.905352	0.007627
35	1	0	-3.076274	-4.000962	0.301261
36	1	0	-5.552953	-3.781737	0.091629
37	6	0	-1.815879	2.836254	-0.509091
38	1	0	-2.014767	3.299959	-1.478149
39	1	0	-1.940149	3.579110	0.281294
40	1	0	-0.799429	2.437369	-0.466352
41	8	0	-4.115905	2.193297	-0.293870
42	6	0	-4.513910	2.598342	1.033942
43	1	0	-3.899061	3.426555	1.397967
44	1	0	-5.545668	2.931783	0.918290
45	1	0	-4.465986	1.754805	1.729072

Sum of electronic and zero-point Energies= -1464.990982
Zero-point correction= 0.354580 (Hartree/Particle)

No imaginary frequency

1B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	2.631477	-0.093585	-0.125639
2	1	0	1.991776	-1.396656	-1.236832
3	6	0	5.107438	0.480874	-0.072290
4	6	0	5.010073	-0.803826	-0.679854
5	6	0	4.520823	1.424239	-0.954991
6	1	0	5.575432	0.702764	0.877395
7	6	0	4.361705	-0.651194	-1.933401
8	1	0	5.388167	-1.730837	-0.271008
9	6	0	4.048881	0.725412	-2.095404
10	1	0	4.417858	2.486426	-0.777008
11	1	0	4.149456	-1.439410	-2.640563
12	1	0	3.521940	1.163953	-2.931688
13	6	0	0.860953	-0.951590	1.522643
14	6	0	1.730267	-2.047420	1.259357
15	6	0	1.604939	0.036337	2.213888
16	1	0	-0.182599	-0.893283	1.236197
17	6	0	3.012395	-1.726102	1.774061
18	1	0	1.453013	-2.966317	0.763717
19	6	0	2.940562	-0.427239	2.357695
20	1	0	1.229339	0.997588	2.538838
21	1	0	3.885840	-2.363641	1.750674
22	1	0	3.744402	0.089387	2.865278
23	17	0	1.113362	1.755168	-0.693672
24	7	0	-4.304858	-1.758713	-0.374366
25	6	0	-3.351170	-0.924892	0.156048
26	8	0	-2.250368	-1.378894	0.473895
27	6	0	-3.647919	0.540760	0.292207
28	6	0	-4.863051	1.076053	0.749501
29	6	0	-2.588433	1.427954	0.059541
30	1	0	-5.701742	0.423119	0.967109
31	7	0	-5.065708	2.382622	0.954554
32	6	0	-2.796559	2.790152	0.249373
33	1	0	-1.623053	1.052432	-0.263136
34	6	0	-4.049087	3.215196	0.694678
35	1	0	-1.999835	3.503250	0.064099
36	1	0	-4.246069	4.273834	0.857114
37	6	0	-4.205344	-3.205568	-0.354393
38	1	0	-3.196905	-3.457396	-0.029669
39	1	0	-4.940843	-3.626884	0.339637
40	1	0	-4.380419	-3.617062	-1.353650
41	8	0	-5.579978	-1.275382	-0.684306
42	6	0	-5.674667	-0.951479	-2.079106
43	1	0	-5.465919	-1.826327	-2.705230
44	1	0	-6.708172	-0.632149	-2.228289
45	1	0	-4.992015	-0.136373	-2.340331

Sum of electronic and zero-point Energies= -1464.996004

Zero-point correction= 0.352832 (Hartree/Particle)

No imaginary frequency

TS_{1B-2B}

Center	Atomic	Atomic	Coordinates (Angstroms)		
--------	--------	--------	-------------------------	--	--

Number	Number	Type	X	Y	Z
1	40	0	1.921206	-0.099281	-0.053200
2	1	0	1.401474	0.714317	-1.601966
3	6	0	4.164941	0.686356	0.882708
4	6	0	4.054663	1.236835	-0.428657
5	6	0	3.188003	1.302908	1.696972
6	1	0	4.884838	-0.054066	1.204015
7	6	0	3.014426	2.200527	-0.414699
8	1	0	4.677632	0.993602	-1.278021
9	6	0	2.459468	2.220525	0.892536
10	1	0	2.989058	1.078453	2.734808
11	1	0	2.704394	2.808293	-1.251639
12	1	0	1.631106	2.829868	1.228114
13	6	0	1.094272	-2.298948	-1.089042
14	6	0	2.017776	-1.737579	-2.015752
15	6	0	1.804500	-2.662786	0.079158
16	1	0	0.026467	-2.374638	-1.233841
17	6	0	3.297769	-1.742905	-1.406667
18	1	0	1.783831	-1.384230	-3.008988
19	6	0	3.165112	-2.300963	-0.100989
20	1	0	1.375332	-3.083486	0.977302
21	1	0	4.217985	-1.400628	-1.859297
22	1	0	3.964908	-2.465303	0.608320
23	17	0	0.435327	-0.323498	1.980417
24	7	0	-2.285117	1.804137	-0.771580
25	6	0	-2.083778	0.461588	-0.622894
26	8	0	-0.970542	-0.035548	-0.825762
27	6	0	-3.228869	-0.402149	-0.184909
28	6	0	-4.522660	-0.329879	-0.723860
29	6	0	-2.951494	-1.423633	0.732900
30	1	0	-4.770865	0.436975	-1.451263
31	7	0	-5.506027	-1.176443	-0.400504
32	6	0	-3.976763	-2.293224	1.092952
33	1	0	-1.953224	-1.505009	1.152671
34	6	0	-5.229368	-2.129745	0.499116
35	1	0	-3.809556	-3.087521	1.813645
36	1	0	-6.050491	-2.797992	0.753854
37	6	0	-1.333123	2.714975	-1.378031
38	1	0	-0.436566	2.146003	-1.625541
39	1	0	-1.767059	3.149529	-2.284641
40	1	0	-1.072869	3.522180	-0.684798
41	8	0	-3.547191	2.356368	-0.535869
42	6	0	-3.647937	2.842703	0.812153
43	1	0	-2.888186	3.605095	1.016930
44	1	0	-4.642548	3.288077	0.879017
45	1	0	-3.556230	2.023148	1.531894

Sum of electronic and zero-point Energies= -1464.988747
Zero-point correction= 0.353609 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

2B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.648312	-0.064080	-0.126065
2	1	0	1.095515	0.432179	-1.804984
3	6	0	3.966505	0.832573	0.518165
4	6	0	3.781583	1.115882	-0.867209

5	6	0	3.053584	1.624517	1.249613
6	1	0	4.687622	0.144344	0.938067
7	6	0	2.757395	2.090216	-0.985001
8	1	0	4.347242	0.697215	-1.687621
9	6	0	2.288839	2.383723	0.324267
10	1	0	2.913320	1.609201	2.319834
11	1	0	2.406160	2.528962	-1.907047
12	1	0	1.494681	3.071745	0.580872
13	6	0	0.752864	-2.375016	-0.864742
14	6	0	1.708199	-1.976003	-1.843123
15	6	0	1.435797	-2.603822	0.353003
16	1	0	-0.310788	-2.483665	-1.027135
17	6	0	2.976117	-1.934686	-1.213290
18	1	0	1.503603	-1.761972	-2.881395
19	6	0	2.806701	-2.305146	0.154658
20	1	0	0.984287	-2.881276	1.293570
21	1	0	3.913658	-1.694547	-1.694391
22	1	0	3.587179	-2.389872	0.898409
23	17	0	0.681588	-0.195319	2.331079
24	7	0	-2.355859	1.984946	-0.532003
25	6	0	-1.809455	0.764034	-0.290072
26	8	0	-0.574901	0.659762	-0.207774
27	6	0	-2.706354	-0.418396	-0.131630
28	6	0	-3.794181	-0.673562	-0.982159
29	6	0	-2.394962	-1.362771	0.856105
30	1	0	-4.051509	0.029485	-1.768938
31	7	0	-4.555931	-1.767100	-0.894317
32	6	0	-3.199863	-2.494279	0.964065
33	1	0	-1.545470	-1.192120	1.514063
34	6	0	-4.261140	-2.649268	0.071019
35	1	0	-3.005946	-3.245350	1.723164
36	1	0	-4.905556	-3.524871	0.128703
37	6	0	-1.596929	3.184505	-0.840012
38	1	0	-0.593356	2.882868	-1.135826
39	1	0	-2.091555	3.702068	-1.665530
40	1	0	-1.531392	3.854959	0.024385
41	8	0	-3.739508	2.149273	-0.496729
42	6	0	-4.188936	2.513157	0.821432
43	1	0	-3.741575	3.458221	1.147033
44	1	0	-5.269461	2.632342	0.724850
45	1	0	-3.962890	1.722560	1.543899

Sum of electronic and zero-point Energies= -1464.992812
Zero-point correction= 0.354151 (Hartree/Particle)
No imaginary frequency

TS_{2B-3B}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.331224	-0.156035	-0.000270
2	1	0	-0.293429	0.330277	-0.924126
3	6	0	3.398536	0.618868	-1.370440
4	6	0	2.244793	0.990769	-2.115697
5	6	0	3.416630	1.379617	-0.182111
6	1	0	4.129321	-0.124595	-1.658172
7	6	0	1.573392	2.015322	-1.397062
8	1	0	1.949486	0.601875	-3.080418
9	6	0	2.280450	2.237373	-0.189395
10	1	0	4.138229	1.300457	0.616814

11	1	0	0.672837	2.514618	-1.724177
12	1	0	2.023473	2.937363	0.592569
13	6	0	0.294058	-2.529522	0.178727
14	6	0	0.318887	-2.197796	-1.207616
15	6	0	1.626728	-2.659290	0.625766
16	1	0	-0.591272	-2.655915	0.783794
17	6	0	1.674740	-2.114089	-1.606405
18	1	0	-0.542997	-2.059631	-1.844304
19	6	0	2.488008	-2.376319	-0.466233
20	1	0	1.939380	-2.861726	1.638944
21	1	0	2.028789	-1.900652	-2.605093
22	1	0	3.568983	-2.397173	-0.438988
23	17	0	2.295719	-0.100745	2.375504
24	7	0	-1.739284	2.022339	0.372881
25	6	0	-1.331607	0.714115	0.479676
26	8	0	-0.406130	0.453491	1.331080
27	6	0	-2.383863	-0.324273	0.170065
28	6	0	-2.958086	-0.533113	-1.090436
29	6	0	-2.813845	-1.128954	1.230656
30	1	0	-2.628510	0.059802	-1.938334
31	7	0	-3.898694	-1.452504	-1.331641
32	6	0	-3.799257	-2.084921	0.991238
33	1	0	-2.369600	-1.003367	2.213241
34	6	0	-4.309393	-2.205378	-0.301757
35	1	0	-4.160742	-2.727037	1.788211
36	1	0	-5.078314	-2.942917	-0.524586
37	6	0	-0.952122	3.153928	0.830807
38	1	0	-0.303349	2.806922	1.633819
39	1	0	-0.357118	3.582121	0.018458
40	1	0	-1.627345	3.921718	1.218451
41	8	0	-2.582326	2.329594	-0.705131
42	6	0	-3.889845	2.698685	-0.242886
43	1	0	-3.849812	3.585153	0.399949
44	1	0	-4.453364	2.931149	-1.148532
45	1	0	-4.366538	1.871974	0.292044

Sum of electronic and zero-point Energies= -1464.977073
Zero-point correction= 0.357957 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

3B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.476634	-0.119701	-0.050583
2	1	0	-1.659879	0.348030	-2.141065
3	6	0	2.854692	-2.285905	0.182958
4	6	0	1.623887	-2.506836	0.868984
5	6	0	2.568623	-2.188515	-1.200014
6	1	0	3.836450	-2.225686	0.633159
7	6	0	0.586376	-2.544429	-0.096394
8	1	0	1.504431	-2.652611	1.934031
9	6	0	1.167334	-2.330351	-1.373018
10	1	0	3.285618	-1.991923	-1.983945
11	1	0	-0.466967	-2.674602	0.110793
12	1	0	0.636766	-2.272663	-2.313789
13	6	0	2.040614	2.142853	1.072774
14	6	0	0.918687	1.643285	1.767200
15	6	0	3.152643	1.287879	1.344404
16	1	0	2.059869	3.011199	0.428991
17	6	0	1.312529	0.450355	2.432236

S12

18	1	0	-0.087086	2.038072	1.711135
19	6	0	2.708307	0.257965	2.199067
20	1	0	4.152068	1.407157	0.948446
21	1	0	0.682897	-0.165108	3.062122
22	1	0	3.312644	-0.545341	2.597503
23	17	0	2.655720	0.940835	-1.965479
24	7	0	-2.165898	1.887326	-0.919203
25	6	0	-1.663254	0.519129	-1.053683
26	8	0	-0.361905	0.343606	-0.577366
27	6	0	-2.634392	-0.465183	-0.417457
28	6	0	-2.586526	-0.779071	0.947113
29	6	0	-3.621201	-1.086307	-1.185428
30	1	0	-1.838681	-0.308839	1.578676
31	7	0	-3.419039	-1.636831	1.549397
32	6	0	-4.499813	-1.980223	-0.574911
33	1	0	-3.700245	-0.871968	-2.248586
34	6	0	-4.356372	-2.221950	0.791271
35	1	0	-5.275432	-2.482749	-1.144454
36	1	0	-5.020998	-2.917306	1.301157
37	6	0	-1.319842	2.884993	-1.577036
38	1	0	-0.301417	2.915521	-1.173598
39	1	0	-1.272131	2.647562	-2.644025
40	1	0	-1.787424	3.865991	-1.463610
41	8	0	-2.185547	2.218228	0.485895
42	6	0	-3.481516	2.694560	0.829616
43	1	0	-4.248118	1.930339	0.662023
44	1	0	-3.433178	2.940479	1.894237
45	1	0	-3.742309	3.596665	0.261579

Sum of electronic and zero-point Energies= -1465.035003
Zero-point correction= 0.357840 (Hartree/Particle)
No imaginary frequency

TS_{3B-4B}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.566903	-0.129090	-0.024028
2	1	0	-1.533816	0.778617	-1.838252
3	6	0	4.211727	0.252332	-0.041421
4	6	0	3.872114	-0.455159	-1.227218
5	6	0	3.638497	1.541443	-0.127576
6	1	0	4.780424	-0.135238	0.793403
7	6	0	3.115811	0.415437	-2.058609
8	1	0	4.172524	-1.464992	-1.474137
9	6	0	2.964968	1.644752	-1.375909
10	1	0	3.680864	2.307107	0.634338
11	1	0	2.700412	0.168828	-3.026430
12	1	0	2.416719	2.506649	-1.731771
13	6	0	0.271248	-1.810899	1.519213
14	6	0	0.397480	-2.458272	0.272257
15	6	0	1.569819	-1.731594	2.111359
16	1	0	-0.642705	-1.434127	1.957543
17	6	0	1.775602	-2.725137	0.055849
18	1	0	-0.398947	-2.651337	-0.432711
19	6	0	2.489896	-2.313168	1.221032
20	1	0	1.799745	-1.275104	3.064562
21	1	0	2.196629	-3.225812	-0.806609
22	1	0	3.558022	-2.395160	1.370448
23	17	0	0.884824	1.587557	1.761807
24	7	0	-2.143771	2.011076	-0.376621

25	6	0	-2.175196	0.848228	-0.967611
26	8	0	0.171030	0.189944	-1.210039
27	6	0	-2.960865	-0.321262	-0.624523
28	6	0	-2.997886	-1.330864	-1.611244
29	6	0	-3.647296	-0.563383	0.581260
30	1	0	-2.442449	-1.192323	-2.536863
31	7	0	-3.666807	-2.474587	-1.487330
32	6	0	-4.334297	-1.763125	0.720893
33	1	0	-3.616805	0.159049	1.384812
34	6	0	-4.323131	-2.677368	-0.335816
35	1	0	-4.867176	-1.993952	1.637335
36	1	0	-4.859000	-3.620726	-0.251800
37	6	0	-1.167708	3.058620	-0.689589
38	1	0	-0.486067	3.125294	0.162847
39	1	0	-0.605501	2.741175	-1.565891
40	1	0	-1.682246	4.004685	-0.873018
41	8	0	-2.808762	2.193945	0.833797
42	6	0	-3.940570	3.071090	0.677200
43	1	0	-4.668028	2.652814	-0.026232
44	1	0	-4.374687	3.133744	1.675588
45	1	0	-3.631416	4.069400	0.353559

Sum of electronic and zero-point Energies= -1464.980566
Zero-point correction= 0.355336 Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

H₂O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.118849
2	1	0	0.000000	0.760074	-0.475396
3	1	0	0.000000	-0.760074	-0.475396

Sum of electronic and zero-point Energies= -76.396776
Zero-point correction= 0.021383 (Hartree/Particle)
No imaginary frequency

6C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.807038	-0.004200	0.131453
2	1	0	-1.643860	-0.431303	1.465633
3	6	0	3.274192	1.952706	0.911609
4	6	0	2.302424	2.507953	0.028434
5	6	0	2.599524	1.519052	2.080503
6	1	0	4.340143	1.895622	0.734982
7	6	0	1.034098	2.401231	0.650617
8	1	0	2.498685	2.952299	-0.937904
9	6	0	1.215903	1.777440	1.914166
10	1	0	3.054287	1.027810	2.928372
11	1	0	0.090724	2.715302	0.225640
12	1	0	0.434315	1.530251	2.620115
13	6	0	2.523301	-1.901899	-1.486788

14	6	0	1.588946	-1.123649	-2.201422
15	6	0	3.692747	-1.110140	-1.271702
16	1	0	2.378973	-2.915803	-1.140508
17	6	0	2.148478	0.168850	-2.391085
18	1	0	0.581726	-1.424518	-2.455728
19	6	0	3.468948	0.158389	-1.845853
20	1	0	4.582363	-1.428970	-0.745614
21	1	0	1.681879	0.994574	-2.913084
22	1	0	4.168399	0.983016	-1.861068
23	17	0	2.506430	-1.680502	1.827977
24	7	0	-2.152878	-1.644229	-0.089501
25	6	0	-1.484469	-0.408756	0.379792
26	8	0	-0.122303	-0.419753	0.093172
27	6	0	-2.178781	0.823159	-0.181357
28	6	0	-1.958017	1.272205	-1.490855
29	6	0	-3.059319	1.559091	0.619356
30	1	0	-1.276671	0.725954	-2.136673
31	7	0	-2.539747	2.356124	-2.018850
32	6	0	-3.673591	2.690699	0.080337
33	1	0	-3.248280	1.248390	1.644825
34	6	0	-3.383141	3.045222	-1.237014
35	1	0	-4.356554	3.292212	0.672727
36	1	0	-3.842798	3.924121	-1.686202
37	6	0	-1.602795	-2.844231	0.560747
38	1	0	-0.525263	-2.943213	0.398318
39	1	0	-1.807948	-2.760440	1.631581
40	1	0	-2.121966	-3.721419	0.168660
41	8	0	-1.899845	-1.775229	-1.504962
42	6	0	-3.122306	-2.034811	-2.184820
43	1	0	-2.850827	-2.173533	-3.234659
44	1	0	-3.606554	-2.946855	-1.813653
45	1	0	-3.820908	-1.193827	-2.099263
46	8	0	-3.266604	-0.595478	3.127571
47	1	0	-3.930993	-0.971881	2.509873
48	1	0	-3.426040	-1.021287	3.977455
49	1	0	-5.197443	-0.669532	0.656360
50	8	0	-4.783150	-1.471848	0.998692
51	1	0	-3.939469	-1.550297	0.490769

Sum of electronic and zero-point Energies= -1617.856018
Zero-point correction= 0.408260 (Hartree/Particle)
No imaginary frequency

TS_{6C-9}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	-1.710535	-0.043198	-0.007031
2	1	0	1.484062	-0.197083	-1.999609
3	6	0	-3.977612	0.839764	-1.042543
4	6	0	-3.093836	1.949960	-0.962814
5	6	0	-3.453809	-0.063186	-1.998188
6	1	0	-4.881049	0.698564	-0.464145
7	6	0	-2.035088	1.735865	-1.886266
8	1	0	-3.219148	2.823259	-0.336602
9	6	0	-2.254346	0.489113	-2.520603
10	1	0	-3.875622	-1.022425	-2.262359
11	1	0	-1.205802	2.407931	-2.061865
12	1	0	-1.612883	0.026078	-3.258326
13	6	0	-1.434164	-0.748588	2.486451
14	6	0	-0.732933	0.466847	2.350077

15	6	0	-2.830636	-0.474934	2.348814
16	1	0	-1.001254	-1.725969	2.646807
17	6	0	-1.679054	1.488578	2.066489
18	1	0	0.340871	0.586267	2.356569
19	6	0	-2.980828	0.903854	2.113669
20	1	0	-3.623825	-1.208971	2.395916
21	1	0	-1.455836	2.537156	1.915813
22	1	0	-3.915196	1.425544	1.957796
23	17	0	-2.122673	-2.532671	-0.299822
24	7	0	2.120944	-1.539174	-0.383808
25	6	0	1.939705	-0.198559	-1.031505
26	8	0	0.115990	-0.065058	-0.481733
27	6	0	2.396328	1.039982	-0.362523
28	6	0	1.920012	2.266095	-0.853211
29	6	0	3.311671	1.076425	0.694882
30	1	0	1.207662	2.271139	-1.674682
31	7	0	2.276745	3.456475	-0.368332
32	6	0	3.678199	2.314045	1.218739
33	1	0	3.751810	0.167298	1.087071
34	6	0	3.136671	3.471244	0.659287
35	1	0	4.382629	2.379684	2.041792
36	1	0	3.407311	4.451836	1.045922
37	6	0	1.449264	-2.616050	-1.169060
38	1	0	0.373194	-2.451040	-1.130479
39	1	0	1.852200	-2.549183	-2.180305
40	1	0	1.713062	-3.576584	-0.727458
41	8	0	1.660490	-1.510077	0.971744
42	6	0	2.327939	-2.502939	1.771832
43	1	0	1.969802	-2.294735	2.780836
44	1	0	2.028893	-3.518676	1.491721
45	1	0	3.415347	-2.394318	1.725587
46	8	0	3.580262	-0.553397	-1.991958
47	1	0	4.611372	-1.155243	-1.016301
48	1	0	3.797879	0.305518	-2.376854
49	1	0	5.284531	-2.525811	-0.570734
50	8	0	4.844193	-1.744777	-0.212204
51	1	0	3.160603	-1.736620	-0.330871

-----Sum of

electronic and zero-point Energies= -1617.735339

Zero-point correction= 0.407528 (Hartree/Particle)

One imaginary frequency, one negative Eigenvalue

6D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	1.710032	-0.016531	0.019241
2	1	0	-1.375671	-0.310166	-2.189398
3	6	0	3.854867	0.474730	-1.328417
4	6	0	3.765117	-0.932225	-1.238241
5	6	0	2.779891	0.931158	-2.150607
6	1	0	4.605723	1.101725	-0.866169
7	6	0	2.611630	-1.348770	-1.964442
8	1	0	4.444305	-1.581726	-0.704187
9	6	0	2.033551	-0.193089	-2.558753
10	1	0	2.569608	1.962991	-2.394063
11	1	0	2.273849	-2.368939	-2.094234
12	1	0	1.139591	-0.175468	-3.166989
13	6	0	0.975640	-0.505817	2.437831
14	6	0	0.917131	-1.745183	1.753690

15	6	0	2.343803	-0.125137	2.534918
16	1	0	0.130828	0.074683	2.784910
17	6	0	2.238582	-2.111251	1.388665
18	1	0	0.016955	-2.292623	1.511528
19	6	0	3.124473	-1.109564	1.888407
20	1	0	2.715586	0.781512	2.990826
21	1	0	2.526660	-3.014645	0.867290
22	1	0	4.202469	-1.107433	1.799797
23	17	0	1.782373	2.413742	0.617389
24	7	0	-2.157667	1.112045	-0.820650
25	6	0	-1.451872	-0.161803	-1.095948
26	8	0	-0.173931	-0.046314	-0.554258
27	6	0	-2.198663	-1.335676	-0.490814
28	6	0	-2.516136	-2.448612	-1.273589
29	6	0	-2.539315	-1.376603	0.866360
30	1	0	-2.271249	-2.448764	-2.335709
31	7	0	-3.120514	-3.550014	-0.810597
32	6	0	-3.175647	-2.512114	1.363157
33	1	0	-2.310368	-0.534905	1.513243
34	6	0	-3.440837	-3.569162	0.488188
35	1	0	-3.461416	-2.581282	2.408336
36	1	0	-3.932963	-4.471119	0.848354
37	6	0	-1.576434	2.251986	-1.544940
38	1	0	-0.542451	2.386593	-1.222011
39	1	0	-1.613822	2.094770	-2.631982
40	1	0	-2.145417	3.144806	-1.278437
41	8	0	-3.481170	0.931255	-1.362089
42	6	0	-4.458236	1.335598	-0.401000
43	1	0	-4.247806	2.341956	-0.022239
44	1	0	-5.409187	1.325801	-0.940764
45	1	0	-4.510397	0.626685	0.435202
46	1	0	-1.759556	1.631061	0.975853
47	8	0	-1.483313	2.019417	1.838292
48	1	0	-0.570776	2.309043	1.676682
49	1	0	-2.512131	3.528198	1.421919
50	8	0	-3.074087	4.187057	0.965651
51	1	0	-3.741979	4.428540	1.618148

Sum of electronic and zero-point Energies= -1617.856510
Zero-point correction= 0.408864 (Hartree/Particle) No
No imaginary frequency

6D'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	-1.570733	-0.294833	-0.011990
2	1	0	1.241356	-0.874305	1.932644
3	6	0	-3.551093	-0.436180	1.594258
4	6	0	-2.868383	-1.676182	1.707714
5	6	0	-2.713839	0.573277	2.147220
6	1	0	-4.544173	-0.287123	1.190867
7	6	0	-1.597309	-1.425115	2.286640
8	1	0	-3.249330	-2.641980	1.406735
9	6	0	-1.511064	-0.031933	2.570973
10	1	0	-2.942033	1.628293	2.188309
11	1	0	-0.841304	-2.170095	2.500479
12	1	0	-0.652912	0.487607	2.975431
13	6	0	-1.236442	-0.742338	-2.526713

14	6	0	-0.740957	-1.888919	-1.862476
15	6	0	-2.648314	-0.701472	-2.332930
16	1	0	-0.636808	-0.006612	-3.046001
17	6	0	-1.827208	-2.531098	-1.214563
18	1	0	0.296987	-2.184682	-1.798703
19	6	0	-3.016194	-1.800937	-1.527071
20	1	0	-3.312598	0.064326	-2.708280
21	1	0	-1.773889	-3.445651	-0.638621
22	1	0	-4.018976	-2.049417	-1.205822
23	17	0	-2.133550	2.040310	-0.650586
24	7	0	1.711450	1.095668	1.758132
25	6	0	1.498295	-0.201029	1.099402
26	8	0	0.418803	-0.098298	0.216087
27	6	0	2.688265	-0.835563	0.374008
28	6	0	2.860203	-2.222262	0.474681
29	6	0	3.614336	-0.136102	-0.413613
30	1	0	2.176205	-2.803952	1.094488
31	7	0	3.819199	-2.921548	-0.141791
32	6	0	4.628853	-0.847394	-1.053206
33	1	0	3.546087	0.942338	-0.499628
34	6	0	4.684834	-2.233364	-0.895773
35	1	0	5.368282	-0.336135	-1.662341
36	1	0	5.460266	-2.815304	-1.390764
37	6	0	2.822136	1.095940	2.711705
38	1	0	2.866721	2.076824	3.190158
39	1	0	2.618261	0.348438	3.485596
40	1	0	3.795786	0.878535	2.252849
41	8	0	2.008057	2.058524	0.729447
42	6	0	1.244314	3.251883	0.937131
43	1	0	1.651980	3.839693	1.770661
44	1	0	1.308165	3.811793	-0.000015
45	1	0	0.198564	3.004642	1.136579
46	1	0	2.146949	1.083469	-2.479480
47	8	0	1.238615	1.364490	-2.316659
48	1	0	0.884799	3.223982	-2.349089
49	1	0	1.078851	1.141709	-1.382013
50	1	0	-0.328398	4.014326	-1.900289
51	8	0	0.592485	4.136689	-2.166737

Sum of electronic and zero-point Energies= -1617.847868
Zero-point correction= 0.408154 (Hartree/Particle)
No imaginary frequency

TS6D'-7D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	-1.576478	-0.284925	0.038929
2	1	0	1.074835	-0.109067	1.678564
3	6	0	-3.041137	-2.369558	-0.636695
4	6	0	-2.066522	-2.156821	-1.659920
5	6	0	-2.362695	-2.753281	0.534450
6	1	0	-4.108584	-2.226572	-0.736490
7	6	0	-0.792153	-2.484570	-1.122138
8	1	0	-2.271895	-1.878233	-2.685738
9	6	0	-0.966146	-2.816466	0.237090
10	1	0	-2.809928	-2.946072	1.500171
11	1	0	0.153113	-2.417944	-1.642454
12	1	0	-0.183656	-3.078231	0.935498

13	6	0	-2.139086	2.253968	-0.262201
14	6	0	-2.454455	1.612960	-1.487603
15	6	0	-3.042675	1.779615	0.718540
16	1	0	-1.315587	2.937642	-0.104197
17	6	0	-3.575277	0.763357	-1.267073
18	1	0	-1.942579	1.764021	-2.428783
19	6	0	-3.935373	0.861510	0.098723
20	1	0	-3.043466	2.050714	1.764869
21	1	0	-4.068822	0.157277	-2.014674
22	1	0	-4.741403	0.330226	0.588052
23	17	0	-1.240090	-0.301853	2.554031
24	7	0	2.309653	1.382040	1.119743
25	6	0	1.821684	0.171161	0.942399
26	8	0	0.212162	0.281074	-0.345288
27	6	0	2.587821	-0.899878	0.280745
28	6	0	2.776786	-2.101620	0.976922
29	6	0	3.122677	-0.794784	-1.009763
30	1	0	2.361141	-2.221229	1.976454
31	7	0	3.459041	-3.145049	0.492364
32	6	0	3.828005	-1.876189	-1.523929
33	1	0	2.947753	0.096218	-1.601657
34	6	0	3.974036	-3.022174	-0.735470
35	1	0	4.253952	-1.841127	-2.521645
36	1	0	4.520995	-3.883749	-1.114232
37	1	0	0.579724	1.670630	-3.020817
38	8	0	0.939089	1.962285	-2.175555
39	1	0	0.630320	1.288034	-1.487057
40	1	0	0.672103	3.526673	-1.328857
41	8	0	0.638532	4.255487	-0.670723
42	1	0	-0.057595	4.848034	-0.977100
43	6	0	1.658663	2.417986	1.918573
44	1	0	1.232658	3.185974	1.265151
45	1	0	0.857384	1.946392	2.489841
46	1	0	2.402226	2.851759	2.591936
47	8	0	3.546631	1.709194	0.574738
48	6	0	3.500750	2.764118	-0.416497
49	1	0	4.550235	2.901890	-0.682391
50	1	0	2.909688	2.465359	-1.284694
51	1	0	3.096466	3.690645	-0.002506

Sum of electronic and zero-point Energies= -1617.824894
Zero-point correction= 0.406799 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

7D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	-1.880673	-0.209891	0.004780
2	1	0	1.195081	-0.100398	0.916590
3	6	0	-3.947456	-1.883011	0.010238
4	6	0	-3.142658	-2.166089	-1.135592
5	6	0	-3.198712	-2.204602	1.156216
6	1	0	-4.940752	-1.455000	-0.003809
7	6	0	-1.923734	-2.737935	-0.681377
8	1	0	-3.441728	-2.047579	-2.169297
9	6	0	-1.937599	-2.726882	0.728290
10	1	0	-3.504899	-2.062578	2.184069
11	1	0	-1.102640	-3.054845	-1.309361
12	1	0	-1.140410	-3.057012	1.380357
13	6	0	-1.891922	2.359980	-0.502397

14	6	0	-2.391835	1.720897	-1.662031
15	6	0	-2.851021	2.195911	0.533474
16	1	0	-0.934038	2.854832	-0.418283
17	6	0	-3.655248	1.152671	-1.341797
18	1	0	-1.887716	1.654330	-2.617069
19	6	0	-3.943360	1.460560	0.015175
20	1	0	-2.751503	2.549701	1.550287
21	1	0	-4.298652	0.610905	-2.022498
22	1	0	-4.829625	1.167926	0.562484
23	17	0	-1.007218	0.125127	2.401778
24	7	0	2.641497	1.282929	1.079275
25	6	0	2.259480	0.084050	0.766308
26	8	0	-0.180005	-0.255158	-0.773382
27	6	0	3.069354	-0.992770	0.225868
28	6	0	2.363559	-2.018589	-0.443931
29	6	0	4.464940	-1.124992	0.362286
30	1	0	1.290023	-1.903415	-0.587163
31	7	0	2.952254	-3.100468	-0.957972
32	6	0	5.072472	-2.258139	-0.161564
33	1	0	5.041710	-0.370597	0.880865
34	6	0	4.278607	-3.210591	-0.808457
35	1	0	6.142782	-2.409889	-0.068203
36	1	0	4.732428	-4.109335	-1.222630
37	6	0	1.790273	2.320384	1.676579
38	1	0	0.865760	1.849167	2.017030
39	1	0	2.342599	2.743300	2.517818
40	1	0	1.578583	3.080634	0.916795
41	8	0	3.958894	1.671193	0.872921
42	6	0	4.102496	2.360491	-0.407120
43	1	0	3.533098	3.291913	-0.415370
44	1	0	5.173485	2.553168	-0.475526
45	1	0	3.757060	1.716831	-1.219362
46	1	0	0.702361	0.689808	-1.594747
47	8	0	1.338910	1.318672	-2.091537
48	1	0	1.214788	1.126672	-3.028044
49	1	0	1.254586	2.941498	-1.553060
50	8	0	1.317576	3.813199	-1.085913
51	1	0	0.612188	4.359933	-1.450158

Sum of electronic and zero-point Energies= -1617.828959
Zero-point correction= 0.406579 (Hartree/Particle)
No imaginary frequency

TS_{7D-8D}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	2.038702	0.177195	-0.015493
2	1	0	-1.330189	0.006458	0.722893
3	6	0	4.231434	1.613361	0.173037
4	6	0	3.496374	2.075825	-0.961522
5	6	0	3.484103	1.917218	1.327069
6	1	0	5.179576	1.093647	0.144464
7	6	0	2.327851	2.729205	-0.486570
8	1	0	3.809663	2.007728	-1.995431
9	6	0	2.298025	2.602297	0.917086
10	1	0	3.744423	1.663464	2.345953
11	1	0	1.553167	3.163304	-1.102681
12	1	0	1.514643	2.951819	1.575409
13	6	0	1.759345	-2.321567	-0.707911
14	6	0	2.365389	-1.662152	-1.805771

S20

15	6	0	2.697044	-2.335409	0.360277
16	1	0	0.758648	-2.734811	-0.689725
17	6	0	3.666799	-1.250953	-1.412225
18	1	0	1.904368	-1.471246	-2.765703
19	6	0	3.873970	-1.678787	-0.069970
20	1	0	2.527292	-2.745993	1.345708
21	1	0	4.385769	-0.734774	-2.034405
22	1	0	4.768825	-1.525531	0.518552
23	17	0	1.010621	-0.249364	2.280766
24	7	0	-2.812658	-1.304514	1.054553
25	6	0	-2.389521	-0.173979	0.561228
26	8	0	0.385693	0.510198	-0.906697
27	6	0	-3.197559	0.958278	0.107964
28	6	0	-2.493679	2.028648	-0.486973
29	6	0	-4.582504	1.104576	0.295110
30	1	0	-1.419510	1.934427	-0.644018
31	7	0	-3.074117	3.157618	-0.896229
32	6	0	-5.186544	2.285999	-0.122841
33	1	0	-5.158314	0.322061	0.771370
34	6	0	-4.397126	3.274108	-0.713392
35	1	0	-6.252208	2.441872	0.010234
36	1	0	-4.846021	4.206316	-1.051749
37	6	0	-1.957871	-2.337297	1.645967
38	1	0	-1.005453	-1.880844	1.922233
39	1	0	-2.469001	-2.716207	2.532711
40	1	0	-1.795253	-3.130875	0.911245
41	8	0	-4.144350	-1.690988	0.929039
42	6	0	-4.408653	-2.294304	-0.369189
43	1	0	-3.654556	-3.044522	-0.618282
44	1	0	-5.394657	-2.745875	-0.251050
45	1	0	-4.433853	-1.524343	-1.145241
46	1	0	-0.487267	-0.154989	-1.289167
47	8	0	-1.518620	-0.819119	-1.520938
48	1	0	-1.966870	-0.416714	-2.276339
49	1	0	-1.482313	-2.476221	-1.486461
50	8	0	-1.524828	-3.452300	-1.278434
51	1	0	-1.076523	-3.901211	-2.004106

Sum of electronic and zero-point Energies= -1617.826376
Zero-point correction= 0.403532 (Hartree/Particle)
One imaginary frequency, one negative Eigenvalue

8D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	2.164541	0.172984	0.006001
2	1	0	-1.568902	-0.066862	0.815511
3	6	0	4.253464	1.667512	0.195910
4	6	0	3.503704	2.142513	-0.922302
5	6	0	3.500426	1.921546	1.363949
6	1	0	5.224261	1.192933	0.153595
7	6	0	2.312595	2.734757	-0.427071
8	1	0	3.811713	2.105038	-1.959187
9	6	0	2.294322	2.577419	0.975169
10	1	0	3.776167	1.653748	2.375146
11	1	0	1.513951	3.145902	-1.027786
12	1	0	1.497041	2.876503	1.641181
13	6	0	1.948638	-2.312423	-0.704575
14	6	0	2.559669	-1.632457	-1.790324
15	6	0	2.866277	-2.303554	0.380267

S21

16	1	0	0.970180	-2.779969	-0.708996
17	6	0	3.836068	-1.179006	-1.370469
18	1	0	2.118549	-1.457029	-2.762760
19	6	0	4.026247	-1.599851	-0.020353
20	1	0	2.687956	-2.725546	1.359034
21	1	0	4.550902	-0.638601	-1.976390
22	1	0	4.905966	-1.425166	0.584816
23	17	0	1.064225	-0.304770	2.195164
24	7	0	-3.194976	-1.224121	1.072385
25	6	0	-2.481080	-0.300782	0.258442
26	8	0	0.519287	0.567643	-1.036197
27	6	0	-3.248933	0.974984	-0.045991
28	6	0	-2.697738	1.924147	-0.921961
29	6	0	-4.469412	1.286275	0.563084
30	1	0	-1.724350	1.743858	-1.374032
31	7	0	-3.283014	3.088211	-1.230991
32	6	0	-5.086831	2.494579	0.248361
33	1	0	-4.919720	0.589638	1.258772
34	6	0	-4.461192	3.354740	-0.654561
35	1	0	-6.037405	2.766865	0.696617
36	1	0	-4.922000	4.304541	-0.921440
37	6	0	-2.455053	-2.315660	1.699933
38	1	0	-1.588982	-1.884342	2.208983
39	1	0	-3.108303	-2.776541	2.444376
40	1	0	-2.097238	-3.083500	1.003602
41	8	0	-4.457412	-1.647070	0.570312
42	6	0	-4.437974	-2.522857	-0.568099
43	1	0	-3.614891	-3.241165	-0.539845
44	1	0	-5.390345	-3.058787	-0.532028
45	1	0	-4.393244	-1.960865	-1.511268
46	1	0	-0.169944	-0.086530	-1.245096
47	8	0	-1.952727	-0.859406	-1.017977
48	1	0	-2.583334	-0.629460	-1.715563
49	1	0	-1.410734	-2.658293	-1.160230
50	8	0	-1.151230	-3.598735	-1.146001
51	1	0	-1.097349	-3.863996	-2.072154

-----Sum of

electronic and zero-point Energies=

-1617.843205

Zero-point correction=

0.408337 (Hartree/Particle)

No imaginary frequency

8D'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	2.564930	-0.078203	-0.113406
2	1	0	-2.485548	0.722586	-1.629738
3	6	0	5.065966	0.105039	-0.755136
4	6	0	4.422056	-0.629635	-1.796081
5	6	0	4.573791	1.429869	-0.791720
6	1	0	5.806228	-0.279127	-0.066294
7	6	0	3.552508	0.256807	-2.481502
8	1	0	4.601113	-1.666573	-2.046997
9	6	0	3.626618	1.520760	-1.849207
10	1	0	4.838437	2.225485	-0.109981
11	1	0	2.892640	-0.003800	-3.297129
12	1	0	3.046736	2.396197	-2.107205
13	6	0	1.391995	-1.454237	1.738028
14	6	0	1.351468	-2.261639	0.576849
15	6	0	2.754329	-1.337590	2.140985
16	1	0	0.541452	-0.998465	2.228231

S22

17	6	0	2.683158	-2.609777	0.230745
18	1	0	0.465451	-2.525869	0.015301
19	6	0	3.549590	-2.053603	1.219531
20	1	0	3.112867	-0.770601	2.988860
21	1	0	2.981626	-3.231333	-0.602861
22	1	0	4.624726	-2.164771	1.256047
23	17	0	2.233372	1.840027	1.447706
24	7	0	-2.705138	1.392195	0.380120
25	6	0	-2.720306	0.305323	-0.640484
26	8	0	0.922312	0.118265	-1.193861
27	6	0	-4.078806	-0.372688	-0.704709
28	6	0	-4.523773	-1.231912	0.307654
29	6	0	-4.923892	-0.180489	-1.799264
30	1	0	-3.892696	-1.419365	1.173340
31	7	0	-5.702052	-1.864960	0.295394
32	6	0	-6.152694	-0.836124	-1.834633
33	1	0	-4.622423	0.477133	-2.610297
34	6	0	-6.495621	-1.663239	-0.764577
35	1	0	-6.832094	-0.710104	-2.671793
36	1	0	-7.448662	-2.189229	-0.757263
37	6	0	-1.536104	2.273671	0.225618
38	1	0	-0.621463	1.696704	0.362179
39	1	0	-1.523462	2.747577	-0.764549
40	1	0	-1.581655	3.047315	0.994298
41	8	0	-3.855516	2.217332	0.097641
42	6	0	-4.644331	2.363093	1.269956
43	1	0	-4.071052	2.819175	2.087672
44	1	0	-5.462895	3.031574	0.990214
45	1	0	-5.057414	1.403374	1.603939
46	1	0	0.043290	-0.217714	-0.933039
47	8	0	-1.672019	-0.596159	-0.343082
48	1	0	-1.724568	-0.829648	0.609228
49	1	0	-2.459828	-0.830890	3.065125
50	8	0	-1.886316	-0.449351	2.389639
51	1	0	-2.328410	0.364932	2.064345

Sum of electronic and zero-point Energies= -1617.856798
Zero-point correction= 0.409308 (Hartree/Particle)
No imaginary frequency

TS_{8D'}-9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	40	0	2.516787	-0.085998	-0.098908
2	1	0	-2.296926	0.337325	-1.633073
3	6	0	4.876969	-0.649413	-1.022001
4	6	0	3.926135	-1.324592	-1.846826
5	6	0	4.715103	0.738071	-1.218645
6	1	0	5.588128	-1.120785	-0.357450
7	6	0	3.221912	-0.342749	-2.591098
8	1	0	3.804401	-2.396288	-1.934199
9	6	0	3.681014	0.928085	-2.184947
10	1	0	5.257229	1.524772	-0.711821
11	1	0	2.405989	-0.533208	-3.273421
12	1	0	3.306315	1.883058	-2.526409
13	6	0	1.352748	-0.802731	2.105007
14	6	0	1.518285	-1.986311	1.340304
15	6	0	2.644350	-0.346267	2.482255
16	1	0	0.407833	-0.334338	2.353009

17	6	0	2.907297	-2.243751	1.215705
18	1	0	0.722408	-2.569157	0.895834
19	6	0	3.605966	-1.225161	1.931343
20	1	0	2.854914	0.546154	3.054249
21	1	0	3.356873	-3.082160	0.700630
22	1	0	4.678485	-1.148587	2.049158
23	17	0	2.376961	2.307173	0.616578
24	7	0	-2.585890	1.385940	0.209483
25	6	0	-2.601551	0.040864	-0.619061
26	8	0	0.777216	-0.219347	-1.006320
27	6	0	-4.012114	-0.525145	-0.655224
28	6	0	-4.379715	-1.581519	0.185840
29	6	0	-4.971688	-0.052668	-1.556810
30	1	0	-3.642682	-2.007119	0.861413
31	7	0	-5.597078	-2.139891	0.202975
32	6	0	-6.238831	-0.629406	-1.561044
33	1	0	-4.727821	0.753260	-2.243137
34	6	0	-6.503232	-1.661326	-0.657794
35	1	0	-7.007160	-0.292103	-2.249725
36	1	0	-7.485522	-2.130113	-0.630309
37	6	0	-1.447315	2.252482	-0.166556
38	1	0	-0.535264	1.655347	-0.170818
39	1	0	-1.630097	2.664263	-1.161675
40	1	0	-1.362084	3.058018	0.563238
41	8	0	-3.773406	2.155302	0.028547
42	6	0	-4.557545	2.189925	1.225562
43	1	0	-3.992448	2.626304	2.057353
44	1	0	-5.406487	2.831832	0.983684
45	1	0	-4.920023	1.193254	1.498570
46	1	0	-0.084536	-0.538219	-0.643303
47	8	0	-1.676054	-0.772350	-0.028382
48	1	0	-1.749851	-0.560394	1.146752
49	1	0	-2.549466	-0.367818	2.780019
50	8	0	-1.926115	0.069984	2.186628
51	1	0	-2.431092	0.963294	1.298851

Sum of electronic and zero-point Energies= -1617.836182
Zero-point correction= 0.403932 (Hartree/Particle)
One imaginary frequency, one negative Eigenval

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	3.466130	1.766155	-2.512052
2	6	0	3.170789	0.745579	-2.305951
3	6	0	1.859679	0.211483	-2.435781
4	6	0	4.038166	-0.321554	-1.928611
5	6	0	1.902870	-1.156891	-2.089834
6	1	0	0.974284	0.767725	-2.712587
7	6	0	3.254806	-1.486714	-1.773769
8	1	0	5.106313	-0.245918	-1.777273
9	1	0	1.055334	-1.828135	-2.040177
10	1	0	3.608727	-2.460663	-1.463483
11	40	0	2.491626	0.141548	0.075489
12	1	0	-3.058488	-0.535533	-0.111947
13	17	0	1.571558	-1.945956	1.132509
14	6	0	4.803353	0.331067	1.195769
15	6	0	4.475890	1.628328	0.699066

S24

16	6	0	3.907198	0.032079	2.249244
17	1	0	5.600903	-0.307203	0.839266
18	6	0	3.388528	2.126229	1.462242
19	1	0	4.991886	2.155379	-0.092507
20	6	0	3.023351	1.134790	2.404556
21	1	0	3.873312	-0.890028	2.811813
22	1	0	2.882102	3.068816	1.307826
23	1	0	2.197404	1.192958	3.099871
24	7	0	-3.704604	-3.369718	0.085599
25	6	0	-2.707279	0.439062	-0.492910
26	8	0	0.882648	1.291454	0.205550
27	6	0	-3.630419	1.560882	-0.283231
28	6	0	-3.305874	2.878081	-0.651223
29	6	0	-4.885546	1.315371	0.291973
30	1	0	-2.337119	3.084440	-1.100473
31	7	0	-4.127907	3.913096	-0.478467
32	6	0	-5.751486	2.388922	0.474033
33	1	0	-5.158924	0.300529	0.571617
34	6	0	-5.325058	3.658394	0.075298
35	1	0	-6.735069	2.254344	0.911959
36	1	0	-5.978869	4.518999	0.204830
37	1	0	0.113949	1.204358	-0.379217
38	8	0	-1.612946	0.531176	-1.051518
39	1	0	-2.804189	-3.062200	-0.302430
40	8	0	-1.044341	-2.295042	-0.967657
41	1	0	-0.410864	-2.370663	-0.234111
42	1	0	-1.115941	-1.334128	-1.111362
43	6	0	-4.648282	-3.561774	-1.006021
44	1	0	-4.815327	-2.661434	-1.618293
45	1	0	-4.245976	-4.350082	-1.650810
46	1	0	-5.612146	-3.895753	-0.610209
47	8	0	-4.163786	-2.206103	0.828935
48	6	0	-4.120070	-2.519513	2.213569
49	1	0	-3.097423	-2.731508	2.550156
50	1	0	-4.496590	-1.635704	2.739241
51	1	0	-4.753684	-3.383861	2.445242

Sum of electronic and zero-point Energies= -1617.858413
Zero-point correction= 0.406912 (Hartree/Particle)
No imaginary frequency