Coordinates for 8

8-HF

H	0.873498	1.162006	1.886500
H	0.873498	-1.162006	1.886500
H	-0.873498	1.162006	1.886500
H	-0.873498	-1.162006	1.886500
C	0.000000	1.272437	-0.107365
C	0.000000	-1.272437	-0.107365
C	0.000000	0.774479	1.373624
C	0.000000	-0.774479	1.373624
C	-1.235357	0.659171	-0.747610
C	-1.235357	-0.659171	-0.747610
C	1.235357	0.659171	-0.747610
C	1.235357	-0.659171	-0.747610
H	0.000000	2.354052	-0.154279
H	0.000000	-2.354052	-0.154279
H	-2.036110	1.271284	-1.122477
H	-2.036110	-1.271284	-1.122477
H	2.036110	-1.271284	-1.122477
H	2.036110	1.271284	-1.122477

8-MP2

H	0.883266	1.165815	1.883991
H	0.883266	-1.165815	1.883991
H	-0.883266	1.165815	1.883991
H	-0.883266	-1.165815	1.883991
H	0.000000	2.369912	-0.152596
H	0.000000	-2.369912	-0.152596
H	-2.046295	1.288279	-1.112220
H	-2.046295	-1.288279	-1.112220
H	2.046295	-1.288279	-1.112220
H	2.046295	1.288279	-1.112220
C	0.000000	1.277238	-0.111609
C	0.000000	-1.277238	-0.111609
C	0.000000	0.771219	1.371629
C	0.000000	-0.771219	1.371629
C	-1.229912	0.671524	-0.745922
C	-1.229912	-0.671524	-0.745922
C	1.229912	0.671524	-0.745922
C	1.229912	-0.671524	-0.745922

8-B3LYP

H	0.882755	1.169613	1.894643
H	0.882755	-1.169613	1.894643
H	-0.882755	1.169613	1.894643
H	-0.882755	-1.169613	1.894643
H	0.000000	2.374462	-0.154991
H	0.000000	-2.374462	-0.154991
H	-2.050665	1.287697	-1.118944
H	-2.050665	-1.287697	-1.118944
H	2.050665	-1.287697	-1.118944
H	2.050665	1.287697	-1.118944
C	0.000000	1.282152	-0.113683
C	0.000000	-1.282152	-0.113683
C	0.000000	0.775535	1.379935
C	0.000000	-0.775535	1.379935
C	-1.238544	0.667752	-0.749493
C	-1.238544	-0.667752	-0.749493
C	1.238544	0.667752	-0.749493
C	1.238544	-0.667752	-0.749493

8-B3PW91

H	0.882937	1.166741	1.888028
H	0.882937	-1.166741	1.888028
H	-0.882937	1.166741	1.888028
H	-0.882937	-1.166741	1.888028
H	0.000000	2.370755	-0.152794
H	0.000000	-2.370755	-0.152794
H	-2.047389	1.286741	-1.115389
H	-2.047389	-1.286741	-1.115389
H	2.047389	-1.286741	-1.115389
H	2.047389	1.286741	-1.115389
C	0.000000	1.278072	-0.113192
C	0.000000	-1.278072	-0.113192
C	0.000000	0.772129	1.373289
C	0.000000	-0.772129	1.373289
C	-1.234487	0.667341	-0.746089
C	-1.234487	-0.667341	-0.746089
C	1.234487	0.667341	-0.746089
C	1.234487	-0.667341	-0.746089

8-SVWN

H	0.889358	1.164914	1.874564
H	0.889358	-1.164914	1.874564
H	-0.889358	1.164914	1.874564
H	-0.889358	-1.164914	1.874564
H	0.000000	2.374078	-0.150673
H	0.000000	-2.374078	-0.150673
H	-2.052052	1.290605	-1.098552
H	-2.052052	-1.290605	-1.098552
H	2.052052	-1.290605	-1.098552
H	2.052052	1.290605	-1.098552
C	0.000000	1.272615	-0.116611
C	0.000000	-1.272615	-0.116611
C	0.000000	0.765014	1.356847
C	0.000000	-0.765014	1.356847
C	-1.226816	0.667906	-0.736897
C	-1.226816	-0.667906	-0.736897
C	1.226816	0.667906	-0.736897
C	1.226816	-0.667906	-0.736897

Coordinates for 9a

9a-HF

H	2.286612	0.632567	0.000000
H	0.722799	0.568899	2.154856
H	0.722799	0.568899	-2.154856
H	-1.791602	0.336662	1.199592
H	-1.791602	0.336662	-1.199592
H	1.260322	2.073587	0.000000
H	-1.099744	1.939965	1.169526
H	-1.099744	1.939965	-1.169526
C	0.412628	0.375186	1.137547
C	0.412628	0.375186	-1.137547
C	1.262862	0.987695	0.000000
C	-0.992194	0.934486	0.776921
C	-0.992194	0.934486	-0.776921
C	0.412628	-1.061410	-0.652186
C	0.412628	-1.061410	0.652186
C	-0.499130	-2.050107	0.000000
H	-1.576657	-1.913337	0.000000
H	-0.212320	-3.088541	0.000000

9a-TCSCF

H	2.296415	0.598222	0.000000
H	0.730003	0.554437	2.152676
H	0.730003	0.554437	-2.152676
H	-1.784655	0.355154	1.201013
H	-1.784655	0.355154	-1.201013
H	1.292769	2.054026	0.000000
H	-1.069153	1.947440	1.168626
H	-1.069153	1.947440	-1.168626
C	0.417801	0.363625	1.135172
C	0.417801	0.363625	-1.135172
C	1.277283	0.967968	0.000000
C	-0.976397	0.940112	0.777503
C	-0.976397	0.940112	-0.777503
C	0.417801	-1.083155	-0.668427
C	0.417801	-1.083155	0.668427
C	-0.559454	-1.997337	0.000000
H	-1.621607	-1.786651	0.000000
H	-0.337412	-3.050426	0.000000

9a-MP2

H	1.621692	-1.792803	0.000000
H	0.310719	-3.063106	0.000000
H	1.783212	0.294436	1.205590
H	1.783212	0.294436	-1.205590
H	-0.729848	0.577327	-2.165930
H	-0.729848	0.577327	2.165930
H	-2.300864	0.619501	0.000000
H	1.104776	1.924317	1.172640
H	1.104776	1.924317	-1.172640
H	-1.270458	2.085963	0.000000
C	-0.424638	-1.064188	-0.675690
C	-0.424638	-1.064188	0.675690
C	0.545075	-2.000565	0.000000
C	-0.424638	0.371679	1.136620
C	-0.424638	0.371679	-1.136620
C	0.988833	0.911352	0.773690
C	0.988833	0.911352	-0.773690
C	-1.270419	0.989261	0.000000

9a-B3LYP

H	2.306450	0.633663	0.000000
H	0.728891	0.577719	2.170740
H	0.728891	0.577719	-2.170740
H	-1.798333	0.317602	1.207581
H	-1.798333	0.317602	-1.207581
H	1.271500	2.092189	0.000000
H	-1.107954	1.941837	1.177996
H	-1.107954	1.941837	-1.177996
C	0.421013	0.374006	1.142589
C	0.421013	0.374006	-1.142589
C	1.273280	0.995721	0.000000
C	-0.997081	0.927988	0.778373
C	-0.997081	0.927988	-0.778373
C	0.421013	-1.067131	-0.665884
C	0.421013	-1.067131	0.665884
C	-0.522461	-2.037992	0.000000
H	-1.607594	-1.869446	0.000000
H	-0.259825	-3.095447	0.000000

9a-B3PW91

C	-0.406173000	-0.389670000	-1.138993000
C	1.025382000	-0.502317000	-0.665869000
C	1.025382000	-0.502317000	0.665869000
H	1.977874000	1.454506000	0.000001000
C	-0.406173000	-0.389672000	1.138993000
C	2.062173000	0.359017000	0.000000000
C	-1.090289000	-1.185554000	-0.000001000
H	-0.635736000	-0.679379000	-2.167307000
C	-0.838438000	1.063033000	-0.774838000
H	-0.635736000	-0.679382000	2.167306000
H	-0.810475000	-2.244456000	-0.000001000
C	-0.838438000	1.063032000	0.774840000
H	-0.164767000	1.811328000	1.205944000
H	-1.839978000	1.256913000	-1.174666000
H	-2.183616000	-1.096452000	-0.000001000
H	-1.839978000	1.256912000	1.174667000
H	-0.164768000	1.811329000	-1.205942000
H	3.096628000	0.015364000	0.000000000

9a-SVWN

C	0.421124000	-0.382333000	1.131902000
C	-0.993540000	-0.548866000	0.668241000
C	-0.993540000	-0.548868000	-0.668241000
H	-1.910376000	1.413897000	-0.000001000
C	0.421125000	-0.382335000	-1.131901000
C	-2.019284000	0.309744000	0.000000000
C	1.137884000	-1.133026000	0.000002000
H	0.676750000	-0.656657000	2.167878000
C	0.757457000	1.081196000	0.767412000
H	0.676752000	-0.656662000	-2.167876000
H	0.901629000	-2.211642000	0.000002000
C	0.757458000	1.081194000	-0.767413000
H	0.028325000	1.788184000	-1.203087000
H	1.749883000	1.342141000	1.174268000
H	2.234693000	-0.992637000	0.000002000
H	1.749884000	1.342139000	-1.174270000
H	0.028324000	1.788186000	1.203083000
H	-3.067957000	-0.017190000	-0.000001000

Coordinates for 9b

9b-HF

H	2.011329	0.663763	0.000000
H	0.444245	0.566932	2.156451
H	0.444245	0.566932	-2.156451
H	-2.062255	0.304596	1.193908
H	-2.062255	0.304596	-1.193908
H	0.988331	2.097277	0.000000
H	-1.395309	1.922150	1.171030
H	-1.395309	1.922150	-1.171030
C	0.130595	0.374719	1.139710
C	0.130595	0.374719	-1.139710
C	0.982924	1.008783	0.000000
C	-1.271869	0.917880	0.779571
C	-1.271869	0.917880	-0.779571
C	0.130595	-1.063452	-0.653989
C	0.130595	-1.063452	0.653989
C	1.056866	-2.032464	0.000000
H	0.783114	-3.074012	0.000000
H	2.133283	-1.882055	0.000000

9b-TCSCF

H	1.999194	0.667309	0.000000
H	0.434913	0.562999	2.152729
H	0.434913	0.562999	-2.152729
H	-2.073266	0.281498	1.194190
H	-2.073266	0.281498	-1.194190
H	0.958905	2.084732	0.000000
H	-1.417062	1.902455	1.171698
H	-1.417062	1.902455	-1.171698
C	0.119540	0.363670	1.137434
C	0.119540	0.363670	-1.137434
C	0.966418	0.997371	0.000000
C	-1.285725	0.899392	0.779770
C	-1.285725	0.899392	-0.779770
C	0.119540	-1.082176	-0.674415
C	0.119540	-1.082176	0.674415
C	1.130816	-1.948796	0.000000
H	0.944194	-3.007895	0.000000
H	2.184858	-1.700145	0.000000

9b-MP2

C	0.123281000	0.369177000	1.139767000
C	0.123281000	-1.066515000	0.678859000
C	0.123281000	-1.066515000	-0.678859000
H	2.178635000	-1.772424000	0.000000000
C	0.123281000	0.369177000	-1.139767000
C	1.102824000	-1.984536000	0.000000000
C	0.975832000	1.001287000	0.000000000
H	0.439802000	0.575829000	2.165955000
C	-1.282386000	0.902203000	0.778094000
H	0.439802000	0.575829000	-2.165955000
H	2.010224000	0.639884000	0.000000000
C	-1.282386000	0.902203000	-0.778094000
H	-2.070362000	0.270896000	-1.197691000
H	-1.415652000	1.913233000	1.177158000
H	0.990252000	2.100548000	0.000000000
H	-1.415652000	1.913233000	-1.177158000
H	-2.070362000	0.270896000	1.197691000
H	0.871268000	-3.046814000	0.000000000

9b-B3LYP

H	2.022929	0.652210	0.000000
H	0.443401	0.574369	2.171754
H	0.443401	0.574369	-2.171754
H	-2.078874	0.295797	1.201366
H	-2.078874	0.295797	-1.201366
H	1.001221	2.109014	0.000000
H	-1.408873	1.931127	1.180869
H	-1.408873	1.931127	-1.180869
C	0.127538	0.372582	1.145360
C	0.127538	0.372582	-1.145360
C	0.987035	1.009499	0.000000
C	-1.283136	0.918469	0.782520
C	-1.283136	0.918469	-0.782520
C	0.127538	-1.069804	-0.667797
C	0.127538	-1.069804	0.667797
C	1.081278	-2.024029	0.000000
H	0.825417	-3.082722	0.000000
H	2.165973	-1.848878	0.000000

9b-B3PW91

C	-0.406173000	-0.389670000	-1.138993000
C	1.025382000	-0.502317000	-0.665869000
C	1.025382000	-0.502317000	0.665869000
H	1.977874000	1.454506000	0.000001000
C	-0.406173000	-0.389672000	1.138993000
C	2.062173000	0.359017000	0.000000000
C	-1.090289000	-1.185554000	-0.000001000
H	-0.635736000	-0.679379000	-2.167307000
C	-0.838438000	1.063033000	-0.774838000
H	-0.635736000	-0.679382000	2.167306000
H	-0.810475000	-2.244456000	-0.000001000
C	-0.838438000	1.063032000	0.774840000
H	-0.164767000	1.811328000	1.205944000
H	-1.839978000	1.256913000	-1.174666000
H	-2.183616000	-1.096452000	-0.000001000
H	-1.839978000	1.256912000	1.174667000
H	-0.164768000	1.811329000	-1.205942000
H	3.096628000	0.015364000	0.000000000

9b-SVWN

C	0.122701000	0.366742000	1.134596000
C	0.122701000	-1.057122000	0.670316000
C	0.122701000	-1.057122000	-0.670316000
H	2.174048000	-1.770535000	0.000000000
C	0.122701000	0.366742000	-1.134596000
C	1.085079000	-1.979887000	0.000000000
C	0.972425000	0.989145000	0.000000000
H	0.440559000	0.581491000	2.167539000
C	-1.272450000	0.900484000	0.772003000
H	0.440559000	0.581491000	-2.167539000
H	2.012076000	0.612574000	0.000000000
C	-1.272450000	0.900484000	-0.772003000
H	-2.069155000	0.268554000	-1.198252000
H	-1.404230000	1.919062000	1.176164000
H	0.999976000	2.097251000	0.000000000
H	-1.404230000	1.919062000	-1.176164000
H	-2.069155000	0.268554000	1.198252000
H	0.859096000	-3.054307000	0.000000000

Coordinates for 10a

10a-HF

H	2.256848	0.552202	0.000000
H	0.622709	0.612218	2.154881
H	0.622709	0.612218	-2.154881
H	1.313207	2.056545	0.000000
C	0.349878	0.410437	1.129367
C	0.349878	0.410437	-1.129367
C	1.258911	0.975242	0.000000
C	-0.991804	1.018032	0.659326
C	-0.991804	1.018032	-0.659326
C	0.349878	-1.040500	-0.651688
C	0.349878	-1.040500	0.651688
C	-0.566470	-2.021767	0.000000
H	-1.640807	-1.861647	0.000000
H	-0.290508	-3.062702	0.000000
H	-1.767114	1.357347	-1.319149
H	-1.767114	1.357347	1.319149

10a-TCSCF

H	2.264793	0.524703	0.000000
H	0.632185	0.604592	2.152638
H	0.632185	0.604592	-2.152638
H	1.341971	2.041480	0.000000
C	0.357570	0.403572	1.127196
C	0.357570	0.403572	-1.127196
C	1.271580	0.960760	0.000000
C	-0.977660	1.013010	0.659626
C	-0.977660	1.013010	-0.659626
C	0.357570	-1.058415	-0.669397
C	0.357570	-1.058415	0.669397
C	-0.623480	-1.963500	0.000000
H	-1.680201	-1.727578	0.000000
H	-0.413361	-3.018747	0.000000
H	-1.757966	1.344697	-1.317743
H	-1.757966	1.344697	1.317743

10a-MP2

H	0.634646	0.614422	2.168200
H	0.634646	0.614422	-2.168200
H	2.271702	0.549314	0.000000
H	-1.770663	1.328966	1.341200
H	-1.770663	1.328966	-1.341200
H	1.305993	2.069729	0.000000
H	-1.680195	-1.744134	0.000000
H	-0.384072	-3.042485	0.000000
C	0.360265	0.404203	1.131800
C	0.360265	0.404203	-1.131800
C	-0.984362	0.998878	0.671400
C	-0.984362	0.998878	-0.671400
C	1.262887	0.976677	0.000000
C	0.360265	-1.045525	-0.675000
C	0.360265	-1.045525	0.675000
C	-0.608787	-1.978324	0.000000

10a-B3LYP

H	2.275814	0.550678	0.000000
H	0.629691	0.615035	2.172221
H	0.629691	0.615035	-2.172221
H	1.320152	2.072400	0.000000
C	0.354310	0.408037	1.136446
C	0.354310	0.408037	-1.136446
C	1.268078	0.979959	0.000000
C	-0.992250	1.021395	0.667115
C	-0.992250	1.021395	-0.667115
C	0.354310	-1.048584	-0.664524
C	0.354310	-1.048584	0.664524
C	-0.586526	-2.019480	0.000000
H	-1.668838	-1.832797	0.000000
H	-0.327960	-3.077528	0.000000
H	-1.772150	1.362067	-1.338326
H	-1.772150	1.362067	1.338326

10a-B3PW91

C	-0.440331000	-0.311792000	-1.132745000
C	1.003210000	-0.456966000	-0.664721000
C	1.003245000	-0.456608000	0.664770000
H	1.976473000	1.474919000	-0.000349000
C	-0.440188000	-0.311230000	1.132933000
C	2.057895000	0.379010000	-0.000120000
H	-0.676011000	-0.564953000	2.168597000
H	-0.772958000	-2.203706000	0.000570000
C	-0.910137000	1.086325000	0.666594000
H	-0.676292000	-0.566047000	-2.168248000
C	-1.098403000	-1.157149000	0.000338000
C	-0.910319000	1.085955000	-0.667054000
H	-2.191088000	-1.097711000	0.000387000
H	-1.167703000	1.897677000	1.338033000
H	-1.168048000	1.896945000	-1.338867000
H	3.085788000	0.017616000	-0.000093000

10a-SVWN

C	-0.441663000	-0.309199000	-1.126732000
C	0.986283000	-0.481119000	-0.666514000
C	0.986310000	-0.481050000	0.666516000
H	1.912187000	1.461459000	-0.000100000
C	-0.441602000	-0.309078000	1.126782000
C	2.025513000	0.358342000	-0.000049000
H	-0.692503000	-0.558767000	2.169339000
H	-0.809343000	-2.188085000	0.000127000
C	-0.864502000	1.093101000	0.667015000
H	-0.692613000	-0.559010000	-2.169248000
C	-1.116141000	-1.126665000	0.000083000
C	-0.864601000	1.093009000	-0.667101000
H	-2.215447000	-1.038359000	0.000104000
H	-1.094750000	1.919823000	1.343289000
H	-1.094940000	1.919641000	-1.343455000
H	3.069835000	0.019258000	-0.000056000

Coordinates for 10b

10b-HF

H	1.966145	0.595109	0.000000
H	0.330709	0.627432	2.156091
H	0.330709	0.627432	-2.156091
H	1.026387	2.092152	0.000000
C	0.056142	0.425598	1.131236
C	0.056142	0.425598	-1.131236
C	0.962593	1.008228	0.000000
C	-1.287903	0.973265	0.661198
C	-1.287903	0.973265	-0.661198
C	0.056142	-1.038015	-0.653108
C	0.056142	-1.038015	0.653108
C	1.007546	-1.987087	0.000000
H	0.757549	-3.034749	0.000000
H	2.080558	-1.813544	0.000000
H	-2.102731	1.224573	-1.313360
H	-2.102731	1.224573	1.313360

10b-TCSCF

H	1.957361	0.611408	0.000000
H	0.324389	0.625987	2.152466
H	0.324389	0.625987	-2.152466
H	0.990534	2.088151	0.000000
C	0.049073	0.416686	1.128947
C	0.049073	0.416686	-1.128947
C	0.946498	1.004400	0.000000
C	-1.302074	0.951569	0.661415
C	-1.302074	0.951569	-0.661415
C	0.049073	-1.052883	-0.672345
C	0.049073	-1.052883	0.672345
C	1.067170	-1.918121	0.000000
H	0.886098	-2.978715	0.000000
H	2.120564	-1.666805	0.000000
H	-2.119103	1.195925	-1.313686
H	-2.119103	1.195925	1.313686

10b-MP2

C	0.051133000	0.424437000	1.134820000
C	0.051133000	-1.038287000	0.676679000
C	0.051133000	-1.038287000	-0.676679000
H	2.117802000	-1.722393000	0.000000000
C	0.051133000	0.424437000	-1.134820000
C	1.044507000	-1.948445000	0.000000000
C	0.952681000	1.008380000	0.000000000
H	0.334207000	0.637326000	2.168135000
C	-1.295175000	0.952470000	0.674709000
H	0.334207000	0.637326000	-2.168135000
H	1.966923000	0.591351000	0.000000000
C	-1.295175000	0.952470000	-0.674709000
H	-2.129700000	1.172038000	-1.332437000
H	-2.129700000	1.172038000	1.332437000
H	1.009096000	2.104152000	0.000000000
H	0.828940000	-3.014898000	0.000000000

10b-B3LYP

H	1.977645	0.587856	0.000000
H	0.332862	0.634304	2.172716
H	0.332862	0.634304	-2.172716
H	1.033280	2.105900	0.000000
C	0.052458	0.427025	1.138575
C	0.052458	0.427025	-1.138575
C	0.965832	1.010595	0.000000
C	-1.295863	0.974380	0.669975
C	-1.295863	0.974380	-0.669975
C	0.052458	-1.044309	-0.665667
C	0.052458	-1.044309	0.665667
C	1.027151	-1.983768	0.000000
H	0.792941	-3.047959	0.000000
H	2.108642	-1.787672	0.000000
H	-2.122389	1.213578	-1.330156
H	-2.122389	1.213578	1.330156

10b-B3PW91

C	0.053636000	0.426100000	1.135035000
C	0.053636000	-1.038928000	0.665753000
C	0.053636000	-1.038928000	-0.665753000
H	2.104727000	-1.781546000	0.000000000
C	0.053636000	0.426100000	-1.135035000
C	1.022554000	-1.975732000	0.000000000
C	0.960272000	1.007187000	0.000000000
H	0.335475000	0.635310000	2.168736000
C	-1.292114000	0.968660000	0.669593000
H	0.335475000	0.635310000	-2.168736000
H	1.972741000	0.584299000	0.000000000
C	-1.292114000	0.968660000	-0.669593000
H	-2.120212000	1.202322000	-1.330202000
H	-2.120212000	1.202322000	1.330202000
H	1.027209000	2.103087000	0.000000000
H	0.785937000	-3.039833000	0.000000000

10b-SVWN

C	0.048557000	0.418923000	1.129224000
C	0.048557000	-1.032642000	0.667449000
C	0.048557000	-1.032642000	-0.667449000
H	2.117451000	-1.704518000	0.000000000
C	0.048557000	0.418923000	-1.129224000
C	1.033067000	-1.938698000	0.000000000
C	0.950337000	0.986011000	0.000000000
H	0.337886000	0.635854000	2.168859000
C	-1.286631000	0.960112000	0.669953000
H	0.337886000	0.635854000	-2.168859000
H	1.965328000	0.543623000	0.000000000
C	-1.286631000	0.960112000	-0.669953000
H	-2.124243000	1.188910000	-1.334287000
H	-2.124243000	1.188910000	1.334287000
H	1.031253000	2.089671000	0.000000000
H	0.832471000	-3.018898000	0.000000000

Coordinates for 11a

11a-HF

C	0.026882	-0.195604	1.322830
C	0.026882	-0.195604	-1.322830
C	-1.429317	-0.177464	0.776933
C	-1.429317	-0.177464	-0.776933
C	0.714293	-1.465051	0.779352
C	0.714293	-1.465051	-0.779352
C	0.714293	0.952457	0.648159
C	0.714293	0.952457	-0.648159
C	0.472979	2.276018	0.000000
H	0.031266	-0.179086	2.406092
H	0.031266	-0.179086	-2.406092
H	1.730655	-1.515235	1.153274
H	1.730655	-1.515235	-1.153274
H	-1.958050	-1.044647	1.161333
H	-1.958050	-1.044647	-1.161333
H	0.195750	-2.339918	1.160222
H	0.195750	-2.339918	-1.160222
H	-1.949518	0.695785	-1.156779
H	-1.949518	0.695785	1.156779
H	-0.515387	2.728753	0.000000
H	1.263497	3.009273	0.000000

11a-TCSCF

C	0.036577	-0.193043	1.318521
C	0.036577	-0.193043	-1.318521
C	-1.416368	-0.182528	0.776925
C	-1.416368	-0.182528	-0.776925
C	0.734254	-1.458487	0.779184
C	0.734254	-1.458487	-0.779184
C	0.734254	0.965580	0.664310
C	0.734254	0.965580	-0.664310
C	0.370806	2.254609	0.000000
H	0.038962	-0.178103	2.402184
H	0.038962	-0.178103	-2.402184
H	1.751125	-1.499999	1.153915
H	1.751125	-1.499999	-1.153915
H	-1.938507	-1.053699	1.160371
H	-1.938507	-1.053699	-1.160371
H	0.224380	-2.338022	1.160920
H	0.224380	-2.338022	-1.160920
H	-1.943740	0.685815	-1.157944
H	-1.943740	0.685815	1.157944
H	-0.651710	2.613588	0.000000
H	1.097836	3.048525	0.000000

11a-MP2

C	1.417563	-0.779382	-0.804208
C	0.193500	-1.322961	-0.038893
C	0.266383	-0.776927	1.415623
C	0.266383	0.776927	1.415623
C	0.193500	1.322961	-0.038894
C	1.417563	0.779381	-0.804208
C	-0.995000	0.648090	-0.653532
C	-0.995000	-0.648090	-0.653531
C	-2.301411	0.000000	-0.330565
H	-0.572679	-1.156746	1.989318
H	1.164862	-1.161272	1.889200
H	-0.572679	1.156747	1.989318
H	1.164862	1.161272	1.889199
H	0.176760	2.406171	-0.042167
H	0.176759	-2.406171	-0.042166
H	1.404262	1.153349	-1.821690
H	2.323080	1.160228	-0.341288
H	2.323080	-1.160228	-0.341288
H	1.404262	-1.153350	-1.821690
H	-2.692179	0.000000	0.683781
H	-3.081278	0.000000	-1.075015

11a-B3LYP

C	0.036346	-0.194649	1.327195
C	0.036346	-0.194649	-1.327195
C	-1.430314	-0.174320	0.777336
C	-1.430314	-0.174320	-0.777336
C	0.723052	-1.473924	0.781968
C	0.723052	-1.473924	-0.781968
C	0.723052	0.957797	0.661627
C	0.723052	0.957797	-0.661627
C	0.435050	2.281207	0.000000
H	0.032347	-0.184773	2.422500
H	0.032347	-0.184773	-2.422500
H	1.748860	-1.525692	1.161523
H	1.748860	-1.525692	-1.161523
H	-1.958676	-1.051816	1.169493
H	-1.958676	-1.051816	-1.169493
H	0.195816	-2.353911	1.169847
H	0.195816	-2.353911	-1.169847
H	-1.952626	0.707055	-1.166106
H	-1.952626	0.707055	1.166106
H	-0.578411	2.705306	0.000000
H	1.211041	3.046882	0.000000

11a-B3PW91

C	-0.773055	-1.441139	0.778473
C	-0.043052	-0.193586	1.323705
C	1.416677	-0.224182	0.774069
C	1.416677	-0.224182	-0.774069
C	-0.043052	-0.193586	-1.323705
C	-0.773055	-1.441139	-0.778473
C	-0.683909	0.979561	-0.661642
C	-0.683909	0.979561	0.661642
C	-0.351474	2.287059	0.000000
H	1.969873	0.638241	1.163316
H	1.914085	-1.119750	1.166530
H	1.969873	0.638241	-1.163316
H	1.914085	-1.119750	-1.166530
H	-0.037627	-0.185457	-2.419253
H	-0.037627	-0.185457	2.419253
H	-1.800178	-1.454816	-1.158315
H	-0.279079	-2.340216	-1.166900
H	-0.279079	-2.340216	1.166900
H	-1.800178	-1.454816	1.158315
H	0.676631	2.675497	0.000000
H	-1.101864	3.078315	0.000000

11a-SVWN

C	-0.691684	-1.475974	0.771069
C	-0.050526	-0.197550	1.315010
C	1.394239	-0.127358	0.766342
C	1.394239	-0.127358	-0.766342
C	-0.050526	-0.197550	-1.315010
C	-0.691684	-1.475974	-0.771069
C	-0.739179	0.935367	-0.664600
C	-0.739179	0.935367	0.664600
C	-0.395012	2.228857	0.000000
H	1.887441	0.780171	1.160044
H	1.954007	-0.991940	1.168123
H	1.887441	0.780171	-1.160044
H	1.954007	-0.991940	-1.168123
H	-0.037188	-0.197475	-2.419800
H	-0.037188	-0.197475	2.419800
H	-1.722397	-1.557212	-1.157379
H	-0.136016	-2.345936	-1.166990
H	-0.136016	-2.345936	1.166990
H	-1.722397	-1.557212	1.157379
H	0.653481	2.591823	0.000000
H	-1.129293	3.046008	0.000000

Coordinates for 12a

12a-HF

C	0.046369	-0.186016	1.308648
C	0.046369	-0.186016	-1.308648
C	1.427380	-0.364358	0.660089
C	1.427380	-0.364358	-0.660089
C	-0.805053	-1.380806	0.778525
C	-0.805053	-1.380806	-0.778525
C	-0.570100	1.013950	-0.648021
C	-0.570100	1.013950	0.648021
C	-0.228665	2.313224	0.000000
H	0.088690	-0.170362	2.389364
H	0.088690	-0.170362	-2.389364
H	-1.817335	-1.298477	1.157330
H	-1.817335	-1.298477	-1.157330
H	2.298639	-0.550779	1.261724
H	2.298639	-0.550779	-1.261724
H	-0.392587	-2.307630	1.160688
H	-0.392587	-2.307630	-1.160688
H	0.794775	2.677923	0.000000
H	-0.960741	3.103988	0.000000

12a-TCSCF

C	0.045051	-0.184285	1.304837
C	0.045051	-0.184285	-1.304837
C	1.430275	-0.286456	0.660080
C	1.430275	-0.286456	-0.660080
C	-0.748872	-1.417554	0.778506
C	-0.748872	-1.417554	-0.778506
C	-0.642242	0.993891	-0.665036
C	-0.642242	0.993891	0.665036
C	-0.252142	2.272055	0.000000
H	0.089029	-0.168149	2.385850
H	0.089029	-0.168149	-2.385850
H	-1.764251	-1.381810	1.157711
H	-1.764251	-1.381810	-1.157711
H	2.312355	-0.413622	1.261413
H	2.312355	-0.413622	-1.261413
H	-0.295888	-2.324932	1.161519
H	-0.295888	-2.324932	-1.161519
H	0.781275	2.596175	0.000000
H	-0.961455	3.081366	0.0000

12a-MP2

C	-0.622078	0.993423	0.670087
C	0.040656	-0.178758	1.312338
C	-0.756591	-1.412051	0.775398
C	-0.756591	-1.412051	-0.775398
C	0.040656	-0.178758	-1.312338
C	-0.622078	0.993423	-0.670087
C	1.421653	-0.299373	-0.671930
C	1.421653	-0.299373	0.671930
C	-0.244181	2.286554	0.000000
H	0.083423	-0.170929	-2.405371
H	0.083423	-0.170929	2.405371
H	2.306176	-0.473110	1.278676
H	2.306176	-0.473110	-1.278676
H	-1.779967	-1.367275	-1.160720
H	-0.297062	-2.324824	-1.166914
H	-0.297062	-2.324824	1.166914
H	-1.779967	-1.367275	1.160720
H	0.802064	2.613792	0.000000
H	-0.965795	3.100276	0.000000

12a-B3LYP

C	0.046499	-0.179772	1.316603
C	0.046499	-0.179772	-1.316603
C	1.430277	-0.354649	0.668016
C	1.430277	-0.354649	-0.668016
C	-0.799032	-1.395006	0.779670
C	-0.799032	-1.395006	-0.779670
C	-0.585327	1.014689	-0.660904
C	-0.585327	1.014689	0.660904
C	-0.227215	2.319114	0.000000
H	0.088647	-0.172016	2.409091
H	0.088647	-0.172016	-2.409091
H	-1.821029	-1.316683	1.164216
H	-1.821029	-1.316683	-1.164216
H	2.305194	-0.556321	1.279077
H	2.305194	-0.556321	-1.279077
H	-0.371912	-2.323640	1.170854
H	-0.371912	-2.323640	-1.170854
H	0.812016	2.673630	0.000000
H	-0.959535	3.125852	0.000000

12a-B3PW91

C	-1.012016	-0.661009	-0.581454
C	0.179277	-1.313632	0.045345
C	1.387630	-0.776304	-0.796597
C	1.387617	0.776161	-0.796742
C	0.179201	1.313649	0.045027
C	-1.012045	0.660830	-0.581626
C	0.355676	0.667753	1.423565
C	0.355802	-0.667395	1.423715
C	-2.310798	-0.000068	-0.223313
H	0.172769	2.406425	0.086775
H	0.172898	-2.406397	0.087355
H	0.560696	-1.278160	2.298440
H	0.560485	1.278748	2.298149
H	1.308857	1.160750	-1.818985
H	2.317218	1.167194	-0.370781
H	2.317263	-1.167239	-0.370617
H	1.308796	-1.161103	-1.818755
H	-2.663343	0.000047	0.816985
H	-3.117694	-0.000181	-0.956081

12a-SVWN

C	-0.996989	-0.663297	-0.597917
C	0.173149	-1.308410	0.039261
C	1.388404	-0.768673	-0.768770
C	1.388416	0.768372	-0.769028
C	0.173075	1.308435	0.038680
C	-0.997017	0.662987	-0.598226
C	0.327475	0.668400	1.407622
C	0.327634	-0.667746	1.407904
C	-2.281125	-0.000094	-0.224754
H	0.174712	2.410502	0.080030
H	0.174829	-2.410458	0.081114
H	0.534342	-1.280897	2.291059
H	0.534070	1.281969	2.290513
H	1.327510	1.158039	-1.799685
H	2.314798	1.166851	-0.322263
H	2.314828	-1.167025	-0.321978
H	1.327355	-1.158691	-1.799286
H	-2.607834	0.000136	0.833986
H	-3.112754	-0.000274	-0.942123

Coordinates for 12b

12b-HF

C	0.087343	-0.272800	1.308068
C	0.087343	-0.272800	-1.308068
C	0.737658	-1.483781	0.661239
C	0.737658	-1.483781	-0.661239
C	-1.386598	-0.235892	0.775528
C	-1.386598	-0.235892	-0.775528
C	0.737658	0.917058	-0.647726
C	0.737658	0.917058	0.647726
C	0.405317	2.222933	0.000000
H	0.114558	-0.297084	2.389064
H	0.114558	-0.297084	-2.389064
H	-1.887721	0.646615	1.160196
H	-1.887721	0.646615	-1.160196
H	1.152055	-2.276157	1.258293
H	1.152055	-2.276157	-1.258293
H	-1.919184	-1.097433	1.161897
H	-1.919184	-1.097433	-1.161897
H	1.146506	3.005642	0.000000
H	-0.610556	2.609861	0.000000

12b-TCSCF

C	0.092622	-0.268788	1.304247
C	0.092622	-0.268788	-1.304247
C	0.755310	-1.475820	0.661357
C	0.755310	-1.475820	-0.661357
C	-1.377484	-0.242349	0.775756
C	-1.377484	-0.242349	-0.775756
C	0.755310	0.929651	-0.663344
C	0.755310	0.929651	0.663344
C	0.328519	2.201892	0.000000
H	0.118583	-0.293896	2.385608
H	0.118583	-0.293896	-2.385608
H	-1.887669	0.634232	1.161834
H	-1.887669	0.634232	-1.161834
H	1.176328	-2.264424	1.258974
H	1.176328	-2.264424	-1.258974
H	-1.901885	-1.109104	1.160891
H	-1.901885	-1.109104	-1.160891
H	1.018091	3.028645	0.000000
H	-0.709028	2.514060	0.000000

12b-MP2

C	-0.738318	0.923696	0.669228
C	-0.103116	-0.272158	1.311762
C	-0.765982	-1.467678	0.674259
C	-0.765982	-1.467678	-0.674259
C	-0.103116	-0.272158	-1.311762
C	-0.738318	0.923696	-0.669228
C	1.373288	-0.243872	-0.770353
C	1.373288	-0.243872	0.770353
C	-0.309749	2.206930	0.000000
H	1.879789	0.644072	1.165500
H	1.894618	-1.120838	1.166103
H	1.879789	0.644072	-1.165500
H	1.894618	-1.120838	-1.166103
H	-0.114082	-0.298084	-2.405294
H	-0.114082	-0.298084	2.405294
H	-1.196705	-2.264934	-1.274354
H	-1.196705	-2.264934	1.274354
H	0.743767	2.512260	0.000000
H	-1.002966	3.045862	0.000000

12b-B3LYP

C	0.097769	-0.274548	1.315311
C	0.097769	-0.274548	-1.315311
C	0.745824	-1.488411	0.669969
C	0.745824	-1.488411	-0.669969
C	-1.390205	-0.233174	0.774944
C	-1.390205	-0.233174	-0.774944
C	0.745824	0.920318	-0.660532
C	0.745824	0.920318	0.660532
C	0.374711	2.225766	0.000000
H	0.113227	-0.301236	2.408177
H	0.113227	-0.301236	-2.408177
H	-1.888774	0.660187	1.168365
H	-1.888774	0.660187	-1.168365
H	1.159963	-2.290351	1.274503
H	1.159963	-2.290351	-1.274503
H	-1.923268	-1.103571	1.170525
H	-1.923268	-1.103571	-1.170525
H	1.101915	3.037957	0.000000
H	-0.663020	2.587155	0.000000

12b-B3PW91

C	0.940946	0.660466	-0.710710
C	-0.270096	1.312664	-0.106291
C	-1.457472	0.669523	-0.792350
C	-1.457471	-0.669538	-0.792339
C	-0.270096	-1.312666	-0.106266
C	0.940946	-0.660479	-0.710698
C	-0.277450	-0.771648	1.374097
C	-0.277448	0.771675	1.374083
C	2.228075	-0.000003	-0.297528
H	0.598874	1.165416	1.902631
H	-1.165026	1.167156	1.878836
H	0.598869	-1.165382	1.902655
H	-1.165031	-1.167118	1.878855
H	-0.296458	-2.405832	-0.120823
H	-0.296457	2.405830	-0.120868
H	-2.245647	-1.273591	-1.233495
H	-2.245649	1.273568	-1.233516
H	2.553648	0.000007	0.752442
H	3.063285	-0.000010	-0.998711

12b-SVWN

C	0.896103	0.662657	-0.757420
C	-0.275968	1.307187	-0.107403
C	-1.490599	0.670088	-0.715623
C	-1.490603	-0.670080	-0.715625
C	-0.275979	-1.307185	-0.107401
C	0.896098	-0.662663	-0.757418
C	-0.186988	-0.763666	1.356809
C	-0.186973	0.763668	1.356808
C	2.172906	-0.000007	-0.344153
H	0.733725	1.160472	1.824078
H	-1.042191	1.168443	1.924015
H	0.733699	-1.160487	1.824086
H	-1.042216	-1.168424	1.924013
H	-0.305647	-2.409625	-0.109513
H	-0.305627	2.409627	-0.109516
H	-2.314079	-1.275995	-1.107968
H	-2.314071	1.276009	-1.107966
H	2.480946	-0.000003	0.722275
H	3.027483	-0.000012	-1.034943

Coordinates for 13

13-HF

H	0.133271	-1.117065	2.378612
H	0.133271	-1.117065	-2.378612
H	-2.082233	-1.299184	1.162751
H	-2.082233	-1.299184	-1.162751
H	1.945040	-2.458591	1.266207
H	1.945040	-2.458591	-1.266207
H	-1.259463	-2.838958	1.161030
H	-1.259463	-2.838958	-1.161030
C	0.091668	-1.143674	1.299677
C	0.091668	-1.143674	-1.299677
C	-1.218065	-1.827270	0.776483
C	-1.218065	-1.827270	-0.776483
C	1.236428	-1.925362	0.659782
C	1.236428	-1.925362	-0.659782
C	0.087488	0.214032	0.658113
C	0.087488	0.214032	-0.658113
C	0.023230	1.617287	-1.125126
C	0.023230	1.617287	1.125126
O	-0.007306	2.065642	2.209564
O	-0.007306	2.065642	-2.209564
O	-0.000664	2.394647	0.000000

13-MP2

H	0.130659	-1.116998	2.397700
H	0.130659	-1.116998	-2.397700
H	-2.086241	-1.251498	1.167900
H	-2.086241	-1.251498	-1.167900
H	1.921659	-2.499998	-1.282300
H	1.921659	-2.499998	1.282300
H	-1.280341	-2.822998	1.166400
H	-1.280341	-2.822998	-1.166400
C	0.111359	0.206402	-0.673400
C	0.111359	0.206402	0.673400
C	0.031159	1.600902	-1.146800
C	0.031159	1.600902	1.146800
C	0.096159	-1.140198	1.306000
C	0.096159	-1.140198	-1.306000
C	-1.227741	-1.803698	0.772900
C	-1.227741	-1.803698	-0.772900
C	1.220659	-1.937698	-0.672200
C	1.220659	-1.937698	0.672200
O	-0.011741	2.057402	2.264700
O	-0.011741	2.057402	-2.264700
O	0.004659	2.419502	0.000000

13-B3LYP

H	0.132742	-1.119262	2.399621
H	0.132742	-1.119262	-2.399621
H	-2.094969	-1.291900	1.170788
H	-2.094969	-1.291900	-1.170788
H	1.941704	-2.485455	1.282963
H	1.941704	-2.485455	-1.282963
H	-1.264782	-2.849804	1.169916
H	-1.264782	-2.849804	-1.169916
C	0.097470	-1.142174	1.309560
C	0.097470	-1.142174	-1.309560
C	-1.227014	-1.829812	0.777064
C	-1.227014	-1.829812	-0.777064
C	1.235981	-1.935884	0.668099
C	1.235981	-1.935884	-0.668099
C	0.094358	0.213237	0.670226
C	0.094358	0.213237	-0.670226
C	0.025169	1.611893	-1.144033
C	0.025169	1.611893	1.144033
O	-0.008231	2.068038	2.253025
O	-0.008231	2.068038	-2.253025
O	-0.001157	2.424639	0.000000

13-B3PW91

C	0.096458	-1.140047	1.306170
C	0.096458	-1.140047	-1.306170
C	-1.222262	-1.821737	0.773540
C	-1.222262	-1.821737	-0.773540
C	1.229798	-1.931987	0.667710
C	1.229798	-1.931987	-0.667710
C	0.095108	0.210633	0.669710
C	0.095108	0.210633	-0.669710
C	0.025898	1.607603	1.139560
C	0.025898	1.607603	-1.139560
H	0.130308	-1.117607	2.396690
H	0.130308	-1.117607	-2.396690
H	-1.262062	-2.842087	-1.166710
H	-1.262062	-2.842087	1.166710
H	-2.090022	-1.283037	1.167900
H	-2.090022	-1.283037	-1.167900
H	1.935778	-2.482597	1.282020
H	1.935778	-2.482597	-1.282020
O	-0.008262	2.064663	2.246480
O	-0.008262	2.064663	-2.246480
O	0.000528	2.415313	0.000000

13-SVWN

H	0.126097	-1.106190	2.402320
H	0.126097	-1.106190	-2.402320
H	-2.083643	-1.243570	1.166910
H	-2.083643	-1.243570	-1.166910
H	1.907547	-2.504200	-1.285000
H	1.907547	-2.504200	1.285000
H	-1.262133	-2.820220	1.166160
H	-1.262133	-2.820220	-1.166160
C	0.097937	-1.129320	1.302370
C	0.097937	-1.129320	-1.302370
C	-1.215003	-1.793560	0.766430
C	-1.215003	-1.793560	-0.766430
C	1.208007	-1.931550	-0.668350
C	1.208007	-1.931550	0.668350
C	0.102887	0.206580	-0.671630
C	0.102887	0.206580	0.671630
C	0.030727	1.592770	-1.134360
C	0.030727	1.592770	1.134360
O	-0.006503	2.050120	2.245430
O	-0.006503	2.050120	-2.245430
O	0.004207	2.400920	0.000000

Coordinates for 9 Transition State

9TS-HF

H	2.119513	0.728931	0.000000
H	0.566912	0.625267	2.162911
H	0.566912	0.625267	-2.162911
H	-1.953659	0.375369	1.197741
H	-1.953659	0.375369	-1.197741
H	1.055334	2.143396	0.000000
H	-1.273350	1.986930	1.167181
H	-1.273350	1.986930	-1.167181
C	0.248992	0.425269	1.149924
C	0.248992	0.425269	-1.149924
C	1.086470	1.055450	0.000000
C	-1.157735	0.979067	0.780813
C	-1.157735	0.979067	-0.780813
C	0.248992	-1.005867	-0.642026
C	0.248992	-1.005867	0.642026
C	0.423554	-2.344172	0.000000
H	-0.389141	-3.061618	0.000000
H	1.391345	-2.835140	0.000000

9TS-B3LYP

H	2.135933	0.733196	0.000000
H	0.569996	0.634154	2.178195
H	0.569996	0.634154	-2.178195
H	-1.965906	0.367300	1.206472
H	-1.965906	0.367300	-1.206472
H	1.060044	2.163441	0.000000
H	-1.282737	1.997059	1.175957
H	-1.282737	1.997059	-1.175957
C	0.252370	0.425134	1.154686
C	0.252370	0.425134	-1.154686
C	1.092885	1.064587	0.000000
C	-1.166104	0.980570	0.783007
C	-1.166104	0.980570	-0.783007
C	0.252370	-1.007858	-0.655293
C	0.252370	-1.007858	0.655293
C	0.423454	-2.354029	0.000000
H	-0.401617	-3.077337	0.000000
H	1.401271	-2.853818	0.000000

Coordinates for 10 Transition State

10TS-HF

H	2.094385	0.624817	0.000000
H	0.469070	0.677906	2.163158
H	0.469070	0.677906	-2.163158
H	1.140776	2.123900	0.000000
C	0.187512	0.472385	1.141734
C	0.187512	0.472385	-1.141734
C	1.093565	1.039795	0.000000
C	-1.144395	1.073221	0.660811
C	-1.144395	1.073221	-0.660811
C	0.187512	-0.982838	-0.640565
C	0.187512	-0.982838	0.640565
C	0.286010	-2.330605	0.000000
H	-0.565378	-3.003073	0.000000
H	1.224609	-2.875627	0.000000
H	-1.938765	1.382904	1.313154
H	-1.938765	1.382904	-1.313154

10TS-B3LYP

H	2.110916	0.621136	0.000000
H	0.474134	0.682602	2.179881
H	0.474134	0.682602	-2.179881
H	1.148440	2.140522	0.000000
C	0.188351	0.473339	1.148265
C	0.188351	0.473339	-1.148265
C	1.101308	1.044864	0.000000
C	-1.146187	1.081622	0.669103
C	-1.146187	1.081622	-0.669103
C	0.188351	-0.987306	-0.652999
C	0.188351	-0.987306	0.652999
C	0.279151	-2.344393	0.000000
H	-0.586897	-3.019624	0.000000
H	1.225782	-2.901395	0.000000
H	-1.947726	1.389733	1.331322
H	-1.947726	1.389733	-1.331322

Coordinates for 11 Transition State

11TS-HF

H	-0.898042	3.096647	0.000000
H	0.897828	3.095158	0.000000
H	-0.000229	-0.176565	2.420323
H	-0.000229	-0.176565	-2.420323
H	-2.145536	-0.462605	1.154506
H	-2.145536	-0.462605	-1.154506
H	2.145837	-0.457077	1.153757
H	2.145837	-0.457077	-1.153757
H	-1.243446	-1.954092	1.156714
H	-1.243446	-1.954092	-1.156714
H	1.248208	-1.951252	1.157052
H	1.248208	-1.951252	-1.157052
C	-0.001809	1.133074	0.638826
C	-0.001809	1.133074	-0.638826
C	-0.000630	2.487535	0.000000
C	-0.000160	-0.192414	1.337888
C	-0.000160	-0.192414	-1.337888
C	-1.244072	-0.934758	0.780464
C	-1.244072	-0.934758	-0.780464
C	1.245568	-0.932055	0.780405
C	1.245568	-0.932055	-0.780405

11TS-B3LYP

H	-0.908680	3.115860	0.000000
H	0.908119	3.115028	0.000000
H	-0.000343	-0.181030	2.436528
H	-0.000343	-0.181030	-2.436528
H	-2.160742	-0.465302	1.163875
H	-2.160742	-0.465302	-1.163875
H	2.160982	-0.463210	1.164109
H	2.160982	-0.463210	-1.164109
H	-1.242426	-1.968093	1.164972
H	-1.242426	-1.968093	-1.164972
H	1.243914	-1.966967	1.164742
H	1.243914	-1.966967	-1.164742
C	-0.000467	1.137874	0.651365
C	-0.000467	1.137874	-0.651365
C	-0.000571	2.500073	0.000000
C	-0.000146	-0.188157	1.342144
C	-0.000146	-0.188157	-1.342144
C	-1.250847	-0.939756	0.782104
C	-1.250847	-0.939756	-0.782104
C	1.251562	-0.938472	0.782249
C	1.251562	-0.938472	-0.782249

Coordinates for 12 Transition State

12TS-HF

C	0.081103	-0.233496	1.322824
C	0.081103	-0.233496	-1.322824
C	1.210642	-1.027128	0.660976
C	1.210642	-1.027128	-0.660976
C	-1.228615	-0.903692	0.779430
C	-1.228615	-0.903692	-0.779430
C	0.081103	1.107203	-0.637917
C	0.081103	1.107203	0.637917
C	0.115299	2.461112	0.000000
H	0.122966	-0.242811	2.402775
H	0.122966	-0.242811	-2.402775
H	-2.091155	-0.367403	1.158693
H	-2.091155	-0.367403	-1.158693
H	1.914244	-1.581040	1.256342
H	1.914244	-1.581040	-1.256342
H	-1.288481	-1.918844	1.156950
H	-1.288481	-1.918844	-1.156950
H	-0.766661	3.092607	0.000000
H	1.028919	3.046284	0.000000

12TS-B3LYP

C	0.086093	-0.230189	1.329736
C	0.086093	-0.230189	-1.329736
C	1.209134	-1.037550	0.669279
C	1.209134	-1.037550	-0.669279
C	-1.238466	-0.904464	0.779993
C	-1.238466	-0.904464	-0.779993
C	0.086093	1.111122	-0.650154
C	0.086093	1.111122	0.650154
C	0.124293	2.473122	0.000000
H	0.121498	-0.246544	2.421435
H	0.121498	-0.246544	-2.421435
H	-2.104235	-0.357347	1.166966
H	-2.104235	-0.357347	-1.166966
H	1.907048	-1.609590	1.273999
H	1.907048	-1.609590	-1.273999
H	-1.296542	-1.927858	1.165728
H	-1.296542	-1.927858	-1.165728
H	-0.766112	3.114743	0.000000
H	1.050566	3.062182	0.000000