Supporting Information for

The Effects of H-Bonding and Sterics on the Photoreactivity of a Trimethyl Butyrophenone Derivative

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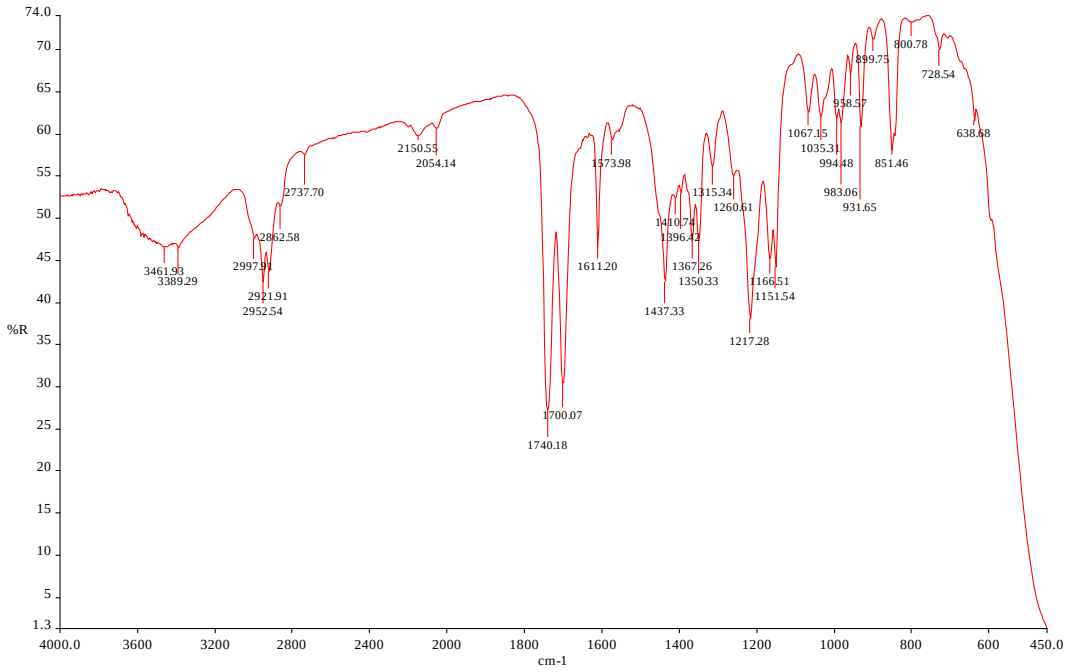
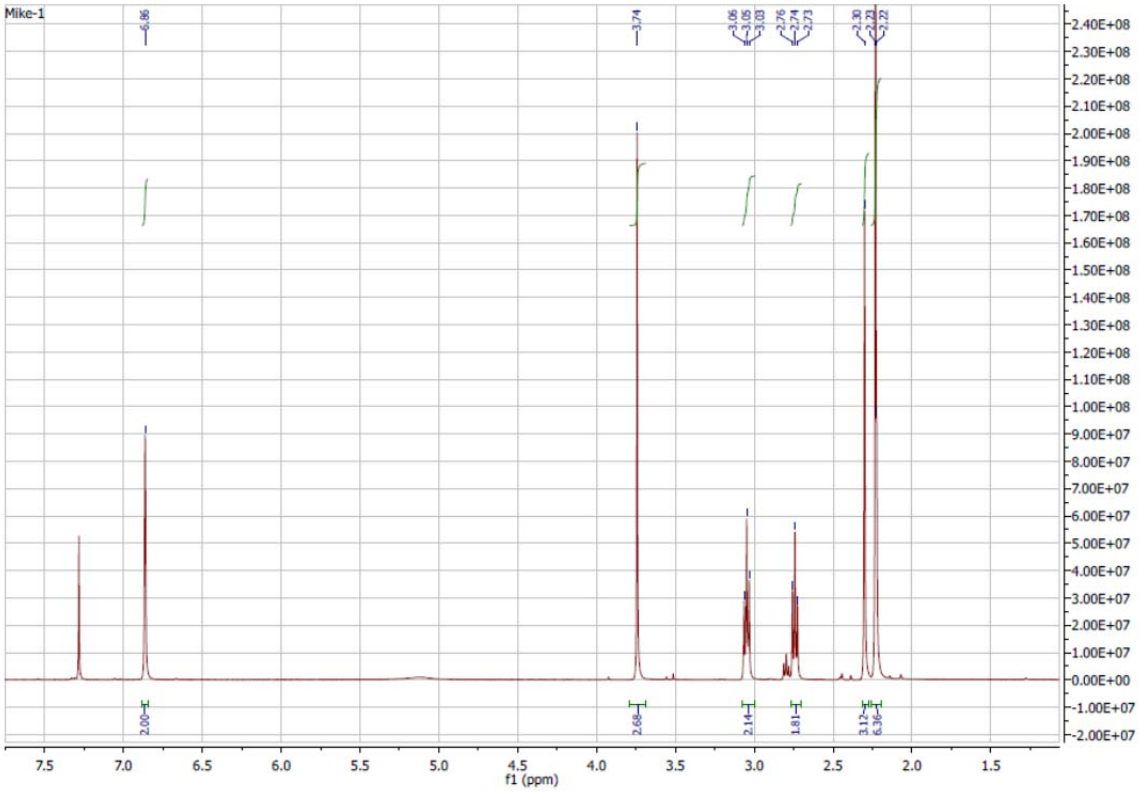
1. IR and NMR Spectra of 1, 4, 5

1.1. IR spectrum of 1



1.2. ^{1}H NMR spectrum of 1



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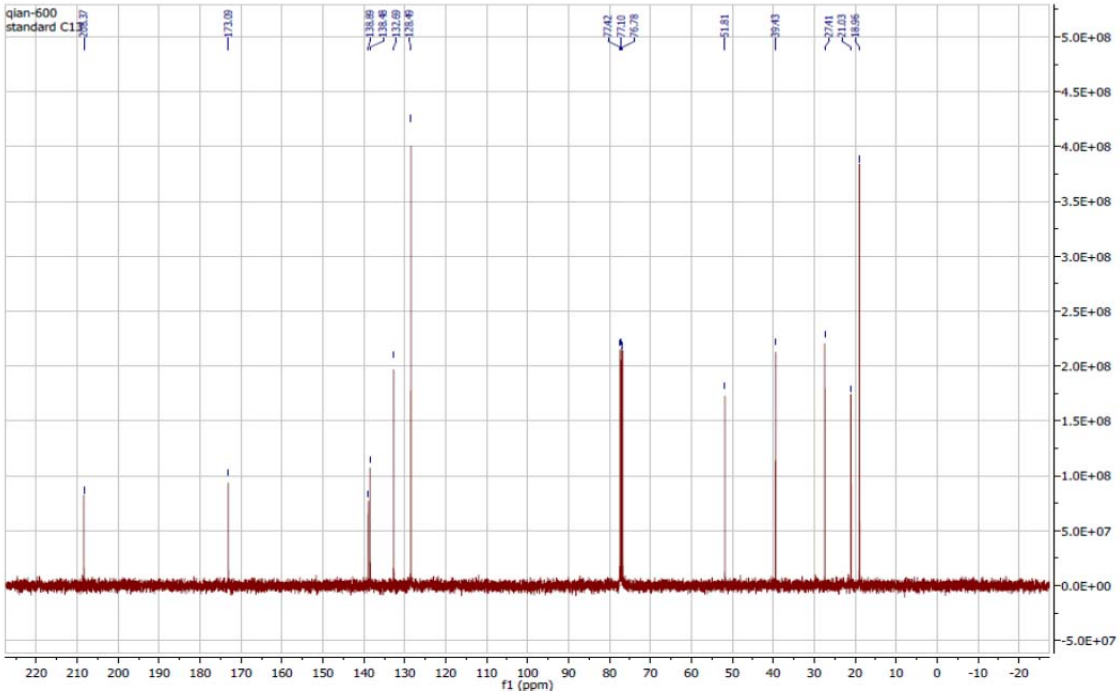
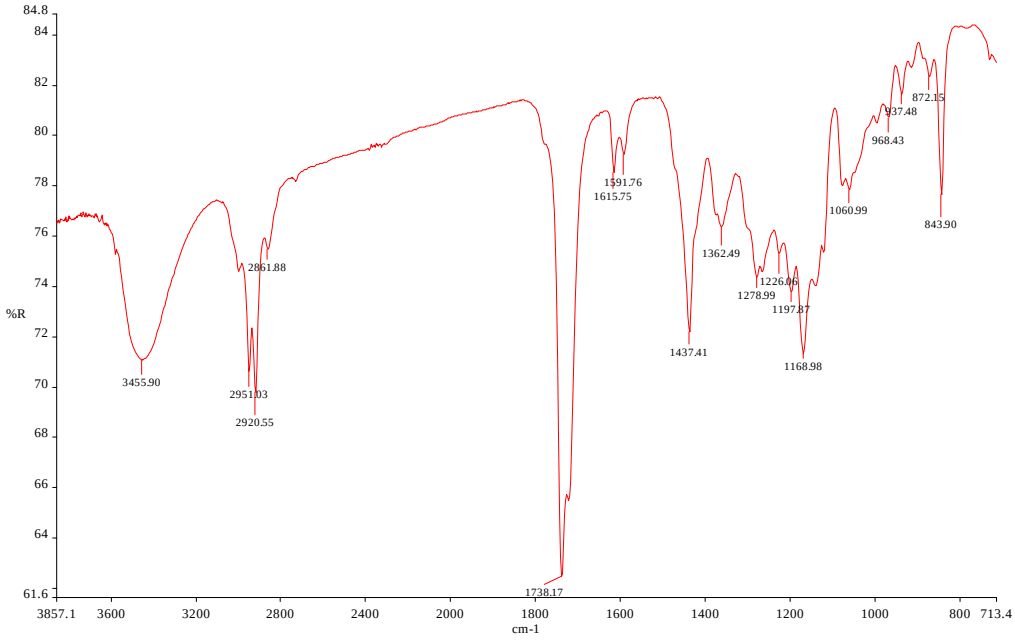


1.4. IR spectrum of 4



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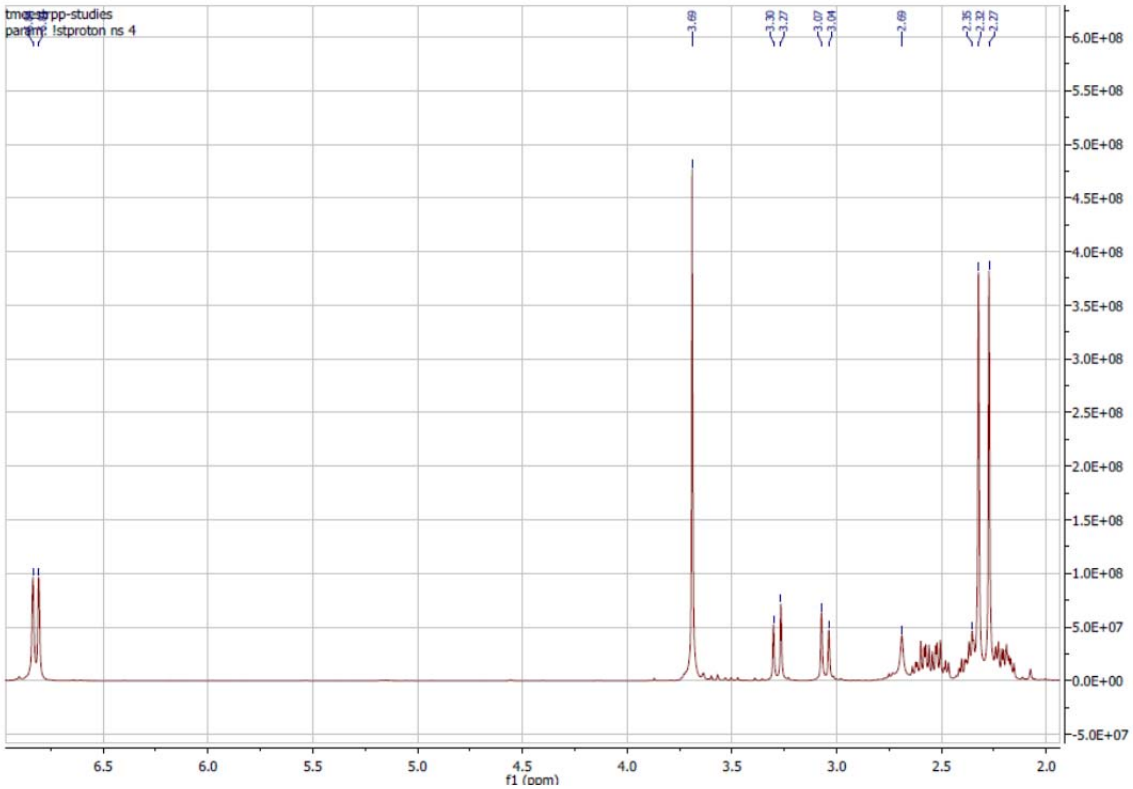

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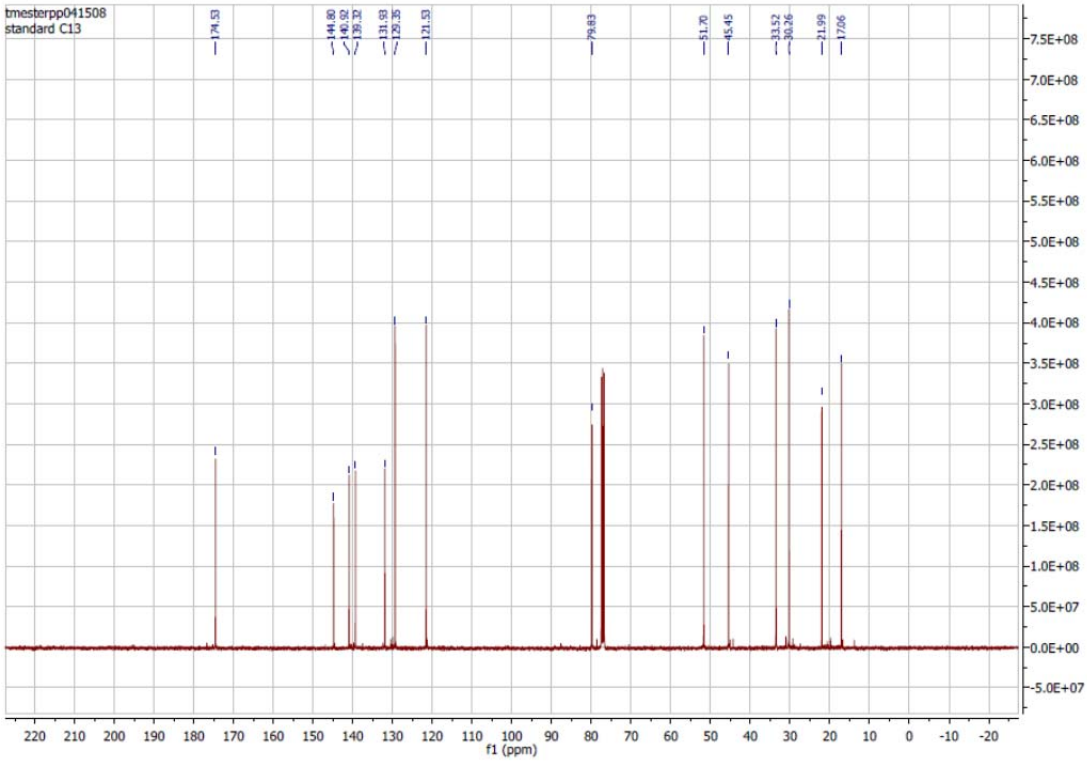

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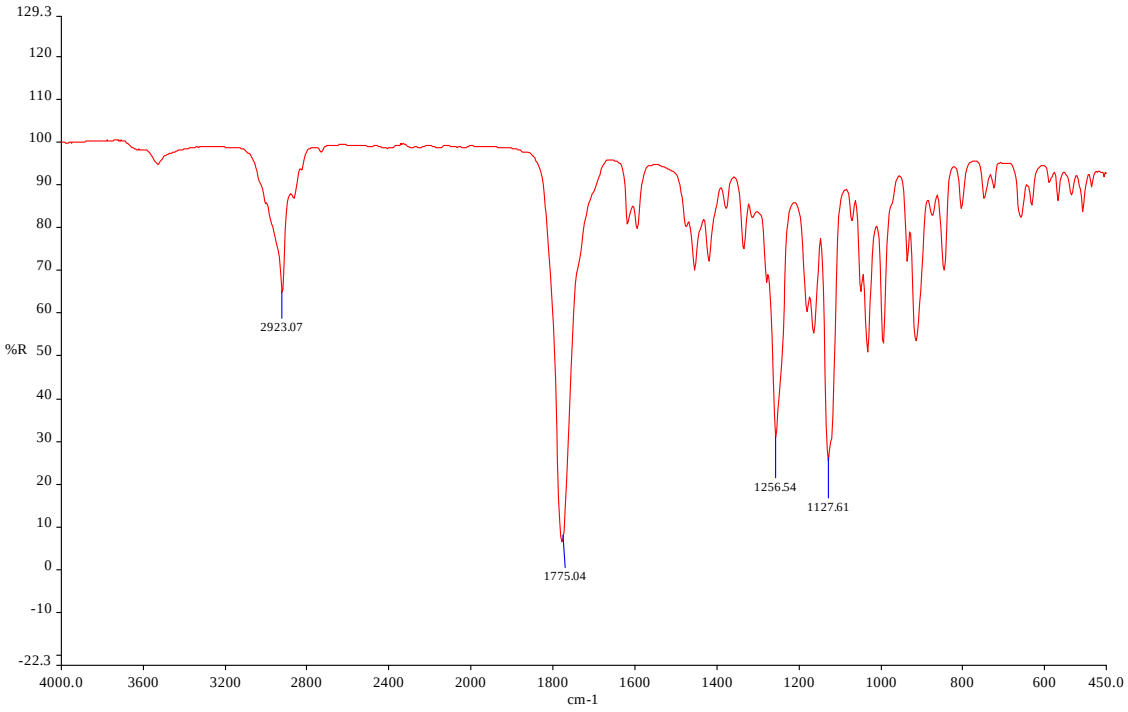
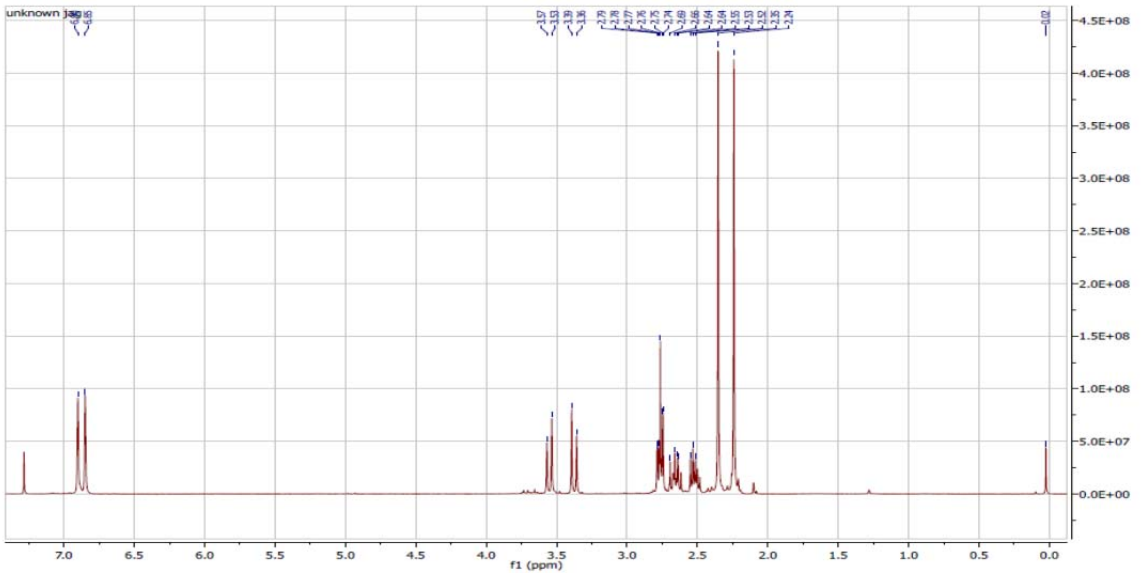
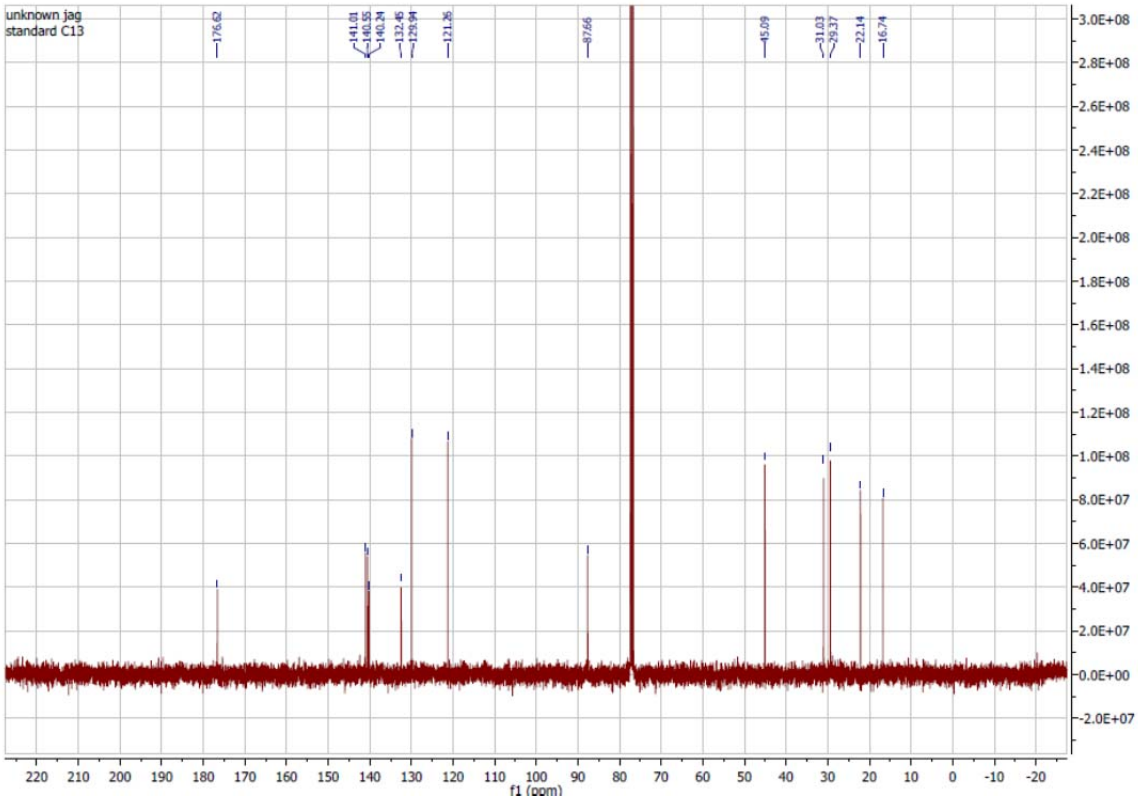


1.8. ^{1}H NMR spectrum of 5



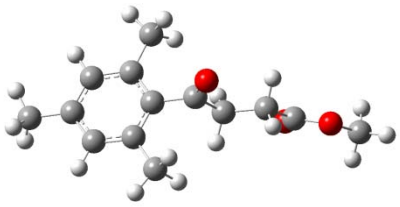
1.9. ^{13}C NMR spectrum of 5



2. Calculations for 1 (B3LYP/ 6-32+G(d))

2.1. Ester 1

E= -770.05398807 a. u.



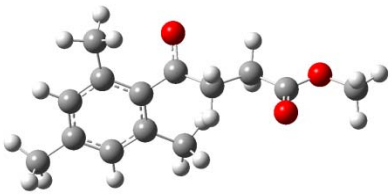
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.198879	-1.369058	-0.064984
2	6	0	1.885383	-1.167784	0.381759
3	6	0	1.363330	0.138694	0.376942
4	6	0	2.151591	1.226475	-0.058889
5	6	0	3.448929	0.974638	-0.512851
6	6	0	3.992882	-0.316674	-0.526743
7	1	0	3.610137	-2.376999	-0.044746
8	1	0	4.055471	1.811175	-0.856435
9	6	0	5.396771	-0.557005	-1.033178
10	1	0	5.448666	-0.444725	-2.124374
11	1	0	6.106813	0.158114	-0.600671
12	1	0	5.743502	-1.566445	-0.788012
13	6	0	1.082259	-2.355531	0.874146
14	1	0	0.454161	-2.780305	0.079254
15	1	0	1.748451	-3.154534	1.215699
16	1	0	0.426236	-2.095129	1.711830
17	6	0	1.621858	2.644735	-0.034243
18	1	0	0.671376	2.738815	-0.575081
19	1	0	1.440382	2.983221	0.991959
20	1	0	2.335127	3.332139	-0.499709
21	6	0	-0.040284	0.407935	0.869750
22	8	0	-0.240257	0.966303	1.937747
23	6	0	-1.182565	0.012711	-0.053925
24	6	0	-2.562033	0.165351	0.581742
25	1	0	-1.021041	-1.008664	-0.418421
26	1	0	-1.103091	0.639343	-0.954411
27	1	0	-2.694477	-0.523307	1.423466
28	1	0	-2.674342	1.168392	1.012273
29	6	0	-3.685589	-0.047107	-0.410754
30	8	0	-3.566732	-0.091245	-1.619643
31	8	0	-4.874862	-0.166602	0.220863
32	6	0	-6.028528	-0.330265	-0.625924
33	1	0	-5.932910	-1.237550	-1.228338

34	1	0	-6.876747	-0.406495	0.054865
35	1	0	-6.140212	0.532621	-1.287983

2.2. T_{1K} of 1

E= -769.94036823 a. u.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.498189	1.172360	0.092160
2	6	0	-3.751083	0.576585	0.208200
3	6	0	-3.946388	-0.810368	0.119628
4	6	0	-2.818052	-1.612686	-0.117043
5	6	0	-1.540170	-1.083364	-0.265471
6	6	0	-1.343345	0.333135	-0.105686
7	1	0	-4.612080	1.216521	0.394025
8	1	0	-2.950180	-2.688743	-0.220829
9	6	0	-0.406744	-2.015789	-0.623823
10	1	0	0.238167	-1.578633	-1.395035
11	1	0	0.232182	-2.260557	0.234553
12	1	0	-0.799823	-2.961828	-1.009808
13	6	0	-2.394642	2.669529	0.280586
14	1	0	-1.582414	2.928647	0.969659
15	1	0	-2.192325	3.196732	-0.657389
16	1	0	-3.329791	3.060746	0.694815
17	6	0	-5.315200	-1.420198	0.289195
18	1	0	-5.520252	-1.647732	1.345475
19	1	0	-6.103857	-0.741234	-0.054156
20	1	0	-5.407892	-2.359784	-0.267395
21	6	0	-0.011132	0.917758	-0.190662
22	8	0	0.043467	2.017761	-0.921419
23	6	0	1.264892	0.490002	0.488896
24	1	0	1.525177	1.239386	1.253177
25	1	0	1.081542	-0.436011	1.037854
26	6	0	2.467177	0.333509	-0.458543
27	1	0	2.252544	-0.391157	-1.254483
28	1	0	2.689512	1.276258	-0.971037
29	6	0	3.714794	-0.130343	0.264924
30	8	0	3.774390	-0.463692	1.431835

31	8	0	4.781639	-0.144728	-0.565860
32	6	0	6.025312	-0.592033	0.007598
33	1	0	6.752645	-0.535786	-0.802703
34	1	0	6.317970	0.058572	0.836001
35	1	0	5.929522	-1.618720	0.371071

2.2.1. TD-DFT of T_{1K} of 1 in the gas phase

Excited State 4: ?Spin -A 2.4606 eV 503.88 nm f=0.0170
64A -> 65A 0.25636
60B -> 63B 0.96206

Excited State 5: ?Spin -A 2.4665 eV 502.68 nm f=0.0114
64A -> 65A 0.93778
64A -> 66A -0.13454
60B -> 63B -0.25919

Excited State 6: ?Spin -A 2.7154 eV 456.60 nm f=0.0014
64A -> 65A 0.14221
64A -> 66A 0.98838

Excited State 7: ?Spin -A 3.1331 eV 395.73 nm f=0.0030
64A -> 67A 0.91584
64A -> 68A -0.36618
64A -> 70A 0.13381

Excited State 8: ?Spin -A 3.1759 eV 390.39 nm f=0.0008
64A -> 67A 0.39167
64A -> 68A 0.89390
64A -> 70A -0.18557

Excited State 9: ?Spin -A 3.2925 eV 376.56 nm f=0.0000
58B -> 63B -0.10870
59B -> 63B 0.99164

Excited State 10: ?Spin -A 3.5075 eV 353.48 nm f=0.0110
62A -> 65A -0.10749
38B -> 63B 0.15387
40B -> 63B 0.16531
44B -> 63B 0.11422
50B -> 63B 0.11593
51B -> 63B 0.36339
55B -> 63B -0.15294
56B -> 63B 0.83698

Excited State 11: ?Spin -A 3.6388 eV 340.72 nm f=0.0115
62A -> 65A -0.12409

63A -> 66A 0.26961
57B -> 63B 0.89105
58B -> 63B -0.18706
61B -> 65B 0.21705
62B -> 64B 0.18779

Excited State 12: ?Spin -A 3.6478 eV 339.89 nm f=0.0002
64A -> 69A 0.95748
64A -> 72A -0.23028

Excited State 13: ?Spin -A 3.6962 eV 335.44 nm f=0.0061
62A -> 65A -0.52693
62A -> 66A 0.15653
63A -> 65A 0.18729
63A -> 66A 0.44171
64A -> 71A 0.10232
56B -> 63B -0.11281
57B -> 63B -0.33254
61B -> 65B 0.49403
62B -> 64B 0.51371
62B -> 66B -0.13951
62B -> 68B -0.19716

Excited State 14: ?Spin -A 3.7425 eV 331.29 nm f=0.0007
52B -> 63B 0.11839
55B -> 63B 0.84217
56B -> 63B 0.15344
58B -> 63B 0.48261

Excited State 15: ?Spin -A 3.7945 eV 326.75 nm f=0.0011
64A -> 70A 0.16137
64A -> 71A 0.94698
64A -> 73A -0.17532
64A -> 74A 0.11951

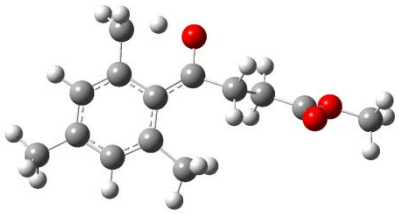
Excited State 16: ?Spin -A 3.9396 eV 314.71 nm f=0.0003
64A -> 68A 0.22698
64A -> 70A 0.93145
64A -> 71A -0.16777
64A -> 75A -0.15376

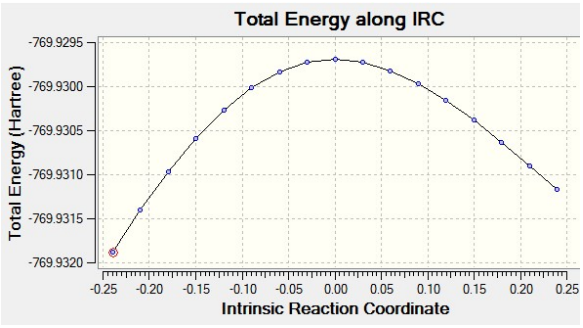
Excited State 17: ?Spin -A 4.0191 eV 308.49 nm f=0.0015
64A -> 69A 0.18508
64A -> 72A 0.77260
64A -> 73A -0.41029
64A -> 74A -0.40427
64A -> 79A 0.12516

2.2.2. TS for intramolecular H abstraction in T_{1K} of 1

E= -769.92968917 a. u.

Imaginary Frequency in IR = 1399.97





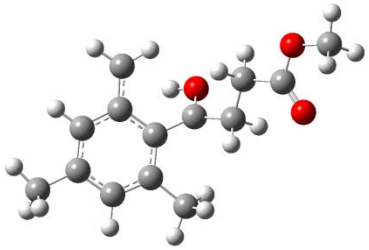
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.462651	1.145448	-0.021522
2	6	0	-3.710717	0.583524	-0.286569
3	6	0	-3.911775	-0.800385	-0.264483
4	6	0	-2.791761	-1.601363	0.015774
5	6	0	-1.511435	-1.102506	0.251455
6	6	0	-1.300102	0.323524	0.214666
7	1	0	-4.552084	1.246379	-0.482417
8	1	0	-2.921504	-2.682816	0.021993
9	6	0	-0.415651	-2.120690	0.485221
10	1	0	0.437501	-1.985047	-0.189412
11	1	0	-0.029996	-2.095395	1.511923
12	1	0	-0.805154	-3.129477	0.315884
13	6	0	-2.335405	2.623616	0.066073
14	1	0	-1.082934	2.757986	-0.125605
15	1	0	-2.878545	3.208226	-0.680435
16	1	0	-2.410729	3.055670	1.071263
17	6	0	-5.266315	-1.414371	-0.523817
18	1	0	-5.667246	-1.902727	0.375124
19	1	0	-5.992743	-0.657517	-0.839237
20	1	0	-5.219255	-2.179278	-1.310004
21	6	0	-0.036281	0.991166	0.322416
22	8	0	0.074881	2.309751	0.033444
23	6	0	1.313540	0.469433	0.757119
24	1	0	1.721925	1.179595	1.487765
25	1	0	1.227696	-0.482332	1.274644
26	6	0	2.312136	0.347452	-0.409885
27	1	0	1.931329	-0.333544	-1.183360
28	1	0	2.451820	1.313727	-0.906693

29	6	0	3.663199	-0.173894	0.035384
30	8	0	3.923424	-0.619712	1.135263
31	8	0	4.569063	-0.098227	-0.966632
32	6	0	5.888514	-0.591543	-0.665624
33	1	0	6.466499	-0.443799	-1.578300
34	1	0	6.324781	-0.028942	0.164015
35	1	0	5.847928	-1.651677	-0.401004

3.8. Biradical 2

2.10.1. Biradical 2 without intramolecular H-atom bonding

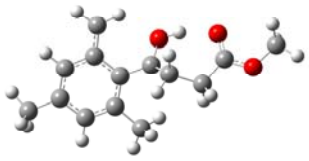


E= -769.95329992 a. u. In gas phase without H-bonding

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.225497	1.167351	-0.419500
2	6	0	-1.976974	1.197096	0.230691
3	6	0	-1.296037	-0.007249	0.495880
4	6	0	-1.907224	-1.258225	0.100218
5	6	0	-3.184027	-1.223400	-0.524954
6	6	0	-3.848047	-0.031625	-0.796962
7	1	0	-3.731227	2.111425	-0.616401
8	1	0	-3.632595	-2.168627	-0.825399
9	6	0	-5.197913	-0.018295	-1.477543
10	1	0	-5.539657	-1.033164	-1.706189
11	1	0	-5.959022	0.456332	-0.844960
12	1	0	-5.164852	0.544025	-2.419500
13	6	0	-1.406201	2.537163	0.640657
14	1	0	-0.694354	2.923801	-0.100980
15	1	0	-2.202198	3.282592	0.742923
16	1	0	-0.871344	2.471317	1.594054
17	6	0	-1.264047	-2.507401	0.271761
18	1	0	-0.264601	-2.598098	0.678331
19	1	0	-1.761059	-3.418963	-0.046217
20	6	0	0.008052	0.001966	1.178325
21	6	0	1.275754	0.616395	0.679545

22	6	0	2.283550	-0.425786	0.147748
23	1	0	1.762438	1.186440	1.484429
24	1	0	1.050142	1.330130	-0.117007
25	1	0	2.528265	-1.160267	0.923397
26	1	0	1.849569	-0.995924	-0.684487
27	6	0	3.571557	0.202264	-0.343450
28	8	0	3.790972	1.393423	-0.438405
29	8	0	4.475759	-0.745605	-0.686304
30	6	0	5.736697	-0.264357	-1.188470
31	1	0	6.235887	0.352384	-0.436260
32	1	0	6.321823	-1.158966	-1.403775
33	1	0	5.585272	0.326286	-2.096126
34	8	0	0.199076	-0.800534	2.289410
35	1	0	-0.656806	-1.144367	2.592884



2.3.2. Biradical 2A with intramolecular H-atom bonding

E= -769.95623958 a. u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.127979	1.278833	0.097846
2	6	0	-3.531010	1.039434	0.123403
3	6	0	-4.075415	-0.232835	-0.006504
4	6	0	-3.192814	-1.308829	-0.183296
5	6	0	-1.797458	-1.131562	-0.231835
6	6	0	-1.242118	0.152758	-0.084973
7	1	0	-4.191183	1.893070	0.268045
8	1	0	-3.596755	-2.313003	-0.302941
9	6	0	-0.922386	-2.344868	-0.465169
10	1	0	-0.136313	-2.130611	-1.198597
11	1	0	-0.424958	-2.682631	0.454699
12	1	0	-1.515890	-3.187335	-0.836596
13	6	0	-1.659932	2.598557	0.288772
14	1	0	-2.371886	3.405678	0.436306
15	1	0	-0.608436	2.848171	0.259617
16	6	0	-5.568585	-0.461857	0.061497
17	1	0	-5.866135	-0.863956	1.039792

18	1	0	-6.122603	0.470211	-0.093337
19	1	0	-5.899405	-1.180961	-0.697468
20	6	0	0.225921	0.329440	-0.093029
21	6	0	1.094728	-0.131957	1.048897
22	1	0	1.385866	0.731523	1.675644
23	1	0	0.487344	-0.775657	1.692779
24	6	0	2.378954	-0.923900	0.698643
25	1	0	2.762576	-1.434711	1.589542
26	1	0	2.153673	-1.712293	-0.032426
27	6	0	3.508972	-0.096989	0.126006
28	8	0	3.395019	0.998321	-0.407300
29	8	0	4.694248	-0.711965	0.255415
30	6	0	5.838966	-0.030311	-0.302017
31	1	0	6.686178	-0.685677	-0.101005
32	1	0	5.705267	0.114375	-1.376888
33	1	0	5.973454	0.939506	0.182988
34	8	0	0.701448	1.308925	-0.925553
35	1	0	1.674421	1.386564	-0.810081

2.3.3. TD-DFT of Biradical 2A

Excited State 1: ?Spin -A 2.5061 eV 494.72 nm f=0.0000
63A -> 65A -0.10762
64A -> 65A 0.99213

Excited State 2: ?Spin -A 2.7484 eV 451.11 nm f=0.0061
63A -> 67A 0.13904
64A -> 66A -0.32535
64A -> 67A 0.69249
62B -> 63B 0.65001
62B -> 64B 0.10513

Excited State 3: ?Spin -A 3.0762 eV 403.04 nm f=0.0043
63A -> 69A 0.26478
64A -> 66A -0.34026
64A -> 67A 0.11370
64A -> 68A -0.16001
64A -> 69A 0.62045
64A -> 70A -0.15839
64A -> 71A 0.10985
61B -> 63B 0.62460
62B -> 63B -0.13359

Excited State 4: ?Spin -A 3.0892 eV 401.35 nm f=0.0368
63A -> 66A -0.11457
63A -> 67A 0.15909
63A -> 69A 0.15626
64A -> 66A 0.79914
64A -> 68A 0.11915

64A -> 69A 0.25298
61B -> 63B 0.24981
62B -> 63B 0.38133

Excited State 5: ?Spin -A 3.1887 eV 388.82 nm f=0.0303
63A -> 67A -0.27815
64A -> 66A 0.29225
64A -> 67A 0.64078
64A -> 68A 0.14602
62B -> 63B -0.56187
62B -> 64B 0.18002

Excited State 6: ?Spin -A 3.5814 eV 346.19 nm f=0.0190
63A -> 69A -0.36466
64A -> 68A -0.43032
64A -> 69A 0.57910
64A -> 71A -0.20154
61B -> 63B -0.45726
62B -> 64B 0.14886

Excited State 7: ?Spin -A 3.6142 eV 343.05 nm f=0.0009
64A -> 66A -0.16753
64A -> 67A -0.18182
64A -> 68A 0.79124
64A -> 69A 0.39677
64A -> 70A 0.23973
64A -> 71A -0.16468
64A -> 72A -0.14572
61B -> 63B -0.11875

Excited State 8: ?Spin -A 3.6828 eV 336.66 nm f=0.0029
63A -> 65A 0.94501
63A -> 67A 0.17072
64A -> 65A 0.10404
64A -> 68A 0.10748
64A -> 71A 0.11878

Excited State 9: ?Spin -A 3.7412 eV 331.40 nm f=0.0176
63A -> 65A -0.20542
63A -> 66A -0.10663
63A -> 67A 0.14068
63A -> 69A -0.20059
64A -> 68A 0.21709
64A -> 70A -0.56834
64A -> 71A 0.65862
64A -> 73A -0.10866
61B -> 63B -0.19411

Excited State 10: ?Spin -A 3.7858 eV 327.50 nm f=0.0285
62A -> 67A 0.17687
63A -> 65A -0.19347

63A -> 66A	-0.29756
63A -> 67A	0.69001
63A -> 68A	0.10932
64A -> 67A	0.14369
64A -> 70A	0.27179
61B -> 63B	-0.13347
61B -> 64B	-0.12362
62B -> 63B	-0.25014
62B -> 64B	-0.32227

Excited State 11: ?Spin -A 3.8157 eV 324.93 nm f=0.0062

63A -> 67A	-0.12569
64A -> 68A	-0.11141
64A -> 69A	0.14422
64A -> 70A	0.66124
64A -> 71A	0.66343
64A -> 73A	0.14223

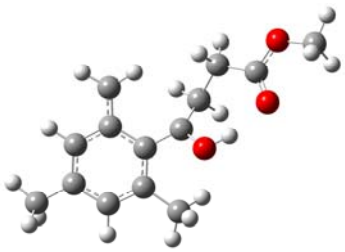
Excited State 12: ?Spin -A 4.0597 eV 305.41 nm f=0.0012

64A -> 68A	0.17372
64A -> 70A	-0.15378
64A -> 72A	0.78985
64A -> 73A	0.51442
64A -> 74A	0.14034

Excited State 13: ?Spin -A 4.1112 eV 301.57 nm f=0.0039

62A -> 67A	0.11516
63A -> 67A	-0.13844
64A -> 70A	-0.13236
64A -> 72A	-0.53317
64A -> 73A	0.69282
64A -> 74A	0.21314
64A -> 75A	0.16326
64A -> 78A	0.10938
64A -> 79A	-0.10567
62B -> 64B	-0.20535

2.3.4. Biradical 2B with intramolecular H-bonding



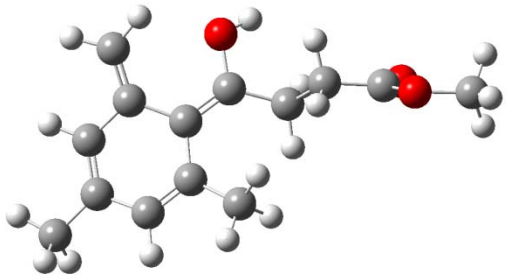
E = -769.95666348 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.867292	-1.229328	-0.221037
2	6	0	-3.283962	-1.324789	-0.144966
3	6	0	-4.093920	-0.208665	0.030859
4	6	0	-3.467177	1.039899	0.152177
5	6	0	-2.067662	1.195162	0.108642
6	6	0	-1.247549	0.066531	-0.086985
7	1	0	-3.738400	-2.307798	-0.255280
8	1	0	-4.081630	1.927314	0.297465
9	6	0	-1.498599	2.586112	0.296062
10	1	0	-0.657437	2.589251	0.997831
11	1	0	-1.120179	2.998250	-0.645289
12	1	0	-2.267040	3.263109	0.684804
13	6	0	-1.119832	-2.407111	-0.454438
14	1	0	-1.624986	-3.361213	-0.571340
15	1	0	-0.045367	-2.390976	-0.587723
16	6	0	-5.600485	-0.325085	0.083155
17	1	0	-6.070506	0.185870	-0.767447
18	1	0	-5.920759	-1.372227	0.060003
19	1	0	-6.005693	0.129386	0.996189
20	6	0	0.225212	0.175197	-0.157487
21	6	0	1.110547	-0.383629	0.926828
22	1	0	1.364731	0.406277	1.659069
23	1	0	0.527559	-1.125615	1.480782
24	6	0	2.426763	-1.076358	0.491434
25	1	0	2.804370	-1.711289	1.299983
26	1	0	2.240221	-1.742866	-0.362804
27	6	0	3.541148	-0.140668	0.079159
28	8	0	3.392406	0.980641	-0.387912
29	8	0	4.752157	-0.685708	0.265180
30	6	0	5.886791	0.105891	-0.150029
31	1	0	6.759096	-0.507271	0.075229
32	1	0	5.826555	0.319249	-1.220052
33	1	0	5.915941	1.044486	0.408533
34	8	0	0.700161	1.196936	-0.934876
35	1	0	1.671836	1.282156	-0.809339

2.4. Z-enol Z-3

2.4.1. Z-enol without intramolecular H-bonding

E= -769.98265634 a. u.

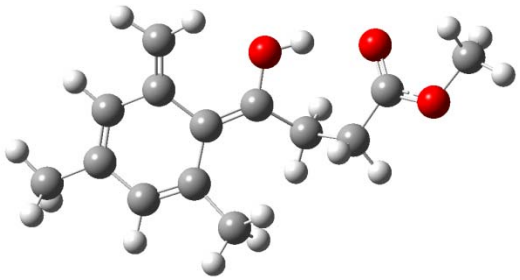


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.754648	-1.592153	-0.053166
2	6	0	1.500454	-1.097416	-0.235665
3	6	0	1.285294	0.365995	-0.135957
4	6	0	2.512338	1.211484	-0.288690
5	6	0	3.779889	0.578415	0.073012
6	6	0	3.913809	-0.761725	0.216566
7	1	0	2.912519	-2.666390	-0.142399
8	1	0	4.646597	1.230736	0.165431
9	6	0	5.223724	-1.424696	0.557776
10	1	0	6.026905	-0.689429	0.673616
11	1	0	5.148450	-1.993709	1.494834
12	1	0	5.525510	-2.136975	-0.222802
13	6	0	0.404290	-2.075391	-0.617458
14	1	0	-0.297850	-1.641558	-1.337082
15	1	0	0.848698	-2.959772	-1.085914
16	1	0	-0.178178	-2.436770	0.239570
17	6	0	2.543201	2.499066	-0.721183
18	1	0	1.673032	3.035396	-1.069152
19	1	0	3.492962	3.029497	-0.742211
20	6	0	0.073949	0.927345	0.173797
21	6	0	-1.198461	0.258734	0.627499
22	6	0	-2.345830	0.344393	-0.401217
23	1	0	-1.531706	0.762257	1.548375
24	1	0	-1.029483	-0.776959	0.913511
25	1	0	-2.424210	1.365460	-0.800187
26	1	0	-2.163474	-0.304512	-1.262319
27	6	0	-3.691869	0.005872	0.209901
28	8	0	-4.002137	0.199322	1.369100
29	8	0	-4.532372	-0.520062	-0.706244
30	6	0	-5.863590	-0.825682	-0.243817
31	1	0	-6.357450	0.080532	0.116557
32	1	0	-6.383518	-1.230153	-1.112403
33	1	0	-5.824657	-1.562171	0.562869
34	8	0	-0.047762	2.299708	0.134410
35	1	0	-0.777050	2.577337	0.713192

2.4.2. Z-3 with intramolecular H bonding

E= -769.98916778 a. u.



Standard orientation:

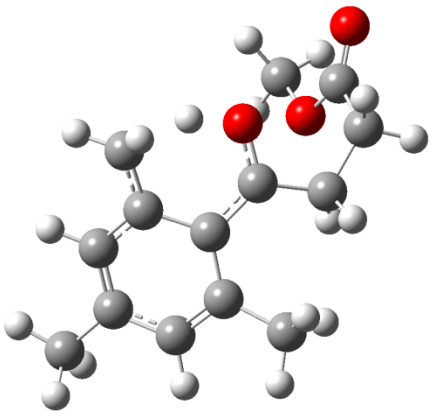
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.166540	-1.252239	-0.092629
2	6	0	1.810339	-1.172931	-0.180484
3	6	0	1.150787	0.148518	-0.073583
4	6	0	2.037949	1.338928	-0.276905
5	6	0	3.463947	1.130064	-0.026943
6	6	0	4.022787	-0.097778	0.093827
7	1	0	3.645312	-2.224119	-0.208415
8	1	0	4.088334	2.021242	0.010368
9	6	0	5.497276	-0.309053	0.326626
10	1	0	6.033693	0.643793	0.387602
11	1	0	5.678204	-0.858867	1.260836
12	1	0	5.948489	-0.900821	-0.482252
13	6	0	1.060632	-2.455318	-0.505333
14	1	0	0.191743	-2.272807	-1.147147
15	1	0	1.724573	-3.141448	-1.041827
16	1	0	0.709906	-2.996828	0.383194
17	6	0	1.643800	2.590584	-0.638203
18	1	0	0.627484	2.853546	-0.885833
19	1	0	2.390234	3.380256	-0.695444
20	6	0	-0.173835	0.304566	0.266024
21	6	0	-1.095663	-0.741404	0.853328
22	6	0	-2.341574	-1.113789	0.014939
23	1	0	-1.435621	-0.360196	1.828036
24	1	0	-0.545412	-1.651033	1.072351
25	1	0	-2.087704	-1.205920	-1.049372
26	1	0	-2.721973	-2.096389	0.317756
27	6	0	-3.489730	-0.131823	0.124325
28	8	0	-3.414347	0.995063	0.593834
29	8	0	-4.629724	-0.639455	-0.362483
30	6	0	-5.784420	0.229245	-0.342982
31	1	0	-5.590286	1.126358	-0.935741
32	1	0	-6.590087	-0.359186	-0.781220
33	1	0	-6.024051	0.513692	0.684326

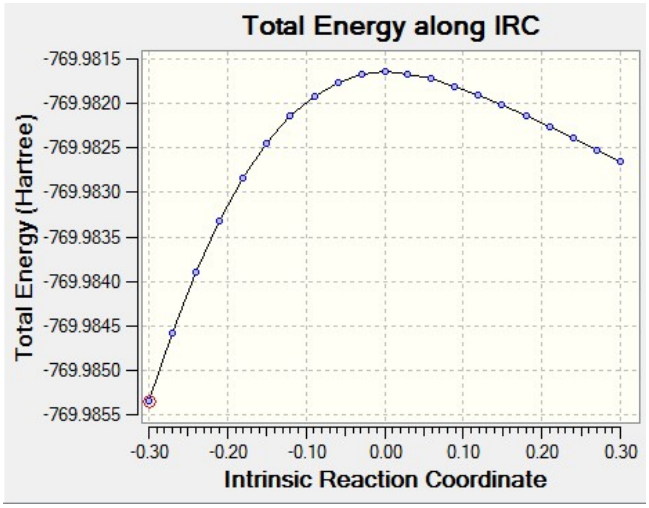
34	8	0	-0.730850	1.545084	0.206111
35	1	0	-1.656471	1.517773	0.531050

2.4.2. Transition State for 1,5-H shift in Z-3

E= -769.98164459 a. u.

Imaginary frequency: 1130 cm^{-1}





Standard orientation:

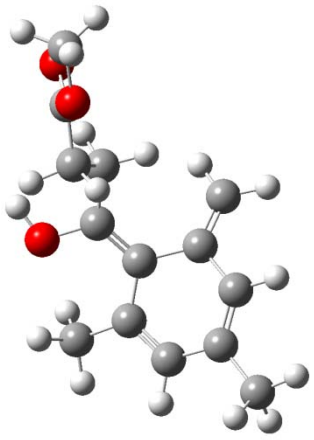
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.876134	0.815256	-0.746656
2	6	0	1.740099	1.315612	-0.159573
3	6	0	0.954495	0.442769	0.698393
4	6	0	1.539380	-0.834869	1.111487
5	6	0	2.634756	-1.330403	0.332829
6	6	0	3.298761	-0.541204	-0.572317
7	1	0	3.487090	1.471857	-1.363648
8	1	0	2.993787	-2.334990	0.547495
9	6	0	-0.441207	0.579623	0.895838
10	6	0	0.973890	-1.618337	2.142155
11	1	0	0.734875	-1.138659	3.093705
12	6	0	-3.317647	-0.051493	-0.298675
13	8	0	-4.351305	-0.599505	0.023002
14	8	0	-2.497182	-0.522542	-1.265371
15	6	0	-2.893461	-1.764460	-1.877135
16	1	0	-2.955404	-2.552988	-1.122744
17	1	0	-3.864918	-1.654526	-2.366577
18	1	0	-2.114931	-1.988356	-2.607032

19	8	0	-1.103822	-0.252809	1.651704
20	1	0	-0.437172	-1.134819	1.849163
21	1	0	1.341734	-2.637290	2.251618
22	6	0	4.502935	-1.040811	-1.330748
23	1	0	5.388158	-0.426658	-1.118492
24	1	0	4.739693	-2.077933	-1.073164
25	1	0	4.332001	-0.990048	-2.414315
26	6	0	1.413532	2.781437	-0.369230
27	1	0	0.643117	2.945135	-1.131144
28	1	0	1.069754	3.258009	0.555535
29	1	0	2.310055	3.313810	-0.702981
30	6	0	-1.332860	1.560279	0.152754
31	1	0	-1.052872	1.588538	-0.903712
32	1	0	-1.153795	2.566895	0.550109
33	6	0	-2.831853	1.262394	0.285085
34	1	0	-3.387869	2.056956	-0.231824
35	1	0	-3.156557	1.279163	1.328081

2.5. E-enol E-3

2.5.1. E-3 without intramolecular H-bonding

E= -769.98463928 a. u.



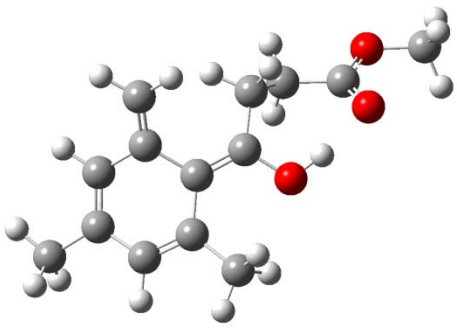
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.476837	0.237895	-0.622886
2	6	0	2.512170	1.095233	-0.189241
3	6	0	1.309025	0.511252	0.448511
4	6	0	1.505784	-0.840640	1.050744
5	6	0	2.443299	-1.718308	0.352551
6	6	0	3.400312	-1.206357	-0.461202

7	1	0	4.353297	0.644530	-1.125510
8	1	0	2.420000	-2.781068	0.587340
9	6	0	4.436907	-2.064660	-1.140049
10	1	0	4.297337	-3.125119	-0.905574
11	1	0	4.392935	-1.949363	-2.231841
12	1	0	5.451993	-1.778676	-0.831560
13	6	0	2.695073	2.583318	-0.388877
14	1	0	2.450756	3.143881	0.520410
15	1	0	3.737342	2.792945	-0.653372
16	1	0	2.052354	2.977767	-1.182153
17	6	0	0.944139	-1.234308	2.220240
18	1	0	0.361348	-0.562542	2.842373
19	1	0	1.101797	-2.241363	2.599442
20	6	0	0.073515	1.092610	0.386448
21	6	0	-1.258757	0.473921	0.730379
22	6	0	-2.151559	0.291228	-0.519656
23	1	0	-1.792624	1.099428	1.460759
24	1	0	-1.116719	-0.496937	1.202488
25	1	0	-2.190848	1.207100	-1.125374
26	1	0	-1.748576	-0.489163	-1.171592
27	6	0	-3.583113	-0.039628	-0.146552
28	8	0	-4.173646	0.407529	0.817369
29	8	0	-4.147882	-0.879962	-1.039240
30	6	0	-5.529756	-1.218157	-0.805069
31	1	0	-6.149676	-0.317902	-0.823932
32	1	0	-5.801884	-1.892307	-1.617406
33	1	0	-5.639684	-1.713266	0.163174
34	8	0	-0.041787	2.346000	-0.180849
35	1	0	-0.915873	2.713122	0.022060

2.5.2. E-3 with intramolecular H-bonding

E= -769.99378093 a. u.

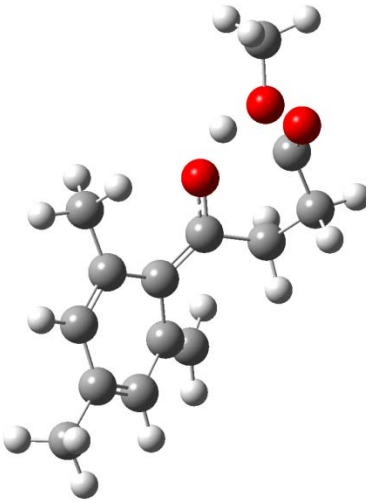


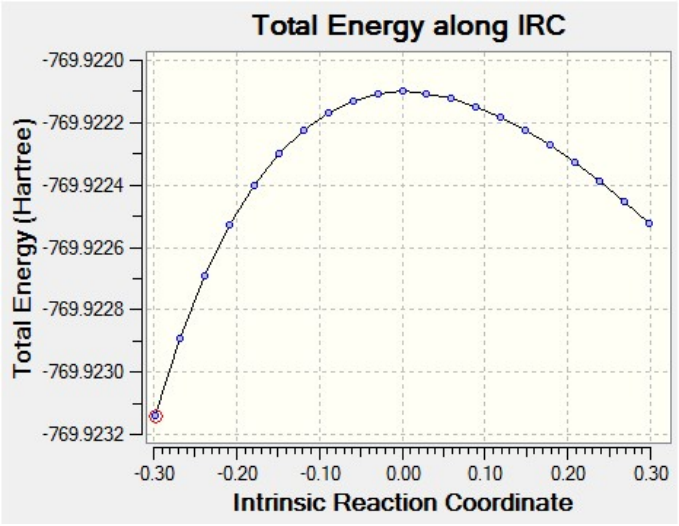
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.262592	1.060631	0.378561
2	6	0	-2.052943	1.289561	-0.206854
3	6	0	-1.198711	0.121544	-0.514912
4	6	0	-1.917475	-1.177504	-0.648386
5	6	0	-3.104722	-1.343143	0.185257
6	6	0	-3.763131	-0.267350	0.686818
7	1	0	-3.888376	1.912318	0.641460
8	1	0	-3.506467	-2.347873	0.306201
9	6	0	-5.035120	-0.393662	1.486414
10	1	0	-5.327456	-1.441170	1.615190
11	1	0	-4.922157	0.052555	2.484181
12	1	0	-5.865222	0.133365	0.995840
13	6	0	-1.632950	2.714384	-0.492892
14	1	0	-1.233183	2.820489	-1.507205
15	1	0	-2.497454	3.379639	-0.389125
16	1	0	-0.847249	3.058793	0.186600
17	6	0	-1.572043	-2.147528	-1.534897
18	1	0	-0.794392	-2.008632	-2.278816
19	1	0	-2.114516	-3.089793	-1.564120
20	6	0	0.173028	0.196516	-0.560440
21	6	0	1.121867	-0.983873	-0.570575
22	6	0	2.184679	-0.969476	0.561050
23	1	0	1.633075	-1.059867	-1.541435
24	1	0	0.539784	-1.899308	-0.460544
25	1	0	1.747801	-0.571806	1.487847
26	1	0	2.496049	-1.994018	0.785699
27	6	0	3.427010	-0.159438	0.266016
28	8	0	3.454993	0.852524	-0.423727
29	8	0	4.518382	-0.659247	0.857743
30	6	0	5.747191	0.080405	0.679251
31	1	0	5.637918	1.092602	1.075959
32	1	0	6.498053	-0.477410	1.238150
33	1	0	6.006436	0.128530	-0.380983
34	8	0	0.776794	1.413958	-0.483715
35	1	0	1.751477	1.327299	-0.583772

2.5.3. Transition state for E-3 forming 6

E= -769.92209602 a. u.
Imaginary frequency: 572 cm^{-1}





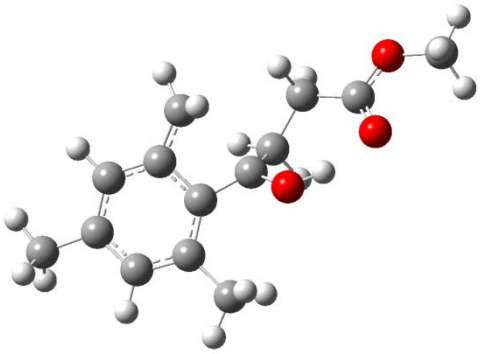
Standard orientation:

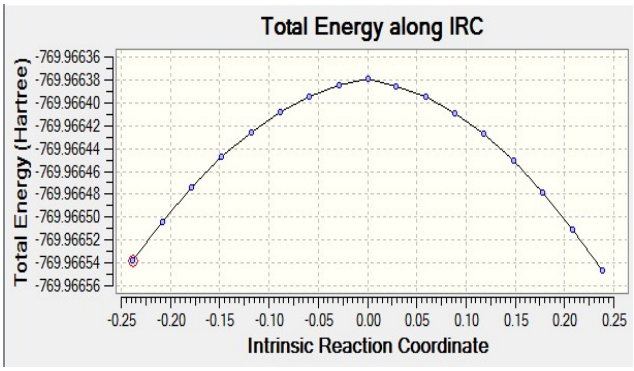
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.828458	-1.373213	0.007416
2	6	0	1.514920	-1.246252	-0.339307
3	6	0	0.927555	0.105466	-0.378474
4	6	0	1.888589	1.238195	-0.472869
5	6	0	3.214598	1.011037	0.091712
6	6	0	3.681076	-0.243018	0.321732
7	1	0	3.260800	-2.370461	0.074828
8	1	0	3.859938	1.876769	0.232114
9	6	0	5.073856	-0.508347	0.835260
10	1	0	5.625524	0.422730	1.003259
11	1	0	5.047406	-1.062969	1.783467
12	1	0	5.647868	-1.120532	0.125860
13	6	0	0.710336	-2.493587	-0.626094
14	1	0	0.161881	-2.411049	-1.571314
15	1	0	1.380093	-3.358953	-0.688413
16	1	0	-0.038405	-2.685625	0.148450
17	6	0	1.621346	2.417629	-1.097581
18	1	0	0.714981	2.589448	-1.667541
19	1	0	2.354820	3.220534	-1.097038
20	6	0	-0.428351	0.322698	-0.235257
21	6	0	-1.093022	1.666690	0.030669
22	6	0	-2.182386	1.444267	1.099271
23	1	0	-1.560134	2.057835	-0.883146
24	1	0	-0.381101	2.421582	0.371463
25	1	0	-1.747894	1.433410	2.105322
26	1	0	-2.947290	2.228653	1.068328
27	6	0	-2.876730	0.127387	0.958271
28	8	0	-3.392036	-0.636505	1.692999

29	8	0	-3.507782	0.092215	-0.665762
30	6	0	-4.604274	-0.824871	-0.860605
31	1	0	-5.528778	-0.292783	-0.629262
32	1	0	-4.598123	-1.128191	-1.910070
33	1	0	-4.496283	-1.695601	-0.208043
34	8	0	-1.333146	-0.661361	-0.201252
35	1	0	-2.547426	-0.344067	-0.871008

2.5.4. Transition state for E-3 forming 4

E= -769.96637873 a. u.
Imaginary frequency in IR= 358.2





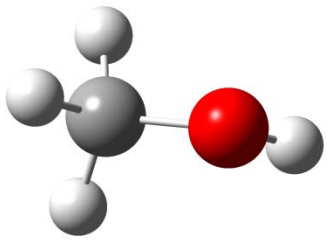
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.535352	0.853668	-0.242812
2	6	0	2.234828	1.286898	-0.004142
3	6	0	1.287448	0.264758	0.257938
4	6	0	1.686536	-1.067580	0.510364
5	6	0	2.990612	-1.485215	0.153344
6	6	0	3.917423	-0.518120	-0.213357
7	1	0	4.289805	1.592131	-0.511527
8	1	0	3.287345	-2.528195	0.250773
9	6	0	-0.160200	0.292707	0.256161
10	6	0	0.608541	-1.747548	1.157998
11	1	0	0.221916	-1.315132	2.074733
12	6	0	-3.437753	-0.171106	-0.211293
13	8	0	-3.361497	0.981653	0.198231
14	8	0	-4.611720	-0.787773	-0.396435
15	6	0	-5.798928	-0.038816	-0.054104
16	1	0	-5.780594	0.233978	1.003802
17	1	0	-5.862459	0.865246	-0.664274
18	1	0	-6.629849	-0.710684	-0.267631
19	8	0	-0.748127	1.326311	0.894496

20	1	0	-1.708705	1.377947	0.668006
21	6	0	-0.948396	-0.336315	-0.881544
22	1	0	-1.166196	0.460293	-1.616619
23	1	0	-0.291262	-1.053742	-1.375029
24	6	0	-2.264650	-1.063320	-0.545429
25	1	0	-2.096651	-1.731299	0.310861
26	1	0	-2.561800	-1.704061	-1.383016
27	1	0	0.488404	-2.831868	1.083571
28	6	0	1.858240	2.744591	-0.116839
29	1	0	1.050486	2.897342	-0.843590
30	1	0	1.494983	3.137579	0.839672
31	1	0	2.717371	3.345957	-0.433053
32	6	0	5.347527	-0.889380	-0.538269
33	1	0	5.625433	-0.558965	-1.547893
34	1	0	6.052223	-0.416896	0.158789
35	1	0	5.500808	-1.972489	-0.485990

2.6. Methanol

E= -115.72519298 a. u.



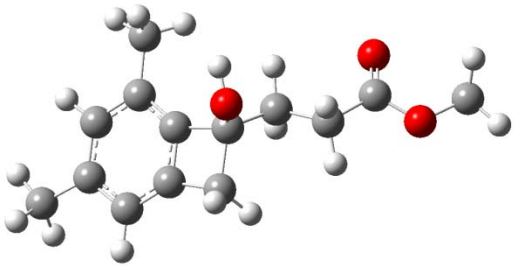
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.668530	-0.020894	0.000000
2	1	0	-1.080351	0.991107	-0.000098
3	1	0	-1.029809	-0.546235	-0.895714
4	1	0	-1.029823	-0.546069	0.895807
5	8	0	0.749368	0.122862	0.000000
6	1	0	1.156215	-0.756339	0.000002

2.7. Cyclobutanol 4

2.7.1. Cyclabutanol 4 without intramolecular H-bonding

E= -770.01041112 a. u.



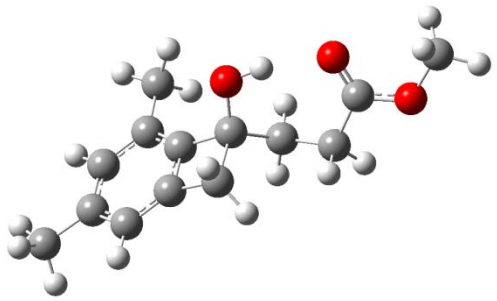
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.525189	0.910871	-0.472667
2	6	0	-2.254383	1.267158	0.022074
3	6	0	-1.440266	0.184970	0.350190
4	6	0	-1.847406	-1.138611	0.205044
5	6	0	-3.095204	-1.484442	-0.290840
6	6	0	-3.955071	-0.420087	-0.633417
7	1	0	-4.212865	1.708590	-0.750622
8	1	0	-3.417794	-2.516794	-0.413712
9	6	0	-5.341427	-0.712380	-1.166988
10	1	0	-5.301904	-1.373910	-2.041531
11	1	0	-5.961303	-1.213015	-0.411661
12	1	0	-5.859014	0.205471	-1.465036
13	6	0	-1.842058	2.711103	0.186961
14	1	0	-2.560660	3.386740	-0.288945
15	1	0	-1.783393	2.991553	1.247729
16	1	0	-0.857376	2.903762	-0.256003
17	6	0	-0.534732	-1.708726	0.723055
18	1	0	0.038866	-2.318708	0.014606
19	1	0	-0.588604	-2.227306	1.685655
20	6	0	-0.050456	-0.210603	0.866891
21	6	0	1.138297	0.210908	-0.005002
22	6	0	2.453474	-0.460389	0.406621
23	1	0	1.259702	1.300382	0.050940
24	1	0	0.910700	-0.017661	-1.054103
25	1	0	2.612594	-0.330981	1.485848
26	1	0	2.431683	-1.541120	0.230604
27	6	0	3.657554	0.126989	-0.298915
28	8	0	3.734532	1.252350	-0.751741
29	8	0	4.680066	-0.758514	-0.346657
30	6	0	5.899577	-0.284161	-0.948213
31	1	0	6.291407	0.571630	-0.391706

32	1	0	6.591491	-1.125481	-0.899024
33	1	0	5.722234	0.011221	-1.985740
34	8	0	0.198893	0.079500	2.249178
35	1	0	0.200051	1.043337	2.367698

2.7.2. Cyclobutanol 4 with intramolecular H bonding

E= -770.01281655 a. u.



Standard orientation:

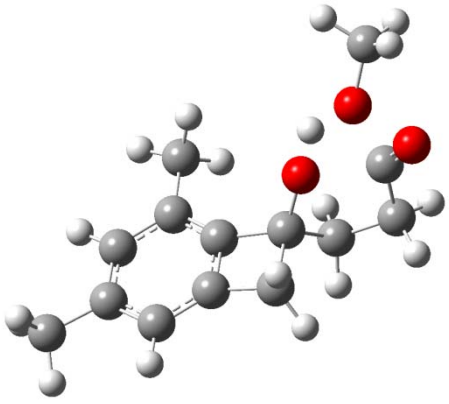
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.588523	0.889490	-0.215202
2	6	0	-2.239026	1.282332	-0.107887
3	6	0	-1.351148	0.232557	0.113134
4	6	0	-1.759571	-1.090707	0.246294
5	6	0	-3.087933	-1.474051	0.131434
6	6	0	-4.022832	-0.445692	-0.108940
7	1	0	-4.339360	1.660646	-0.384050
8	1	0	-3.417396	-2.506556	0.235067
9	6	0	-5.493694	-0.780012	-0.243451
10	1	0	-5.680083	-1.417721	-1.117669
11	1	0	-5.862677	-1.323219	0.635854
12	1	0	-6.102127	0.123571	-0.356475
13	6	0	-1.811881	2.725627	-0.222750
14	1	0	-2.670851	3.402027	-0.152516
15	1	0	-1.099964	2.986949	0.568065
16	1	0	-1.316715	2.920818	-1.183921
17	6	0	-0.355805	-1.608524	0.518969
18	1	0	0.034377	-2.348605	-0.193141
19	1	0	-0.178418	-1.962567	1.539938
20	6	0	0.129483	-0.093718	0.321149
21	6	0	1.011929	0.132051	-0.923669
22	6	0	2.345149	-0.643195	-1.004645
23	1	0	1.197524	1.208824	-1.030577
24	1	0	0.423629	-0.171645	-1.797729
25	1	0	2.192321	-1.689886	-0.704097

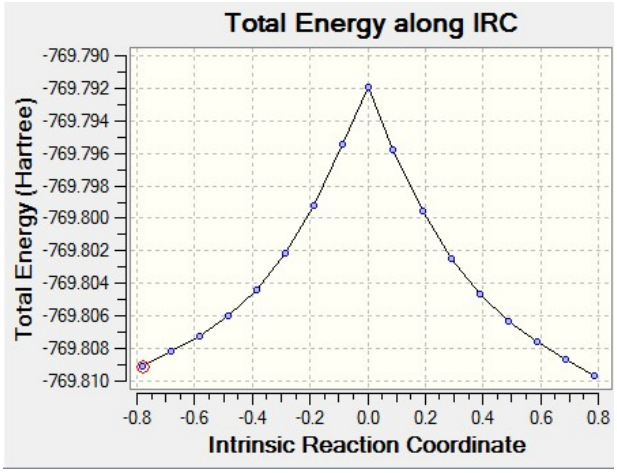
26	1	0	2.693403	-0.680144	-2.041972
27	6	0	3.483865	-0.116927	-0.157904
28	8	0	3.372696	0.460911	0.912464
29	8	0	4.679216	-0.386727	-0.709879
30	6	0	5.840989	0.014836	0.047233
31	1	0	5.849289	-0.483847	1.019645
32	1	0	6.694891	-0.294960	-0.555056
33	1	0	5.840491	1.097729	0.193396
34	8	0	0.638009	0.526634	1.485559
35	1	0	1.616272	0.527641	1.457482

2.7.2. Transition state for 4 forming 5

E= -769.93987843 a. u.

Imaginary frequency: 1234 cm^{-1}





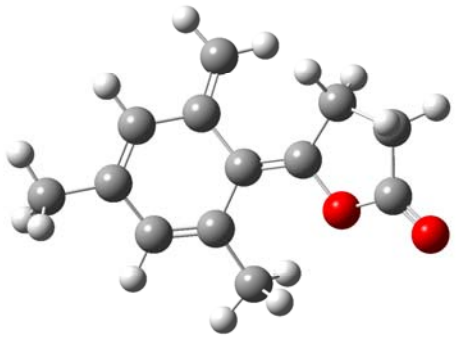
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.067279	1.163404	0.083298
2	6	0	1.669753	1.246363	0.234110
3	6	0	1.002414	0.030961	0.083445
4	6	0	1.658673	-1.162691	-0.203713
5	6	0	3.037733	-1.239970	-0.339317
6	6	0	3.754129	-0.035148	-0.195415
7	1	0	3.652589	2.076048	0.189794
8	1	0	3.559140	-2.170941	-0.553639
9	6	0	5.257756	-0.020622	-0.370334
10	1	0	5.717979	-0.925155	0.043897
11	1	0	5.532526	0.025646	-1.433088

12	1	0	5.712010	0.845567	0.122938
13	6	0	0.975932	2.555667	0.523439
14	1	0	1.699804	3.364721	0.667776
15	1	0	0.311885	2.843836	-0.301478
16	1	0	0.356167	2.494601	1.426677
17	6	0	0.377742	-1.983350	-0.241019
18	1	0	0.296912	-2.802729	0.485068
19	1	0	0.085761	-2.346895	-1.231683
20	6	0	-0.369662	-0.638279	0.151064
21	6	0	-1.094958	-0.635243	1.512806
22	6	0	-2.507774	-1.161472	1.244860
23	1	0	-1.147768	0.388121	1.899792
24	1	0	-0.565579	-1.245083	2.251827
25	1	0	-2.530058	-2.256798	1.193212
26	1	0	-3.232335	-0.841108	2.000043
27	6	0	-2.983588	-0.674536	-0.102279
28	8	0	-3.792423	-1.080282	-0.869352
29	8	0	-2.946844	1.117348	0.042995
30	6	0	-3.923429	1.785801	-0.756263
31	1	0	-4.442338	1.063745	-1.399026
32	1	0	-4.644627	2.274421	-0.093341
33	1	0	-3.432603	2.539634	-1.381235
34	8	0	-1.326354	-0.227467	-0.816230
35	1	0	-1.936508	0.810281	-0.494939

2.8. Lactone 6

E= -654.25186299 a. u.



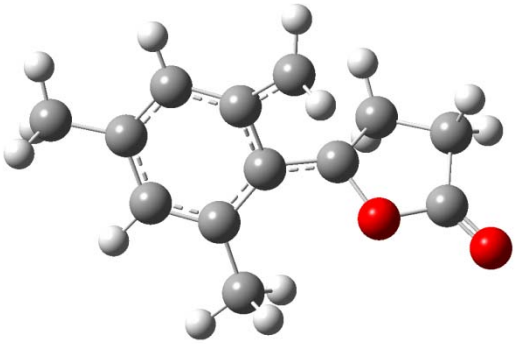
Standard orientation:

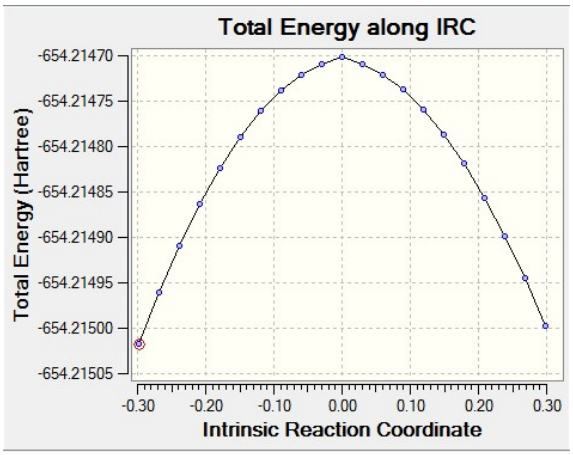
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.207006	-1.294095	-0.023957
2	6	0	-0.899357	-1.199682	-0.386890
3	6	0	-0.263108	0.136589	-0.349329
4	6	0	-1.182709	1.313016	-0.351753
5	6	0	-2.513840	1.091871	0.204920
6	6	0	-3.018760	-0.155120	0.372144
7	1	0	-2.679699	-2.274998	-0.023458
8	1	0	-3.126451	1.969500	0.402393
9	6	0	-4.412375	-0.407387	0.887224
10	1	0	-4.930813	0.528204	1.120880
11	1	0	-5.014186	-0.955166	0.149130
12	1	0	-4.391538	-1.021071	1.798173
13	6	0	-0.150794	-2.445911	-0.802296
14	1	0	0.576233	-2.766677	-0.049555
15	1	0	-0.860594	-3.264090	-0.962999
16	1	0	0.410322	-2.290470	-1.730562
17	6	0	-0.868072	2.531441	-0.861526
18	1	0	0.047763	2.730711	-1.404242
19	1	0	-1.576640	3.352884	-0.791333
20	6	0	1.076694	0.325259	-0.200346
21	6	0	1.886196	1.582313	0.025118
22	1	0	1.325730	2.321779	0.604853
23	1	0	2.146351	2.055344	-0.931157
24	6	0	3.185704	-0.410969	0.337352
25	8	0	4.072979	-1.215222	0.439034
26	8	0	1.946935	-0.762101	-0.157333
27	6	0	3.156578	1.059006	0.709805
28	1	0	4.081897	1.548375	0.397785
29	1	0	3.097398	1.126265	1.803674

2.8.2. Transition State for 6 forming 5

E= -654.21470115 a. u.

Imaginary frequency: 399 cm^{-1}



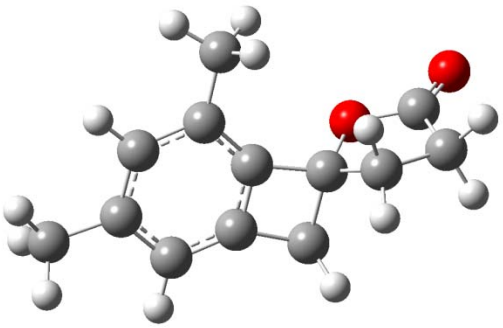


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.438015	1.157777	0.084349
2	6	0	-1.063055	1.281042	-0.061275
3	6	0	-0.353411	0.053840	-0.177022
4	6	0	-1.030171	-1.171943	-0.404140
5	6	0	-2.416781	-1.268654	-0.129023
6	6	0	-3.120543	-0.096980	0.101384
7	1	0	-3.025797	2.060693	0.244156
8	1	0	-2.933069	-2.224389	-0.194612
9	6	0	-4.616103	-0.112358	0.323103
10	1	0	-5.141845	0.450603	-0.459132
11	1	0	-5.009578	-1.134012	0.323038
12	1	0	-4.879393	0.350036	1.283408
13	6	0	-0.372852	2.621222	0.000308
14	1	0	0.166695	2.835859	-0.929316
15	1	0	-1.096485	3.424924	0.170843
16	1	0	0.369398	2.656242	0.807687
17	6	0	-0.112127	-2.106448	-0.956502
18	1	0	0.469342	-1.808850	-1.820218
19	1	0	-0.233959	-3.184717	-0.830145
20	6	0	1.026531	-0.272422	-0.002177
21	6	0	1.669315	-0.965686	1.193740
22	6	0	3.143898	-0.994492	0.784535
23	1	0	1.236182	-1.934337	1.430087
24	1	0	1.554076	-0.308511	2.073002
25	1	0	3.861272	-0.945384	1.606505
26	1	0	3.378126	-1.877059	0.173261
27	6	0	3.265043	0.233004	-0.102621
28	8	0	4.236362	0.840742	-0.461198
29	8	0	1.987971	0.595694	-0.514618

2.9. Lactone 5

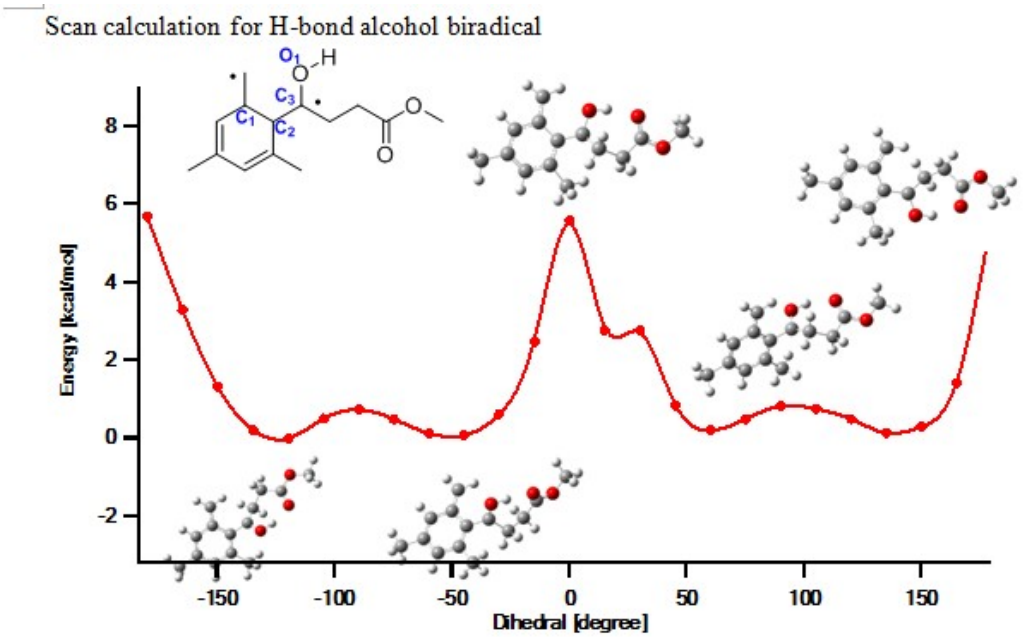
E= -654.27533369 a. u.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.580892	1.037655	-0.018727
2	6	0	-1.196258	1.275680	0.070674
3	6	0	-0.418216	0.118709	0.063289
4	6	0	-0.956453	-1.161464	-0.036206
5	6	0	-2.322624	-1.389906	-0.108198
6	6	0	-3.150558	-0.248943	-0.103648
7	1	0	-3.251838	1.895533	-0.024011
8	1	0	-2.753765	-2.386540	-0.178058
9	6	0	-4.651684	-0.405074	-0.218673
10	1	0	-4.943433	-0.680179	-1.241093
11	1	0	-5.024290	-1.192924	0.446785
12	1	0	-5.172939	0.524118	0.034049
13	6	0	-0.625095	2.669449	0.161133
14	1	0	0.150792	2.829485	-0.596652
15	1	0	-1.402854	3.426724	0.017576
16	1	0	-0.163596	2.850820	1.141043
17	6	0	0.404291	-1.846090	-0.016379
18	1	0	0.707151	-2.304543	-0.963828
19	1	0	0.595584	-2.548839	0.804194
20	6	0	1.004536	-0.391478	0.178862
21	6	0	1.822733	-0.112999	1.453198
22	6	0	3.266335	-0.293014	0.975110
23	1	0	1.533035	-0.773674	2.274915
24	1	0	1.655268	0.920883	1.776965
25	1	0	4.003527	0.341981	1.472361
26	1	0	3.609387	-1.332099	1.065270
27	6	0	3.187220	0.049249	-0.508251
28	8	0	4.087566	0.310397	-1.266762
29	8	0	1.882179	0.016928	-0.906065

2.10. Rotational barrier for 2.



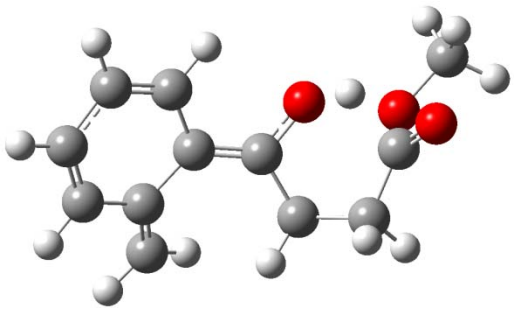
Rotation around **C1-C2-C3-O1**

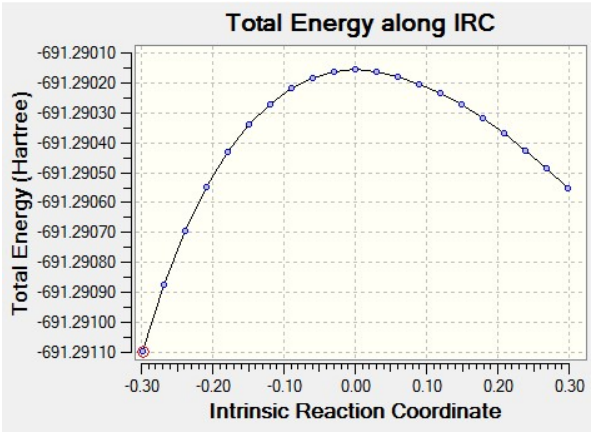
3. Calculation for 7 (B3LYP/6-32+G(d))

3.1. Transition state E-10 forming 12

E= -691.29015396 a. u.

Imaginary frequency 545 cm^{-1}





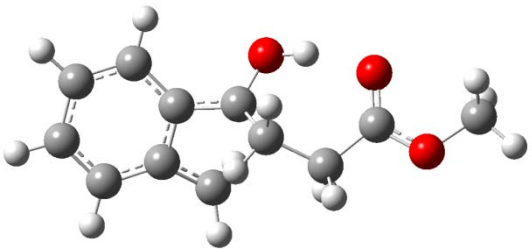
Standard orientation:

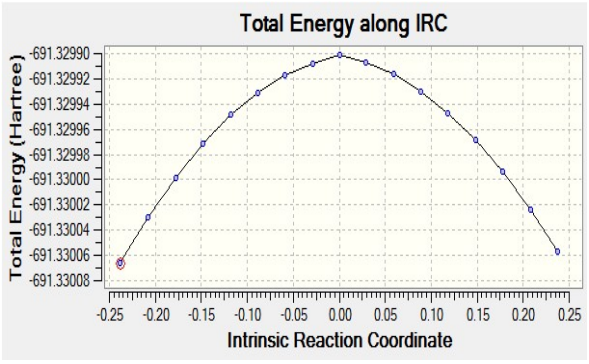
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.036272	-1.923948	0.090196
2	6	0	1.754449	-1.546605	-0.162467
3	6	0	1.364533	-0.146892	-0.203143
4	6	0	2.448562	0.865470	-0.245028
5	6	0	3.769060	0.397183	0.174429
6	6	0	4.054123	-0.922875	0.313701
7	1	0	3.295460	-2.977012	0.163413
8	1	0	4.548899	1.146119	0.296090
9	6	0	2.322904	2.142706	-0.707752
10	1	0	1.427306	2.517326	-1.188489
11	1	0	3.172228	2.820575	-0.677678
12	6	0	0.016048	0.150630	-0.130392
13	6	0	-0.590152	1.520389	0.108889
14	6	0	-1.802964	1.345950	1.045092
15	1	0	-0.920048	1.973890	-0.836374
16	1	0	0.131494	2.210179	0.555773
17	1	0	-1.485151	1.307371	2.093027
18	1	0	-2.520540	2.167686	0.939312
19	6	0	-2.544956	0.066944	0.817392
20	8	0	-3.175336	-0.668622	1.487694
21	8	0	-2.993597	0.061625	-0.862362
22	6	0	-4.119717	-0.783404	-1.181754
23	1	0	-5.024505	-0.180819	-1.084946
24	1	0	-3.998803	-1.117758	-2.214514
25	1	0	-4.159458	-1.639125	-0.502255
26	8	0	-0.918217	-0.801256	-0.174915
27	1	0	-2.048861	-0.431319	-0.970703
28	1	0	0.968363	-2.286724	-0.266860
29	1	0	5.061842	-1.237652	0.575886

3.2. Transition state for E-10 forming 11

E= -691.32990113 a. u.

Imaginary frequency: 354 cm^{-1}



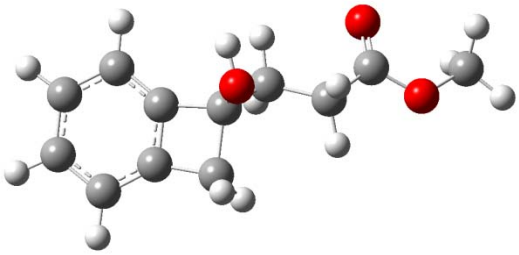


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.042056	-1.082159	-0.410314
2	6	0	-2.730931	-1.448200	-0.127783
3	6	0	-1.818453	-0.411116	0.145169
4	6	0	-2.251396	0.915368	0.376120
5	6	0	-3.557339	1.288555	-0.020762
6	6	0	-4.434631	0.280572	-0.400016
7	1	0	-4.768913	-1.842055	-0.686110
8	1	0	-3.892430	2.321134	0.052970
9	6	0	-0.371847	-0.423882	0.192484
10	6	0	-1.205397	1.615867	1.057223
11	1	0	-0.855277	1.196030	1.994361
12	6	0	2.910177	0.056091	-0.171814
13	8	0	2.824422	-1.096181	0.237240
14	8	0	4.086476	0.678476	-0.315325
15	6	0	5.264625	-0.063357	0.071745
16	1	0	5.208643	-0.334679	1.128679
17	1	0	5.355437	-0.967791	-0.534347
18	1	0	6.098956	0.612990	-0.112131
19	8	0	0.194428	-1.458319	0.844192
20	1	0	1.162443	-1.507510	0.649718
21	6	0	0.443811	0.207071	-0.923281
22	1	0	0.684921	-0.591246	-1.648922
23	1	0	-0.202509	0.919983	-1.437326
24	6	0	1.745484	0.941752	-0.550637
25	1	0	1.548647	1.616435	0.294026
26	1	0	2.067038	1.576395	-1.383849
27	1	0	-1.093129	2.700377	0.977479
28	1	0	-5.460487	0.532810	-0.659782
29	1	0	-2.408222	-2.484059	-0.192424

3.4. Cyclobutanol 11 without H bonding

E= -691.37381703 a. u.

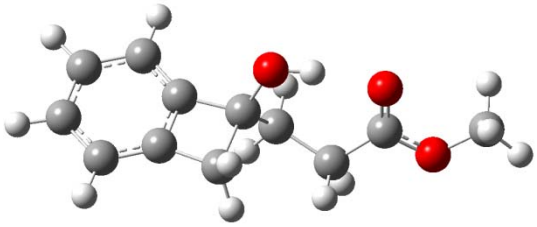


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.994887	1.377507	-0.286070
2	6	0	-2.737360	1.443480	0.338942
3	6	0	-1.971833	0.285355	0.283509
4	6	0	-2.408059	-0.875517	-0.351964
5	6	0	-3.642889	-0.950877	-0.983716
6	6	0	-4.434456	0.210271	-0.931712
7	1	0	-4.643770	2.249976	-0.275472
8	1	0	-3.998670	-1.845475	-1.489420
9	6	0	-1.139930	-1.653786	-0.029430
10	1	0	-0.546583	-1.984848	-0.890400
11	1	0	-1.258171	-2.486935	0.670640
12	6	0	-0.625286	-0.334938	0.676895
13	6	0	0.616060	0.333331	0.076508
14	6	0	1.896762	-0.482925	0.282787
15	1	0	0.743471	1.325425	0.529429
16	1	0	0.446522	0.506924	-0.993818
17	1	0	1.993376	-0.756982	1.342153
18	1	0	1.873401	-1.425546	-0.274347
19	6	0	3.147115	0.281574	-0.098129
20	8	0	3.265293	1.491166	-0.098002
21	8	0	4.157859	-0.558557	-0.420918
22	6	0	5.417206	0.061982	-0.742385
23	1	0	5.786539	0.638096	0.110382
24	1	0	6.093559	-0.761459	-0.973518
25	1	0	5.305674	0.725124	-1.604314
26	8	0	-0.453379	-0.581692	2.077342
27	1	0	-0.466429	0.268515	2.546592
28	1	0	-5.414553	0.208711	-1.402932
29	1	0	-2.407213	2.358394	0.826243

3.5. Cyclobutanol 11 with intermolecular H-bonding

E= -691.37596285 a. u.



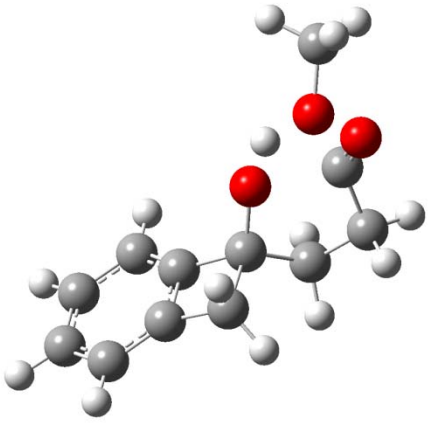
Standard orientation:

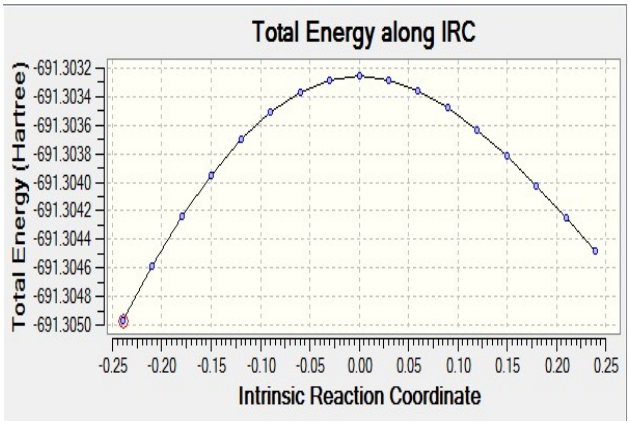
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.098204	-1.076376	-0.501406
2	6	0	2.741420	-1.426319	-0.391360
3	6	0	1.883697	-0.408391	0.004851
4	6	0	2.327794	0.877526	0.302228
5	6	0	3.665198	1.239351	0.191273
6	6	0	4.547168	0.225203	-0.221494
7	1	0	4.822025	-1.828236	-0.807282
8	1	0	4.031763	2.238165	0.417255
9	6	0	0.944799	1.384056	0.681735
10	1	0	0.556107	2.224572	0.090913
11	1	0	0.801583	1.594880	1.746575
12	6	0	0.416136	-0.078794	0.290289
13	6	0	-0.483680	-0.114103	-0.960997
14	6	0	-1.811629	0.672732	-0.905747
15	1	0	-0.678469	-1.162950	-1.221079
16	1	0	0.095221	0.309290	-1.790068
17	1	0	-1.650712	1.657687	-0.443785
18	1	0	-2.167726	0.876172	-1.920872
19	6	0	-2.945709	0.020652	-0.144736
20	8	0	-2.826053	-0.729132	0.812122
21	8	0	-4.144357	0.385926	-0.629305
22	6	0	-5.301534	-0.129924	0.063191
23	1	0	-5.295692	0.198584	1.105469
24	1	0	-6.158981	0.281877	-0.468798
25	1	0	-5.308085	-1.221931	0.025412
26	8	0	-0.089962	-0.836255	1.368247
27	1	0	-1.067840	-0.854903	1.330527
28	1	0	5.607299	0.447759	-0.319547
29	1	0	2.405299	-2.438951	-0.600187

3.6. Transition State for 11 forming 8

E= -691.30325697 a. u.

Imaginary frequency: 1216 cm^{-1}





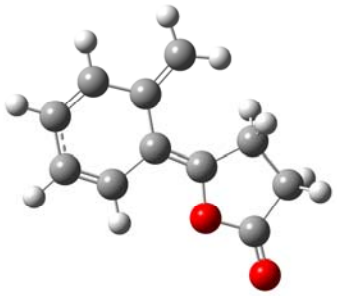
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.445488	1.543662	0.224440
2	6	0	2.051787	1.493922	0.397895
3	6	0	1.448622	0.277262	0.104823
4	6	0	2.165191	-0.832506	-0.340229
5	6	0	3.544765	-0.799866	-0.503866
6	6	0	4.172668	0.423688	-0.212075
7	1	0	3.977945	2.468397	0.433629
8	1	0	4.123027	-1.655430	-0.844833
9	6	0	0.930180	-1.713746	-0.466276
10	1	0	0.907900	-2.620275	0.152068
11	1	0	0.640310	-1.966487	-1.491287
12	6	0	0.116235	-0.470626	0.098520
13	6	0	-0.577135	-0.661489	1.463430
14	6	0	-1.975309	-1.209270	1.164275
15	1	0	-0.657562	0.307809	1.968020
16	1	0	-0.008136	-1.330836	2.116597
17	1	0	-1.959035	-2.291013	0.984384
18	1	0	-2.690547	-1.008384	1.968146
19	6	0	-2.506763	-0.587914	-0.104518
20	8	0	-3.315182	-0.936825	-0.898857
21	8	0	-2.530806	1.168798	0.240173
22	6	0	-3.548068	1.888632	-0.459897
23	1	0	-4.044037	1.230562	-1.183814

24	1	0	-4.278886	2.256340	0.267024
25	1	0	-3.097227	2.735693	-0.987421
26	8	0	-0.871978	0.006466	-0.797454
27	1	0	-1.526865	0.977564	-0.342189
28	1	0	5.250331	0.510950	-0.329358
29	1	0	1.500549	2.367110	0.739011

3.7. Lactone 12.

E= -575.61889623a. u.



Standard orientation:

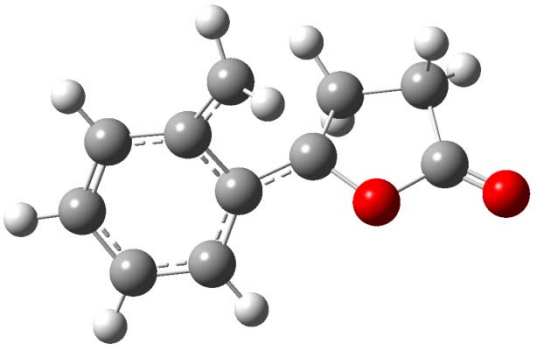
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.877430	-1.423080	-0.000043
2	6	0	-1.521663	-1.442882	-0.000053
3	6	0	-0.720557	-0.222155	-0.000016
4	6	0	-1.448594	1.081816	0.000014
5	6	0	-2.910302	1.004676	0.000052
6	6	0	-3.591918	-0.165540	0.000024
7	1	0	-3.435853	-2.355456	-0.000087
8	1	0	-3.446804	1.950618	0.000097
9	6	0	-0.876033	2.316601	0.000021
10	1	0	0.190356	2.485748	-0.000013
11	1	0	-1.515720	3.195614	0.000058
12	6	0	0.633201	-0.374166	0.000000
13	6	0	1.446374	-1.656525	-0.000038
14	1	0	1.219363	-2.268489	-0.880758
15	1	0	1.219178	-2.268682	0.880491
16	6	0	2.813411	0.345349	-0.000012
17	8	0	3.692435	1.163208	-0.000098
18	8	0	1.482742	0.716070	-0.000040
19	6	0	2.904444	-1.169959	0.000171
20	1	0	3.473322	-1.485225	0.880497
21	1	0	3.473708	-1.485457	-0.879818
22	1	0	-4.678790	-0.169570	0.000049

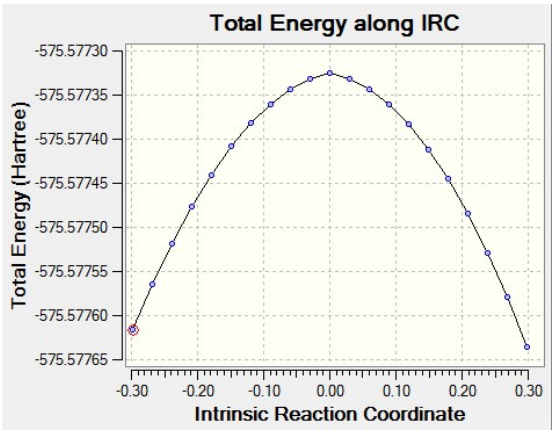
23	1	0	-1.005775	-2.398137	-0.000124

3.8. Transition state for 12 forming 8

E= -575.57732438 a. u.

Imaginary frequency: 395 cm^{-1}





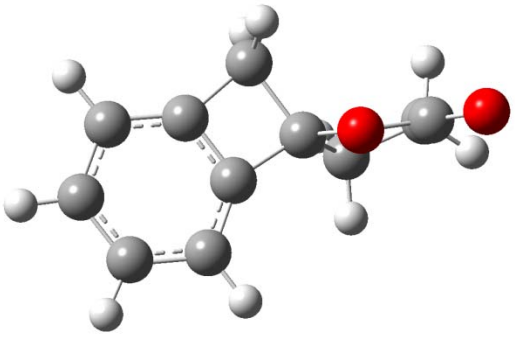
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.810712	-1.510767	0.221553
2	6	0	1.436766	-1.535965	0.033546
3	6	0	0.789539	-0.289343	-0.111071
4	6	0	1.525997	0.904152	-0.326545
5	6	0	2.907080	0.928599	-0.009046
6	6	0	3.528239	-0.283446	0.247192
7	1	0	3.347217	-2.439097	0.399621
8	1	0	3.479120	1.852245	-0.059615
9	6	0	0.667626	1.867733	-0.926364
10	1	0	0.116702	1.580971	-1.813529
11	1	0	0.819932	2.942104	-0.802557
12	6	0	-0.584857	0.083555	0.002366
13	6	0	-1.249807	0.805519	1.168422
14	6	0	-2.712846	0.844200	0.719021
15	1	0	-0.812761	1.773513	1.400162
16	1	0	-1.164796	0.161282	2.060311
17	1	0	-3.451259	0.812589	1.522961
18	1	0	-2.923081	1.721441	0.091711
19	6	0	-2.824884	-0.393016	-0.155568
20	8	0	-3.791737	-0.994366	-0.533842

21	8	0	-1.539243	-0.775474	-0.527912
22	1	0	4.599002	-0.307919	0.435173
23	1	0	0.876378	-2.465730	0.078763

3.9. Lactone 8

E= -575.63795788 a. u.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.035608	-1.305147	0.090468
2	6	0	1.648408	-1.477923	0.224817
3	6	0	0.882869	-0.327728	0.078756
4	6	0	1.436649	0.922108	-0.192096
5	6	0	2.808235	1.108682	-0.312795
6	6	0	3.599505	-0.043529	-0.166847
7	1	0	3.693331	-2.165282	0.187336
8	1	0	3.261891	2.075209	-0.517640
9	6	0	0.086021	1.625206	-0.240218
10	1	0	-0.225908	1.962282	-1.234487
11	1	0	-0.081244	2.430767	0.485397
12	6	0	-0.531060	0.216467	0.150314
13	6	0	-1.318961	0.108766	1.468630
14	6	0	-2.772250	0.239703	1.005248
15	1	0	-1.005439	0.863840	2.194597
16	1	0	-1.147666	-0.878381	1.914201
17	1	0	-3.499911	-0.323461	1.594444
18	1	0	-3.108487	1.284386	0.973825
19	6	0	-2.730518	-0.284087	-0.425605
20	8	0	-3.648670	-0.626872	-1.127034
21	8	0	-1.433193	-0.313693	-0.853440
22	1	0	1.221484	-2.457911	0.421728
23	1	0	4.679807	0.037969	-0.259643
