Mechanism of the photochemical isomerization and oxidation of 2-butenedial: A Theoretical Study

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Supplementary Materials

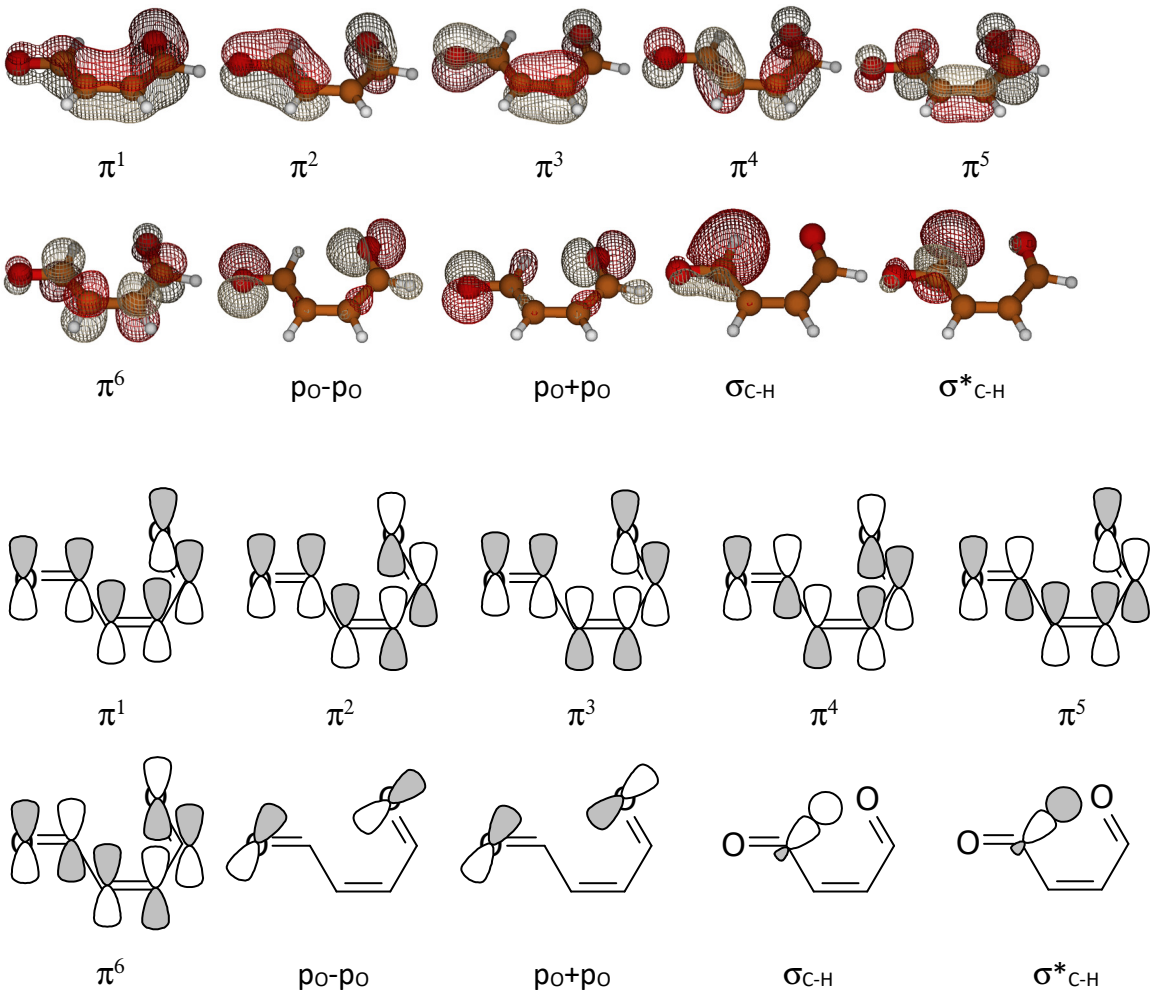


Figure S1. Active orbitals

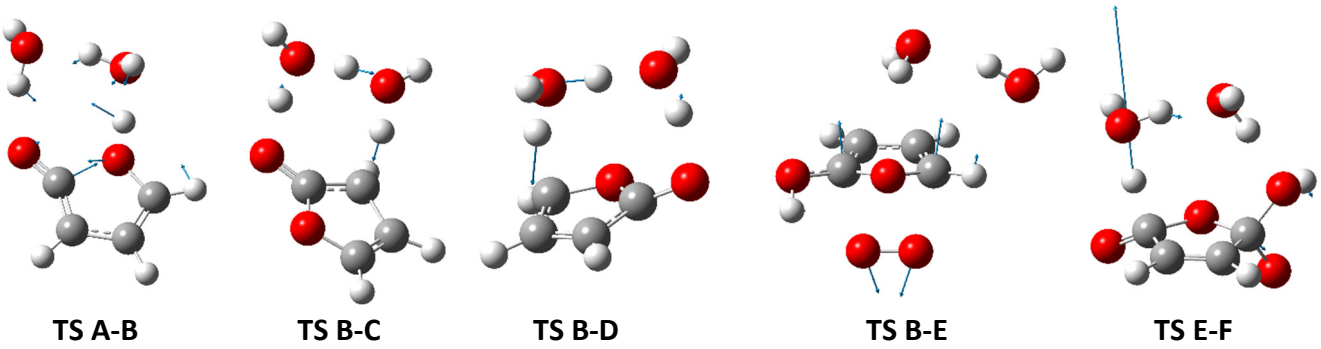
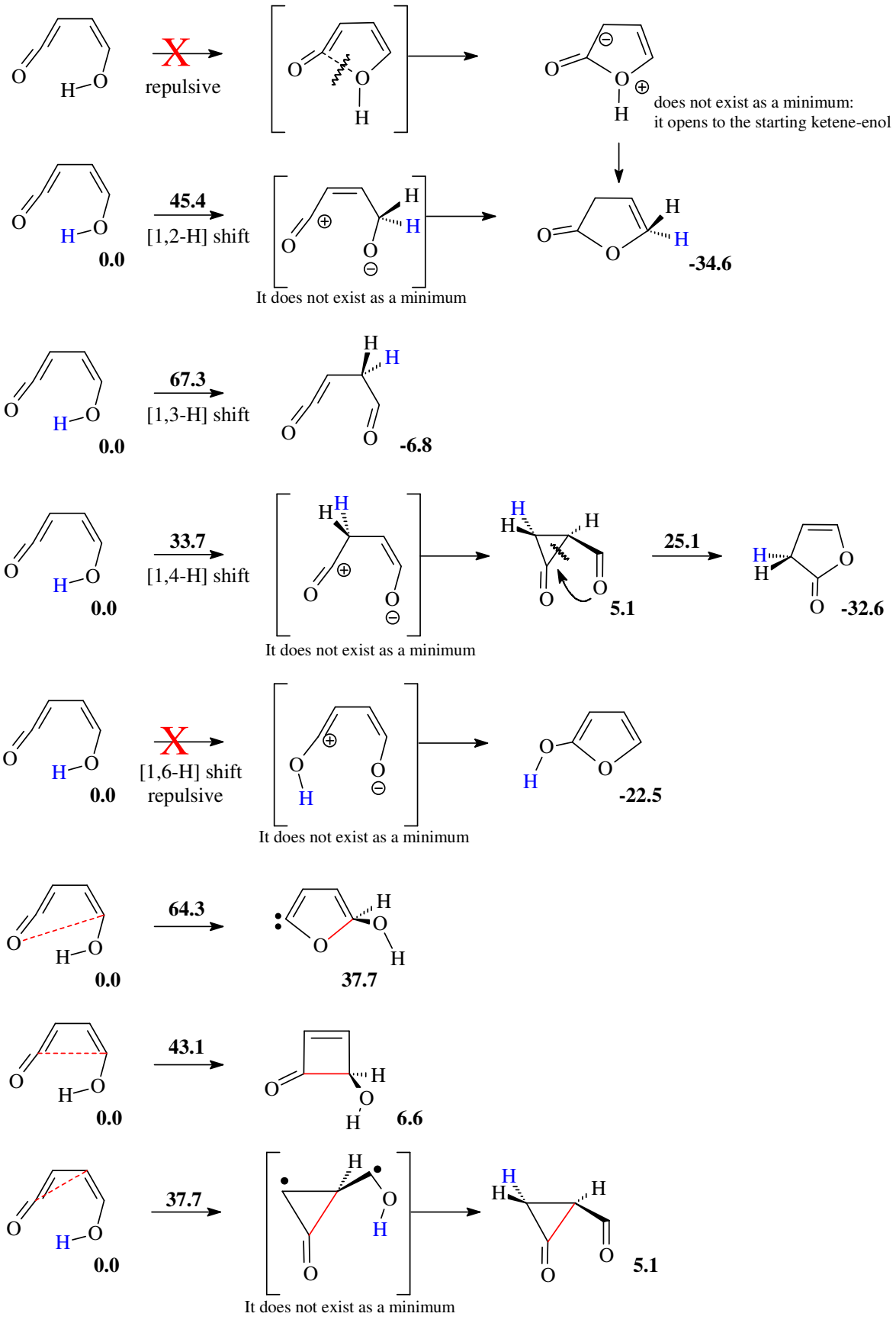


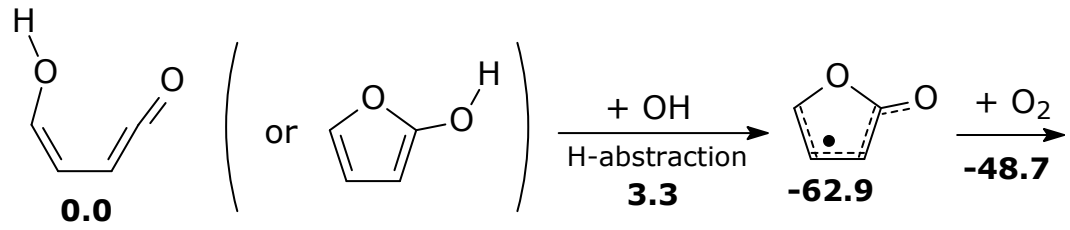
Figure S2. Displacement vectors for the transition structures.

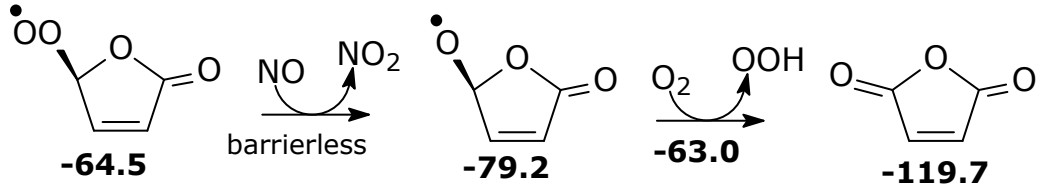
Formation of furanones



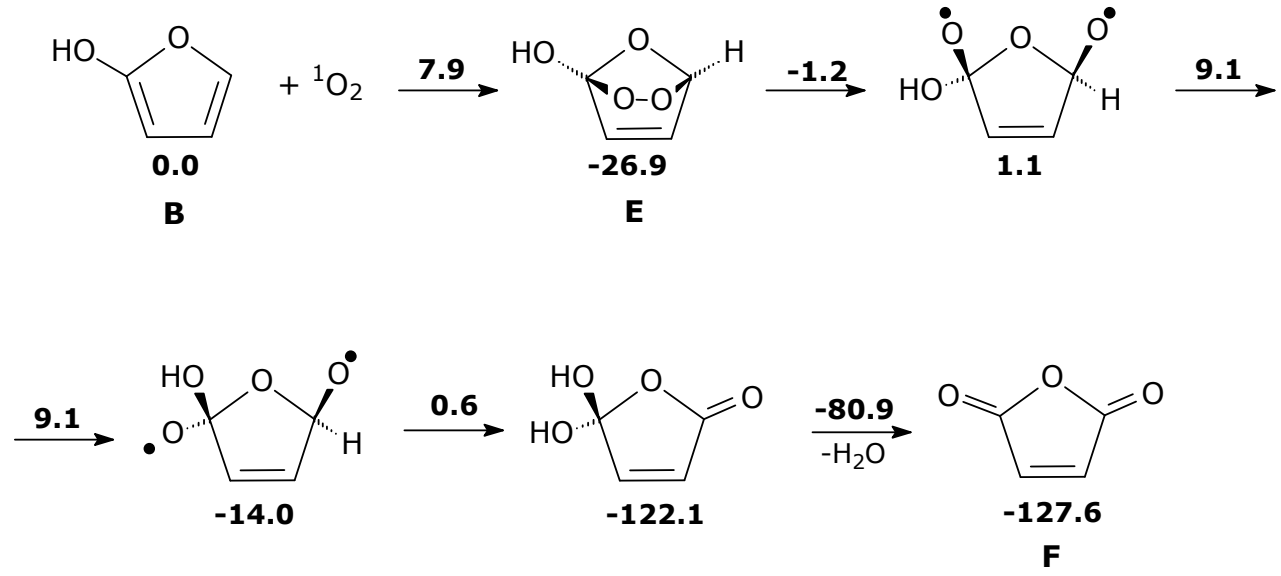
Scheme S1. Attempts to form furanones form ketene-enol, in the ground state. M06-2X/6-31G(d) potential energies in kcal mol^{-1}.

Possible formation of maleic anhydride if the hydroxyl radical had a major role and NOx concentration were substantial.





Scheme S2. Formation of maleic anhydride form ketene-enol **A** (or 2-furanol **B**), initiated by OH. ΔG(298K) M06-2X/cc-pVTZ in kcal mol^{-1}.



Scheme S3. Formation of maleic anhydride form ketene-enol in the gas phase, initiated by $^1O_2$, without intervention of water molecules. ΔG(298K) M06-2X/cc-pVTZ in kcal mol^{-1}.

Cartesian coordinates and energies

Formation of furanones without water molecules:

A

Atom	X	Y	Z (Angstrom)
8	2.142733	-0.668503	-0.000002
8	-0.939391	-1.272032	-0.000003
6	1.331917	0.152744	0.000000
6	0.479153	1.159488	0.000004
6	-0.973665	1.052283	-0.000002
6	-1.637058	-0.097448	-0.000001
1	-1.534099	-2.023099	0.000033
1	-1.535363	1.972664	-0.000008
1	-2.716220	-0.156261	-0.000006
1	0.956866	2.128581	0.000012

Energy -305.216208 (Hartree)

Frequencies (cm-1):

103.18 150.41 212.77 269.22 479.16 536.65 591.82 618.85
741.80 828.88 921.98 949.66 1084.24 1150.33 1226.15 1284.52
1413.37 1461.13 1764.24 2238.80 3220.36 3224.50 3257.09 3926.22

TS A–B

Atom	X	Y	Z (Angstrom)
8	-1.967494	0.023086	-0.097644
8	-0.123675	-0.984478	0.136748
6	-0.757545	0.321361	0.077214
6	0.247301	1.235290	0.059178
6	1.485765	0.499095	-0.050225
6	1.264654	-0.824738	-0.073283
1	-1.167272	-1.223046	-0.223980
1	0.120117	2.299514	0.009894
1	2.467468	0.939140	-0.114171
1	1.867994	-1.710525	-0.061880

Energy -305.141098 (Hartree)

Frequencies (cm-1):

1648.25i 220.91 527.04 573.94 616.21 655.67 730.44 742.25
780.17 860.54 918.27 953.99 1015.84 1058.28 1129.86 1184.92
1302.96 1370.13 1609.78 1800.55 2256.02 3267.03 3315.78 3338.36

B

Atom	X	Y	Z (Angstrom)
8	-2.002732	0.089243	0.000031
8	-0.021374	-1.045085	0.000004
6	-0.664845	0.134841	-0.000015
6	0.194892	1.176821	-0.000007
6	1.500686	0.576194	0.000008
6	1.321220	-0.758144	0.000003
1	-2.281408	-0.832205	-0.000160
1	-0.065590	2.218658	-0.000043
1	2.447546	1.087248	0.000003
1	1.980587	-1.605239	-0.000014

Energy -305.243573 (Hartree)

Frequencies (cm-1):

173.63 299.20 430.87 620.57 680.39 697.39 739.22 796.20
896.17 901.56 988.66 1024.38 1106.17 1174.19 1200.81 1281.89
1327.94 1475.05 1600.03 1715.78 3282.28 3308.04 3318.61 3873.39

TS B–C

Atom	X	Y	Z (Angstrom)
8	1.564690	0.169298	0.535997
8	0.215042	-0.985112	-0.642180
6	0.709233	0.259902	-0.393812

```
  6    -0.370324     1.205803    -0.336800
  6    -1.334302     0.418541     0.225032
  6    -0.818697    -0.919208     0.322607
  1     0.606022    -0.485422     1.193709
  1    -1.433901    -1.804649     0.397152
  1    -2.254153     0.750566     0.679872
  1    -0.271295     2.275778    -0.323435
Energy         -305.084168  (Hartree)
Frequencies (cm-1):
 1862.31i    365.84    459.10    608.46    650.39    692.14    761.73    825.63
923.22    941.87    992.17   1026.77   1085.41   1131.52   1144.17   1191.43
1328.70   1385.65   1497.04   1525.64   1721.19   3227.93   3258.11   3300.20
```

C

```
 Atom      X            Y            Z (Angstrom)
  8     2.005502    -0.029346     0.000031
  8     0.049450    -1.131093    -0.000032
  6     0.819609     0.009309    -0.000001
  6    -0.115136     1.207330    -0.000025
  6    -1.464188     0.558967     0.000024
  6    -1.277499    -0.750623     0.000010
  1     0.088972     1.820534     0.878483
  1    -2.415812     1.060710     0.000072
  1    -1.978416    -1.568045     0.000034
  1     0.088926     1.820413    -0.878632
Energy         -305.256241  (Hartree)
Frequencies (cm-1):
   172.08    444.62    501.52    577.39    684.09    740.01    832.18    867.06
950.87    973.60    993.44   1094.34   1138.74   1169.44   1190.48   1290.93
1385.70   1443.96   1710.44   1938.03   3088.16   3124.45   3272.69   3295.97
```

TS B–D

```
 Atom      X            Y            Z (Angstrom)
  8    -2.044741    -0.046791     0.020288
  8    -0.006691    -1.112834    -0.084435
  6    -0.869454     0.111612    -0.036381
  6     0.056643     1.188906    -0.019665
  6     1.348311     0.735562     0.024613
  6     1.434794    -0.653369     0.052393
  1     0.530883    -1.310666     0.871933
  1     2.226373     1.364040     0.040462
  1    -0.274591     2.211824    -0.019849
  1     2.107026    -1.284458    -0.505138
Energy         -305.139832  (Hartree)
Frequencies (cm-1):
 1687.54i    220.73    473.11    527.84    553.23    632.64    677.43    735.19
792.72    819.05    858.12    974.73   1085.78   1097.67   1118.03   1136.87
1278.43   1450.50   1566.01   1921.74   2458.25   3240.78   3263.12   3294.87
```

D

```
 Atom      X            Y            Z (Angstrom)
  8    -2.028810    -0.037266     0.000000
  8    -0.045353    -1.092452     0.000005
  6    -0.838676     0.019065     0.000000
  6     0.055988     1.202992    -0.000003
  6     1.310566     0.779790     0.000005
  6     1.320848    -0.716902    -0.000004
  1     1.807930    -1.129003     0.886016
  1    -0.325354     2.210048     0.000001
  1     2.210465     1.376011     0.000006
  1     1.807913    -1.128982    -0.886043
Energy         -305.259922  (Hartree)
Frequencies (cm-1):
```

206.80 359.82 504.66 683.88 707.87 801.93 840.24 900.98
962.48 988.54 1046.28 1079.84 1152.82 1179.89 1225.46 1362.68
1388.26 1503.74 1693.75 1909.12 3068.66 3105.64 3245.65 3282.68

Formation of furanones with 1 water molecule:

A

Atom	X	Y	Z (Angstrom)
6	-1.446569	0.775397	0.488447
6	-0.112953	1.375604	0.541915
6	0.921176	1.031405	-0.195433
8	1.878749	0.743263	-0.779975
6	-1.776661	-0.309204	-0.209750
8	-0.904326	-1.031969	-0.960123
1	0.073104	2.236807	1.168827
1	-2.218076	1.279624	1.050029
1	-2.802311	-0.653869	-0.253771
1	-0.159191	-1.334336	-0.406940
8	1.116087	-1.736053	0.823582
1	1.957256	-1.429334	0.470882
1	0.915173	-1.140033	1.552023

Energy -381.654788 (Hartree)
Frequencies (cm-1):
30.56 86.42 113.07 142.94 189.42 210.94 270.57 339.45
364.68 471.29 525.70 590.53 625.62 669.57 774.77 850.00
941.78 957.50 1091.55 1149.83 1262.85 1396.26 1413.55 1450.86
1625.38 1729.04 2222.63 3196.50 3214.19 3240.63 3561.71 3838.03
3930.76

TS A–B

Atom	X	Y	Z (Angstrom)
6	-1.177230	-1.254028	-0.077439
8	0.070375	-0.672013	-0.324586
6	-0.038595	0.818437	-0.096580
6	-1.363737	1.002783	0.167948
6	-2.040191	-0.263599	0.178640
8	1.041426	1.413861	-0.169168
8	2.376535	-0.688558	0.165301
1	1.101711	-0.971076	-0.033770
1	2.143363	0.299707	0.052672
1	2.704521	-0.817462	1.059665
1	-1.251985	-2.315929	-0.210524
1	-1.793799	1.966530	0.365876
1	-3.091982	-0.409641	0.358281

Energy -381.634683 (Hartree)
Frequencies (cm-1):
461.39i 78.12 266.53 342.37 439.40 469.44 539.59 568.84
597.71 621.62 702.22 709.99 746.27 828.93 914.02 995.86
1021.58 1048.31 1124.85 1178.29 1202.54 1254.66 1353.13 1403.32
1592.28 1633.83 1836.30 1945.19 2854.36 3271.92 3304.27 3325.37
3903.18

B

Atom	X	Y	Z (Angstrom)
6	-1.497982	0.958164	0.046766
6	-0.182224	0.648956	-0.014249
8	-0.000383	-0.694079	-0.055264
6	-1.251746	-1.265664	-0.020108
6	-2.187407	-0.301618	0.041604
8	0.901991	1.411747	-0.043730
8	2.844270	-0.516415	-0.038342

```
  1    -1.911936     1.948163     0.087073
  1    -3.251448    -0.456962     0.079194
  1    -1.278791    -2.338400    -0.047811
  1     3.346897    -0.677492     0.763325
  1     1.704023     0.850445    -0.057358
  1     2.140387    -1.174811    -0.049810
Energy         -381.685522  (Hartree)
Frequencies (cm-1):
    28.87    118.07    154.79    198.36    239.43    296.03    434.40    507.29
613.64    672.98    701.77    704.30    728.62    793.59    896.20    900.63
979.37   1024.99   1113.01   1185.97   1229.54   1300.30   1372.14   1487.30
1606.33   1620.39   1724.01   3281.42   3307.85   3320.87   3516.57   3834.77
3947.64
```

TS B–C

```
 Atom      X            Y            Z (Angstrom)
  6    -1.606534    -0.099648    -0.522374
  6    -0.668250    -1.097337    -0.687599
  6     0.354172    -0.820549     0.253657
  8    -0.116454     0.094473     1.146375
  6    -1.196279     0.737604     0.526952
  8     1.594702    -0.957019     0.191237
  8     1.118941     1.436153    -0.576019
  1    -0.575006    -1.808425    -1.488350
  1    -2.473373     0.083186    -1.138588
  1    -1.825385     1.315566     1.184288
  1     1.195184     1.520738    -1.533726
  1     1.574636     0.526209    -0.275721
  1     0.027776     1.453461    -0.264464
Energy         -381.613341  (Hartree)
Frequencies (cm-1):
 1074.07i    163.68    315.02    374.42    419.35    464.90    512.64    650.26
690.79    709.74    783.27    820.72    847.74    919.24    944.98    992.90
1050.16   1104.52   1152.08   1194.13   1253.36   1267.63   1347.33   1451.09
1536.03   1616.29   1688.37   1702.84   2231.10   3244.00   3259.60   3294.13
3864.29
```

C

```
 Atom      X            Y            Z (Angstrom)
  6     2.140802     0.120630     0.000109
  6     1.458188     1.252651    -0.000014
  6     0.002968     0.907234    -0.000137
  6     0.038011    -0.606964    -0.000062
  8     1.341048    -1.011580     0.000085
  8    -0.861078    -1.394200    -0.000114
  8    -2.914813     0.558545     0.000053
  1    -0.556738     1.253702     0.869627
  1     1.879045     2.242739    -0.000018
  1     3.198162    -0.080550     0.000226
  1    -3.853801     0.368158     0.000649
  1    -2.471170    -0.301098    -0.000003
  1    -0.556570     1.253625    -0.870040
Energy         -381.694476  (Hartree)
Frequencies (cm-1):
    25.91     86.35    124.27    171.27    186.61    379.28    443.41    504.46
518.89    579.67    689.55    746.85    835.82    881.64    942.74    968.86
998.23   1091.36   1163.32   1180.33   1186.91   1304.94   1386.92   1423.46
1642.87   1708.78   1900.15   3096.35   3126.57   3274.32   3297.49   3760.72
3948.63
```

TS B–D

```
 Atom      X            Y            Z (Angstrom)
  6     1.439162     1.138271     0.091130
```

6	0.064149	0.852902	0.490414
6	-0.073105	-0.553349	0.285648
8	1.061341	-1.050264	-0.240603
6	1.969379	-0.009159	-0.335419
8	-1.106083	-1.258635	0.344860
8	-2.296859	0.628038	-0.549497
1	-0.393031	1.313818	1.357318
1	1.943474	2.088038	0.130974
1	2.932282	-0.277802	-0.729117
1	-2.932583	1.079021	0.014135
1	-2.010516	-0.341120	-0.105084
1	-1.204331	1.012948	-0.296947

Energy -381.637076 (Hartree)

Frequencies (cm-1):

1552.63i	111.34	276.24	414.08	469.71	513.69	566.85	605.25
619.95	715.63	728.52	784.89	860.35	889.20	908.98	968.63
1033.43	1100.53	1174.58	1188.55	1273.17	1328.20	1396.46	1441.47
1526.57	1573.84	1649.20	1777.13	2094.23	3192.89	3279.41	3313.14
3893.00							

D

Atom	X	Y	Z (Angstrom)
6	-2.184425	-0.113743	-0.015220
6	-1.283421	-1.307187	0.000336
6	-0.021462	-0.903271	0.012511
6	-0.020324	0.577576	0.006280
8	-1.307443	1.002932	-0.011981
8	0.903738	1.342604	0.015786
8	3.054530	-0.532000	0.061633
1	0.897456	-1.467016	0.024019
1	-1.651041	-2.321976	0.001668
1	-2.828467	-0.063342	0.864426
1	3.720586	-0.381266	-0.610598
1	2.523413	0.277333	0.081545
1	-2.810748	-0.072277	-0.908002

Energy -381.698858 (Hartree)

Frequencies (cm-1):

33.24	68.88	128.33	172.19	208.63	326.76	362.75	517.67
585.41	695.30	711.65	806.71	848.55	916.47	964.59	1007.46
1045.94	1085.66	1152.03	1206.45	1224.61	1363.01	1393.60	1500.92
1647.28	1691.42	1872.08	3074.24	3112.89	3246.77	3273.48	3745.53
3944.88							

TS C–D

Atom	X	Y	Z (Angstrom)
6	0.806260	-1.047780	-0.611835
6	0.878537	-0.965165	0.759609
6	-0.195624	-0.167859	1.202062
6	-1.082583	0.014825	0.073141
8	-0.391729	-0.504234	-1.036966
8	-2.152770	0.543213	-0.064456
8	1.380061	1.525719	-0.265601
1	-0.488920	0.028494	2.218092
1	1.680382	-1.371232	1.357589
1	1.304665	-1.711449	-1.297394
1	2.175549	1.833209	0.186193
1	1.521697	0.463415	-0.535950
1	0.682589	1.235846	0.469792

Energy -381.604311 (Hartree)

Frequencies (cm-1):

968.42i	131.51	239.16	404.52	443.27	480.38	517.22	522.92
610.67	654.67	716.04	764.00	785.12	850.38	886.74	926.26
1018.83	1107.30	1114.77	1162.94	1220.12	1301.52	1336.72	1446.00

1536.09 1632.82 1756.15 1860.25 2550.29 3240.58 3274.47 3287.07
3855.87

Formation of furanones with 2 water molecules:

A

Atom	X	Y	Z (Angstrom)
8	0.948718	2.056997	0.243327
8	-0.316058	-0.735348	-0.020283
6	1.583566	1.093340	0.127366
6	2.370044	0.048065	-0.012827
6	1.923639	-1.339393	-0.102642
6	0.642310	-1.691768	-0.094049
1	-1.215974	-1.092046	0.127391
8	-2.034491	1.513567	-0.399319
1	-1.186416	1.079239	-0.557848
1	-1.813677	2.284114	0.128925
8	-2.953826	-0.970620	0.339642
1	-2.908490	-0.009245	0.185560
1	-3.564634	-1.313441	-0.315352
1	0.313928	-2.720721	-0.150118
1	2.681832	-2.101380	-0.180278
1	3.421341	0.295246	-0.052306

Energy -458.101961 (Hartree)
Frequencies (cm-1):
21.14 34.72 83.88 107.53 123.00 166.20 187.44 209.78
227.39 246.48 282.21 305.63 378.81 469.47 499.86 530.52
607.10 622.23 715.80 756.96 808.91 855.02 930.48 955.05
1101.67 1144.72 1255.95 1383.84 1419.27 1453.43 1632.26 1648.25
1758.73 2218.81 3213.15 3223.84 3258.39 3483.34 3638.21 3814.74
3934.20 3935.09

TS A-B

Atom	X	Y	Z (Angstrom)
8	-0.529914	-1.566459	-0.239557
8	0.485583	0.592357	-0.592500
6	0.514005	-0.993323	-0.067131
6	1.789772	-1.062470	0.386118
6	2.497709	0.184952	0.271778
6	1.726226	1.134397	-0.259466
1	-0.350460	1.102104	-0.232349
8	-2.987307	-0.506498	0.133232
1	-2.181321	-1.052557	0.025428
1	-3.550179	-0.706674	-0.617156
8	-1.580794	1.687229	0.272943
1	-2.245439	0.946848	0.219126
1	-1.543580	1.959835	1.193066
1	1.901903	2.161346	-0.524153
1	2.178374	-1.978853	0.791808
1	3.523886	0.333579	0.563495

Energy -458.087519 (Hartree)
Frequencies (cm-1):
164.01i 25.40 63.23 93.90 202.58 260.19 267.30 301.54
366.90 373.02 418.62 501.16 553.09 581.32 625.02 647.90
683.46 711.64 721.30 854.21 916.41 1011.59 1031.77 1065.03
1112.81 1154.65 1179.08 1343.87 1404.61 1520.16 1641.49 1660.10
1667.96 1916.84 2406.61 3179.94 3267.75 3291.03 3301.89 3531.84
3914.51 3930.55

B

Atom	X	Y	Z (Angstrom)
8	0.287579	-1.514350	-0.569949
8	-0.341948	0.574395	0.136735
6	-0.688379	-0.693340	-0.224983
6	-2.032926	-0.840096	-0.202621
6	-2.560269	0.432775	0.201821
6	-1.510818	1.249382	0.401896
1	1.339438	1.381088	-0.459963
8	2.528053	-0.922949	0.719815
1	1.111793	-1.339247	-0.046730
1	2.517626	-0.840105	1.675349
8	2.296885	1.508652	-0.507690
1	2.674102	-0.026503	0.363088
1	2.513238	1.546891	-1.441781
1	-3.595795	0.692803	0.335252
1	-2.568178	-1.741248	-0.437066
1	-1.402419	2.268003	0.723888

Energy -458.128841 (Hartree)

Frequencies (cm-1):

28.87	30.52	75.70	141.91	213.56	218.57	240.30	267.16	
303.34	321.43	432.95	469.09	532.19	619.17	677.40	700.33	
731.20	766.12	804.37	897.55	899.48	953.96	975.81	1025.56	
1114.99	1187.82	1228.59	1301.07	1373.89	1458.00	1606.62	1626.35	
1642.17	1725.72	3230.83	3281.01	3306.27	3316.83	3593.59	3778.23	
3932.32	3935.58							

TS B-C

Atom	X	Y	Z (Angstrom)
8	0.553405	-1.547782	0.191732
8	-1.478923	-0.968843	-0.553724
6	-0.375990	-0.715448	0.193925
6	-0.506037	0.573152	0.780216
6	-1.850059	1.012336	0.421317
6	-2.359931	0.080103	-0.387004
1	0.567974	1.234581	-0.099228
8	2.711250	-0.394264	0.145482
1	1.820304	-0.976080	0.248165
1	3.281964	-0.847435	-0.480231
8	1.526631	1.549589	-0.619340
1	2.205017	0.686630	-0.307351
1	1.826483	2.383486	-0.243646
1	-3.288219	-0.006959	-0.921082
1	-2.336049	1.926589	0.715625
1	-0.024274	0.788735	1.723818

Energy -458.092767 (Hartree)

Frequencies (cm-1):

1155.93i	50.17	85.96	119.35	266.22	377.37	404.75	432.69	
485.50	544.70	596.29	608.06	655.06	662.73	727.67	752.73	
787.41	871.91	887.30	905.70	964.72	1021.10	1108.08	1143.06	
1182.55	1203.14	1250.60	1316.21	1401.30	1451.99	1569.85	1614.70	
1658.12	1674.95	1727.76	1839.26	2216.75	3216.58	3272.67	3306.74	
3881.52	3909.18							

C

Atom	X	Y	Z (Angstrom)
8	0.634777	-1.582979	0.532089
8	-0.233152	-0.258623	-1.046761
6	-0.245313	-0.853532	0.182891
6	-1.501420	-0.433412	0.909938
6	-2.159319	0.460732	-0.093470
6	-1.377762	0.516510	-1.156293
1	-1.199229	0.085385	1.819366

8	2.758791	0.043187	-0.462530
1	2.290079	-0.745071	-0.150985
1	2.496218	0.120062	-1.383168
8	0.834314	1.605173	0.900946
1	1.591356	1.197408	0.446525
1	1.203948	2.019193	1.682387
1	-1.466934	1.054383	-2.083944
1	-3.089046	0.986585	0.033119
1	-2.081343	-1.313794	1.188353

Energy -458.137219 (Hartree)

Frequencies (cm-1):

63.45	86.66	101.50	136.59	157.73	177.89	213.85	218.74	
236.47	262.26	427.82	437.52	510.90	552.34	587.75	690.60	
739.08	777.39	840.58	878.28	942.42	971.78	994.59	1091.84	
1161.78	1180.05	1189.25	1298.64	1386.90	1428.58	1647.18	1658.80	
1717.47	1900.73	3093.93	3137.80	3276.21	3299.66	3649.83	3761.92	
3921.96	3935.65							

TS B–D

Atom	X	Y	Z (Angstrom)
8	-0.728427	-1.815938	-0.038150
8	0.309828	-0.168441	1.072962
6	0.254020	-1.058051	0.044556
6	1.341770	-0.796463	-0.828667
6	1.983409	0.322086	-0.342591
6	1.285990	0.794783	0.776288
1	0.212780	1.622028	0.029726
8	-2.384973	0.075363	-0.094052
1	-1.836809	-0.800343	-0.042639
1	-2.849038	0.163021	0.743018
8	-0.775442	1.865704	-0.452561
1	-1.524923	1.056651	-0.272673
1	-0.641690	1.972179	-1.400223
1	1.697142	1.297902	1.637259
1	2.842288	0.815100	-0.772101
1	1.541242	-1.354168	-1.725477

Energy -458.088214 (Hartree)

Frequencies (cm-1):

1009.27i	68.42	110.93	175.22	295.75	343.29	363.48	427.26	
451.47	518.12	540.41	579.67	659.41	715.81	735.67	763.51	
813.65	862.42	910.77	946.26	991.02	1047.09	1095.43	1102.20	
1162.23	1197.49	1286.05	1337.78	1444.04	1456.99	1530.09	1584.75	
1640.69	1709.79	1723.85	1793.63	2592.82	3238.73	3253.24	3298.54	
3879.15	3903.10							

D

Atom	X	Y	Z (Angstrom)
8	-0.587713	-1.736989	-0.345242
8	0.211892	-0.140561	1.002233
6	0.281523	-0.950748	-0.079662
6	1.545654	-0.668768	-0.786094
6	2.140424	0.341030	-0.169017
6	1.300358	0.775220	0.986679
1	0.901575	1.778533	0.829482
8	-2.751874	-0.010973	0.301605
1	-2.225942	-0.798565	0.091441
1	-2.591042	0.128991	1.238024
8	-0.834882	1.686345	-0.891325
1	-1.579497	1.189120	-0.509287
1	-1.149843	2.003002	-1.739030
1	1.848190	-1.209771	-1.665908
1	3.067130	0.824816	-0.436860
1	1.822287	0.720887	1.942542

Energy -458.142888 (Hartree)
Frequencies (cm-1):
52.22 79.54 91.70 148.69 176.98 182.48 210.68 222.04
251.98 281.89 363.40 431.64 514.26 587.73 680.25 714.46
784.90 807.62 843.25 918.12 965.43 978.66 1040.85 1081.40
1148.40 1205.73 1237.97 1368.38 1399.67 1478.16 1650.26 1655.70
1691.64 1864.18 3081.53 3128.71 3248.48 3288.09 3628.20 3732.83
3920.07 3939.45

Formation of maleic anhydride without water molecules:

Singlet O_2

Atom	X	Y	Z (Angstrom)
8	0.000000	0.000000	0.594632
8	0.000000	0.000000	-0.594632

Energy -150.298750 (Hartree)
Frequencies (cm-1):
1753.05

B

Atom	X	Y	Z (Angstrom)
6	-1.468769	0.642813	-0.000003
6	-1.362997	-0.699590	-0.000007
8	-0.043845	-1.066139	-0.000002
6	0.667212	0.064979	0.000007
6	-0.128411	1.161422	0.000008
8	1.992640	-0.137049	0.000020
1	2.435243	0.715417	-0.000189
1	-2.383409	1.209287	-0.000004
1	-2.071198	-1.506432	-0.000009
1	0.186793	2.189490	0.000024

Energy -305.242255 (Hartree)
Frequencies (cm-1):
223.03 303.35 438.74 621.36 687.54 699.67 741.52 777.95
890.90 902.35 995.29 1028.14 1111.94 1169.69 1206.68 1275.30
1340.23 1506.29 1597.94 1676.65 3281.42 3293.57 3320.30 3903.11

TS B-E

Atom	X	Y	Z (Angstrom)
8	1.267927	-1.314343	-0.111419
6	1.097854	0.556595	0.789668
8	-0.160829	0.214667	1.151668
6	-0.881063	0.288549	0.021570
8	0.114028	-1.463270	-0.588321
6	-0.203110	1.026368	-0.946189
6	1.071856	1.207488	-0.438063
8	-2.154602	-0.058955	0.068757
1	-2.234134	-0.877174	0.576221
1	1.927374	1.626909	-0.936334
1	1.847849	0.494134	1.555622
1	-0.586504	1.257332	-1.922908

Energy -455.522928 (Hartree)
Frequencies (cm-1):
598.57i 157.41 201.38 262.65 314.81 362.60 447.69 534.86
594.52 616.49 706.28 785.38 852.58 893.21 926.48 973.70
1058.04 1119.30 1168.12 1208.21 1292.20 1303.73 1396.14 1496.71
1518.63 1632.60 3290.47 3308.66 3318.73 3821.05

E

Atom	X	Y	Z (Angstrom)
6	-1.213932	-0.193540	-0.561669
8	0.032357	-0.215750	-1.198522
6	0.742618	0.129638	-0.028096
6	0.031426	1.368477	0.464471
6	-1.233304	1.163615	0.123784
8	2.078248	0.156412	-0.139331
1	2.376750	-0.726334	-0.392924
1	-2.116006	1.718156	0.396110
1	-2.033575	-0.515115	-1.191804
1	0.479274	2.122701	1.089870
8	0.334166	-0.944457	0.865304
8	-1.028181	-1.172272	0.486026

Energy -455.583838 (Hartree)

Frequencies (cm-1):

305.05	323.90	392.71	426.25	461.54	555.19	684.17	702.06	
736.18	753.55	843.62	878.78	904.33	949.28	977.15	990.95	
1002.09	1052.91	1081.23	1145.72	1278.46	1305.45	1338.13	1366.77	
1488.30	1674.54	3204.63	3261.59	3285.45	3829.50			

TS E-int1

Atom	X	Y	Z (Angstrom)
6	-0.153246	1.360741	-0.435905
6	1.122346	1.257246	-0.109996
6	1.261894	-0.115493	0.545122
8	-0.004740	-0.328535	1.120225
6	-0.782054	0.052596	0.004340
8	1.416941	-1.091452	-0.437547
8	-2.115231	0.071664	0.242360
8	-0.504237	-0.934886	-0.978843
1	-2.381911	-0.816497	0.512496
1	1.947947	1.904943	-0.354975
1	2.066103	-0.261702	1.268601
1	-0.667651	2.108391	-1.017044

Energy -455.531103 (Hartree)

Frequencies (cm-1):

501.50i	270.05	330.79	383.56	419.76	444.80	518.92	620.69	
669.08	696.40	758.06	834.13	864.44	926.53	970.60	991.45	
1010.10	1044.36	1068.41	1115.23	1248.41	1277.18	1311.96	1329.22	
1448.43	1695.91	3104.18	3257.66	3281.67	3827.42			

intermediate1

Atom	X	Y	Z (Angstrom)
6	1.371739	-0.103626	0.490010
8	0.161621	-0.819984	0.489094
6	-0.878901	-0.036664	-0.062571
6	-0.261959	1.309422	-0.318180
6	1.019191	1.272799	-0.010419
8	-1.953198	0.038343	0.806230
1	-2.248316	-0.863851	0.985702
1	1.748200	2.062081	-0.106994
1	1.802037	-0.115329	1.495126
1	-0.843304	2.118222	-0.730707
8	-1.399378	-0.643666	-1.179498
8	2.196075	-0.806282	-0.395347

Energy -455.542077 (Hartree)

Frequencies (cm-1):

77.01	188.79	279.59	353.61	359.92	385.43	485.61	554.69	
612.51	691.02	770.66	835.30	863.76	972.94	1002.16	1035.75	
1098.68	1117.68	1123.16	1146.84	1200.31	1313.22	1361.72	1433.22	
1442.65	1723.77	3071.30	3248.34	3272.61	3825.04			

TS int1-int2

Atom	X	Y	Z (Angstrom)
6	1.096737	1.220327	0.026617
6	1.410442	-0.220790	0.401911
8	0.155217	-0.881117	0.379432
6	-0.847264	-0.011568	-0.001858
6	-0.193672	1.319556	-0.215457
8	2.320738	-0.732959	-0.436803
8	-1.966214	-0.039659	0.834088
8	-1.667264	-0.484303	-1.027672
1	-2.468722	-0.594362	-0.123295
1	1.867637	1.970090	-0.039656
1	1.825770	-0.301513	1.419403
1	-0.761960	2.184939	-0.516085

Energy -455.515655 (Hartree)

Frequencies (cm-1):

1905.35i 79.92 182.81 329.83 376.86 461.79 500.13 577.43
587.46 635.01 758.88 796.37 857.68 903.76 939.38 986.35
991.08 1050.97 1097.54 1128.35 1165.77 1199.70 1265.72 1332.44
1383.41 1720.91 2274.16 2973.85 3258.76 3281.98

intermediate2

Atom	X	Y	Z (Angstrom)
6	1.044035	1.229216	-0.068728
6	1.373163	-0.168852	0.436170
8	0.119895	-0.821277	0.533613
6	-0.902573	-0.015434	0.022976
6	-0.245021	1.294575	-0.325303
8	2.245696	-0.755978	-0.397066
8	-1.922209	0.076442	0.945121
8	-1.523606	-0.564238	-1.088499
1	1.808745	1.975148	-0.209594
1	1.835073	-0.157388	1.435801
1	-0.816625	2.123382	-0.711091
1	-1.803032	-1.457761	-0.851148

Energy -455.556831 (Hartree)

Frequencies (cm-1):

71.27 173.64 251.48 337.44 359.58 402.14 498.50 556.04
583.25 688.61 753.10 798.54 875.08 906.37 992.10 1029.70
1087.58 1094.19 1114.51 1128.42 1171.18 1213.18 1294.88 1335.02
1433.02 1722.18 2984.76 3255.36 3279.43 3828.81

TS int2-int3

Atom	X	Y	Z (Angstrom)
6	-0.898288	-0.041923	-0.031341
6	-0.401402	1.394584	-0.089364
6	0.912301	1.317064	-0.006746
6	1.232852	-0.188868	0.000705
8	0.122479	-0.781892	-0.650970
8	2.375513	-0.689774	-0.110060
8	-0.895739	-0.479265	1.316658
8	-2.135250	-0.249293	-0.548512
1	1.674208	2.070566	0.099152
1	0.903005	-0.416851	1.176580
1	-1.051175	2.254498	-0.095058
1	-2.334833	-1.191567	-0.477120

Energy -455.526325 (Hartree)

Frequencies (cm-1):

1607.18i 261.60 292.23 304.12 356.44 407.14 461.84 505.40
594.86 634.06 682.17 704.44 771.71 825.11 864.58 892.75
953.20 981.53 1044.86 1046.92 1149.42 1268.33 1300.53 1406.46
1432.65 1676.87 1706.80 3260.62 3287.40 3829.23

intermediate3

Atom	X	Y	Z (Angstrom)
6	1.028907	1.254540	-0.054435
6	1.393964	-0.186621	0.021131
8	0.233561	-0.910332	0.029056
6	-0.894522	-0.034217	0.013277
6	-0.287382	1.349020	-0.058277
8	2.469370	-0.690898	0.054623
8	-1.637865	-0.147144	1.153390
8	-1.697009	-0.371091	-1.067399
1	-2.116842	-0.983622	1.111298
1	1.775186	2.030175	-0.093805
1	-0.915708	2.224719	-0.095843
1	-1.132894	-0.611882	-1.809191

Energy -455.733132 (Hartree)

Frequencies (cm-1):

115.18 198.08 248.00 301.84 403.10 412.33 459.86 567.29
576.18 686.69 723.88 747.50 858.92 872.47 959.41 1007.53
1038.67 1086.23 1138.75 1174.05 1242.76 1336.73 1376.18 1461.02
1714.47 1927.23 3258.25 3284.40 3838.05 3873.71

TS int3-F

Atom	X	Y	Z (Angstrom)
6	0.818163	0.041850	-0.239821
6	0.208746	1.380964	0.056519
6	-1.101563	1.239467	0.149978
6	-1.425638	-0.200870	-0.029916
8	-0.244126	-0.865755	-0.280811
8	-2.471437	-0.757181	0.019879
8	1.804397	-0.128618	-1.040484
8	1.706797	-0.404485	1.099242
1	2.308744	-0.516627	0.096621
1	-1.865934	1.976758	0.329423
1	0.817983	2.266898	0.130961
1	1.375900	-1.247185	1.439822

Energy -455.662271 (Hartree)

Frequencies (cm-1):

1656.36i 120.04 191.41 301.38 384.67 398.18 484.45 551.13
580.74 674.53 707.54 763.00 832.41 873.34 893.98 929.32
958.08 1005.43 1076.46 1107.08 1292.15 1333.16 1342.80 1560.43
1704.92 1939.62 2076.93 3265.84 3288.18 3818.20

F

Atom	X	Y	Z (Angstrom)
6	0.661714	1.255844	0.000000
6	1.121775	-0.162477	-0.000000
8	-0.000000	-0.964313	0.000000
6	-0.661714	1.255844	-0.000000
6	-1.121775	-0.162476	-0.000000
8	-2.222913	-0.597813	0.000000
1	-1.356309	2.079547	0.000000
1	1.356310	2.079547	0.000000
8	2.222913	-0.597813	0.000000

Energy -379.295342 (Hartree)

Frequencies (cm-1):

166.40 271.13 413.70 566.74 650.47 653.68 715.46 797.77
883.09 893.25 961.60 1014.93 1076.54 1089.83 1311.70 1336.73
1693.55 1910.43 1978.87 3265.64 3286.84

Formation of maleic anhydride with 2 water molecules:

Singlet O_2

Atom	X	Y	Z (Angstrom)
8	0.000000	0.000000	0.594632
8	0.000000	0.000000	-0.594632

Energy -150.298750 (Hartree)

Frequencies (cm-1):

1753.05

B

Atom	X	Y	Z (Angstrom)
6	-1.277937	-0.368040	-0.230405
6	-1.650436	0.646763	0.582602
6	-0.703042	1.697852	0.310284
6	0.146793	1.231612	-0.628465
8	-0.206006	-0.047482	-0.969317
8	-1.770620	-1.601892	-0.393163
8	2.839992	-0.219541	-0.695931
8	1.254301	-0.668482	1.674274
1	-2.481282	0.649382	1.263090
1	-1.290483	-2.033488	-1.108648
1	1.026437	1.608555	-1.114029
1	0.611924	-1.369572	1.806762
1	0.724684	0.128292	1.546862
1	3.724516	-0.085671	-0.351548
1	2.323868	-0.521788	0.065275
1	-0.673269	2.674351	0.761230

Energy -458.116742 (Hartree)

Frequencies (cm-1):

39.66	51.81	96.77	107.22	134.93	151.82	175.28	192.55
201.91	256.98	302.23	323.29	432.36	454.20	624.18	665.85
692.92	699.14	768.50	801.37	900.95	906.72	993.63	1022.38
1108.01	1177.00	1203.42	1281.51	1328.21	1476.02	1591.48	1617.55
1649.73	1712.35	3281.56	3305.53	3331.50	3750.37	3817.29	3858.71
3933.47	3938.48						

TS B–E

Atom	X	Y	Z (Angstrom)
6	-0.304258	-0.631286	1.052562
6	0.610398	0.376370	1.326274
6	1.079576	0.791456	0.082359
8	0.332436	0.261666	-0.903736
6	-0.335670	-0.769232	-0.329966
8	1.889781	1.792593	-0.221465
8	2.295951	-0.914423	-0.083670
8	1.469072	-1.828057	-0.325747
8	-3.259433	-1.041880	-0.157135
8	-2.358862	1.689805	-0.086696
1	2.409463	1.542940	-0.997268
1	-0.817946	-1.277170	1.741547
1	-0.976054	-1.351551	-0.965412
1	1.018699	0.688012	2.270361
1	-3.133614	-0.081464	-0.150362
1	-4.207441	-1.181024	-0.178478
1	-1.841849	1.838585	-0.883148
1	-1.703084	1.540180	0.602976

Energy -608.395070 (Hartree)

Frequencies (cm-1):

580.96i	24.61	42.10	58.44	111.94	128.90	159.11	163.94
195.95	201.64	204.64	212.72	267.68	293.92	314.04	361.60
437.95	455.08	531.13	595.79	614.59	652.15	705.59	792.16
870.66	891.89	924.78	971.55	1055.99	1119.15	1169.17	1200.86

1288.83 1303.10 1387.19 1495.21 1508.10 1627.15 1629.12 1645.38
3293.89 3307.10 3326.32 3735.90 3814.07 3837.26 3932.46 3941.56

E

Atom	X	Y	Z (Angstrom)
8	1.033648	-1.717263	-0.456810
6	-0.173078	-0.938026	-0.344751
8	0.248851	0.300198	-0.878229
6	1.292740	0.455328	0.076033
8	2.051511	-0.751660	-0.160899
6	-0.356749	-0.627470	1.130666
6	0.583825	0.269252	1.397735
8	2.068984	1.536691	-0.088645
8	-3.130096	-0.832573	-0.021125
8	-2.176536	1.799740	-0.305602
1	2.532125	1.451252	-0.932173
1	-1.037802	-1.146746	1.783025
1	-0.972578	-1.411795	-0.897417
1	0.926475	0.676140	2.334608
1	-2.979799	0.121809	-0.123635
1	-4.008487	-0.997728	-0.366903
1	-1.312233	1.513963	-0.632651
1	-1.999026	2.157525	0.567532

Energy -608.462134 (Hartree)
Frequencies (cm-1):
34.28 51.53 80.13 132.08 143.72 169.91 211.46 222.41
283.93 308.40 337.29 369.42 396.45 433.85 463.70 555.36
572.49 686.90 706.42 729.50 742.64 757.67 832.91 877.87
912.88 955.44 986.96 1000.36 1008.31 1042.80 1079.55 1131.63
1267.88 1314.62 1335.49 1358.05 1483.11 1639.13 1645.78 1672.51
3232.68 3266.58 3292.20 3667.73 3776.07 3822.80 3926.43 3939.48

TS E-F

Atom	X	Y	Z (Angstrom)
6	-1.279200	-0.428015	-0.085686
6	-1.041954	0.005304	1.338103
6	-0.223130	1.042351	1.357022
6	0.205747	1.383772	-0.039435
8	-0.471015	0.417240	-0.872793
8	0.382000	2.546502	-0.476736
8	-0.924183	-1.779065	-0.255938
8	-2.506969	-0.201011	-0.595895
1	-1.275151	-2.043510	-1.116543
1	0.111981	1.621888	2.202353
1	1.414097	0.911196	-0.099053
1	-1.548456	-0.467842	2.164591
8	2.644763	0.279766	-0.197177
1	2.406852	-0.686797	-0.102643
1	2.958617	0.422316	-1.096385
8	1.779043	-2.151469	0.109117
1	0.811484	-2.097109	-0.014399
1	1.922682	-2.576312	0.957433

Energy -608.428119 (Hartree)
Frequencies (cm-1):
1452.69i 37.37 68.38 83.40 122.44 184.45 224.27 253.25
312.83 323.33 345.31 365.45 384.73 431.98 462.38 474.56
508.87 555.32 592.74 620.82 692.51 737.18 756.74 822.25
835.96 875.16 976.11 988.43 1001.28 1027.53 1123.83 1138.03
1180.93 1209.21 1305.15 1328.38 1434.97 1537.24 1626.10 1649.07
1699.73 3112.95 3248.13 3272.11 3558.53 3818.20 3881.87 3927.16

F

Atom	X	Y	Z (Angstrom)
6	0.732436	1.129604	0.370587
8	0.308939	0.675887	-0.854766
6	-1.075360	0.585626	-0.836627
6	-1.532678	1.040410	0.504579
6	-0.463652	1.377158	1.209445
8	-1.688744	0.215111	-1.778847
8	1.888932	1.273854	0.619933
8	-2.196399	-1.717729	0.608611
8	0.616313	-1.686056	0.892595
8	2.719510	-1.112649	-0.817181
1	-2.441261	-1.941831	-0.291885
1	-0.386078	1.735591	2.221723
1	2.812216	-0.222317	-0.451238
1	-2.573596	1.032844	0.775880
1	1.357839	-1.633920	0.259257
1	2.350681	-0.972973	-1.693625
1	-1.238616	-1.860279	0.656661
1	0.965946	-2.121259	1.672550

Energy -608.618856 (Hartree)

Frequencies (cm-1):

35.49	58.99	64.39	104.20	117.78	142.48	154.75	174.49	
186.19	208.36	224.62	256.20	279.06	293.23	295.79	380.52	
420.17	468.83	533.31	574.60	643.29	652.98	669.75	714.72	
784.88	815.69	872.99	900.83	966.44	994.70	1079.19	1098.30	
1320.95	1339.54	1645.34	1649.20	1660.45	1690.82	1889.51	1968.82	
3279.67	3305.02	3561.15	3722.21	3789.08	3917.21	3925.29	3929.71	

Formation of maleic anhydride with OH:

Triplet O_2

Atom	X	Y	Z (Angstrom)
8	0.000000	0.000000	0.594932
8	0.000000	0.000000	-0.594932

Energy -150.321735 (Hartree)

Frequencies (cm-1):

1758.25

OH

Atom	X	Y	Z (Angstrom)
8	0.000000	0.000000	0.107936
1	0.000000	0.000000	-0.863486

Energy -75.730487 (Hartree)

Frequencies (cm-1):

3776.00

OOH

Atom	X	Y	Z (Angstrom)
8	0.055050	-0.600572	0.000000
8	0.055050	0.708417	0.000000
1	-0.880808	-0.862760	0.000000

Energy -150.904168 (Hartree)

Frequencies (cm-1):

1254.95 1459.86 3700.76

NO

Atom	X	Y	Z (Angstrom)
7	0.000000	0.000000	-0.606661
8	0.000000	0.000000	0.530829

Energy -129.891119 (Hartree)

Frequencies (cm-1): 2074.35

NO_2

Atom	X	Y	Z (Angstrom)
7	0.000000	0.000000	0.315041
8	0.000000	1.090464	-0.137830
8	0.000000	-1.090464	-0.137830

Energy -205.070765 (Hartree)

Frequencies (cm-1):

784.74 1470.98 1786.94

A

Atom	X	Y	Z (Angstrom)
6	-0.973626	1.052301	-0.000005
6	-1.637087	-0.097394	-0.000005
8	-0.939506	-1.272029	0.000004
6	0.479191	1.159458	0.000009
6	1.331959	0.152714	0.000000
8	2.142786	-0.668537	-0.000007
1	0.956936	2.128539	0.000024
1	-1.535291	1.972703	-0.000014
1	-2.716254	-0.156131	-0.000014
1	-1.534250	-2.023064	0.000026

Energy -305.216208 (Hartree)

Frequencies (cm-1):

103.19 150.40 212.64 269.23 479.16 536.67 591.83 618.86
741.80 828.88 921.99 949.66 1084.24 1150.33 1226.14 1284.51
1413.37 1461.13 1764.24 2238.73 3220.35 3224.48 3257.08 3926.26

TS Habs

Atom	X	Y	Z (Angstrom)
6	0.557250	1.568910	-0.140568
6	1.662833	0.660434	-0.355195
6	1.655180	-0.637445	-0.090583
8	1.742891	-1.766513	0.113517
6	-0.642401	1.189639	0.315519
8	-0.849070	-0.094688	0.655690
8	-2.980889	-0.802656	-0.389990
1	-2.763535	-0.557121	-1.302893
1	2.598291	1.013005	-0.764925
1	0.729434	2.613488	-0.348120
1	-1.459505	1.884984	0.461185
1	-1.805315	-0.332719	0.545979

Energy -380.952265 (Hartree)

Frequencies (cm-1):

1314.23i 30.81 66.21 133.99 155.69 193.97 254.21 293.42
479.45 486.79 536.80 596.27 624.70 776.07 842.91 936.07
961.85 1099.06 1155.42 1231.46 1262.40 1409.60 1463.20 1627.73
2179.90 2693.58 3200.45 3225.85 3250.37 3790.90

rad

Atom	X	Y	Z (Angstrom)
6	-1.403051	0.650773	0.000003
6	-1.265611	-0.727757	-0.000001
8	0.013077	-1.105380	0.000000
6	-0.126744	1.173749	-0.000001
6	0.804700	0.069171	0.000000
8	1.999578	-0.003141	-0.000001
1	0.186755	2.202361	0.000004
1	-2.339416	1.181160	-0.000010
1	-2.004342	-1.510970	0.000001

Energy -304.625857 (Hartree)

Frequencies (cm-1):

259.76 500.25 534.97 689.70 710.48 764.34 803.63 819.06
884.23 924.02 1046.87 1101.69 1123.54 1225.99 1367.51 1423.56

1521.12   1816.71   3273.46   3287.61   3300.91

TS rad+O_2

Atom	X	Y	Z (Angstrom)
6	0.328076	1.483335	-0.377870
6	0.617116	0.797598	0.836693
8	-0.339820	-0.078000	1.129159
6	-0.739138	0.866130	-0.924192
6	-1.219145	-0.146721	0.020768
8	-2.143910	-0.890219	0.014849
1	-1.220789	1.044216	-1.869553
1	0.936725	2.267769	-0.794010
1	1.276822	1.084612	1.637652
8	1.910802	-0.553626	-0.001533
8	1.208651	-1.277986	-0.680785

Energy -454.943896 (Hartree)
Frequencies (cm-1):
494.09i 114.51 141.45 215.24 302.32 404.78 500.63 569.93
703.52 716.51 808.69 818.69 864.87 874.86 966.27 1050.92
1098.07 1118.70 1228.59 1367.87 1407.33 1514.71 1591.40 1903.12
3270.95 3282.41 3298.21

peroxyl rad

Atom	X	Y	Z (Angstrom)
6	-0.112795	1.488161	0.125162
6	0.677306	0.254961	0.459114
8	-0.216010	-0.812590	0.352510
6	-1.352395	1.129427	-0.156277
6	-1.455168	-0.350001	-0.026959
8	-2.385786	-1.065762	-0.187919
1	-2.192933	1.737120	-0.445817
1	0.327921	2.472242	0.116716
1	1.153990	0.243819	1.437703
8	1.716639	0.110592	-0.518410
8	2.656324	-0.680798	-0.085535

Energy -454.971637 (Hartree)
Frequencies (cm-1):
71.48 124.05 214.15 351.65 460.01 500.73 565.91 702.93
717.64 825.28 856.52 903.46 999.24 1017.98 1043.63 1089.97
1146.89 1179.57 1258.75 1340.68 1378.92 1384.50 1707.27 1939.09
3134.34 3258.41 3287.89

oxyl radical

Atom	X	Y	Z (Angstrom)
6	0.705035	1.221260	0.126383
6	1.115681	-0.227292	0.356220
8	-0.090191	-0.967481	0.244031
6	-0.595142	1.255147	-0.095798
6	-1.134820	-0.131864	-0.021423
8	-2.255283	-0.505896	-0.149527
1	-1.226500	2.103830	-0.300359
1	1.427965	2.020555	0.136640
1	1.516564	-0.378143	1.371012
8	2.062655	-0.582842	-0.519452

Energy -379.813215 (Hartree)
Frequencies (cm-1):
127.07 230.81 388.44 489.11 554.86 696.55 707.15 779.88
849.54 897.32 920.73 1002.25 1061.59 1096.26 1122.70 1168.71
1197.89 1321.01 1350.98 1699.20 1925.01 2983.75 3260.91 3283.52

TS Habs by O_2

Atom	X	Y	Z (Angstrom)
6	1.831225	-0.409043	-0.028475
8	0.629426	-0.714006	0.546636
6	-0.263289	0.375444	0.378213
6	0.532984	1.451215	-0.319386
6	1.747727	0.981790	-0.551370
8	-1.141117	0.584375	1.246546
8	2.743878	-1.169990	-0.070276
1	2.588275	1.466800	-1.019514
1	0.103347	2.414072	-0.544325
1	-1.019946	-0.008964	-0.553420
8	-2.306592	-0.537331	-1.012227
8	-3.021040	-0.446591	-0.055259

Energy -530.121399 (Hartree)

Frequencies (cm-1):

1335.42i 60.70 96.13 139.83 184.88 232.18 321.54 402.33
522.96 541.13 600.71 684.23 724.41 799.24 854.71 884.31
921.30 1002.30 1049.45 1064.98 1088.12 1231.15 1254.23 1332.22
1615.48 1686.12 1687.83 1920.07 3259.53 3282.07

Anhydride

Atom	X	Y	Z (Angstrom)
6	0.661714	1.255844	0.000000
6	1.121775	-0.162477	-0.000000
8	-0.000000	-0.964313	0.000000
6	-0.661714	1.255844	-0.000000
6	-1.121775	-0.162476	-0.000000
8	-2.222913	-0.597813	0.000000
1	-1.356309	2.079547	0.000000
1	1.356310	2.079547	0.000000
8	2.222913	-0.597813	0.000000

Energy -379.295342 (Hartree)

Frequencies (cm-1):

166.40 271.13 413.70 566.74 650.47 653.68 715.46 797.77
883.09 893.25 961.60 1014.93 1076.54 1089.83 1311.70 1336.73
1693.55 1910.43 1978.87 3265.64 3286.84

S1 - First excited state

2-butenedial

Atom	X	Y	Z (Angstrom)
C	-1.101424	0.000000	-0.863990
C	-0.063582	0.000000	-1.869102
O	1.134633	0.000000	-1.633114
C	-0.910054	0.000000	0.547255
C	0.288818	0.000000	1.185044
O	0.398237	0.000000	2.528802
H	-1.796521	0.000000	1.156906
H	1.262501	0.000000	0.679930
H	-2.113111	0.000000	-1.225175
H	-0.399141	0.000000	-2.903409

Energy -303.48573585 (Hartree)

Frequencies (cm-1):

178.99 188.44 222.79 337.36 408.74 513.74 677.56 742.47
874.77 970.42 985.75 1002.91 1140.09 1225.72 1299.45 1406.42 1538.34
1562.70 1651.74 1750.53 3129.72 3231.92 3353.87 3380.59

TS ring closure

Atom	X	Y	Z (Angstrom)
C	-0.431143	0.182898	-0.927672
C	-0.139350	1.267949	0.048409
O	0.419340	-0.136722	-1.823221
O	-0.158124	-1.262794	0.257420
C	0.178821	0.790334	1.316513
C	0.131307	-0.583614	1.394459
H	0.202194	-1.209476	2.260504
H	0.411327	1.407992	2.161605
H	-0.161801	2.299171	-0.242309
H	-1.495469	-0.034863	-1.152629

Energy -303.4393962 (Hartree)

Frequencies (cm-1):

848.56i 163.24 315.71 438.30 515.82 563.77 650.23 690.66 879.60 899.89 903.40 1022.71 1096.03 1153.92 1255.44 1351.73 1405.87 1460.95 1528.50 1614.01 2977.08 3402.70 3415.38 3434.27

Cyclic intermediate – conical intersection

Atom	X	Y	Z (Angstrom)
C	0.077691	-0.328755	0.809312
C	1.222892	-0.091199	-0.130555
O	-0.013548	0.306936	1.924862
O	-1.160742	-0.106883	-0.163730
C	0.743906	0.115105	-1.396605
C	-0.660826	0.126266	-1.355400
H	-1.356979	0.274385	-2.154275
H	1.324797	0.271127	-2.283106
H	2.242601	-0.163577	0.186293
H	-0.058736	-1.429384	1.001604

Energy -303.45989428 (Hartree)

TS H-transfer

Atom	X	Y	Z (Angstrom)
C	-1.102687	0.000000	-0.977294
C	0.079520	0.000000	-1.707912
O	1.264818	0.000000	-1.185807
C	-1.114660	0.000000	0.419966
C	0.130398	0.000000	1.097464
O	0.429289	0.000000	2.261676
H	-2.026338	0.000000	0.986640
H	-2.025941	0.000000	-1.523586
H	0.072752	0.000000	-2.784030
H	1.009655	0.000000	0.158990

Energy -303.4755490 (Hartree)

Frequencies (cm-1):

1292.30i 222.43 388.34 421.79 521.96 553.54 558.71 835.47 873.42 881.52 948.00 1048.81 1173.78 1188.93 1235.19 1373.81 1503.89 1567.31 1604.79 1724.95 1852.36 3361.51 3391.66 3407.55

Ketene-enol – conical intersection

Atom	X	Y	Z (Angstrom)
C	-1.115614	0.000000	-0.859220
C	-0.109487	0.000000	-1.792514
O	1.209426	0.000000	-1.569061
C	-1.014595	0.000000	0.549742
C	0.210815	0.000000	1.264909
O	0.500482	0.000000	2.423036
H	-1.914927	0.000000	1.138103
H	-2.110404	0.000000	-1.265301

```
 H    -0.332155     0.000000    -2.840164
 H     1.392429     0.000000    -0.613104
Energy    -303.5073118        (Hartree)
```

Ketene-enol - ground state

```
 Atom      X            Y            Z (Angstrom)
 C    -1.081513    -0.219250    -0.800812
 C    -0.079280    -0.283169    -1.695876
 O     1.161787     0.235210    -1.571197
 C    -1.002475     0.420317     0.530998
 C    -0.093464     0.062805     1.424258
 O     0.705014    -0.251878     2.206972
 H    -1.721324     1.150251     0.850996
 H    -2.018979    -0.666311    -1.074956
 H    -0.195748    -0.791260    -2.632416
 H     1.195724     0.801849    -0.783594
Energy     -303.55904586      (Hartree)
```

S2 - Second excited state

2-butenedial

```
 Atom      X            Y            Z (Angstrom)
 C    -1.078306     0.000000    -0.851517
 C    -0.145095     0.000000    -1.877670
 O     1.136337     0.000000    -1.722350
 C    -0.868093     0.000000     0.566390
 C     0.338972     0.000000     1.254911
 O     0.369405     0.000000     2.539508
 H    -1.752512     0.000000     1.177665
 H     1.315675     0.000000     0.747957
 H    -2.102899     0.000000    -1.175004
 H    -0.477722     0.000000    -2.902935
Energy       -303.47017495    (Hartree)
Frequencies (cm-1):
    122.12   182.16   208.51   337.11   469.44   525.29   746.68   823.95
859.09   870.81   918.70  1029.31  1204.76  1255.50  1339.16  1377.31  1505.03
1515.14  1597.71  3083.19  3323.25  3360.61  3378.20  4353.57
```

2-butenedial - conical intersection

```
 Atom      X            Y            Z (Angstrom)
 C    -0.992252     0.000000    -0.738913
 C    -0.270230     0.000000    -1.926573
 O     0.972483     0.000000    -2.206733
 C    -0.647916     0.000000     0.664467
 C     0.507477     0.000000     1.442007
 O     0.264192     0.000000     2.708012
 H    -1.525846     0.000000     1.295455
 H     1.555589     0.000000     1.139570
 H    -2.054079     0.000000    -0.915924
 H    -0.888131     0.000000    -2.814688
Energy      -303.47502427     (Hartree)
```

TS H-transfer

```
 Atom      X            Y            Z (Angstrom)
 C    -1.073623     0.000000    -1.048246
 C     0.074165     0.000000    -1.741526
 O     1.297981     0.000000    -1.155462
 C    -1.101879     0.000000     0.413539
```

C	0.053049	0.000000	1.089125
O	0.420065	0.000000	2.314591
H	-2.039748	0.000000	0.934354
H	-1.997687	0.000000	-1.592140
H	0.158700	0.000000	-2.811469
H	1.015745	0.000000	0.407644

Energy -303.43373387 (Hartree)

Frequencies (cm-1):

2080.73i 92.86 279.87 280.36 464.96 518.14 581.56 587.42 647.38
862.01 899.11 1042.48 1121.18 1142.46 1246.68 1378.09 1482.21 1504.71
1629.05 1716.62 1829.96 3363.95 3389.94 3407.36

TS ring closure

Atom	X	Y	Z (Angstrom)
C	-0.406989	0.144630	-0.839484
C	-0.149331	1.239922	0.133432
O	0.394266	-0.041214	-1.861540
O	-0.147973	-1.191641	0.152777
C	0.188026	0.727916	1.374679
C	0.130044	-0.656444	1.340762
H	0.217466	-1.350808	2.151046
H	0.401356	1.297425	2.257288
H	-0.209577	2.274275	-0.138003
H	-1.479663	-0.001876	-1.091167

Energy -303.44696585 (Hartree)

Frequencies (cm-1):

114.64i 78.79 387.62 481.76 531.83 594.26 750.17 889.64
897.34 997.62 1058.23 1135.40 1175.01 1299.25 1362.71 1449.41 1458.03
1544.35 1641.81 2031.32 2950.94 3410.75 3422.60 3441.01