

## Theoretical study of the gas-phase ozonolysis of b-pinene (C<sub>10</sub>H<sub>16</sub>)

### - Supporting Information -

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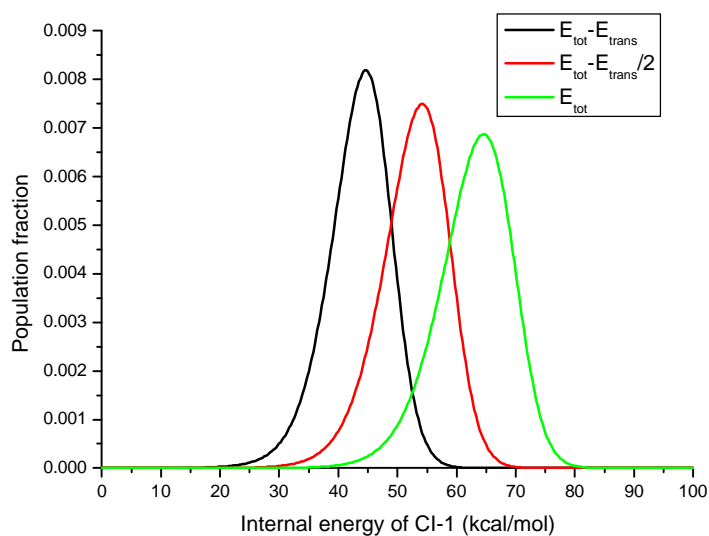
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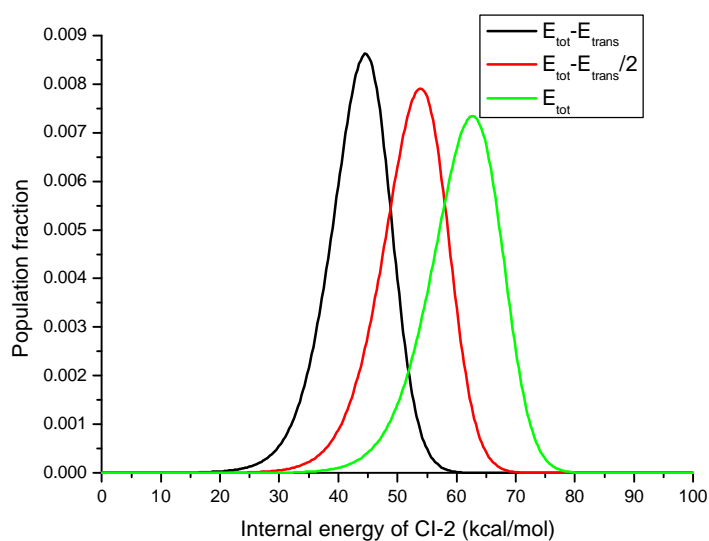
#### Content:

- p. 2: figures SI-10a and 10b
- p. 3: figures SI-11
- p. 4: figures SI-12
- p. 5: tables SI-1 and SI-2
- p. 6-53: quantum chemical data for the triplet potential energy surface
- p. 54-61 quantum chemical data for the triplet potential energy surface

**Figure SI-10a:** Nascent energy distribution of CI-1 after partitioning of the energy available in the primary ozonide at the moment of decomposition.



**Figure SI-10b:** Nascent energy distribution of CI-2 after partitioning of the energy available in the primary ozonide at the moment of decomposition.



**Figure SI-11:** decomposition of triplet bis(oxy) radicals formed after inter-system crossing from the dioxirane intermediate.

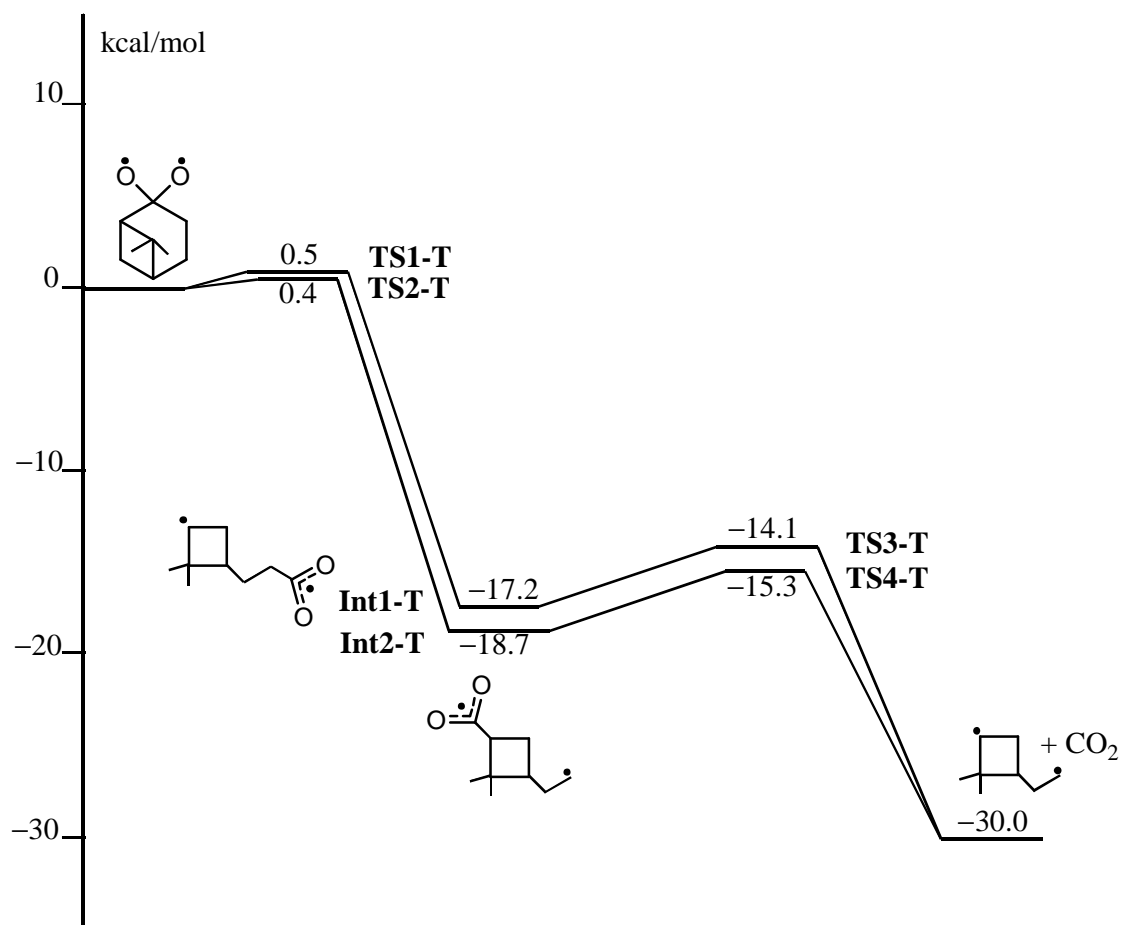
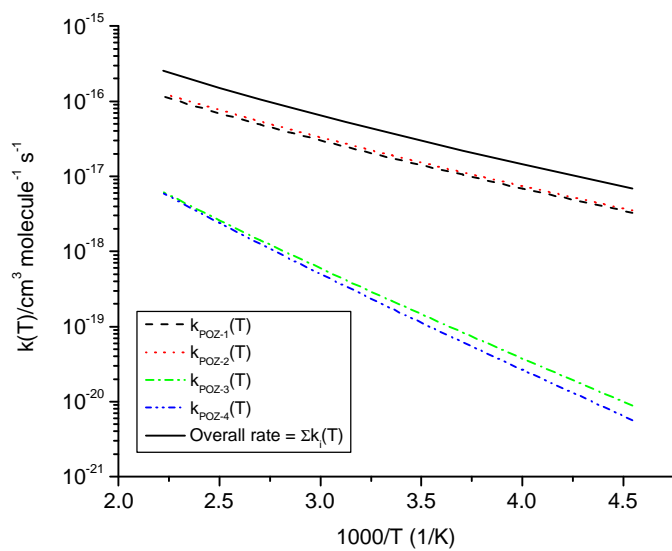


Figure SI-12: Temperature dependent rate coefficients for the formation of the 4 primary ozonides. POZ-1 and POZ-2 correspond to the two envelope conformers of the *anti*-POZ, while POZ-3 and POZ-4 correspond to the conformers of the *syn*-POZ.



**Table SI-1:** Barrier heights (kcal/mol) for decomposition of the primary ozonide (POZ) in the  $\alpha$ -pinene ozonolysis reaction, calculated at different levels of theory.

Structure	B3LYP <sup>a)</sup>	MPW1B95 <sup>b)</sup>	CBS-QB3
POZ	0.0	0.0	0.0
TS1 (POZ $\rightarrow$ CI-1a)	15.6	21.6	16.7
TS2 (POZ $\rightarrow$ CI-1b)	19.2	24.7	20.4
TS3 (POZ $\rightarrow$ CI-2a)	16.2	22.1	17.4
TS4 (POZ $\rightarrow$ CI-2b)	17.3	23.1	17.9

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)

b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)

**Table SI-2:** Barrier heights (kcal/mol) for decomposition of the primary ozonide (POZ) in the  $\beta$ -pinene ozonolysis reaction, calculated at different levels of theory.

Structure	B3LYP <sup>a)</sup>	MPW1B95 <sup>b)</sup>	CBS-QB3
POZ	0.0	0.0	0.0
TS1 (POZ $\rightarrow$ HCHO + CI-1)	13.5	18.7	14.3
TS2 (POZ $\rightarrow$ HCHO + CI-2)	12.9	18.0	13.5
TS3 (POZ $\rightarrow$ H <sub>2</sub> COO + nopinone)	17.9	24.5	19.1
TS4 (POZ $\rightarrow$ H <sub>2</sub> COO + nopinone)	17.9	24.7	19.1

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)

b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)

## Stationary points on singlet PES

### b-pinene

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E(RB+HF-LYP/CBSB7) (Hartree): -390.755805894

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.076391	-0.283651	0.195405
C	-0.028839	-0.552164	-0.904927
C	-1.392652	-0.530847	-0.265076
C	-0.504263	1.646069	0.785574
C	0.735091	1.233313	-0.024114
C	0.298960	0.864569	-1.470155
C	2.482518	-0.638288	-0.308766
C	0.886653	-0.899749	1.581163
H	0.109283	-1.423924	-1.549236
H	-0.715108	2.706245	0.613798
H	-0.296689	1.543220	1.854496
H	1.554140	1.947068	0.104969
H	-0.521381	1.432211	-1.914315
H	1.128599	0.847925	-2.174927
H	2.698739	-0.235057	-1.299620
H	2.608728	-1.724722	-0.357767
H	3.240390	-0.248201	0.378819
H	1.037249	-1.983173	1.535918
H	-0.107534	-0.731647	1.994764
H	1.621049	-0.493502	2.285236
C	-1.748553	0.802974	0.382515
H	-2.331644	1.374842	-0.347558
H	-2.411777	0.646919	1.236837
C	-2.217685	-1.577436	-0.272303
H	-1.955614	-2.500721	-0.778253
H	-3.184159	-1.546231	0.220941

Rotational constants (GHz): 1.8990400 1.2814300 1.1415800

Vibrational harmonic frequencies (cm-1):

110.9946	167.6246	186.8931
209.3300	228.5696	298.0401
358.2761	383.5765	392.8894
421.6608	451.7118	478.3689
531.9950	612.8603	643.4610
731.6827	772.4174	796.1268
828.8116	859.4843	888.0075
905.2204	915.0215	934.2963
948.6117	966.9923	988.0876
1006.3643	1027.1191	1060.8236
1076.5130	1099.3247	1128.5823
1165.8117	1209.2385	1219.8837
1227.0274	1237.5768	1260.2395
1284.5736	1286.3258	1311.2148
1322.0152	1344.8248	1368.3206
1403.3850	1422.5598	1450.4988
1480.2338	1486.1271	1486.8406
1502.8051	1506.3032	1516.5979
1525.6685	1706.1061	3016.0651
3020.2862	3022.1462	3030.7096
3045.7992	3057.3973	3058.4071
3065.9635	3068.2234	3074.8242
3076.0476	3100.7684	3117.9143
3122.7049	3123.6969	3201.3874

Zero-point correction (Hartree): 0.235417

O3: UB3LYP/6-311G(d,p)

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -225.473809652

Point group : C2V  
Cartesian coordinates (Angs):  
O 0.000000 1.088099 -0.225319  
O 0.000000 0.000000 0.450637  
O 0.000000 -1.088099 -0.225319  
Rotational constants (GHz): 103.7265200 13.3434700 11.8226000  
Vibrational harmonic frequencies (cm-1):  
709.9044 1020.3796 1048.2558  
Zero-point correction (Hartree): 0.006330

O3: UMPW1B95/6-31+G(d,p)

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E(UmPW+HF-B95/6-31+G(d,p)) (Hartree): -225.345928869  
Point group : C2V  
Cartesian coordinates (Angs):  
O 0.000000 1.075328 -0.223535  
O 0.000000 0.000000 0.447070  
O 0.000000 -1.075328 -0.223535  
Rotational constants (GHz): 105.3884400 13.6622900 12.0944000  
Vibrational harmonic frequencies (cm-1):  
725.1136 1094.2254 1193.9475  
Zero-point correction (Hartree): 0.006865

POZ-1

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.316395885  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 1.601227 -0.614012 -0.007227  
C 0.296610 -0.270488 -0.822292  
C -0.830252 0.252951 0.075487  
C 1.166002 1.702092 0.977539  
C 1.908239 0.919738 -0.113022  
C 1.061821 0.943697 -1.415257  
C 2.572343 -1.459694 -0.845125  
C 1.515683 -1.241806 1.387629  
H -0.095445 -1.029592 -1.503475  
H 1.370248 2.769813 0.855233  
H 1.556241 1.428289 1.961751  
H 2.961084 1.210827 -0.167051  
H 0.478331 1.840990 -1.627617  
H 1.633513 0.684879 -2.304416  
H 2.719131 -1.070282 -1.853555  
H 2.203839 -2.486344 -0.937722  
H 3.553095 -1.502143 -0.360578  
H 1.196995 -2.286945 1.328375  
H 0.835755 -0.724781 2.065805  
H 2.505017 -1.233053 1.856992  
C -0.373516 1.478783 0.912747  
H -0.839393 2.345621 0.440644  
H -0.802408 1.424864 1.915558  
C -1.559278 -0.900259 0.847587  
H -1.570916 -0.757132 1.927810  
H -1.127798 -1.871974 0.593389  
O -2.916423 -0.835140 0.422130  
O -2.761799 -0.377839 -0.940743  
O -1.913100 0.761847 -0.753830  
Rotational constants (GHz): 1.3796900 0.6490900 0.6082300  
Vibrational harmonic frequencies (cm-1):  
67.9725 100.7924 150.0194  
208.9750 214.3521 228.7527  
270.7521 308.2792 325.0215  
362.3098 381.2008 400.2627  
408.8693 427.0253 467.7375  
519.4986 568.6358 634.1672  
694.0188 705.4092 739.5640  
785.7631 795.4753 828.0876

859.4422	885.5855	917.5046
921.9674	928.2603	950.3128
960.2188	965.5616	988.7308
1003.9298	1022.6274	1032.8824
1041.5981	1061.2137	1102.8053
1124.1888	1145.5418	1178.1515
1210.0090	1219.1377	1232.6276
1239.5164	1255.6403	1271.8049
1282.0461	1297.9389	1320.6697
1335.8998	1357.1489	1366.5828
1376.2652	1407.2232	1426.7592
1486.5699	1489.9318	1494.1091
1504.2630	1509.8614	1510.9475
1520.7569	1527.7158	3019.9402
3025.8625	3033.1340	3045.2614
3049.9524	3059.1475	3061.8567
3064.0882	3072.4141	3074.3625
3078.5674	3094.7554	3105.0816
3107.3811	3124.2887	3126.8139

Zero-point correction (Hartree): 0.249391

**POZ-2**

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.315585243  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.678054	-0.542736	-0.014080
C	0.349006	-0.306447	-0.821120
C	-0.821249	0.119914	0.069851
C	1.041545	1.738606	0.984872
C	1.848460	1.014561	-0.100390
C	1.001594	0.981136	-1.399505
C	2.715443	-1.280966	-0.875399
C	1.650652	-1.217684	1.360886
H	0.019226	-1.083762	-1.514552
H	1.010602	2.803246	0.735016
H	1.556438	1.664110	1.947339
H	2.870572	1.399846	-0.156043
H	0.339805	1.827286	-1.589188
H	1.586842	0.788311	-2.296824
H	2.811456	-0.866148	-1.879579
H	2.446009	-2.336991	-0.977812
H	3.701256	-1.234721	-0.402027
H	1.403521	-2.280182	1.265573
H	0.943427	-0.773866	2.060983
H	2.641629	-1.160573	1.822766
C	-0.410053	1.185468	1.126355
H	-1.139600	1.993361	1.051267
H	-0.535819	0.764034	2.125728
C	-1.621726	-1.074226	0.686039
H	-1.884120	-0.876376	1.729583
H	-1.099126	-2.026376	0.595032
O	-2.793246	-1.176502	-0.108832
O	-3.066611	0.217748	-0.355379
O	-1.797951	0.670384	-0.863577

Rotational constants (GHz): 1.4329200 0.6352800 0.5918400  
 Vibrational harmonic frequencies (cm-1):

57.9317	71.1989	158.8134
180.5856	191.1711	215.7738
256.2538	277.5492	301.7101
367.6452	382.8000	393.5133
414.8757	430.8687	481.6013
506.2291	570.2549	630.8715
700.2967	707.3793	742.6356
782.8069	790.5651	824.5520
861.7228	878.6661	912.7189
920.8584	924.8673	947.2840
953.2955	964.7421	997.4528



1008.0076	1021.9767	1034.2354
1038.3436	1064.3969	1114.3120
1133.5170	1147.7282	1178.0396
1209.5221	1217.6092	1234.3355
1241.1886	1257.6362	1265.9448
1281.1158	1294.6441	1311.9889
1337.2015	1354.7595	1372.2150
1377.4172	1404.7747	1424.4848
1483.1552	1487.5830	1491.7395
1498.7730	1507.7387	1510.4576
1518.9883	1526.8473	3020.0224
3025.9515	3029.3738	3035.6722
3049.0508	3054.3990	3061.9577
3064.1815	3069.8321	3077.0310
3077.8177	3096.9802	3106.5882
3123.4747	3124.8630	3129.2738

Zero-point correction (Hartree): 0.248996

**POZ-3**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.316114749

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.612157	-0.581842	-0.001267
C	0.287343	-0.312338	-0.797199
C	-0.839032	0.258851	0.068087
C	1.157085	1.784896	0.863474
C	1.885513	0.949933	-0.194999
C	1.007376	0.892572	-1.473748
C	2.578006	-1.445502	-0.828809
C	1.561156	-1.159495	1.415048
H	-0.095165	-1.122833	-1.422226
H	1.231973	2.840671	0.584920
H	1.663252	1.684862	1.827412
H	2.927839	1.264408	-0.298800
H	0.409058	1.779725	-1.701804
H	1.556462	0.610442	-2.369944
H	2.686223	-1.106053	-1.860515
H	2.230870	-2.483049	-0.856242
H	3.573355	-1.441125	-0.373475
H	1.202868	-2.192215	1.391881
H	0.909471	-0.612388	2.093742
H	2.566923	-1.165995	1.849094
C	-0.344706	1.390685	1.014939
H	-0.974101	2.271038	0.875300
H	-0.542246	1.050908	2.032328
C	-2.068692	0.639102	-0.834403
H	-2.375741	1.679298	-0.728070
H	-1.865529	0.404058	-1.883646
O	-3.146526	-0.148433	-0.343266
O	-2.449846	-1.334858	0.103906
O	-1.418971	-0.762074	0.921022

Rotational constants (GHz): 1.3892700 0.6574500 0.6061300

Vibrational harmonic frequencies (cm-1):

44.3066	79.1980	147.7200
172.3653	196.3518	214.9106
255.4522	278.2730	297.8255
361.4867	383.6953	391.3642
414.3495	429.4186	457.7618
523.0302	569.0327	641.8183
696.7981	707.5756	736.0638
782.9089	797.3233	826.8046
860.4033	876.4321	915.8905
919.6605	921.9341	948.4157
957.0226	966.5976	997.4978
1001.9924	1019.5705	1025.7403
1050.6234	1076.4315	1091.1765

1119.9582	1146.8906	1186.9480
1206.9300	1220.8832	1230.6563
1240.6238	1257.2138	1272.7824
1282.0418	1291.8516	1313.2270
1339.2479	1354.0345	1368.3358
1378.4241	1407.1665	1428.0930
1484.6066	1486.0653	1495.6923
1503.9054	1505.6508	1510.6487
1514.5486	1521.8643	3021.4079
3027.6163	3029.2908	3034.3235
3040.5083	3050.6854	3061.9397
3063.7633	3066.6358	3076.6357
3084.3214	3098.7589	3100.4764
3119.9074	3122.2032	3133.6042

Zero-point correction (Hartree): 0.248857

#### POZ-4

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.317131209

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.612511	-0.597719	0.019543
C	-0.352703	-0.208127	0.877752
C	0.831869	0.261577	0.025168
C	-1.083790	1.627307	-1.120177
C	-1.902941	0.943054	-0.014650
C	-1.139510	1.057393	1.335270
C	-2.639496	-1.359175	0.873887
C	-1.456149	-1.349493	-1.303887
H	-0.012698	-0.930845	1.623812
H	-1.318556	2.696056	-1.139456
H	-1.377528	1.231669	-2.095355
H	-2.952037	1.250368	-0.043202
H	-0.572613	1.973362	1.519651
H	-1.768815	0.866057	2.201766
H	-2.835802	-0.890754	1.839924
H	-2.291367	-2.379059	1.064335
H	-3.593186	-1.429281	0.341305
H	-1.129160	-2.376642	-1.122272
H	-0.731981	-0.902067	-1.981884
H	-2.422635	-1.392943	-1.818376
C	0.443345	1.455509	-0.886771
H	0.823043	2.369092	-0.420620
H	0.986921	1.350088	-1.828030
C	2.090526	0.594350	0.892099
H	2.601305	1.485068	0.514241
H	1.856731	0.702306	1.951742
O	2.924647	-0.543567	0.763242
O	2.738416	-0.836679	-0.632518
O	1.295255	-0.891071	-0.730347

Rotational constants (GHz): 1.3986900 0.6495400 0.6093000

Vibrational harmonic frequencies (cm-1):

61.3525	104.2118	147.6878
194.3082	212.2122	220.7976
268.3765	306.9885	324.1575
359.0436	383.1220	395.2670
427.6357	433.7962	482.1030
491.8277	562.5394	637.1266
694.7660	707.2070	728.3988
779.1236	788.5459	827.2328
858.7738	883.5665	903.8357
915.5961	929.0095	953.7572
966.4813	967.7543	983.5770
1014.6409	1022.9703	1028.8314
1053.5185	1064.6195	1098.0814
1119.5523	1141.3259	1191.8210
1208.4243	1222.4655	1230.9719

1239.8851	1248.3074	1264.5961
1276.0899	1297.9708	1321.6636
1337.2995	1357.5558	1371.6182
1379.2889	1406.6422	1426.5546
1481.3408	1486.8224	1488.7433
1495.1114	1505.8108	1506.7461
1518.5006	1525.0651	3019.8866
3025.6365	3028.9973	3035.6226
3042.9542	3050.4789	3056.8970
3063.5802	3069.3881	3077.0319
3084.8976	3092.2083	3097.9912
3120.4175	3129.3553	3132.9647

Zero-point correction (Hartree): 0.249143

**CI-1**

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.800361271  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.340797	-0.409758	0.214626
C	0.213896	-0.539085	-0.894573
C	-1.094947	-0.197939	-0.286760
C	0.103485	1.794019	0.707088
C	1.257264	1.133991	-0.066782
C	0.774145	0.790832	-1.502217
C	2.666255	-1.016086	-0.264245
C	1.042270	-0.937485	1.618543
H	0.161359	-1.445846	-1.497848
H	0.010770	2.834601	0.384840
H	0.340962	1.821467	1.773684
H	2.183102	1.704597	0.040767
H	0.055243	1.466234	-1.970269
H	1.585937	0.602305	-2.201471
H	2.952201	-0.693786	-1.266560
H	2.608823	-2.108554	-0.268560
H	3.472913	-0.729062	0.417501
H	0.998015	-2.030833	1.610458
H	0.100141	-0.578123	2.034054
H	1.840750	-0.647114	2.308759
C	-1.247563	1.059123	0.487270
H	-1.990460	1.666810	-0.045799
H	-1.773428	0.798539	1.413034
O	-3.285628	-0.609533	0.104126
O	-2.074365	-0.981331	-0.455413

Rotational constants (GHz): 1.8660600 0.8699600 0.8081700  
 Vibrational harmonic frequencies (cm-1):

75.2957	163.3666	181.4999
189.9938	225.1594	262.9550
271.1592	299.4813	369.4473
385.9850	411.8201	428.5024
460.2371	528.6437	581.9405
622.2011	675.2887	771.6298
782.8986	827.0507	852.9829
880.7312	887.1679	930.5552
951.3270	960.4299	969.6982
1001.4738	1016.8823	1055.4392
1066.2030	1100.7421	1122.8934
1162.5923	1189.5585	1206.7284
1233.9633	1237.6189	1248.9165
1263.8149	1296.1682	1308.9472
1319.3865	1358.0217	1380.5087
1407.4634	1428.2271	1450.1451
1487.5269	1489.7567	1504.2890
1507.6410	1515.9727	1521.9893
1554.5691	3021.1065	3024.2855
3029.8850	3040.6454	3044.2882
3060.3960	3067.5028	3077.2626

3078.7718	3084.8398	3099.0153
3107.0366	3114.1180	3132.8712

Zero-point correction (Hartree): 0.214984

**CI-2**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.796884488  
Electronic state : 1-A  
Cartesian coordinates (Angs):

C	1.013762	-0.624064	0.230764
C	-0.076897	-0.341269	-0.908484
C	-1.165807	0.380442	-0.221169
C	0.616817	1.882845	0.696158
C	1.481732	0.851434	-0.050726
C	0.926856	0.691850	-1.493193
C	2.037834	-1.665922	-0.234346
C	0.514308	-1.016288	1.621484
H	-0.459581	-1.182435	-1.481225
H	0.965067	2.891138	0.457725
H	0.728560	1.757410	1.775678
H	2.546522	1.061496	0.077479
H	0.520188	1.578541	-1.983682
H	1.631099	0.216577	-2.172142
H	2.429037	-1.472458	-1.234119
H	1.588894	-2.662730	-0.237394
H	2.887015	-1.683583	0.456559
H	0.013202	-1.985851	1.575315
H	-0.198615	-0.309592	2.048805
H	1.355745	-1.098537	2.316904
C	-0.888821	1.758929	0.297024
H	-1.110709	2.475540	-0.502481
H	-1.564407	1.990573	1.121685
O	-2.489261	-1.477231	-0.301613
O	-2.272079	-0.158248	0.071091

Rotational constants (GHz): 1.5112400 1.1075600 0.8801900  
Vibrational harmonic frequencies (cm-1):

75.4748	141.9144	161.7989
206.3993	222.4808	271.2202
286.7862	301.6233	374.8305
382.5906	413.7760	443.1967
454.4604	550.2608	581.2394
636.7706	658.4209	769.7052
792.7288	813.4154	849.0282
881.8458	905.9363	931.1224
944.8562	957.5765	967.4001
1001.9893	1015.5618	1047.7229
1071.7053	1091.9272	1115.3240
1166.1616	1194.0640	1212.2144
1229.9852	1236.5342	1249.5127
1270.0992	1288.2949	1311.9247
1328.7752	1348.2492	1379.3917
1408.1601	1427.6840	1469.8100
1485.9941	1486.9104	1504.0133
1506.5096	1518.1813	1526.0752
1555.7683	3019.7286	3025.7435
3032.7982	3045.9692	3060.8432
3068.2320	3081.7385	3085.0037
3096.3319	3101.4909	3110.2222
3112.5850	3131.8208	3139.2077

Zero-point correction (Hartree): 0.215371

**HP**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.823940003  
Electronic state : 1-A  
Cartesian coordinates (Angs):

C	1.364478	-0.425922	0.215532
C	0.197433	-0.517930	-0.846576
C	-1.090529	-0.059098	-0.203932
C	0.190063	1.820384	0.663286
C	1.326985	1.116819	-0.104147
C	0.813432	0.743266	-1.524108
C	2.651866	-1.092685	-0.291270
C	1.113501	-0.897096	1.647156
H	0.070503	-1.440219	-1.415880
H	0.089871	2.850642	0.297490
H	0.449350	1.903858	1.727053
H	2.268341	1.667100	-0.021074
H	0.113156	1.430858	-2.000647
H	1.616226	0.503889	-2.219358
H	2.912812	-0.815917	-1.313615
H	2.554659	-2.182462	-0.257443
H	3.494957	-0.817554	0.350670
H	1.054983	-1.989955	1.682552
H	0.190812	-0.501961	2.070159
H	1.944196	-0.594023	2.293454
C	-1.119326	1.071583	0.501945
H	-2.021402	1.425686	0.980105
H	-3.854127	-0.231103	-0.541318
O	-3.330946	-0.533600	0.214836
O	-2.115524	-0.936996	-0.462269
Rotational constants (GHz): 1.8843200 0.8388200 0.7850000			
Vibrational harmonic frequencies (cm-1):			
81.0336	154.1598	169.4109	
179.6441	190.2522	232.6603	
254.5491	267.4353	321.0796	
342.6054	392.3729	417.8284	
435.5698	471.4480	576.8503	
597.8261	656.9623	696.5977	
796.8878	813.0243	833.1105	
856.7566	893.9617	897.5965	
939.4806	950.2407	963.2929	
968.7248	991.4483	1021.2331	
1059.9297	1073.4173	1105.1740	
1120.6506	1124.4530	1181.5276	
1205.1222	1230.7127	1233.9936	
1249.4585	1264.7993	1293.2795	
1325.6213	1355.9486	1363.2830	
1381.3349	1402.2600	1420.8689	
1484.3016	1484.8436	1495.9982	
1502.3429	1516.6054	1521.5856	
1724.6486	2994.1631	3012.0064	
3017.7536	3024.4319	3050.9784	
3067.9819	3068.2104	3076.0543	
3085.7728	3105.1385	3123.1505	
3127.2054	3214.3191	3760.9880	
Zero-point correction (Hartree): 0.214636			

**DIO**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.825652708

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.226491	-0.374747	0.126825
C	0.038019	-0.419270	-0.903752
C	-1.260751	-0.203239	-0.166300
C	0.021764	1.755606	0.898382
C	1.118897	1.187182	-0.015142
C	0.533202	0.956358	-1.437972
C	2.524215	-0.921511	-0.484472
C	1.032083	-1.015884	1.503379
H	-0.045558	-1.275041	-1.575372
H	-0.041192	2.838686	0.759574
H	0.291606	1.593664	1.945197

H	2.048343	1.755508	0.076070
H	-0.218348	1.661896	-1.799175
H	1.298318	0.847824	-2.204035
H	2.739039	-0.512490	-1.473144
H	2.472369	-2.010452	-0.579140
H	3.374112	-0.684442	0.163418
H	0.980419	-2.104486	1.410248
H	0.124402	-0.693247	2.014627
H	1.880818	-0.779003	2.153493
C	-1.362145	1.120959	0.584118
H	-1.937051	1.790926	-0.060862
H	-1.964226	0.966406	1.480666
O	-2.437234	-0.648668	-0.779034
O	-1.841979	-1.339892	0.411289
Rotational constants (GHz):	1.7039700	1.0490100	0.9449900
Vibrational harmonic frequencies (cm-1):			
100.2448	160.3970		190.0075
205.7185	225.7813		295.9062
314.2194	370.9269		381.0116
397.5596	415.8116		441.9282
465.4492	526.7999		584.0754
651.3704	727.5165		778.0465
819.6680	846.2310		857.3813
888.1720	897.2368		931.2424
952.2371	957.9773		971.1270
1009.5010	1019.9504		1052.4602
1071.7102	1099.9445		1132.5523
1170.1268	1208.6839		1216.8591
1226.5655	1235.3097		1256.5048
1265.5306	1286.3574		1287.7469
1320.2779	1345.5147		1368.7592
1408.6463	1425.3693		1427.4183
1478.3022	1487.2487		1490.5967
1506.3819	1507.4650		1518.8296
1525.0152	3021.6436		3027.4394
3037.3115	3052.7600		3055.6511
3065.0534	3071.7749		3076.8803
3083.5379	3090.4287		3102.0675
3105.0942	3111.7336		3130.1800
Zero-point correction (Hartree):	0.215823		

**LAC-1**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.944049239

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.210693	-0.164405	0.251309
C	0.200879	-0.786268	-0.794259
C	-1.162405	-1.082317	-0.195759
C	-0.342175	1.934698	0.395458
C	0.820362	1.243755	-0.330434
C	0.357556	0.520696	-1.624743
C	2.653201	-0.531581	-0.124165
C	0.999614	-0.452702	1.737758
H	0.519779	-1.712375	-1.271080
H	-0.417644	2.970668	0.043319
H	-0.135292	1.990645	1.468070
H	1.656836	1.941129	-0.431442
H	-0.512931	0.907128	-2.154606
H	1.163051	0.411730	-2.350221
H	2.874984	-0.349956	-1.178196
H	2.845283	-1.588885	0.080027
H	3.358674	0.057719	0.470125
H	1.218047	-1.503435	1.950684
H	-0.017900	-0.256421	2.075084
H	1.681278	0.154296	2.342785
C	-1.721772	1.317886	0.155056
H	-2.054748	1.504963	-0.869320

H	-2.449781	1.783117	0.819980
O	-1.609079	-2.197618	-0.157056
O	-1.869091	-0.090994	0.429990
Rotational constants (GHz):	1.5017400	1.1543600	0.9274100
Vibrational harmonic frequencies (cm <sup>-1</sup> ):			
87.7888	167.2293	193.1153	
209.8880	223.0826	261.3526	
316.5682	340.8225	362.4714	
388.4153	402.7524	436.0715	
458.3628	541.3946	632.0325	
648.0451	725.2274	750.6747	
788.8820	839.0689	874.9726	
916.5282	924.3427	948.8292	
959.6583	968.3320	1009.7395	
1026.8889	1058.8517	1084.1373	
1095.8791	1136.8607	1158.6608	
1169.5436	1218.5607	1223.7637	
1248.6733	1257.9256	1267.9301	
1300.4107	1303.0236	1330.4780	
1355.3291	1390.4757	1404.4848	
1424.3476	1426.4581	1481.8152	
1489.1235	1494.4874	1500.4365	
1509.8131	1520.0477	1530.8316	
1810.4185	3019.0630	3021.1459	
3026.5266	3043.7096	3046.9278	
3066.1247	3077.2560	3079.6727	
3084.2858	3097.0633	3101.6720	
3104.9990	3120.6023	3122.4261	
Zero-point correction (Hartree): 0.217808			

#### LAC-2

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.945694983

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.286272	-0.318447	0.241385
C	0.493627	-0.481182	-1.095164
C	-1.811530	-0.406876	-0.142378
C	-0.382550	1.566960	0.946464
C	0.899373	1.208616	0.187098
C	0.655297	1.036669	-1.340409
C	2.790060	-0.512464	-0.003642
C	0.858591	-1.165844	1.437335
H	0.912755	-1.159760	-1.838084
H	-0.469567	2.656935	1.000096
H	-0.303945	1.220275	1.981157
H	1.704179	1.889993	0.476481
H	-0.182932	1.560527	-1.799419
H	1.545599	1.240741	-1.935566
H	3.155095	0.064834	-0.856591
H	3.018246	-1.566111	-0.191191
H	3.360154	-0.197865	0.875681
H	1.091996	-2.218923	1.255392
H	-0.207085	-1.110110	1.660515
H	1.402427	-0.854969	2.335184
C	-1.691864	1.045261	0.320886
H	-1.937908	1.650794	-0.558373
H	-2.516207	1.181687	1.020841
O	-2.793975	-1.058446	0.091807
O	-0.850582	-0.965831	-0.933753
Rotational constants (GHz):	1.8164100	0.9746500	0.8957500
Vibrational harmonic frequencies (cm <sup>-1</sup> ):			
81.2307	147.2314	189.0002	
214.1556	232.8772	271.9099	
301.5463	331.5386	361.1693	
375.3274	425.0158	471.8311	
484.3988	522.9558	572.9943	
650.6244	689.4892	747.3090	

797.4211	832.5366	884.2327
888.3353	894.1239	953.0787
955.9349	969.5813	998.8209
1019.1598	1053.3149	1065.1685
1108.1198	1147.7139	1158.5067
1175.1126	1190.4270	1228.7267
1241.1572	1246.7069	1266.3702
1279.5915	1302.1830	1344.3927
1369.5261	1385.0901	1399.6571
1407.7630	1427.7596	1471.9122
1485.9578	1489.9569	1499.9453
1504.6585	1510.4595	1516.3933
1809.9633	3021.9881	3028.5216
3029.1900	3034.4958	3050.0097
3064.2062	3076.5789	3080.1085
3085.9084	3093.2553	3096.4028
3109.3418	3113.7054	3121.7142

Zero-point correction (Hartree): 0.217236

#### ACID

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.927157805  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.932571	-0.023589	0.152415
C	1.365091	-1.225150	0.903245
C	-2.428659	0.070123	0.238933
C	-0.324977	0.896808	-1.088873
C	0.686540	-0.238492	-0.830497
C	0.323552	-1.399506	0.086942
C	3.282346	-0.292463	-0.525339
C	1.990297	1.287884	0.939253
H	1.729388	-1.765607	1.770941
H	-0.823406	0.706430	-2.050538
H	0.225286	1.828269	-1.258923
H	1.051716	-0.579951	-1.806416
H	-2.343947	-0.367276	-1.630438
H	-0.479640	-2.126150	0.053140
H	3.258992	-1.223657	-1.097744
H	4.079795	-0.376762	0.219943
H	3.550839	0.521927	-1.206544
H	2.178845	2.140837	0.278627
H	2.809618	1.251405	1.664164
H	1.073050	1.480657	1.496969
C	-1.389607	1.158940	-0.009887
H	-1.955600	2.057476	-0.286204
H	-0.943027	1.363566	0.961299
O	-2.829683	-0.650345	-0.846842
O	-2.924670	-0.139466	1.308663

Rotational constants (GHz): 2.1575000 0.6403700 0.6287000  
 Vibrational harmonic frequencies (cm-1):

41.0141	45.6784	80.5910
116.1941	180.8167	233.6733
254.1416	269.7867	280.5659
330.1056	358.4639	389.3152
424.4610	469.7156	504.8128
565.4237	604.0787	629.0973
657.4472	751.4801	798.1088
809.5881	866.2797	893.4620
927.7969	944.2118	957.9783
974.9957	989.9548	1012.5172
1027.6181	1068.6169	1113.5340
1149.7722	1177.6626	1189.4895
1212.0472	1229.7314	1258.9041
1267.7273	1310.4260	1326.6196
1348.4526	1367.0115	1389.9008
1399.7830	1420.0070	1464.7908



1484.8543	1492.3735	1499.5416
1508.8858	1513.2015	1638.1109
1857.6273	2974.7523	3011.7405
3015.2966	3022.2704	3025.4750
3045.9099	3070.7385	3076.5361
3088.0893	3110.9489	3131.5652
3161.8292	3197.0545	3802.3417

Zero-point correction (Hartree): 0.213722

**HC1 (formed by CO2-loss)**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -313.324867242

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.766824	0.116998	-0.000002
C	0.313024	-0.399943	-1.026137
C	1.509178	0.544995	0.784656
C	0.313022	-0.399935	1.026139
C	0.635504	-1.526143	0.000006
C	-2.078411	-0.681923	-0.000001
C	-1.138394	1.603395	-0.000003
H	0.048770	-0.619699	-2.062344
H	2.432839	0.136481	1.201814
H	1.365898	1.539155	1.212547
H	0.048764	-0.619684	2.062347
H	1.656670	-1.916719	0.000008
H	-0.067460	-2.354835	0.000008
H	-1.944971	-1.763217	-0.000014
H	-2.675473	-0.425297	-0.881323
H	-2.675463	-0.425317	0.881334
H	-1.742781	1.842226	-0.881535
H	-0.280493	2.274475	-0.000029
H	-1.742739	1.842238	0.881556
C	1.509182	0.544986	-0.784658
H	2.432844	0.136463	-1.201806
H	1.365910	1.539142	-1.212562

Rotational constants (GHz): 3.0899800 2.1340600 1.7725400

Vibrational harmonic frequencies (cm-1):

150.6809	204.4784	221.7532
314.5073	350.1899	392.6236
412.5788	489.2911	512.5865
630.8304	666.4971	792.9972
829.9941	841.8620	852.7104
896.2314	928.2651	932.9587
953.7631	971.9732	987.7650
1001.8496	1023.1459	1027.9910
1083.4308	1109.3249	1141.8348
1185.9332	1196.0831	1219.5652
1225.0730	1250.1299	1253.5507
1258.2798	1291.0874	1309.0489
1332.2734	1406.1284	1424.8747
1484.2497	1485.4785	1501.3276
1505.4682	1516.8970	1521.7962
1535.1147	3018.0011	3024.9952
3045.0126	3049.4501	3053.5441
3064.6139	3071.7644	3077.2444
3079.0764	3083.8643	3093.8696
3116.8863	3129.5185	3145.5897

Zero-point correction (Hartree): 0.202023

**HC2 (formed by CO2-loss)**

-----  
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -313.31665858

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-0.863865	-0.313170	0.030945
C	-1.596536	0.995670	0.318210
C	1.712221	0.564477	0.233912

C	0.339817	0.638512	-0.438448
C	-0.584474	1.781858	-0.053675
C	-1.471293	-1.148123	-1.101130
C	-0.620081	-1.177474	1.271269
H	-2.601114	1.188926	0.681920
H	1.595161	0.527328	1.321671
H	2.240149	1.502937	0.023026
H	0.480211	0.565873	-1.525451
H	-0.452861	2.858229	-0.095090
H	-1.655478	-0.535152	-1.987689
H	-2.426070	-1.587253	-0.792632
H	-0.805490	-1.969330	-1.386527
H	0.038213	-2.023957	1.052384
H	-1.569895	-1.586735	1.631371
H	-0.181078	-0.602299	2.089049
C	2.574377	-0.609136	-0.244437
H	2.741797	-0.556877	-1.324850
H	2.102379	-1.571501	-0.030435
H	3.553080	-0.605878	0.243370
Rotational constants (GHz):	2.7153400	1.6744400	1.3738900
Vibrational harmonic frequencies (cm-1):			
97.5190	123.8354		193.4592
240.4120	254.9160		260.7850
288.6406	339.1136		347.0625
376.2718	438.2475		549.1576
648.1016	729.9895		764.0348
838.8779	866.2028		916.9156
946.5288	953.8406		965.3387
990.2512	1008.2558		1051.6197
1070.6047	1099.0551		1134.5872
1186.2198	1191.4046		1239.2383
1253.0780	1283.7802		1320.1376
1341.6882	1384.5304		1396.7741
1412.2974	1417.3216		1482.6416
1488.7081	1493.9698		1500.7667
1505.4753	1508.8116		1515.2904
1639.1522	2992.0579		3010.6529
3011.5214	3020.7396		3024.4931
3048.7129	3069.1212		3074.7565
3084.0567	3085.4441		3093.1527
3101.0299	3148.2983		3181.2895
Zero-point correction (Hartree):	0.198201		

### H<sub>2</sub>CO

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -114.536341384  
 Point group : C2V  
 Electronic state : 1-A1  
 Cartesian coordinates (Angs):

O	0.000000	0.000000	0.674024
C	0.000000	0.000000	-0.525922
H	0.000000	0.938531	-1.118330
H	0.000000	-0.938531	-1.118330

Rotational constants (GHz): 284.6461200 39.0463600 34.3362800  
 Vibrational harmonic frequencies (cm-1):

1202.0395	1270.0158	1539.0889
1827.0102	2870.2323	2919.4757

Zero-point correction (Hartree): 0.026490

### H<sub>2</sub>COO

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -189.633443828  
 Point group : CS  
 Electronic state : 1-A'  
 Cartesian coordinates (Angs):

O	0.000000	0.455955	0.000000
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C	1.071840	-0.206448	0.000000
H	1.979889	0.382038	0.000000
H	1.020866	-1.290205	0.000000
O	-1.178974	-0.187598	0.000000

Rotational constants (GHz): 81.4771000 12.3770900 10.7448500  
 Vibrational harmonic frequencies (cm-1):  
 534.6570 ( A') 674.7096 ( A") 909.8832 ( A")  
 933.3384 ( A') 1241.0006 ( A') 1397.1386 ( A')  
 1527.3225 ( A') 3120.1615 ( A') 3276.9189 ( A')  
 Zero-point correction (Hartree): 0.031018

**RAD-1**

-----  
 E(UB+HF-LYP/6-311G(d,p)) (Hartree): -426.047897835  
 Electronic state : 2-A  
 Cartesian coordinates (Angs):

C	1.053123	-0.249098	0.200429
C	-0.068820	-0.652174	-0.835129
C	-1.442003	-0.572610	-0.178330
C	-0.582952	1.684451	0.638613
C	0.658568	1.233390	-0.149592
C	0.189827	0.715849	-1.537282
C	2.454533	-0.604781	-0.315702
C	0.932067	-0.737244	1.645355
H	0.035395	-1.583707	-1.392494
H	-0.941544	2.649095	0.249936
H	-0.338844	1.874108	1.693816
H	1.450760	1.985535	-0.112517
H	-0.671401	1.213356	-1.990181
H	0.990681	0.664096	-2.272886
H	2.626218	-0.290530	-1.346474
H	2.614781	-1.686149	-0.267151
H	3.218452	-0.128045	0.307225
H	1.093245	-1.818710	1.692525
H	-0.042630	-0.535446	2.091933
H	1.693493	-0.263331	2.273639
C	-1.672780	0.663054	0.539127
H	-2.632720	0.806383	1.023833
O	-2.278158	-1.471459	-0.249517

Rotational constants (GHz): 1.9807200 1.2698800 1.1695700  
 Vibrational harmonic frequencies (cm-1):  
 120.8989 175.6949 200.8874  
 218.2165 225.1938 295.5183  
 356.4678 386.7359 416.5414  
 433.7010 472.1122 492.0248  
 577.7297 617.1896 665.5376  
 731.4668 776.2376 827.2638  
 856.7665 879.9908 907.2100  
 935.5738 948.9141 962.3884  
 972.0480 1014.8303 1057.7756  
 1065.2678 1070.6651 1118.8390  
 1153.3764 1199.7325 1211.8516  
 1228.5407 1239.3487 1250.9332  
 1286.9079 1292.9859 1310.2342  
 1366.7925 1377.4111 1404.0072  
 1424.3287 1459.1975 1485.3980  
 1488.5846 1501.9399 1512.7072  
 1518.5668 1626.3898 2979.5238  
 2994.4776 3019.6022 3025.4167  
 3052.4905 3059.7960 3074.0926  
 3080.3034 3094.6912 3103.3334  
 3104.8169 3124.1516 3177.2336  
 Zero-point correction (Hartree): 0.198221

**RAD-2**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -426.020140323  
Electronic state : 2-A  
Cartesian coordinates (Angs):

C	1.080587	-0.290303	0.123034
C	0.005988	-0.340989	-0.993570
C	-1.351054	-0.613089	-0.426908
C	-0.649089	1.408051	1.033223
C	0.627507	1.227553	0.192301
C	0.229088	1.137589	-1.314272
C	2.517341	-0.434864	-0.399690
C	0.903082	-1.185474	1.348449
H	-0.929986	2.464968	1.027815
H	-0.443462	1.147998	2.074964
H	1.409433	1.944455	0.467192
H	-0.627656	1.721538	-1.654095
H	1.068305	1.311016	-1.986361
H	2.715163	0.177641	-1.280173
H	2.718367	-1.475660	-0.666616
H	3.228596	-0.142607	0.379577
H	1.086699	-2.229289	1.078372
H	-0.095429	-1.136597	1.784658
H	1.622707	-0.912334	2.126673
C	-1.820834	0.547553	0.483863
H	-2.489549	1.161179	-0.129590
H	-2.439690	0.118949	1.274118
O	-2.009899	-1.610928	-0.596889

Rotational constants (GHz): 1.9459900 1.3018200 1.1535800  
Vibrational harmonic frequencies (cm-1):

84.6633	167.4406	187.7469
201.3604	229.0977	285.7419
373.9579	376.6550	410.6690
424.3938	450.6861	480.5463
548.7106	612.2396	655.8067
750.7352	762.0224	819.9295
864.7710	884.6709	933.1223
948.4844	966.9543	969.4924
998.4565	1019.9395	1020.7763
1064.9392	1089.5959	1121.2073
1172.1378	1189.2709	1209.3499
1210.0333	1236.4499	1258.1841
1271.6014	1293.7247	1321.0706
1355.7730	1404.6044	1425.8862
1461.3875	1484.7849	1488.1616
1504.1370	1506.5870	1514.2661
1521.1735	1781.8916	3017.4451
3025.4242	3031.0510	3034.6360
3044.4601	3069.6689	3071.6047
3082.9989	3088.8261	3098.3766
3111.4658	3113.9288	3123.2437

Zero-point correction (Hartree): 0.198721

**RAD-3(a)**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.77686192  
Electronic state : 1-A  
Cartesian coordinates (Angs):

C	-2.485273	0.009943	-0.127488
C	1.131742	1.396420	-0.197434
C	1.827398	0.264231	-0.039206
C	-0.242250	-0.981717	0.572846
C	-0.994631	0.020069	-0.340887
C	-0.369899	1.426452	-0.173217
C	-3.365061	-0.683362	-1.119186
C	-3.064667	0.326548	1.216534
H	1.678264	2.319980	-0.360675
H	-0.703991	-1.970473	0.504634
H	-0.339466	-0.657352	1.614634
H	-0.803372	-0.288762	-1.376487

H	-0.736207	2.087873	-0.965907
H	-0.708053	1.880122	0.767798
H	-2.983731	-0.588961	-2.140384
H	-4.386147	-0.287480	-1.098493
H	-3.451395	-1.764922	-0.912573
H	-4.032144	0.833201	1.123686
H	-2.412578	0.961848	1.821166
H	-3.253739	-0.586292	1.806472
C	1.246974	-1.088955	0.210942
H	1.396259	-1.712640	-0.678579
H	1.814443	-1.579969	1.006160
O	3.890014	-0.741578	-0.016714
O	3.211968	0.393585	-0.124396
Rotational constants (GHz):	2.7483100	0.5253600	0.4949900
Vibrational harmonic frequencies (cm-1):			
42.1432	63.2100		95.8734
121.4860	123.1329		150.4658
181.6332	244.9994		254.5199
281.6244	310.1622		385.2777
420.9086	447.9044		487.3148
519.2765	562.4546		652.7710
763.6041	794.6258		829.6693
855.1558	917.8143		940.2785
943.5069	965.3834		981.6655
1012.6580	1036.5669		1044.9383
1067.2812	1083.1425		1090.1522
1164.8865	1167.2066		1194.0925
1240.8857	1273.6546		1294.7247
1318.5708	1326.2076		1341.4044
1362.1544	1391.7880		1398.8353
1402.9139	1418.1801		1469.0725
1472.0094	1475.5746		1477.5589
1483.4410	1495.7038		1500.7882
1689.6198	2924.7062		2940.3321
2998.9644	3008.7809		3022.8620
3025.2121	3028.8237		3029.6075
3041.7349	3067.6290		3074.2465
3076.2643	3083.1502		3165.0599
Zero-point correction (Hartree):	0.210772		

**RAD-3(b)**

-----  
 E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.77500172  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	2.480797	-0.184039	-0.123703
C	-1.300382	-1.050877	-0.091282
C	-1.821982	0.171134	0.001085
C	0.409188	1.161877	0.509229
C	1.003228	0.010029	-0.342504
C	0.185083	-1.282746	-0.101523
C	3.454255	0.277288	-1.161563
C	3.014768	-0.492759	1.240915
H	-1.973867	-1.896295	-0.163787
H	1.006288	2.068899	0.381865
H	0.461478	0.890836	1.569182
H	0.855192	0.286225	-1.394242
H	0.434272	-2.018745	-0.873828
H	0.481087	-1.745723	0.848967
H	3.031626	0.231758	-2.169263
H	4.370583	-0.323933	-1.149434
H	3.774163	1.321422	-0.996533
H	3.884184	-1.158400	1.187152
H	2.273423	-0.965917	1.889695
H	3.359551	0.416464	1.761795
C	-1.051138	1.449211	0.129007
H	-1.100793	2.000977	-0.817878

H	-1.530017	2.086031	0.879965
O	-3.993292	-0.620288	-0.161031
O	-3.202967	0.426749	-0.002922
Rotational constants (GHz):	2.8100200	0.5166000	0.4896100
Vibrational harmonic frequencies (cm-1):			
40.2598	54.2621	73.1999	
103.2806	115.1949	153.3958	
181.5306	233.7797	258.0966	
281.2818	313.1785	386.0336	
408.0601	438.5284	491.5016	
524.1074	532.1747	671.9402	
778.7863	794.0491	840.2853	
863.3848	925.6339	938.4346	
941.8993	966.8006	978.7507	
1012.2597	1037.0682	1044.3926	
1050.7717	1077.3263	1098.2685	
1162.1822	1170.7707	1193.6104	
1245.2754	1273.8549	1294.6798	
1318.9865	1327.0304	1342.7654	
1360.2259	1390.7106	1397.9656	
1401.8621	1418.4916	1468.3001	
1473.4594	1477.4239	1481.1740	
1484.1697	1495.3352	1501.0803	
1691.4263	2924.7238	2940.2911	
2998.2313	3007.8269	3013.4817	
3022.3396	3024.4527	3028.7537	
3040.2630	3054.3078	3073.2809	
3077.2081	3083.1399	3191.3924	
Zero-point correction (Hartree): 0.210636			

### Nopinone

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -426.698631617  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.071802	-0.237819	0.190451
C	0.004183	-0.560616	-0.930883
C	-1.361346	-0.640177	-0.282578
C	-0.619939	1.597380	0.799312
C	0.641007	1.258886	-0.009012
C	0.228826	0.887313	-1.459782
C	2.500511	-0.499637	-0.304761
C	0.904962	-0.892455	1.563551
H	0.171653	-1.420955	-1.580384
H	-0.915085	2.628989	0.586179
H	-0.395658	1.555930	1.868750
H	1.417969	2.015806	0.129342
H	-0.630303	1.407288	-1.889831
H	1.053104	0.937631	-2.169028
H	2.702723	-0.059761	-1.282908
H	2.689311	-1.574959	-0.377795
H	3.224906	-0.081958	0.402094
H	1.103437	-1.966335	1.495281
H	-0.093436	-0.776108	1.987918
H	1.620090	-0.469103	2.276531
C	-1.789756	0.635075	0.456566
H	-2.507133	1.129792	-0.207747
H	-2.361642	0.335224	1.336705
O	-2.070180	-1.618647	-0.339036
Rotational constants (GHz):	1.9181100	1.2830900	1.1535800
Vibrational harmonic frequencies (cm-1):			
85.9999	164.9212	189.9077	
208.2671	232.2345	279.5665	
366.3380	384.3323	413.4705	
429.9263	471.1144	485.9213	
548.8573	616.9042	648.5250	
753.1696	786.6555	832.5946	

869.3926	887.5725	928.2693
944.3719	956.4748	968.1896
1002.2234	1013.9088	1040.8654
1070.8278	1091.5440	1122.9491
1166.2433	1201.3653	1210.2016
1220.4881	1234.2511	1251.4413
1263.6064	1276.6922	1306.6882
1313.3687	1336.1077	1368.9091
1407.4821	1425.7038	1459.5949
1487.5639	1487.8658	1503.2964
1506.5423	1516.1955	1524.8407
1796.0950	3020.2690	3025.9812
3029.8781	3037.6760	3051.9582
3061.0247	3066.3834	3075.2140
3081.9355	3090.1128	3093.3367
3103.3041	3105.7405	3125.2619

Zero-point correction (Hartree): 0.211933

**TS1**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.23161984  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	-1.905835	0.397187	-0.186328
C	-0.442479	0.268177	-0.797198
C	0.547708	0.335181	0.327608
C	-1.007251	-1.417522	1.388240
C	-1.776921	-1.141961	0.089722
C	-0.786483	-1.216713	-1.104787
C	-2.940167	0.708589	-1.276747
C	-2.139161	1.351394	0.985439
H	-0.175285	0.935981	-1.617907
H	-0.894755	-2.497679	1.517882
H	-1.584925	-1.061443	2.245950
H	-2.697883	-1.729687	0.040664
H	0.035941	-1.929182	-1.042651
H	-1.283947	-1.332854	-2.065761
H	-2.839385	0.073994	-2.158230
H	-2.849693	1.749027	-1.604386
H	-3.953258	0.571905	-0.884453
H	-2.047018	2.390679	0.653589
H	-1.439228	1.212130	1.809871
H	-3.151713	1.222679	1.382269
C	0.404301	-0.751891	1.378098
H	1.162248	-1.514409	1.172377
H	0.651029	-0.350680	2.364462
C	1.339628	1.438850	0.551248
H	1.778038	1.620984	1.523784
H	1.345027	2.259218	-0.153143
O	3.354329	0.883586	-0.098735
O	3.194197	-0.391613	-0.251026
O	2.224570	-0.673025	-1.064750

Rotational constants (GHz): 1.4643300 0.5377000 0.5263400  
 Vibrational harmonic frequencies (cm-1):

-177.3435	50.8271	82.8131
108.1357	174.5628	182.6097
189.6840	207.9155	219.0210
238.4962	285.4889	369.3563
386.6583	397.6937	415.9949
454.0794	461.5938	487.8041
547.4425	621.7808	654.9246
743.2877	755.1304	783.0061
804.2428	826.1306	852.5981
887.7600	919.9734	925.6735
945.7836	954.6411	968.0934
984.8369	1005.5785	1029.9581

1061.1866	1070.8719	1075.4177
1090.9183	1103.5351	1119.4657
1164.6260	1204.1938	1220.0317
1232.6136	1236.2002	1259.6345
1280.4786	1289.7581	1311.0187
1312.6887	1347.0833	1368.2404
1405.9370	1424.7222	1439.8192
1475.9324	1486.2453	1489.8766
1504.8642	1507.2592	1515.8327
1523.5079	1562.1857	3018.9350
3024.7990	3031.0859	3038.4680
3051.2367	3059.4232	3070.4579
3075.8267	3077.3082	3077.9402
3084.4362	3110.0915	3111.9009
3133.0307	3154.5411	3248.0456

Zero-point correction (Hartree): 0.244619

**TS2**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.23267133

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.869942	-0.475739	-0.137461
C	0.374650	-0.412910	-0.686743
C	-0.541113	-0.176749	0.478535
C	1.134511	1.690530	1.022740
C	1.815161	1.089981	-0.215475
C	0.758039	0.941115	-1.344769
C	2.820350	-1.080845	-1.179716
C	2.138284	-1.148297	1.208667
H	0.039532	-1.238902	-1.318031
H	1.076101	2.776930	0.910118
H	1.745848	1.504130	1.910438
H	2.752995	1.603644	-0.444869
H	-0.030205	1.690429	-1.410530
H	1.200735	0.807847	-2.329941
H	2.694947	-0.654454	-2.176008
H	2.664185	-2.161418	-1.258394
H	3.860499	-0.918491	-0.878778
H	1.988884	-2.230171	1.131188
H	1.495131	-0.788775	2.012159
H	3.176915	-0.981975	1.513381
C	-0.302233	1.119501	1.223933
H	-1.039666	1.834547	0.846323
H	-0.529109	0.990899	2.285218
C	-1.346173	-1.167921	0.993230
H	-1.744327	-1.091604	1.995870
H	-1.394089	-2.140979	0.520699
O	-3.355574	-0.666134	0.332438
O	-3.105565	-0.263201	-0.869973
O	-2.324722	0.770128	-0.898276

Rotational constants (GHz): 1.4162300 0.5377000 0.5313200

Vibrational harmonic frequencies (cm-1):

-167.5415	52.4461	81.9667
104.5064	170.1445	175.3639
190.7783	203.4864	223.0274
232.1781	287.8607	371.7477
386.5251	391.6890	415.4692
447.5430	454.6983	485.9546
541.8169	617.9576	654.1551
740.1680	750.6274	786.9818
809.7376	825.3718	849.6158
889.6083	918.0631	938.7364
948.1895	952.4800	966.2371
981.9726	1004.9176	1029.1101
1058.0932	1074.1490	1077.3091
1095.2096	1102.2771	1119.5873



1162.8555	1202.8186	1216.2173
1223.4094	1236.2319	1255.7339
1278.2091	1289.8976	1309.1858
1311.1568	1344.5115	1366.5150
1404.5516	1423.4094	1441.0018
1477.9190	1485.8001	1487.2541
1503.7797	1504.5918	1515.7638
1524.1597	1564.2801	3018.3699
3023.9730	3031.6574	3039.1063
3051.3329	3060.8629	3065.7794
3070.4699	3077.1998	3078.7142
3086.0266	3106.3583	3110.1708
3136.3154	3150.6557	3242.7015

Zero-point correction (Hartree): 0.244417

**TS1b**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.22804754

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.508484	0.744780	-0.044440
C	-0.505656	-0.036631	-0.982998
C	0.575504	-0.798429	-0.272784
C	-1.357506	-1.430959	1.305456
C	-2.145651	-0.659341	0.234458
C	-1.653636	-1.102170	-1.165270
C	-2.430953	1.644560	-0.884797
C	-1.010902	1.573633	1.139669
H	-0.133492	0.479118	-1.870770
H	-1.697652	-2.471316	1.298308
H	-1.588778	-1.036425	2.298458
H	-3.220153	-0.691333	0.436758
H	-1.344288	-2.142655	-1.285615
H	-2.334182	-0.841065	-1.973649
H	-2.847497	1.148033	-1.762429
H	-1.882667	2.525962	-1.231338
H	-3.269163	1.996037	-0.275167
H	-0.446295	2.441564	0.793346
H	-0.365052	1.026368	1.821896
H	-1.871807	1.937409	1.711696
C	0.184657	-1.386306	1.066941
H	0.618860	-2.384405	1.165434
H	0.673666	-0.779045	1.834551
C	1.697050	-1.233023	-0.938316
H	2.270036	-2.071085	-0.566120
H	1.890854	-0.921181	-1.956940
O	3.388193	-0.048431	-0.187923
O	2.836058	1.115981	-0.139183
O	1.835885	1.168367	0.678865

Rotational constants (GHz): 1.2788700 0.6077200 0.5386500

Vibrational harmonic frequencies (cm-1):

-143.6485	55.9911	82.4246
116.1968	155.5841	174.3374
204.1055	205.6243	227.0268
257.3910	278.1896	327.8356
392.6187	410.6087	418.7186
433.5560	447.9675	509.3129
552.5129	598.4669	664.7239
741.6721	761.6968	785.2372
804.8752	832.1350	856.8432
878.2022	916.3157	923.8573
937.7890	950.7406	966.8025
992.2463	1005.5465	1019.0724
1059.1341	1063.3259	1085.2632
1105.2851	1106.8078	1130.4994
1161.0047	1206.4264	1206.7946
1228.2649	1237.9483	1257.1450

1273.3116	1295.6546	1307.2589
1310.3316	1343.3383	1371.3082
1406.6041	1427.2891	1442.1442
1475.1173	1486.0610	1490.5240
1504.0647	1507.4212	1515.4808
1522.0735	1565.5584	3023.0990
3028.8311	3029.4401	3039.5096
3047.8698	3058.9169	3060.9997
3070.3281	3077.1286	3079.0802
3095.1959	3103.5091	3125.8908
3150.3408	3151.7106	3243.6554

Zero-point correction (Hartree): 0.244591

**TS2b**

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.22692343  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	-1.547816	0.708264	-0.055880
C	-0.563486	-0.088319	-1.001971
C	0.591625	-0.746730	-0.305978
C	-1.224362	-1.364802	1.416871
C	-2.102945	-0.700519	0.344899
C	-1.666556	-1.212023	-1.050214
C	-2.558297	1.509838	-0.895008
C	-1.029288	1.629140	1.048123
H	-0.260283	0.386575	-1.936445
H	-1.519345	-2.415402	1.501097
H	-1.415950	-0.910282	2.392396
H	-3.162122	-0.765181	0.610426
H	-1.315635	-2.243758	-1.121784
H	-2.402854	-1.036077	-1.832177
H	-3.010042	0.933246	-1.703505
H	-2.069934	2.381224	-1.341698
H	-3.368991	1.875910	-0.257212
H	-0.588447	2.533296	0.621917
H	-0.267987	1.178902	1.679781
H	-1.866911	1.933897	1.685689
C	0.299755	-1.280783	1.085045
H	0.769719	-2.261188	1.197854
H	0.805434	-0.634968	1.810403
C	1.698309	-1.172162	-1.002884
H	2.322831	-1.969236	-0.621180
H	1.832930	-0.894207	-2.038970
O	3.395070	0.132265	-0.470618
O	2.864131	0.779445	0.514286
O	1.757793	1.365269	0.188256

Rotational constants (GHz): 1.3113800 0.6019500 0.5420800  
 Vibrational harmonic frequencies (cm-1):

-159.6751	49.9984	71.8014
110.5106	162.9702	177.3190
188.8093	208.4342	224.5969
256.9216	266.8734	326.7442
389.1313	408.8778	413.0818
439.4615	453.4411	508.2520
554.9766	596.6099	664.5727
742.3727	758.6451	780.0040
799.3404	829.9243	855.9940
875.4127	913.7819	923.1139
925.3299	951.4022	967.1080
989.7107	1004.9966	1018.4426
1056.4493	1062.1674	1080.2392
1097.1200	1106.7690	1129.0878
1160.0724	1205.5916	1207.1231
1228.6668	1237.7803	1256.4543
1272.3944	1293.6702	1307.7355
1311.6148	1343.8048	1370.0247

1406.4711	1428.3622	1440.5955
1472.5370	1481.5326	1488.1901
1502.4751	1503.9504	1510.5678
1517.7226	1562.2267	3021.7642
3027.7016	3027.7671	3032.4468
3047.1499	3057.8736	3060.8410
3075.2095	3077.9218	3081.2467
3089.7274	3102.2853	3126.2735
3150.4213	3155.3363	3248.7033

Zero-point correction (Hartree): 0.244295

**TS3**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.31233620

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.576585	-0.607992	0.035642
C	0.189675	-0.414499	-0.686241
C	-0.843464	0.310703	0.186446
C	1.236597	1.875646	0.570060
C	1.859634	0.869262	-0.404857
C	0.874659	0.650620	-1.583174
C	2.451864	-1.614783	-0.727644
C	1.653861	-0.960914	1.524761
H	-0.265191	-1.286591	-1.159112
H	1.291572	2.871211	0.120019
H	1.827682	1.921206	1.489457
H	2.896949	1.131534	-0.632048
H	0.258336	1.496920	-1.891064
H	1.342521	0.221059	-2.467314
H	2.474326	-1.431747	-1.802732
H	2.084098	-2.634267	-0.573684
H	3.483278	-1.575106	-0.362730
H	1.313968	-1.987373	1.698694
H	1.072463	-0.303031	2.171218
H	2.693862	-0.908125	1.863174
C	-0.247642	1.545477	0.917457
H	-0.891602	2.392789	0.679199
H	-0.349310	1.391885	1.994570
C	-1.656080	-0.633396	1.083019
H	-2.242371	-0.068837	1.817953
H	-1.058316	-1.405398	1.565766
O	-2.487056	-1.304339	0.158004
O	-2.912921	-0.256493	-0.761467
O	-1.913323	0.817472	-0.647059

Rotational constants (GHz): 1.3383600 0.6741200 0.6191100

Vibrational harmonic frequencies (cm-1):

-134.4542	76.3239	151.6061
185.5803	196.4405	216.9693
230.7660	275.0166	281.1044
326.7944	363.9307	386.8890
405.5295	426.0666	474.5450
500.8316	567.0629	627.1931
698.5419	706.8892	761.9034
772.4180	782.5959	827.6472
852.7997	880.3800	886.6426
924.2557	929.2689	952.9042
961.3476	968.9912	992.0600
1021.7666	1030.6006	1038.4105
1054.3385	1069.5159	1119.2704
1137.1749	1155.1210	1183.4072
1208.5161	1221.3366	1235.3794
1244.2408	1257.7539	1264.6431
1283.7911	1293.8217	1314.1513
1341.6369	1350.8859	1371.4259
1380.1250	1405.9477	1425.1002
1485.0681	1486.7510	1491.0258

1494.9950	1509.0254	1510.6277
1518.8813	1524.5232	3016.7358
3018.5064	3024.5041	3029.5893
3047.3163	3052.1126	3061.8730
3068.2152	3070.4120	3076.5427
3083.2136	3098.5317	3108.3690
3113.3922	3126.0703	3136.3188

Zero-point correction (Hartree): 0.248667

**TS4**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.29355387

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.532253	-0.621590	-0.014840
C	0.137544	-0.346460	-0.695806
C	-0.829194	0.401199	0.200558
C	1.251257	1.817037	0.738156
C	1.842815	0.882649	-0.329216
C	0.848661	0.783962	-1.515544
C	2.361698	-1.578435	-0.888909
C	1.652961	-1.113010	1.431558
H	-0.358690	-1.157170	-1.222415
H	1.268401	2.839443	0.349534
H	1.878757	1.813401	1.633591
H	2.882088	1.144152	-0.546566
H	0.255457	1.668186	-1.753910
H	1.296191	0.406924	-2.432674
H	2.358895	-1.311890	-1.946266
H	1.975391	-2.598655	-0.805252
H	3.402789	-1.588014	-0.551869
H	1.303757	-2.146113	1.522790
H	1.109970	-0.513165	2.160137
H	2.706992	-1.105451	1.728091
C	-0.212525	1.435402	1.131239
H	-0.864071	2.311571	1.132395
H	-0.235558	1.047493	2.151646
C	-1.844114	-0.916607	1.094920
H	-2.290365	-0.323499	1.911405
H	-0.962363	-1.504587	1.389930
O	-2.606254	-1.412168	0.204322
O	-2.491109	0.058728	-1.242101
O	-1.924611	0.922502	-0.416379

Rotational constants (GHz): 1.2449600 0.6834200 0.6328100

Vibrational harmonic frequencies (cm-1):

-422.6775	100.8438	129.6326
156.7239	193.1104	204.6553
222.8194	243.7749	259.9140
276.7075	294.6310	380.8339
396.7466	407.1396	413.8020
470.1667	490.5509	537.0602
571.3188	590.4344	657.3026
678.0633	762.9983	793.6828
827.7964	864.9948	872.5598
880.5905	917.9161	946.7542
957.8171	966.5293	989.8906
1017.4066	1050.1336	1059.8550
1081.5771	1112.6415	1123.7527
1133.8562	1151.3764	1196.5744
1209.9242	1219.4778	1228.0210
1237.7720	1252.7309	1269.3977
1285.4943	1290.4497	1309.3503
1334.6974	1363.3700	1380.1627
1384.2359	1405.4299	1425.6263
1479.7100	1489.9469	1492.5680
1505.3348	1508.2467	1516.7540
1520.7190	1538.5330	2921.0038

2998.5683	3023.7825	3029.8178
3034.3157	3053.3237	3058.1513
3067.5458	3072.2999	3073.2599
3083.7154	3094.6601	3110.3000
3130.6441	3131.2029	3140.2220

Zero-point correction (Hartree): 0.246169

**TS5**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.29215673

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.725611	0.476404	-0.078094
C	-0.523269	-0.018215	-0.970412
C	0.775381	-0.126190	-0.208420
C	-0.756020	-1.238504	1.554745
C	-1.783706	-1.002164	0.438609
C	-1.169913	-1.444127	-0.914541
C	-2.931575	0.833224	-0.963025
C	-1.551059	1.599141	0.946522
H	-0.373615	0.452005	-1.943932
H	-0.733252	-2.307603	1.784980
H	-1.081317	-0.734706	2.468640
H	-2.765717	-1.395161	0.715087
H	-0.484249	-2.293185	-0.906609
H	-1.906083	-1.595105	-1.701406
H	-3.137264	0.090913	-1.735319
H	-2.766508	1.792964	-1.462501
H	-3.831735	0.930149	-0.348625
H	-1.327835	2.549507	0.452244
H	-0.768875	1.408465	1.680329
H	-2.485491	1.734688	1.500526
C	0.687122	-0.775688	1.175435
H	1.377147	-1.622082	1.141506
H	1.104363	-0.116918	1.936612
C	1.700535	1.513569	-0.017744
H	1.067743	1.876717	0.801906
H	1.504454	1.993973	-0.991105
O	2.894132	1.177652	0.276036
O	2.896537	-0.762261	-0.393991
O	1.743946	-0.624057	-1.028392

Rotational constants (GHz): 1.4093600 0.6289800 0.5820200

Vibrational harmonic frequencies (cm-1):

-432.9360	68.6259	120.1531
143.9595	195.4171	209.4230
221.0322	254.4003	273.8864
294.7208	305.9608	328.7487
385.8820	407.7787	435.0478
461.9926	500.7382	545.1504
571.8808	592.5238	638.8640
694.2177	763.6042	790.0096
825.0751	863.2129	863.8608
883.4887	918.2790	941.3295
965.6638	970.6549	993.7189
1018.0333	1046.1533	1057.1072
1090.0014	1111.3725	1117.0428
1133.8235	1144.7904	1193.2495
1212.2066	1215.8614	1225.6473
1239.1762	1247.2557	1265.3432
1278.9868	1284.8186	1309.2690
1338.6156	1363.3293	1376.9841
1379.1752	1405.1605	1428.0331
1483.2490	1488.8310	1491.9657
1505.0873	1508.2780	1518.2077
1524.6073	1539.6987	2928.0775
3022.8674	3025.9327	3029.5754
3036.9124	3056.0411	3063.9498

3070.3308	3072.8232	3076.0504
3081.9426	3083.3806	3104.5388
3107.2153	3117.5248	3135.0736

Zero-point correction (Hartree): 0.246003

**TS6**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.28565147

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.553827	-0.682852	0.029057
C	0.286723	-0.288069	-0.818815
C	-0.785903	0.535604	-0.076879
C	1.330462	1.760673	0.805967
C	2.000172	0.802767	-0.195006
C	1.177506	0.793145	-1.508256
C	2.435704	-1.673906	-0.751812
C	1.451780	-1.211015	1.464799
H	-0.185812	-1.049310	-1.442120
H	1.464160	2.782044	0.437348
H	1.844148	1.708253	1.770665
H	3.075021	0.997167	-0.256762
H	0.675278	1.717306	-1.798521
H	1.728329	0.409374	-2.365394
H	2.587124	-1.387185	-1.792919
H	1.983640	-2.670945	-0.747294
H	3.421886	-1.755521	-0.283595
H	1.007950	-2.212488	1.481508
H	0.879877	-0.574673	2.138784
H	2.455916	-1.305569	1.890968
C	-0.192298	1.485207	1.019664
H	-0.772163	2.406364	0.961605
H	-0.347258	1.082198	2.022365
C	-1.818157	-0.680839	0.969684
H	-2.323764	0.055707	1.585706
H	-1.177768	-1.419376	1.436705
O	-2.561042	-1.209685	0.007152
O	-3.346245	-0.290670	-0.528823
O	-1.712145	1.021900	-0.812014

Rotational constants (GHz): 1.3146600 0.6322700 0.5758900

Vibrational harmonic frequencies (cm-1):

-412.6865	82.2169	113.1276
138.5679	191.6870	199.1611
224.3115	257.2482	274.1203
279.8422	313.5877	347.5553
393.6490	416.4969	433.5173
480.8582	496.3412	524.1468
566.2268	599.3017	614.8583
681.8909	740.7077	798.0163
821.3534	868.2570	874.9103
891.4757	923.1312	944.1810
961.9446	969.2703	986.5009
1004.9700	1031.1417	1045.2180
1063.6757	1100.8515	1105.6598
1129.8122	1156.0979	1161.1267
1211.3552	1221.1991	1228.1339
1234.6668	1250.3748	1258.6378
1270.5505	1282.3438	1309.5090
1309.6064	1339.9241	1366.9779
1403.1433	1414.2241	1425.2969
1478.6809	1486.8509	1489.9648
1494.9298	1507.0559	1513.6556
1519.5945	1527.4428	3017.8537
3024.2532	3028.0154	3046.3933
3051.3675	3064.2708	3066.2206
3070.2055	3075.7169	3083.5844
3107.5705	3110.4057	3114.9769

3124.9224                      3126.6808                      3247.1979  
Zero-point correction (Hartree): 0.246294

**TS7**

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -616.28533649

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.656651	0.606026	-0.028601
C	-0.480631	0.108338	-0.952609
C	0.780418	-0.403444	-0.206699
C	-1.059406	-1.529767	1.270689
C	-1.958463	-0.916834	0.184936
C	-1.322677	-1.182690	-1.202501
C	-2.740473	1.299872	-0.873396
C	-1.421057	1.477395	1.209400
H	-0.195714	0.713027	-1.815980
H	-1.156541	-2.617978	1.212690
H	-1.424478	-1.241559	2.260983
H	-3.004509	-1.198192	0.338131
H	-0.762115	-2.109207	-1.333309
H	-2.021157	-1.074150	-2.030799
H	-2.989150	0.757621	-1.786535
H	-2.413012	2.303206	-1.164490
H	-3.661332	1.408737	-0.291743
H	-1.075601	2.477812	0.927845
H	-0.711017	1.057139	1.920841
H	-2.366443	1.609172	1.745748
C	0.447811	-1.139546	1.127249
H	1.079652	-2.027952	1.135968
H	0.757922	-0.540663	1.985859
C	1.667614	1.226702	0.221057
H	1.215003	1.707689	1.078922
H	1.595610	1.701582	-0.751839
O	2.864688	0.731146	0.515610
O	3.410403	0.176735	-0.553294
O	1.674155	-0.933205	-0.953496

Rotational constants (GHz):    1.4090400            0.5995200            0.5603900

Vibrational harmonic frequencies (cm-1):

-419.7762	80.5808	95.4138
138.2774	198.5876	202.7281
228.6149	257.9366	276.9722
286.1402	309.2929	347.8025
387.4237	414.9855	437.6845
483.7881	494.2449	518.2771
563.8347	596.4249	616.7673
673.1241	739.3182	795.5771
822.7505	868.1704	879.0460
888.4246	925.1707	947.2336
960.8158	968.5097	987.4938
1007.0741	1037.1428	1042.0369
1062.6471	1091.2122	1107.2941
1126.4588	1153.4281	1157.8857
1210.2951	1222.1144	1232.2232
1234.7444	1246.8983	1262.5532
1266.6481	1271.7504	1300.3114
1309.6634	1340.0959	1367.2631
1405.4776	1410.6722	1426.5496
1479.0475	1484.6873	1490.3115
1494.9454	1508.0946	1509.9240
1521.2163	1525.8951	3018.9833
3024.7457	3028.7571	3047.1800
3054.3151	3063.9418	3067.5767
3068.6235	3075.9780	3076.7051
3104.6011	3106.3970	3117.1425
3122.6446	3127.0182	3248.0502

Zero-point correction (Hartree): 0.246157

**TS8a**

-----  
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.77253875  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 1.273572 -0.460069 0.192857  
C 0.310868 -0.273940 -1.065689  
C -1.051036 -0.021703 -0.528113  
C -0.021040 1.621163 1.004709  
C 1.237326 1.111079 0.270665  
C 0.970904 1.122955 -1.261731  
C 2.646578 -0.992723 -0.237958  
C 0.782308 -1.284802 1.381946  
H 0.324718 -1.029150 -1.852338  
H -0.073991 2.709279 0.900467  
H 0.068782 1.418126 2.077387  
H 2.139974 1.605241 0.638856  
H 0.332517 1.916495 -1.654024  
H 1.880135 1.069144 -1.856434  
H 3.067464 -0.465441 -1.094896  
H 2.581512 -2.053733 -0.496664  
H 3.355850 -0.896659 0.590126  
H 0.715504 -2.342489 1.109407  
H -0.195584 -0.976757 1.751268  
H 1.493659 -1.203873 2.210160  
C -1.296516 0.970880 0.448186  
H -2.125917 1.645102 0.226951  
H -2.247666 0.134591 0.909610  
O -3.073326 -0.627879 0.140333  
O -1.981017 -0.907985 -0.726471  
Rotational constants (GHz): 1.8566600 0.9216500 0.8451200  
Vibrational harmonic frequencies (cm-1):  
-1581.0977 105.0884 180.0214  
189.4973 221.6918 249.7879  
284.1333 328.9738 373.0887  
386.5431 409.7663 425.3423  
451.6177 490.3905 580.2040  
623.3324 668.4177 718.3594  
776.0844 832.1420 848.7294  
860.4350 880.9817 894.0311  
934.9110 954.8126 966.6839  
984.7298 1000.2133 1022.4729  
1054.1435 1082.7441 1101.9412  
1119.0330 1158.6382 1197.3456  
1224.6254 1227.4124 1241.3406  
1249.5057 1287.3193 1294.8202  
1305.8112 1360.3376 1402.8120  
1407.1366 1427.0618 1442.7078  
1483.1946 1488.9808 1497.4644  
1504.2684 1515.2361 1519.2506  
1536.3780 1826.3800 3022.9843  
3024.1594 3030.0451 3052.7929  
3058.8835 3070.4637 3077.2612  
3083.9656 3091.1922 3097.7162  
3111.6883 3123.3575 3134.6584  
Zero-point correction (Hartree): 0.210907

**TS8b**

-----  
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.77105442  
Electronic state : 1-A  
Cartesian coordinates (Angs):  
C 1.436868 -0.228847 0.271278  
C 0.231946 -0.903517 -0.489267  
C -1.053341 -0.401141 0.065806



C	-0.055928	1.863863	0.017268
C	1.101116	1.045520	-0.591911
C	0.530399	0.087576	-1.673385
C	2.776110	-0.863196	-0.132369
C	1.390051	-0.135198	1.797090
H	0.223887	-1.978785	-0.671724
H	-0.356894	2.637957	-0.697052
H	0.290701	2.390152	0.911986
H	1.940453	1.687347	-0.870865
H	-0.325423	0.430199	-2.256570
H	1.287102	-0.308155	-2.347627
H	2.896876	-0.977401	-1.210725
H	2.880568	-1.854187	0.319870
H	3.604787	-0.246421	0.228475
H	1.498759	-1.129825	2.241348
H	0.465431	0.297338	2.177415
H	2.221110	0.476809	2.161828
C	-1.255354	0.966495	0.357129
H	-2.508055	0.771876	-0.094966
H	-1.744225	1.168267	1.311961
O	-3.262412	-0.343862	0.172596
O	-2.110872	-1.150450	-0.039244
Rotational constants (GHz): 2.0058600 0.8444100 0.8111700			
Vibrational harmonic frequencies (cm-1):			
-1589.5130	112.1469	173.0987	
193.8690	211.9385	238.0334	
274.3194	312.3489	361.6315	
386.3737	419.5635	424.8920	
459.0081	486.0690	576.0493	
611.5929	679.1225	731.1056	
801.8194	813.2953	851.3533	
862.1187	886.8911	896.3314	
932.9840	942.1316	958.5462	
968.6097	1010.5532	1016.3956	
1063.9885	1086.5643	1090.0104	
1124.5362	1155.1323	1201.3516	
1211.9143	1228.7617	1242.3812	
1250.0144	1283.7633	1293.5306	
1310.5460	1360.5450	1400.5812	
1404.9248	1424.4123	1444.5432	
1484.7749	1487.6985	1496.8138	
1503.9219	1514.4751	1519.0265	
1537.7494	1825.1573	3022.7187	
3023.6363	3028.8828	3052.8287	
3059.6552	3073.2309	3074.9777	
3082.8547	3089.7976	3096.5912	
3105.3446	3125.1160	3133.9524	
Zero-point correction (Hartree): 0.210751			

#### TS9a

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.76686709

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.135363	-0.486566	0.184003
C	-0.051861	-0.414449	-0.863219
C	-1.262280	0.151965	-0.221182
C	0.357476	1.908109	0.718351
C	1.326945	1.045550	-0.103282
C	0.703556	0.807313	-1.501361
C	2.296673	-1.326262	-0.364105
C	0.818923	-0.958789	1.602552
H	-0.292432	-1.298054	-1.446612
H	0.447517	2.949328	0.396867
H	0.633807	1.882667	1.775117
H	2.345993	1.436730	-0.049061
H	0.101632	1.609933	-1.934553
H	1.418847	0.469821	-2.248845

H	2.585216	-1.053711	-1.380739
H	2.030042	-2.386799	-0.364986
H	3.177408	-1.203850	0.274089
H	0.524158	-2.010128	1.587771
H	0.002415	-0.413288	2.075336
H	1.705149	-0.858990	2.238202
C	-1.112146	1.434831	0.546868
H	-1.733357	2.178423	0.031572
H	-1.610994	1.278429	1.508212
O	-2.120220	-1.661825	0.086941
O	-2.456193	-0.282015	-0.393706
Rotational constants (GHz):	1.5685300	1.0781100	0.8929500
Vibrational harmonic frequencies (cm <sup>-1</sup> ):			
-400.7046	88.1588		143.7058
173.3245	196.3544		221.0109
259.0001	302.4251		348.7813
383.1132	394.5896		417.0939
450.0622	463.4746		522.6492
603.3305	641.5945		757.4344
764.9232	779.4165		832.7306
851.9104	879.7280		909.7187
947.2970	959.3676		961.8609
996.0739	1013.6604		1037.9685
1063.0605	1096.5375		1122.3460
1160.5889	1201.8188		1204.1757
1226.8542	1231.5242		1248.2620
1266.4128	1284.0362		1296.8282
1309.8051	1343.6041		1373.9848
1407.7574	1426.5434		1439.7600
1481.7004	1485.8737		1502.0669
1503.8858	1511.3926		1517.0806
1523.6110	3023.4467		3025.2056
3031.3283	3043.6442		3055.0603
3060.6537	3063.3093		3082.0405
3084.5200	3098.6054		3103.4955
3120.5119	3126.7591		3151.8863
Zero-point correction (Hartree):	0.213238		

### TS9b

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 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.76602127  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.252406	-0.382946	0.248433
C	-0.128977	-0.766367	-0.448740
C	-1.202487	0.022122	0.207592
C	0.400522	2.004767	-0.085663
C	1.241945	0.871519	-0.690098
C	0.367076	0.056353	-1.681576
C	2.340549	-1.392937	-0.139497
C	1.286858	-0.195776	1.766996
H	-0.404049	-1.809972	-0.557708
H	0.322844	2.824572	-0.804615
H	0.900491	2.410912	0.797290
H	2.210566	1.239851	-1.037662
H	-0.394229	0.589875	-2.253020
H	0.946405	-0.559856	-2.365595
H	2.384677	-1.587724	-1.211841
H	2.173758	-2.348338	0.366241
H	3.321458	-1.018121	0.170350
H	1.125388	-1.155048	2.267638
H	0.534966	0.497488	2.146820
H	2.266696	0.178511	2.080605
C	-1.020014	1.507308	0.290014
H	-1.774050	1.896013	-0.408647
H	-1.359801	1.843539	1.274613
O	-2.697295	-1.202181	-0.440402

O	-2.238003	-0.466064	0.781748	
Rotational constants (GHz):	1.6501200	0.9731200	0.8812000	
Vibrational harmonic frequencies (cm <sup>-1</sup> ):				
-389.6622		85.2758		166.9613
188.4174		196.9153		219.2875
258.0742		274.9821		367.6829
384.6214		408.1570		419.5284
451.0731		468.2691		508.0700
586.2625		657.7511		752.8247
760.0991		785.7280		824.2281
851.4174		887.4595		920.0594
944.9598		956.5159		962.9929
992.9948		1014.5595		1048.3463
1066.1128		1090.6429		1119.7271
1155.7989		1193.8489		1206.4559
1224.7042		1233.7971		1254.0363
1261.5414		1286.1488		1301.1993
1308.2309		1346.2402		1373.6407
1406.2365		1425.3216		1436.8666
1486.1209		1487.6383		1503.8406
1505.5792		1514.6728		1521.6301
1526.8967		3010.1291		3023.2975
3028.9516		3042.9455		3058.4374
3061.5961		3072.7842		3078.7617
3080.3012		3084.8545		3107.5879
3109.9467		3134.8205		3164.2041
Zero-point correction (Hartree): 0.213325				

**TS10a**

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.76365808  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.303621	-0.399670	0.145274	
C	0.137651	-0.390628	-0.963041	
C	-1.128311	-0.223050	-0.201856	
C	0.062073	1.705871	0.920273	
C	1.207567	1.163417	0.051093	
C	0.688753	0.993997	-1.403101	
C	2.607385	-0.950071	-0.445450	
C	1.037733	-1.092442	1.481835	
H	0.090250	-1.224542	-1.662196	
H	0.013979	2.793240	0.818061	
H	0.260422	1.498199	1.974904	
H	2.134553	1.719961	0.210248	
H	-0.031881	1.723991	-1.774381	
H	1.486358	0.889150	-2.135126	
H	2.865943	-0.508168	-1.408427	
H	2.540585	-2.033365	-0.579675	
H	3.434413	-0.750474	0.243469	
H	0.981345	-2.175884	1.343208	
H	0.109981	-0.780463	1.961673	
H	1.858869	-0.889275	2.176643	
C	-1.312211	1.100386	0.495048	
H	-1.801899	1.778664	-0.206479	
H	-2.016835	0.964605	1.314868	
O	-3.101482	-0.539554	-0.357725	
O	-1.842474	-1.267007	0.013070	
Rotational constants (GHz):	1.8074300	0.9414700	0.8450500	
Vibrational harmonic frequencies (cm <sup>-1</sup> ):				
-419.5221		101.2948		164.7713
180.5188		202.5537		222.6305
298.7254		311.6026		361.7476
383.2967		404.8371		426.0803
456.1875		492.6748		547.6329
605.1129		638.0405		746.6737
771.8051		790.7266		816.9863

844.6705	892.6449	919.4335
936.7202	954.1911	968.0617
998.6696	1015.0795	1048.7771
1070.0763	1075.1091	1102.2688
1157.8807	1186.8100	1202.2460
1226.7640	1230.3050	1242.7296
1259.3851	1281.0386	1305.5108
1314.4568	1339.6692	1364.6128
1409.0505	1428.0868	1456.8810
1482.8829	1487.0267	1501.4808
1505.2243	1515.3836	1521.8957
1525.6984	3024.9033	3031.1207
3042.4981	3061.2697	3063.9302
3076.9935	3081.3582	3082.0406
3088.0653	3110.0541	3110.4875
3118.9893	3125.0398	3138.1185

Zero-point correction (Hartree): 0.213805

### TS10b

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.76390577  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.166527	-0.511367	0.151460
C	0.223400	-0.111063	-1.095330
C	-1.140634	0.080948	-0.545524
C	-0.007271	1.521388	1.191872
C	1.229589	1.032949	0.416150
C	0.987742	1.248158	-1.102920
C	2.502719	-1.075916	-0.348761
C	0.617312	-1.442178	1.231300
H	0.222497	-0.766382	-1.966617
H	0.078048	2.593737	1.386604
H	-0.060120	1.024976	2.163546
H	2.155974	1.413931	0.852850
H	0.437128	2.136576	-1.415549
H	1.897572	1.180771	-1.694221
H	2.988270	-0.457711	-1.104763
H	2.360390	-2.074953	-0.769713
H	3.192913	-1.168456	0.495690
H	0.592994	-2.470978	0.861044
H	-0.398795	-1.202141	1.539083
H	1.279498	-1.418445	2.103708
C	-1.306807	1.252823	0.386908
H	-1.480957	2.107416	-0.285421
H	-2.187995	1.133445	1.005702
O	-2.486656	-1.109112	0.385161
O	-2.102454	-0.641668	-0.995520

Rotational constants (GHz): 1.6732000 1.0243200 0.9047900  
 Vibrational harmonic frequencies (cm-1):

-406.7588	114.7402	152.3029
184.2974	212.6542	231.8835
296.2246	346.7574	384.0634
390.8718	401.9466	434.9028
458.7119	485.3715	544.2952
608.5441	647.7435	732.8682
756.8214	793.1700	817.8399
848.9824	898.9368	922.7025
946.2275	963.6096	973.2309
999.6359	1016.1340	1047.6399
1069.8987	1078.1251	1100.5886
1158.8133	1186.0603	1205.4151
1222.2700	1233.9910	1246.6887
1261.0994	1281.2836	1309.9564
1316.0429	1341.4428	1368.1641
1410.5439	1434.0644	1463.9480
1477.5396	1490.3686	1499.9625

1506.5170	1512.1363	1521.3173
1530.0581	2975.4885	3021.5110
3030.4832	3046.0732	3063.1655
3075.2824	3080.2338	3085.1544
3087.8029	3100.8994	3111.2816
3134.7242	3137.9705	3180.8788

Zero-point correction (Hartree): 0.214080

### TS11

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E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.75227547

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.961497	-0.595915	0.234407
C	-0.126148	-0.257852	-0.959272
C	-1.149893	0.406342	-0.252075
C	0.503787	1.913339	0.725849
C	1.409162	0.892502	0.000782
C	0.905406	0.774229	-1.461818
C	1.991296	-1.621762	-0.244941
C	0.458097	-1.014778	1.613627
H	-1.088381	-1.360355	-1.053844
H	0.862990	2.923501	0.514931
H	0.554168	1.776932	1.808361
H	2.466513	1.117065	0.180055
H	0.528524	1.682919	-1.938899
H	1.636712	0.320705	-2.128650
H	2.377836	-1.406922	-1.241248
H	1.543224	-2.618088	-0.268494
H	2.840747	-1.650267	0.447066
H	-0.044338	-1.982033	1.552998
H	-0.248261	-0.313272	2.059767
H	1.306090	-1.112439	2.299828
C	-0.994879	1.797876	0.248184
H	-1.173224	2.498863	-0.571881
H	-1.715255	2.027102	1.035074
O	-2.018207	-1.652391	-0.374159
O	-2.181455	-0.306059	0.108718

Rotational constants (GHz): 1.4568000 1.2331100 0.9339800

Vibrational harmonic frequencies (cm-1):

-1292.5706	135.1856	148.0091
176.1208	215.6515	235.2125
290.5763	302.3949	378.9110
385.6040	387.2888	432.2525
463.6500	498.3754	564.4285
624.0728	642.1219	682.4711
750.0659	802.1297	827.5495
851.8155	882.3892	889.2074
921.4171	945.4824	955.0406
984.9732	998.9605	1024.6189
1065.3482	1083.8633	1117.4390
1133.1236	1164.9627	1185.4441
1196.3115	1213.3075	1230.4375
1235.1036	1267.0258	1298.1554
1317.6482	1337.3818	1405.5279
1409.7532	1421.6588	1457.8942
1467.2275	1484.0033	1486.5163
1502.7460	1506.1232	1518.1317
1530.2868	1911.7937	3019.8565
3025.0738	3031.1118	3047.5082
3051.1737	3057.3771	3084.2896
3085.8545	3096.8875	3105.8572
3108.8085	3116.2566	3123.4349

Zero-point correction (Hartree): 0.210267

### TS12

-----  
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.79103231

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.247471	-0.309147	0.065357
C	0.037785	-0.353299	-0.931844
C	-1.288766	-0.347965	-0.166567
C	-0.104881	1.611410	1.090793
C	0.999816	1.242043	0.091977
C	0.379757	1.108301	-1.328616
C	2.568217	-0.666640	-0.631481
C	1.164030	-1.104492	1.371175
H	0.013806	-1.136385	-1.692077
H	-0.265918	2.693073	1.069686
H	0.216589	1.365038	2.106451
H	1.878655	1.880210	0.216809
H	-0.451436	1.767874	-1.588086
H	1.118004	1.157261	-2.126816
H	2.718050	-0.126616	-1.568024
H	2.604443	-1.737131	-0.855513
H	3.414573	-0.435374	0.023077
H	1.244677	-2.176102	1.166881
H	0.233927	-0.952879	1.922386
H	1.991123	-0.832724	2.035858
C	-1.442007	0.893876	0.761892
H	-2.120290	1.588844	0.258685
H	-1.965093	0.547873	1.654544
O	-2.412943	-0.422560	-0.978580
O	-1.587013	-1.583375	0.408582

Rotational constants (GHz): 1.6805400 1.0505300 0.9666100

Vibrational harmonic frequencies (cm-1):

-849.4995	84.8383	157.8268
190.0815	202.9934	229.9387
285.3844	287.7358	364.0907
382.0416	383.8520	411.7143
455.0299	481.5177	502.3166
579.8240	643.7983	692.4254
773.2974	820.5368	853.0105
882.0019	906.0384	934.1985
955.7570	956.5938	962.9284
1007.4387	1020.2090	1025.8011
1059.7796	1076.9627	1103.6659
1135.5523	1180.7683	1185.2066
1213.3668	1221.2623	1233.9850
1249.6600	1262.9619	1285.4858
1305.5551	1325.7254	1342.2324
1364.5358	1404.6299	1428.2975
1472.2886	1483.9968	1489.6237
1503.3586	1506.9349	1514.2864
1519.0359	3020.3172	3025.5463
3033.3846	3042.1938	3053.9068
3062.4525	3068.6925	3076.0578
3080.5459	3082.2359	3097.6700
3101.8675	3103.2339	3123.5790

Zero-point correction (Hartree): 0.212494

### TS13

CASSCF(4,4)/3-21G(d)

Final geometry

-----

C	-0.9344986284	1.2856925103	-0.8213474461
C	1.5630182230	1.6592082266	0.6862780734
C	1.2115583526	-0.4914970373	3.5152146830
C	-0.2203488260	-3.4573947321	-0.2171270944
C	0.3081681368	-1.1727895624	-1.9206081840
C	2.9492088267	-0.0098723421	-1.2575669873

C	-0.9881046957	3.4075682126	-2.8420555445
C	-3.5302801053	1.1730769503	0.4212845318
H	2.1795960209	3.4435399496	1.4063338895
H	0.5599657301	-5.1439409392	-1.0824165011
H	-2.2397979924	-3.7424532716	-0.0706060365
H	-0.0841790852	-1.5744563177	-3.8832480816
H	4.3931953506	-1.2329926862	-0.5256377977
H	3.7171618961	1.1275352521	-2.7687204142
H	0.7778469621	3.6097121208	-3.8497318272
H	-1.4444075086	5.2000548200	-1.9606913953
H	-2.4527815909	2.9695732069	-4.2068970978
H	-3.9616661840	2.9774441741	1.2882423841
H	-3.6479079709	-0.2340606718	1.8774906257
H	-4.9346607513	0.7914464532	-1.0241781386
C	0.9727635891	-3.1925959475	2.4633091385
H	2.8546954599	-3.9733388800	2.4385645344
H	-0.1401157612	-4.2722777585	3.7965244597
O	3.6914592954	0.3133350578	3.8236196694
O	-0.5999233499	0.5397032568	4.7095562091

Total Molecular Energy

electronic	vibrational	total	energy
-495.822992	0.229195	-495.593797	Hartrees
-108820568.37	50302.54	-108770265.83	cm-1
-1301783.08	601.75	-1301181.33	kJ/mol
-311133.62	143.82	-310989.80	kcal/mol

Rotational constants

A	B	C
1618.0723	1075.8548	1031.9928 MHz
0.053973	0.035887	0.034424 cm-1

Vibrational Frequencies and IR Intensities

mode	irrep	frequency	IR intensity		
		cm-1	hartrees	km/mol	(D/A)**2/amu
1	A	3416.15	0.015565	8.032	0.1901
2	A	3374.96	0.015377	3.617	0.0856
3	A	3367.62	0.015344	2.796	0.0662
4	A	3312.41	0.015092	9.011	0.2133
5	A	3295.47	0.015015	31.499	0.7455
6	A	3275.91	0.014926	21.255	0.5030
7	A	3267.38	0.014887	35.327	0.8361
8	A	3264.35	0.014873	10.839	0.2565
9	A	3261.70	0.014861	12.033	0.2848
10	A	3255.47	0.014833	0.959	0.0227
11	A	3252.06	0.014817	19.493	0.4613
12	A	3217.20	0.014659	26.831	0.6350
13	A	3208.25	0.014618	40.452	0.9574
14	A	3200.84	0.014584	9.586	0.2269
15	A	1686.81	0.007686	10.186	0.2411
16	A	1678.91	0.007650	12.890	0.3051
17	A	1669.60	0.007607	10.552	0.2497
18	A	1666.40	0.007593	9.082	0.2149
19	A	1655.22	0.007542	8.270	0.1957
20	A	1649.87	0.007517	6.582	0.1558
21	A	1640.02	0.007472	5.452	0.1290
22	A	1595.05	0.007268	14.345	0.3395
23	A	1569.32	0.007150	6.684	0.1582

24	A	1520.77	0.006929	0.379	0.0090
25	A	1502.26	0.006845	1.434	0.0339
26	A	1460.02	0.006652	1.225	0.0290
27	A	1440.38	0.006563	3.638	0.0861
28	A	1399.75	0.006378	1.246	0.0295
29	A	1380.39	0.006290	3.807	0.0901
30	A	1368.73	0.006236	2.685	0.0635
31	A	1341.90	0.006114	2.488	0.0589
32	A	1329.25	0.006057	15.553	0.3681
33	A	1324.39	0.006034	5.262	0.1245
34	A	1281.24	0.005838	16.758	0.3966
35	A	1258.25	0.005733	0.418	0.0099
36	A	1239.96	0.005650	66.580	1.5757
37	A	1194.32	0.005442	17.695	0.4188
38	A	1160.60	0.005288	4.890	0.1157
39	A	1133.59	0.005165	5.115	0.1210
40	A	1124.25	0.005122	8.697	0.2058
41	A	1118.91	0.005098	6.955	0.1646
42	A	1101.07	0.005017	0.433	0.0102
43	A	1066.25	0.004858	1.989	0.0471
44	A	1019.84	0.004647	6.602	0.1562
45	A	1002.63	0.004568	14.801	0.3503
46	A	960.55	0.004377	3.934	0.0931
47	A	935.64	0.004263	0.565	0.0134
48	A	905.05	0.004124	4.712	0.1115
49	A	863.28	0.003933	2.884	0.0682
50	A	854.48	0.003893	6.924	0.1639
51	A	790.32	0.003601	19.390	0.4589
52	A	716.52	0.003265	3.097	0.0733
53	A	667.10	0.003040	6.934	0.1641
54	A	577.55	0.002631	13.828	0.3273
55	A	575.43	0.002622	37.327	0.8834
56	A	482.48	0.002198	6.009	0.1422
57	A	472.49	0.002153	26.513	0.6275
58	A	451.83	0.002059	3.392	0.0803
59	A	418.62	0.001907	0.879	0.0208
60	A	393.48	0.001793	2.463	0.0583
61	A	363.45	0.001656	35.049	0.8295
62	A	339.04	0.001545	2.012	0.0476
63	A	285.51	0.001301	2.464	0.0583
64	A	265.65	0.001210	1.831	0.0433
65	A	241.97	0.001102	0.132	0.0031
66	A	216.76	0.000988	3.147	0.0745
67	A	173.86	0.000792	1.281	0.0303
68	A	104.31	0.000475	0.901	0.0213
69	A	1162.24i	0.005296i		

Printout of CI-coefficients larger than 0.05000 for root 1

(this is the reference state)

Printout of coefficients in interval 0.3162 to 1.000

```

=====
Coefficient of CSF no.      1 is 0.92512972
Occupation and spin coupling
    1  2
    2  2
Coefficient of CSF no.      2 is -0.35584473
Occupation and spin coupling
    1  3
    2  2
    
```

#### TS14

**CASSCF(4,4)/3-21G(d)**

Final geometry



```

-----
C      0.3609307428      -0.8617323334      -1.4741935670
C      0.1172554488      -2.1087273345      1.2213850580
C      1.3722019452      -0.5401109263      3.2938874520
C     -1.5348820145      3.0717713763      0.8077395185
C     -2.0830417781      0.6676261263      -0.7349618840
C     -2.7487958998      -1.5066468304      1.1429799487
C     -0.2923042757      -2.8192329638      -3.5273809253
C      2.8145930977      0.5241987764      -2.2426051992
H      0.7143936607      -4.0552132931      1.3779424253
H     -3.1998341959      3.5321350764      1.9018402658
H     -1.1555111239      4.6487676595      -0.4565008481
H     -3.4012626121      1.0769577592      -2.2402318794
H     -3.5854107343      -0.9637869297      2.9115121896
H     -3.8405659515      -2.9887728849      0.2708216138
H     -2.0155990901      -3.8417131271      -3.1285838540
H      1.2340893583      -4.1777973078      -3.6975333162
H     -0.5122396597      -1.8745333847      -5.3348793990
H      4.1891622135      0.4471849465      -0.7381883021
H      2.4431424484      2.4813176078      -2.7288384763
H      3.6491113888      -0.3577902313      -3.8915302145
C      0.7539680074      2.9169808368      2.5446789035
H      0.6032901115      3.9077909007      4.3011209015
H      2.5126569775      3.2479640312      1.6215409379
O     -0.1734849049      0.0755890217      5.3311501080
O      3.7781285305      -0.5022100265      3.4688304320
    
```

Total Molecular Energy

```

-----
electronic      vibrational      total      energy
-495.820140      0.229668      -495.590472      Hartrees
-108819942.37      50406.32      -108769536.05      cm-1
-1301775.59      602.99      -1301172.60      kJ/mol
-311131.83      144.12      -310987.71      kcal/mol
    
```

Rotational constants

```

-----
A      B      C
1667.1993      1075.1901      996.9985 MHz
0.055612      0.035864      0.033256 cm-1
    
```

Vibrational Frequencies and IR Intensities

```

-----
mode  irrep      frequency      IR intensity
-----
cm-1      hartrees      km/mol      (D/A)**2/amu
-----
1      A      3482.68      0.015868      2.298      0.0544
2      A      3383.28      0.015415      5.333      0.1262
3      A      3364.43      0.015329      5.700      0.1349
4      A      3313.97      0.015100      2.009      0.0476
5      A      3303.91      0.015054      45.773      1.0833
6      A      3279.23      0.014941      10.313      0.2441
7      A      3266.97      0.014885      12.251      0.2899
8      A      3264.41      0.014874      30.481      0.7214
9      A      3261.26      0.014859      18.808      0.4451
10     A      3249.87      0.014807      32.256      0.7634
11     A      3245.62      0.014788      13.845      0.3277
12     A      3204.27      0.014600      31.445      0.7442
    
```

13	A	3194.56	0.014555	21.124	0.4999
14	A	3183.65	0.014506	7.948	0.1881
15	A	1709.65	0.007790	13.443	0.3182
16	A	1681.26	0.007660	4.021	0.0952
17	A	1678.51	0.007648	15.094	0.3572
18	A	1674.63	0.007630	6.916	0.1637
19	A	1658.17	0.007555	2.265	0.0536
20	A	1648.29	0.007510	14.646	0.3466
21	A	1636.39	0.007456	0.429	0.0102
22	A	1588.28	0.007237	14.536	0.3440
23	A	1572.36	0.007164	8.714	0.2062
24	A	1521.62	0.006933	1.808	0.0428
25	A	1456.14	0.006635	3.216	0.0761
26	A	1439.35	0.006558	4.498	0.1064
27	A	1430.57	0.006518	5.457	0.1291
28	A	1407.34	0.006412	7.257	0.1717
29	A	1400.01	0.006379	1.643	0.0389
30	A	1373.74	0.006259	23.717	0.5613
31	A	1341.99	0.006115	0.980	0.0232
32	A	1338.22	0.006097	6.652	0.1574
33	A	1304.84	0.005945	15.777	0.3734
34	A	1297.37	0.005911	7.374	0.1745
35	A	1262.18	0.005751	3.406	0.0806
36	A	1234.44	0.005625	19.940	0.4719
37	A	1206.71	0.005498	3.671	0.0869
38	A	1178.49	0.005370	3.015	0.0714
39	A	1136.80	0.005180	6.048	0.1431
40	A	1133.52	0.005165	5.974	0.1414
41	A	1114.72	0.005079	25.302	0.5988
42	A	1082.32	0.004931	1.406	0.0333
43	A	1045.79	0.004765	1.937	0.0458
44	A	1044.88	0.004761	14.750	0.3491
45	A	1023.38	0.004663	5.004	0.1184
46	A	994.39	0.004531	1.930	0.0457
47	A	947.69	0.004318	6.860	0.1624
48	A	920.45	0.004194	0.476	0.0113
49	A	861.80	0.003927	6.131	0.1451
50	A	848.28	0.003865	2.054	0.0486
51	A	783.59	0.003570	23.089	0.5464
52	A	681.91	0.003107	0.523	0.0124
53	A	667.39	0.003041	2.634	0.0623
54	A	627.15	0.002857	26.353	0.6237
55	A	550.88	0.002510	0.340	0.0081
56	A	513.02	0.002337	42.844	1.0139
57	A	489.69	0.002231	7.334	0.1736
58	A	443.79	0.002022	2.821	0.0668
59	A	420.68	0.001917	2.690	0.0637
60	A	393.95	0.001795	24.730	0.5853
61	A	379.75	0.001730	3.740	0.0885
62	A	320.45	0.001460	2.653	0.0628
63	A	295.46	0.001346	0.279	0.0066
64	A	270.72	0.001233	0.223	0.0053
65	A	242.32	0.001104	0.868	0.0205
66	A	226.30	0.001031	1.334	0.0316
67	A	160.46	0.000731	1.993	0.0472
68	A	152.47	0.000695	2.962	0.0701
69	A	1341.45i	0.006112i		

Printout of CI-coefficients larger than 0.05000 for root 1

(this is the reference state)

Printout of coefficients in interval 0.3162 to 1.000

=====

Coefficient of CSF no. 1 is 0.92029299

Occupation and spin coupling

1	2
2	2

Coefficient of CSF no. 2 is -0.36831083  
 Occupation and spin coupling  
     1    3  
     2    2

=====

**DIO**

**CASSCF(4,4)/3-21G(d)**

Final geometry

-----

C	0.6352544511	-1.2006679770	-1.1738910861
C	-0.6708438629	-1.6048589803	1.4594987603
C	0.2208915754	0.4398513132	3.1972293478
C	-0.8192975365	3.3608779515	-0.5318976161
C	-1.5063685545	0.7878372017	-1.6932142700
C	-3.1973821150	-0.6942158487	0.2285022402
C	0.3492642810	-3.5436810080	-2.8629602707
C	3.4000569842	-0.3465597579	-1.2263780454
H	-0.5527044897	-3.4339982668	2.3463947937
H	-2.3564672180	4.6773011881	-0.8480964561
H	0.8336094895	4.1222812887	-1.4654189536
H	-2.1561078608	0.9672468847	-3.6206548351
H	-4.4667841457	0.3996791838	1.3954810104
H	-4.2231386674	-2.2276896217	-0.6347863873
H	-1.5712329652	-4.2436107658	-2.9130087820
H	1.5615748048	-5.0510788303	-2.1830316992
H	0.9102261354	-3.0861704745	-4.7820938545
H	4.6085202612	-1.8772855417	-0.5961166448
H	3.7708615481	1.2635069728	-0.0272190608
H	3.9339270519	0.1468000905	-3.1444000083
C	-0.3496541870	3.1271224732	2.3677987935
H	-2.0293890927	3.7076174865	3.3802357034
H	1.1788952851	4.3302812717	2.9915822608
O	-0.1132478410	-0.0218025089	5.9532020267
O	2.6095366687	0.0012162752	4.3832430334

Total Molecular Energy

-----

electronic	vibrational	total	energy
-495.879923	0.231342	-495.648580	Hartrees
-108833063.24	50773.77	-108782289.46	cm-1
-1301932.55	607.39	-1301325.16	kJ/mol
-311169.35	145.17	-311024.18	kcal/mol

Rotational constants

-----

A	B	C
1689.0847	1046.6813	947.2671 MHz
0.056342	0.034914	0.031597 cm-1

Vibrational Frequencies and IR Intensities

-----

mode	irrep	frequency	IR intensity		
		cm-1	hartrees	km/mol	(D/A)**2/amu
1	A	3325.88	0.015154	25.250	0.5976
2	A	3307.81	0.015072	8.231	0.1948
3	A	3295.44	0.015015	20.546	0.4862
4	A	3292.46	0.015002	17.085	0.4043
5	A	3275.94	0.014926	38.440	0.9097

6	A	3268.78	0.014894	33.894	0.8021
7	A	3260.45	0.014856	29.678	0.7024
8	A	3258.04	0.014845	12.113	0.2867
9	A	3254.34	0.014828	29.777	0.7047
10	A	3246.27	0.014791	7.372	0.1745
11	A	3244.79	0.014784	3.214	0.0761
12	A	3222.31	0.014682	25.485	0.6031
13	A	3202.37	0.014591	32.465	0.7683
14	A	3194.61	0.014556	16.179	0.3829
15	A	1689.01	0.007696	7.124	0.1686
16	A	1682.75	0.007667	10.575	0.2503
17	A	1670.19	0.007610	7.631	0.1806
18	A	1667.74	0.007599	9.832	0.2327
19	A	1660.09	0.007564	3.991	0.0945
20	A	1653.32	0.007533	2.380	0.0563
21	A	1638.27	0.007465	7.940	0.1879
22	A	1589.67	0.007243	9.117	0.2158
23	A	1569.81	0.007153	9.544	0.2259
24	A	1522.20	0.006936	11.468	0.2714
25	A	1500.56	0.006837	8.693	0.2057
26	A	1470.82	0.006702	5.997	0.1419
27	A	1451.90	0.006615	1.535	0.0363
28	A	1416.53	0.006454	1.855	0.0439
29	A	1402.03	0.006388	1.915	0.0453
30	A	1383.79	0.006305	4.527	0.1071
31	A	1379.11	0.006284	9.162	0.2168
32	A	1347.34	0.006139	7.389	0.1749
33	A	1341.49	0.006112	4.388	0.1038
34	A	1334.52	0.006081	4.904	0.1161
35	A	1293.51	0.005894	3.666	0.0868
36	A	1267.18	0.005774	20.281	0.4800
37	A	1245.38	0.005674	4.686	0.1109
38	A	1199.71	0.005466	2.566	0.0607
39	A	1151.83	0.005248	6.362	0.1506
40	A	1145.53	0.005219	0.607	0.0144
41	A	1116.77	0.005088	1.884	0.0446
42	A	1103.98	0.005030	0.538	0.0127
43	A	1054.91	0.004807	0.709	0.0168
44	A	1036.92	0.004725	2.976	0.0704
45	A	1015.95	0.004629	4.355	0.1031
46	A	986.04	0.004493	0.843	0.0200
47	A	956.10	0.004356	4.666	0.1104
48	A	943.29	0.004298	2.816	0.0666
49	A	881.66	0.004017	2.357	0.0558
50	A	870.62	0.003967	1.657	0.0392
51	A	825.90	0.003763	1.392	0.0330
52	A	779.75	0.003553	0.860	0.0204
53	A	696.63	0.003174	0.310	0.0073
54	A	662.46	0.003018	1.242	0.0294
55	A	601.61	0.002741	3.822	0.0905
56	A	535.95	0.002442	0.469	0.0111
57	A	489.62	0.002231	4.351	0.1030
58	A	456.72	0.002081	0.455	0.0108
59	A	428.78	0.001954	3.076	0.0728
60	A	407.28	0.001856	4.168	0.0986
61	A	401.92	0.001831	0.745	0.0176
62	A	376.67	0.001716	3.233	0.0765
63	A	322.61	0.001470	2.112	0.0500
64	A	307.49	0.001401	0.855	0.0202
65	A	250.65	0.001142	0.078	0.0018
66	A	232.30	0.001058	1.077	0.0255
67	A	209.36	0.000954	0.408	0.0097
68	A	166.16	0.000757	0.603	0.0143
69	A	105.63	0.000481	3.006	0.0711

Printout of CI-coefficients larger than 0.05000 for root 1

(this is the reference state)

```

Printout of coefficients in interval 0.3162 to 1.000
=====
Coefficient of CSF no.      1 is -0.94614911
Occupation and spin coupling
    1  2
    2  2
Printout of coefficients in interval 0.1000 to 0.3162
=====
Coefficient of CSF no.      2 is 0.28576636
Occupation and spin coupling
    1  3
    2  2
Coefficient of CSF no.      5 is 0.11703516
Occupation and spin coupling
    2  4
    2  2
    
```

=====  
**SB (Singlet Biradical)**

**CASSCF(4,4)/3-21G(d)**

Final geometry

```

-----
C      0.4338568455      -1.1027947113      -1.3377360316
C     -0.0007825338      -1.7138365448       1.5268260271
C      1.0988383795       0.3405370372       3.2271045107
C     -1.2038726852       3.2414535779      -0.0800594111
C     -1.9509417339       0.6398129041      -1.1066128520
C     -2.8445907947      -1.0384524171       1.1540035196
C     -0.1314808283      -3.4492199752      -2.9581757164
C      2.9308404585       0.0481032587      -2.2363330405
H      0.5096747741      -3.5713369339       2.1991794843
H     -2.8984880439       4.3528668910       0.2202550892
H     -0.0667993682       4.2314571913      -1.4623808461
H     -3.1577609204       0.7884497351      -2.7475181091
H     -3.7505876778      -0.1014350975       2.7211400748
H     -3.9581172743      -2.6411655706       0.5701889292
H     -1.8892091643      -4.3567893705      -2.4414290046
H      1.3798959556      -4.8206514170      -2.7562037411
H     -0.2483822084      -2.9130164493      -4.9341557994
H      4.4371576549      -1.3297361037      -2.0595160742
H      3.4884315438       1.6925770215      -1.1762382816
H      2.7593152020       0.5641642326      -4.2146390002
C      0.2579698003       3.0599947705       2.4819201232
H     -0.9402945885       3.7357445325       3.9896954347
H      1.9170507899       4.2512549802       2.4401060552
O      0.0616805691      -0.1003835928       5.7712451292
O      3.7665958486       0.1924020512       3.2093335307
    
```

Total Molecular Energy

```

-----
          electronic      vibrational      total      energy
          -495.861652      0.230654      -495.630998      Hartrees
          -108829053.26      50622.76      -108778430.50      cm-1
          -1301884.58      605.58      -1301279.00      kJ/mol
          -311157.88      144.74      -311013.15      kcal/mol
    
```

Rotational constants

```

-----
          A          B          C
          1651.1744      1052.0441      996.7914 MHz
          0.055077      0.035092      0.033249 cm-1
    
```

Vibrational Frequencies and IR Intensities

mode	irrep	frequency		IR intensity	
		cm-1	hartrees	km/mol	(D/A)**2/amu
1	A	3336.88	0.015204	20.461	0.4842
2	A	3332.58	0.015184	16.271	0.3851
3	A	3298.02	0.015027	16.819	0.3980
4	A	3287.60	0.014979	28.489	0.6742
5	A	3277.03	0.014931	21.258	0.5031
6	A	3270.41	0.014901	18.164	0.4299
7	A	3262.10	0.014863	37.878	0.8964
8	A	3256.66	0.014838	10.367	0.2453
9	A	3254.06	0.014827	20.350	0.4816
10	A	3253.14	0.014822	28.576	0.6763
11	A	3243.95	0.014781	1.864	0.0441
12	A	3219.79	0.014670	24.415	0.5778
13	A	3202.37	0.014591	42.051	0.9952
14	A	3194.32	0.014554	13.968	0.3306
15	A	1686.76	0.007685	8.053	0.1906
16	A	1683.00	0.007668	9.271	0.2194
17	A	1670.88	0.007613	10.697	0.2532
18	A	1668.61	0.007603	8.813	0.2086
19	A	1659.96	0.007563	2.763	0.0654
20	A	1652.89	0.007531	1.419	0.0336
21	A	1640.73	0.007476	8.718	0.2063
22	A	1591.59	0.007252	8.331	0.1972
23	A	1570.62	0.007156	8.853	0.2095
24	A	1523.55	0.006942	2.532	0.0599
25	A	1503.63	0.006851	2.835	0.0671
26	A	1466.87	0.006684	0.748	0.0177
27	A	1454.95	0.006629	3.121	0.0739
28	A	1425.33	0.006494	0.381	0.0090
29	A	1411.65	0.006432	0.316	0.0075
30	A	1394.66	0.006355	14.114	0.3340
31	A	1375.37	0.006267	3.924	0.0929
32	A	1343.86	0.006123	0.980	0.0232
33	A	1341.56	0.006113	0.089	0.0021
34	A	1295.89	0.005905	4.130	0.0977
35	A	1270.29	0.005788	6.243	0.1478
36	A	1253.45	0.005711	1.243	0.0294
37	A	1217.61	0.005548	6.275	0.1485
38	A	1174.31	0.005351	3.039	0.0719
39	A	1146.71	0.005225	1.452	0.0344
40	A	1111.13	0.005063	3.962	0.0938
41	A	1103.01	0.005026	2.721	0.0644
42	A	1073.14	0.004890	8.169	0.1933
43	A	1055.00	0.004807	7.252	0.1716
44	A	1027.15	0.004680	5.042	0.1193
45	A	1014.37	0.004622	10.655	0.2522
46	A	995.03	0.004534	1.496	0.0354
47	A	968.64	0.004413	1.063	0.0252
48	A	923.79	0.004209	0.899	0.0213
49	A	910.71	0.004149	6.391	0.1513
50	A	869.96	0.003964	1.646	0.0389
51	A	830.87	0.003786	0.931	0.0220
52	A	783.11	0.003568	0.641	0.0152
53	A	683.57	0.003115	0.158	0.0037
54	A	638.56	0.002910	0.780	0.0185
55	A	580.71	0.002646	6.185	0.1464
56	A	530.08	0.002415	0.164	0.0039
57	A	481.00	0.002192	3.757	0.0889
58	A	452.13	0.002060	1.180	0.0279
59	A	417.18	0.001901	2.980	0.0705
60	A	403.26	0.001837	1.646	0.0389
61	A	383.87	0.001749	6.362	0.1506

62	A	349.82	0.001594	7.215	0.1707
63	A	315.08	0.001436	0.465	0.0110
64	A	291.16	0.001327	0.131	0.0031
65	A	248.60	0.001133	0.064	0.0015
66	A	234.68	0.001069	1.062	0.0251
67	A	208.95	0.000952	0.257	0.0061
68	A	174.75	0.000796	0.738	0.0175
69	A	72.61	0.000331	1.002	0.0237

Printout of CI-coefficients larger than 0.05000 for root 1

(this is the reference state)

Printout of coefficients in interval 0.3162 to 1.000

=====

Coefficient of CSF no. 1 is 0.73573246

Occupation and spin coupling

1 2

2 2

Coefficient of CSF no. 2 is -0.66440043

Occupation and spin coupling

1 3

2 2

### TS15

-----

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.81537143

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.167084	-0.384402	0.092949
C	-0.073895	-0.632850	-0.807109
C	-1.623775	-0.798519	-0.140848
C	0.273311	2.019717	0.663362
C	1.086493	1.115342	-0.346362
C	0.239560	0.665827	-1.562728
C	2.422217	-1.029995	-0.540245
C	1.135076	-0.737615	1.575345
H	-0.086902	-1.564006	-1.377017
H	0.249185	3.013868	0.196718
H	0.820663	2.064376	1.606499
H	2.030615	1.631334	-0.534536
H	-0.608243	1.273776	-1.876700
H	0.873616	0.491589	-2.435562
H	2.527675	-0.797367	-1.601896
H	2.368136	-2.116838	-0.438269
H	3.326315	-0.686948	-0.027923
H	1.182162	-1.819971	1.709353
H	0.209831	-0.415677	2.053856
H	1.990682	-0.292686	2.095997
C	-1.092291	1.560646	0.850166
H	-1.854654	1.745123	0.106713
H	-1.429286	1.113798	1.777220
O	-2.483804	-0.230063	-0.817224
O	-1.616505	-1.558597	0.822020

Rotational constants (GHz): 1.4680200 1.0435500 0.9197500

Vibrational harmonic frequencies (cm-1):

-243.4746	89.8584	118.0509
148.0197	195.0389	203.4637
216.1989	239.9465	271.3366
314.3477	333.6007	356.7025
370.1500	416.6542	460.3185
470.4545	548.3383	567.3440
651.6072	694.7802	764.9795
813.0827	842.9052	871.2070
919.3257	925.4832	957.6918

983.2950	998.2877	1016.6558
1019.2041	1043.7893	1068.0075
1121.3170	1133.9098	1157.9389
1169.4109	1183.7555	1207.4422
1230.7291	1255.1472	1270.6172
1291.4910	1306.7112	1343.4648
1400.5295	1422.2673	1463.1424
1476.7076	1485.2061	1490.6157
1503.0119	1507.0224	1528.6273
1747.0871	2995.7756	3020.1351
3026.6710	3053.2913	3069.1479
3076.1647	3088.3413	3093.0321
3097.7237	3103.5485	3112.7412
3117.7755	3170.8492	3279.1554

Zero-point correction (Hartree): 0.209342

### TS16

-----  
 E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.84263511

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.355832	0.381268	-0.103556
C	1.074545	-0.045234	1.291366
C	-1.914305	0.338036	0.304964
C	-0.559212	-1.050359	-1.374494
C	0.760732	-1.031510	-0.564774
C	0.703536	-1.388635	0.952447
C	2.912715	0.316299	-0.230310
C	0.861679	1.718450	-0.645698
H	1.178054	0.466613	2.242769
H	-0.598647	-2.001977	-1.914737
H	-0.482760	-0.275078	-2.144048
H	1.511186	-1.594052	-1.123932
H	-0.397625	-1.199781	1.311578
H	1.091136	-2.287051	1.429001
H	3.329509	-0.619672	0.147725
H	3.378917	1.147988	0.302719
H	3.165703	0.401077	-1.290223
H	1.359376	2.537533	-0.117750
H	-0.211800	1.852529	-0.534785
H	1.119788	1.804072	-1.705444
C	-1.910995	-0.884945	-0.634396
H	-2.127512	-1.788786	-0.057650
H	-2.695700	-0.761872	-1.382402
O	-2.371656	1.407190	-0.072931
O	-1.294192	0.117590	1.430916

Rotational constants (GHz): 1.7462600 0.9215400 0.8661200

Vibrational harmonic frequencies (cm-1):

-982.8960	112.2031	115.4687
155.8194	185.2730	195.8702
229.4644	266.9371	283.1459
296.0900	356.4643	392.5376
414.4508	447.2626	479.9777
603.2315	621.8822	648.9457
746.4864	757.4000	827.5696
856.7893	867.7858	884.7225
906.5864	928.6612	961.2867
977.0581	1006.8394	1011.8415
1044.1439	1086.0820	1116.2619
1127.4043	1168.4790	1185.2758
1198.7874	1228.9861	1245.6197
1289.9908	1295.2106	1328.4292
1346.1057	1363.6526	1372.0834
1391.4290	1402.9160	1433.8432
1482.7291	1485.5402	1490.8437
1493.8114	1503.4972	1520.8746
1706.8271	2128.5242	3023.9417



3028.0525	3031.5213	3039.8815
3057.4520	3067.3670	3084.4258
3100.8857	3103.9982	3108.2721
3126.1136	3151.5958	3194.0045

Zero-point correction (Hartree): 0.209803

**TS17**

-----  
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.82396482  
Electronic state : 1-A  
Cartesian coordinates (Angs):

C	-1.597632	0.178953	-0.180675
C	-0.430334	-0.231623	-1.016206
C	2.237956	0.148243	-0.316672
C	0.202932	-0.050141	1.691918
C	-0.896265	-0.764035	0.900735
C	-0.221151	-1.510667	-0.312149
C	-2.903136	-0.505787	-0.693731
C	-1.938615	1.647740	0.085048
H	0.143655	0.279275	-1.782360
H	0.826487	-0.804766	2.179518
H	-0.247700	0.554833	2.489055
H	-1.581022	-1.350601	1.518422
H	0.806941	-1.860551	-0.216523
H	-0.856899	-2.321352	-0.679757
H	-2.773516	-1.558645	-0.938909
H	-3.274051	0.011725	-1.581353
H	-3.660148	-0.425377	0.090085
H	-2.848431	1.707347	0.687875
H	-2.135037	2.165131	-0.858652
H	-1.158956	2.190762	0.610531
C	1.086571	0.824094	0.810718
H	1.924921	1.202840	1.405167
H	0.609713	1.704475	0.395058
O	2.639295	-0.949202	0.052412
O	2.483466	0.959733	-1.193921

Rotational constants (GHz): 1.9453500 0.7808000 0.7559500  
Vibrational harmonic frequencies (cm-1):

-247.8142	82.9123	101.8515
122.5398	173.7125	213.6812
221.1171	243.6867	268.6759
315.0769	372.6440	379.0952
408.0607	430.5892	462.6399
517.3753	595.0608	603.8818
680.3823	711.9035	766.9822
807.5515	816.9467	874.8040
898.7106	933.6998	950.6773
970.1921	982.3081	1006.8219
1013.9822	1069.9167	1073.7448
1098.9857	1145.8789	1151.3423
1167.2212	1211.9690	1232.3570
1258.1129	1275.8475	1287.8558
1317.2754	1344.8200	1359.4020
1397.8130	1421.8727	1450.8458
1465.4453	1482.1611	1487.7866
1491.7422	1508.2737	1519.0053
1846.2700	3008.3651	3036.2233
3039.9781	3042.5450	3043.6047
3063.7191	3069.7059	3091.6670
3097.1385	3105.3360	3135.8174
3155.8672	3176.6708	3188.3242

Zero-point correction (Hartree): 0.210157

**TS18**

-----  
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -501.82188139

Electronic state : 1-A

Cartesian coordinates (Angs):

C	2.016223	0.438926	0.133003
C	2.998443	-0.724315	0.255039
C	-3.260010	0.157982	-0.006266
C	-0.304755	-0.984780	-0.059942
C	1.082334	-0.628729	-0.613086
C	2.207531	-1.614848	-0.346413
C	2.491872	1.580651	-0.771489
C	1.519286	0.981862	1.476037
H	3.999804	-0.773591	0.670852
H	-0.245669	-1.147447	1.020416
H	-0.603695	-1.944099	-0.498906
H	0.978712	-0.380352	-1.676535
H	-2.228572	-0.786091	0.277185
H	2.316376	-2.665259	-0.593815
H	2.854010	1.200548	-1.730526
H	3.310679	2.133304	-0.299489
H	1.682857	2.291208	-0.969195
H	0.708440	1.705296	1.346991
H	2.335939	1.498689	1.990100
H	1.171752	0.186237	2.138416
C	-1.373279	0.100282	-0.396986
H	-1.455037	0.216356	-1.477220
H	-1.110304	1.051933	0.059834
O	-3.444440	-0.925264	0.616659
O	-3.803206	1.121649	-0.401345

Rotational constants (GHz): 2.1434800 0.4877800 0.4484800

Vibrational harmonic frequencies (cm-1):

-2045.8885	37.6122	45.5333
66.5901	125.5550	154.7970
209.7020	229.5639	247.8647
268.7603	280.2652	349.4251
353.7804	378.5263	435.7579
485.8601	562.0787	595.0287
625.2010	652.0754	728.5254
747.2280	772.7047	859.8317
883.9470	940.7882	947.8188
952.3685	969.3662	991.1738
1010.9542	1048.9398	1076.5751
1113.5622	1139.4198	1172.8220
1187.0669	1205.5683	1236.8094
1251.5844	1293.7894	1306.1747
1319.0970	1344.1666	1374.9992
1400.7884	1419.6944	1455.9021
1482.6690	1487.9732	1495.8989
1504.5376	1513.6710	1639.4194
1833.8504	2096.5982	3008.8666
3016.0192	3017.5725	3024.0995
3061.7776	3074.5095	3078.7169
3082.3466	3087.9942	3100.4394
3151.0745	3155.2338	3187.8541

Zero-point correction (Hartree): 0.205848

**TS19**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.75730869

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.504928	-0.529481	0.203543
C	-0.138089	0.175542	-1.348753
C	-1.200160	0.111944	-0.476075
C	0.164783	1.407500	1.235883
C	1.307748	0.984759	0.292795
C	0.870085	1.292318	-1.147132
C	2.670665	-1.034390	-0.597059
C	1.063991	-1.449309	1.300402

H	-0.186157	-0.399775	-2.266438
H	0.153743	2.499848	1.269888
H	0.374757	1.073304	2.254728
H	2.228518	1.503192	0.599649
H	0.444517	2.295006	-1.276556
H	1.693285	1.202022	-1.854886
H	2.904404	-0.421207	-1.468184
H	2.510321	-2.062711	-0.932439
H	3.574919	-1.046631	0.034580
H	1.034586	-2.484712	0.950968
H	0.085446	-1.204607	1.712202
H	1.783026	-1.417478	2.136452
C	-1.238428	0.888248	0.799264
H	-1.945912	1.717175	0.683930
H	-1.702992	0.243052	1.548654
O	-3.193229	-0.827235	0.138638
O	-2.179972	-0.745171	-0.759857
Rotational constants (GHz): 1.7142900 0.8265900 0.7908000			
Vibrational harmonic frequencies (cm-1):			
-399.4928	75.2825	97.8351	
131.0913	144.3403	159.8080	
213.7138	259.9755	279.5811	
315.7837	367.6621	396.6859	
406.1037	452.6417	477.6161	
568.7060	601.8466	683.8842	
772.1600	805.9634	813.9215	
842.2408	911.1222	930.1708	
934.9813	967.2158	976.5635	
987.8564	1010.5554	1037.7751	
1047.9663	1075.0331	1085.5567	
1137.4574	1166.9351	1196.8567	
1219.7051	1239.3413	1261.4120	
1286.5158	1305.3900	1329.4504	
1341.1615	1368.3209	1392.9246	
1397.8391	1412.8089	1464.1456	
1470.4107	1477.1222	1488.3341	
1495.9033	1508.0451	1518.1826	
1544.7403	2947.8530	2952.7808	
2970.1065	3012.2352	3031.5565	
3049.9055	3057.1781	3065.6218	
3069.2561	3085.3237	3105.1886	
3116.2295	3124.2683	3178.7120	
Zero-point correction (Hartree): 0.211006			

## TS20

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 E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.75633545  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.374352	-0.557334	0.295609
C	-0.474576	-0.169735	-1.181421
C	-1.292911	0.305630	-0.197894
C	0.540032	1.846717	0.638806
C	1.381975	0.883469	-0.220169
C	0.685567	0.719263	-1.586367
C	2.275679	-1.544859	-0.382481
C	1.002199	-0.888387	1.706024
H	-0.748618	-1.076388	-1.702645
H	0.769739	2.869429	0.329971
H	0.832802	1.768788	1.687852
H	2.406972	1.277175	-0.293232
H	0.377555	1.672536	-2.033926
H	1.324279	0.219701	-2.313987
H	2.419985	-1.345357	-1.445083
H	1.906198	-2.567415	-0.269403
H	3.274525	-1.516314	0.085178
H	0.923194	-1.968734	1.844172

H	0.054719	-0.442390	2.016501	
H	1.770701	-0.525675	2.408872	
C	-0.999000	1.607378	0.490785	
H	-1.432751	2.424079	-0.096566	
H	-1.503491	1.624314	1.458849	
O	-2.579078	-1.591676	-0.193805	
O	-2.337887	-0.361651	0.312067	
Rotational constants (GHz):	1.4766300	0.9631700	0.8296900	
Vibrational harmonic frequencies (cm-1):				
-332.4145	71.1861		96.8723	
128.2908	150.2760		154.3095	
220.6829	266.3988		284.1555	
305.6767	364.0056		380.5947	
413.1823	443.9181		503.7315	
568.8609	598.4443		708.5708	
777.3432	805.9334		826.6847	
837.4031	915.2356		921.5591	
931.2304	961.3276		976.0190	
992.7975	1019.4316		1027.4501	
1037.4430	1066.3431		1081.2209	
1136.8846	1160.1463		1201.0830	
1217.3973	1251.7695		1268.0681	
1287.3499	1298.3651		1330.4791	
1338.6140	1359.0381		1384.3851	
1398.6741	1412.2908		1467.7964	
1478.4476	1482.3968		1486.9859	
1494.2804	1506.5168		1518.1834	
1533.3207	2946.9448		2953.9893	
2968.4472	3009.3514		3024.0657	
3052.9807	3059.3189		3064.0653	
3078.3372	3094.3823		3099.4741	
3105.6153	3114.4901		3217.3600	
Zero-point correction (Hartree):	0.211045			

### TS21

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 E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.77897569  
 Electronic state : 1-A  
 Cartesian coordinates (Angs):

C	1.484880	-0.202957	0.092441	
C	0.169078	-0.868114	-0.466083	
C	-1.009444	-0.530397	0.431338	
C	-0.099849	1.799339	0.336941	
C	0.937545	1.115300	-0.570691	
C	0.181991	0.213952	-1.591466	
C	2.736386	-0.728940	-0.624255	
C	1.750687	-0.232438	1.599863	
H	0.172837	-1.927474	-0.724364	
H	-0.604357	2.615658	-0.198121	
H	0.369069	2.281299	1.208356	
H	1.670676	1.832809	-0.947564	
H	-0.797302	0.544509	-1.937387	
H	0.798390	-0.066883	-2.443847	
H	2.638643	-0.739503	-1.710638	
H	2.957382	-1.750743	-0.301067	
H	3.603230	-0.108103	-0.375513	
H	1.984036	-1.252984	1.919381	
H	0.906973	0.106258	2.202888	
H	2.613589	0.394675	1.847444	
O	-1.967978	-1.314405	0.640808	
C	-1.122416	0.823272	0.807471	
H	-1.981715	1.128429	1.389712	
O	-3.102508	-0.080231	-0.519414	
H	-3.940713	-0.234954	-0.993783	
Rotational constants (GHz):	1.9306500	0.8466700	0.8296300	
Vibrational harmonic frequencies (cm-1):				
-433.1361	93.3067		115.7493	

183.5778	199.7091	222.6732
234.6014	293.3938	320.3343
336.0066	361.1845	388.0308
423.4079	443.6953	468.8119
498.7184	597.0008	628.5315
688.8641	757.6548	790.2895
835.4882	842.8670	854.4295
889.6378	916.8371	942.3688
956.9016	968.1027	973.4601
1018.4960	1061.9299	1068.3906
1089.8994	1123.0178	1155.6948
1198.7237	1210.4179	1231.7651
1248.6779	1256.6376	1286.0042
1298.6832	1316.4042	1366.6584
1404.4892	1413.4421	1423.2599
1452.6039	1486.5907	1490.5409
1502.5018	1507.5599	1513.7616
1519.8202	2982.3367	3008.8729
3019.4928	3025.4748	3059.0496
3073.3410	3076.2555	3079.9421
3096.1179	3103.3398	3108.3290
3132.3910	3220.4483	3671.9750

Zero-point correction (Hartree): 0.210797

## Stationary points on triplet PES

### Triplet Biradical

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.80286294

Electronic state : 3-A

Cartesian coordinates (Angs):

C	1.232042	-0.280500	0.060626
C	0.048958	-0.312648	-0.965012
C	-1.360635	-0.411632	-0.156005
C	-0.168239	1.550741	1.164864
C	0.943296	1.260010	0.148108
C	0.326142	1.171395	-1.278692
C	2.553884	-0.581611	-0.670420
C	1.188223	-1.126691	1.332312
H	0.028543	-1.072942	-1.744045
H	-0.343108	2.629736	1.214513
H	0.154907	1.245123	2.163387
H	1.807515	1.912096	0.298195
H	-0.529413	1.806094	-1.510813
H	1.061374	1.285483	-2.074609
H	2.683244	0.001023	-1.583500
H	2.609908	-1.640947	-0.936902
H	3.397633	-0.358105	-0.010037
H	1.276779	-2.187815	1.086404
H	0.268912	-1.005976	1.906102
H	2.027739	-0.862355	1.984419
C	-1.496209	0.855790	0.777438
H	-2.133729	1.549379	0.229246
H	-2.051674	0.524802	1.655550
O	-2.274624	-0.454888	-1.120803
O	-1.458300	-1.616952	0.476151

Rotational constants (GHz): 1.6433100 1.0677000 0.9938900

Vibrational harmonic frequencies (cm-1):

102.5072	170.0186	197.5138
207.4968	224.4215	266.4786
303.6597	324.8700	366.5363
376.8880	391.3176	421.3327
448.5291	462.0957	527.3298
582.0499	585.5599	658.6582
707.9981	801.3904	820.4660
863.5166	877.4204	907.6585
951.6725	962.9184	965.3275
972.5865	1007.8758	1020.8366
1042.0363	1086.8353	1097.4896
1118.3291	1139.3150	1159.2148
1209.2175	1223.1078	1228.6529
1239.0301	1247.3775	1258.1345
1288.2970	1318.3073	1334.7164
1368.2723	1402.7823	1428.5047
1477.3183	1482.0121	1486.3181
1501.5030	1505.1139	1510.6685
1519.3742	3023.2468	3028.5322
3035.2719	3058.8062	3066.8603
3072.3027	3078.2775	3082.1233
3088.9793	3108.2962	3111.3364
3115.0017	3119.7002	3124.1735

Zero-point correction (Hartree): 0.212466

### Int1-T-B3LYP

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.83626097

Electronic state : 3-A

Cartesian coordinates (Angs):

C	2.203907	-0.230757	0.074233
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C	2.574238	0.984026	-0.742954
C	-3.020417	-0.082262	0.049734
C	-0.488176	-0.280622	0.097358
C	0.810218	0.484244	0.332623
C	1.208298	1.597739	-0.692335
C	3.038275	-0.462756	1.342532
C	2.140929	-1.527925	-0.753929
H	3.486979	1.261841	-1.258112
H	-0.531277	-1.154530	0.756076
H	-0.525286	-0.663494	-0.926145
H	0.804844	0.892210	1.348638
H	0.649496	1.538718	-1.639836
H	1.136465	2.634910	-0.342948
H	3.113153	0.449832	1.939641
H	4.053994	-0.780551	1.086832
H	2.590731	-1.244438	1.966253
H	3.152300	-1.835313	-1.035903
H	1.567503	-1.400163	-1.674589
H	1.691554	-2.345552	-0.180842
C	-1.719891	0.600493	0.348763
H	-1.687955	1.501189	-0.276383
H	-1.762637	0.952421	1.384808
O	-3.136942	-1.139359	-0.615938
O	-4.141076	0.351838	0.430483
Rotational constants (GHz): 2.4104300 0.4805500 0.4550400			
Vibrational harmonic frequencies (cm-1):			
14.1255	46.9991	75.7451	
85.8387	102.3773	205.5536	
211.9033	225.8184	230.8629	
269.1247	282.7836	345.8931	
395.3110	431.8016	447.7841	
513.7986	552.1060	614.2830	
628.0400	761.7631	787.5027	
869.7776	878.1388	901.3784	
919.3830	944.3437	949.9367	
995.1115	1001.1770	1011.9589	
1047.5598	1096.7157	1103.3634	
1119.2180	1161.7324	1191.0480	
1210.6921	1219.8665	1249.9651	
1266.3293	1279.6282	1309.1090	
1327.2302	1364.3247	1391.5611	
1397.1464	1414.6711	1455.1125	
1464.7560	1483.0717	1488.4925	
1496.5237	1504.8940	1509.6494	
1580.7930	2951.6267	3009.0359	
3011.4695	3019.6581	3025.2730	
3032.9429	3036.1355	3060.0146	
3072.5964	3080.1046	3081.9552	
3088.0543	3098.1658	3174.9682	
Zero-point correction (Hartree): 0.208626			

**Int2-T-B3LYP**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.83418052

Electronic state : 3-A

Cartesian coordinates (Angs):

C	-0.198450	0.895428	0.085011
C	0.855991	0.094641	-0.792542
C	2.025896	-0.495882	-0.087660
C	-2.680468	-0.191450	-0.230557
C	-1.306723	0.217754	-0.802518
C	-0.279757	-0.852250	-1.250861
C	-0.099831	2.414567	-0.025848
C	-0.201296	0.465302	1.554075
H	1.227844	0.731314	-1.599120
H	-3.313076	-0.435763	-1.100833
H	-3.142134	0.691399	0.225095

H	-1.496465	0.891287	-1.645556
H	-0.311597	-1.749481	-0.631202
H	-0.277642	-1.148376	-2.300675
H	-0.082017	2.739555	-1.070045
H	0.808169	2.785213	0.459845
H	-0.955797	2.893492	0.460935
H	0.705638	0.818459	2.054750
H	-0.253014	-0.617724	1.675034
H	-1.058788	0.900369	2.074406
C	-2.712109	-1.336793	0.722031
H	-3.183727	-1.252684	1.692246
H	-2.342705	-2.312124	0.429163
O	2.065441	-1.661717	0.379830
O	3.091533	0.136363	0.151317
Rotational constants (GHz): 1.6803200 0.8147500 0.7031000			
Vibrational harmonic frequencies (cm-1):			
40.9021	56.6592	74.2378	
102.5742	134.5768	182.8691	
206.3813	236.1376	256.0970	
271.2526	291.6744	341.9077	
363.4106	415.3983	440.6729	
485.7237	583.0850	600.2344	
614.5298	666.9306	731.2974	
789.2331	795.6917	896.6655	
918.6789	957.4362	963.0032	
969.6041	992.0307	1006.8887	
1039.4208	1092.7816	1124.2564	
1124.8670	1144.0908	1169.2690	
1185.7344	1219.0788	1245.6464	
1255.4828	1279.6579	1305.1619	
1330.6763	1349.2120	1393.2650	
1406.9923	1429.2918	1460.8227	
1475.3757	1482.5361	1492.1204	
1496.8798	1505.3024	1510.4455	
1573.5080	2934.5257	3015.5126	
3023.8681	3029.0027	3039.9877	
3065.0610	3068.0777	3077.7212	
3085.6115	3087.8459	3111.1107	
3117.1627	3142.9027	3242.7057	
Zero-point correction (Hartree): 0.208495			

**HC-Triplet biradical (formed by CO<sub>2</sub>-loss)**

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E(UB+HF-LYP/CBSB7) (Hartree): -313.21375644

Electronic state : 3-A

Cartesian coordinates (Angs):

C	0.910290	-0.186806	-0.070063
C	0.999025	1.097414	-0.859130
C	-1.654262	-0.265143	0.858282
C	-0.314295	0.477542	0.696145
C	-0.226813	1.713867	-0.258452
C	2.117198	-0.476219	0.838721
C	0.599775	-1.430858	-0.919745
H	1.711240	1.446312	-1.599095
H	-2.268243	0.350897	1.540654
H	-1.474481	-1.198073	1.404970
H	0.017939	0.761390	1.698748
H	-1.073208	1.818701	-0.951189
H	-0.103335	2.685574	0.237106
H	2.379100	0.396611	1.442710
H	2.994974	-0.748581	0.243829
H	1.900961	-1.309112	1.517202
H	1.466413	-1.681883	-1.539925
H	-0.254718	-1.270481	-1.579539
H	0.381231	-2.297078	-0.285709
C	-2.443770	-0.546136	-0.373567
H	-2.629894	0.227752	-1.108175



H	-2.970864	-1.483999	-0.494730	
Rotational constants (GHz):	2.8034400	1.6795800	1.4505300	
Vibrational harmonic frequencies (cm-1):				
34.3086	84.2963		123.9875	
196.7739	207.9397		222.2900	
245.7376	280.4356		286.3546	
351.2852	402.7990		420.3797	
476.6029	575.4651		622.1074	
689.9885	793.0344		869.8238	
888.0040	917.4725		941.4217	
948.3548	961.4386		998.9988	
1010.2575	1047.2394		1117.7318	
1120.8041	1147.3674		1189.4319	
1209.7012	1235.4482		1255.6995	
1271.3052	1313.1759		1334.5691	
1381.2704	1389.4684		1412.3369	
1454.7852	1462.4920		1472.2952	
1482.1053	1484.8149		1500.4631	
1505.8434	2908.1839		2978.5366	
2999.6722	3007.4012		3013.5218	
3030.0623	3044.9688		3066.7097	
3073.2328	3085.1303		3098.9601	
3141.3648	3168.8803		3239.1662	
Zero-point correction (Hartree):	0.191807			

**TS1-T**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.80195205

Electronic state : 3-A

Cartesian coordinates (Angs):

C	1.260443	-0.286411	0.060886	
C	0.126309	-0.340874	-0.982696	
C	-1.475454	-0.407506	-0.111450	
C	-0.167400	1.544164	1.151169	
C	0.946146	1.252787	0.137876	
C	0.342052	1.139416	-1.295364	
C	2.609660	-0.558523	-0.643380	
C	1.212872	-1.135380	1.331307	
H	0.005516	-1.131962	-1.717802	
H	-0.321793	2.625134	1.221052	
H	0.145664	1.215899	2.145662	
H	1.802775	1.915980	0.280767	
H	-0.528465	1.745829	-1.546504	
H	1.082122	1.271705	-2.087440	
H	2.749255	0.033800	-1.548834	
H	2.692524	-1.614631	-0.914428	
H	3.429766	-0.321980	0.041343	
H	1.316069	-2.194475	1.081684	
H	0.282940	-1.028715	1.887479	
H	2.043385	-0.862843	1.990936	
C	-1.512453	0.892873	0.752397	
H	-2.099055	1.593065	0.155126	
H	-2.106314	0.646095	1.634794	
O	-2.328500	-0.480249	-1.102818	
O	-1.489931	-1.581773	0.474280	
Rotational constants (GHz):	1.6608200	1.0348900	0.9658900	
Vibrational harmonic frequencies (cm-1):				
-251.2379	109.5291		165.6759	
191.1810	206.1388		225.7555	
243.4690	307.2399		319.9489	
378.8781	388.9698		408.9736	
432.9095	447.2231		502.3071	
542.0579	615.2251		665.9008	
730.6222	795.7466		816.2776	
862.9985	872.1026		906.2169	
947.3432	951.4062		965.2519	
966.7346	1004.6323		1014.3969	

1021.6513	1066.7689	1101.5548
1115.6786	1144.9477	1176.0405
1205.3754	1219.4345	1231.1897
1236.4211	1250.0308	1273.1911
1297.3293	1324.7427	1340.6896
1372.0477	1399.6105	1427.4721
1469.9623	1481.7887	1485.2568
1496.7813	1504.4401	1507.4570
1518.8822	3025.2598	3030.7663
3036.3706	3057.7870	3058.9478
3067.2105	3069.4412	3085.0162
3091.2214	3102.6320	3109.2294
3112.6858	3128.1771	3146.7344

Zero-point correction (Hartree): 0.211358

**TS2-T**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.80077577

Electronic state : 3-A

Cartesian coordinates (Angs):

C	1.249535	-0.290661	0.062272
C	0.048407	-0.400423	-0.933366
C	-1.333605	-0.535163	-0.246059
C	-0.118875	1.623511	1.079695
C	0.961788	1.251675	0.050783
C	0.314496	1.066717	-1.350211
C	2.573981	-0.619653	-0.646363
C	1.221304	-1.044996	1.393674
H	0.086741	-1.182192	-1.695891
H	-0.283076	2.707310	1.037650
H	0.234197	1.390248	2.086803
H	1.824058	1.916840	0.142285
H	-0.551887	1.680283	-1.603789
H	1.034180	1.141450	-2.163469
H	2.687536	-0.106548	-1.603020
H	2.646109	-1.694956	-0.834963
H	3.420529	-0.334970	-0.013725
H	1.304441	-2.121255	1.221930
H	0.310841	-0.888414	1.971372
H	2.072568	-0.739150	2.011973
C	-1.464139	0.958402	0.817870
H	-2.140650	1.547480	0.206640
H	-1.977725	0.546800	1.680562
O	-2.390964	-0.417851	-1.014472
O	-1.532188	-1.572072	0.537706

Rotational constants (GHz): 1.6476600 1.0392600 0.9692500

Vibrational harmonic frequencies (cm-1):

-392.8672	79.6401	152.8526
191.9837	204.4485	222.0839
255.4714	292.4518	323.5006
339.4992	377.9445	407.6771
420.1491	473.3615	513.5951
560.2718	582.4540	656.3443
693.8678	748.8577	819.0328
840.2199	879.9809	907.0083
935.4665	956.6030	958.6393
978.5780	1008.5320	1021.3276
1047.9305	1080.5938	1088.4624
1129.4403	1133.8629	1168.2857
1188.8200	1215.1968	1227.9642
1233.9338	1253.3779	1267.7634
1283.0283	1295.0545	1323.0308
1363.8799	1404.3864	1429.5444
1469.4363	1482.8721	1488.1248
1497.8385	1505.5908	1512.8416
1516.1928	3010.8260	3021.5363
3026.6694	3058.2374	3065.1973

3072.0614	3074.1781	3079.7173
3086.5445	3102.0926	3118.1238
3119.2166	3124.5397	3195.6703

Zero-point correction (Hartree): 0.210876

**TS3-T**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.83030852  
Electronic state : 3-A  
Cartesian coordinates (Angs):

C	-2.182820	0.230613	0.091365
C	-2.541368	-0.925191	-0.812059
C	3.021272	0.138564	-0.034799
C	0.504598	0.282875	0.148522
C	-0.790780	-0.506334	0.317088
C	-1.176270	-1.541615	-0.789539
C	-3.030331	0.375678	1.363228
C	-2.108742	1.581278	-0.644603
H	-3.445723	-1.160357	-1.362228
H	0.535610	1.109044	0.866895
H	0.569163	0.726087	-0.847000
H	-0.799602	-0.983129	1.302178
H	-0.605979	-1.413499	-1.722862
H	-1.108462	-2.601312	-0.515065
H	-3.111480	-0.574906	1.896655
H	-4.043214	0.710011	1.117342
H	-2.591093	1.114191	2.042926
H	-3.116695	1.907465	-0.917706
H	-1.522778	1.517889	-1.563872
H	-1.667917	2.357154	-0.010192
C	1.733376	-0.615125	0.357602
H	1.701982	-1.493552	-0.296452
H	1.793181	-0.980528	1.386191
O	3.136608	0.896150	-0.969262
O	3.968317	-0.191027	0.799558

Rotational constants (GHz): 2.3307700 0.4854300 0.4721000  
Vibrational harmonic frequencies (cm-1):

-630.6736	30.0547	46.2531
83.1881	88.2734	102.3905
207.2773	226.3869	229.5602
229.7682	269.5239	287.9680
345.6740	395.4328	434.9298
453.1688	504.6992	616.8060
651.5041	709.3035	761.6818
803.2848	868.3544	884.3547
900.1673	941.0892	947.9769
991.2009	993.9737	999.8006
1026.8146	1049.5954	1092.3797
1107.5162	1184.9766	1185.1842
1210.4164	1211.3166	1248.7748
1261.3939	1266.5644	1303.5842
1319.6922	1345.1405	1376.5975
1391.6960	1412.8921	1457.6875
1466.5870	1481.8943	1487.2826
1496.4795	1503.5538	1509.1514
1662.0152	2956.3006	3009.8991
3011.6620	3019.0661	3028.6424
3038.0530	3038.8692	3072.5731
3075.8407	3080.5100	3088.3421
3095.7972	3104.1589	3173.7307

Zero-point correction (Hartree): 0.206987

**TS4-T**

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E(UB+HF-LYP/6-311G(d,p)) (Hartree): -501.82910222  
Electronic state : 3-A

Cartesian coordinates (Angs):

C	-0.157980	0.894898	0.151613
C	0.902263	0.111870	-0.720712
C	1.989754	-0.624333	0.004111
C	-2.632498	-0.143967	-0.327155
C	-1.235227	0.278338	-0.825515
C	-0.220155	-0.792854	-1.299695
C	-0.016594	2.413076	0.095689
C	-0.257549	0.420057	1.601699
H	1.308145	0.781555	-1.481023
H	-3.227979	-0.350742	-1.234240
H	-3.109461	0.726775	0.136655
H	-1.380009	1.001323	-1.634853
H	-0.280081	-1.721922	-0.734669
H	-0.167916	-1.009609	-2.366674
H	0.050067	2.773960	-0.934624
H	0.883209	2.739198	0.626889
H	-0.875248	2.899909	0.569166
H	0.618388	0.751803	2.168003
H	-0.318287	-0.663968	1.687765
H	-1.141624	0.853441	2.077275
C	-2.713371	-1.319178	0.584880
H	-3.352617	-1.304182	1.457810
H	-2.232238	-2.255981	0.333451
O	1.845889	-1.673985	0.589872
O	3.063335	0.092860	-0.122425

Rotational constants (GHz): 1.6581600 0.8399900 0.7266200

Vibrational harmonic frequencies (cm-1):

-232.8128	44.4081	55.6947
77.0248	108.4212	156.8256
184.9734	212.1104	237.8513
266.9460	276.0954	301.0647
357.7276	370.9774	441.0016
475.7520	512.2835	589.0794
602.3814	652.8732	723.2518
767.9736	794.5405	835.8662
883.4154	929.6608	951.7724
958.5210	975.0802	1003.1900
1010.6937	1068.5501	1099.7841
1123.9395	1136.2709	1169.0923
1178.2335	1217.2332	1241.7169
1245.3143	1267.8729	1304.1564
1308.4601	1341.3913	1391.2380
1406.9501	1428.9570	1457.7691
1472.2742	1481.1921	1490.3183
1495.0815	1503.3451	1509.6522
1718.4473	2918.6607	3015.7316
3028.7100	3030.4857	3037.1279
3070.0104	3077.5341	3078.0082
3084.6568	3085.4245	3131.9904
3138.8528	3147.3739	3246.5281

Zero-point correction (Hartree): 0.207099

