SUPPORTING INFORMATION

Substituent effects on the rate of formation of azomethine ylides.

A computational investigation.

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Energies in hartrees. Entropies in e.u. Unique imaginary frequencies for transition states (last entry) in cm^{-1}.

1 TS: E(HF) = -132.9731736; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.06424470; $E_{\alpha,\beta}$ = -0.43071506.
GS: E(HF) = -133.0764840; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.06074692; $E_{\alpha,\beta}$ = -0.41418843.

2 TS: E(HF) = -231.8590954; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.09539804. $E_{\alpha,\beta}$ = -0.5894450.
GS: E(HF) = -231.9611539; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ =-0.09106686; $E_{\alpha,\beta}$ = -0.5688007.

3 TS: E(HF) = -330.7224368; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1265345; $E_{\alpha,\beta}$ = -0.7522558.

GS: E(HF) = -330.8494111; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1217177; $E_{\alpha,\beta}$ = -0.7236328.

4 TS: E(HF) = -330.7509637; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1249954; $E_{\alpha,\beta}$ = -0.1213261.
GS: E(HF) = -330.8428943; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1213261; $E_{\alpha,\beta}$ = -0.7238220.

5 TS: E(HF) = =-330.7206697; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1270207; $E_{\alpha,\beta}$ = -0.7538292.

GS: E(HF) = =-330.839483; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1214898; $E_{\alpha,\beta}$ = -0.7239380.

6 TS: E(HF) = -429.591384; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1580039; $E_{\alpha,\beta}$ = -0.9123923.
E(MP2) = -430.8197841. TC = 0.052169. S = 76.292. -606.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.052814	-0.636208	-0.377709
2	6	0	-0.777009	-0.016490	0.306325
3	1	0	0.713993	-0.729465	-1.403694
4	7	0	0.169722	-0.936300	0.635343
5	1	0	0.431954	-1.168693	1.587931
6	9	0	1.923017	0.405086	-0.203663
7	9	0	-1.807756	-0.350457	-0.495979
8	9	0	-0.558464	1.319643	0.232605

GS: E(HF) = -429.7260775; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1522915; $E_{\alpha,\beta}$ = -0.8793555.
E(MP2) = -430.9100161. TC = 0.052169. S = 72.912.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.202499	-0.650188	1.017955
2	1	0	0.112928	-1.587180	1.266871
3	6	0	-0.823036	-0.478454	-0.291646
4	6	0	0.508993	0.037238	0.017608
5	1	0	-0.946904	-1.325211	-0.961265
6	9	0	-1.916797	0.342400	-0.308216
7	9	0	1.593263	-0.558339	-0.557057
8	9	0	0.783059	1.339384	0.222266

7 TS: E(HF) =-528.4609306; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1896662; $E_{\alpha,\beta}$ = -1.0794960.
E(MP2) = -529.9197591. TC = 0.042788. S = 77.359. -120.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.104481	0.113072	-0.128621
2	6	0	-1.104677	-0.112916	-0.128936
3	7	0	-0.000073	-0.001529	0.663167
4	1	0	-0.000239	-0.001521	1.701683
5	9	0	2.144768	0.660242	0.530261
6	9	0	1.523164	-0.984258	-0.796910
7	9	0	-1.522287	0.986207	-0.795044
8	9	0	-2.145431	-0.660937	0.528525

GS: E(HF) = =-528.6074072; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0870415; $E_{\alpha,\beta}$ = -0.5508833.
MP2=-530.0092453. S = 76.904.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.731981	-0.031591	0.019339
2	6	0	0.731981	-0.031588	0.019338
3	7	0	0.000000	-0.080508	1.244813
4	1	0	-0.000009	0.749987	1.839382
5	9	0	1.498264	-1.093778	-0.284092
6	9	0	-1.498266	-1.093773	-0.284101
7	9	0	1.387984	1.104477	-0.315082
8	9	0	-1.387981	1.104479	-0.315074

8 TS: E(HF) = =-591.9066081; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0907129; $E_{\alpha,\beta}$ = -0.5642077.
E(MP2)=-592.6522418.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.082909	-0.043345	0.553524
2	6	0	-1.956097	-0.420804	-0.216353

3	1	0	-0.182900	-0.508426	1.522682
4	1	0	-2.970498	-0.386347	0.175760
5	1	0	-1.629166	-1.247516	-0.833800
6	7	0	-1.087249	0.634509	-0.029129
7	1	0	-1.093267	1.588132	-0.390250
8	17	0	1.512977	-0.064854	-0.134913

GS: E(HF) = HF=-592.0052914; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.087046; $E_{\alpha,\beta}$ = -0.5508833.
E(MP2) = =-592.730258.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.219895	-0.718821	-0.382474
2	1	0	-1.884472	-1.297456	0.133513
3	6	0	-0.259381	-0.103311	0.506578
4	6	0	-1.343806	0.720502	-0.058620
5	1	0	-0.272983	-0.351755	1.563123
6	1	0	-2.133788	1.051602	0.611158
7	1	0	-1.125975	1.376214	-0.894228
8	17	0	1.386800	0.032353	-0.083764

9 TS: E(HF) = HF=-1050.8122527; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1174402; $E_{\alpha,\beta}$ = -0.7022318.
E(MP2)= -1051.749365.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016685	-0.127577	0.025038
2	6	0	1.825451	-1.103285	-0.414874
3	1	0	2.866315	-0.930914	-0.153540
4	1	0	1.525457	-1.340089	-1.426909
5	7	0	0.829984	-1.044375	0.550256
6	1	0	0.666608	-1.634838	1.371465
7	17	0	-1.675645	-0.478830	-0.101298
8	17	0	0.386169	1.573044	0.024605

GS: E(HF) = =-1050.9206303; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1128502; $E_{\alpha,\beta}$ = -0.6797526.
E(MP2)=-1051.8260834.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.121790	1.529991	-0.671074
2	6	0	-0.004378	0.222572	-0.003865
3	7	0	0.051559	1.396904	0.811912
4	1	0	0.961059	1.507750	1.263992
5	17	0	1.385423	-0.857136	-0.032836
6	17	0	-1.523575	-0.645846	-0.005266
7	1	0	1.077132	1.760155	-1.134922
8	1	0	-0.755008	1.989070	-1.115090

10 TS: E(HF) = -1050.8362899. $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1171584; $E_{\alpha,\beta}$ = -0.6981609. E(MP2)=-1051.7687677.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.932170	-0.179716	0.456941
2	6	0	-0.932170	-0.179718	-0.456940
3	7	0	0.000000	0.688328	0.000000
4	1	0	0.000000	1.712606	-0.000002
5	1	0	0.720466	-0.877990	1.253244
6	17	0	2.573066	-0.077009	-0.079068
7	17	0	-2.573067	-0.077009	0.079068
8	1	0	-0.720464	-0.877994	-1.253239

GS: E(HF) = =-1050.9278637; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1122154; $E_{\alpha,\beta}$ = -0.6772567. E(MP2) = -1051.8295514.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.033454	1.349936	0.095035
2	1	0	-0.521442	1.866214	-0.590751
3	6	0	0.558009	0.104074	-0.441361
4	6	0	-0.565084	0.093334	0.511350

5	1	0	0.354530	-0.160865	-1.474444
6	1	0	-0.420772	-0.172290	1.552440
7	17	0	-2.155434	-0.368050	-0.071990
8	17	0	2.178725	-0.347659	0.038318

11 TS: E(HF) = -1050.819831; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1174331; $E_{\alpha,\beta}$ = -0.7012569. MP2=-1051.7559542

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213062	0.875101	0.126794
2	6	0	0.850026	0.651515	0.483232
3	7	0	-0.018735	1.277714	-0.361588
4	1	0	0.208778	1.836296	-1.187748
5	1	0	-2.013520	1.573845	0.350421
6	17	0	-1.766681	-0.775521	-0.028469
7	17	0	1.963911	-0.535616	-0.080060
8	1	0	0.761199	0.775481	1.553274

GS: E(HF) = =-1050.9237605; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1124518; $E_{\alpha,\beta}$ = -0.6778688. MP2=-1051.8265329.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000093	1.382711	-0.653866
2	1	0	0.000048	2.401275	-0.581781
3	6	0	-0.740341	0.712609	0.397585
4	6	0	0.740405	0.712554	0.397614
5	1	0	1.249214	1.298233	1.158474
6	17	0	1.681464	-0.683203	-0.056743
7	17	0	-1.681534	-0.683139	-0.056738
8	1	0	-1.249110	1.298365	1.158361

12 TS: E(HF) = =-2704.7676279; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1510553; $E_{\alpha,\beta}$ = -0.7756407.

E(MP2)=-2705.8453793.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675996	0.004474	0.603860
2	6	0	-2.500931	-0.447811	-0.230445
3	1	0	-0.811211	-0.411984	1.591110
4	1	0	-3.531797	-0.410745	0.116320
5	1	0	-2.129380	-1.303062	-0.780284
6	7	0	-1.658505	0.631826	-0.062914
7	1	0	-1.660329	1.563155	-0.478335
8	35	0	1.108680	-0.034289	-0.064254

GS: E(HF) = =-2704.8640316; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1465729; $E_{\alpha,\beta}$ = -0.7562652.
E(MP2)=-2705.9134427

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.815822	-0.047174	0.592468
2	6	0	-1.840222	0.697581	-0.162624
3	1	0	-0.837000	-0.149165	1.671025
4	1	0	-1.512711	1.213672	-1.060438
5	1	0	-2.687359	1.136796	0.354083
6	7	0	-1.807399	-0.789342	-0.148347
7	1	0	-1.431261	-1.163257	-1.020629
8	35	0	1.001611	0.016712	-0.042419

13 TS: E(HF) = =-5276.535317; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2380939; $E_{\alpha,\beta}$ = -1.1245175.
E(MP2)=-5278.1360225.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013167	0.498908	0.046677
2	6	0	-0.858205	2.356004	-0.433865
3	1	0	-1.808559	2.831900	-0.204591

4	1	0	-0.450215	2.352538	-1.435949
5	7	0	-0.120034	1.725398	0.556030
6	1	0	0.316017	2.102680	1.402715
7	35	0	1.697230	-0.310926	-0.046732
8	35	0	-1.468338	-0.731771	0.008696

GS: E(HF) = HF=-5276.6399567; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2334707; $E_{\alpha,\beta}$ = -1.1022088. E(MP2)=-5278.2091069.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.048073	1.874523	-0.679791
2	6	0	-0.004752	0.574003	0.006591
3	1	0	-0.849572	2.269968	-1.131456
4	1	0	0.988137	2.151977	-1.136843
5	7	0	-0.020647	1.753926	0.808698
6	1	0	0.877580	1.918516	1.255954
7	35	0	1.585959	-0.499838	-0.014383
8	35	0	-1.618289	-0.451851	-0.003027

1 **$R^1 = CH_3$. (see S43.)**

2 **$R^1 = CH_3$.**

TS: E(HF) = -270.9034668; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1138042; $E_{\alpha,\beta}$ = -0.7217554. E(MP2) = -271.8528308. TC = 0.093709. S = 74.736.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.776532	-0.393959	0.368090
2	6	0	-0.970572	-1.304875	-0.179185
3	1	0	1.096181	-0.938497	1.244269
4	1	0	-1.866868	-1.649221	0.336989
5	1	0	-0.588084	-1.846113	-1.033544
6	7	0	-0.471433	-0.043275	0.078299
7	9	0	1.816459	0.292936	-0.239689
8	6	0	-1.113558	1.259979	-0.003776
9	1	0	-1.170079	1.602024	-1.040662
10	1	0	-2.127336	1.155736	0.395687

11	1	0	-0.546328	1.975697	0.595590

GS: E(HF) = 270.9985413; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1095686; $E_{\alpha,\beta}$ = -0.7021727. E(MP2) \MP2=-271.9198514= -594.6759795. TC = 0.097215. S = 71.613.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.597876	-0.103801	0.398901
2	7	0	-0.501109	-0.049485	-0.498241
3	6	0	0.057579	1.215189	0.032704
4	1	0	-0.515752	1.758141	0.784330
5	1	0	0.580978	1.819687	-0.700117
6	6	0	-1.794200	-0.475302	0.029756
7	1	0	-2.583334	0.005976	-0.552371
8	1	0	-1.879308	-1.558667	-0.085738
9	1	0	-1.932530	-0.215142	1.090965
10	9	0	1.800633	-0.529317	-0.134955
11	1	0	0.464489	-0.516265	1.397049

3 **R^1 = CH_3.**

TS: E(HF) = -369.7665889; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1450493; $E_{\alpha,\beta}$ = -0.8850451. E(MP2) -370.9417327. TC = 0.086577. S = 78.102. -253.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.637345	0.096011	-0.200843
2	6	0	1.012937	1.366982	-0.439114
3	1	0	1.678215	1.953662	0.190178
4	1	0	0.793065	1.661558	-1.454553
5	7	0	0.673309	0.074367	-0.040690
6	9	0	-1.242280	-1.083984	-0.524248
7	9	0	-1.447556	0.734798	0.692245
8	6	0	1.565196	-1.002419	0.393453
9	1	0	1.954954	-1.550682	-0.467311
10	1	0	2.394390	-0.525390	0.923216
11	1	0	1.030013	-1.680476	1.060338

GS: E(HF) = -369.8858258; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1402017; $E_{\alpha,\beta}$ = -0.8572428.
E(MP2) = -371.0234722. TC = 0.089576. S = 75.625.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.536700	-0.018011	0.044664
2	9	0	-0.591643	1.234289	0.591669
3	6	0	0.105010	-1.091586	0.794875
4	7	0	0.673208	-0.492865	-0.468931
5	1	0	0.578534	-0.809538	1.734686
6	1	0	-0.228943	-2.119350	0.701415
7	9	0	-1.657109	-0.192764	-0.703256
8	6	0	1.870955	0.339393	-0.357584
9	1	0	2.740124	-0.319113	-0.401518
10	1	0	1.899528	1.021453	-1.209884
11	1	0	1.901472	0.924101	0.570375

4 **R^1 = CH_3.**

TS: E(HF) = -369.7822736; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1448539; $E_{\alpha,\beta}$ = -0.8814612.
E(MP2)= -370.9534427. TC = 0.086422. S = 83.153. -524.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.997807	-0.539891	0.435668
2	6	0	-0.939281	-0.643848	-0.356544
3	1	0	0.872024	-1.389329	1.089631
4	1	0	-0.849232	-1.390239	-1.130671
5	7	0	-0.000373	0.248414	-0.020113
6	9	0	2.228059	-0.444852	-0.177958
7	9	0	-2.209206	-0.479122	0.149199
8	6	0	-0.058672	1.711168	-0.004178
9	1	0	-0.589837	2.055012	-0.894113
10	1	0	-0.568879	2.058852	0.897058
11	1	0	0.969731	2.077993	-0.011969

GS: E(HF) = =-369.8795532; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1396462; $E_{\alpha,\beta}$ = -0.8568897.
E(MP2) = -371.0157355. TC = 0.090014. S = 77.154.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.785632	-0.006134	0.366207
2	7	0	0.164388	0.639127	-0.473526
3	6	0	0.143690	-0.797159	-0.449755
4	9	0	1.145426	-1.454702	0.257758
5	9	0	-2.115739	0.149050	0.024265
6	6	0	1.263273	1.421201	0.090231
7	1	0	2.057363	1.490941	-0.655427
8	1	0	0.884521	2.422907	0.300249
9	1	0	1.672739	0.982592	1.007262
10	1	0	-0.661227	0.001314	1.448215
11	1	0	-0.099280	-1.328217	-1.363928

5 $\mathbf{R^1 = CH_3}$**.**

TS: E(HF)= -369.8775273; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1397928; $E_{\alpha,\beta}$ = -0.8569893.
E(MP2) = -370.9424127. TC = 0.086250. S = 79.855. -358.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.108813	0.464956	0.400994
2	6	0	0.585426	-0.722453	0.630671
3	7	0	0.216355	0.539241	0.257166
4	9	0	1.055224	-1.579699	-0.333425
5	1	0	0.113846	-1.210218	1.477024
6	1	0	-1.736039	1.201921	0.892446
7	9	0	-1.836559	-0.332634	-0.474642
8	6	0	1.072164	1.579354	-0.300685
9	1	0	2.081939	1.430507	0.089411
10	1	0	1.077354	1.531420	-1.392877
11	1	0	0.687773	2.551540	0.020549

GS: E(HF)= -369.8775273; $E_{\alpha,\alpha} = E_{\beta,\beta}$ -0.1397928; $E_{\alpha,\beta}$ = -0.8569893.
E(MP2) = -371.0141022. TC = 0.090049. S = 77.302.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.664458	0.000014	-0.383713

2	6	0	0.240976	-0.736809	0.432912
3	6	0	0.240982	0.736804	0.432981
4	1	0	-0.118538	-1.302961	1.291675
5	9	0	1.222599	-1.437362	-0.229191
6	9	0	1.222554	1.437378	-0.229218
7	6	0	-2.100186	-0.000015	-0.124196
8	1	0	-2.534720	0.889212	-0.584998
9	1	0	-2.534861	-0.888694	-0.585926
10	1	0	-2.339247	-0.000562	0.948885
11	1	0	-0.118438	1.302887	1.291852

6 R^1 = CH_3•

TS: E(HF) = =-468.6513005; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1739622; $E_{\alpha,\beta}$ = -1.0359635. E(MP2) = -470.0351885. TC = 0.080282. S = 86.301. -580.8.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.270433	-0.628710	-0.490895
2	6	0	1.028683	-0.194783	-0.078551
3	1	0	-1.030316	-1.688946	-0.545471
4	7	0	-0.238585	0.193516	-0.100093
5	9	0	-2.421511	-0.400355	0.256497
6	9	0	2.036133	0.692565	-0.036787
7	9	0	1.390531	-1.451566	0.212220
8	6	0	-0.519637	1.633440	0.073127
9	1	0	-0.075851	2.191984	-0.750986
10	1	0	-1.600650	1.749053	0.064661
11	1	0	-0.101143	1.967820	1.022989

GS: E(HF) = -468.7642667; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1706187; $E_{\alpha,\beta}$ = -1.0124804. E(MP2) = -470.1179848. TC = 0.082452. S = 81.433.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.431072	-0.584466	-0.498457
2	6	0	0.594753	-0.639372	0.516419

3	6	0	0.050793	0.623521	0.014760
4	1	0	0.348918	-0.973933	1.524089
5	9	0	1.815495	-1.124280	0.117752
6	9	0	-0.746524	1.360717	0.846844
7	9	0	0.697900	1.470619	-0.814595
8	6	0	-1.787677	-1.089343	-0.296938
9	1	0	-2.437360	-0.644320	-1.051882
10	1	0	-1.765711	-2.170702	-0.437980
11	1	0	-2.177400	-0.852127	0.699514

7 $\mathbf{R^1 = CH_3}$**.**

TS: E(HF) =-567.5025506; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2079301; $E_{\alpha,\beta}$ = -1.2118529. E(MP2) = -569.1302637. TC = 0.073527. S = 87.238. -125.0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.101622	-0.405248	0.138317
2	6	0	1.109964	-0.401886	-0.142291
3	7	0	0.000424	0.393005	-0.026908
4	9	0	-2.175889	0.295139	0.566741
5	9	0	-1.468329	-1.183532	-0.907105
6	9	0	1.454023	-1.151654	0.932773
7	9	0	2.199733	0.276921	-0.567598
8	6	0	-0.015466	1.878775	-0.001347
9	1	0	0.035797	2.231806	1.030285
10	1	0	0.850533	2.228468	-0.559047
11	1	0	-0.932390	2.226983	-0.474251

GS: E(HF)= -567.6466538; $E_{\alpha,\alpha} = E_{\beta,\beta}$ -0.2015726; $E_{\alpha,\beta}$ = -1.1685622. E(MP2)= -569.2183613. TC = 0.074899. S = 85.643.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.732959	-0.323883	0.044369
2	7	0	0.000002	0.581232	-0.757010
3	6	0	0.732958	-0.323888	0.044368
4	9	0	-1.380093	0.139274	1.146604
5	9	0	1.524719	-1.229054	-0.569057

6	9	0	1.380091	0.139272	1.146602
7	9	0	-1.524725	-1.229042	-0.569062
8	6	0	0.000008	2.039451	-0.629898
9	1	0	0.888812	2.420261	-1.133421
10	1	0	-0.888938	2.420239	-1.133187
11	1	0	0.000138	2.356744	0.416851

8 $\mathbf{R^1 = CH_3}$**.**

TS: E(HF) =-630.9506285; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1093317; $E_{\alpha,\beta}$ = -0.6971710.
E(MP2)= - 631.8664629. TC = 0.092709. S = 77.316. -476.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.255886	-0.504575	0.538904
2	6	0	-1.446236	-1.220775	-0.299150
3	1	0	0.382933	-1.188235	1.366054
4	1	0	-2.396910	-1.596316	0.080975
5	1	0	-0.954027	-1.715839	-1.128907
6	7	0	-0.937113	-0.023318	0.158397
7	17	0	1.742611	0.114707	-0.145584
8	6	0	-1.397126	1.339616	-0.029387
9	1	0	-1.118672	1.718782	-1.018363
10	1	0	-2.487629	1.333925	0.056843
11	1	0	-0.965432	1.975288	0.747353

GS: E(HF) = -631.0410536; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1050776001D; $E_{\alpha,\beta}$ = -0.6789517.
E(MP2) = -631.9301605. TC = 0.096186. S = 73.961.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.904836	-0.072631	-0.497105
2	6	0	0.582910	1.274691	-0.002401
3	6	0	-0.153148	0.079179	0.461712
4	1	0	0.125419	1.934654	-0.732298
5	1	0	1.271315	1.743043	0.701641
6	1	0	0.009817	-0.280600	1.475334
7	17	0	-1.791989	-0.259550	-0.068718
8	6	0	2.132205	-0.679253	0.011100

9	1	0	2.032883	-1.766242	-0.044083
10	1	0	2.962991	-0.366475	-0.625974
11	1	0	2.355731	-0.391318	1.050862

9 $R^1 = CH_3$•

TS: E(HF) = -1089.8569161; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1363001; $E_{\alpha,\beta}$ -0.8358637.
E(MP2) = -1090.9653802. TC = 0.084244. S = 83.778. -347.9.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.187458	-0.029005	0.160539
2	6	0	1.333190	-1.135838	1.035223
3	1	0	1.795156	-2.098181	0.818266
4	1	0	1.077733	-0.847346	2.047199
5	7	0	1.122632	-0.215783	0.020222
6	17	0	-0.809107	1.596496	0.251798
7	17	0	-1.377159	-1.190951	-0.371261
8	6	0	2.090669	0.455054	-0.835438
9	1	0	2.470037	1.363694	-0.357780
10	1	0	2.918480	-0.243703	-0.986104
11	1	0	1.628281	0.700479	-1.794212

GS: E(HF) =-1089.9571031; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1318726; $E_{\alpha,\beta}$ = -0.8141888.
E(MP2) = -1091.0350372. TC = 0.087295. S = 80.484.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.535939	-0.841181	1.237397
2	6	0	0.179749	-0.096478	0.179176
3	1	0	-0.074486	-1.707499	1.702534
4	1	0	-1.218176	-0.260787	1.859386
5	7	0	-0.861056	-0.987421	-0.195151
6	17	0	-0.057936	1.648165	0.079405
7	17	0	1.803204	-0.552777	-0.312815
8	6	0	-2.137659	-0.493086	-0.700431
9	1	0	-2.009554	-0.206644	-1.746583
10	1	0	-2.853069	-1.315734	-0.641736
11	1	0	-2.523768	0.365478	-0.136433

10 $R^1 = CH_3$.

TS: E(HF) = -1089.8801655; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1360511; $E_{\alpha,\beta}$ = -0.8320935.
E(MP2) = -1090.9843613. TC = 0.084846. S = 86.000. -394.301.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.917392	-0.435408	0.456103
2	6	0	-0.909490	-0.475171	-0.469552
3	7	0	0.005279	0.426842	-0.050108
4	1	0	0.693015	-1.125164	1.257925
5	17	0	2.575077	-0.379831	-0.067641
6	17	0	-2.553709	-0.396970	0.088478
7	1	0	-0.694345	-1.204478	-1.237576
8	6	0	-0.048461	1.882235	0.003152
9	1	0	-0.571738	2.250745	-0.881400
10	1	0	-0.562820	2.214015	0.909925
11	1	0	0.979047	2.252666	0.009435

GS: E(HF) = -1089.9648253; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1310966; $E_{\alpha,\beta}$ = -0.8113941.
E(MP2)= -1091.0384127. TC = 0.087858. S = 81.654.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.019713	0.963019	0.485423
2	6	0	0.651875	-0.015803	-0.356461
3	6	0	-0.439932	-0.407062	0.558309
4	1	0	0.434861	-0.009066	-1.423567
5	1	0	-0.246233	-0.923424	1.492660
6	17	0	-1.983641	-0.901903	-0.135147
7	17	0	2.333168	-0.411859	-0.046637
8	6	0	-0.773664	2.023885	-0.129706
9	1	0	-1.508198	2.371293	0.599670
10	1	0	-0.093927	2.843872	-0.369577
11	1	0	-1.296121	1.704026	-1.039661

11 $R^1 = CH_3$.

TS: E(HF) =-1089.8652701; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1362738; $E_{\alpha,\beta}$ -0.8346836.
E(MP2) = -1090.9725015. TC = 0.084602. S = 84.598. -412.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.197104	0.537346	0.564639
2	6	0	0.790162	-0.009955	0.812433
3	7	0	0.042023	1.000740	0.293551
4	1	0	-1.952995	1.164440	1.032679
5	17	0	-1.886346	-0.839529	-0.277647
6	17	0	1.824174	-0.980444	-0.179709
7	1	0	0.691243	-0.306775	1.847333
8	6	0	0.463577	2.118362	-0.536618
9	1	0	-0.239846	2.940306	-0.373396
10	1	0	1.468734	2.420324	-0.233443
11	1	0	0.455829	1.841536	-1.595693

GS: E(HF) = =-1089.9630547; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1311755; $E_{\alpha,\beta}$ = -0.8116820.
E(MP2)= -1091.0370878. TC = 0.087767. S = 81.298.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.074459	-0.000010	-0.413878
2	6	0	-0.260345	-0.741579	0.514485
3	6	0	-0.260357	0.741575	0.514485
4	1	0	-0.743772	1.245639	1.350764
5	17	0	1.056878	1.693347	-0.122476
6	17	0	1.056906	-1.693329	-0.122476
7	1	0	-0.743751	-1.245652	1.350764
8	6	0	-2.520995	-0.000020	-0.212993
9	1	0	-2.934876	0.889563	-0.693196
10	1	0	-2.934865	-0.889602	-0.693211
11	1	0	-2.805666	-0.000031	0.850343

12 $R^1 = CH_3$.

TS: E(HF) = -2743.8110933; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1698774; $E_{\alpha,\beta}$ = -0.9091908.
E(MP2) = -2745.0600392. TC = 0.092147. S = 80.407. -510.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.357843	-0.552686	0.613688
2	6	0	-2.038000	-1.169110	-0.353570
3	1	0	-0.301061	-1.283882	1.407544
4	1	0	-3.025751	-1.510263	-0.042911
5	1	0	-1.503418	-1.676241	-1.149369
6	7	0	-1.502305	-0.012787	0.174662
7	35	0	1.335492	0.041800	-0.072944
8	6	0	-1.858196	1.377935	-0.033311
9	1	0	-1.479034	1.738111	-0.995809
10	1	0	-2.950026	1.444297	-0.029404
11	1	0	-1.442554	1.977637	0.779530

GS: E(HF) = =-2743.8988392; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1655337; $E_{\alpha,\beta}$ = -0.8905023. E(MP2)= -2745.120409. TC = 0.095778. S = 76.814.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.384519	-1.172346	0.513462
2	6	0	-0.434991	-0.739313	-0.537009
3	1	0	-1.970723	-2.080153	0.401606
4	1	0	-1.127560	-0.894520	1.535271
5	7	0	-1.700025	-0.082222	-0.427561
6	6	0	-1.797011	1.280505	0.082769
7	1	0	-1.511301	1.971375	-0.713827
8	1	0	-2.839220	1.460483	0.355147
9	1	0	-1.158044	1.460004	0.956903
10	35	0	1.212902	0.107138	0.044152
11	1	0	-0.245417	-1.304542	-1.442842

13 **R^1 = CH_3.**

TS: E(HF) = -5315.579906; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2570558; $E_{\alpha,\beta}$ = -1.2582594. E(MP2) = -5317.3522771. TC = 0.083456. S = 89.885. -346.4.

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.000441	0.283196	0.214293
2	6	0	0.534522	2.051899	1.152083
3	1	0	1.359850	2.751549	1.023414
4	1	0	0.209400	1.732739	2.134112
5	7	0	-0.169204	1.590395	0.052612
6	35	0	-1.515522	-0.866849	0.092014
7	35	0	1.657344	-0.596419	-0.157203
8	6	0	-0.894598	2.334317	-0.965967
9	1	0	-1.926012	2.519061	-0.650295
10	1	0	-0.376536	3.289737	-1.093943
11	1	0	-0.882953	1.772071	-1.902389

GS: E(HF) = =-5315.6756263; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2526767; $E_{\alpha,\beta}$ = -1.2370700. E(MP2) = -5317.4180498. TC = 0.086382. S = 86.448.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.314408	1.346414	1.307593
2	6	0	-0.005894	0.378900	0.237319
3	1	0	-0.483067	1.827530	1.866850
4	1	0	1.257194	1.189988	1.832684
5	7	0	0.367349	1.686065	-0.132871
6	6	0	1.634922	1.968992	-0.796590
7	1	0	1.555697	1.652784	-1.839065
8	1	0	1.793254	3.048555	-0.759818
9	1	0	2.484639	1.455898	-0.328793
10	35	0	1.222352	-1.098357	0.013738
11	35	0	-1.817774	-0.134301	-0.137500

14 TS: E(HF) = -158.2845428; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.07266217; $E_{\alpha,\beta}$ = -0.5036735. E(MP2)= -158.9335407.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.078509	-0.903965	0.085974
2	6	0	-0.191763	0.938017	0.228216
3	1	0	-0.212286	1.844347	-0.374496
4	1	0	-0.337303	1.100432	1.293243
5	7	0	-1.001568	-0.173814	-0.325267
6	1	0	-1.927308	-0.390519	0.041359
7	1	0	-0.077154	-1.691608	0.841402
8	5	0	1.301163	-0.016077	-0.152986
9	1	0	2.209127	-0.119767	0.624926
10	1	0	1.529606	0.349887	-1.269776

GS: E(HF) = -158.3335866; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.07010907; $E_{\alpha,\beta}$ = -0.4975095.
E(MP2) = -158.9713143.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.912498	-0.740683	-0.036311
2	1	0	-0.642188	-1.192435	-0.913152
3	6	0	-0.830970	0.692910	-0.170083
4	6	0	0.281044	-0.059250	0.554825
5	1	0	-1.517394	1.260411	0.449248
6	1	0	-0.618582	1.123821	-1.145734
7	1	0	0.225280	-0.016245	1.638559
8	5	0	1.603317	0.016367	-0.205877
9	1	0	1.600268	-0.204243	-1.384960
10	1	0	2.623071	0.329683	0.331150

15 TS: E(HF) = =-139.8043327; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0672443; $E_{\alpha,\beta}$ = -0.4485762.
GS: E(HF) = -139.8994718; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0639313; $E_{\alpha,\beta}$ = -0.4320218.

16 TS: E(HF) = =-359.6756380; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1621211; $E_{\alpha,\beta}$ = -0.9998139.
GS: E(HF) = -359.7720901; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1564237; $E_{\alpha,\beta}$ = -0.9714646.

17 TS: E(HF) = -505.5113459; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.19330466; $E_{\alpha,\beta}$ = -1.1405759. E(MP2) = -508.0385311. TC = 0.069958. -550.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.792473	-0.592081	0.584984
2	6	0	1.023611	-0.342405	-0.434884
3	1	0	2.369703	-0.627886	1.581341
4	7	0	2.237913	0.304271	-0.294045
5	1	0	2.711982	0.885209	-0.978518
6	1	0	3.674785	-1.184893	0.339399
7	6	0	-0.201802	0.337542	-0.120784
8	6	0	-1.414623	-0.229181	0.009903
9	9	0	-0.136177	1.687457	0.048250
10	9	0	-2.545602	0.426870	0.249421
11	9	0	-1.608403	-1.545127	-0.112381
12	1	0	0.991824	-1.368383	-0.786822

GS: E(HF) = =-506.6041612; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1890914; $E_{\alpha,\beta}$ = -1.1238172. E(MP2)= -508.1061612.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.382284	-0.000506	-0.611113
2	6	0	1.094685	-0.563480	-0.129243
3	1	0	3.034501	-0.661690	-1.176390
4	1	0	2.436896	1.050214	-0.872765
5	1	0	0.892071	-1.608396	-0.353183
6	6	0	-0.105222	0.275314	-0.031522
7	6	0	-1.363835	-0.165693	-0.012892
8	7	0	2.176844	-0.252079	0.825416
9	1	0	2.642435	-1.112956	1.119339
10	9	0	-1.680903	-1.464605	-0.073049
11	9	0	-2.444401	0.605370	0.054792
12	9	0	0.092939	1.617409	0.042002

18 TS: E(HF) = HF=-362.584976; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1829613; $E_{\alpha,\beta}$ = -1.1277753.
GS: E(HF) = =-362.6752185; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1786817; $E_{\alpha,\beta}$ = -1.1113974.

19 TS: E(HF) = -461.4637475; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2135238; $E_{\alpha,\beta}$ = -1.2847335.
GS: E(HF) = =-461.5507638; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2091769; $E_{\alpha,\beta}$ = -1.2685433.

20 TS: E(HF) = =-322.6477903; $E_{\alpha,\alpha} = E_{\beta,\beta}$ =-0.1496973; $E_{\alpha,\beta}$ = -0.9375519.
GS: E(HF) = -322.7371304; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1449454; $E_{\alpha,\beta}$ = -0.9210022.

21 TS: E(HF) =-566.1056051; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2718998; $E_{\alpha,\beta}$ = -1.5939967.
E(MP2)= -568.2434017. TC = 0.160789. -536.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.324475	-0.334466	0.658883
2	6	0	-2.673963	0.565301	-0.224092
3	1	0	-3.859398	-0.521887	1.619292
4	7	0	-3.534250	-0.500808	-0.452573
5	1	0	-3.833899	-0.845776	-1.361085
6	1	0	-5.390524	-0.113128	0.594259
7	6	0	-1.253922	0.366508	-0.100378
8	6	0	-0.695156	-0.927874	-0.127947
9	6	0	-0.385602	1.472958	0.011050
10	6	0	0.683385	-1.114848	-0.091632
11	1	0	-1.360274	-1.787974	-0.167586
12	6	0	0.992507	1.304892	0.057196
13	1	0	-0.803007	2.478082	0.052551
14	6	0	1.505647	0.007323	-0.000764
15	1	0	1.121064	-2.107837	-0.114914
16	1	0	1.665477	2.152860	0.133210
17	1	0	-3.102954	1.560779	-0.123873
18	7	0	2.957498	-0.180988	0.049570
19	8	0	3.675809	0.832449	-0.035932
20	8	0	3.387972	-1.342613	0.172842

GS: E(HF) = -566.1943993; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2676976; $E_{\alpha,\beta}$ = -1.5783528.
E(MP2) = -568.3081475. TC = 0.165057.

Standard orientation:

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

1	6	0	-2.786581	0.445780	-0.257673
2	6	0	-3.659284	0.015617	0.872327
3	1	0	-4.560638	0.590385	1.072865
4	1	0	-3.196046	-0.447554	1.738705
5	7	0	-3.584456	-0.787818	-0.358061
6	1	0	-4.406840	-0.637985	-0.945329
7	6	0	-1.312543	0.281993	-0.195904
8	6	0	-0.485649	1.413703	-0.202771
9	6	0	-0.731468	-0.989632	-0.104082
10	6	0	0.899726	1.291653	-0.118062
11	1	0	-0.927729	2.405588	-0.284631
12	6	0	0.652122	-1.134788	-0.014148
13	1	0	-1.378068	-1.863412	-0.116605
14	6	0	1.442736	0.012093	-0.020808
15	1	0	1.548705	2.161334	-0.122187
16	1	0	1.115181	-2.114254	0.049700
17	1	0	-3.133213	1.310494	-0.824038
18	7	0	2.901158	-0.130948	0.069870
19	8	0	3.571891	0.899505	0.262765
20	8	0	3.379033	-1.273474	-0.050817

22 TS: E(HF) =-188.0354484; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -.09052388; $E_{\alpha,\beta}$ = -0.5786241. E(MP2) =-188.7951203.
GS: E(HF) = =-188.1235281; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -.0864521; $E_{\alpha,\beta}$ = -0.5633482. E(MP2) = -188.8597804.

23 TS: E(HF) =-284.8829948; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1275901; $E_{\alpha,\beta}$ = -0.8144852.
GS: E(HF) = -284.8829948; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1275901; $E_{\alpha,\beta}$ = -0.8144852.

24 TS: E(HF) = -246.8755389; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1124875; $E_{\alpha,\beta}$ = -0.7262445.
GS: E(HF) = -246.9884767; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1077608; $E_{\alpha,\beta}$ = -0.7042309.

25 TS: E(HF) = -569.5603406; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1186335; $E_{\alpha,\beta}$ = -0.7491188. E(MP2)=-570.5467265. TC = 0.103550. S = 80.277. -530.9.

Standard orientation:

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

1	6	0	-2.360409	0.308030	0.484919
2	6	0	-0.448192	0.361006	-0.285070
3	1	0	-2.007944	0.128243	1.494857
4	1	0	-0.344350	1.437496	-0.376601
5	7	0	-1.641992	-0.221183	-0.576578
6	1	0	-1.777508	-1.096637	-1.083040
7	1	0	-3.282334	0.859107	0.310595
8	6	0	2.247349	0.587658	-0.061811
9	1	0	3.172685	0.126484	0.289282
10	1	0	2.352653	0.838504	-1.118696
11	1	0	2.067886	1.493290	0.522256
12	16	0	0.917523	-0.611149	0.198072

GS: E(HF) = -569.652372; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1143832; $E_{\alpha,\beta}$ = -0.7323295.
E(MP2)= -570.613468. S = 77.629. TC = 0.107645.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.859781	-0.525316	-0.070094
2	1	0	2.577904	-0.607399	0.651648
3	6	0	1.498305	0.884007	-0.310972
4	6	0	0.619747	0.003679	0.501050
5	1	0	1.221954	1.099646	-1.337882
6	1	0	2.055026	1.663093	0.205131
7	1	0	0.594646	0.176231	1.577148
8	16	0	-0.868940	-0.706461	-0.171934
9	6	0	-1.950208	0.718889	0.096594
10	1	0	-2.939511	0.454572	-0.284186
11	1	0	-2.044051	0.960660	1.158167
12	1	0	-1.588457	1.594335	-0.448457

26 TS: E(HF) = -266.1041481; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1280096; $E_{\alpha,\beta}$ = -0.8470309.
E(MP2)= -267.2071982. TC = 0.149438. S = 81.911. -381.714.

Standard orientation:

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

1	6	0	2.267153	-0.006918	0.550338
2	6	0	0.373502	-0.643853	-0.106994
3	1	0	1.891806	0.586316	1.374803
4	1	0	0.392671	-1.675358	0.230341
5	7	0	1.508918	-0.098635	-0.605029
6	1	0	1.616733	0.377609	-1.504014
7	1	0	3.275128	-0.415142	0.589621
8	7	0	-0.862037	-0.024447	-0.291534
9	6	0	-2.003466	-0.789655	0.187359
10	1	0	-2.920902	-0.364508	-0.228456
11	1	0	-1.917761	-1.824420	-0.150240
12	1	0	-2.076413	-0.773484	1.287519
13	6	0	-0.949046	1.388346	0.069197
14	1	0	-1.094001	1.514137	1.155317
15	1	0	-0.031854	1.902225	-0.223560
16	1	0	-1.792429	1.846686	-0.454789

GS: E(HF) = -266.1948778; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1238260; $E_{\alpha,\beta}$ = -0.8312604. E(MP2)=-267.2737903. TC = 0.153172. S = 79.102.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.615143	0.780632	-0.144856
2	1	0	-2.199498	1.159581	0.603235
3	6	0	-1.737868	-0.695631	-0.194188
4	6	0	-0.556312	-0.054259	0.421086
5	1	0	-1.631118	-1.108002	-1.191357
6	1	0	-2.464058	-1.183495	0.451494
7	7	0	0.679247	-0.026498	-0.295095
8	1	0	-0.479378	-0.076760	1.518899
9	6	0	1.491957	-1.184902	0.050243
10	1	0	2.400850	-1.179795	-0.557492
11	1	0	1.787791	-1.197027	1.116236
12	1	0	0.930982	-2.098165	-0.166211
13	6	0	1.385606	1.226157	-0.056900
14	1	0	1.676845	1.352905	1.003170
15	1	0	2.291596	1.249928	-0.668642
16	1	0	0.736965	2.053701	-0.351132

27 TS: E(HF) = -208.6715466; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1023853; $E_{\alpha,\beta}$ = -0.6495748.

E(MP2) = -209.5258921.

GS: E(HF) = -208.7626309; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -.0981726; $E_{\alpha,\beta}$ = -0.6337159.
E(MP2) = -209.5926921.

28 TS: E(HF) = -307.5213325; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1329829; $E_{\alpha,\beta}$ = -0.8075062.
E(MP2) = -308.5948046.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.812832	-0.333918	0.534318
2	6	0	2.525421	0.622641	-0.074356
3	1	0	3.566050	0.502397	0.231835
4	1	0	2.098214	1.613207	-0.169589
5	7	0	1.749136	-0.432805	-0.480495
6	1	0	2.019852	-1.259978	-1.004251
7	6	0	-0.564476	-0.148231	0.257588
8	6	0	-1.754047	0.019733	0.041810
9	1	0	1.150282	-0.423805	1.561889
10	9	0	-3.021858	0.181829	-0.201397

GS: E(HF) = -307.6137359; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1287409; $E_{\alpha,\beta}$ = -0.7911090.
E(MP2)= -308.6623268.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.949326	0.756743	-0.102671
2	6	0	-0.972284	-0.161769	0.544255
3	1	0	-1.584588	1.487898	-0.816075
4	7	0	-1.839549	-0.637647	-0.557919
5	1	0	-2.599779	-1.202912	-0.173672
6	1	0	-2.818902	1.057757	0.476548
7	1	0	-1.224595	-0.498950	1.547956
8	6	0	0.440081	-0.070957	0.267419
9	6	0	1.633702	-0.013121	0.051712
10	9	0	2.910185	0.061597	-0.188180

29 TS: E(HF) = -339.8565159; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1570622; $E_{\alpha,\beta}$ = -0.9775002.
E(MP2)= -341.1481406.

GS: E(HF) = =-339.9486066; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1529398; $E_{\alpha,\beta}$ = -0.9607989.
E(MP2)= -341.2152853.

30 TS: E(HF) = -754.560161; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1941279; $E_{\alpha,\beta}$ = -1.1037940.
E(MP2)= -756.052211.
GS: E(HF) = -754.6559273; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ -0.1903402; $E_{\alpha,\beta}$ = -1.0852695.
E(MP2)= -756.1218773.

31 TS: E(HF) = - 307.5213325; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1329829; $E_{\alpha,\beta}$ = -0.8075062.
E(MP2)= =-308.5948046. TC = 0.075343. S = 78.266.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.812832	-0.333918	0.534318
2	6	0	2.525421	0.622641	-0.074356
3	1	0	3.566050	0.502397	0.231835
4	1	0	2.098214	1.613207	-0.169589
5	7	0	1.749136	-0.432805	-0.480495
6	1	0	2.019852	-1.259978	-1.004251
7	6	0	-0.564476	-0.148231	0.257588
8	6	0	-1.754047	0.019733	0.041810
9	1	0	1.150282	-0.423805	1.561889
10	9	0	-3.021858	0.181829	-0.201397

GS: E(HF) = -307.6137359; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1287409; $E_{\alpha,\beta}$ = -0.7911090.
E(MP2) = -308.6623268. TC = 0.079400. S = 76.048.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.949326	0.756743	-0.102671
2	6	0	-0.972284	-0.161769	0.544255
3	1	0	-1.584588	1.487898	-0.816075
4	7	0	-1.839549	-0.637647	-0.557919
5	1	0	-2.599779	-1.202912	-0.173672
6	1	0	-2.818902	1.057757	0.476548
7	1	0	-1.224595	-0.498950	1.547956

8	6	0	0.440081	-0.070957	0.267419
9	6	0	1.633702	-0.013121	0.051712
10	9	0	2.910185	0.061597	-0.188180

32 TS: E(HF) = -530.5179304; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0996560; $E_{\alpha,\beta}$ = -6156968. E(MP2) = -531.3329394. TC = 0.071751. S = 71.132. -527.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.931315	-0.440415	-0.243004
2	6	0	-0.088739	-0.039437	0.582780
3	1	0	-1.547189	-1.223158	-0.887415
4	1	0	-0.221171	-0.550562	1.528208
5	7	0	-1.121611	0.647652	0.034844
6	1	0	-1.091611	1.577569	-0.384305
7	1	0	-2.954764	-0.480480	0.124541
8	16	0	1.474310	-0.034334	-0.219062
9	1	0	2.197385	-0.428468	0.841405

GS: E(HF) = -530.6114495; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -.0953114; $E_{\alpha,\beta}$ = -0.5982542. E(MP2) =-531.4003267.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.369878	0.706601	-0.153764
2	6	0	0.272119	-0.017943	0.531872
3	1	0	2.175354	1.102760	0.460552
4	1	0	0.340376	-0.132158	1.611525
5	7	0	1.233223	-0.755310	-0.289301
6	1	0	1.150181	1.258306	-1.061329
7	16	0	-1.391864	-0.057548	-0.124531
8	1	0	-1.784117	1.098245	0.438022
9	1	0	1.903484	-1.251157	0.300178

33 TS: E(HF) = =-320.6573607; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1424674; $E_{\alpha,\beta}$ = -0.8539911.

E(MP2) = =-321.7962868.
GS: E(HF) = =-320.7466276; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1388047; $E_{\alpha,\beta}$ = -0.8389655.
E(MP2) = =-321.8632026.

34 TS: E(HF) = =-224.7314103; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1074208; $E_{\alpha,\beta}$ = -0.6648143.
E(MP2) = =-225.6110663.
GS: E(HF) -224.8217519; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1042265; $E_{\alpha,\beta}$ = -0.6532382.
E(MP2) = - 225.6834432.

35 TS: E(HF) = =-245.7427014; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1118144; $E_{\alpha,\beta}$ = -0.6956549.
E(MP2) = =-246.6619852.
GS: E(HF) = =-245.8262541; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1083103; $E_{\alpha,\beta}$ = -0.6824799.
E(MP2) = =-246.7253548.

36 TS: E(HF) = =-207.8649254; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0946088; $E_{\alpha,\beta}$ = -0.5898583.
E(MP2) = =-208.6440015.
GS: E(HF) = =-207.957462; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -.090457933; $E_{\alpha,\beta}$ = -0.5724007.
E(MP2) = -208.7107786.

37 TS: E(HF) = =-289.1545365; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1427573; $E_{\alpha,\beta}$ = -0.9704288.
E(MP2) = =-290.4104800.
GS: E(HF) =-289.2535245; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1387795; $E_{\alpha,\beta}$ = -0.9533348.
E(MP2) = =-290.4844184.

38 TS: E(HF) = -755.0852491; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1917808; $E_{\alpha,\beta}$ = -1.1010810.
E(MP2) = -756.5698918.
GS: E(HF) = -755.1791647; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1888229; $E_{\alpha,\beta}$ = -1.0877377.
E(MP2) = -756.6445484.

39 TS: E(HF) = -423.0776565; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0898334; $E_{\alpha,\beta}$ = -0.6090219.
E(MP2) =-423.8663452.
GS: E(HF) = =-423.1764063; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.08614029; $E_{\alpha,\beta}$ = -0.5920159.

E(MP2) =-423.9407029.

40 TS: E(HF) = -359.6893622; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1590924; $E_{\alpha,\beta}$ = -0.9821700. E(MP2) = -360.9897172.
GS: E(HF) = -359.7828052; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1561925; $E_{\alpha,\beta}$ = -0.9701484. E(MP2) = =-361.0653387.

41 TS: E(HF) = -294.2283253; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0800223; $E_{\alpha,\beta}$ = -0.5158171. E(MP2) = -294.9041869.
GS: E(HF) = -294.2894894; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0818782; $E_{\alpha,\beta}$ = -0.5243034. E(MP2) = -294.9775492.

42 TS: E(HF) = -540.2504588; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1489538; $E_{\alpha,\beta}$ = 1.0083297. E(MP2 MP2=-541.5566962.
GS: E(HF) = -540.3490995; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1453275; $E_{\alpha,\beta}$ = -0.9919704. E(MP2) = =-541.6317251.

43 TS: E(HF) =-172.0241897; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0837706; $E_{\alpha,\beta}$ = -0.5646062. E(MP2) = -172.7563373.
GS: E(HF) = -172.1250439; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0798414; $E_{\alpha,\beta}$ = -0.5476437. E(MP2) = =-246.7253548.

44 TS: E(HF) = -320.0902932; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1461689; $E_{\alpha,\beta}$ = -0.8604448. E(MP2) = -321.2430758.
GS: E(HF) = -320.1919025; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1424405; $E_{\alpha,\beta}$ = -0.8423503. E(MP2) = -321.319134.

45 TS: E(HF) = -468.6946115; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1748732; $E_{\alpha,\beta}$ = -1.0288843. E(MP2) = -470.0732423.
GS: E(HF) = -468.7941517; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1714459; $E_{\alpha,\beta}$ = -1.0127827. E(MP2) = -470.1498262.

46 TS(in): E(HF) =-270.9029280; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1136588; $E_{\alpha,\beta}$ = -0.7201564. E(MP2) = -271.8504020. TC = -0.094103

GS: E(HF) = -271.004715; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1094558; $E_{\alpha,\beta}$ = -0.7022087. E(MP2) = -271.9258354.

47 TS: E(HF) = -592.1968184; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.3024036; $E_{\alpha,\beta}$ = -1.8266379. E(MP2) = -594.6282636.

GS: E(HF) = -592.2708409; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2971128; $E_{\alpha,\beta}$ = -1.8109128. E(MP2)= -594.6759795.

48 TS: E(HF) = -358.5134377; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1599601; $E_{\alpha,\beta}$ = -0.9621396. E(MP2) = -359.7954977.

GS: E(HF) = -358.5833567; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1557360; $E_{\alpha,\beta}$ = -0.9497706. E(MP2)= -359.8445995.

49 TS: E(HF) = -439.4966015; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2213039; $E_{\alpha,\beta}$ = -1.3701738. E(MP2) =-441.3093833. TC = 0.191354. S = 98.429. -322.9.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.236291	-0.284985	0.035902
2	6	0	-0.482048	0.644340	-0.648632
3	1	0	-1.764619	-0.433869	1.010757
4	1	0	-0.835725	1.672626	-0.615798
5	7	0	-1.410006	-0.283798	-1.092676
6	1	0	-1.133534	-1.126148	-1.596940
7	6	0	0.856799	0.305932	-0.259475
8	6	0	1.263934	-1.040063	-0.120697
9	6	0	1.807440	1.323716	-0.016777
10	6	0	2.579431	-1.350518	0.225242
11	1	0	0.537407	-1.841956	-0.245331
12	6	0	3.115772	1.005653	0.329146
13	1	0	1.504698	2.365985	-0.113226
14	6	0	3.512419	-0.333898	0.446855

15	1	0	2.875813	-2.392260	0.332280
16	1	0	3.835315	1.802445	0.507007
17	1	0	4.536423	-0.579667	0.719296
18	6	0	-3.635554	-0.010254	-0.053583
19	6	0	-4.456575	0.096588	1.022787
20	1	0	-4.043467	0.098328	-1.059421
21	1	0	-5.523332	0.259824	0.908483
22	1	0	-4.070895	0.022218	2.037019

GS: E(HF) = -439.5763543; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2159466; $E_{\alpha,\beta}$ = 1.3528898. E(MP2)= -441.3611374. TC = 0.195187. S = 98.481.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.411336	1.365060	-0.728403
2	1	0	2.082094	1.475294	-1.493817
3	6	0	1.841319	0.279173	0.181674
4	6	0	0.739728	0.060300	-0.809851
5	1	0	1.538342	0.453573	1.213838
6	1	0	0.998668	-0.579583	-1.655652
7	6	0	-0.678229	-0.006301	-0.377727
8	6	0	-1.379463	-1.214019	-0.496400
9	6	0	-1.317906	1.108394	0.178781
10	6	0	-2.704763	-1.307250	-0.067971
11	1	0	-0.887096	-2.082743	-0.932836
12	6	0	-2.642043	1.011339	0.612694
13	1	0	-0.770794	2.045375	0.251761
14	6	0	-3.338860	-0.194347	0.492451
15	1	0	-3.241709	-2.248211	-0.169144
16	1	0	-3.134262	1.883242	1.038978
17	1	0	-4.371631	-0.265340	0.826671
18	6	0	3.145274	-0.374257	-0.010010
19	6	0	3.973619	-0.692611	0.998005
20	1	0	3.432812	-0.603057	-1.038682
21	1	0	4.925433	-1.181080	0.816592
22	1	0	3.716739	-0.475405	2.031238

50 TS: E(HF = -821.5180793; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2096271; $E_{\alpha,\beta}$ = -1.2616264. E(MP2) = -823.1989600.

GS: E(HF) = -821.6027092; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2045925; $E_{\alpha,\beta}$ = -1. 2434567. E(MP2) = -823.2553509.

51 TS: E(HF) =-586.3812222; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2571448; $E_{\alpha,\beta}$ = -1.5492786. E(MP2) = -588.4447905. TC =0.165172. S = 110.451. -146.819.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.699084	-0.116168	0.015281
2	6	0	-1.107390	-0.950910	0.656972
3	1	0	0.563659	0.943932	0.168034
4	1	0	-0.814528	-1.433654	1.579029
5	7	0	-0.284794	-0.936146	-0.422965
6	1	0	-0.342409	-1.475630	-1.297427
7	8	0	-2.478915	-0.909565	0.451915
8	6	0	-3.081715	0.233277	-0.058003
9	8	0	-4.220750	0.149197	-0.466370
10	6	0	-2.262146	1.495238	-0.025582
11	1	0	-1.767064	1.611564	0.942237
12	1	0	-1.492366	1.470981	-0.802629
13	1	0	-2.930627	2.335167	-0.215241
14	8	0	1.994471	-0.585487	-0.184557
15	6	0	3.023367	0.313160	0.009097
16	8	0	2.843185	1.475068	0.325430
17	6	0	4.342938	-0.362429	-0.207052
18	1	0	4.489137	-1.132570	0.555409
19	1	0	4.360344	-0.852464	-1.183420
20	1	0	5.138659	0.378987	-0.140872

GS: E(HF) = -586.4667301; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2520732; $E_{\alpha,\beta}$ -1.528265377D. E(MP2) = -588.4991420. TC = 0.168251. S = 107.897.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.366641	-1.416244	0.722820
2	1	0	-0.044515	-2.259003	0.238328
3	6	0	-0.441902	-0.273845	-0.185343
4	6	0	0.677200	-0.410247	0.761704

5	1	0	-0.233459	-0.426851	-1.243945
6	1	0	0.718148	0.179452	1.673577
7	8	0	1.917918	-0.826350	0.238545
8	8	0	-1.405289	0.702761	0.098039
9	6	0	2.822611	0.137374	-0.184587
10	8	0	3.860616	-0.243424	-0.682168
11	6	0	-2.747149	0.420731	-0.113980
12	8	0	-3.553800	1.284247	0.157285
13	6	0	2.442536	1.576976	0.035763
14	1	0	1.459896	1.807213	-0.384019
15	1	0	2.409784	1.802635	1.106244
16	1	0	3.202188	2.200047	-0.435059
17	6	0	-3.084372	-0.937233	-0.665527
18	1	0	-2.561784	-1.124529	-1.608359
19	1	0	-2.792934	-1.712526	0.047467
20	1	0	-4.159939	-0.973123	-0.835758

52 TS: E(HF) = -1025.0376272; E□,□ = E□□□ = -0.2987391; E□□□ = -1.7282272. E(MP2) = -594.6282636. TC = 0.152832. S = 109.317. -339.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.396909	-0.312941	-0.462595
2	6	0	1.713097	0.537283	0.376914
3	1	0	3.063892	-0.424945	-1.486079
4	1	0	2.149319	1.534104	0.399045
5	7	0	2.563989	-0.539916	0.578369
6	1	0	2.767756	-1.047788	1.440164
7	6	0	0.298032	0.351033	0.205256
8	6	0	-0.263673	-0.940128	0.118095
9	6	0	-0.566048	1.465748	0.156228
10	6	0	-1.640033	-1.118754	0.022625
11	1	0	0.395263	-1.805987	0.106482
12	6	0	-1.941404	1.306004	0.048016
13	1	0	-0.147433	2.469511	0.213411
14	6	0	-2.458217	0.009820	-0.009283
15	1	0	-2.079273	-2.109373	-0.039181
16	1	0	-2.610164	2.159902	0.011642
17	17	0	5.077988	0.014815	-0.228992

18	7	0	-3.907650	-0.169772	-0.122950
19	8	0	-4.605469	0.847451	-0.291665
20	8	0	-4.355970	-1.328434	-0.042346

GS: E(HF) = -1025.1200265; $E_{\square,\square}$ = $E_{\square\square\square}$ = -0.2937303; $E_{\square\square\square}$ -0.7110904. E(MP2 MP2=-1027.4185777. TC = 0.156597. S = 111.626

. Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.887151	0.344387	-0.412784
2	6	0	1.939217	-0.109848	0.637845
3	1	0	2.524927	0.710903	-1.368266
4	1	0	2.313146	-0.916054	1.269252
5	7	0	2.638892	1.194604	0.730189
6	1	0	3.404817	1.157950	1.407059
7	6	0	0.471445	-0.069865	0.433742
8	6	0	-0.254980	-1.268720	0.405877
9	6	0	-0.198169	1.145550	0.240770
10	6	0	-1.632327	-1.265490	0.198198
11	1	0	0.258675	-2.216581	0.558896
12	6	0	-1.574250	1.169367	0.018598
13	1	0	0.368665	2.072169	0.282444
14	6	0	-2.265184	-0.039927	-0.001167
15	1	0	-2.207403	-2.185584	0.183687
16	1	0	-2.107061	2.102840	-0.131613
17	7	0	-3.716662	-0.022789	-0.225658
18	8	0	-4.342931	-1.080461	-0.032254
19	8	0	-4.230398	1.047887	-0.596672
20	17	0	4.431637	-0.476498	-0.578132

53 TS: E(HF) = =-461.4711535; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2138897; $E_{\alpha,\beta}$ = -1.2848270. E(MP2) = =-463.1837601. TC = 0.148608. S = 92.119. -232.3.

GS: E(HF) = -461.5574839; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2088258; $E_{\alpha,\beta}$ = -1.2665304. E(MP2)= -463.2416660. TC = 0.152651. S = 91.529.

54 TS: E(HF) =-592.1803853; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.3043072; $E_{\alpha,\beta}$ = -1.8341361. E(MP2) = =-594.6231359.

GS: E(HF) =-592.2679334; $\mathbf{E_{\alpha,\alpha} = E_{\beta,\beta}}$ = -0.2988710; $\mathbf{E_{\alpha,\beta}}$ = -1.8154075. **E(MP2) =** =-594.6810831.

55 TS: E(HF) =-1280.4254216; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2371381; $E_{\alpha,\beta}$ = -1.400941. E(MP2) = =-1282.3006397.

GS: E(HF) = =-1280.5141608; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2319038; $E_{\alpha,\beta}$ = -1.3810263. E(MP2)= =-1282.3589948.

56 TS: E(HF)= -821.5025844; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2108496; $E_{\alpha,\beta}$ = -1.2673126. E(MP2) = -823.1915965.

GS: E(HF) =-821.5962426; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2050462; $E_{\alpha,\beta}$ = -1.2456288. E(MP2) = -823.2519638.

57 TS: E(HF) = -506.5113459; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1933047; $E_{\alpha,\beta}$ = -1.1405759. E(MP2) = -508.0385311. TC = -0.0848840. S = 88.504. -550.678.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.915421	-0.634542	0.487977
2	6	0	1.028948	-0.417440	-0.579568
3	1	0	2.415834	-1.041285	1.359438
4	7	0	2.244009	0.362691	-0.177361
5	1	0	2.747575	0.831034	-0.922924
6	1	0	3.726991	-1.215503	0.032487
7	6	0	-0.128696	0.264255	-0.127264
8	6	0	-1.370940	-0.261435	0.072156
9	9	0	-0.153511	1.667503	0.104393
10	9	0	-2.518483	0.472043	0.160574
11	9	0	-1.690990	-1.563779	-0.081332

GS: E(HF) = -506.6041612; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1890914; $E_{\alpha,\beta}$ = -1.1238172. E(MP2) = -508.1061612. TC = 0.089004. = 86.039.

Standard orientation:

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

1	6	0	2.382284	-0.000506	-0.611113
2	6	0	1.094685	-0.563480	-0.129243
3	1	0	3.034501	-0.661690	-1.176390
4	1	0	2.436896	1.050214	-0.872765
5	1	0	0.892071	-1.608396	-0.353183
6	6	0	-0.105222	0.275314	-0.031522
7	6	0	-1.363835	-0.165693	-0.012892
8	7	0	2.176844	-0.252079	0.825416
9	1	0	2.642435	-1.112956	1.119339
10	9	0	-1.680903	-1.464605	-0.073049
11	9	0	-2.444401	0.605370	0.054792
12	9	0	0.092939	1.617409	0.042002

58 TS: E(HF) = -796.1614722; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2182353; $E_{\alpha,\beta}$ = -1.3127627. E(MP2) = =-797.9107056. TC = 0.151448. S = 96.638. -385.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.451903	1.264446	0.474536
2	6	0	1.530105	0.734327	0.392014
3	1	0	1.671527	0.731430	1.469581
4	7	0	0.712697	1.731287	-0.078770
5	1	0	0.829473	2.253735	-0.946500
6	6	0	2.355144	-0.105067	-0.438013
7	6	0	3.259108	-0.961562	0.085940
8	1	0	2.221725	-0.037208	-1.515647
9	1	0	3.887819	-1.578953	-0.547044
10	1	0	3.366635	-1.079468	1.161554
11	16	0	-1.095275	-0.314942	0.051819
12	8	0	-0.318196	-0.837102	-1.090815
13	8	0	-1.309653	-1.135238	1.259513
14	6	0	-2.727742	0.084957	-0.567937
15	1	0	-3.301593	0.581451	0.217029
16	1	0	-2.630266	0.718601	-1.450792
17	1	0	-3.200784	-0.864665	-0.829141
18	1	0	-1.074497	1.871252	1.134410

GS: E(HF) = - 796.2442642; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2145189; $E_{\alpha,\beta}$ = -1.3007224. E(MP2)= -797.9740245. TC = 0.153591. S = 96.680.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.174009	-0.519988	-0.616104
2	6	0	1.376113	-0.303909	0.240467
3	1	0	0.227996	-0.505152	-1.702768
4	1	0	1.187203	0.168342	1.205765
5	6	0	2.690838	-0.047869	-0.372849
6	6	0	3.564236	0.842919	0.120657
7	1	0	2.929831	-0.630527	-1.261634
8	1	0	4.524679	1.015025	-0.353576
9	1	0	3.346722	1.417493	1.017455
10	7	0	0.803554	-1.652256	0.052060
11	1	0	0.260492	-1.910298	0.884680
12	16	0	-1.392722	0.043770	0.019163
13	8	0	-2.460797	-0.459416	-0.858324
14	8	0	-1.375448	-0.275007	1.461417
15	6	0	-1.327669	1.815455	-0.158410
16	1	0	-0.503577	2.207543	0.439259
17	1	0	-1.206277	2.060893	-1.215284
18	1	0	-2.283599	2.197883	0.207777

1 0 -2.283599 2.197883 0.207777

59 TS: E(HF) = -345.7752928; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1428047; $E_{\alpha,\beta}$ = -0.8815406.
E(MP2) = -346.9424429. TC = 0.099564. S = 82.690. -479.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.560447	-0.237487	0.364206
2	6	0	-0.462707	-0.103474	-0.293408
3	1	0	1.500390	-0.659080	1.356768
4	1	0	-0.436076	-1.081075	-0.761264
5	7	0	0.672660	0.629653	-0.139209
6	1	0	0.775737	1.634579	-0.320578
7	9	0	2.834139	-0.219682	-0.163890
8	8	0	-1.579391	0.332018	0.371009

9	6	0	-2.786788	-0.277580	-0.100622
10	1	0	-2.732050	-1.367315	0.002743
11	1	0	-3.586178	0.109868	0.529577
12	1	0	-2.968273	-0.012311	-1.146901

GS: E(HF) = =-345.8746706; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1377715; $E_{\alpha,\beta}$ = -0.8582907. E(MP2) = MP2 -347.0085044. TC = 0.103059. S = 78.475.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.000724	-0.145194	-0.399079
2	6	0	0.122122	0.277229	0.456455
3	1	0	-0.833572	-0.353850	-1.451926
4	1	0	0.167566	0.004901	1.511241
5	7	0	-0.944349	1.200040	0.099862
6	1	0	-0.658083	1.877648	-0.608993
7	8	0	1.353507	0.498297	-0.161907
8	9	0	-2.036138	-0.911527	0.101675
9	6	0	2.223547	-0.630913	-0.022163
10	1	0	1.795482	-1.514822	-0.508565
11	1	0	3.158617	-0.355373	-0.507978
12	1	0	2.407950	-0.848145	1.036088

60 TS: E(HF) = -306.7432521; $E_{□,□} = E_{□□□}$ = -0.1255777; $E_{□□□}$ = -0.7502401. E(MP2)= -307.7446478. TC = 0.068907. S = 73.962.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.986013	-0.303618	0.305561
2	6	0	-1.017699	-0.192164	-0.418568
3	1	0	0.936308	-0.943297	1.174194
4	1	0	-0.874591	-1.036616	-1.080001
5	7	0	0.032153	0.575319	-0.030267
6	1	0	0.041757	1.600485	0.030411
7	9	0	2.268896	-0.033646	-0.121889
8	8	0	-2.202970	0.000590	0.265177
9	1	0	-2.934736	-0.375017	-0.259102

GS: E(HF) = -306.8430713; $\mathbf{E_{\alpha,\alpha}} = \mathbf{E_{\beta,\beta}}$ = -0.1205460; $\mathbf{E_{\alpha,\beta}}$ = -0.7264227. **E(MP2)** = -307.8105862. **TC** = 0.072255. S = 70.796.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.608864	-0.078652	-0.403574
2	6	0	0.591466	-0.123519	0.447614
3	1	0	-0.531471	-0.298287	-1.464201
4	1	0	0.537230	-0.426441	1.491006
5	7	0	-0.066207	1.134765	0.138937
6	1	0	0.444357	1.690187	-0.549790
7	8	0	1.829642	-0.316907	-0.186600
8	1	0	2.120974	-1.235907	-0.040743
9	9	0	-1.848932	-0.436070	0.091081

61 TS: E(HF) = =-286.7806043; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1409360; $E_{\alpha,\beta}$ = -0.9151665. E(MP2) = -287.977643. TC = 0.141460. S = 82.777. -487.9.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.569765	-1.111984	0.591596
2	6	0	0.141997	-0.263429	-0.231293
3	1	0	-1.182057	-1.287377	1.588571
4	7	0	-0.712940	-1.368950	-0.451927
5	1	0	-1.052972	-1.603123	-1.382948
6	1	0	-2.629909	-0.906646	0.445205
7	6	0	1.547276	-0.553220	-0.061426
8	6	0	2.471038	0.344072	0.356808
9	1	0	1.849178	-1.577089	-0.289608
10	1	0	3.522429	0.080480	0.417392
11	1	0	2.191377	1.349436	0.659314
12	6	0	-0.301095	1.120934	-0.415390
13	6	0	-1.363136	1.759023	0.117904
14	1	0	0.326831	1.681441	-1.115254
15	1	0	-1.646384	2.749218	-0.230860
16	1	0	-1.945800	1.323933	0.922481

GS: E(HF) = -286.8735749; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1355325; $E_{\alpha,\beta}$ = -0.8983838.
E(MP2)= -288.0430239. TC = 0.145366. S = 83.161.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.787617	-1.284556	0.742587
2	6	0	0.014780	-0.316218	-0.084289
3	1	0	1.789196	-1.002522	1.057014
4	1	0	0.254573	-1.934979	1.429859
5	6	0	-1.464883	-0.323931	0.021400
6	6	0	-2.226205	0.774235	0.146275
7	1	0	-1.922469	-1.312835	-0.005678
8	1	0	-3.305996	0.697552	0.225219
9	1	0	-1.796804	1.771264	0.177642
10	7	0	0.552203	-1.575525	-0.683819
11	1	0	1.397245	-1.352901	-1.218212
12	6	0	0.652036	0.960016	-0.499686
13	6	0	1.506758	1.670939	0.252030
14	1	0	0.370939	1.325620	-1.488814
15	1	0	1.945507	2.593561	-0.116176
16	1	0	1.781765	1.361014	1.255978

62 TS: E(HF) = -804.4021771; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2863815; $E_{\alpha,\beta}$ = -1.6310535.
E(MP2) = \MP2=-806.6059937. TC = 0.087367. S = 101.367. -427.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.730204	0.742573	-0.660961
2	6	0	1.204929	1.189963	-0.417001
3	1	0	-0.762302	0.838951	-1.741686
4	1	0	1.909778	1.858574	-0.916196
5	7	0	0.011246	1.623137	0.072608
6	1	0	-0.239100	2.392167	0.690164
7	6	0	-1.764448	-0.132536	-0.025581

8	6	0	1.761916	-0.134827	-0.013538
9	9	0	-1.814103	0.051541	1.312770
10	9	0	-1.567552	-1.450265	-0.264910
11	9	0	-3.001393	0.167161	-0.522520
12	9	0	0.982736	-0.801201	0.862732
13	9	0	1.998763	-0.959311	-1.069457
14	9	0	2.977077	0.053998	0.588268

GS: HF= -804.4966103; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.2823518$; $E_{\alpha,\beta} = -1.6132268$.
E(MP2)= -806.6745409. TC = 0.091234. S = 97.189.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.017661	1.887206	0.149113
2	1	0	0.005761	1.587963	1.129908
3	6	0	-0.729420	0.917711	-0.664829
4	6	0	0.753392	0.913395	-0.665043
5	1	0	-1.215746	1.351454	-1.534314
6	1	0	1.253418	1.340477	-1.530887
7	6	0	1.589845	-0.155622	-0.029819
8	6	0	-1.589465	-0.149884	-0.028662
9	9	0	2.817836	0.339104	0.269311
10	9	0	1.769240	-1.200217	-0.869620
11	9	0	1.058733	-0.627598	1.120185
12	9	0	-1.550011	-0.124640	1.323710
13	9	0	-1.249269	-1.396794	-0.428340
14	9	0	-2.881327	0.049707	-0.390621

63 TS: E(HF) =-804.4002522; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.2867220$; $E_{\alpha,\beta} = -1.6324227$.
E(MP2)= -806.6061191. TC = 0.087274. S = 100.621.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.740455	0.708856	0.701077
2	6	0	0.740349	0.708743	-0.701036
3	7	0	0.000047	1.609957	0.000031
4	1	0	-0.000250	2.628737	-0.000349

5	6	0	-1.759778	-0.135478	0.010566
6	6	0	1.759779	-0.135485	-0.010546
7	1	0	-0.824255	0.741701	1.787913
8	1	0	0.824084	0.741499	-1.787883
9	9	0	-1.593695	-1.463256	0.236523
10	9	0	-1.813588	0.052728	-1.327764
11	9	0	-3.000692	0.173738	0.502854
12	9	0	3.000696	0.174083	-0.502620
13	9	0	1.593959	-1.463232	-0.236839
14	9	0	1.813400	0.052444	1.327817

GS: E(HF) = -804.4966103; $\mathbf{E}_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2823518; $E_{\alpha,\beta}$ **=** -1.6132268.
E(MP2) = -806.6745409. **TC =** 0.091234. S = 97.189.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.017661	1.887206	0.149113
2	1	0	0.005761	1.587963	1.129908
3	6	0	-0.729420	0.917711	-0.664829
4	6	0	0.753392	0.913395	-0.665043
5	1	0	-1.215746	1.351454	-1.534314
6	1	0	1.253418	1.340477	-1.530887
7	6	0	1.589845	-0.155622	-0.029819
8	6	0	-1.589465	-0.149884	-0.028662
9	9	0	2.817836	0.339104	0.269311
10	9	0	1.769240	-1.200217	-0.869620
11	9	0	1.058733	-0.627598	1.120185
12	9	0	-1.550011	-0.124640	1.323710
13	9	0	-1.249269	-1.396794	-0.428340
14	9	0	-2.881327	0.049707	-0.390621

64 TS: E(HF) = =-408.8304158; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1627064; $E_{\alpha,\beta}$ = -1.0094442.
E(MP2)= -410.1652729. TC = 0.118157. S = 86.684. -497.0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.854542	0.294505	0.605087
2	6	0	-1.092322	0.815519	0.295728

3	1	0	0.907078	0.720662	1.602845
4	1	0	-1.681581	1.687742	0.597200
5	7	0	0.106045	0.967580	-0.344190
6	1	0	0.398792	1.693333	-0.994357
7	6	0	-1.754763	-0.506950	0.330675
8	1	0	-2.157969	-0.769865	1.311492
9	1	0	-1.096792	-1.296524	-0.038200
10	6	0	1.827155	-0.747193	0.195407
11	1	0	2.251103	-1.273206	1.053841
12	1	0	1.415759	-1.458141	-0.524965
13	9	0	2.919054	-0.110160	-0.477442
14	9	0	-2.895318	-0.468990	-0.540325

GS: E(HF) = =-408.9254724; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1583607; $E_{\alpha,\beta}$ = -0.9912358. E(MP2) = -410.2334297. TC = 0.121880. S = 84.538.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.747200	0.521645	0.533422
2	6	0	0.747143	0.521597	0.533116
3	1	0	-1.236684	1.176472	1.251039
4	1	0	1.236653	1.176495	1.250644
5	6	0	-1.557065	-0.686588	0.188159
6	1	0	-1.831902	-1.256685	1.080428
7	1	0	-1.068029	-1.343502	-0.534075
8	6	0	1.557013	-0.686586	0.187658
9	1	0	1.831263	-1.257234	1.079764
10	1	0	1.068327	-1.343021	-0.535231
11	9	0	-2.763470	-0.262709	-0.411073
12	9	0	2.763843	-0.262559	-0.410679
13	7	0	-0.000244	1.258225	-0.495425
14	1	0	-0.000625	0.746905	-1.382954

65 TS: E(HF) = -592.1675226; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.3044146; $E_{\alpha,\beta}$ = -1.8354903. E(MP2) = -594.6118422. TC = 0.241065. S = 111.180. -467.254.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.061168	0.878776	0.165296
2	6	0	-0.504197	2.828539	-0.370122

3	7	0	0.106484	2.180458	0.674811
4	1	0	0.044439	2.432025	1.659990
5	6	0	1.312460	0.157809	0.011236
6	6	0	1.353442	-1.163142	-0.489729
7	6	0	2.535028	0.788297	0.329218
8	6	0	2.565191	-1.839820	-0.607478
9	1	0	0.429569	-1.657236	-0.781376
10	6	0	3.742931	0.100025	0.221303
11	1	0	2.521969	1.829528	0.644724
12	6	0	3.766227	-1.217315	-0.246755
13	1	0	2.575417	-2.857245	-0.993979
14	1	0	4.673243	0.602080	0.480605
15	1	0	4.710517	-1.748589	-0.345361
16	1	0	0.051105	2.871081	-1.301887
17	6	0	-1.237636	0.167999	0.045330
18	6	0	-1.477549	-0.867622	0.972517
19	6	0	-2.240443	0.465078	-0.889027
20	6	0	-2.691630	-1.553740	0.985045
21	1	0	-0.707453	-1.114862	1.702285
22	6	0	-3.463771	-0.214803	-0.870870
23	1	0	-2.045155	1.220613	-1.646168
24	6	0	-3.693094	-1.225299	0.064213
25	1	0	-2.861548	-2.338110	1.720255
26	1	0	-4.231201	0.037823	-1.600002
27	1	0	-4.641671	-1.757987	0.073869
28	1	0	-1.433376	3.388969	-0.257703

GS: E(HF) = -592.2666491; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2989258; $E_{\alpha,\beta}$ = -1.8160077. E(MP2)= -594.6805086. TC = 0.245254. S = 110.656.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.032982	1.041220	-0.112360
2	6	0	0.063457	2.323664	-0.871908
3	7	0	0.132649	2.337950	0.603707
4	1	0	-0.787359	2.574436	0.987227
5	6	0	1.267775	0.196379	-0.057725
6	6	0	1.286447	-1.050721	-0.700611
7	6	0	2.424018	0.652591	0.587771
8	6	0	2.445861	-1.828126	-0.697820
9	1	0	0.390078	-1.416660	-1.198521

10	6	0	3.582564	-0.129036	0.589336
11	1	0	2.397349	1.615345	1.092196
12	6	0	3.598926	-1.369720	-0.053086
13	1	0	2.448486	-2.794588	-1.198132
14	1	0	4.473954	0.231456	1.099286
15	1	0	4.501499	-1.977153	-0.049310
16	1	0	0.987322	2.611504	-1.366639
17	6	0	-1.257278	0.297015	-0.005955
18	6	0	-1.599175	-0.283140	1.225586
19	6	0	-2.117043	0.136208	-1.099117
20	6	0	-2.790998	-0.994456	1.365245
21	1	0	-0.920607	-0.171912	2.070881
22	6	0	-3.309193	-0.582316	-0.961885
23	1	0	-1.846026	0.559491	-2.064869
24	6	0	-3.648919	-1.146346	0.270000
25	1	0	-3.049624	-1.436170	2.325419
26	1	0	-3.969792	-0.703615	-1.818019
27	1	0	-4.577246	-1.703081	0.377537
28	1	0	-0.853126	2.666007	-1.347839

66 TS: E(HF)= -560.3360929; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.2453012$; $E_{\alpha,\beta} = -1.4482152$.
E(MP2) = -562.2749106. TC = 0.141749. S = 94.453. -145.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.537473	0.109152	0.091717
2	6	0	-0.583190	0.859474	-0.211847
3	1	0	-0.840586	1.908745	-0.113491
4	7	0	-1.561013	0.037480	-0.795607
5	1	0	-1.548303	-0.423965	-1.717596
6	9	0	-3.813661	0.074436	-0.361861
7	6	0	0.763700	0.391793	-0.070283
8	6	0	1.081495	-0.975365	-0.222104
9	6	0	1.812004	1.306043	0.176645
10	6	0	2.409104	-1.400618	-0.181472
11	1	0	0.278935	-1.702579	-0.333992
12	6	0	3.130949	0.869540	0.237259
13	1	0	1.578959	2.362636	0.304192
14	6	0	3.439128	-0.484677	0.050476
15	1	0	2.639497	-2.456939	-0.304904
16	1	0	3.927545	1.586511	0.425200

17	1	0	4.472097	-0.822050	0.097189
18	9	0	-2.483601	-0.604077	1.249672

GS: E(HF) = =-560.4435719; $\mathbf{E_{\alpha,\alpha}}$ **=** $\mathbf{E_{\beta,\beta}}$ **=** -0.2396257; $\mathbf{E_{\alpha,\beta}}$ **=** -1.4222311. **E(MP2)** = -562.3450544. **TC =** 0.144898. S = 94.618.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.931626	0.576448	-0.655100
2	6	0	-2.028954	-0.050649	0.076773
3	1	0	-1.151388	0.952397	-1.652835
4	7	0	-1.790240	1.299115	0.393005
5	1	0	-1.282763	1.372788	1.279741
6	6	0	0.485779	0.244289	-0.351382
7	6	0	0.941788	-1.079131	-0.402571
8	6	0	1.383004	1.276412	-0.044833
9	6	0	2.284927	-1.364900	-0.147261
10	1	0	0.247015	-1.882165	-0.638880
11	6	0	2.724379	0.987238	0.211980
12	1	0	1.029257	2.306339	-0.015834
13	6	0	3.176514	-0.334603	0.163002
14	1	0	2.634282	-2.394246	-0.185295
15	1	0	3.416228	1.792281	0.449443
16	1	0	4.221129	-0.560553	0.364365
17	9	0	-3.214010	-0.352117	-0.509938
18	9	0	-1.763429	-1.004691	1.014895

67 TS: E(HF) = -211.0730391; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1032539; $E_{\alpha,\beta}$ = -0.6989520. E(MP2) = -211.9785324.

GS: E(HF) = -211.1745573; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0989948; $E_{\alpha,\beta}$ = -0.6812918. E(MP2) = -212.4065201.

68 TS: E(HF) = -211.0629068; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1034748; $E_{\alpha,\beta}$ = -0.7016034. E(MP2) = -211.9714600.

GS: E(HF) = -211.1705564; $E_{□,□}$ = $E_{□□□}$ = -0.099000; $E_{□□□}$ = -0.6812863. E(MP2) = -212.0527279.

69 TS: E(HF) = -248.9234412; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1204270; $E_{\alpha,\beta}$ = -0.8043859.

E(MP2)= - 249.9686813. TC = 0.135790. S = 80.162. -572.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.957371	1.364230	0.092438
2	6	0	-0.276107	-0.105938	-0.624550
3	1	0	0.771850	2.119475	-0.662303
4	1	0	-0.535333	-0.421838	-1.641719
5	7	0	1.071475	0.061946	-0.320776
6	1	0	1.113730	1.661007	1.134512
7	6	0	1.951670	-0.938243	0.245210
8	1	0	2.984005	-0.584569	0.177314
9	1	0	1.706490	-1.147777	1.296483
10	1	0	1.839485	-1.860852	-0.331850
11	6	0	-1.328173	-0.030705	0.358493
12	6	0	-2.636612	-0.241300	0.085552
13	1	0	-1.019440	0.155636	1.389548
14	1	0	-3.382062	-0.254262	0.873214
15	1	0	-2.987944	-0.388704	-0.932623

GS: E(HF) = -249.0154384; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1162777; $E_{\alpha,\beta}$ = -0.7881765.
E(MP2) = -250.0361704. **TC =** 0.139762. S = 79.046.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777561	1.225191	0.251974
2	6	0	0.178150	0.078190	0.319932
3	1	0	-1.403642	1.403749	1.126782
4	1	0	-0.516596	2.110378	-0.321562
5	1	0	0.143731	-0.509017	1.241302
6	6	0	1.480581	0.107710	-0.367285
7	6	0	2.600769	-0.428686	0.141200
8	1	0	1.495585	0.598277	-1.340040
9	1	0	3.544672	-0.381488	-0.391973
10	1	0	2.604407	-0.929382	1.106158
11	7	0	-1.022379	0.015068	-0.526650
12	6	0	-2.085183	-0.846101	-0.018125
13	1	0	-3.038977	-0.511673	-0.435962
14	1	0	-1.895549	-1.871588	-0.346539

15	1	0	-2.157514	-0.832557	1.082197

70 **See S7.**

71 TS: HF = -362.5737253; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.1823734$; $E_{\alpha,\beta} = -1.1284277$.
E(MP2) = =-364.0668998. TC = 0.154962. S = 87.836. -597.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.488831	1.005347	-0.193594
2	6	0	2.488684	-1.005390	0.193796
3	1	0	3.135786	1.285501	0.629266
4	1	0	2.510991	-1.567296	1.130421
5	1	0	3.136015	-1.285687	-0.628717
6	7	0	1.575663	-0.000023	-0.000202
7	1	0	2.511672	1.567331	-1.130155
8	6	0	0.178630	-0.000012	-0.000080
9	6	0	-0.514341	1.212232	0.101032
10	6	0	-0.514402	-1.212225	-0.101201
11	6	0	-1.909091	1.206517	0.082181
12	1	0	0.045331	2.138404	0.218079
13	6	0	-1.909144	-1.206472	-0.082095
14	1	0	0.045222	-2.138424	-0.218282
15	6	0	-2.611859	0.000038	0.000054
16	1	0	-2.449602	2.147797	0.155875
17	1	0	-2.449698	-2.147728	-0.155787
18	1	0	-3.699212	0.000056	0.000158

GS: E(HF)= -362.6671104; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.1785166$; $E_{\alpha,\beta} = -1.1115080$.
E(MP2) = -364.1356516. TC = 0.159215. S = 85.756.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.481195	0.744471	0.294580
2	6	0	2.481198	-0.744466	0.294597
3	1	0	3.267681	1.294332	-0.213275

4	1	0	2.043708	1.239158	1.160395
5	1	0	2.043712	-1.239135	1.160422
6	1	0	3.267686	-1.294336	-0.213245
7	7	0	1.571098	-0.000009	-0.577780
8	6	0	0.191797	-0.000004	-0.260719
9	6	0	-0.505540	-1.211125	-0.156432
10	6	0	-0.505533	1.211122	-0.156428
11	6	0	-1.882999	-1.207243	0.068945
12	1	0	0.035233	-2.150048	-0.258851
13	6	0	-1.882992	1.207248	0.068945
14	1	0	0.035246	2.150042	-0.258844
15	6	0	-2.578665	0.000004	0.181129
16	1	0	-2.415085	-2.152768	0.151199
17	1	0	-2.415072	2.152775	0.151201
18	1	0	-3.651556	0.000007	0.357754

72 TS: E(HF) = HF=-231.783036; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0955758D; $E_{\alpha,\beta}$ = -0.5961798.
E(MP2) = MP2=-232.570367. TC = 0.062158. S = 66.538. -746.9.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.652935	1.088553	0.039030
2	6	0	-0.863787	-0.978359	0.106562
3	1	0	-1.231272	1.643047	-0.693417
4	1	0	-1.037350	-1.871882	-0.489264
5	1	0	-1.332070	-0.896332	1.087649
6	7	0	-0.043562	-0.032358	-0.370333
7	1	0	-0.471866	1.504366	1.034066
8	9	0	1.497536	-0.090429	0.086639

GS: E(HF) =-231.8854764; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0901770; $E_{\alpha,\beta}$ = -0.5758729.
E(MP2) = -232.6417034. TC – 0.066123. S = 64.460.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.823278	-0.739974	0.159898
2	6	0	-0.823277	0.739973	0.159900
3	1	0	-1.529065	-1.298909	-0.445062

4	1	0	-0.431722	-1.246149	1.034674
5	1	0	-0.431721	1.246152	1.034675
6	1	0	-1.529054	1.298914	-0.445066
7	7	0	0.176299	0.000000	-0.636737
8	9	0	1.396311	-0.000001	0.151017

73 TS: E(HF)= -359.6808244; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1593587; $E_{\alpha,\beta}$ = -0.9891531. E(MP2) = -360.9886951. TC = 0.118237. S = 85.001. -524.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183093	0.695061	-0.026290
2	6	0	-1.560980	-1.362497	0.043042
3	1	0	-2.892404	0.545098	-0.828904
4	1	0	-1.349464	-2.096390	-0.731210
5	1	0	-2.192111	-1.596723	0.890689
6	7	0	-1.052275	-0.086834	-0.033267
7	1	0	-2.347097	1.431818	0.756789
8	6	0	0.266140	0.364216	-0.006689
9	8	0	0.577509	1.542865	-0.012930
10	8	0	1.106383	-0.687820	0.023279
11	6	0	2.504306	-0.323477	0.001647
12	1	0	2.748365	0.272729	0.881498
13	1	0	3.037234	-1.271815	0.013278
14	1	0	2.732023	0.242940	-0.902322

GS: E(HF) = -359.7828552; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1553687; $E_{\alpha,\beta}$ = -0.9678884. E(MP2)= -361.0614812. TC = 0.122703. S = 83.733.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.990590	-0.061061	-0.558751
2	6	0	-2.152244	0.431860	0.165547
3	6	0	-1.757114	-1.007469	0.246923
4	1	0	-2.987636	0.731119	-0.458982
5	1	0	-1.958599	1.065096	1.027625
6	1	0	-1.299316	-1.355227	1.169531
7	1	0	-2.300028	-1.758684	-0.317720
8	6	0	0.278465	0.346148	-0.156540

9	8	0	0.606137	1.497903	0.091678
10	8	0	1.121473	-0.713493	-0.150451
11	6	0	2.494438	-0.372650	0.136353
12	1	0	2.573143	0.088383	1.121912
13	1	0	3.028415	-1.320285	0.105619
14	1	0	2.875997	0.314412	-0.620242

74 TS: E(HF) = -591.8619091\; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0895774; $E_{\alpha,\beta}$ = -0.5650470. E(MP2) = -592.6061109. TC = 0.062232. S = 69.014. -549.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208218	1.035439	0.020603
2	6	0	-1.266090	-1.004612	0.097348
3	1	0	-1.905590	1.356858	-0.745036
4	1	0	-1.403036	-1.867766	-0.554329
5	1	0	-1.718249	-1.013178	1.087075
6	7	0	-0.414410	-0.021299	-0.272545
7	1	0	-1.041046	1.657619	0.905005
8	17	0	1.400861	-0.009965	0.029847

GS: E(HF) = -591.959125; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ -0.0856498; $E_{\alpha,\beta}$ = -0.5490040. E(MP2)= -592.6794287. TC =0.059597. S = 70.510.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.252354	-0.741150	0.173095
2	6	0	-1.252351	0.741153	0.173094
3	1	0	-1.975349	-1.295249	-0.416358
4	1	0	-0.878905	-1.244443	1.059458
5	1	0	-0.878898	1.244450	1.059454
6	1	0	-1.975345	1.295252	-0.416362
7	7	0	-0.271503	-0.000002	-0.650284
8	17	0	1.331603	0.000000	0.069921

75 TS: E(HF) = -172.0156652; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0828012; $E_{\alpha,\beta}$ = -0.5640067.

E(MP2) = -172.7452744. TC = 0.100383. S = 69.314. -648.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807416	1.040867	-0.015019
2	6	0	-0.870519	-1.004612	0.083346
3	1	0	-1.582216	1.187032	-0.756282
4	1	0	-1.044839	-1.804582	-0.637770
5	1	0	-1.401142	-1.009811	1.030678
6	7	0	0.049103	-0.010251	-0.178144
7	6	0	1.480583	-0.028671	0.030722
8	1	0	1.732541	0.109504	1.091094
9	1	0	1.858744	-1.001823	-0.295784
10	1	0	1.943436	0.766252	-0.560046
11	1	0	-0.666128	1.779685	0.780825

GS: E(HF) = -172.1137344; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0794431; $E_{\alpha,\beta}$ = -0.5477858.
E(MP2) = -172.8204067. TC = 0.104015. S = 66.340.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.154273	0.000024	-0.571480
2	6	0	0.895050	-0.743594	0.126589
3	6	0	0.894602	0.743750	0.126608
4	1	0	1.584762	-1.290423	-0.508382
5	1	0	0.621376	-1.244689	1.054540
6	1	0	0.620765	1.244483	1.054726
7	6	0	-1.449144	-0.000142	0.100303
8	1	0	-2.006987	0.888660	-0.207007
9	1	0	-2.006423	-0.889557	-0.206242
10	1	0	-1.360872	0.000381	1.199922
11	1	0	1.584237	1.290890	-0.508194

76 TS: E(HF)= -401.6081363; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2008127; $E_{\alpha,\beta}$ = 1.2627212.
E(MP2) = -403.2724832.TC = 0.185575. S = 96.415. -642.7.

Standard orientation:

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.106052	-0.091502	1.367840
2	6	0	-3.407835	0.309094	-0.178460
3	1	0	-2.320658	0.771808	1.984400
4	1	0	-3.755218	1.214794	-0.677815
5	1	0	-4.127775	-0.433776	0.152224
6	7	0	-2.059343	0.085918	0.013227
7	1	0	-1.840918	-1.046129	1.833584
8	6	0	-1.107352	-0.518184	-0.910592
9	1	0	-1.273800	-1.605708	-0.973764
10	1	0	-1.329509	-0.093351	-1.898710
11	6	0	0.305340	-0.234555	-0.479981
12	6	0	1.184468	-1.273661	-0.159844
13	6	0	0.752059	1.090442	-0.384098
14	6	0	2.495330	-0.998087	0.241964
15	1	0	0.843086	-2.306260	-0.222969
16	6	0	2.057365	1.369788	0.020011
17	1	0	0.063432	1.902474	-0.613526
18	6	0	2.933540	0.324354	0.332481
19	1	0	3.170141	-1.815137	0.488369
20	1	0	2.393892	2.402001	0.091534
21	1	0	3.951554	0.541728	0.648163

GS: E(HF) = -401.7078100; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1972856; $E_{\alpha,\beta}$ = -1.2457385.
E(MP2)= 403.3481198. TC = 0.189869. S = 93.943.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.379567	0.308400	1.127211
2	6	0	-3.352851	-0.036176	0.056312
3	1	0	-2.429220	-0.185367	2.092569
4	1	0	-1.991797	1.326450	1.146811
5	1	0	-3.625722	0.749920	-0.646854
6	1	0	-4.118712	-0.785079	0.232612
7	7	0	-1.976878	-0.541249	0.003907
8	6	0	-1.113376	0.130197	-0.971367
9	1	0	-1.240000	-0.388985	-1.930115
10	1	0	-1.405350	1.185978	-1.123596
11	6	0	0.316030	0.066286	-0.507526
12	6	0	1.056552	1.231404	-0.279830
13	6	0	0.914224	-1.178294	-0.265842

14	6	0	2.377574	1.159465	0.173557
15	1	0	0.600267	2.203975	-0.462195
16	6	0	2.230701	-1.253584	0.190185
17	1	0	0.333593	-2.085244	-0.423295
18	6	0	2.966434	-0.084028	0.410719
19	1	0	2.942610	2.073297	0.345522
20	1	0	2.685131	-2.224872	0.374996
21	1	0	3.993033	-0.143352	0.765681

77 TS: E(HF) = -207.7984942; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0940233; $E_{\alpha,\beta}$ = -0.5955294. E(MP2) = -208.5820702. TC = 0.074610. S = 66.836. -698.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.672449	1.093048	0.012092
2	6	0	-0.885711	-0.973646	0.070305
3	1	0	-1.322785	1.474761	-0.765782
4	1	0	-1.055836	-1.823650	-0.588649
5	1	0	-1.398595	-0.924617	1.027654
6	7	0	0.035433	-0.031189	-0.261490
7	1	0	-0.490055	1.665891	0.925089
8	8	0	1.430640	-0.128090	0.171424
9	1	0	1.923076	0.134249	-0.633658

GS: E(HF)= -207.9012626; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0898842; $E_{\alpha,\beta}$ = -0.5783125. E(MP2)= -208.6593437. TC = 0.078742. = 67.396.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858793	0.741649	0.135881
2	1	0	-1.542990	1.296776	-0.497550
3	1	0	-0.518861	1.243216	1.035719
4	6	0	-0.858804	-0.741652	0.135919
5	1	0	-0.518880	-1.243179	1.035781
6	1	0	-1.543000	-1.296795	-0.497497
7	7	0	0.182902	-0.000012	-0.594408
8	8	0	1.383164	0.000048	0.236932

9	1	0	2.083691	-0.000301	-0.441849

78 TS: E(HF) = -224.6989962; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1077419; $E_{\alpha,\beta}$ = -0.6735149. E(MP2) = -225.587995. TC = 0.069682. S = 71.913. -544.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.165495	-1.067459	0.052092
2	6	0	-1.165419	1.067499	-0.052023
3	1	0	-1.849187	-1.101115	0.888684
4	1	0	-1.143198	1.840450	0.712884
5	1	0	-1.849273	1.101317	-0.888473
6	7	0	-0.292554	-0.000014	-0.000116
7	1	0	-1.143620	-1.840451	-0.712785
8	6	0	1.055738	-0.000032	-0.000026
9	7	0	2.240602	-0.000022	0.000036

GS: E(HF) = =-224.8115192; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1040740; $E_{\alpha,\beta}$ = -0.6520236. E(MP2) = -225.671691. TC = 0.074239. S = 69.275.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213600	-0.739799	0.197381
2	6	0	-1.213533	0.739855	0.197338
3	1	0	-1.939078	-1.280527	-0.399944
4	1	0	-0.841888	-1.252377	1.079624
5	1	0	-0.841772	1.252452	1.079548
6	1	0	-1.938962	1.280615	-0.400019
7	7	0	-0.215829	-0.000043	-0.616566
8	6	0	1.051638	-0.000062	-0.134892
9	7	0	2.189353	0.000025	0.199684

79 TS: E(HF) = -187.4532112; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0915224; $E_{\alpha,\beta}$ = -0.5724306. E(MP2) = -188.2072625. TC = 0.077272. S = 65.003. -287.0.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.463578	0.068091	0.443908
2	6	0	1.292369	-0.557427	-0.035425
3	1	0	1.100527	-1.187383	-0.906592
4	1	0	2.309995	-0.578091	0.368934
5	7	0	0.652123	0.766065	-0.050722
6	1	0	0.429025	1.124703	-0.985123
7	1	0	-2.233421	-0.652507	0.221032
8	7	0	-1.522936	-0.160695	-0.332366
9	1	0	-0.483184	-0.008293	1.532466

GS: E(HF) = =-187.4801976; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.09170198; $E_{\alpha,\beta}$ = -0.5743280. E(MP2)= -188.2379296. TC = 0.077272. S = 65.864.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.897642	-0.661159	-0.112769
2	6	0	0.321506	-0.065623	0.449740
3	1	0	-1.634912	-1.161168	0.517334
4	1	0	0.337527	0.015721	1.547196
5	7	0	-0.929749	0.828327	-0.026882
6	1	0	-0.575894	1.160458	-0.932205
7	1	0	-0.772230	-1.116651	-1.095682
8	7	0	1.493518	-0.125774	-0.285312
9	1	0	2.155946	0.544465	0.126886

80 TS: E(HF) = \HF=-207.335778; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0944854; $E_{\alpha,\beta}$ = -0.5775746. E(MP2)= -208.1023235. TC = 0.062981. S = 67.190. -319.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542814	0.048162	0.427491
2	6	0	-1.369332	-0.495752	-0.011195
3	1	0	-2.401052	-0.361506	0.324126

4	1	0	-1.233113	-1.159216	-0.869416
5	7	0	-0.575260	0.740179	-0.061127
6	1	0	-0.368857	1.100800	-0.998237
7	8	0	1.558663	-0.248084	-0.254924
8	1	0	0.519652	-0.091118	1.513036

GS: E(HF) = -207.3533118; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0947797; $E_{\alpha,\beta}$ = -0.5794308.
E(MP2) = -208.122302. TC = 0.065349. S = 64.335.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.915126	-0.653767	-0.131780
2	6	0	0.344266	-0.066771	0.434831
3	1	0	-1.695415	-1.112950	0.479588
4	1	0	0.382398	-0.062663	1.540636
5	7	0	-0.829374	0.838444	0.005227
6	1	0	-0.501619	1.196563	-0.898262
7	1	0	-0.813230	-1.078501	-1.130286
8	8	0	1.482330	-0.061042	-0.230821

81 TS: E(HF)= -591.6130822; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.3066262; $E_{\alpha,\beta}$ = -1.8291475.
E(MP2)= -594.0554823. TC = 0.225899. S = 111.594. -447.4.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.730589	-0.254166	-0.561661
2	6	0	-0.730686	-0.255057	0.561341
3	1	0	0.297116	0.357511	-1.373897
4	1	0	-0.297211	0.355540	1.374411
5	7	0	-0.000062	-1.303232	-0.000909
6	6	0	-2.140571	-0.047807	0.304845
7	6	0	-2.793813	-0.801623	-0.697183
8	6	0	-2.906664	0.907393	1.013598
9	6	0	-4.158662	-0.641185	-0.938377
10	1	0	-2.187660	-1.516615	-1.252785
11	6	0	-4.266802	1.071427	0.764567
12	1	0	-2.414861	1.508164	1.780861
13	6	0	-4.906748	0.300693	-0.219454

14	1	0	-4.643822	-1.240559	-1.709748
15	1	0	-4.835630	1.811290	1.328985
16	1	0	-5.969294	0.434150	-0.419810
17	6	0	2.140472	-0.047002	-0.304587
18	6	0	2.793842	-0.802369	0.696175
19	6	0	2.906505	0.909359	-1.011780
20	6	0	4.158884	-0.642898	0.936930
21	1	0	2.187843	-1.518495	1.250487
22	6	0	4.266806	1.072545	-0.763134
23	1	0	2.414608	1.511459	-1.777942
24	6	0	4.906867	0.300271	0.219612
25	1	0	4.644096	-1.243521	1.707295
26	1	0	4.835443	1.813654	-1.326105
27	1	0	5.969691	0.432559	0.419259

GS: E(HF) = HF=-591.652352; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.3031735; $E_{\alpha,\beta}$ = -1.8184303.
E(MP2) = -594.0771295. TC = 0.227899. S = 112.076.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.490992	0.645369	0.573601
2	6	0	0.490978	0.645162	-0.573833
3	1	0	0.088403	0.282796	-1.543166
4	7	0	-0.000050	1.866616	-0.000432
5	6	0	1.880973	0.180404	-0.328705
6	6	0	2.483888	-0.815879	-1.113999
7	6	0	2.637735	0.761027	0.702503
8	6	0	3.790884	-1.242548	-0.862849
9	1	0	1.910864	-1.262219	-1.928560
10	6	0	3.938981	0.329373	0.965820
11	1	0	2.162278	1.565863	1.264358
12	6	0	4.527015	-0.672711	0.182828
13	1	0	4.240041	-2.016013	-1.486642
14	1	0	4.509084	0.788230	1.774299
15	6	0	-1.880945	0.180474	0.328693
16	6	0	-2.637340	0.760189	-0.703315
17	6	0	-2.484254	-0.814839	1.114922
18	6	0	-3.938582	0.328509	-0.966540
19	1	0	-2.161603	1.564398	-1.265827
20	6	0	-3.791276	-1.241490	0.863877
21	1	0	-1.911537	-1.260391	1.930130

22	6	0	-4.526995	-0.672652	-0.182636
23	1	0	-4.508381	0.786615	-1.775656
24	1	0	-4.240779	-2.014149	1.488416
25	1	0	-5.545723	-1.003618	-0.382397
26	1	0	-0.088384	0.283565	1.543119
27	1	0	5.545670	-1.003732	0.382752

82 TS: E(HF) = -361.9915386.; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1874780; $E_{\alpha,\beta}$ = -1.1308894.
E(MP2) = -363.4973841. TC = 0.140583. S = 85.849. -675.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.970192	-0.106892	0.655438
2	6	0	-1.551770	0.593014	-0.308334
3	1	0	-2.384300	-0.312522	1.566587
4	1	0	-1.835851	1.649894	-0.389445
5	7	0	-2.511908	-0.409913	-0.601293
6	6	0	-0.153725	0.301564	-0.159224
7	6	0	0.285054	-1.045324	-0.085100
8	6	0	0.833957	1.309823	-0.008898
9	6	0	1.642789	-1.356518	0.006142
10	1	0	-0.478136	-1.819120	-0.165899
11	6	0	2.184895	0.995032	0.096510
12	1	0	0.519822	2.355450	-0.028654
13	6	0	2.606373	-0.346473	0.124386
14	1	0	1.951915	-2.402699	0.036499
15	1	0	2.919657	1.795870	0.194653
16	1	0	3.663978	-0.592995	0.213649
17	1	0	-4.038008	0.130157	0.856141

GS: E(HF) = =-362.0395664; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1842050; $E_{\alpha,\beta}$ = -1.1194190.
E(MP2) = -363.5273955. TC = 0.142675. S = 85.620.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.650052	0.586849	-0.207808
2	6	0	2.610212	-0.105687	0.708142
3	1	0	2.177279	-0.793906	1.460727

4	7	0	2.567815	-0.421646	-0.689639
5	6	0	0.199323	0.293149	-0.092258
6	6	0	-0.243404	-1.041319	-0.089883
7	6	0	-0.772383	1.306787	-0.035427
8	6	0	-1.600570	-1.348992	0.015129
9	1	0	0.524243	-1.808308	-0.199110
10	6	0	-2.134473	1.005025	0.058355
11	1	0	-0.446065	2.348259	-0.058324
12	6	0	-2.559054	-0.328504	0.083960
13	1	0	-1.920468	-2.391840	0.018545
14	1	0	-2.868681	1.810954	0.095501
15	1	0	-3.619702	-0.568457	0.155716
16	1	0	1.842002	1.657996	-0.425121
17	1	0	3.438468	0.492982	1.138278

83 TS: E(HF) = HF=-460.8744563; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2178501; $E_{\alpha,\beta}$ = -1.2874074.
E(MP2) = -462.5975641. T = 0.133167. S = 90.617. -672.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.401748	-0.251912	0.681870
2	6	0	-2.036516	0.553586	-0.283138
3	1	0	-2.797732	-0.427208	1.587165
4	1	0	-2.387715	1.591105	-0.343660
5	7	0	-2.928308	-0.506679	-0.581122
6	6	0	-0.619268	0.345966	-0.162743
7	6	0	-0.103254	-0.974812	-0.120172
8	6	0	0.310868	1.408156	-0.020758
9	6	0	1.272271	-1.218588	-0.061662
10	1	0	-0.822409	-1.789701	-0.195929
11	6	0	1.682935	1.178844	0.053308
12	1	0	-0.060585	2.434176	-0.017397
13	6	0	2.137105	-0.138662	0.043049
14	1	0	1.670506	-2.231838	-0.049693
15	1	0	2.396239	1.995980	0.145799
16	1	0	-4.482215	-0.093716	0.889173
17	9	0	3.503079	-0.371946	0.141541

GS: E(HF) = -460.9237781; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2145700; $E_{\alpha,\beta}$ = -1.2756973.

E(MP2) = -462.6286155. TC = 0.135420. S = 89.990

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128617	0.529478	-0.196714
2	6	0	3.024787	-0.224593	0.733368
3	1	0	2.533034	-0.878713	1.480354
4	7	0	2.979032	-0.540207	-0.665744
5	6	0	0.658798	0.329214	-0.102934
6	6	0	0.138120	-0.976519	-0.117055
7	6	0	-0.249483	1.398998	-0.045102
8	6	0	-1.235738	-1.213952	-0.033078
9	1	0	0.861387	-1.785548	-0.226503
10	6	0	-1.631719	1.187623	0.026040
11	1	0	0.136110	2.419529	-0.053940
12	6	0	-2.091752	-0.121545	0.033305
13	1	0	-1.646076	-2.221969	-0.040548
14	1	0	-2.340391	2.012629	0.063330
15	1	0	2.392050	1.584842	-0.415085
16	1	0	3.889194	0.311452	1.173265
17	9	0	-3.458700	-0.345889	0.099151

84 TS: E(HF) HF=-224.1605448; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1113358; $E_{\alpha,\beta}$ = -0.6658109.
E(MP2) MP2 = -225.0490274. TC = 0.056072. S = 69.371. -714.8.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376698	0.726866	0.179940
2	6	0	-0.189081	-0.695037	0.264878
3	1	0	-1.644973	0.724419	1.243202
4	1	0	-0.142177	-1.612598	0.876218
5	7	0	-1.298796	-0.427889	-0.564611
6	1	0	-1.432631	1.726433	-0.297019
7	6	0	1.076277	-0.072361	0.064740
8	7	0	2.178337	0.342880	-0.132495

GS: E(HF) = =-224.2115876; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1085192; $E_{\alpha,\beta}$ = -0.6559526.
E(MP2)= -225.0845788. TC = 0.058438. S = 69.219.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.248677	-0.715207	-0.488400
2	6	0	-1.351330	0.644699	-0.048139
3	6	0	-0.290643	-0.255816	0.498027
4	1	0	-2.138163	0.958624	0.664796
5	1	0	-1.039651	1.479275	-0.701210
6	1	0	-0.362528	-0.577359	1.551280
7	6	0	1.091862	-0.014568	0.112494
8	7	0	2.225964	0.128574	-0.210051

85 TS: E(HF)= -468.1129328; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1787348; $E_{\alpha,\beta}$ = -1.0313612. E(MP2) = -469.5017637. TC = 0.064017. S = 80.479. -649.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.387537	-0.390520	0.082420
2	6	0	0.695666	-0.042122	-0.576927
3	1	0	2.109567	-1.200986	0.762115
4	1	0	0.759672	-0.375068	-1.614446
5	7	0	1.673847	0.787435	-0.000896
6	1	0	3.427087	-0.464701	-0.306750
7	6	0	-0.672595	-0.029941	-0.043219
8	9	0	-1.233767	1.230324	0.098133
9	9	0	-1.565094	-0.730504	-0.833089
10	9	0	-0.809684	-0.577131	1.222925

GS: E(HF) = -468.1741669; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1757087; $E_{\alpha,\beta}$ = -1.0182531. E(MP2) = -469.5438374. TC = 0.066735. S = 78.959.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.782417	0.860822	0.127364

2	6	0	-1.911391	-0.572822	0.007283
3	6	0	-0.770239	0.152448	-0.600989
4	1	0	-2.637464	-1.019138	-0.698422
5	1	0	-1.729612	-1.229797	0.873276
6	1	0	-0.682724	0.225382	-1.702833
7	6	0	0.594199	-0.001856	-0.023814
8	9	0	1.363920	1.135340	-0.161992
9	9	0	0.631990	-0.309584	1.299181
10	9	0	1.343124	-0.988958	-0.654794

86 TS: E(HF) =-132.3626352; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0683269; $E_{\alpha,\beta}$ = -0.4332811.
E(MP2) = - 132.9325703. TC = 0.055142. S = 59.931. -752.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.939506	-0.256672	-0.036796
2	6	0	0.939506	-0.256673	0.036795
3	1	0	-1.079809	-0.870847	-0.930187
4	1	0	1.790598	-0.291556	-0.676783
5	1	0	1.079812	-0.870838	0.930194
6	7	0	0.000000	0.772124	0.000000
7	1	0	-1.790599	-0.291556	0.676785

GS: E(HF) =- 132.4236029; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.0653177; $E_{\alpha,\beta}$ = -0.4207598.
E(MP2)= -132.9749981. TC = 0.057894. S = 59.244.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000035	0.919518	0.000000
2	6	0	0.000035	-0.317615	0.743723
3	6	0	0.000035	-0.317615	-0.743723
4	1	0	-0.912280	-0.656226	1.274294
5	1	0	0.911945	-0.656395	1.274864
6	1	0	0.911945	-0.656395	-1.274864
7	1	0	-0.912280	-0.656226	-1.274294

87 TS: E(HF) = =-529.9881738; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1010062; $E_{\alpha,\beta}$ = -0.6033550.
E(MP2)= - 530.7935414. TC = 0.061946. S = 67.778. -318.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004178	0.112047	0.562252
2	6	0	-1.908282	-0.475997	-0.233301
3	1	0	-2.794893	-0.546906	0.397533
4	1	0	-1.400074	-1.400393	-0.505926
5	7	0	-1.087200	0.699257	-0.064492
6	1	0	-0.832793	1.205043	-0.912833
7	1	0	-0.220029	-0.220007	1.575924
8	16	0	1.520810	-0.109302	-0.129810

GS: E(HF) = =-530.0511662; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0979227; $E_{\alpha,\beta}$ = -0.5943093.
E(MP2)= -530.8413211. TC = 0.065329. S = 66.803.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.347613	-0.664542	-0.183049
2	6	0	-0.224066	-0.027625	0.550869
3	1	0	-2.188999	-1.115840	0.343327
4	1	0	-0.308367	-0.015608	1.637831
5	7	0	-1.286763	0.817703	-0.078524
6	1	0	-0.862284	1.179046	-0.937891
7	1	0	-1.093131	-1.125190	-1.135026
8	16	0	1.430637	-0.030833	-0.097843

88 TS: E(HF) = =-306.0956917|; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1296644; $E_{\alpha,\beta}$ = -0.7573796.
E(MP2) = -307.1124002.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.570214	-0.463599	0.309512
2	6	0	-1.028715	-1.149128	-0.120815

3	1	0	0.860191	-0.704224	1.329550
4	1	0	-1.924934	-1.346547	0.496688
5	1	0	-0.958732	-1.693721	-1.060005
6	7	0	-0.528334	0.155620	-0.065825
7	8	0	-1.110266	1.329578	0.019732
8	9	0	1.928327	0.188321	-0.177278

GS: E(HF) = =-306.1763633; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1238982; $E_{\alpha,\beta}$ = -0.7362818. E(MP2)= -307.1604417. TC = 0.056886. S = 69.450.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.491471	-0.115466	0.385281
2	6	0	0.091384	1.188896	0.059794
3	1	0	-0.323672	-0.604423	1.339335
4	1	0	0.755680	1.640737	0.792842
5	1	0	-0.404097	1.842555	-0.652988
6	7	0	0.597074	-0.122047	-0.533390
7	8	0	1.777198	-0.570781	0.075984
8	9	0	-1.780499	-0.433208	-0.113754

89 TS: E(HF) = =-549.7160167; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2644421; $E_{\alpha,\beta}$ = -1.5549886. E(MP2) = -551.7998896. TC = 0.159120. S = 101.939. -489.2.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.965858	1.474035	-1.027973
2	6	0	0.466094	1.018773	0.275278
3	1	0	1.347223	1.741681	-1.882267
4	1	0	0.606396	1.890186	0.918240
5	7	0	1.586326	0.408204	-0.261826
6	6	0	-0.853857	0.465911	0.105029
7	6	0	-1.053334	-0.675101	-0.700815
8	6	0	-1.982682	1.057083	0.711340
9	6	0	-2.320443	-1.240910	-0.830421
10	1	0	-0.183351	-1.125008	-1.176001

11	6	0	-3.250714	0.496983	0.567943
12	1	0	-1.846133	1.945814	1.328614
13	6	0	-3.431523	-0.651174	-0.214300
14	1	0	-2.449151	-2.136406	-1.437556
15	1	0	-4.106682	0.964882	1.053792
16	1	0	-4.421684	-1.090709	-0.325203
17	1	0	2.943496	1.944591	-0.892950
18	6	0	2.498066	-0.608702	0.355403
19	8	0	3.626139	-0.624295	-0.190348
20	8	0	1.971463	-1.252436	1.289999

GS: E(HF) = -549.7900377; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2600688; $E_{\alpha,\beta}$ = -0.1538986.
E(MP2)= -551.8491618. TC = 0.162771. S = 101.998.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.281248	-0.052275	1.536842
2	6	0	0.542557	-0.600989	0.343587
3	1	0	0.752992	0.609939	2.225222
4	1	0	0.854955	-1.585957	-0.008404
5	7	0	1.523471	0.456487	0.203491
6	1	0	2.061386	-0.667920	1.984611
7	6	0	-0.884462	-0.268024	0.109792
8	6	0	-1.286619	1.060988	-0.084456
9	6	0	-1.861532	-1.274168	0.113583
10	6	0	-2.635450	1.373556	-0.268809
11	1	0	-0.512839	1.825930	-0.112522
12	6	0	-3.210233	-0.964732	-0.078488
13	1	0	-1.555490	-2.311063	0.253287
14	6	0	-3.604479	0.364527	-0.263178
15	1	0	-2.932352	2.409729	-0.426946
16	1	0	-3.954689	-1.760103	-0.080925
17	1	0	-4.654824	0.609462	-0.413669
18	6	0	2.825504	0.076775	-0.440963
19	8	0	2.697457	-0.513337	-1.543448
20	8	0	3.837212	0.435916	0.211878

90 TS: E(HF) = -663.6231395; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.3119404; $E_{\alpha,\beta}$ = -1.8474695.
E(MP2)= 666.09449. TC = 0.194729. S = 117.696. -493.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.800052	1.133578	1.381017
2	6	0	-1.415849	1.094328	-0.115813
3	1	0	-2.117903	1.310961	2.210124
4	1	0	-1.704761	2.047628	-0.563345
5	7	0	-2.409472	0.275081	0.392576
6	6	0	-0.039367	0.671219	-0.169481
7	6	0	0.346245	-0.578926	0.361831
8	6	0	0.963233	1.489703	-0.732096
9	6	0	1.667284	-1.013519	0.283134
10	1	0	-0.427521	-1.215252	0.787728
11	6	0	2.290204	1.067556	-0.794150
12	1	0	0.684170	2.457679	-1.149674
13	6	0	2.642823	-0.180456	-0.273961
14	1	0	1.950862	-1.997136	0.655497
15	1	0	3.062335	1.692317	-1.240747
16	1	0	-3.824386	1.513190	1.425692
17	6	0	-3.284813	-0.710080	-0.321231
18	8	0	-4.340927	-0.946843	0.310562
19	8	0	-2.804791	-1.115420	-1.402973
20	8	0	3.973158	-0.600206	-0.356501
21	6	0	4.650022	-0.483816	0.896100
22	1	0	5.673273	-0.826647	0.727376
23	1	0	4.658159	0.559851	1.235394
24	1	0	4.174185	-1.105927	1.663113

GS: E(HF) = -663.6976291; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.3074937; $E_{\alpha,\beta}$ = -1.8311630.
E(MP2) = -666.1437797. TC = 0.198434. S = 117.855.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.097945	-0.178248	1.540059
2	6	0	-1.442321	0.590588	0.422224
3	1	0	-1.495121	-0.873473	2.127218

4	1	0	-1.851099	1.580085	0.209159
5	7	0	-2.324622	-0.526306	0.153098
6	1	0	-2.920431	0.296246	2.075271
7	6	0	0.003070	0.424209	0.127967
8	6	0	0.510278	-0.816554	-0.284846
9	6	0	0.893743	1.496250	0.282180
10	6	0	1.875363	-0.986134	-0.523524
11	1	0	-0.198926	-1.627539	-0.439804
12	6	0	2.261491	1.337499	0.044961
13	1	0	0.507753	2.470800	0.581135
14	6	0	2.748331	0.090319	-0.348177
15	1	0	2.264903	-1.941281	-0.873126
16	1	0	2.956231	2.168932	0.150819
17	6	0	-3.672170	-0.190523	-0.419065
18	8	0	-3.625988	0.548249	-1.434802
19	8	0	-4.629396	-0.726493	0.193172
20	8	0	4.113475	-0.053389	-0.607028
21	6	0	4.789971	-0.736517	0.449843
22	1	0	5.841095	-0.790350	0.159077
23	1	0	4.692116	-0.182723	1.392056
24	1	0	4.392243	-1.748817	0.586035

91 TS: E(HF) = -648.590881; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2945699; $E_{\alpha,\beta}$ = -1.7104262. E(MP2) = -650.8904471. TC = 0.155672. S = 107.427. -517.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.039568	1.045647	-1.471172
2	6	0	0.522550	1.110687	-0.155059
3	1	0	1.476873	0.887702	-2.388913
4	1	0	0.642422	2.161969	0.118400
5	7	0	1.663484	0.359497	-0.353170
6	6	0	-0.812173	0.566586	-0.051901
7	6	0	-1.175356	-0.756353	-0.370250
8	6	0	-1.876443	1.399754	0.361416
9	6	0	-2.468090	-1.245040	-0.234747
10	6	0	-3.182878	0.937741	0.502222
11	1	0	-1.640086	2.434792	0.608310
12	6	0	-3.489189	-0.392851	0.196033
13	1	0	-2.658651	-2.286118	-0.485023

14	1	0	-3.964154	1.616960	0.839458
15	1	0	-4.503200	-0.771612	0.307811
16	1	0	2.990754	1.586258	-1.506569
17	6	0	2.550263	-0.279809	0.662035
18	8	0	3.714007	-0.460614	0.233053
19	8	0	1.972591	-0.515060	1.747464
20	9	0	-0.236737	-1.628801	-0.832986

GS: E(HF) = -648.6642416; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2905082; $E_{\alpha,\beta}$ = -1.6957718. E(MP2)= -650.94103. TC = 0.151807. S = 106.552.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.479901	1.142843	0.981279
2	6	0	0.666796	-0.099274	0.740852
3	1	0	1.031213	2.129154	0.904893
4	1	0	1.003710	-0.982809	1.285824
5	7	0	1.615535	0.390028	-0.249362
6	1	0	2.289717	1.052863	1.706384
7	6	0	-0.769106	-0.175573	0.382794
8	6	0	-1.543006	0.874888	-0.121319
9	6	0	-1.421780	-1.416637	0.483133
10	6	0	-2.878883	0.740788	-0.480199
11	6	0	-2.760942	-1.589794	0.128379
12	1	0	-0.840028	-2.264458	0.840911
13	6	0	-3.494763	-0.507348	-0.362742
14	1	0	-3.410361	1.609814	-0.860370
15	1	0	-3.221664	-2.571938	0.214374
16	1	0	-4.538333	-0.625667	-0.647440
17	6	0	2.861277	-0.434915	-0.403754
18	8	0	2.647845	-1.666521	-0.549164
19	8	0	3.918880	0.241602	-0.388890
20	9	0	-0.999307	2.123593	-0.253906

92 TS: E(HF) = -320.1024501; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1448337; $E_{\alpha,\beta}$ = -0.8550032. E(MP2) = -321.2471209. TC = 0.074178. S = 77.090. -646.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.443938	1.016412	-0.021519
2	6	0	-1.479907	-1.004387	0.066177
3	1	0	-2.126981	1.174703	-0.851218
4	1	0	-1.553976	-1.830106	-0.647560
5	1	0	-1.995415	-1.097233	1.019082
6	7	0	-0.548479	-0.012892	-0.094920
7	1	0	-1.339630	1.800535	0.734614
8	6	0	0.931134	-0.005949	-0.012571
9	8	0	1.411630	1.153160	0.020678
10	8	0	1.439822	-1.152424	0.006447

GS: E(HF) = -320.1805378; $E_{\alpha,\alpha} = E_{\beta,\beta} =$ -0.1423042; $E_{\alpha,\beta}$ = -0.842726. E(MP2) = -321.23076187. TC = 0.078050. S = 76.081.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.476689	0.005566	0.738601
2	6	0	-1.476689	0.005566	-0.738599
3	1	0	-1.175323	0.932542	1.219884
4	1	0	-2.166632	-0.631147	1.289515
5	1	0	-1.175323	0.932544	-1.219876
6	1	0	-2.166639	-0.631140	-1.289510
7	7	0	-0.423971	-0.718637	0.000001
8	6	0	0.908374	0.021562	-0.000005
9	8	0	0.849063	1.283103	-0.000108
10	8	0	1.891153	-0.754167	0.000107

GS: E(HF) = -284.1843498; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1423041; $E_{\alpha,\beta}$ = -0.8424726. E(MP2) = -285.2724699. TC = 0.078050. S = 76.081.

Standard orientation:

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

1	6	0	-1.476689	0.005566	0.738601
2	6	0	-1.476689	0.005566	-0.738599
3	1	0	-1.175323	0.932542	1.219884
4	1	0	-2.166632	-0.631147	1.289515
5	1	0	-1.175323	0.932544	-1.219876
6	1	0	-2.166639	-0.631140	-1.289510
7	7	0	-0.423971	-0.718637	0.000001
8	6	0	0.908374	0.021562	-0.000005
9	8	0	0.849063	1.283103	-0.000108
10	8	0	1.891153	-0.754167	0.000107

93 TS: E(HF) = -284.1145473; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = 0.1338950; $E_{\alpha,\beta}$ = -0.8315811. E(MP2) = -285.2139187. TC = 0.061031. S = 64.875. -869.6514

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150776	-0.380802	-0.501091
2	6	0	1.355189	-1.135044	0.393703
3	1	0	-0.381660	-1.031992	-1.346613
4	1	0	2.261111	-1.734761	0.219716
5	1	0	0.861869	-1.279251	1.365891
6	7	0	1.152961	0.030609	-0.331706
7	8	0	1.466189	1.327649	0.021142
8	6	0	-1.231448	0.261758	0.224827
9	6	0	-2.545889	-0.004901	0.050996
10	1	0	-0.903174	0.992676	0.963750
11	1	0	-3.315025	0.481496	0.646703
12	1	0	-2.885824	-0.709699	-0.707252

GS: E(HF) = -284.1843498; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1317989; $E_{\alpha,\beta}$ = -0.8245221. E(MP2) = 285.2724699. TC = 0.064381. S = 64.309.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.925035	1.118611	0.271127
2	6	0	0.123184	0.061556	0.358434
3	1	0	-1.617046	1.195165	1.108072
4	1	0	-0.697928	2.045361	-0.259383
5	1	0	0.042398	-0.616176	1.205893

6	6	0	1.409274	0.186387	-0.305724
7	6	0	2.568994	-0.373483	0.104863
8	1	0	1.404313	0.757209	-1.237032
9	1	0	3.486434	-0.270124	-0.468989
10	1	0	2.621511	-0.956793	1.021370
11	7	0	-1.123825	-0.083992	-0.558131
12	8	0	-2.053926	-0.940640	-0.004402

94 TS: E(HF) = -436.8155701; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2153633; $E_{\alpha,\beta}$ = -1.2889302. E(MP2) = -438.5352271. TC = 0.146425. S = 90.547. -835.132.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.415044	-0.604601	1.067550
2	6	0	1.199636	-0.876653	-0.344474
3	1	0	1.652822	-0.406007	1.839400
4	1	0	1.355490	-1.894473	-0.713639
5	7	0	2.308596	-0.070331	-0.197926
6	6	0	-0.175132	-0.393283	-0.248736
7	6	0	-0.436182	0.964415	0.038932
8	6	0	-1.256717	-1.296098	-0.283356
9	6	0	-1.746589	1.390397	0.262354
10	1	0	0.419910	1.640768	0.020849
11	6	0	-2.565507	-0.857961	-0.080296
12	1	0	-1.060248	-2.350019	-0.486209
13	6	0	-2.817667	0.489265	0.207892
14	1	0	-1.936785	2.441563	0.479148
15	1	0	-3.389869	-1.570338	-0.119309
16	1	0	-3.838562	0.834466	0.368657
17	1	0	3.396325	-0.941701	1.441001
18	8	0	2.442428	1.230647	-0.645452

GS: E(HF) = -436.8827798; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ =-0.2136032; $E_{\alpha,\beta}$ = -1.2838776. E(MP2) = -438.593864. TC = 0.148628. S = 92.015.

Standard orientation:

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

1	7	0	2.207048	-0.390166	-0.456012
2	6	0	1.206321	0.517983	0.348884
3	6	0	2.143477	-0.429972	1.013829
4	1	0	1.539069	1.552919	0.302565
5	1	0	3.017002	-0.003957	1.506021
6	1	0	1.723291	-1.333852	1.462372
7	8	0	3.291254	0.317417	-0.901930
8	6	0	-0.215227	0.248909	0.192685
9	6	0	-1.151976	1.301711	0.140462
10	6	0	-0.699712	-1.064094	0.016098
11	6	0	-2.512452	1.057285	-0.048884
12	1	0	-0.796224	2.325253	0.258832
13	6	0	-2.060561	-1.308138	-0.179194
14	1	0	0.012565	-1.885818	-0.003350
15	6	0	-2.979364	-0.253125	-0.209592
16	1	0	-3.211505	1.893001	-0.082186
17	1	0	-2.406130	-2.331916	-0.322744
18	1	0	-4.040473	-0.447148	-0.359717

95 TS: E(HF) = -207.2015344; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0970109; $E_{\alpha,\beta}$ = -0.5925366. E(MP2) = -207.988093. TC = 0.061031. S = 64.875. -875.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642911	1.013221	0.015976
2	6	0	-0.882884	-0.878081	0.073452
3	1	0	-1.289365	1.416272	-0.759123
4	1	0	-1.082798	-1.768048	-0.546421
5	1	0	-1.190434	-0.961624	1.124022
6	7	0	0.171465	-0.043161	-0.260924
7	1	0	-0.392309	1.659884	0.881958
8	8	0	1.488677	-0.106899	0.073683

GS: E(HF) = -207.2779066; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.0941074; $E_{\alpha,\beta}$ = -0.5828583. E(MP2)= -208.0489798. TC = 0.064381. S = 64.309.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.805310	0.743932	0.136276
2	6	0	0.805310	-0.743932	0.136276

3	1	0	1.507310	1.299539	-0.486161
4	1	0	0.455336	1.239573	1.038123
5	1	0	0.455335	-1.239571	1.038125
6	1	0	1.507311	-1.299539	-0.486159
7	7	0	-0.269755	0.000000	-0.575233
8	8	0	-1.462591	0.000000	0.160925

96 TS: E(HF) = HF=-418.9879117; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.1766852$; $E_{\alpha,\beta} = -1.0177280$. E(MP2) = -420.3590108. TC = 0.067075. S = 80.930. -278.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.385552	0.186361	0.339217
2	6	0	-0.154890	1.840640	0.040943
3	1	0	-1.825221	0.375195	1.307901
4	1	0	0.632400	2.364629	0.579770
5	1	0	-0.762011	2.363674	-0.686979
6	7	0	-0.129909	0.462084	-0.009723
7	9	0	-2.104700	-0.777363	-0.367205
8	6	0	1.126345	-0.424059	-0.014113
9	8	0	2.150546	0.249042	-0.246373
10	8	0	0.885839	-1.618975	0.243364

GS: E(HF)= -419.0812367; $E_{\alpha,\alpha} = E_{\beta,\beta} = -0.1721073$; $E_{\alpha,\beta} = -0.9958535$. E(MP2) = -420.4213049. TC = 0.070654. S = 79.737.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.137519	-0.116675	0.371863
2	6	0	-0.764253	1.300289	0.182136
3	1	0	-0.923850	-0.674864	1.279072
4	1	0	-0.191224	1.801632	0.961262
5	1	0	-1.388852	1.941169	-0.436696
6	7	0	-0.106605	0.186905	-0.522547
7	6	0	1.290953	-0.189642	-0.094299
8	8	0	2.079039	0.784200	-0.033055
9	8	0	1.433751	-1.417756	0.116054
10	9	0	-2.354138	-0.585740	-0.174222

97 TS: = -436.8806922; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2160361; $E_{\alpha,\beta}$ = -1.2920959.
E(MP2) = -438.6048605. TC = 0.146210. S = 92.850 -701.8.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.917045	-0.906666	0.395033
2	6	0	2.949261	0.929354	-0.276421
3	1	0	3.603355	-1.408162	-0.280085
4	1	0	3.095401	1.415590	-1.249346
5	1	0	3.364184	1.416965	0.603788
6	7	0	1.990464	-0.044120	-0.124677
7	1	0	2.798297	-1.300321	1.415360
8	6	0	0.586102	-0.021545	-0.044829
9	6	0	-0.145028	-1.213539	-0.180469
10	6	0	-0.108864	1.190784	0.096022
11	6	0	-1.534019	-1.202361	-0.105207
12	1	0	0.396237	-2.150141	-0.331182
13	6	0	-1.499403	1.204719	0.141979
14	1	0	0.461513	2.112284	0.229329
15	6	0	-2.303855	0.013299	0.011155
16	1	0	-2.093988	-2.131839	-0.213093
17	1	0	-2.031923	2.148831	0.261370
18	8	0	-3.586720	0.030171	0.026627

GS: E(HF) = HF=-436.9625204; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2128115; $E_{\alpha,\beta}$ = -1.2794269.
E(MP2) = -438.6675704. TC = 0.150015. S = 91.512.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.017838	0.000179	-0.582422
2	6	0	-2.871368	0.743383	0.351915
3	6	0	-2.871330	-0.743550	0.351513
4	1	0	-3.690897	1.297113	-0.099937
5	1	0	-2.370039	1.237063	1.183208
6	1	0	-2.369982	-1.237649	1.182547
7	1	0	-3.690837	-1.297081	-0.100624
8	6	0	-0.610181	0.000096	-0.273231
9	6	0	0.107093	1.202890	-0.204287
10	6	0	0.106968	-1.202768	-0.204226

11	6	0	1.487939	1.205442	-0.006568
12	1	0	-0.431691	2.150094	-0.285854
13	6	0	1.487819	-1.205450	-0.006525
14	1	0	-0.431906	-2.149924	-0.285748
15	6	0	2.272698	-0.000043	0.076043
16	1	0	2.027270	2.151820	0.052145
17	1	0	2.027054	-2.151880	0.052227
18	8	0	3.549759	-0.000101	0.233899

98 TS: E(HF) = -895.843488; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2420314; $E_{\alpha,\beta}$ = -1.4204983.
E(MP2) = -897.7480493. TC = 0.139195. S = 100.602. -614.2669

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.323161	-0.238295	-0.353114
2	6	0	0.525341	0.555198	0.339113
3	1	0	1.985381	-0.416871	-1.365524
4	1	0	0.769928	1.609913	0.310975
5	7	0	1.540130	-0.302288	0.739179
6	1	0	1.415089	-1.103707	1.370414
7	6	0	-0.806102	0.085241	0.142580
8	6	0	-1.080590	-1.297974	0.058849
9	6	0	-1.871969	1.073581	-0.026875
10	6	0	-2.383295	-1.779961	-0.069719
11	1	0	-0.247939	-2.005258	0.091906
12	6	0	-3.192489	0.516527	-0.137085
13	6	0	-3.433986	-0.852779	-0.183034
14	1	0	-2.573028	-2.850085	-0.144579
15	1	0	-4.014135	1.226272	-0.239044
16	1	0	-4.460862	-1.210042	-0.287134
17	17	0	4.061778	-0.009405	-0.191875
18	8	0	-1.648251	2.332057	-0.034212

GS: E(HF) = -895.9264496; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.2391611; $E_{\alpha,\beta}$ = -1.409567.
E(MP2)= -897.8143399. TC = 0.142913. S = 96.201.

Standard orientation:

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

1	6	0	0.793134	-0.496742	0.524495
2	6	0	1.844032	0.280612	-0.160103
3	1	0	1.094550	-1.485005	0.874178
4	1	0	1.570316	1.006625	-0.917325
5	7	0	1.560504	0.588331	1.220974
6	1	0	0.961474	1.428756	1.178543
7	6	0	-0.645040	-0.351833	0.198936
8	6	0	-1.452905	-1.494904	0.230089
9	6	0	-1.209641	0.953471	-0.055611
10	6	0	-2.820221	-1.443174	-0.058777
11	1	0	-0.985916	-2.457164	0.456352
12	6	0	-2.609195	0.960493	-0.353338
13	6	0	-3.391065	-0.192456	-0.335296
14	1	0	-3.429057	-2.345673	-0.030453
15	1	0	-3.058848	1.932692	-0.556810
16	1	0	-4.456798	-0.120075	-0.560997
17	17	0	3.428685	-0.451022	-0.509233
18	8	0	-0.495186	2.037012	-0.034465

99 TS: E(HF)= -330.1572705; $E_{\alpha,\alpha} = E_{\beta,\beta} =$ -0.1297535; $E_{\alpha,\beta}$ = -0.7524767. E(MP2) = -331.1692544. TC = 0.042011. S = 68.847. -411.3284.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.214831	-0.077389	0.165159
2	6	0	-1.728787	-0.014704	0.244165
3	1	0	-2.618811	0.368240	-0.269029
4	1	0	-1.854193	-0.273912	1.289871
5	7	0	-0.731723	-0.653376	-0.540151
6	9	0	1.495044	-0.712262	0.129207
7	9	0	0.580379	1.271358	-0.095399

GS: E(HF) = -330.2452983; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1268457; $E_{\alpha,\beta}$ = -0.7340798. E(MP2)= -331.2330697. TC = 0.044286. S = 68.938.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.954625	0.000000	0.936535
2	6	0	0.028033	0.000002	0.068385

3	6	0	-1.260939	-0.000004	-0.572227
4	1	0	-1.665680	0.919308	-1.013054
5	1	0	-1.665671	-0.919326	-1.013046
6	9	0	0.967291	-1.105252	-0.083698
7	9	0	0.967283	1.105255	-0.083701

100 TS: E(HF) = -754.559376; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1948777; $E_{\alpha,\beta}$ = -1.1053833. E(MP2)= -756.0545148. TC = 0.077288. S = 83.393. -565.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.603949	-0.461718	-0.082726
2	6	0	-0.756257	0.049842	0.747185
3	1	0	-2.157881	-1.374079	-0.463885
4	1	0	-0.914862	-0.321756	1.753651
5	7	0	-1.791645	0.659769	0.092274
6	1	0	-1.576612	1.359274	-0.619816
7	1	0	-3.627202	-0.454647	0.293638
8	16	0	0.833091	-0.033853	-0.035870
9	8	0	0.865921	1.269220	-0.776377
10	8	0	1.805314	-0.148217	1.086628
11	8	0	0.784997	-1.222787	-0.938044

GS: E(HF) = -754.6559273; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1903402; $E_{\alpha,\beta}$ = -1.0852695. E(MP2)= -756.1218773. TC = 0.081153. S = 80.828.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.004137	-0.693092	-0.019031
2	6	0	-0.907145	0.105123	-0.596976
3	1	0	-2.769010	-1.079421	-0.691146
4	1	0	-1.788925	-1.287739	0.862064
5	1	0	-0.908189	0.289588	-1.670440
6	7	0	-1.927721	0.768842	0.223750
7	1	0	-2.573599	1.268723	-0.391636
8	16	0	0.773080	-0.006966	0.035707
9	8	0	1.368760	-1.033564	-0.873734

10	8	0	1.329482	1.364209	-0.145751
11	8	0	0.630782	-0.447367	1.450690

101 TS: E(HF) = -510.935042; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2314975; $E_{\alpha,\beta}$ = -1.3938452. E(MP2)= -512.7918824. TC = 0.145446. S = 103.485. -623.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.472108	0.060416	-0.898845
2	6	0	1.917020	-0.773756	0.881730
3	1	0	2.972693	0.914321	-0.454609
4	1	0	1.565775	-0.355224	1.825108
5	1	0	2.596637	-1.618178	0.881468
6	7	0	1.332188	-0.445424	-0.305091
7	1	0	2.799191	-0.315413	-1.872767
8	6	0	-0.043194	-0.080133	-0.567284
9	1	0	-0.156999	-0.037249	-1.660656
10	6	0	-1.058399	-1.123522	0.016822
11	8	0	-0.990504	-1.242101	1.273939
12	8	0	-1.826223	-1.669600	-0.824119
13	6	0	-0.386290	1.283063	0.006741
14	8	0	0.433407	1.980517	0.607507
15	6	0	-1.819980	1.723045	-0.175407
16	1	0	-1.899051	2.795455	0.019518
17	1	0	-2.183340	1.481020	-1.178803
18	1	0	-2.441237	1.168037	0.535214

GS: E(HF) = =-511.0310378; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.2277983; $E_{\alpha,\beta}$ = -1.3772282. E(MP2)= -512.8638627. TC = 0.149391. S = 101.355.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.136119	-0.423977	0.494795
2	6	0	-2.050644	-1.405994	-0.114798
3	6	0	-2.450983	0.018274	0.053538
4	1	0	-2.428125	-2.171447	0.559141
5	1	0	-1.805060	-1.754333	-1.117650

6	1	0	-2.480120	0.655554	-0.826446
7	1	0	-3.131107	0.311456	0.848464
8	6	0	-0.037898	0.008495	-0.376840
9	1	0	-0.308939	-0.095628	-1.444619
10	6	0	0.362003	1.507835	-0.147533
11	8	0	-0.573369	2.291319	0.166775
12	8	0	1.586810	1.740502	-0.375911
13	6	0	1.125632	-0.923064	-0.119023
14	8	0	1.530399	-1.708449	-0.984263
15	6	0	1.736666	-0.876154	1.257362
16	1	0	2.392151	-1.739498	1.398368
17	1	0	2.307422	0.053921	1.335648
18	1	0	0.947228	-0.855508	2.014490

102 TS: E(HF) = =-754.560161; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1941279; $E_{\alpha,\beta}$ = -1.1037940. E(MP2) = -756.052211. TC = 0.076617. S = 84.024. -658.5.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.855497	-1.032559	-0.036954
2	6	0	1.887226	1.014510	0.047023
3	1	0	2.618569	-1.198255	-0.788768
4	1	0	2.001035	1.852839	-0.642434
5	1	0	2.345751	1.063193	1.030597
6	7	0	0.992166	0.009555	-0.227368
7	1	0	1.678126	-1.784185	0.737562
8	16	0	-0.758726	0.004273	0.003590
9	8	0	-0.938227	-0.044533	1.477779
10	8	0	-1.147773	1.284882	-0.630348
11	8	0	-1.152171	-1.235418	-0.705335

GS: E(HF) = =-754.6588421; $E_{\alpha,\alpha} = E_{\beta,\beta}$ = -0.1906868; $E_{\alpha,\beta}$ = -1.0863670. E(MP2)= -756.1265829. TC = 0.080740. S = 80.205.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.857418	-0.000003	-0.730187
2	6	0	-1.882442	0.743758	0.008914

3	6	0	-1.882448	-0.743757	0.008913
4	1	0	-2.576467	1.299415	-0.617462
5	1	0	-1.570871	1.228055	0.931533
6	1	0	-1.570880	-1.228059	0.931530
7	1	0	-2.576476	-1.299407	-0.617466
8	16	0	0.733989	0.000000	0.020057
9	8	0	1.328052	-1.257037	-0.493663
10	8	0	1.328037	1.257051	-0.493645
11	8	0	0.486680	-0.000012	1.494220

103 TS: E(HF) = -359.0520394; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1591931; $E_{\alpha,\beta}$ = -0.9764782. E(MP2)= -360.3469038. TC = 0.103693. S = 84.365. -593.3.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.185523	0.682788	0.051954
2	6	0	1.463333	-1.527308	0.125915
3	1	0	2.911252	0.434367	0.817194
4	1	0	2.296926	-1.633269	-0.599090
5	7	0	1.099956	-0.180229	-0.053917
6	1	0	2.469690	1.289527	-0.806947
7	6	0	-0.192482	0.311877	-0.009195
8	8	0	-0.517415	1.498810	0.021576
9	8	0	-1.105104	-0.699449	-0.082660
10	6	0	-2.456643	-0.256500	0.039321
11	1	0	-2.729863	0.403784	-0.788310
12	1	0	-3.053506	-1.169311	0.013997
13	1	0	-2.612429	0.276479	0.981273

GS: E(HF) = =-359.1318025; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1585145; $E_{\alpha,\beta}$ = -0.9717201. E(MP2)= -360.4205517. TC = 0.107056. S = 84.034.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.992735	-0.224665	-0.505390
2	6	0	-2.177086	0.413357	0.045882
3	6	0	-1.849149	-0.980157	0.551607
4	1	0	-2.938915	0.610927	-0.716302
5	1	0	-2.003443	1.263331	0.705717

6	1	0	-2.427296	-1.704281	-0.052476
7	6	0	0.223040	0.265704	-0.149398
8	8	0	0.544060	1.432401	0.114709
9	8	0	1.177503	-0.729463	-0.213274
10	6	0	2.484752	-0.298775	0.158304
11	1	0	2.491232	0.097429	1.177410
12	1	0	3.108259	-1.192907	0.094643
13	1	0	2.857467	0.473887	-0.521117

104 TS: E(HF) = -320.0902932; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1461689; $E_{\alpha,\beta}$ = -0.8604448.
E(MP2) = -321.2430758. TC = 0.074828. S = 75.760. -547.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.212416	-0.200460	0.474093
2	6	0	0.293354	-0.536286	-0.344250
3	1	0	1.799793	-0.471961	1.442296
4	1	0	0.450885	-1.564157	-0.656679
5	7	0	1.351919	0.323453	-0.506230
6	1	0	1.084023	1.311179	-0.512480
7	1	0	3.201374	-0.558517	0.186717
8	6	0	-1.056387	0.000572	0.023625
9	8	0	-2.003087	-0.842250	0.101251
10	8	0	-1.083889	1.271792	0.169117

GS: E(HF) = =-320.1919025; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1424405; $E_{\alpha,\beta}$ = -0.8423503.
E(MP2) = -321.319134. TC = 0.079113. S = 73.899.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.549732	0.242710	-0.700997
2	1	0	-1.129216	1.180818	-0.682123
3	6	0	-1.538183	-0.242228	0.690699
4	6	0	-0.443504	-0.625345	-0.236233
5	1	0	-2.324813	-0.953034	0.934035
6	1	0	-1.281589	0.469951	1.471296
7	1	0	-0.438376	-1.626696	-0.659350
8	6	0	0.921455	0.028991	-0.012745
9	8	0	0.888975	1.293520	0.130808

10	8	0	1.908963	-0.760835	0.018291

105 TS: E(HF) = =-527.9440454; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1907715; $E_{\alpha,\beta}$ = -1.0685196. E(MP2) = -529.3941081. TC = 0.028865. S = 77.337. -186.1.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.005002	0.125155	-0.061706
2	6	0	-1.005005	-0.125142	-0.061698
3	7	0	0.000002	-0.000012	0.822767
4	9	0	2.178765	0.610351	0.510229
5	9	0	1.431448	-0.987576	-0.789064
6	9	0	-1.431453	0.987595	-0.789040
7	9	0	-2.178760	-0.610369	0.510215

GS: E(HF) = =-528.0522451; $E_{\alpha,\alpha}$ = $E_{\beta,\beta}$ = -0.1883030; $E_{\alpha,\beta}$ = -1.0456504. E(MP2)= -529.4745017. TC = 0.030151. S = 77.326.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.202319	0.417963	0.000000
2	6	0	0.094838	0.032989	0.706214
3	6	0	0.094838	0.032989	-0.706214
4	9	0	0.094838	-1.128402	1.522870
5	9	0	0.094838	-1.128402	-1.522870
6	9	0	-0.625632	0.943868	1.522733
7	9	0	-0.625632	0.943868	-1.522733

Aziridine	C_2 — N	C_3 — N	C_2 — C_3	C_2 — X	C_n — X^b

.

Selected Wiberg Bond Indices for Haloaziridines

1	1.165	1.139	0.756	—	—
2	1.266	1.131	0.661	0.804[a]	—
3	1.253	1.168	0.627	0.818[a]	0.822[b]
4	1.177	1.177	0.656	0.814[a]	0.814[a]
5	1.128	1.204	0.662	0.822[a]	0.803[b]
6	0.823	1.106	0.711	0.823[a]	0.857[a]; 0.849[b]
7	1.209	0.838	0.496	0.838[a]; 0.844[b]	0.884[a]; 0.838[b]
8	1.202	1.129	0.685	1.030	—
9	1.029	1.146	0.624	1.029	1.020
10	1.178	1.178	0.613	1.043	1.043
11	1.159	1.068	0.624	1.019 [a]	1.067 [a]
12	1.026	1.130	0.692	1.017	0.933; 0.929
13	1.203	1.152	0.629	1.007	0.990

(a) outward rotation (b) inward rotation (c) $C_n = C_2$ or C_3 depending on structure.

Transition State Distances in Conrotatory Cleavage of Aziridines

(a) Average bond distances (Å) (From March, J. *Advanced Organic Chemistry*, 4th Ed. Wiley: New York, NY, 1992, p. 21) :

$C(sp^3) – F = 1.38.$
$C(sp^3) – Cl = 1.78.$
$C(sp^3) – Br = 1.94.$
$C(sp^3) – N = 1.47.$
$C(sp^2) – N = 1.28.$
(b) Outward rotation. (c) Inward rotation.

3-Substituted Cyclobutenes

TS: Cyclobutene

E = -155.5332896. TC = 0.088999. S = 63.814. -748.115.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.878813	-1.107448	0.417088
2	6	0	0.684273	0.733767	0.092241
3	6	0	1.058771	-0.626725	-0.125909
4	6	0	-0.684188	0.733875	-0.092332
5	6	0	-1.058692	-0.626772	0.125920
6	1	0	1.343572	1.537120	0.416284
7	1	0	-1.343957	1.536944	-0.416063
8	1	0	0.844856	-1.072169	-1.090570
9	1	0	-0.845639	-1.071826	1.090946
10	1	0	-1.878627	-1.107487	-0.417210

GS: Cyclobutene

E = -155.5881075. TC = 0.091683. S = 64.059.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.698694	-0.782194	0.000000
2	6	0	-0.811205	-0.675348	-0.000000
3	6	0	-0.812705	0.673675	-0.000000
4	6	0	0.696929	0.783690	-0.000000
5	1	0	1.143959	-1.238711	0.890696
6	1	0	1.143957	-1.238712	-0.890696
7	1	0	-1.599004	-1.424853	0.000000
8	1	0	-1.602147	1.421443	-0.000000
9	1	0	1.141479	1.240946	0.890666
10	1	0	1.141481	1.240948	-0.890665

TS:3,3-Difluorocyclobutene

E = -353.7284644. TC = 0.074259. S = 72.909. -647.9.

Standard orientation:

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.946344	-1.583353	0.673518
2	6	0	-1.594261	0.384808	-0.246107
3	6	0	-1.406063	-0.635981	0.714596
4	6	0	-0.381052	1.045331	-0.390350
5	6	0	0.538912	0.052067	0.008630
6	1	0	-2.500370	0.541461	-0.829511
7	1	0	-0.141321	2.079657	-0.623822
8	1	0	-1.014600	-0.365132	1.688052
9	9	0	0.804772	-1.050082	-0.741925
10	9	0	1.712719	0.411195	0.583163

GS:3,3-Difluorocyclobutene

E = -353.7971133. TC = 0.077138. S = 72.616.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.361946	-0.023503	0.000000
2	6	0	-0.719284	-1.059652	0.000000
3	6	0	-1.678426	-0.111335	0.000000
4	6	0	-0.724157	1.074752	0.000000
5	1	0	-0.700013	-2.143908	-0.000001
6	1	0	-2.762990	-0.159180	0.000000
7	1	0	-0.725686	1.698774	0.898104
8	1	0	-0.725686	1.698774	-0.898103
9	9	0	1.192994	-0.020890	-1.099405
10	9	0	1.192995	-0.020891	1.099405

TS:3-Fluorocyclobutene (out)

E = -254.6396845. TC = 0.082154. S = 68.424. -607.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.863248	-1.683833	0.367054
2	6	0	1.428461	0.446315	-0.008016
3	6	0	1.220527	-0.953334	-0.132208
4	6	0	0.163538	1.010333	-0.069577
5	6	0	-0.639607	-0.073251	0.349485
6	1	0	-0.589164	-0.492868	1.346730

7	1	0	2.370888	0.933803	0.234686
8	1	0	-0.181798	1.992881	-0.379133
9	1	0	0.718400	-1.327204	-1.016645
10	9	0	-1.913231	-0.222574	-0.154532

GS:3-Fluorocyclobutene

E = -254.6873232. TC = 0.084838. S = 68.754.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.518462	1.063434	0.023806
2	6	0	1.457802	-0.105154	-0.204666
3	6	0	0.526373	-1.050358	0.043184
4	6	0	-0.501606	-0.031305	0.439707
5	1	0	0.793184	1.792842	0.794018
6	1	0	0.203520	1.587328	-0.882492
7	1	0	2.515625	-0.149758	-0.449797
8	1	0	0.521273	-2.135931	0.040462
9	1	0	-0.797720	-0.022408	1.492847
10	9	0	-1.693563	-0.036864	-0.311913

TS:3-Acetylcyclobutene (in)

E = -307.8807557. TC = 0.130589. S = 82.246. -616.9.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.718619	0.772039	1.990658
2	6	0	1.819893	0.457200	0.084123
3	6	0	1.084351	0.059467	1.245556
4	6	0	1.404399	-0.413623	-0.896381
5	6	0	0.162858	-0.936650	-0.408934
6	1	0	2.487211	1.314885	0.015389
7	1	0	1.899773	-0.712913	-1.817956
8	1	0	1.206617	-0.952769	1.618121
9	1	0	-0.093667	-1.995785	-0.527491
10	6	0	-1.046739	-0.136128	-0.077690
11	8	0	-2.041490	-0.719002	0.372754
12	6	0	-1.139127	1.340809	-0.408692
13	1	0	-1.566264	1.869779	0.446705

14	1	0	-0.190307	1.792838	-0.694690
15	1	0	-1.843869	1.437481	-1.240657

GS:3-Acetylcyclobutene

E = -307.9286730. TC = 0.133003. S = 83.434.

Standard orientation:

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	6	0	0.251776	-0.559576	0.456153
2	6	0	1.262460	0.478117	0.900966
3	6	0	2.069194	0.303457	-0.166023
4	6	0	1.196856	-0.760267	-0.792206
5	1	0	1.310111	1.111625	1.783816
6	1	0	3.015246	0.744765	-0.470197
7	1	0	1.627254	-1.765375	-0.852483
8	1	0	0.743542	-0.514385	-1.759829
9	1	0	0.170946	-1.450886	1.088131
10	6	0	-1.140671	-0.107979	0.084770
11	8	0	-2.096254	-0.880530	0.181147
12	6	0	-1.312997	1.303009	-0.422584
13	1	0	-0.543727	1.561153	-1.156870
14	1	0	-2.306820	1.411196	-0.859687
15	1	0	-1.206234	2.005585	0.411487

TS:3-Phenylcyclobutene (out)

E = -386.0746826. TC = 0.174254. S = 89.771. -593.262.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.406675	-1.207548	1.514778
2	6	0	-3.245020	0.305258	-0.103221
3	6	0	-2.800533	-0.427518	1.043012
4	6	0	-2.101914	0.523202	-0.837731
5	6	0	-1.180320	-0.476334	-0.361465
6	1	0	-1.466798	-1.514390	-0.521306
7	1	0	-4.280131	0.533879	-0.354753
8	1	0	-1.878576	1.286927	-1.582108
9	1	0	-2.064009	0.025505	1.699074

10	6	0	0.248029	-0.228403	-0.176072
11	6	0	1.181593	-1.279837	-0.223055
12	6	0	0.711555	1.073886	0.085321
13	6	0	2.542244	-1.031596	-0.050951
14	1	0	0.832095	-2.294307	-0.412998
15	6	0	2.074749	1.324484	0.245418
16	1	0	-0.008586	1.887635	0.163306
17	6	0	2.993471	0.272262	0.183739
18	1	0	3.253728	-1.853585	-0.096280
19	1	0	2.420518	2.337559	0.440703
20	1	0	4.055308	0.465908	0.319616

GS:3-Phenylcyclobutene (out)

E = -386.1186058. TC = 0.176668. S = 91.375.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.515982
3	6	0	1.345319	0.000000	1.620146
4	6	0	1.573555	0.030890	0.125072
5	1	0	-0.354590	-0.945023	-0.433690
6	1	0	-0.814465	-0.007062	2.237755
7	1	0	2.030120	-0.030215	2.464709
8	1	0	2.089087	-0.835037	-0.308456
9	1	0	2.018984	0.949949	-0.271490
10	6	0	-0.638159	1.158071	-0.709464
11	6	0	-1.199044	0.990694	-1.982935
12	6	0	-0.635915	2.440757	-0.141320
13	6	0	-1.754538	2.072311	-2.670828
14	1	0	-1.212479	-0.000991	-2.434448
15	6	0	-1.188557	3.524829	-0.826106
16	1	0	-0.208651	2.586903	0.849782
17	6	0	-1.745092	3.345617	-2.095961
18	1	0	-2.189814	1.921487	-3.656705
19	1	0	-1.183425	4.512233	-0.368548
20	1	0	-2.178239	4.189840	-2.627938

TS: Cyclobut-3-en-ol (out)

E = -230.6449418. TC = 0.094718. S = 69.207. -590.4.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.808939	-1.740627	0.364578
2	6	0	1.461018	0.411374	-0.011186
3	6	0	1.189927	-0.983849	-0.127294
4	6	0	0.220450	1.018572	-0.043401
5	6	0	-0.646253	-0.039855	0.348594
6	1	0	2.430629	0.865812	0.187224
7	1	0	-0.089160	2.017437	-0.342006
8	1	0	0.677633	-1.335933	-1.015851
9	1	0	-0.569395	-0.451412	1.350818
10	8	0	-1.891094	-0.139629	-0.234128
11	1	0	-2.480742	-0.675695	0.327979

GS: Cyclobut-3-en-ol

E = -230.6848836. TC = 0.097004. S = 70.391.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.497630	0.030691	0.442954
2	6	0	0.546272	1.054970	0.047120
3	6	0	1.472449	0.112433	-0.222580
4	6	0	0.540539	-1.052793	0.041336
5	1	0	0.546651	2.142371	0.031942
6	1	0	2.519988	0.156832	-0.510189
7	1	0	0.830036	-1.759470	0.827377
8	1	0	0.220827	-1.603495	-0.847811
9	8	0	-1.683840	-0.064030	-0.344275
10	1	0	-2.271913	0.677684	-0.113907
11	1	0	-0.744649	0.026512	1.513813

TS: Cyclobut-3-enylborane (In)

E = -180.9248471. TC = 0.102797. S = 68.244. -454.7.

Standard orientation:

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

1	6	0	0.919273	-0.844827	-0.086071
2	6	0	-0.487185	-0.938721	0.254188
3	6	0	1.138577	0.493752	-0.198784
4	6	0	-0.067873	1.100318	0.378280
5	1	0	1.617580	-1.671985	-0.181129
6	1	0	1.990207	1.027287	-0.613150
7	1	0	-0.157864	1.042712	1.462301
8	1	0	-0.459329	2.046886	-0.006420
9	1	0	-0.788231	-1.561660	1.107401
10	5	0	-1.476426	-0.035163	-0.457705
11	1	0	-1.277017	0.284121	-1.593433
12	1	0	-2.559969	0.145324	0.027272

GS: Cyclobut-3-enylborane (In)

E = -180.9407838. TC = 0.104039. S = 71.298.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.526517	-0.386377	0.520124
2	6	0	-0.775555	-0.959392	0.024635
3	6	0	-1.322898	0.228403	-0.302037
4	6	0	-0.150465	1.044853	0.181035
5	1	0	0.750964	-0.506054	1.584687
6	1	0	-1.115068	-1.988354	-0.063448
7	1	0	-2.247782	0.525829	-0.789699
8	1	0	-0.290351	1.638116	1.088923
9	1	0	0.337872	1.678684	-0.575165
10	5	0	1.716130	-0.173058	-0.432955
11	1	0	1.576528	-0.327770	-1.611072
12	1	0	2.741595	0.279914	-0.011987

TS: Cyclobutene 3-Anion (In.)

E = -154.8932091. TC = 0.073072. S = 63.927. -601.255.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.989680	-1.114120	0.259842
2	6	0	0.753033	0.618111	0.077128

3	6	0	1.082549	-0.704441	-0.266723
4	6	0	-0.655760	0.749447	-0.011511
5	6	0	-1.079485	-0.606630	0.077140
6	1	0	1.454858	1.380601	0.449755
7	1	0	-1.233624	1.556858	-0.466925
8	1	0	-0.854430	-1.180722	0.971336
9	1	0	-1.958508	-0.981542	-0.470206

GS: Cyclobutene 3-Anion

E = -154.9390792. TC = 0.0.075498. S = 63.794.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.085851	-1.052054	-0.128263
2	6	0	-1.025475	-0.000725	0.000036
3	6	0	-0.087314	1.051884	0.127903
4	6	0	1.031357	0.000727	0.000038
5	1	0	-0.109096	-2.042879	0.344280
6	1	0	-2.123229	-0.001498	0.000297
7	1	0	-0.112421	2.043145	-0.343511
8	1	0	1.673891	-0.118137	0.887920
9	1	0	1.674553	0.120376	-0.887271

Aziridine + Ethyne Transition State

E = -210.7308532. TC = 0.103978. S = 75.338. -205.04

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.826049	1.211936	0.195335
2	6	0	1.619042	0.617910	-0.060707
3	6	0	1.619129	-0.617970	-0.060570
4	6	0	-0.826143	-1.211888	0.195427
5	1	0	-1.466365	0.000011	-1.261934
6	1	0	-0.643274	1.287552	1.259843
7	1	0	-1.189766	2.072040	-0.352333
8	1	0	1.905922	1.646362	-0.079756
9	1	0	1.905466	-1.646548	-0.080616
10	1	0	-0.643335	-1.287443	1.259933
11	1	0	-1.189882	-2.072020	-0.352189

12	7	0	-1.170662	0.000016	-0.287123

Azomethine Produced from Aziridine

E = -133.5751276. TC = 0.0719170. S = 65.510.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.231674	-0.187684	-0.000396
2	6	0	1.231657	-0.187695	0.000195
3	1	0	-1.332855	-1.263876	0.000369
4	1	0	2.079748	0.478048	-0.000622
5	1	0	1.332812	-1.263877	0.000003
6	7	0	0.000020	0.350526	0.000049
7	1	0	0.000022	1.370218	-0.000127
8	1	0	-2.079761	0.478080	0.001243

Ethyne

E = -77.1505690. TC = 0.028936. S = 49.000.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.609380
2	1	0	0.000000	0.000000	1.676725
3	6	0	0.000000	0.000000	-0.609380
4	1	0	0.000000	0.000000	-1.676725

Azomethine Ylide from **86 (2-Aza-allyl Anion.)**

E = -132.9933223. TC = 0.056389. S = 62.830.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.177744	-0.145343	-0.000058
2	6	0	-1.177744	-0.145343	0.000057
3	1	0	1.265404	-1.244015	0.000108
4	1	0	-2.089792	0.446181	-0.000128
5	1	0	-1.265405	-1.244015	-0.000107
6	7	0	0.000000	0.477113	0.000000
7	1	0	2.089792	0.446181	0.000130

Aziridine Anion + Ethene Transition State.

E = -211.3890752. TC = 0.113756. S = 75.899. -168.6.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.912898	1.146650	0.165815
2	6	0	1.449421	0.692055	-0.048832
3	6	0	1.449444	-0.692399	-0.048741
4	6	0	-0.913517	-1.146469	0.165742
5	1	0	-0.766884	1.199697	1.256882
6	1	0	-1.200586	2.079595	-0.322490
7	1	0	1.709798	1.252368	0.846649
8	1	0	1.709572	-1.252620	0.846865
9	1	0	-0.767422	-1.199674	1.256786
10	1	0	-1.201566	-2.079244	-0.322667
11	7	0	-1.266321	0.000195	-0.429657
12	1	0	1.473230	-1.251425	-0.979068
13	1	0	1.473404	1.250913	-0.979260

2-Acetoxyaziridine + Acetylene Transition State

E = -438.1679763. TC = 0.149908. S = 109.035. -22.7.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.095256	-0.564507	0.443207
2	6	0	2.091766	1.915088	-0.352053
3	6	0	3.156272	1.330860	-0.220655
4	6	0	2.273923	-1.674170	0.225334
5	1	0	0.750083	-1.619028	-1.093646
6	1	0	0.209002	-0.370217	1.507703
7	1	0	1.207958	2.493750	-0.498973
8	1	0	4.091579	0.830871	-0.104847
9	1	0	2.611439	-1.395123	1.213894
10	1	0	2.938701	-2.070153	-0.527230
11	7	0	1.034527	-1.311898	-0.161252
12	8	0	-1.188010	-0.888766	-0.029943
13	6	0	-2.167795	0.078098	-0.078221
14	8	0	-3.238684	-0.215937	-0.572977

15	6	0	-1.840636	1.408467	0.540369
16	1	0	-1.802763	1.315692	1.630843
17	1	0	-0.862279	1.756731	0.206774
18	1	0	-2.624566	2.115375	0.269721

Azomethine Ylide from 2-Acetoxyaziridine

E = -285.9335687. TC = 0.114554. S = 81.168.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.774483	0.183281	0.465330
2	6	0	3.165947	0.053735	-0.120404
3	1	0	1.592064	-0.813072	-1.027068
4	1	0	0.932689	0.613559	1.450858
5	1	0	3.488316	0.710108	0.677006
6	1	0	3.797995	-0.172810	-0.965489
7	7	0	1.847266	-0.203672	-0.246802
8	8	0	-0.315734	-0.682773	0.308085
9	6	0	-1.549921	-0.144464	-0.015750
10	8	0	-2.488299	-0.906097	-0.131552
11	6	0	-1.621498	1.348870	-0.186534
12	1	0	-1.377798	1.859131	0.749277
13	1	0	-0.907012	1.690281	-0.939254
14	1	0	-2.638916	1.600937	-0.485834

2-Phenylaziridine + Acetylene Transition State

E = -441.2671512. TC = 0.189934. S = 99.625. -283.429.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.411121	-1.241402	0.095430
2	6	0	-2.511017	0.763839	1.396508
3	6	0	-1.742650	1.546931	0.815767
4	6	0	-0.922266	0.280164	-1.114106
5	1	0	-2.728320	-0.348659	-1.654477
6	1	0	-1.683981	-1.617078	0.798074
7	1	0	-3.354063	-1.764444	-0.019572

8	1	0	-3.169959	0.376405	2.145633
9	1	0	-1.152733	2.406978	0.575999
10	1	0	-0.974779	0.916859	-1.994442
11	7	0	-1.981687	-0.560000	-0.994828
12	6	0	0.390230	0.057299	-0.528697
13	6	0	1.327555	1.107863	-0.602241
14	6	0	0.814712	-1.161656	0.032311
15	6	0	2.613084	0.969468	-0.084409
16	1	0	1.032902	2.050563	-1.063960
17	6	0	2.103541	-1.299431	0.550924
18	1	0	0.148905	-2.019945	0.045278
19	6	0	3.009050	-0.236930	0.502552
20	1	0	3.311190	1.801990	-0.147358
21	1	0	2.406309	-2.252874	0.979901
22	1	0	4.009631	-0.346667	0.914491

Azomethine Ylide from 2-Phenylaziridine

E = -364.1146369. TC = 0.159280. S = 88.185.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.905633	0.910201	0.302101
2	6	0	-1.378181	-0.994848	-0.222864
3	1	0	-2.161867	1.596015	0.659323
4	1	0	-1.486238	-2.045552	-0.445903
5	7	0	-2.551635	-0.345362	-0.045386
6	1	0	-3.349655	-0.939510	-0.241565
7	1	0	-3.955952	1.081471	0.456775
8	6	0	-0.067262	-0.423862	-0.093748
9	6	0	1.022934	-1.304656	0.099577
10	6	0	0.219871	0.954355	-0.221018
11	6	0	2.328340	-0.833993	0.180014
12	1	0	0.828953	-2.367687	0.187267
13	6	0	1.533358	1.419661	-0.135649
14	1	0	-0.568812	1.658008	-0.442262
15	6	0	2.593464	0.536871	0.075137
16	1	0	3.139932	-1.533679	0.335112
17	1	0	1.725833	2.480066	-0.241454
18	1	0	3.607894	0.906028	0.149105

Transition State for *trans*-2,3-diphenyl-l-aziridinecarboxylate.

E(B3LYP) = -784.2492856. TC = 0.244871. S = 125.304.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.816857	-0.254069	-0.609543
2	6	0	0.816860	-0.254064	0.609508
3	1	0	-0.388874	-0.865257	-1.406298
4	1	0	0.388868	-0.865239	1.406269
5	7	0	0.000008	0.669235	-0.000030
6	6	0	2.217955	-0.446241	0.303478
7	6	0	2.873651	0.292873	-0.708908
8	6	0	2.972355	-1.415680	1.005726
9	6	0	4.219675	0.075097	-0.990637
10	1	0	2.312349	1.050029	-1.246902
11	6	0	4.318486	-1.630648	0.719495
12	1	0	2.483535	-1.996887	1.786240
13	6	0	4.954757	-0.887069	-0.283346
14	1	0	4.705029	0.664191	-1.766618
15	1	0	4.876219	-2.380447	1.278386
16	1	0	6.006001	-1.053425	-0.509068
17	6	0	-0.000020	2.174735	-0.000000
18	8	0	-0.877524	2.663728	-0.734915
19	8	0	0.877467	2.663733	0.734933
20	6	0	-2.217948	-0.446244	-0.303492
21	6	0	-2.972352	-1.415695	-1.005721
22	6	0	-2.873634	0.292876	0.708894
23	6	0	-4.318478	-1.630668	-0.719469
24	1	0	-2.483539	-1.996907	-1.786234
25	6	0	-4.219653	0.075094	0.990645
26	1	0	-2.312332	1.050044	1.246872
27	6	0	-4.954739	-0.887083	0.283374
28	1	0	-4.876214	-2.380476	-1.278345
29	1	0	-4.705000	0.664193	1.766626
30	1	0	-6.005979	-1.053443	0.509112

Ground State for *trans*-2,3-diphenyl-1-carboxylate.

E(B3LYP) = -784.2787768. TC = 0.247587. S = 124.552.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.373149	-0.072949	-0.721905
2	6	0	-0.662521	0.263688	0.354371
3	7	0	-0.136209	1.268174	-0.523198
4	6	0	1.739445	-0.544210	-0.340414
5	6	0	2.482379	0.008004	0.719585
6	6	0	2.303149	-1.612497	-1.057447
7	6	0	3.737575	-0.505350	1.047793
8	1	0	2.084185	0.849317	1.279017
9	6	0	3.559536	-2.128278	-0.727865
10	1	0	1.747246	-2.040773	-1.890083
11	6	0	4.284545	-1.576527	0.331484
12	1	0	4.297641	-0.055510	1.865090
13	1	0	3.971751	-2.955906	-1.302605
14	1	0	5.266081	-1.968664	0.590663
15	1	0	-0.003911	-0.570196	-1.621076
16	6	0	-2.088743	-0.158185	0.222710
17	6	0	-2.660821	-1.031584	1.161848
18	6	0	-2.884019	0.287784	-0.844944
19	6	0	-3.985954	-1.456503	1.036041
20	1	0	-2.058702	-1.376020	2.001057
21	6	0	-4.208269	-0.136492	-0.973810
22	1	0	-2.442350	0.983805	-1.553392
23	6	0	-4.767318	-1.012772	-0.036216
24	1	0	-4.410013	-2.131310	1.777633
25	1	0	-4.810935	0.225069	-1.805216
26	1	0	-5.800425	-1.339921	-0.135826
27	1	0	-0.279470	0.251389	1.377084
28	6	0	0.711067	2.411236	-0.023662
29	8	0	0.424499	2.802182	1.130079
30	8	0	1.549647	2.802732	-0.855749

Table A Effect of strain energy in kJ/mol on the relative rates of thermolysis of haloaziridines. See text for details

Aziridines[a] $R^1 = H$	R^2	R^3	R^4	R^5	k_{rel}	***Strain Energy***	k_{rel}^{SE}
1	H	H	H	H	1.00E+00	114.2	1.00E+00
2	F	H	H	H	1.37E+03	149.0	1.21E+06
3	F	F	H	H	1.19E-05	176.1	7.05E+10
4	F	H	H	F	1.30E+05	148.1	8.65E+05
5	F	H	F	H	1.13E+00	167.8	2.41E+09
6	F	F	F	H	5.33E-06	—	—
7	F	F	F	F	4.93E-07	192.9	6.03E+13
8	Cl	H	H	H	4.39E+04	138.5	1.78E+04
9	Cl	Cl	H	H	7.22E+00	140.2	3.50E+04
10	Cl	H	H	Cl	2.10E+08	110.9	2.59E-01
11	Cl	H	Cl	H	8.07E+03	122.6	2.92E+01
12	Br	H	H	H	1.66E+05	151.0	2.82E+06
13	Br	Br	H	H	3.07E+02	166.9	1.72E+09

Table B Free energies of activation in kJ/mol for aziridines and N-methylaziridines as a function of halogen substitution. See the text for details

	MP2			*SCS-MP2*	
Aziridines	ΔG_{act} ($R^1 = H$)	ΔG_{act} ($R^1 = CH_3$)	$\Delta\Delta G_{act}$	$\Delta G_{act}^{a,b}$ ($R^1 = H$)	ΔG_{act}^{a} ($R^1 = CH_3$)
1	194.6 [194.6]	182.9	-11.7	200.4	192.2
2	176.7 [176.7]	163.2	-13.5	184.5	170.7
3	222.7 [195.8]	204.0	-18.7	226.0	208. 6
4	165.4 [158.8]	147.0	-18.4	141.3	158.0
5	194.3 [195.8]	175.4	-18.9	197.4	182.5
6	224.7 [177.9]	205.8	-18.9	230.6	209.8
7	230.6 [197.0]	225.8	-4.8	230.3	226.9
8	168.1 [168.1]	154.2	-13.9	175.9	162.8
9	189.7 [181.3]	171.1	-18.6	196.2	178.3
10	147.1 [141.6]	128.9	-18.2	156.4	139.5
11	172.3 [181.3]	157.4	-14.9	180.4	166.3
12	164.8 [164.8]	144.8	-20.0	173.0	153.6
13	180.4 [175.0]	161.0	-19.4	187.3	168.5

Table C NBO Atomic Charge Differences Relative to 1. See text for details

	R_2	R_3	C_2	R_4	R_5	C_3	R_1	N
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	-0.624	-0.004	0.659	0.002	0.006	-0.080	-0.002	0.034
3	-0.610	-0.620	1.194	0.050	0.028	-0.019	-0.016	-0.009
4	-0.617	-0.003	0.571	0.017	-0.629	0.633	0.013	0.014
5	-0.613	-0.010	0.583	-0.625	-0.006	0.645	0.026	0.000
6	-0.583	-0.602	1.184	-0.615	0.001	0.645	0.026	-0.057
7	-0.599	-0.606	1.159	-0.586	-0.611	1.220	-0.008	0.029
8	-0.238	0.034	0.159	0.019	-0.004	-0.005	0.004	0.029
9	-0.185	-0.194	0.235	0.028	0.001	0.076	-0.002	0.039
10	-0.222	0.037	0.116	0.057	-0.319	0.263	0.006	0.059
11	-0.199	0.041	0.182	-0.243	0.025	0.146	0.003	0.044
12	-0.191	0.039	0.085	0.021	-0.002	0.010	0.006	0.031
13	-0.119	-0.126	0.071	0.030	0.004	0.102	0.002	0.034

Selected Wiberg Bond Indices for Haloaziridines

Aziridine	C_2 — N	C_3 — N	C_2 — C_3	C_2 — X	C_n — X^b
1	1.165	1.139	0.756	—	—
2	1.266	1.131	0.661	0.804[a]	—
3	1.253	1.168	0.627	0.818[a]	0.822[b]
4	1.177	1.177	0.656	0.814[a]	0.814[a]
5	1.128	1.204	0.662	0.822[a]	0.803[b]
6	0.823	1.106	0.711	0.823[a]	0.857[a]; 0.849[b]
7	1.209	0.838	0.496	0.838[a]; 0.844[b]	0.884[a]; 0.838[b]
8	1.202	1.129	0.685	1.030	—
9	1.029	1.146	0.624	1.029	1.020
10	1.178	1.178	0.613	1.043	1.043
11	1.159	1.068	0.624	1.019[a]	1.067[a]
12	1.026	1.130	0.692	1.017	0.933; 0.929
13	1.203	1.152	0.629	1.007	0.990

(a) outward rotation (b) inward rotation (c) $C_n = C_2$ or C_3 depending on structure.

Transition State Distances in Conrotatory Cleavage of Aziridines

(a) Average bond distances (Å) (From March, J. *Advanced Organic Chemistry*, 4th Ed. Wiley: New York, NY, 1992, p. 21) :

$C(sp^3) – F = 1.38.$
$C(sp^3) – Cl = 1.78.$
$C(sp^3) – Br = 1.94.$
$C(sp^3) – N = 1.47.$
$C(sp^2) – N = 1.28.$

(b) Outward rotation. (c) Inward rotation.

Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry