Benzoxyl Radical Decomposition Kinetics: Formation of Benzaldehyde + H, Phenyl + CH_2O, and Benzene + HCO

Supporting Information

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Molecular geometries (Cartesian coordinates)

benzoxyl

	x	*y*	*z*
C	2.261410	0.283400	-0.012146
C	1.348350	1.335610	0.010199
C	-0.019962	1.077000	0.026057
C	-0.485198	-0.236932	0.017873
C	0.432451	-1.289180	-0.006725
C	1.800210	-1.031720	-0.020743
H	3.327120	0.486231	-0.024745
H	1.702500	2.361440	0.014229
H	-0.741545	1.885820	0.039512
H	0.076095	-2.316310	-0.016845
H	2.505370	-1.856220	-0.040782
C	-1.973400	-0.530938	0.045122
H	-2.245650	-1.025850	1.006980
H	-2.239000	-1.316210	-0.694091
O	-2.821010	0.517211	-0.080260

α-hydroxybenzyl

	x	*y*	*z*
C	2.273590	0.295504	0.000188
C	1.344770	1.339610	-0.000050
C	-0.014873	1.080380	-0.000261
C	-0.505885	-0.255588	-0.000194
C	0.459822	-1.303060	-0.000044
C	1.812490	-1.027550	0.000151
H	3.336660	0.507066	0.000357
H	1.689850	2.368780	-0.000127
H	-0.702127	1.922930	-0.000719
H	0.112935	-2.331950	-0.000028
H	2.524140	-1.847100	0.000284
C	-1.872860	-0.578127	-0.000226
H	-2.548880	1.207430	0.001673
H	-2.222770	-1.602500	-0.000680
O	-2.896520	0.308541	0.000233

1-oxaspiro[2.5]octa-4,7-dien-5-yl

	x	*y*	*z*
C	-2.145130	-0.000077	-0.014000
C	-1.437000	1.221540	-0.011861
C	-0.069513	1.245120	-0.023586
C	0.701037	0.000035	-0.047917
C	-0.069474	-1.245020	-0.023801
C	-1.437120	-1.221510	-0.011978
H	-3.228760	0.000051	-0.000542
H	-1.988440	2.156380	0.006541
H	0.484258	2.177320	-0.002206
H	0.484295	-2.177200	-0.002544
H	-1.988360	-2.156460	0.006664
C	2.093340	0.000128	-0.593443
H	2.480000	-0.919197	-1.036790
O	1.932630	-0.000333	0.803013
H	2.479110	0.920456	-1.035720

phenoxymethyl

	x	*y*	*z*
C	-2.231310	0.278257	0.060056
C	-1.759290	-1.034740	0.072961
C	-0.396697	-1.293750	0.002977
C	0.503568	-0.230403	-0.079640
C	0.045583	1.086940	-0.106430
C	-1.324960	1.330050	-0.032868
H	-3.295700	0.476945	0.115959
H	-2.456160	-1.863600	0.140288
H	-0.008205	-2.305470	0.016543
H	0.746919	1.905000	-0.211946
H	-1.681630	2.354590	-0.057647
C	2.781220	0.352514	0.140703
O	1.830480	-0.569579	-0.158140
H	3.784760	-0.027698	0.003812
H	2.557510	1.083640	0.911557

2,5-cyclohexadien-4-formyl-1-yl

	x	*y*	*z*
C	-2.147840	0.001992	-0.362188
C	-1.486120	1.223110	-0.086367
C	-0.206828	1.252050	0.384795
C	0.604849	-0.001841	0.563092
C	-0.210014	-1.253470	0.384087
C	-1.489250	-1.220990	-0.086939
H	-3.164880	0.003384	-0.734865
H	-2.022530	2.156790	-0.228300
H	0.281089	2.194870	0.609653
H	0.275317	-2.197730	0.608519
H	-2.028090	-2.153190	-0.229352
C	1.742980	-0.001822	-0.492221
O	2.914060	0.001048	-0.230047
H	1.131290	-0.002647	1.528210
H	1.368590	-0.004085	-1.539040

benzaldehyde

	x	*y*	*z*
C	0.588570	-2.146940	0.000000
C	-0.742418	-1.722740	0.000000
C	-1.037670	-0.367013	0.000000
C	0.000000	0.573640	0.000000
C	1.329530	0.143876	0.000000
C	1.625130	-1.215390	0.000000
H	0.816679	-3.207950	0.000000
H	-1.544090	-2.453780	0.000000
H	-2.060610	-0.007257	0.000000
H	2.128340	0.880583	0.000000
H	2.657250	-1.549090	0.000000
C	-0.304818	2.020840	0.000000
H	0.595883	2.676290	0.000000
O	-1.417920	2.492950	0.000000

phenyl

	x	*y*	*z*
C	0.000000	0.000137	-1.320970
C	0.000000	1.211720	-0.631043
C	0.000000	1.224340	0.770789
C	0.000000	-0.000009	1.395230
C	0.000000	-1.224140	0.770505
C	0.000000	-1.211690	-0.631340
H	0.000000	0.000043	-2.405790
H	0.000000	2.150480	-1.176980
H	0.000000	2.159020	1.321250
H	0.000000	-2.158960	1.320810
H	0.000000	-2.150330	-1.177440

benzene

	x	*y*	*z*
C	0.000000	1.393100	0.000000
C	1.206460	0.696551	0.000000
C	1.206460	-0.696551	0.000000
C	0.000000	-1.393100	0.000000
C	-1.206460	-0.696551	0.000000
C	-1.206460	0.696551	0.000000
H	0.000000	2.478100	0.000000
H	2.146090	1.239050	0.000000
H	2.146090	-1.239050	0.000000
H	-2.146090	-1.239050	0.000000
H	-2.146090	1.239050	0.000000
H	0.000000	-2.478100	0.000000

CH_2O

	x	*y*	*z*
C	0.000000	0.000000	-0.525459
H	0.000000	0.937280	-1.121920
H	0.000000	-0.937280	-1.121920
O	0.000000	0.000000	0.674574

HC•O

		x	*y*	*z*
1	C	0.062345	0.585162	0.000000
2	H	-0.872833	1.216930	0.000000
3	O	0.062345	-0.590988	0.000000

TS1

	x	*y*	*z*
C	-2.255290	-0.236400	0.002021
C	-1.378960	-1.323460	0.032767
C	-0.007255	-1.110400	0.025356
C	0.495743	0.194582	-0.012559
C	-0.384362	1.279720	-0.044669
C	-1.758440	1.065360	-0.037788
H	-3.327070	-0.405675	0.007637
H	-1.771160	-2.334580	0.060949
H	0.696669	-1.934870	0.043799
H	0.013641	2.290500	-0.074198
H	-2.440910	1.908060	-0.063948
C	1.967420	0.426510	-0.049812
H	2.069320	0.918422	1.685930
H	2.257640	1.490920	-0.205502
O	2.803590	-0.463524	-0.118321

TS2

	x	*y*	*z*
C	-2.265200	-0.296391	-0.001664
C	-1.341150	-1.342710	0.001587
C	0.020921	-1.075850	0.007680
C	0.481056	0.251535	0.003588
C	-0.455587	1.298410	-0.005231
C	-1.817000	1.024790	-0.004931
H	-3.328860	-0.509497	-0.004888
H	-1.687960	-2.370970	-0.002142
H	0.750635	-1.877160	0.006368
H	-0.105953	2.326830	-0.015244
H	-2.531570	1.841230	-0.013014
C	1.908880	0.550705	0.024833
H	2.616650	0.135161	0.967869
H	2.219360	1.564130	-0.254946
O	2.859520	-0.446584	-0.104897

TS3

	x	*y*	*z*
C	2.252320	0.306640	0.024679
C	1.325460	1.349670	-0.029977
C	-0.033538	1.071100	-0.065912
C	-0.476482	-0.260294	-0.040560
C	0.459866	-1.301480	0.017418
C	1.819740	-1.019290	0.046703
H	3.314230	0.528438	0.048971
H	1.668890	2.378550	-0.047652
H	-0.771905	1.862960	-0.115692
H	0.111209	-2.330120	0.040949
H	2.542670	-1.826770	0.089389
C	-1.906430	-0.565977	-0.052168
H	-2.929020	1.294830	1.188870
H	-2.169020	-1.639920	0.002701
O	-2.801580	0.281235	-0.076078

TS4

	x	*y*	*z*
C	-2.251780	-0.269811	-0.039128
C	-1.774420	1.047530	-0.047000
C	-0.418805	1.305270	0.000016
C	0.508990	0.225139	0.056577
C	0.014997	-1.110510	0.051860
C	-1.345830	-1.338140	0.004602
H	-3.318140	-0.461235	-0.076185
H	-2.474420	1.874810	-0.101083
H	-0.044835	2.324620	-0.014127
H	0.735960	-1.919120	0.063639
H	-1.716410	-2.358000	-0.011642
C	2.004970	0.470915	-0.007287
O	2.846730	-0.430180	-0.131776
H	1.356930	0.453029	1.168330
H	2.258350	1.544990	-0.092561

TS5

	x	*y*	*z*
C	2.231460	0.250626	-0.067850
C	1.743010	-1.058550	-0.090489
C	0.380195	-1.291220	-0.013025
C	-0.521321	-0.209638	0.122062
C	-0.018190	1.111770	0.075568
C	1.345240	1.331520	0.005497
H	3.299560	0.430129	-0.127835
H	2.431410	-1.892420	-0.176714
H	-0.010586	-2.304430	-0.033717
H	-0.728000	1.930300	0.106446
H	1.729930	2.345890	-0.006782
C	-1.990930	-0.448738	-0.026792
O	-2.808660	0.417649	-0.212670
H	-0.991224	-0.443555	1.883160
H	-2.278590	-1.521720	0.026974

TS6

	x	*y*	*z*
C	-2.3764200	-0.3060400	-0.0000160
C	-1.4460800	-1.3451200	-0.0000090
C	-0.0735890	-1.0644200	0.0000010
C	0.2658860	0.2649020	0.0000040
C	-0.5928010	1.3358100	-0.0000020
C	-1.9600800	1.0244200	-0.0000120
H	-3.4367000	-0.5348840	-0.0000240
H	-1.7811500	-2.3778000	-0.0000120
H	0.6780850	-1.8447800	0.0000060
H	-0.2508210	2.3650700	0.0000010
H	-2.6907400	1.8273800	-0.0000180
C	2.5827300	0.5637240	0.0000350
H	2.4541500	1.1471400	0.9338610
H	2.4541700	1.1472200	-0.9337410
O	3.0218900	-0.5711230	-0.0000100

TS7

	x	*y*	*z*
C	2.146400	-0.000034	0.059239
C	1.444160	-1.217920	0.002677
C	0.075156	-1.235430	-0.108701
C	-0.669822	-0.000024	-0.159487
C	0.075275	1.235430	-0.108529
C	1.444210	1.218000	0.002624
H	3.226600	-0.000066	0.150280
H	1.990920	-2.154290	0.046114
H	-0.476402	-2.168130	-0.145133
H	-0.476806	2.167880	-0.143624
H	1.991140	2.154310	0.045101
C	-2.113950	0.000209	-0.514587
H	-2.522430	0.913703	-0.959992
O	-1.952420	-0.000216	0.866084
H	-2.522200	-0.913037	-0.960839

TS8

	x	*y*	*z*
C	2.145880	0.000013	0.168919
C	1.451550	1.210910	0.047731
C	0.086080	1.226690	-0.161947
C	-0.635235	-0.000009	-0.207214
C	0.086097	-1.226690	-0.161941
C	1.451570	-1.210890	0.047740
H	3.218250	0.000021	0.326472
H	1.992990	2.150220	0.097757
H	-0.460668	2.154110	-0.288981
H	-0.460635	-2.154120	-0.288975
H	1.993030	-2.150190	0.097776
C	-2.178970	0.000017	0.733949
O	-1.974790	-0.000028	-0.641735
H	-2.463080	-0.942696	1.193260
H	-2.463380	0.942699	1.193140

TS9

	x	*y*	*z*
C	-2.363430	0.283374	0.000002
C	-1.458950	1.345040	-0.000003
C	-0.081457	1.090710	-0.000006
C	0.296630	-0.225722	-0.000003
C	-0.539193	-1.312830	0.000004
C	-1.912120	-1.037370	0.000007
H	-3.429070	0.486086	0.000004
H	-1.820200	2.369200	-0.000003
H	0.646758	1.898180	-0.000002
H	-0.158445	-2.328410	0.000006
H	-2.625770	-1.855960	0.000013
C	3.087550	0.325114	0.000022
O	2.290060	-0.617325	-0.000032
H	3.446060	0.779787	0.938554
H	3.446050	0.779885	-0.938465

TS10

	x	*y*	*z*
C	-1.984800	0.388459	-0.531754
C	-1.137680	1.365610	-0.003339
C	-0.003418	1.007330	0.711152
C	0.368440	-0.366770	0.834086
C	-0.579068	-1.347150	0.403782
C	-1.701660	-0.970405	-0.302259
H	-2.873200	0.674313	-1.083380
H	-1.380940	2.415820	-0.130525
H	0.639563	1.769420	1.137730
H	-0.377013	-2.395980	0.593424
H	-2.389760	-1.728260	-0.663822
C	1.814770	-0.230774	-0.615968
O	2.917600	0.111276	-0.354155
H	1.100730	-0.642229	1.586500
H	1.280350	-0.061048	-1.580880

Vibrational frequnecies (cm^{-1})

benzoxyl

3205.12	3195.81	3182.75	3172.13	3154.47
2887.29	2838.98	1642.49	1627.15	1525.18
1481.86	1365.39	1346.66	1328.30	1305.57
1212.30	1193.36	1181.76	1124.16	1102.33
1077.69	1047.03	1013.94	996.55	962.63
926.88	873.75	801.69	769.37	717.86
628.49	607.58	555.18	437.87	420.14
410.22	216.29	187.11	41.89	

α-hydroxybenzyl

3809.90	3216.39	3201.86	3183.62	3176.55
3165.29	3139.37	1603.44	1572.05	1533.74
1491.43	1460.38	1358.20	1350.33	1336.02
1240.14	1195.53	1175.72	1148.51	1104.99
1035.73	983.81	970.34	938.60	859.45
819.26	798.30	753.16	686.07	658.26
622.97	600.53	494.35	435.75	413.15
332.14	223.33	204.90	78.14	

1-oxaspiro[2.5]octa-4,7-dien-5-yl

3205.91	3194.93	3193.35	3174.43	3170.92
3140.82	3054.38	1586.39	1544.18	1516.76
1464.69	1425.63	1337.57	1313.15	1274.43
1187.38	1162.13	1154.85	1139.98	1099.71
1003.88	993.48	968.07	952.43	944.21
903.06	824.32	766.81	749.11	718.46
655.12	597.28	553.62	440.13	434.86
413.52	332.98	274.21	115.47	

phenoxymethyl

3271.31	3211.30	3205.74	3197.52	3182.32
3174.34	3124.55	1640.38	1626.96	1524.15
1489.10	1471.51	1353.86	1330.57	1315.63
1195.73	1191.97	1179.24	1154.97	1099.48
1044.38	1011.45	982.47	954.35	911.51
848.21	798.41	779.92	710.46	662.62
624.37	561.90	519.74	455.08	424.33
346.85	247.73	218.89	105.25	

2,5-cyclohexadien-4-formyl-1-yl

3208.68	3187.01	3186.52	3167.18	3165.11
2997.30	2894.41	1825.81	1595.09	1537.16
1447.64	1398.76	1391.48	1342.81	1294.52
1222.03	1195.80	1170.45	1121.20	1054.27
1000.35	992.46	990.73	968.99	965.15
936.95	890.86	794.88	754.57	664.58
620.72	589.42	576.24	424.23	408.95
343.60	271.47	73.26	45.66	

benzaldehyde

3205.92	3197.79	3187.43	3175.50	3165.32
2872.89	1799.67	1639.57	1623.19	1520.72
1485.51	1428.94	1353.69	1332.18	1228.11
1187.78	1183.79	1100.58	1047.53	1044.29
1014.02	1005.24	976.42	943.08	876.47
839.12	773.58	710.28	660.92	625.87
470.46	441.31	418.60	241.21	219.51
124.15				

phenyl

3,196.95	3,187.86	3,185.07	3,170.72	3,163.94
1,629.84	1,571.60	1,468.05	1,460.18	1,328.11
1,298.26	1,176.71	1,175.88	1,074.96	1,051.23
1,019.61	989.80	982.60	957.82	896.22
826.43	730.65	678.53	613.87	595.89
427.19	401.51			

benzene

3202.45	3191.59	3191.59	3175.40	3175.40
3165.67	1636.02	1636.02	1512.23	1512.23
1362.24	1340.81	1198.29	1198.29	1173.67
1062.56	1062.56	1017.58	1014.83	1008.10
959.82	959.82	871.12	871.12	721.77
697.97	616.93	616.93	411.71	411.71

CH_2O

2929.65	2882.00	1846.22	1544.39	1272.64
1201.99				

HC•O

2636.76	1947.71	1116.69		

TS1

3206.71	3198.61	3187.87	3176.40	3164.37
2855.93	1687.11	1637.25	1618.49	1518.75
1481.72	1399.77	1351.99	1328.56	1217.34
1185.96	1182.82	1100.32	1043.80	1037.70
1013.68	1003.46	972.95	941.15	873.35
829.74	777.31	710.77	655.35	625.07
502.06	452.32	420.63	406.12	350.39
218.40	189.41	114.82		

TS2

3207.76	3197.74	3184.97	3174.68	3164.88
3050.92	2377.76	1626.98	1609.28	1517.15
1482.97	1388.59	1348.91	1322.07	1244.22
1192.20	1181.00	1138.11	1093.19	1044.21
1008.57	995.55	962.61	956.47	925.12
864.12	827.39	790.94	711.40	653.12
626.13	603.92	460.35	427.20	415.32
229.11	202.27	121.91		

TS3

3209.85	3199.54	3188.85	3176.98	3167.33
2942.26	1662.12	1633.00	1608.27	1519.60
1479.71	1406.18	1354.14	1331.67	1236.79
1189.36	1184.10	1102.75	1044.07	1012.52
1009.10	993.22	970.00	934.74	870.67
842.01	773.20	707.66	664.24	625.31
528.14	474.77	436.94	417.69	253.27
219.69	168.14	120.63		

TS4

3213.47	3203.64	3187.56	3179.14	3169.73
2931.71	1646.09	1600.72	1567.19	1502.82
1482.50	1457.06	1358.62	1342.98	1305.52
1196.34	1174.64	1118.28	1099.01	1090.82
1027.40	995.67	988.04	973.15	956.78
889.99	830.94	792.57	754.60	685.03
628.73	614.00	485.34	421.00	409.17
272.32	201.12	150.70		

TS5

3209.85	3200.82	3188.93	3178.95	3169.49
2890.41	1810.02	1617.55	1590.86	1501.68
1478.62	1420.93	1346.75	1321.04	1215.42
1180.64	1176.40	1102.49	1036.73	1031.99
1003.66	997.96	968.85	930.03	859.44
825.91	771.91	696.89	651.09	619.78
494.14	453.07	439.06	398.80	352.05
243.15	203.27	135.61		

TS6

3209.06	3197.58	3188.38	3175.90	3168.44
2933.79	2894.06	1711.02	1636.81	1569.41
1518.79	1468.60	1464.99	1328.48	1296.65
1256.78	1176.62	1175.23	1114.81	1075.38
1048.54	1018.16	986.50	964.48	948.42
898.59	822.83	736.53	675.85	602.53
595.03	457.76	405.61	390.89	264.37
93.46	81.57	32.96		

TS7

3205.96	3198.42	3195.04	3178.91	3174.06
3086.66	3017.49	1581.36	1551.45	1526.42
1473.69	1446.61	1339.83	1326.70	1282.01
1216.50	1189.22	1163.92	1149.22	1106.82
1027.73	1014.99	985.56	969.48	945.55
940.22	853.78	788.84	751.56	733.69
650.43	606.57	486.83	423.43	421.21
333.82	236.56	153.34		

TS8

3227.22	3205.80	3199.11	3195.81	3177.53
3172.31	3095.48	1592.20	1565.38	1487.86
1474.40	1469.35	1338.71	1305.79	1228.46
1173.31	1171.00	1147.81	1094.27	1080.17
1026.80	996.45	968.65	945.78	863.27
813.29	786.91	777.80	717.87	667.95
614.79	516.01	501.52	430.16	422.11
360.57	211.51	166.08		

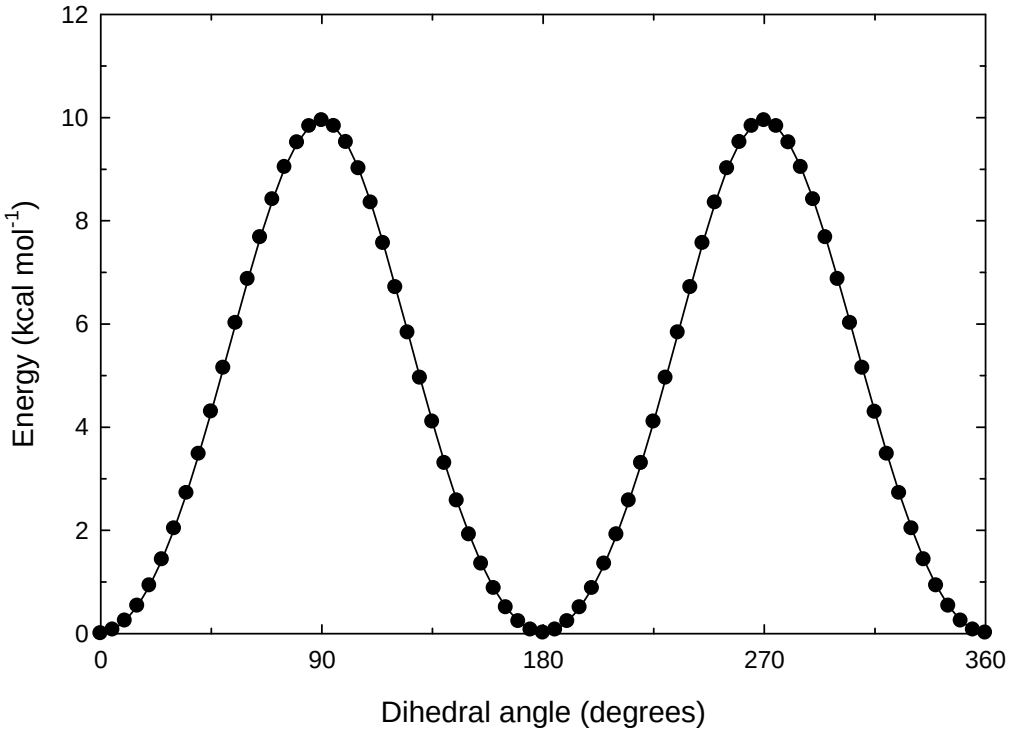
TS9

3196.28	3189.14	3173.23	3165.77	3148.77
3020.26	2948.20	1649.53	1602.60	1573.51
1480.41	1470.24	1431.42	1336.32	1299.98
1238.59	1175.43	1171.39	1074.87	1049.89
1020.86	1014.39	981.85	958.08	942.79
892.05	835.65	734.03	685.77	601.13
583.58	431.48	402.56	305.58	173.77
89.43	87.23	44.90		

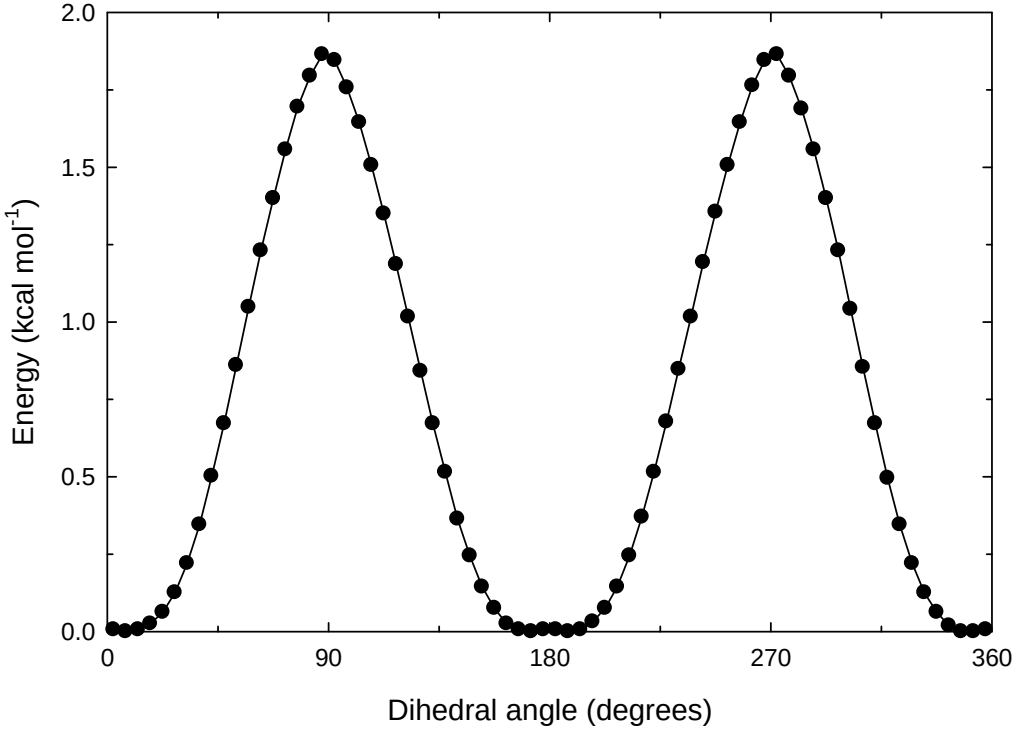
TS10

3202.94	3193.63	3190.06	3174.27	3170.49
3160.94	2801.66	1857.67	1599.53	1557.20
1494.13	1479.81	1358.87	1321.59	1197.19
1176.16	1170.37	1168.98	1051.11	1039.07
1026.07	1002.20	978.37	967.31	954.06
870.21	838.12	739.93	702.02	621.66
609.68	597.31	423.19	367.62	291.37
161.93	109.77	83.70		

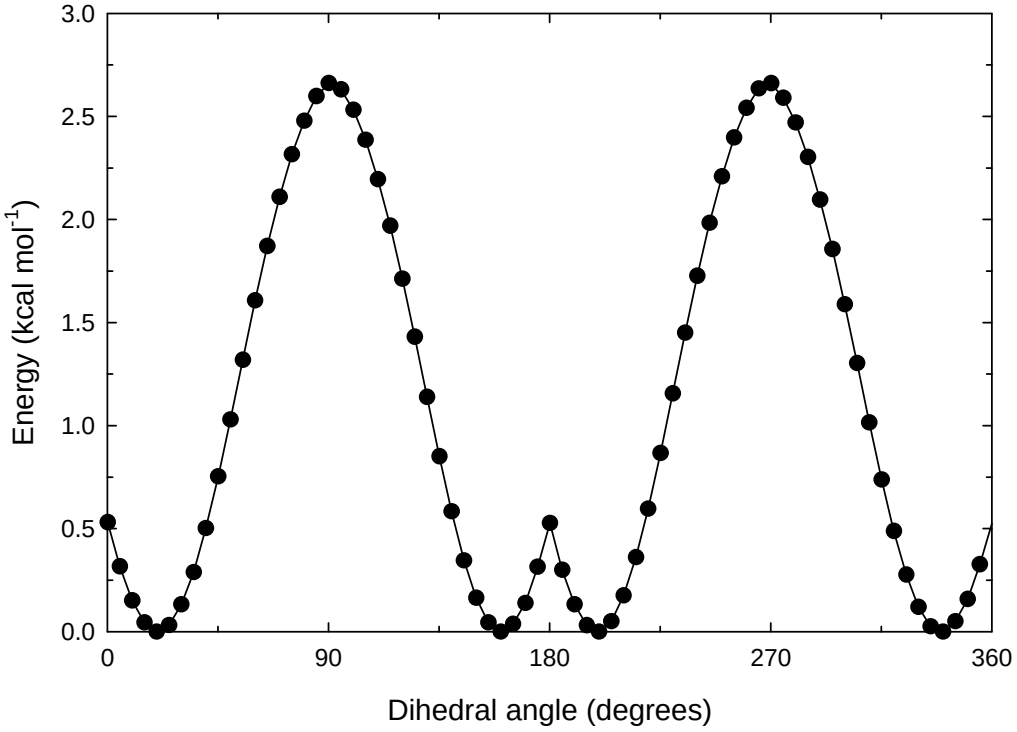
Internal rotor potentials (B3LYP/6-31G(d))



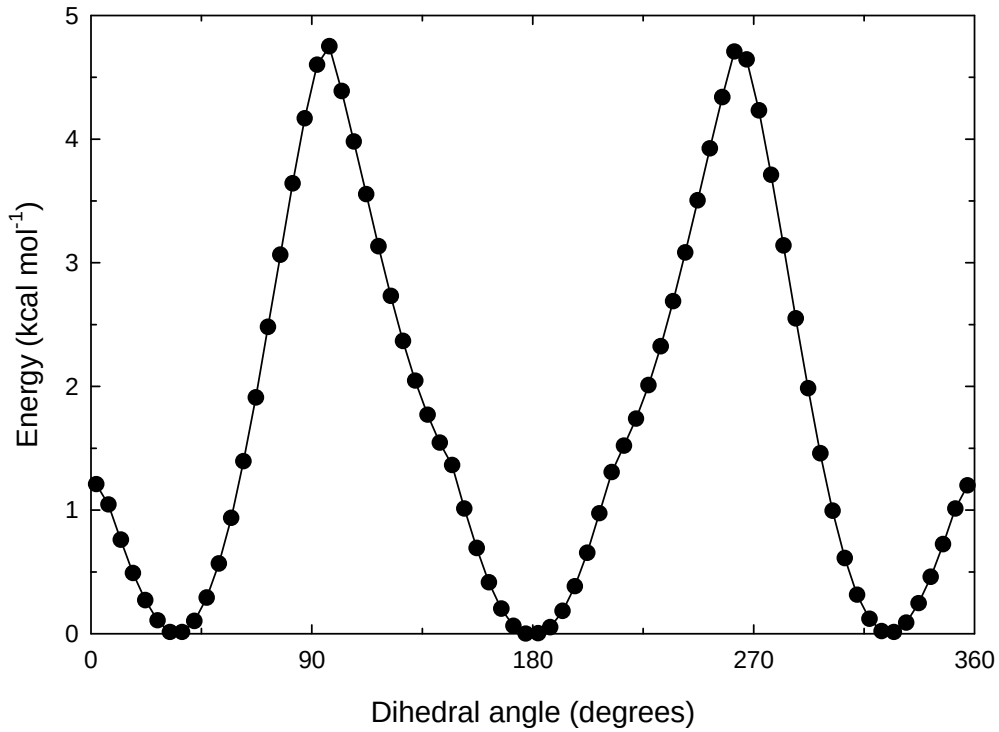
Benzaldehyde


2.0
1.5
1.0
0.5
0.0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

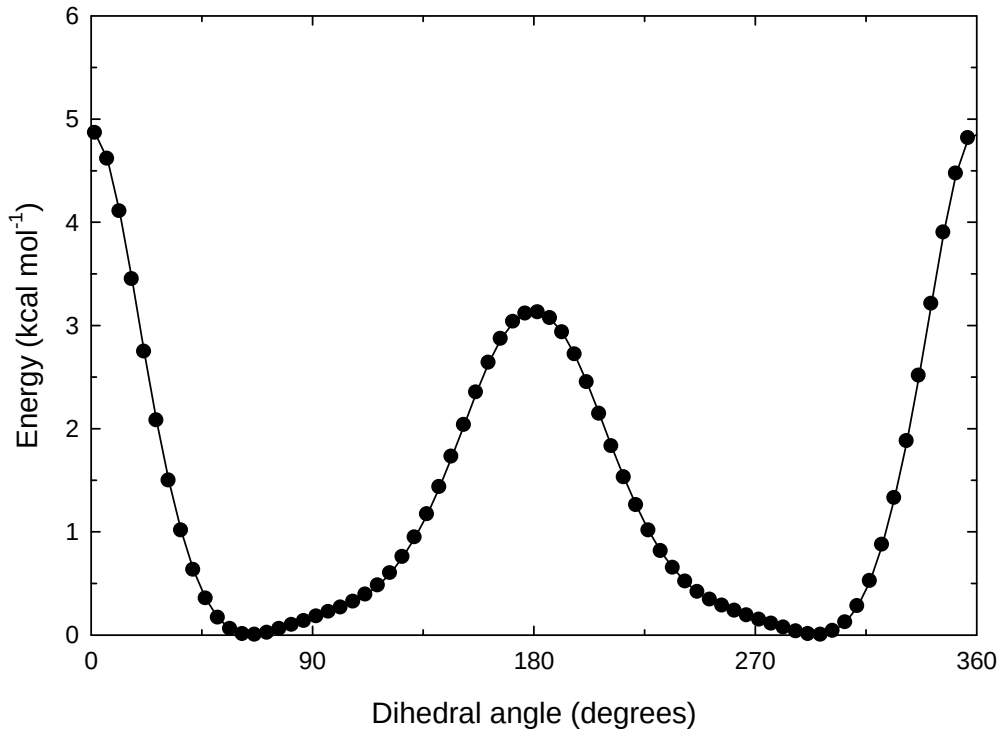
Benzoxyl



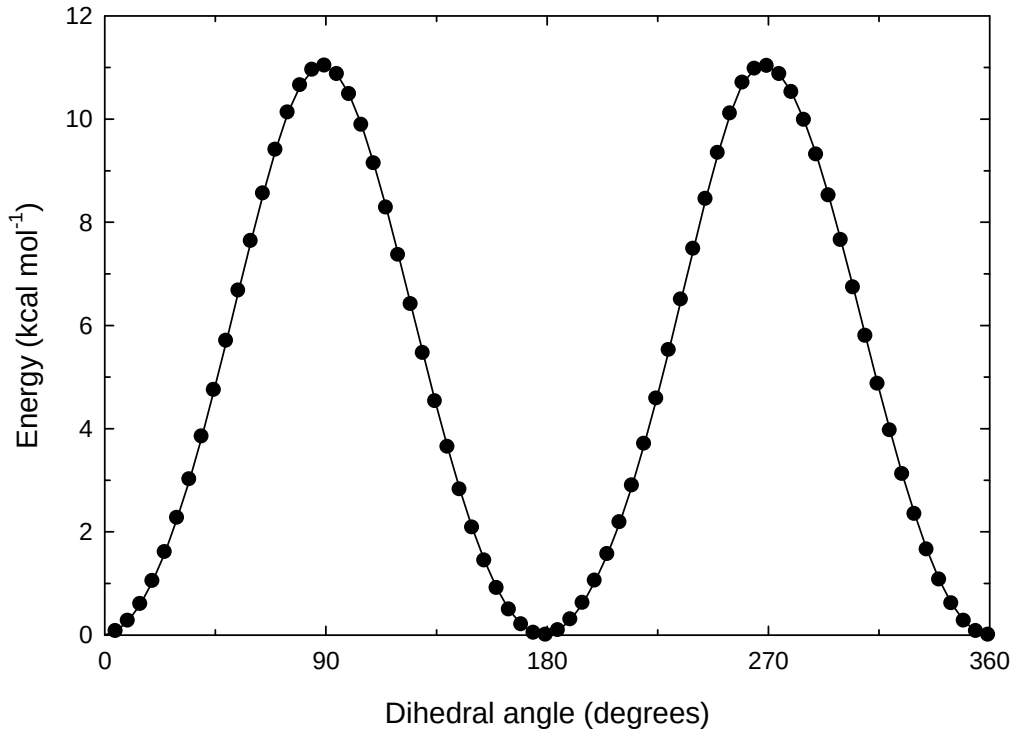
Phenoxymethyl (C--O)



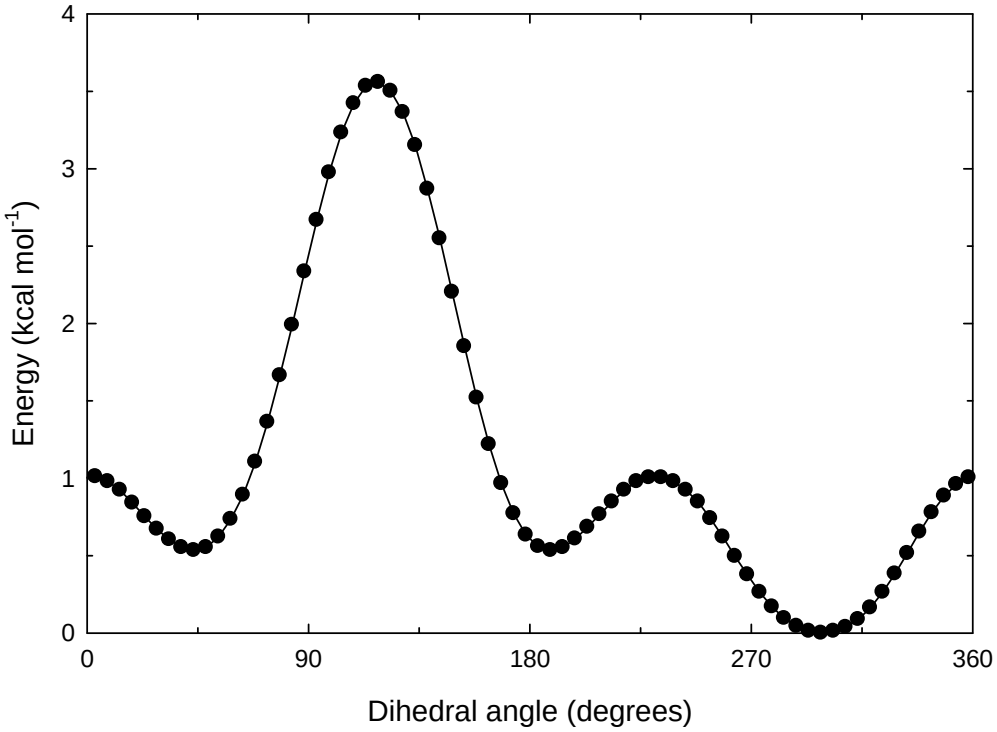
Phenoxymethyl (O--C)



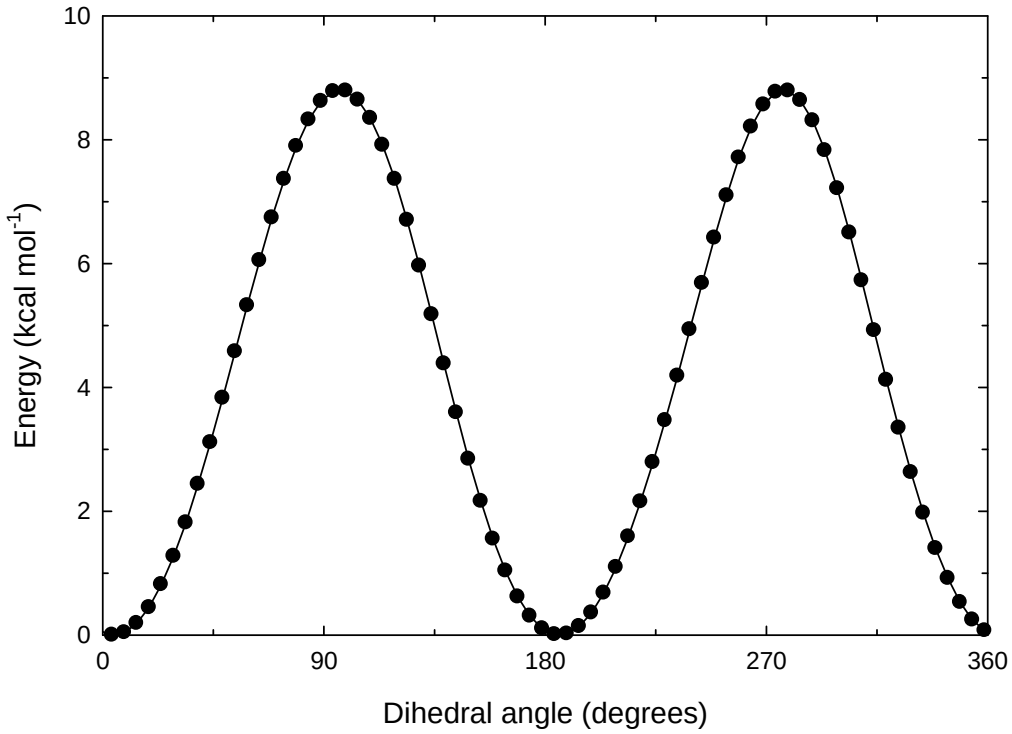
α-Hydroxybenzyl (C--O)



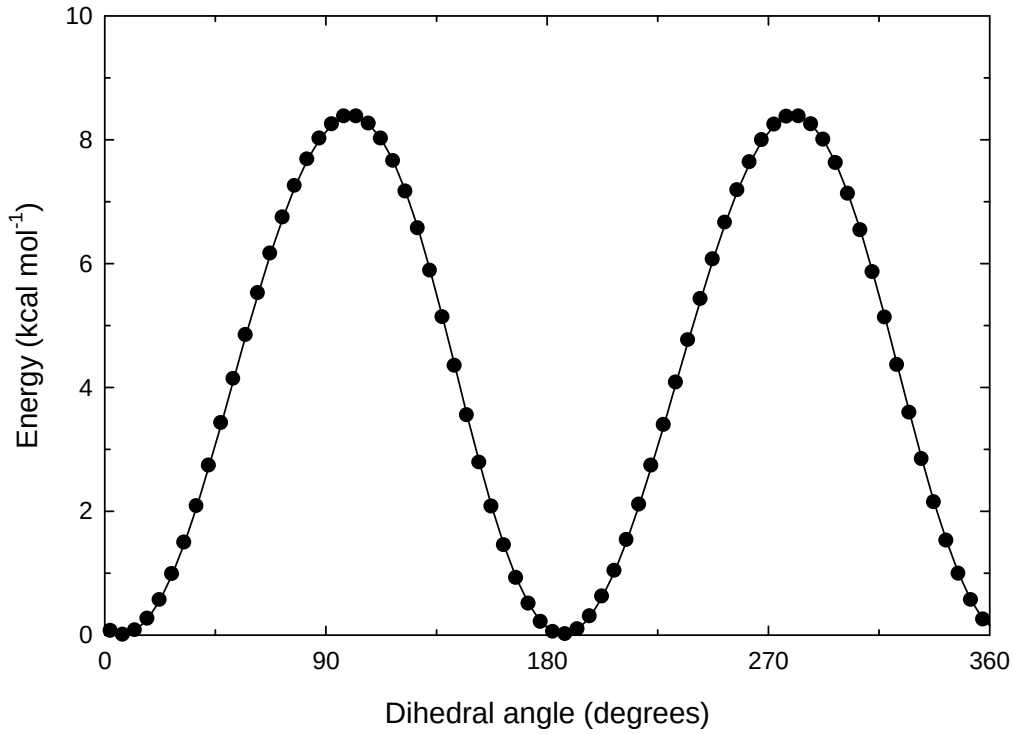
α–Hydroxybenzyl (C--C)



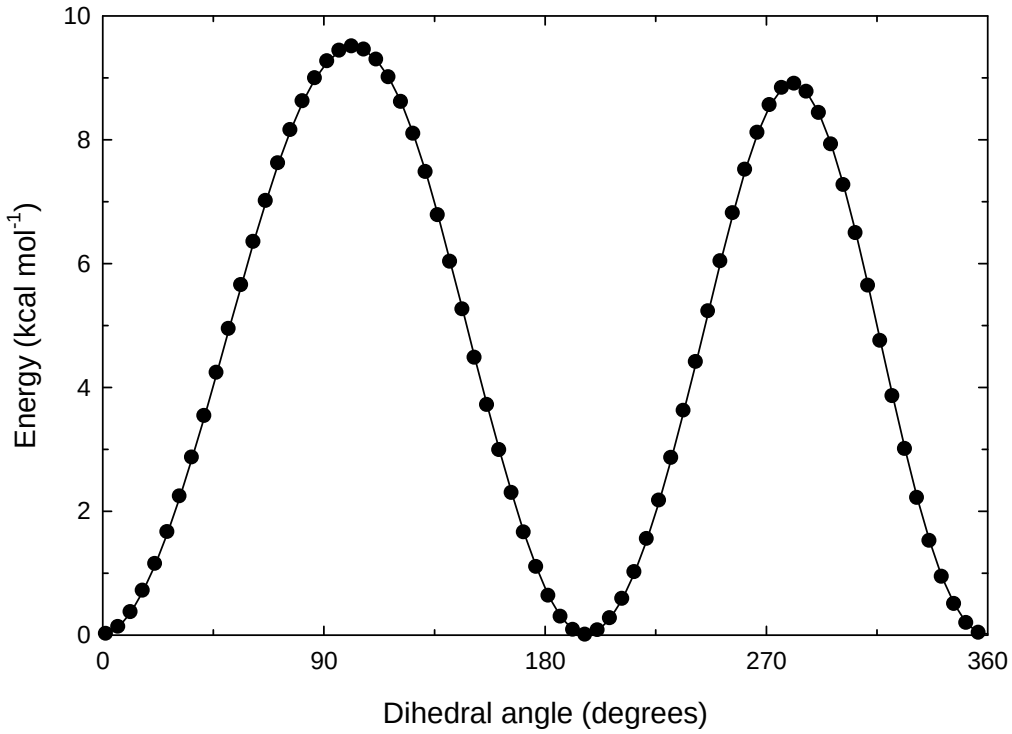
2,5-cyclohexadien-4-formyl-1-yl


10
8
6
4
2
0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

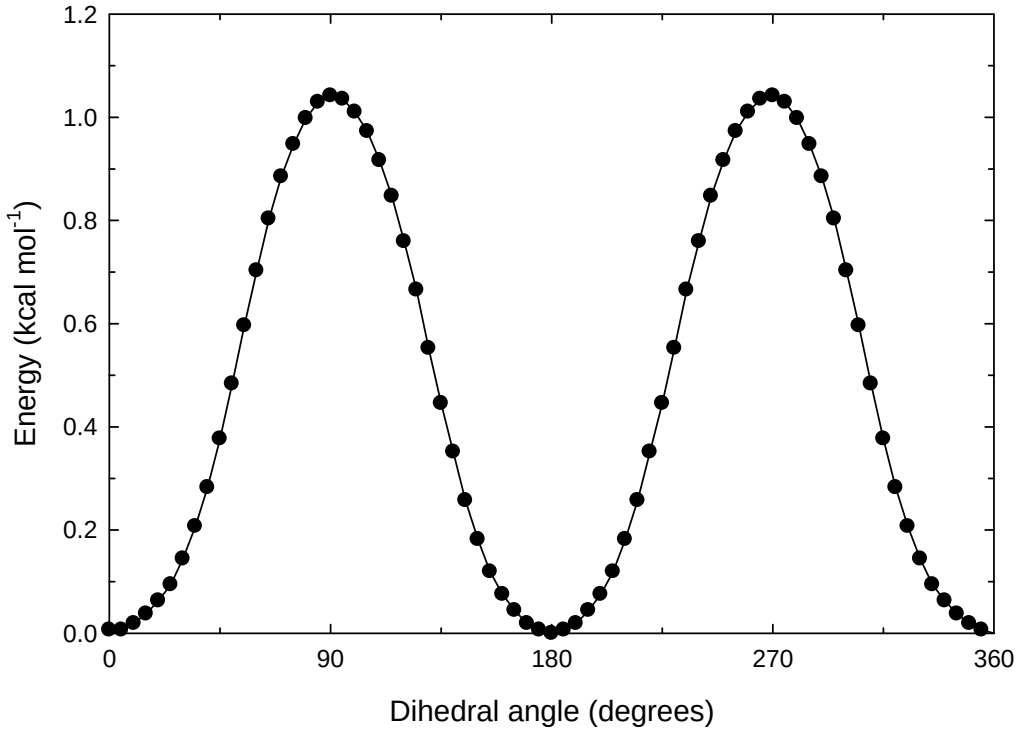
TS1


10
8
6
4
2
0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

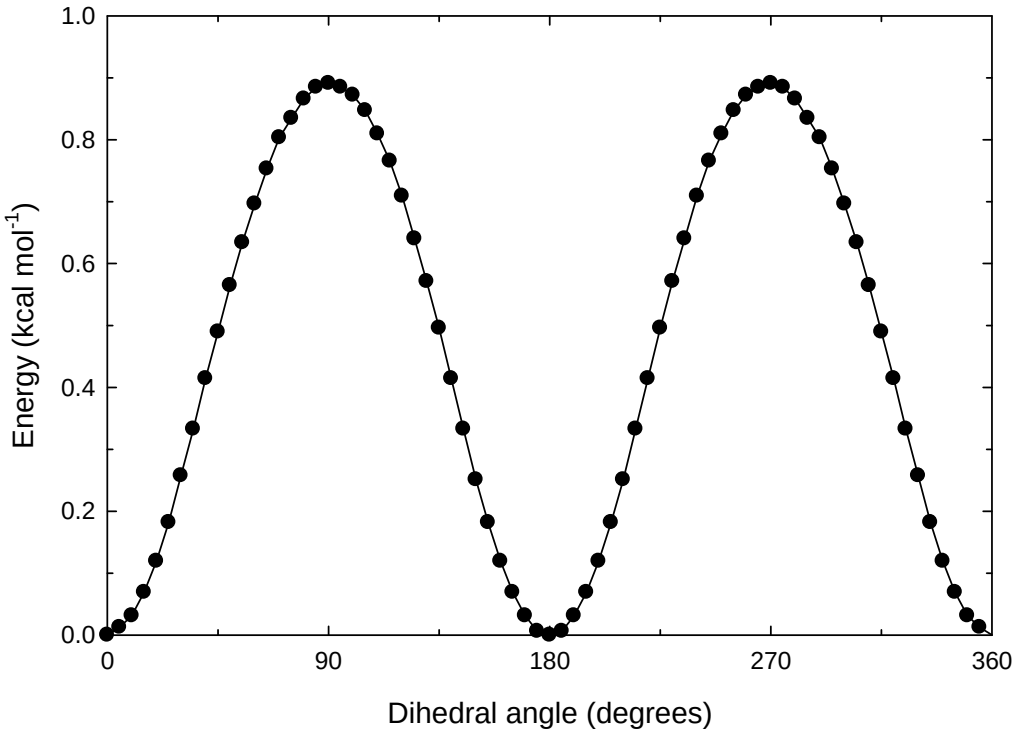
TS2


10
8
6
4
2
0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

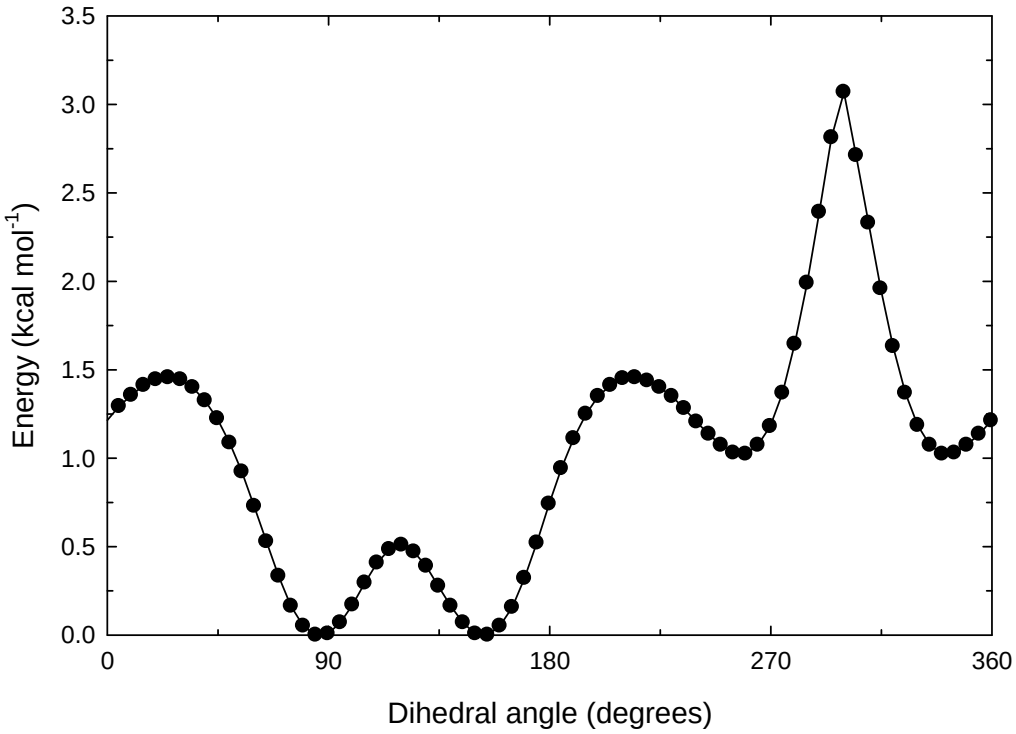
TS5


1.2
1.0
0.8
0.6
0.4
0.2
0.0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

TS6


1.0
0.8
0.6
0.4
0.2
0.0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

TS9


3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Energy (kcal mol-1)
0
90
180
270
360
Dihedral angle (degrees)

TS10

Energies and enthalpies (G3X, hartrees)

	E_0	H_{298}
benzoxyl	-345.84757048	-345.83976848
α-hydroxybenzyl	-345.87963296	-345.87165096
1-oxaspiro[2.5]octa-4,7-dien-5-yl	-345.83154811	-345.82412611
phenoxymethyl	-345.84736602	-345.83957802
2,5-cyclohexadien-4-formyl-1-yl	-345.85607824	-345.84801424
benzaldehyde	-345.32832995	-345.32109095
phenyl	-231.37494637	-231.36962637
benzene	-232.05533592	-232.04998892
CH_2O	-114.43328799	-114.42947699
HC•O	-113.79373132	-113.78993032
TS1	-345.81970698	-345.81173198
TS2	-345.80306081	-345.79554481
TS3	-345.81921994	-345.81116194
TS4	-345.81380769	-345.80647569
TS5	-345.81599029	-345.80809329
TS6	-345.79969932	-345.79118132
TS7	-345.82960883	-345.82247583
TS8	-345.81687712	-345.80957212
TS9	-345.78664729	-345.77788229
TS10	-345.82966248	-345.82154848

Apparent rate parameters (0.01 - 100 atm, 300 - 2000 K)

***P* = 0.01 atm:**

	A' (s^{-1})	n	E_a (kcal mol^{-1})
benzoxyl → benzaldehyde + H	3.04×10^{32}	-6.665	21.88
benzoxyl → phenyl + CH_2O	4.59×10^{43}	-9.513	39.05
benzoxyl → benzene + HC•O	2.57×10^{31}	-6.215	25.76

***P* = 0.1 atm:**

	A' (s^{-1})	n	E_a (kcal mol^{-1})
benzoxyl → benzaldehyde + H	6.13×10^{31}	-6.261	22.36
benzoxyl → phenyl + CH_2O	2.88×10^{38}	-7.786	37.77
benzoxyl → benzene + HC•O	5.27×10^{31}	-6.153	26.88

***P* = 1 atm:**

	A' (s^{-1})	n	E_a (kcal mol^{-1})
benzoxyl → benzaldehyde + H	5.26×10^{28}	-5.081	22.25
benzoxyl → phenyl + CH_2O	7.21×10^{33}	-6.210	36.85
benzoxyl → benzene + HC•O	2.37×10^{32}	-6.095	28.81

***P* = 10 atm:**

	A' (s^{-1})	n	E_a (kcal mol^{-1})
benzoxyl → benzaldehyde + H	1.68×10^{22}	-2.901	20.76
benzoxyl → phenyl + CH_2O	1.32×10^{27}	-4.009	35.07
benzoxyl → benzene + HC•O	3.82×10^{31}	-5.663	29.84

***P* = 100 atm:**

	A' (s^{-1})	n	E_a (kcal mol^{-1})
benzoxyl → benzaldehyde + H	2.44×10^{17}	-1.307	19.54
benzoxyl → phenyl + CH_2O	1.08×10^{27}	-2.057	33.31
benzoxyl → benzene + HC•O	2.04×10^{28}	-4.576	29.20