Supplementary Information

An Ab Initio RRKM-Based Master Equation Study for Kinetics of OH-Initiated Oxidation of 2-Methyltetrahydrofuran and Its Implications in Kinetic Modeling

Tam V.-T. Mai [1,2,†], Thanh Q. Bui [3,†], Nguyen Thi Ai Nhung [3,*], Phan Tu Quy [4], Krishna Prasad Shrestha [5,‡], Fabian Mauss [5], Binod Raj Giri [6,*] and Lam K. Huynh [7,8,*]

[1] Institute of Fundamental and Applied Sciences, Duy Tan University, 06 Tran Nhat Duat, Tan Dinh Ward, District 1, Ho Chi Minh City 700000, Vietnam
[2] Faculty of Natural Sciences, Duy Tan University, Da Nang City 550000, Vietnam
[3] Department of Chemistry, University of Sciences, Hue University, Hue City 530000, Vietnam
[4] Department of Natural Sciences & Technology, Tay Nguyen University, Buon Ma Thuot City 630000, Vietnam
[5] Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology, Siemens-Halske-Ring 8, 03046 Cottbus, Germany
[6] Physical Science and Engineering Division, Clean Combustion Research Center, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia
[7] School of Chemical and Environmental Engineering, International University, Quarter 6, Linh Trung Ward, Thu Duc City, Ho Chi Minh City 700000, Vietnam
[8] Vietnam National University, Ho Chi Minh City 700000, Vietnam
* Correspondence: ntanhung@hueuni.edu.vn (N.T.A.N.); binod.giri@kaust.edu.sa (B.R.G.); hklam@hcmiu.edu.vn (L.K.H.); Tel.: +84-(8)-2211-4046 (ext. 3233) (L.K.H.); Fax: +84-(8)-3724-4271 (L.K.H.)
† These authors contributed equally to this work.
‡ Current address: Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

Contents

Table S1: Optimized geometries, electronic energies at 0 K ($E_{elec}^{0\,K}$), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at CCSD(T)/cc-pVTZ//M06-2X/aug-cc-pVTZ level of theory for the title reaction.

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
OH	8	0.000000000	0.000000000	0.107999000	-75.637723	0.008530	3742.0378 (3737.8)[1]		
($C_{\infty v}$)	1	0.000000000	0.000000000	-0.863995000					
H_2O	8	0.000000000	0.000000000	0.116332000	-76.332140	0.021565	1615.7190	3873.1681	3977.2474
(C_{2v})	1	0.000000000	0.762680000	-0.465326000			(1595.0; 3657.0[2]; 3756.0[1])		
	1	0.000000000	-0.762680000	-0.465326000					
2MTHF	6	1.359420000	-0.833589000	0.167257000	-271.304799	0.145654	45.9007	198.9607	241.7856
(C_1)	8	-0.016915000	-1.130708000	-0.051144000			321.6648	472.9320	564.5336
	6	-0.730955000	0.054869000	-0.395401000			661.9380	833.1459	879.1904
	6	0.118034000	1.189529000	0.162632000			888.9693	920.2310	944.3517
	6	1.528959000	0.665808000	-0.091771000			994.3893	1021.6762	1068.1326
	1	1.607918000	-1.090231000	1.199633000			1152.2294	1168.3976	1181.5757
	1	1.972108000	-1.445694000	-0.495743000			1204.9369	1227.3689	1268.3241
	1	-0.768082000	0.138844000	-1.489675000			1308.7387	1339.2186	1362.9386
	1	-0.087281000	2.144638000	-0.316830000			1396.3646	1399.8296	1422.9779
	1	-0.069778000	1.288067000	1.234277000			1485.9086	1488.4901	1501.7979
	1	1.810933000	0.843931000	-1.129853000			1504.1545	1540.0299	2996.4629
	1	2.285478000	1.115172000	0.547558000			3053.4140	3064.1249	3067.6243
	6	-2.135363000	-0.037456000	0.153997000			3080.3042	3097.6805	3135.1959
	1	-2.705986000	0.853177000	-0.110192000			3139.0330	3143.7821	3146.1076
	1	-2.646925000	-0.909459000	-0.250195000					
	1	-2.103637000	-0.127747000	1.239886000					
RC	6	0.769120000	-0.766597000	-0.123486000	-346.955251	0.157496	67.5885	84.5772	112.7911
(C_1)	8	0.017971000	-0.020735000	-1.084381000			157.0109	233.0870	253.0762
	6	-1.343030000	-0.386907000	-0.881629000			322.8405	453.4482	492.6279
	6	-1.513502000	-0.549168000	0.639698000			575.3928	596.7120	679.8552
	6	-0.063705000	-0.654837000	1.154919000			803.2187	861.2955	905.0323
	1	0.793942000	-1.812035000	-0.456659000			918.2873	941.0198	1001.3474
	1	-1.966397000	0.393724000	-1.311455000			1043.6887	1079.3276	1139.8243
	1	-1.540976000	-1.327298000	-1.403842000			1166.2272	1176.4978	1229.9926
	1	-2.014930000	0.314701000	1.069086000			1257.4769	1281.8835	1301.9181
	1	-2.101403000	-1.433719000	0.874393000			1325.7270	1366.3804	1390.1562
	1	0.221027000	0.253389000	1.689053000			1398.7135	1428.6246	1491.7927

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	0.094384000	-1.501643000	1.819383000			1494.0771	1502.0461	1513.3208
	8	-0.162083000	2.395508000	0.293215000			1528.8135	3007.5952	3045.1472
	1	-0.001145000	1.743806000	-0.424275000			3065.8949	3075.5715	3103.9203
	6	2.169404000	-0.211059000	-0.038297000			3130.1950	3137.1276	3140.1763
	1	2.748412000	-0.774396000	0.692941000			3149.1828	3155.1112	3547.1860
	1	2.671136000	-0.276275000	-1.002273000					
	1	2.139126000	0.832965000	0.275753000					
TS1 (C_1)	6	1.463583000	0.069377000	-0.882896000	-346.946041	0.153706	-625.7975	51.9506	64.4149
	8	0.059066000	-0.069497000	-1.124038000			126.4005	202.3738	228.5237
	6	-0.618821000	-0.326123000	0.087476000			277.4985	313.9585	442.7778
	6	0.433495000	-0.871989000	1.037379000			563.9336	649.7834	663.1653
	6	1.656132000	-0.054226000	0.629304000			832.6715	877.6092	884.9834
	1	1.978842000	-0.726363000	-1.424146000			921.3035	944.1358	979.0006
	1	1.798876000	1.029730000	-1.274486000			1021.5887	1031.3445	1087.5553
	1	-0.958531000	0.680097000	0.511488000			1164.2304	1179.8193	1191.6683
	1	0.155537000	-0.752279000	2.081940000			1227.6980	1260.5203	1283.6131
	1	0.583134000	-1.935411000	0.831792000			1295.6237	1347.9050	1357.2538
	1	1.612218000	0.928672000	1.096675000			1397.8581	1408.9772	1481.1227
	1	2.602096000	-0.523622000	0.888262000			1484.6560	1495.0628	1501.5612
	8	-0.951432000	2.245005000	0.407851000			1535.8429	1956.6451	3057.8345
	1	-0.764950000	2.172815000	-0.543213000			3062.8799	3063.8880	3094.1175
	6	-1.840775000	-1.171345000	-0.163873000			3107.9338	3137.5791	3142.5922
	1	-2.389344000	-1.326064000	0.764234000			3151.7563	3152.9318	3762.7979
	1	-2.499741000	-0.685672000	-0.881317000					
	1	-1.540896000	-2.140127000	-0.566076000					
TS2a (C_1)	6	1.449317000	-0.678847000	-0.660750000	-346.941814	0.153159	-987.6041	69.4333	134.3607
	8	0.056050000	-0.774887000	-0.949444000			146.2876	201.8288	225.7041
	6	-0.631788000	-0.775296000	0.296137000			311.4897	389.7924	463.6943
	6	0.119156000	0.281449000	1.081958000			545.5848	697.7311	759.1570
	6	1.571541000	0.033301000	0.706357000			825.2120	872.2465	899.5954
	1	1.883997000	-1.680706000	-0.623663000			914.0041	933.7682	1000.4778
	1	1.916997000	-0.126353000	-1.472939000			1035.0072	1063.5521	1084.9447
	1	-0.482246000	-1.750188000	0.786268000			1161.9835	1169.1599	1193.0773
	1	-0.185527000	1.313442000	0.597106000			1206.6262	1243.9258	1269.0586
	1	-0.107823000	0.352902000	2.143097000			1284.6432	1311.8142	1344.7193
	1	2.138506000	0.958938000	0.642017000			1384.7360	1394.6731	1423.6140

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	2.056921000	-0.610990000	1.439581000			1490.2744	1493.2578	1500.6427
	8	-0.297384000	2.212463000	-0.469148000			1531.7653	1619.2842	2969.0366
	1	-0.295276000	1.534143000	-1.167224000			3054.3760	3073.2120	3086.0102
	6	-2.104627000	-0.536981000	0.068897000			3123.4318	3142.5923	3144.2845
	1	-2.515839000	-1.309122000	-0.578736000			3147.8459	3155.1900	3736.0751
	1	-2.636788000	-0.561568000	1.019356000					
	1	-2.263840000	0.437133000	-0.391718000					
TS2b (C_1)	6	0.042953000	1.452563000	-0.498016000	-346.940355	0.153069	-1002.2764	75.7373	111.6627
	8	0.240078000	0.210267000	-1.175850000			141.1508	199.5973	210.4501
	6	0.616449000	-0.767530000	-0.209290000			310.8319	407.8069	435.5955
	6	-0.255615000	-0.408238000	0.979228000			620.7577	714.2494	771.2196
	6	-0.256347000	1.113404000	0.977038000			823.3336	871.5684	905.8197
	1	0.937132000	2.072533000	-0.592053000			913.0506	940.7253	989.1461
	1	-0.783760000	1.962407000	-0.988980000			1021.3468	1052.1156	1085.6162
	1	0.357654000	-1.738888000	-0.631294000			1095.6309	1159.0120	1174.7941
	1	-1.341269000	-0.753394000	0.687275000			1212.5678	1245.2509	1252.5322
	1	-0.014609000	-0.894832000	1.921689000			1284.5007	1310.9763	1340.4255
	1	-1.210288000	1.517233000	1.308085000			1372.1371	1399.8548	1404.5163
	1	0.518880000	1.504106000	1.636620000			1487.9172	1491.6358	1500.5330
	8	-2.425668000	-0.848210000	-0.192915000			1533.8655	1646.9705	3046.5590
	1	-1.931211000	-0.570649000	-0.984047000			3061.7453	3076.2382	3097.8721
	6	2.105427000	-0.708664000	0.097164000			3122.6255	3125.9296	3127.9265
	1	2.379763000	-1.491733000	0.803852000			3133.0280	3142.4826	3740.3790
	1	2.677447000	-0.847071000	-0.818849000					
	1	2.377776000	0.254615000	0.531079000					
TS3a (C_1)	6	1.137655000	-0.409654000	0.019908000	-346.941923	0.153449	-983.3379	58.6392	125.7745
	8	0.256691000	-0.404105000	-1.108834000			143.1145	257.2315	285.6182
	6	-0.915450000	-1.093785000	-0.716184000			343.0822	408.6677	460.5922
	6	-1.176193000	-0.562115000	0.677077000			535.1456	657.7336	781.7737
	6	0.221828000	-0.432242000	1.268191000			830.8888	880.2149	907.7900
	1	1.725785000	-1.332741000	-0.019656000			913.7854	959.2494	996.1269
	1	-1.702980000	-0.874668000	-1.433849000			1032.4268	1072.7913	1087.1109
	1	-0.736591000	-2.177183000	-0.697059000			1154.1931	1157.2915	1176.3134
	1	-1.587451000	0.528483000	0.519982000			1214.4671	1241.9522	1268.9146
	1	-1.915584000	-1.090788000	1.273328000			1292.3520	1311.3398	1350.4705
	1	0.325645000	0.478494000	1.856571000			1382.1740	1392.6926	1422.8751

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	0.458236000	-1.278565000	1.913023000			1491.1056	1492.9607	1501.1728
	8	-1.556114000	1.798322000	-0.072341000			1513.5765	1652.0980	3004.1993
	1	-0.911234000	1.563961000	-0.762922000			3026.6004	3063.5355	3082.4997
	6	2.050364000	0.790328000	-0.070947000			3126.8360	3135.9475	3137.5702
	1	2.773273000	0.775742000	0.744374000			3144.8749	3148.8731	3731.9009
	1	2.590984000	0.789733000	-1.016028000					
	1	1.466081000	1.708595000	0.003361000					
TS3b (C_1)	6	-0.899102000	-0.511751000	-0.270524000	-346.940806	0.153149	-975.7793	50.9011	118.0245
	8	-0.250432000	0.567752000	-0.966029000			127.3200	251.8839	271.7122
	6	0.426506000	1.375838000	-0.017474000			362.4641	393.5687	459.0685
	6	0.928765000	0.379799000	1.001670000			516.4054	671.8782	795.9545
	6	-0.240498000	-0.580149000	1.123158000			834.2318	869.8618	907.4358
	1	-0.682210000	-1.415260000	-0.842197000			913.8544	959.1713	983.9630
	1	1.212037000	1.923690000	-0.534180000			1025.2511	1043.7992	1086.7261
	1	-0.261901000	2.094571000	0.445969000			1131.5126	1153.0105	1178.5938
	1	1.805666000	-0.202302000	0.471521000			1205.3240	1230.2383	1282.5178
	1	1.331320000	0.784420000	1.926941000			1285.2142	1307.4675	1355.7226
	1	0.067943000	-1.589875000	1.384032000			1375.3739	1396.4177	1412.0497
	1	-0.937045000	-0.229003000	1.888676000			1486.1394	1490.0523	1500.6100
	8	2.389228000	-0.872921000	-0.604506000			1519.1197	1636.2193	3009.1181
	1	1.742358000	-0.579439000	-1.269797000			3058.7515	3060.4625	3077.2893
	6	-2.395566000	-0.278663000	-0.219838000			3129.3668	3130.4860	3138.8997
	1	-2.808245000	-0.212790000	-1.224847000			3146.4074	3149.0263	3735.8162
	1	-2.888408000	-1.095123000	0.309397000					
	1	-2.612512000	0.652012000	0.306820000					
TS4a (C_1)	6	-0.976392000	0.711388000	0.443304000	-346.943185	0.153680	-721.8573	62.1017	79.0519
	8	0.010291000	-0.001141000	1.194040000			103.4447	177.1481	244.5902
	6	0.476473000	-1.087741000	0.432631000			274.2281	352.8668	431.5253
	6	-0.527793000	-1.336011000	-0.699645000			644.4911	678.8224	722.6866
	6	-1.680008000	-0.382743000	-0.355634000			804.3246	837.6832	885.0968
	1	-1.635682000	1.175655000	1.176041000			915.0720	947.9282	980.5235
	1	1.491082000	-0.829817000	-0.014292000			1026.0379	1054.9234	1092.3879
	1	0.645678000	-1.934354000	1.097708000			1117.3332	1167.2054	1223.9834
	1	-0.082626000	-1.081957000	-1.660584000			1226.2777	1245.5553	1302.3819
	1	-0.843116000	-2.375691000	-0.744021000			1325.0419	1335.5757	1371.1108
	1	-2.188012000	0.004200000	-1.236725000			1387.3669	1414.1614	1443.3992

Species	Cartesian coordinate (Å)				$E_{elec}^{0\ K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-2.412905000	-0.883087000	0.276121000			1484.7242	1493.7173	1504.8623
	8	2.658223000	0.124887000	-0.397437000			1510.8467	1889.5126	3053.6243
	1	2.420123000	0.728841000	0.325676000			3074.3108	3082.7469	3096.7534
	6	-0.331486000	1.774467000	-0.429877000			3103.0465	3127.2581	3134.1203
	1	-1.095549000	2.349604000	-0.953108000			3134.5392	3141.1446	3751.9927
	1	0.255093000	2.458379000	0.183191000					
	1	0.333031000	1.322100000	-1.167505000					
TS4b (C_1)	6	0.858678000	-0.378654000	-0.275540000	-346.944365	0.153822	-720.2306	52.7329	60.6151
	8	0.047455000	-0.449811000	0.898281000			94.8836	159.5153	230.0948
	6	-0.963895000	0.511119000	0.765053000			261.3309	317.3224	472.4637
	6	-0.425159000	1.635364000	-0.135221000			579.1332	671.6299	711.1800
	6	0.962989000	1.118961000	-0.542052000			770.0668	864.8673	883.2470
	1	0.313808000	-0.857529000	-1.099722000			917.9744	944.9893	989.1730
	1	-1.860406000	0.033121000	0.247520000			1034.6095	1080.1268	1102.5760
	1	-1.297527000	0.814611000	1.755620000			1165.5851	1173.9354	1224.5907
	1	-1.069791000	1.765496000	-1.002490000			1232.0296	1261.0294	1306.9093
	1	-0.376006000	2.585922000	0.391081000			1319.6809	1360.9242	1370.9717
	1	1.214921000	1.341264000	-1.576644000			1396.7488	1425.6809	1428.5337
	1	1.737461000	1.539201000	0.101060000			1486.1088	1489.6949	1502.5958
	8	-2.510641000	-1.102847000	-0.599550000			1509.1991	1947.6908	3008.5196
	1	-2.003105000	-1.779353000	-0.121317000			3068.0717	3079.5553	3097.9334
	6	2.162936000	-1.090653000	-0.017012000			3120.3869	3136.9539	3142.7843
	1	1.991486000	-2.139878000	0.217556000			3148.1256	3149.9076	3767.5360
	1	2.802775000	-1.032658000	-0.897107000					
	1	2.678576000	-0.625763000	0.823225000					
TS5 (C_1)	6	-1.321407000	1.019655000	-0.374889000	-346.940455	0.152787	-1115.9075	53.6060	91.2708
	8	-0.182475000	0.448131000	-1.022808000			158.9474	219.0353	314.2150
	6	0.108166000	-0.838634000	-0.467308000			370.0125	393.4764	476.9706
	6	-0.656341000	-0.887333000	0.850213000			563.9547	653.9154	755.6514
	6	-1.904500000	-0.078753000	0.508837000			844.5086	884.0785	888.7690
	1	-0.992109000	1.870215000	0.229109000			930.0111	939.4009	956.9562
	1	-2.014505000	1.378148000	-1.134721000			1009.8776	1036.5584	1059.4434
	1	-0.286524000	-1.603149000	-1.150281000			1143.6103	1171.6517	1194.7301
	1	-0.867185000	-1.905857000	1.169164000			1207.8868	1225.0252	1275.6389
	1	-0.072471000	-0.383994000	1.622978000			1308.6668	1314.6735	1341.9945
	1	-2.608395000	-0.689222000	-0.057834000			1353.1872	1394.0017	1403.4066

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-2.418256000	0.319901000	1.380394000			1455.2298	1487.1134	1501.2949
	6	1.598152000	-1.004827000	-0.351044000			1530.0866	1534.9815	2992.7198
	1	1.887652000	-1.904203000	0.189565000			3041.9271	3076.6717	3082.5197
	1	2.117010000	-0.924890000	-1.303177000			3103.4959	3112.5256	3141.5228
	1	1.992418000	-0.084210000	0.301616000			3148.2722	3177.4046	3744.9657
	8	2.040155000	1.193188000	0.737718000					
	1	1.456514000	1.536059000	0.039043000					
PC1 (C_1)	6	-0.665203000	-1.007156000	0.943788000	-346.9902578	0.156318	47.3646	59.3110	124.5372
	8	-0.009238000	0.273338000	0.946079000			138.1284	168.0050	176.7777
	6	0.857153000	0.350662000	-0.124583000			222.7764	265.8919	313.0034
	6	0.945418000	-0.980583000	-0.794609000			352.6164	503.7227	569.5667
	6	-0.414363000	-1.589762000	-0.442357000			640.3204	812.4599	883.5283
	1	-0.213032000	-1.616274000	1.728898000			906.4600	937.3057	946.0881
	1	-1.717746000	-0.848832000	1.167274000			999.4456	1023.3006	1068.8118
	1	-2.078234000	1.762109000	-1.241622000			1106.5581	1183.9236	1216.9788
	1	1.122237000	-0.900325000	-1.865873000			1254.1993	1270.8053	1280.0560
	1	1.762616000	-1.581290000	-0.368817000			1344.3253	1360.1803	1404.6118
	1	-1.176140000	-1.229832000	-1.132427000			1419.3490	1471.2650	1481.4862
	1	-0.419073000	-2.676966000	-0.440020000			1489.7734	1497.4346	1526.5725
	8	-2.336770000	1.311963000	-0.435248000			1632.0386	2975.2822	2991.2808
	1	-1.528852000	1.259788000	0.090848000			3065.5733	3097.1156	3097.7170
	6	1.976589000	1.306996000	0.038612000			3118.1487	3140.4858	3144.3883
	1	2.486145000	1.458316000	-0.911749000			3156.4244	3793.3595	3937.0672
	1	1.616567000	2.270477000	0.398637000					
	1	2.716022000	0.939475000	0.763099000					
PC2 (C_1)	6	1.230240000	-0.688764000	-0.827116000	-346.9809593	0.155681	54.3122	85.6147	146.0368
	8	-0.044122000	-0.102579000	-1.074593000			160.5524	202.4440	223.5776
	6	-0.956706000	-0.679328000	-0.137351000			242.7924	297.4608	320.2358
	6	-0.117920000	-0.889920000	1.080206000			362.9888	495.5373	571.3663
	6	1.323592000	-0.842756000	0.699227000			661.7039	677.7244	859.0433
	1	1.282517000	-1.665364000	-1.318066000			866.1196	915.3002	948.0267
	1	1.986196000	-0.031677000	-1.249311000			1004.2975	1038.3556	1052.5863
	1	-1.294398000	-1.648966000	-0.540156000			1083.1749	1149.3149	1153.9705
	1	0.393248000	2.195805000	1.073346000			1208.3106	1266.8659	1299.0365
	1	-0.506966000	-1.227682000	2.027292000			1304.1569	1340.7523	1375.5939
	1	1.834396000	0.016556000	1.143469000			1400.7435	1411.2001	1477.4046

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	1.877367000	-1.737524000	0.990228000			1488.8646	1498.4456	1520.7231
	8	0.732006000	2.386871000	0.195877000			1644.8937	2941.4291	3039.0539
	1	0.363113000	1.691185000	-0.366671000			3043.5966	3068.4343	3083.3567
	6	-2.157360000	0.229519000	0.028096000			3144.2275	3147.1222	3150.7510
	1	-2.662138000	0.365307000	-0.926924000			3242.6153	3745.0860	3920.9943
	1	-2.860437000	-0.209258000	0.735148000					
	1	-1.847041000	1.204778000	0.403007000					
PC3 (C_1)	6	0.913691000	-0.661679000	-0.141752000	-346.9818076	0.155318	61.3776	78.2587	138.9862
	8	-0.015402000	-0.111448000	-1.082775000			162.3043	199.3614	222.3904
	6	-1.282285000	-0.699468000	-0.813616000			247.7392	287.3661	323.5450
	6	-1.280284000	-0.930057000	0.660661000			337.1551	481.0489	558.8430
	6	0.114249000	-0.778739000	1.165559000			611.2943	734.6577	851.7521
	1	1.185184000	-1.667348000	-0.485200000			897.6909	909.2656	950.3606
	1	-2.058090000	-0.014658000	-1.163378000			978.1734	1012.6951	1061.3896
	1	-1.386722000	-1.638299000	-1.377895000			1088.1228	1146.8706	1162.3309
	1	-1.380637000	1.999231000	0.756399000			1212.2724	1231.4379	1282.5090
	1	-2.119629000	-1.308582000	1.220097000			1323.8634	1361.6206	1386.7980
	1	0.237121000	0.134678000	1.760159000			1392.7719	1427.4972	1470.7724
	1	0.449544000	-1.616377000	1.779552000			1492.9323	1501.5473	1506.6586
	8	-0.665752000	2.384713000	0.244590000			1644.7260	2974.6894	3008.8368
	1	-0.392709000	1.683691000	-0.363883000			3019.7996	3066.7165	3072.9885
	6	2.134330000	0.222504000	-0.078474000			3087.2069	3141.1722	3150.7574
	1	2.855990000	-0.190690000	0.625914000			3250.7265	3747.7638	3917.6439
	1	2.607134000	0.295072000	-1.056345000					
	1	1.853837000	1.221802000	0.255791000					
PC4 (C_1)	6	-1.254035000	0.598609000	0.187576000	-346.986457	0.156228	55.8206	78.0427	118.3595
	8	-0.624555000	-0.088401000	1.287142000			150.2362	162.2033	213.1404
	6	0.186491000	-1.059249000	0.787461000			256.0954	287.9094	356.5437
	6	-0.096024000	-1.317884000	-0.663995000			419.2494	450.1908	602.9676
	6	-1.361075000	-0.473858000	-0.896639000			674.2497	751.3146	821.2083
	1	-2.226914000	0.919923000	0.555218000			867.3055	925.5053	954.9276
	1	2.165903000	-0.127209000	0.319344000			960.1286	1019.2282	1065.6263
	1	0.492602000	-1.799202000	1.512272000			1096.6794	1128.7716	1208.9447
	1	0.726366000	-0.978878000	-1.300251000			1223.0111	1233.6188	1301.4273
	1	-0.252447000	-2.375190000	-0.875877000			1318.9184	1336.5231	1379.2246
	1	-1.410556000	-0.043058000	-1.894110000			1411.2581	1419.8178	1483.6390

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-2.251626000	-1.079117000	-0.733045000			1495.8179	1503.8728	1506.9323
	8	2.821468000	0.245273000	-0.287088000			1621.1235	3045.8888	3061.2299
	1	3.461246000	0.693564000	0.269475000			3090.0651	3104.2663	3110.7548
	6	-0.416972000	1.794232000	-0.225586000			3138.7854	3144.3105	3148.8376
	1	-0.933295000	2.359693000	-1.001346000			3214.4441	3726.1316	3931.6845
	1	-0.248699000	2.449379000	0.627776000					
	1	0.551809000	1.474019000	-0.612791000					
PC5 (C_1)	6	-1.073970000	1.015830000	-0.655524000	-346.9746056	0.155438	50.8957	76.3996	102.7625
	8	-0.002992000	0.149461000	-1.054646000			127.3467	181.6808	194.7995
	6	-0.061456000	-1.063254000	-0.298150000			213.2700	324.7327	367.1287
	6	-0.730410000	-0.658527000	1.012271000			452.2359	556.5691	571.3238
	6	-1.786569000	0.325182000	0.513430000			572.4944	671.3330	840.5317
	1	-0.634455000	1.967454000	-0.354141000			869.5353	900.0461	916.3840
	1	-1.732808000	1.184971000	-1.507021000			947.4557	1016.3157	1067.5325
	1	-0.724455000	-1.766719000	-0.829912000			1086.0701	1150.6658	1175.4174
	1	-1.145800000	-1.508625000	1.549458000			1210.3892	1221.9441	1271.4168
	1	0.002721000	-0.153387000	1.642516000			1304.8938	1334.2703	1346.7581
	1	-2.665621000	-0.214148000	0.160483000			1380.8342	1401.8014	1453.7341
	1	-2.104860000	1.034296000	1.273395000			1485.9434	1503.6183	1537.8231
	6	1.294582000	-1.644490000	-0.183455000			1649.4414	2935.8014	3071.9220
	1	1.497454000	-2.373976000	0.585705000			3082.2445	3085.7880	3113.8955
	1	1.987182000	-1.544654000	-1.005434000			3142.8193	3151.1220	3175.3949
	1	2.648739000	0.939674000	0.762847000			3283.0619	3726.6370	3925.1182
	8	1.948213000	1.540871000	0.501444000					
	1	1.457070000	1.064014000	-0.183710000					
P1 (C_1)	6	1.334954000	-0.843146000	0.165267000	-270.647357	0.132088	121.8876	166.1173	201.9049
	8	-0.046182000	-1.118467000	-0.082302000			303.7417	344.0915	568.6478
	6	-0.734097000	0.061667000	-0.233750000			643.6899	811.3360	881.9887
	6	0.147421000	1.206897000	0.143060000			907.7212	940.7154	945.0089
	6	1.532119000	0.633394000	-0.169282000			999.2943	1021.4087	1080.6018
	1	1.539500000	-1.043111000	1.219814000			1105.0805	1181.7605	1216.8683
	1	1.935258000	-1.516566000	-0.443047000			1253.4641	1266.7448	1286.8553
	1	-0.081813000	2.116440000	-0.409674000			1339.1951	1358.1716	1404.7038
	1	0.060050000	1.439875000	1.215090000			1420.1167	1471.1000	1481.3105
	1	1.753034000	0.753641000	-1.229147000			1490.1280	1498.2540	1532.2794
	1	2.335117000	1.084435000	0.408880000			2967.7913	2986.0774	3057.3094

Species	Cartesian coordinate (Å)				$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	-2.189528000	-0.019475000	0.027927000			3091.8734	3096.8885	3115.7890
	1	-2.685135000	0.892785000	-0.301105000			3127.4771	3143.2398	3149.2065
	1	-2.630049000	-0.864784000	-0.499924000					
	1	-2.401722000	-0.151001000	1.098203000					
P2	6	1.382993000	-0.768015000	0.054206000	-270.637339	0.130685	104.4240	212.3590	216.5447
(C_1)	8	0.013286000	-1.102293000	-0.083605000			245.8811	336.2689	478.1201
	6	-0.749512000	-0.009480000	0.422560000			645.3867	679.9741	859.2057
	6	0.118020000	1.182705000	0.181273000			875.3629	915.4714	949.2307
	6	1.466588000	0.731015000	-0.259396000			1003.4201	1033.8850	1047.6688
	1	1.715027000	-0.957841000	1.081563000			1087.6246	1141.9732	1160.4611
	1	1.953081000	-1.397906000	-0.624358000			1200.9384	1260.8702	1298.6571
	1	-0.904838000	-0.159019000	1.504198000			1306.3833	1339.1417	1370.8757
	1	-0.197780000	2.203156000	0.323301000			1400.4149	1402.8120	1474.1036
	1	1.617717000	0.893512000	-1.332678000			1487.3754	1498.1440	1522.1108
	1	2.288106000	1.225158000	0.261850000			2940.3398	3012.9448	3022.9613
	6	-2.098935000	0.019138000	-0.269291000			3066.1775	3087.0978	3137.5455
	1	-2.627045000	-0.918370000	-0.101529000			3143.9143	3147.7348	3250.4266
	1	-2.704471000	0.836707000	0.120930000					
	1	-1.961013000	0.160768000	-1.340543000					
P3	6	0.685485000	-0.002761000	0.382698000	-270.637876	0.130548	154.0155	168.3260	232.7882
(C_1)	8	-0.070411000	-1.094821000	-0.130074000			243.3125	323.7279	474.3841
	6	-1.444671000	-0.766802000	-0.001033000			605.7555	737.1681	856.2046
	6	-1.492719000	0.722468000	-0.066900000			900.3003	911.3974	950.1487
	6	-0.099610000	1.244613000	-0.045846000			973.9215	1010.7707	1058.7671
	1	0.683970000	-0.058442000	1.479792000			1093.5186	1158.2105	1161.4399
	1	-1.992508000	-1.266787000	-0.803295000			1206.9527	1223.2112	1279.1273
	1	-1.837863000	-1.146833000	0.954696000			1326.5367	1360.3160	1387.3128
	1	-2.394051000	1.307722000	-0.136422000			1393.2885	1425.7036	1471.5743
	1	0.231430000	1.569644000	-1.041112000			1487.6314	1501.5335	1506.4583
	1	0.047127000	2.084469000	0.635426000			2962.9325	2990.7385	3003.2899
	6	2.097625000	-0.094486000	-0.140284000			3064.8510	3066.7213	3086.4103
	1	2.694422000	0.736807000	0.234920000			3140.6146	3148.5295	3255.9163
	1	2.563259000	-1.026838000	0.174446000					
	1	2.090848000	-0.059364000	-1.229670000					
P4	6	-0.767352000	0.012106000	-0.537604000	-270.645220	0.131967	159.6434	172.4504	235.8177
(C_1)	8	0.043983000	-1.168786000	-0.447361000			355.9184	440.2502	486.5841

Species	Cartesian coordinate (Å)				$E_{elec}^{0\ K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	1.143130000	-0.876695000	0.306849000			675.4260	748.8208	819.0782
	6	1.331036000	0.601547000	0.455830000			871.1651	923.1115	953.6176
	6	0.245498000	1.157130000	-0.482786000			955.3720	1021.8025	1063.3647
	1	-1.282124000	-0.044337000	-1.495291000			1083.0153	1123.9761	1201.1017
	1	1.919504000	-1.623975000	0.279351000			1217.4747	1234.1663	1295.1741
	1	1.165751000	0.930390000	1.486189000			1314.0603	1333.3794	1376.2977
	1	2.331306000	0.932123000	0.174575000			1408.6320	1414.1266	1482.6854
	1	-0.199863000	2.083707000	-0.126731000			1490.7289	1500.5522	1506.7760
	1	0.661135000	1.329625000	-1.474516000			3032.7366	3063.4500	3085.6838
	6	-1.768504000	0.039932000	0.602725000			3095.6016	3109.2484	3138.2903
	1	-2.428824000	0.901681000	0.506166000			3144.5980	3150.0843	3242.5913
	1	-2.371664000	-0.866182000	0.598486000					
	1	-1.249938000	0.103133000	1.560577000					
P5 (C_1)	6	-1.315400000	-0.818387000	-0.165841000	-270.630852	0.130600	68.5373	131.1941	215.5910
	8	0.047621000	-1.136624000	0.101934000			308.2708	440.4125	488.1806
	6	0.791955000	0.047223000	0.388868000			565.6626	658.9658	834.3397
	6	-0.057792000	1.185099000	-0.199858000			877.5707	898.2565	922.3909
	6	-1.467903000	0.680748000	0.087654000			950.5479	1008.5385	1061.1284
	1	-1.533736000	-1.066762000	-1.207491000			1107.3448	1156.1067	1159.0846
	1	-1.956034000	-1.424455000	0.475013000			1196.7120	1211.4547	1266.4048
	1	0.842813000	0.182073000	1.477889000			1298.5701	1336.8646	1340.1017
	1	0.172162000	2.147965000	0.250611000			1378.5615	1399.5093	1456.8866
	1	0.121415000	1.247443000	-1.274694000			1485.9812	1500.6016	1540.2284
	1	-1.726288000	0.867436000	1.130491000			2992.3784	3051.4743	3074.9910
	1	-2.231030000	1.134098000	-0.541185000			3081.4356	3102.8478	3139.8862
	6	2.156854000	-0.070497000	-0.163565000			3147.8200	3180.0698	3291.6781
	1	2.975661000	0.481970000	0.269187000					
	1	2.307791000	-0.621884000	-1.078839000					

Frequencies in the parentheses ("( )") are taken from experimental studies.

Table S2: T1 diagnostics for the species involved in 2MTHF + OH reaction calculated at CCSD(T)/cc-pVTZ based on the M06-2X/aug-cc-pVTZ geometries.

No.	Species	T1 diagnostics
1	2MTHF	0.00988196
2	OH	0.00704816
3	**RC**	0.01033272
4	**TS1**	0.01689595
5	**TS2a**	0.01639799
6	**TS2b**	0.01606206
7	**TS3a**	0.01620179
8	**TS3b**	0.01609799
9	**TS4a**	0.01691631
10	**TS4b**	0.01695069
11	**TS5**	0.01588828
12	**PC1**	0.01278459
13	**PC2**	0.01143563
14	**PC3**	0.01129848
15	**PC4**	0.01326695
16	**PC5**	0.01080681
17	**P1**	0.01358125
18	**P2**	0.01164737
19	**P3**	0.01147930
20	**P4**	0.01354334
21	**P5**	0.01132015
22	H_2O	0.00651823

Table S3: Calculated global rate constants, k_{tot}, of the 2MTHF + OH → products over the range of temperature 200 – 2000 K at different pressures, including the HIR treatments and Eckart quantum tunneling effects. Units are in cm^3/molecule/s. The $k_{tot}(T, P)$ at different pressures are fitted as the double-modified Arrhenius formats.

T (K)	0.76 Torr	7.6 Torr	76 Torr	760 Torr	7600 Torr
200	8.18E-11	8.18E-11	8.25E-11	8.83E-11	1.25E-10
240	4.81E-11	4.81E-11	4.84E-11	5.04E-11	6.40E-11
298	**2.36E-11**	**2.35E-11**	**2.36E-11**	**2.41E-11**	**2.72E-11**
300	2.31E-11	2.30E-11	2.31E-11	2.35E-11	2.64E-11
400	8.68E-12	8.68E-12	8.68E-12	8.73E-12	9.00E-12
440	6.45E-12	6.46E-12	6.44E-12	6.47E-12	6.60E-12
500	4.57E-12	4.57E-12	4.58E-12	4.58E-12	4.63E-12
600	3.43E-12	3.44E-12	3.44E-12	3.44E-12	3.45E-12
700	3.40E-12	3.40E-12	3.40E-12	3.39E-12	3.40E-12
800	3.93E-12	3.94E-12	3.94E-12	3.94E-12	3.93E-12
900	4.89E-12	4.90E-12	4.90E-12	4.89E-12	4.89E-12
1000	6.23E-12	6.23E-12	6.23E-12	6.24E-12	6.23E-12
1100	7.94E-12	7.93E-12	7.93E-12	7.95E-12	7.94E-12
1200	1.00E-11	1.00E-11	1.00E-11	1.00E-11	1.00E-11
1300	1.25E-11	1.25E-11	1.25E-11	1.25E-11	1.25E-11
1400	1.54E-11	1.54E-11	1.54E-11	1.54E-11	1.54E-11
1500	1.87E-11	1.88E-11	1.88E-11	1.87E-11	1.87E-11
1600	2.26E-11	2.26E-11	2.25E-11	2.26E-11	2.26E-11
1700	2.69E-11	2.69E-11	2.69E-11	2.69E-11	2.69E-11
1800	3.17E-11	3.17E-11	3.17E-11	3.17E-11	3.17E-11
1900	3.70E-11	3.70E-11	3.70E-11	3.70E-11	3.70E-11
2000	4.29E-11	4.29E-11	4.29E-11	4.29E-11	4.29E-11

- $k(T) = 1.26\times10^{2}\times T^{-4.90}\times\exp[-418.0\ K/T] + 7.10\times10^{-23}\times T^{3.51}\times\exp[945.2\ K/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 0.76 Torr**; error = 0.7 %).
- $k(T) = 9.72\times10^{1}\times T^{-4.87}\times\exp[-406.6\ K/T] + 7.09\times10^{-23}\times T^{3.51}\times\exp[945.2\ K/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 7.6 Torr**; error = 0.7 %).
- $k(T) = 9.45\times10^{1}\times T^{-4.86}\times\exp[-402.2\ K/T] + 6.88\times10^{-23}\times T^{3.51}\times\exp[950.7\ K/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 76 Torr**; error = 0.7 %).
- $k(T) = 3.55\times10^{1}\times T^{-4.72}\times\exp[-340.0\ K/T] + 8.21\times10^{-23}\times T^{3.49}\times\exp[918.8\ K/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 760 Torr**; error = 0.7 %).
- $k(T) = 1.96\times T^{-4.33}\times\exp[-104.5\ K/T] + 6.95\times10^{-23}\times T^{3.51}\times\exp[941.9\ K/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 7600 Torr**; error = 1.1 %).

Table S4: The calculated Eckart tunneling factor via tight transition state channels over the wide range of temperature 200 – 2000 K.

T (K)	via TS1	via TS2a	via TS2b	via TS3a	via TS3b	via TS4a	via TS4b	via TS5
200	2.44	13.20	16.00	13.40	13.30	3.66	3.53	28.90
250	1.75	4.63	5.05	4.62	4.57	2.20	2.17	7.35
300	**1.47**	**2.79**	**2.93**	**2.78**	**2.75**	**1.71**	**1.70**	**3.78**
400	1.25	1.76	1.80	1.75	1.74	1.35	1.35	2.07
500	1.15	1.44	1.45	1.43	1.43	1.21	1.21	1.59
600	1.11	1.29	1.30	1.29	1.28	1.15	1.14	1.39
700	1.08	1.21	1.22	1.21	1.20	1.11	1.11	1.28
800	1.06	1.16	1.16	1.16	1.15	1.08	1.08	1.21
900	1.05	1.13	1.13	1.12	1.12	1.06	1.06	1.17
1000	1.04	1.10	1.10	1.10	1.10	1.05	1.05	1.13
1100	1.03	1.08	1.09	1.08	1.08	1.04	1.04	1.11
1200	1.03	1.07	1.07	1.07	1.07	1.04	1.04	1.09
1300	1.02	1.06	1.06	1.06	1.06	1.03	1.03	1.08
1400	1.02	1.05	1.06	1.05	1.05	1.03	1.03	1.07
1500	1.02	1.05	1.05	1.05	1.05	1.02	1.02	1.06
1600	1.02	1.04	1.04	1.04	1.04	1.02	1.02	1.06
1700	1.01	1.04	1.04	1.04	1.04	1.02	1.02	1.05
1800	1.01	1.03	1.03	1.03	1.03	1.02	1.02	1.05
1900	1.01	1.03	1.03	1.03	1.03	1.02	1.02	1.04
2000	1.01	1.03	1.03	1.03	1.03	1.01	1.01	1.04

Table S5: Calculated overall rate constants, k_{tot}, of the 2MTHF + OH → products over the range of temperature 200 – 2000 K at P = 760 Torr with and without HIR treatments based on M06-2X/aug-cc-pVTZ level of theory. Units are in cm^3/molecule/s.

T (K)	2MTHF + OH → products (k_{tot})		HIR factor
	With HIR	Without HIR	
200	8.83E-11	8.09E-11	1.09
240	5.04E-11	4.74E-11	1.06
298	2.41E-11	2.36E-11	1.02
300	2.35E-11	2.31E-11	1.02
400	8.73E-12	8.89E-12	0.98
440	6.47E-12	6.56E-12	0.98
500	4.58E-12	4.56E-12	1.01
600	3.44E-12	3.10E-12	1.11
700	3.39E-12	2.69E-12	1.26
800	3.94E-12	2.75E-12	1.43
900	4.89E-12	3.07E-12	1.59
1000	6.24E-12	3.60E-12	1.73
1100	7.95E-12	4.25E-12	1.87
1200	1.00E-11	5.04E-12	1.99
1300	1.25E-11	5.96E-12	2.09
1400	1.54E-11	7.02E-12	2.19
1500	1.87E-11	8.20E-12	2.29
1600	2.26E-11	9.51E-12	2.38
1700	2.69E-11	1.10E-11	2.45
1800	3.17E-11	1.25E-11	2.53
1900	3.70E-11	1.43E-11	2.59
2000	4.29E-11	1.62E-11	2.65

Table S6: Calculated NASA coefficients for the thermodynamic properties of various species in the reaction of OH radicals with 2MTHF.

oh O 1H 1 G 300.000 2500.000 1500.000 1
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1.00522902E+04 5.41837124E+00 3.87657025E+00-1.35782277E-03 1.62653697E-06 3
-5.14676941E-10 2.70765002E-14 9.82537593E+03-3.08896856E-01 4
2mthf C 5O 1H 10 G 300.000 2500.000 1500.000 1
5.85692741E+00 4.41809893E-02-2.18955532E-05 5.30616329E-09-5.11618235E-13 2
-4.29778615E+02-7.18572649E+00-5.32334471E+00 7.48293718E-02-5.34263436E-05 3
1.96151761E-08-2.90724173E-12 1.79282047E+03 5.10119692E+01 4
rc C 5O 2H 11 G 300.000 2500.000 1500.000 1
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2.83542108E-08-4.97806827E-12 8.41122924E+03 4.34389779E+01 4
ts1 C 5O 2H 11 G 300.000 2500.000 1500.000 1
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ts5 C 5O 2H 11 G 300.000 2500.000 1500.000 1
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h2o O 1H 2 G 300.000 2500.000 1500.000 1
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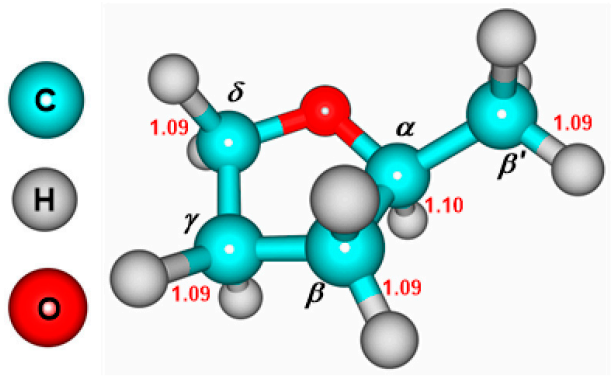

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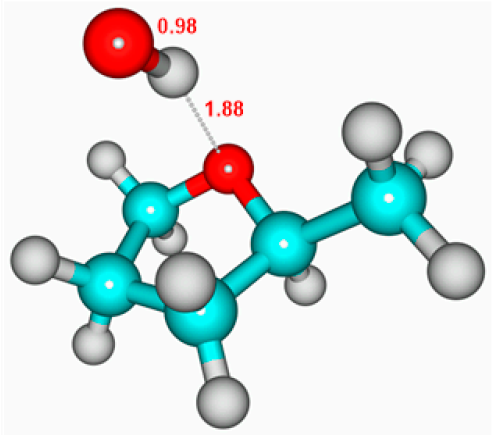

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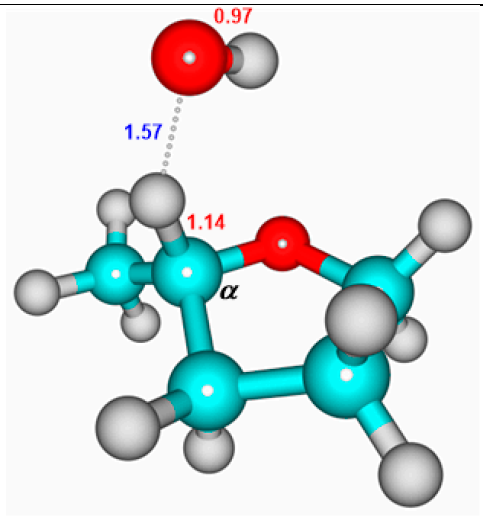

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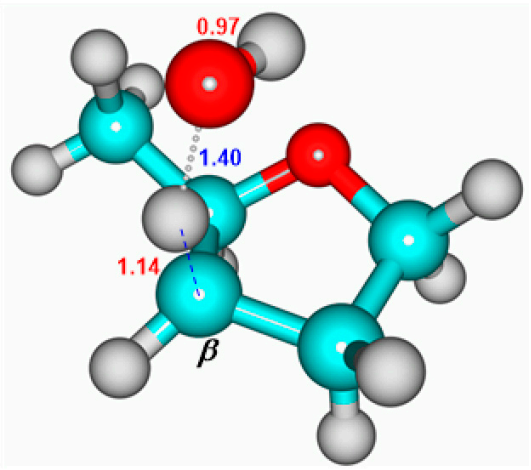

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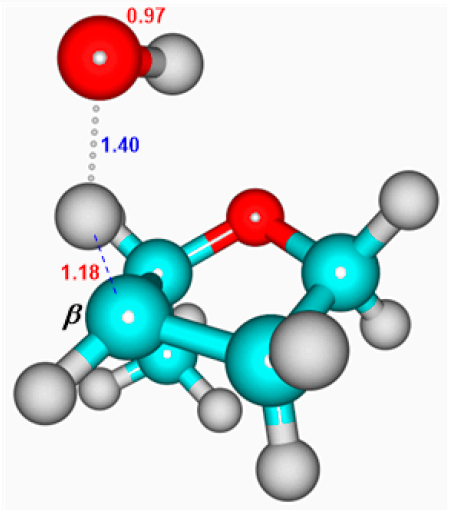

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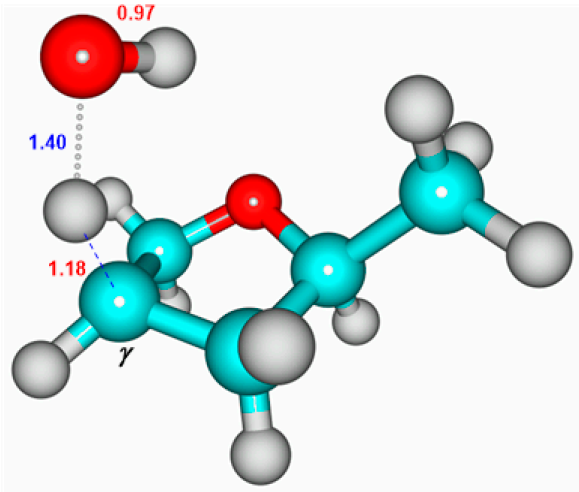

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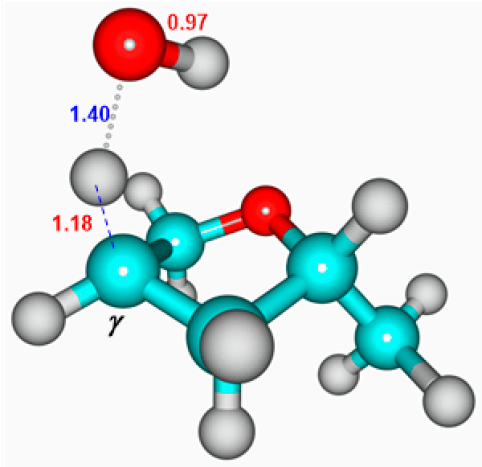

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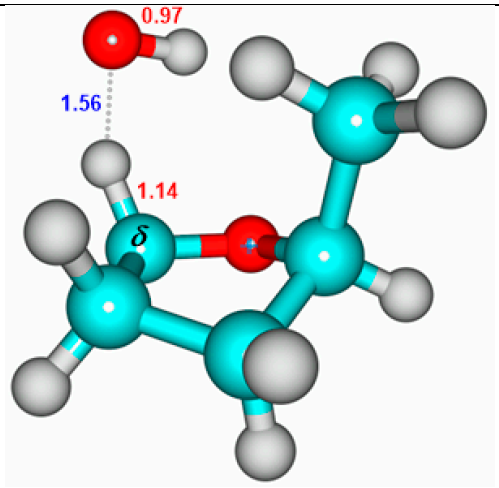

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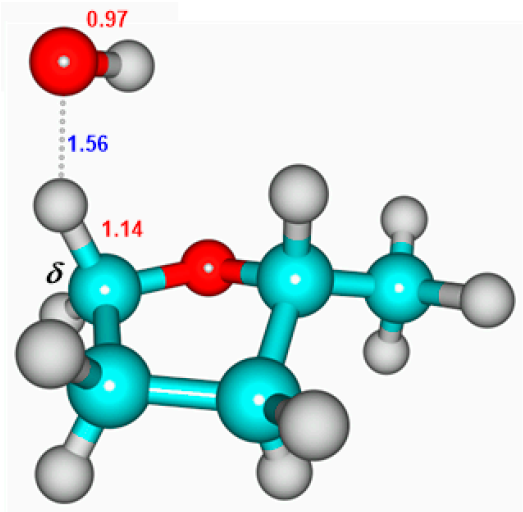

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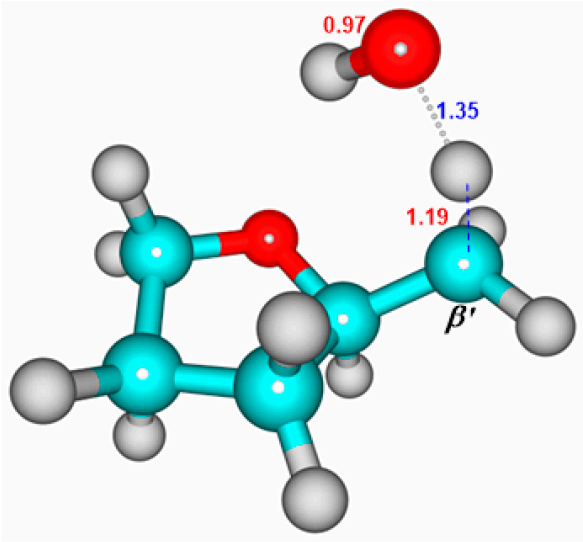

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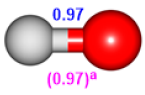

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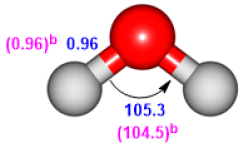

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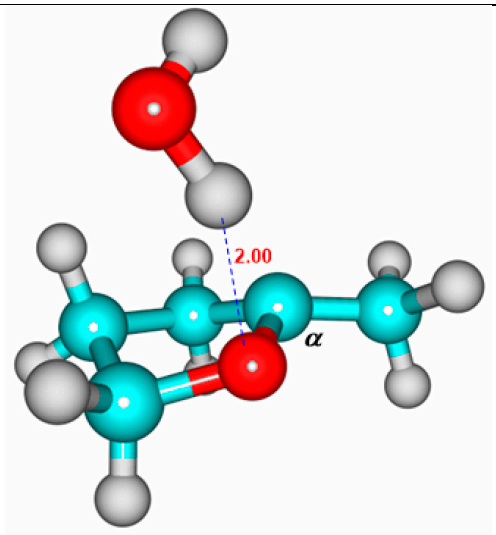

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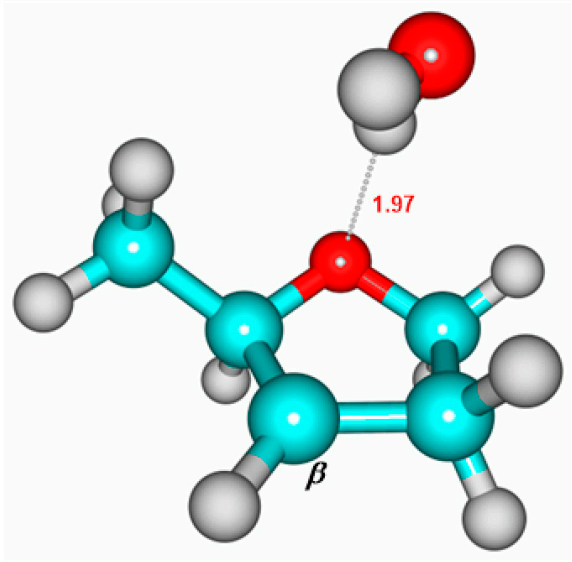

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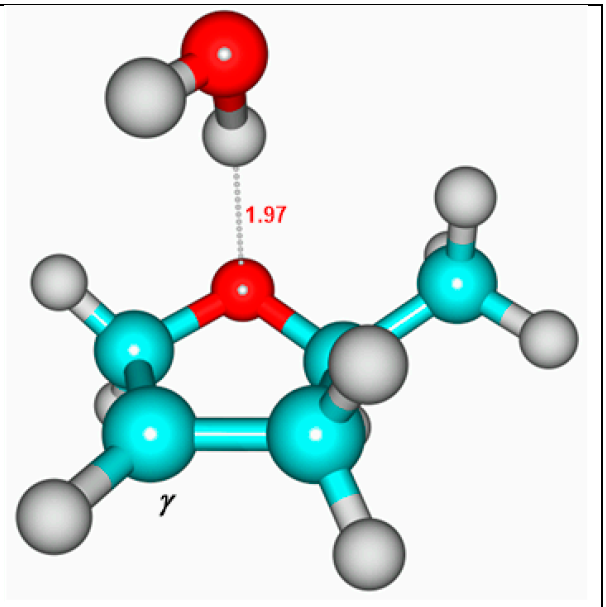

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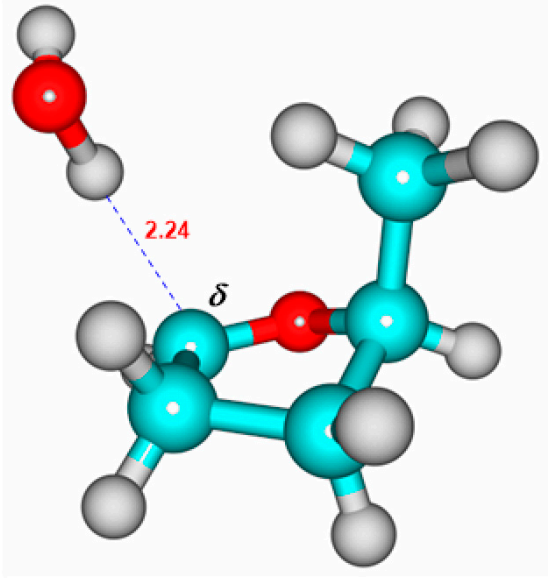

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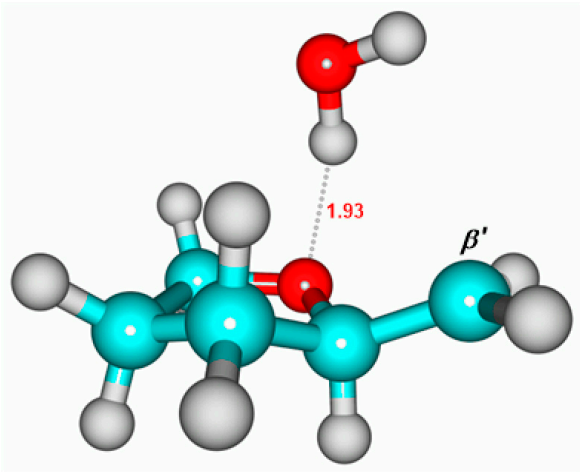

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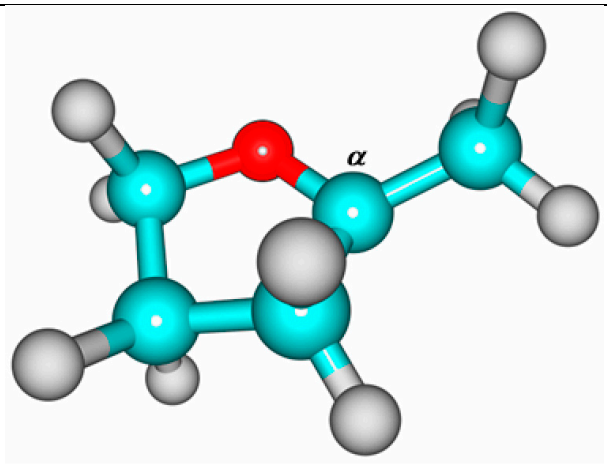

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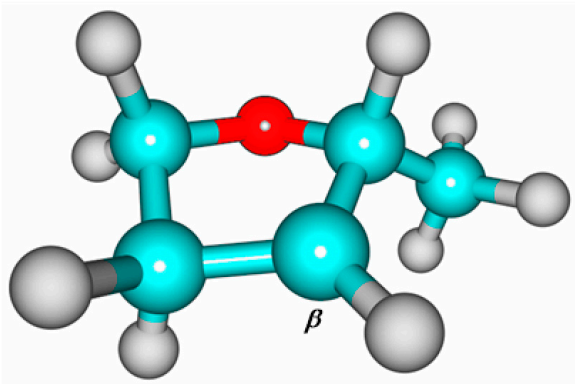

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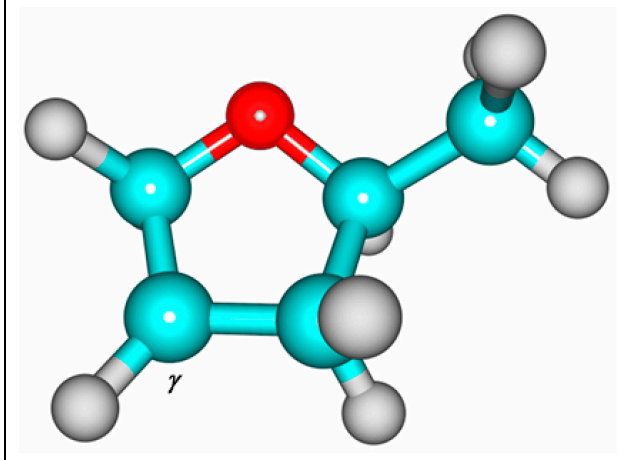
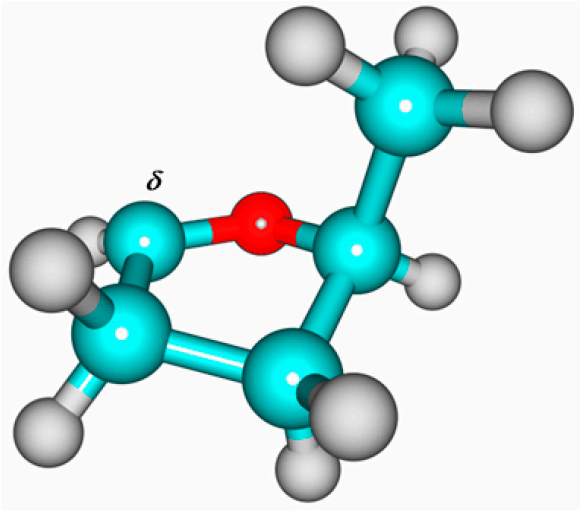
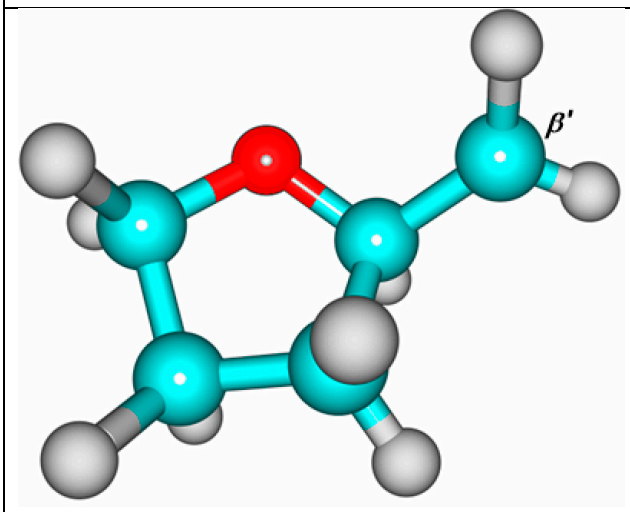


P3

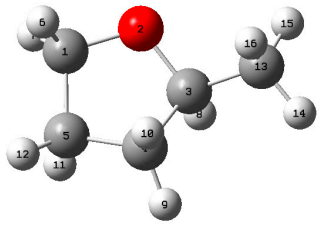
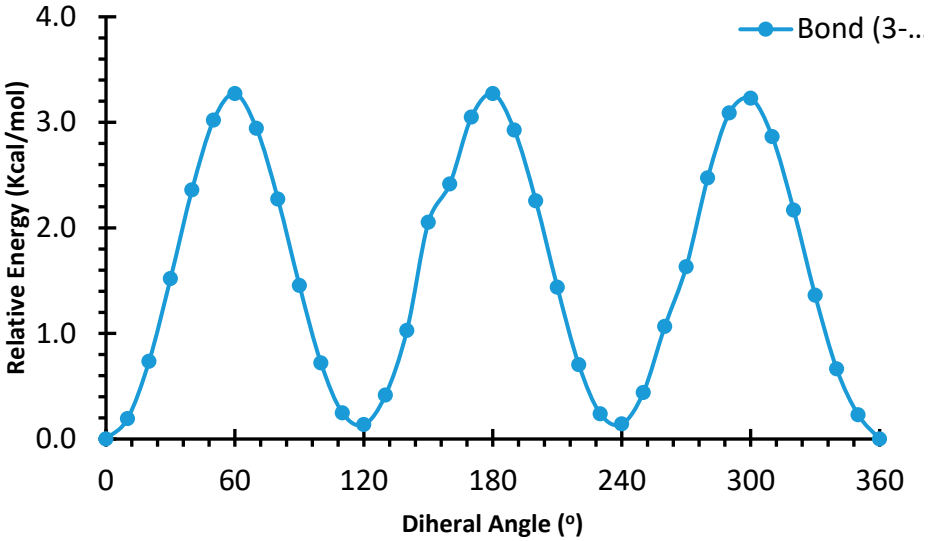
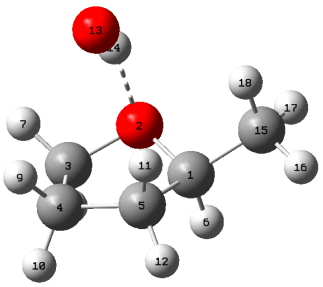
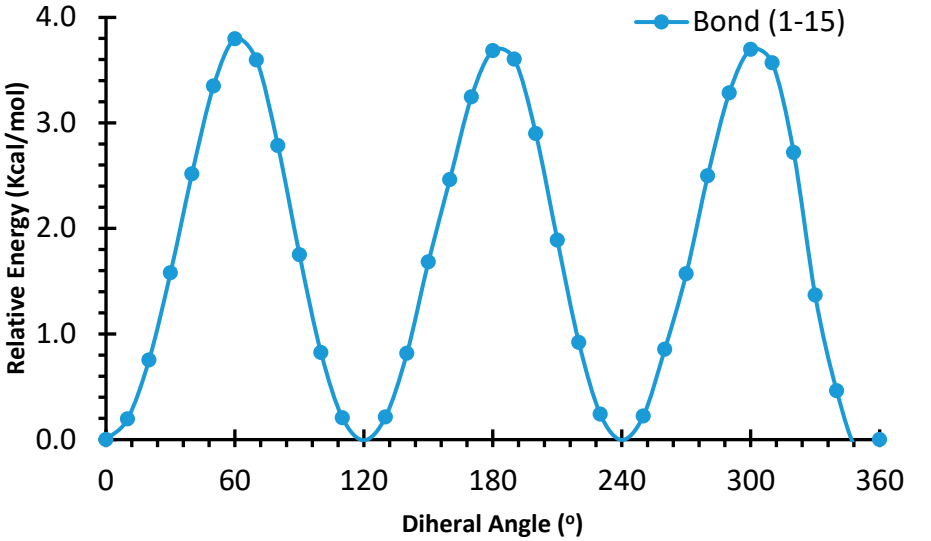
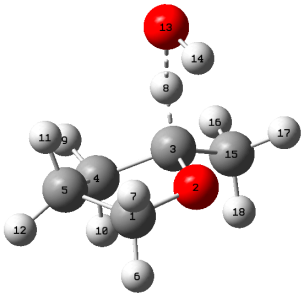
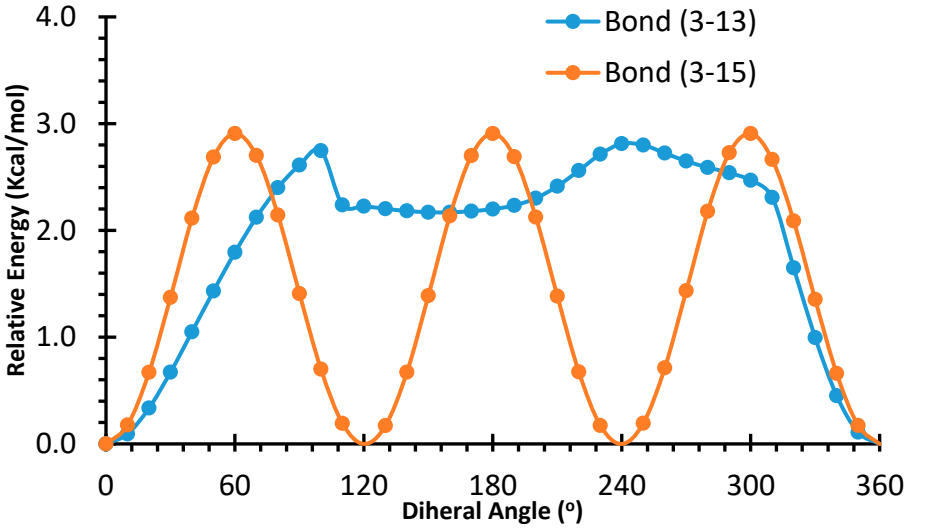


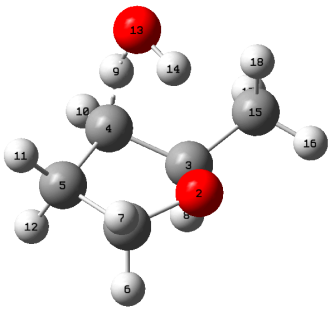
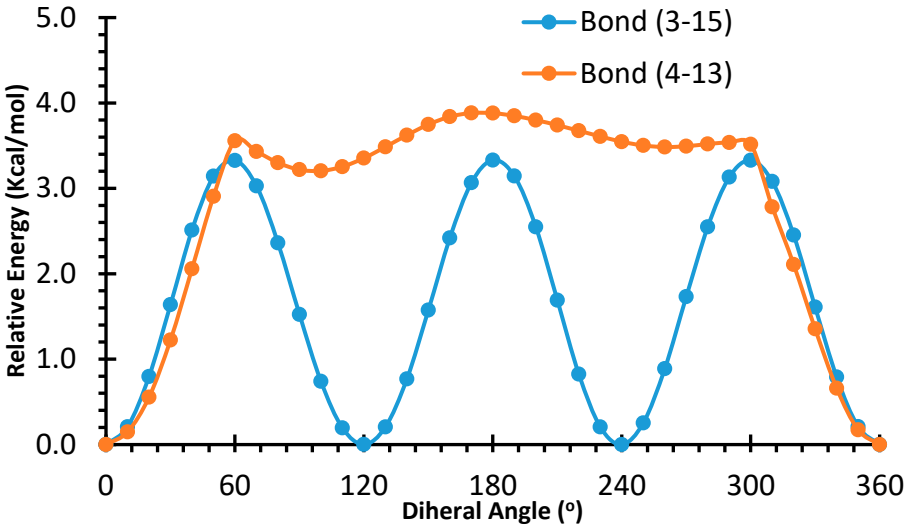
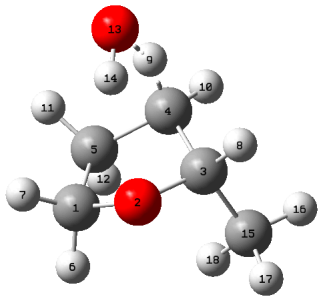
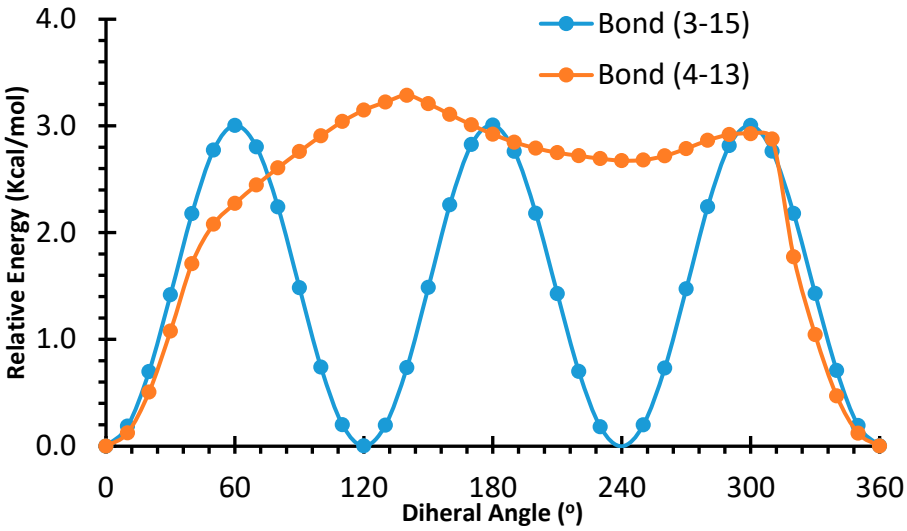
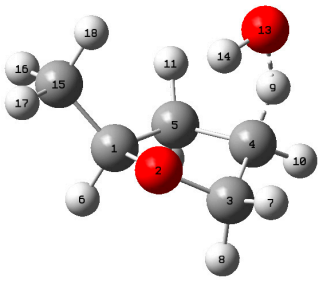
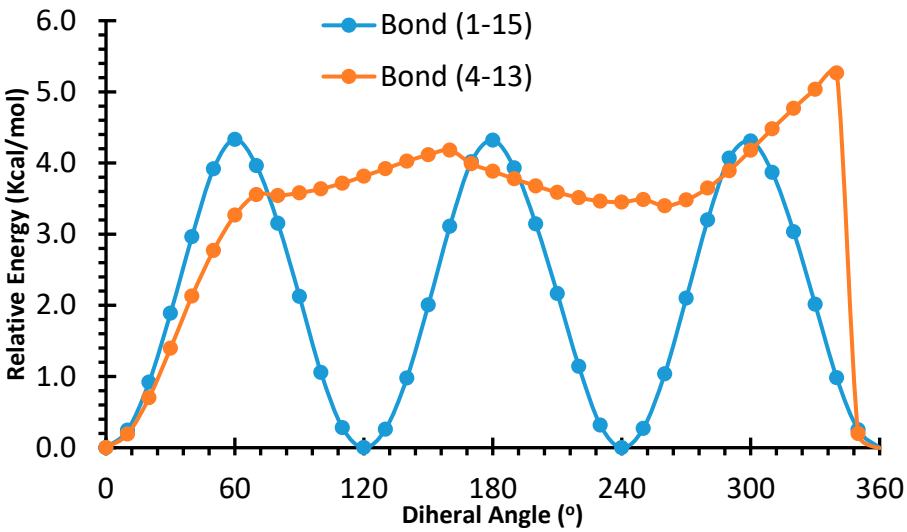
P4

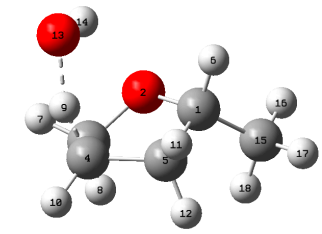
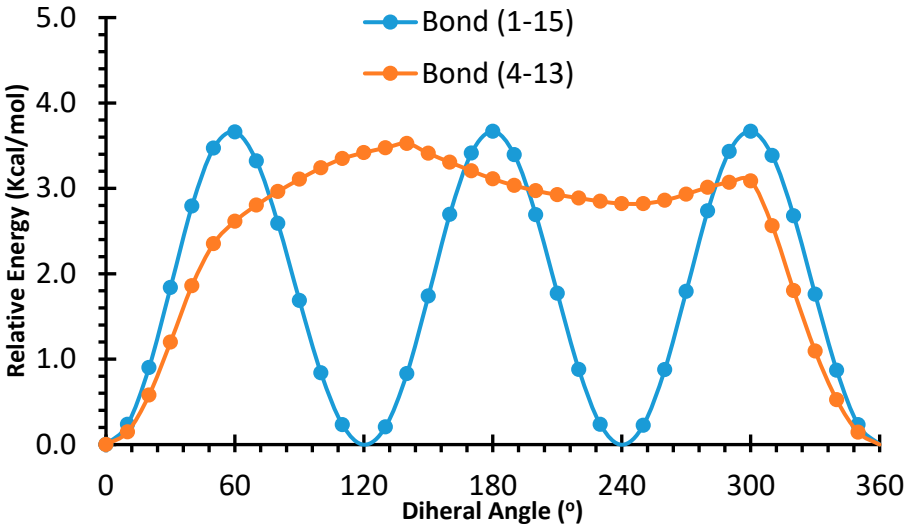
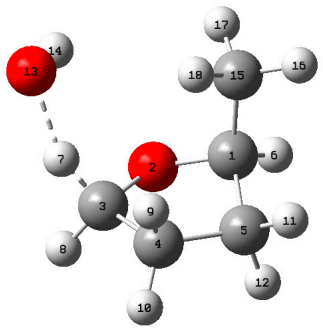
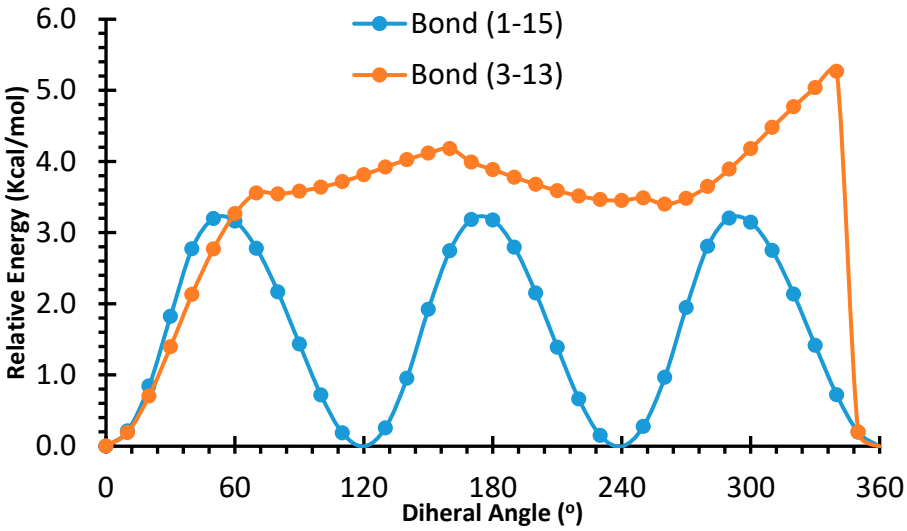
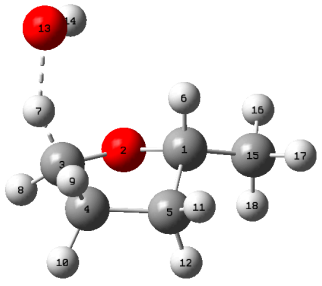
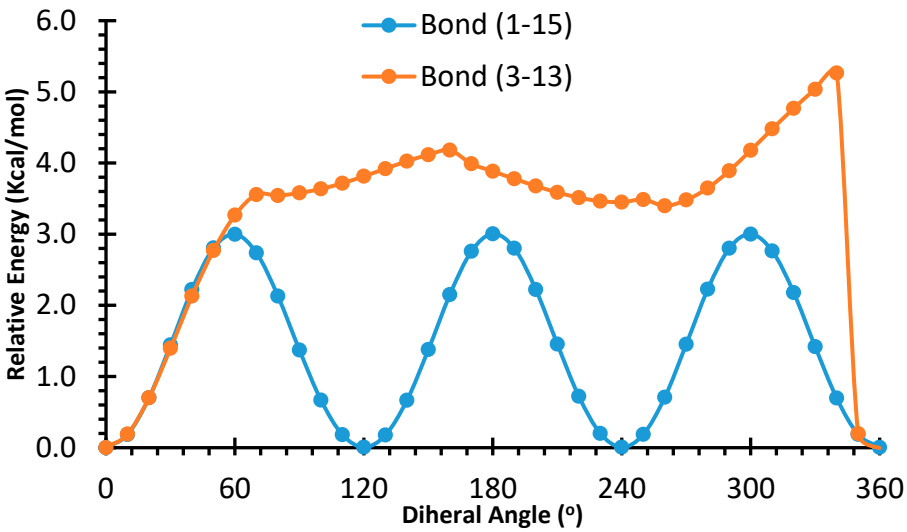


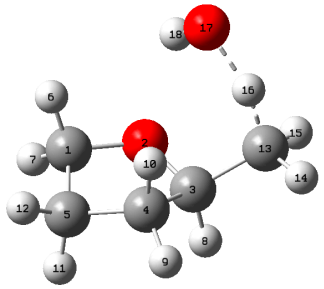
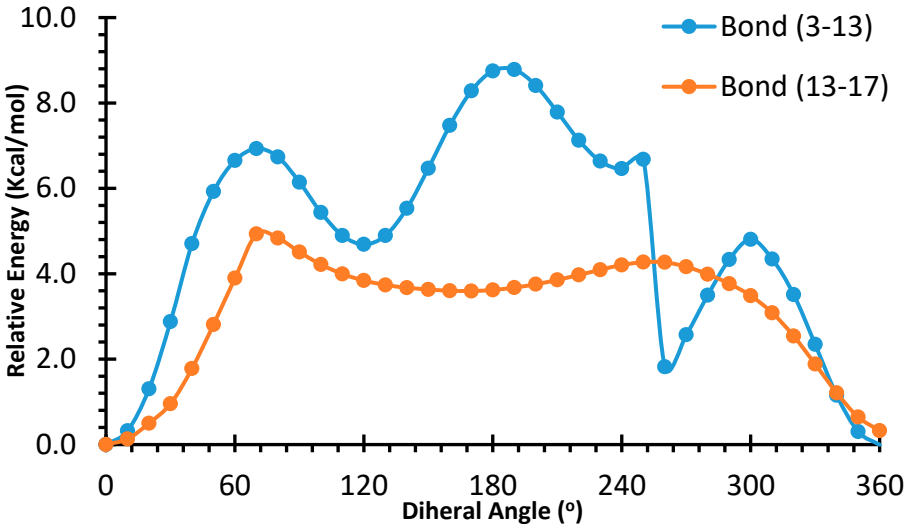
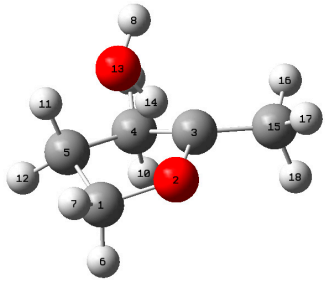
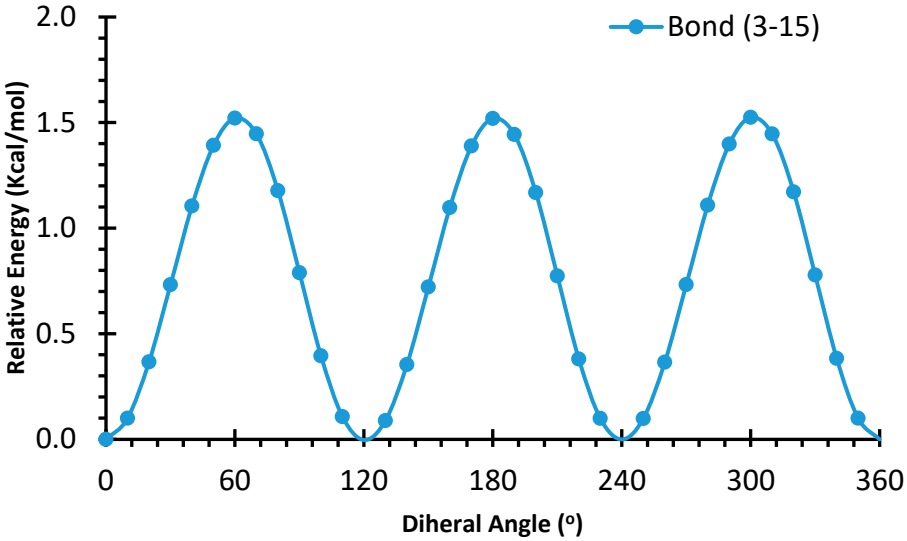
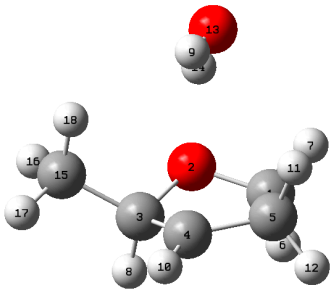
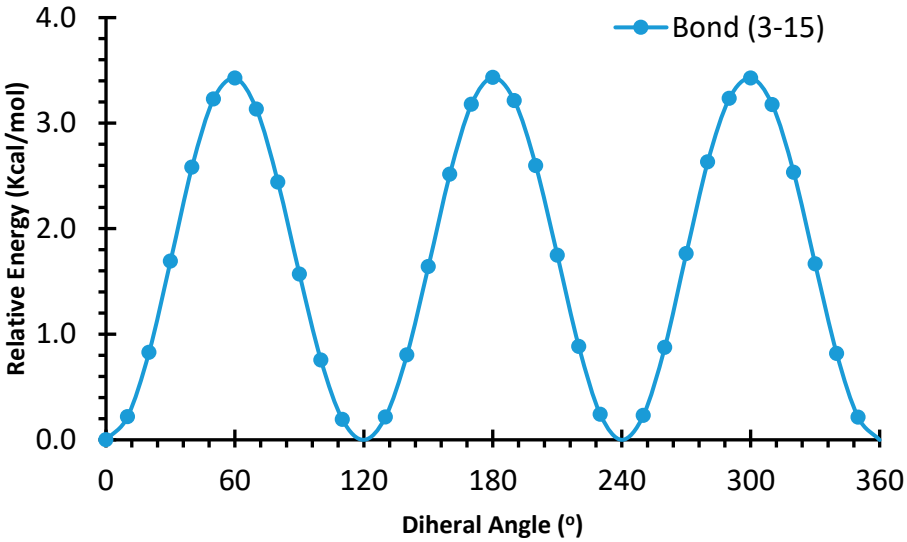
P5

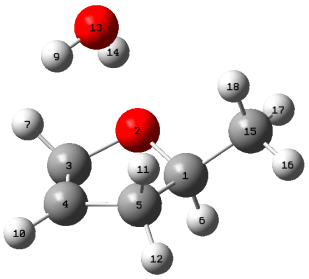
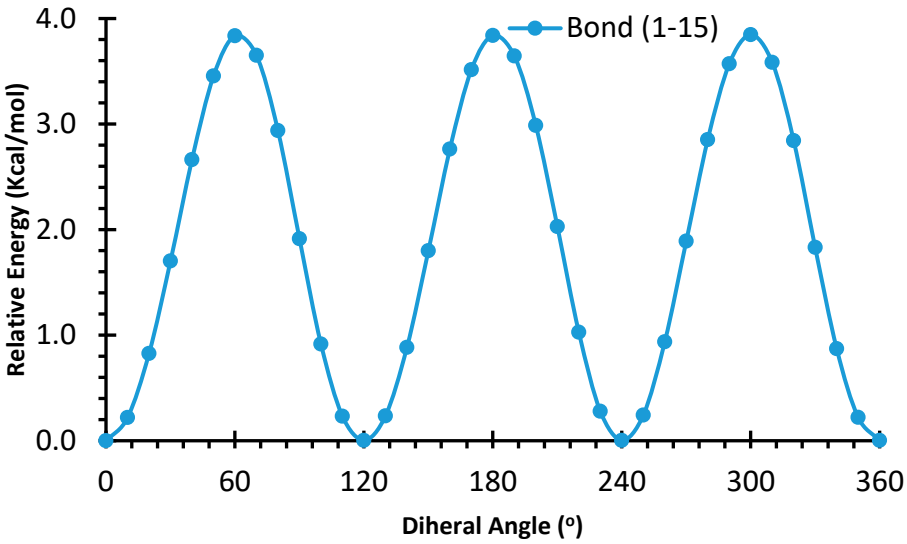
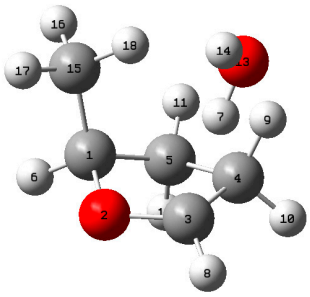
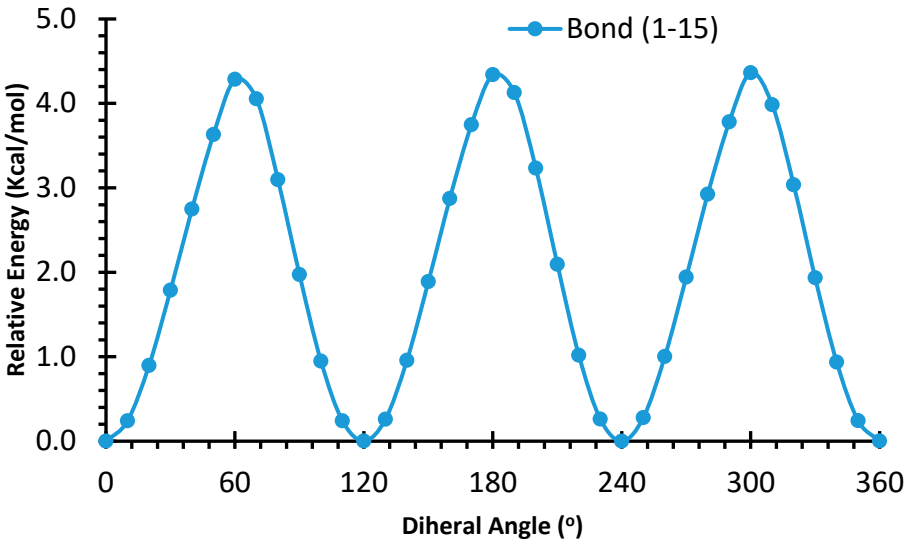
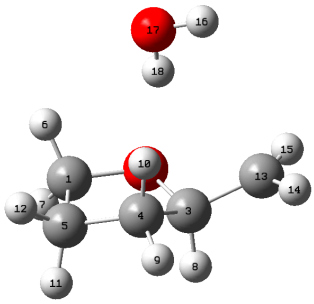
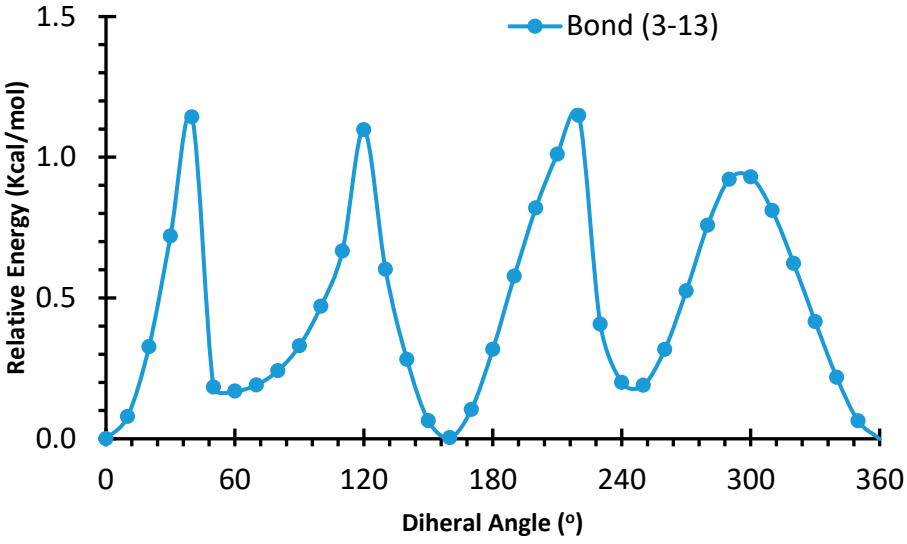
Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the title reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree (°), respectively. [a, b] are taken from the experimental data[1, 3], respectively.

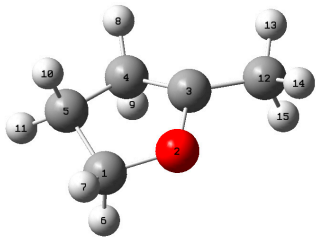
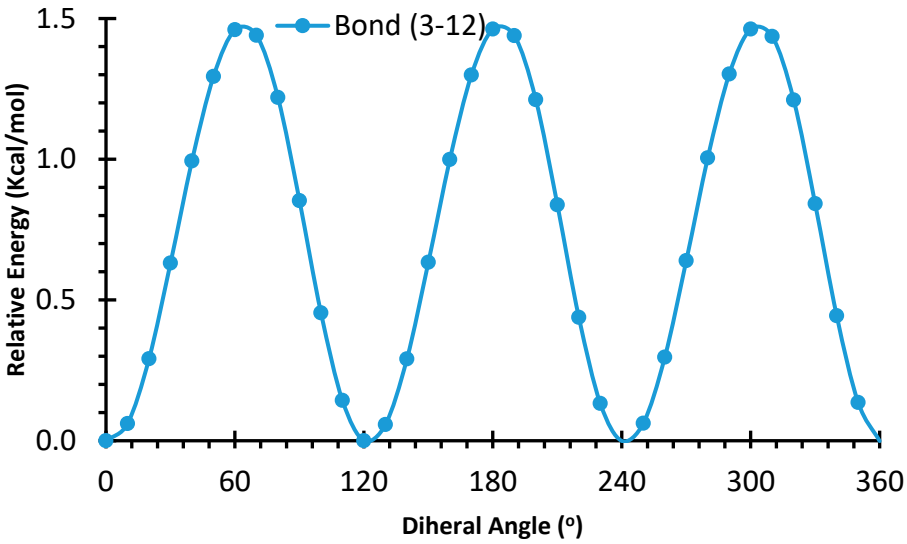
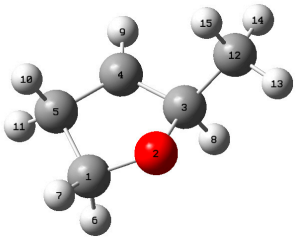
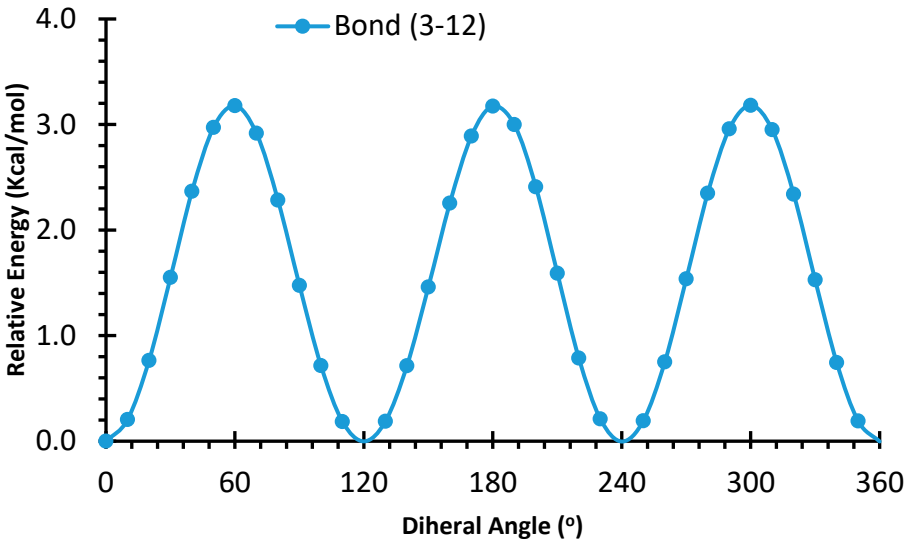
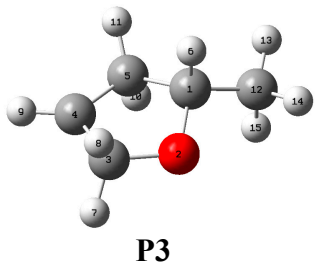
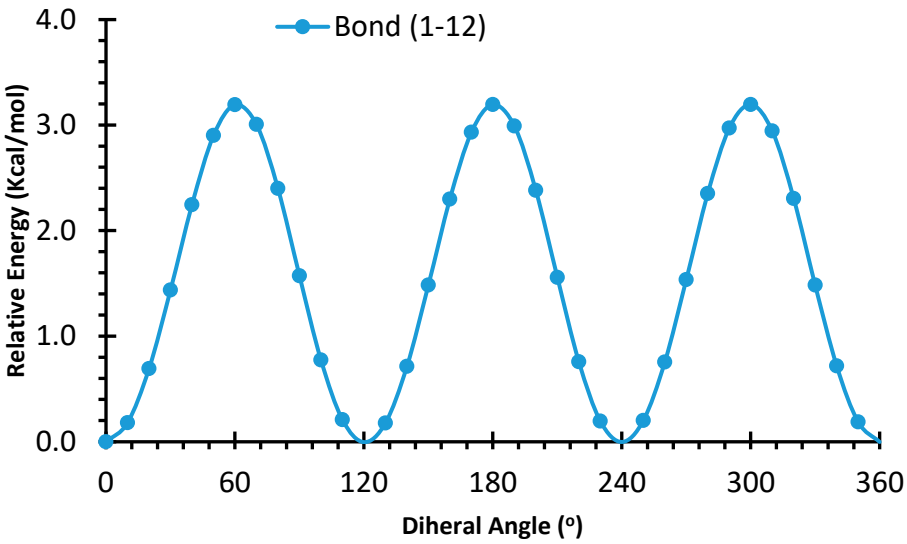
Species	Potential energy surfaces for the internal rotations
 2MTHF	
 RC	
 TS1	

Species	Potential energy surfaces for the internal rotations
 TS2a	
 TS2b	
 TS3a	

Species	Potential energy surfaces for the internal rotations
 TS3b	
 TS4a	
 TS4b	

Species	Potential energy surfaces for the internal rotations
 TS5	
 PC1	
 PC2	

Species	Potential energy surfaces for the internal rotations
 PC3	
 PC4	
 PC5	

Species	Potential energy surfaces for the internal rotations
 P1	
 P2	
 P3	

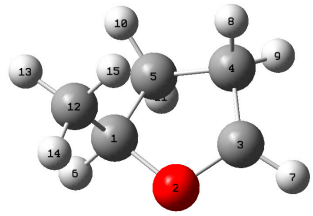
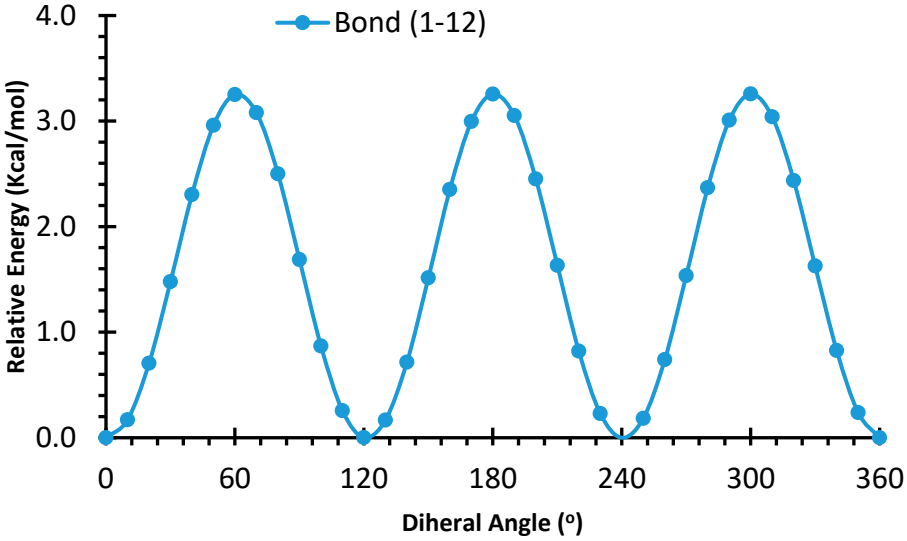
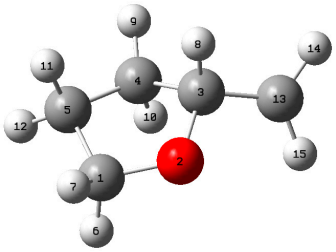
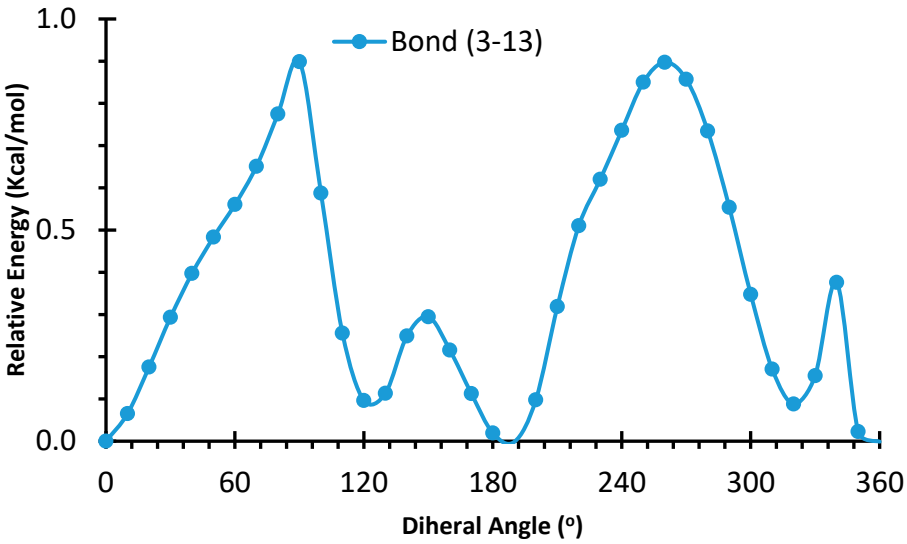
Species	Potential energy surfaces for the internal rotations
 P4	
 P5	

Figure S2: Hindrance potentials for the species involved in the 2MTHF + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

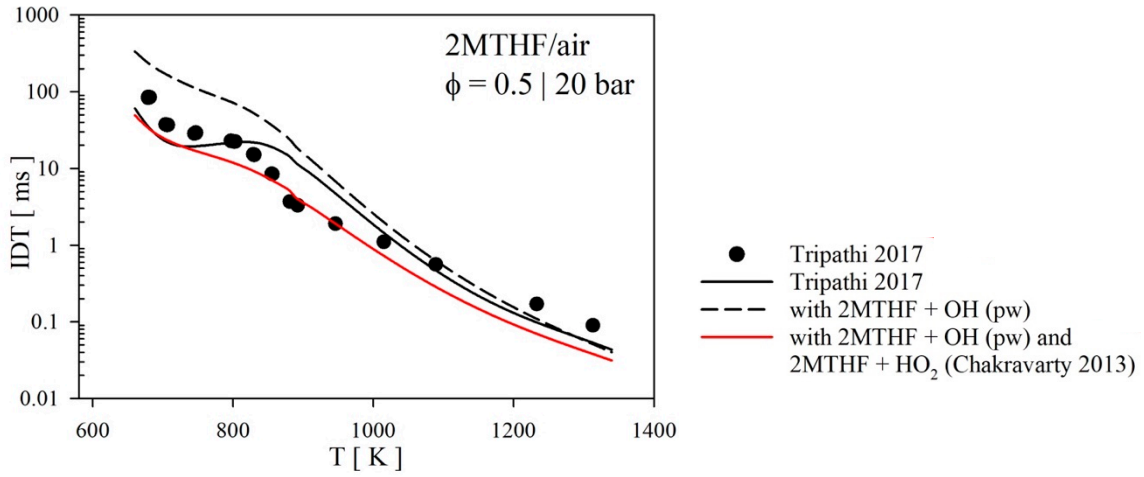
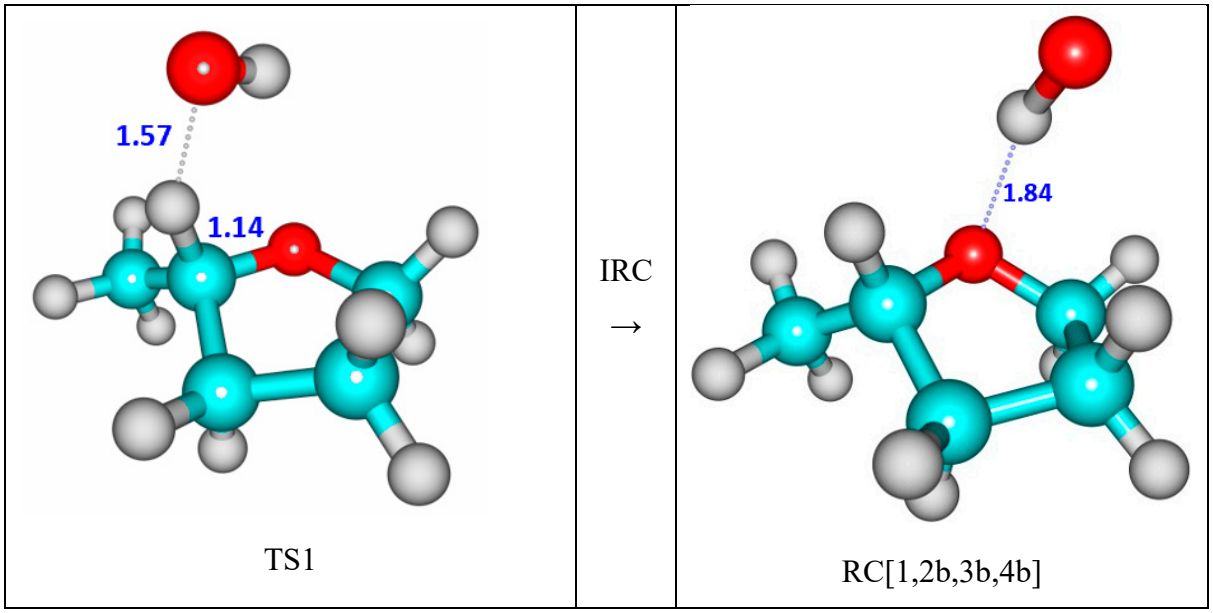
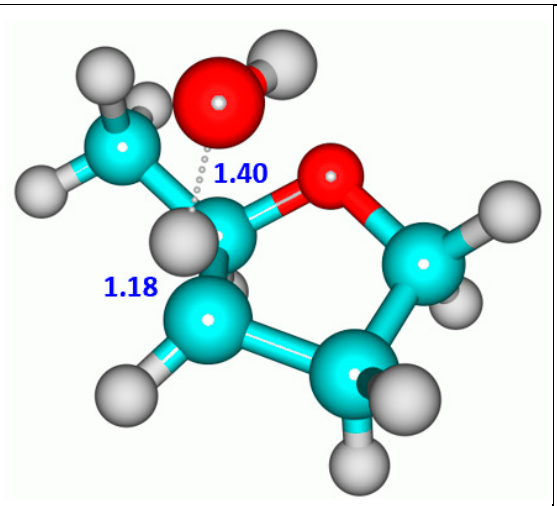
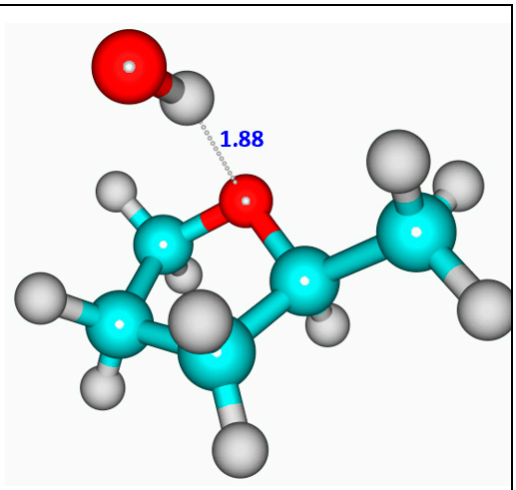
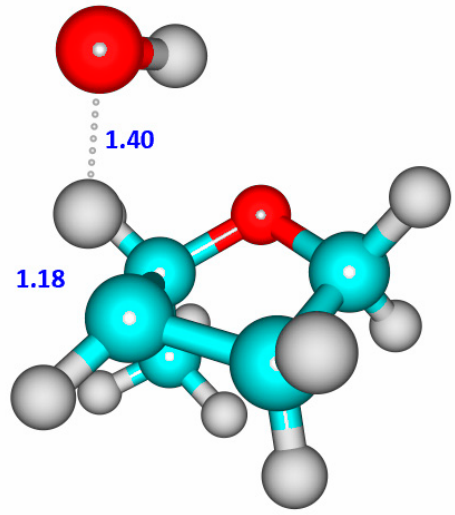
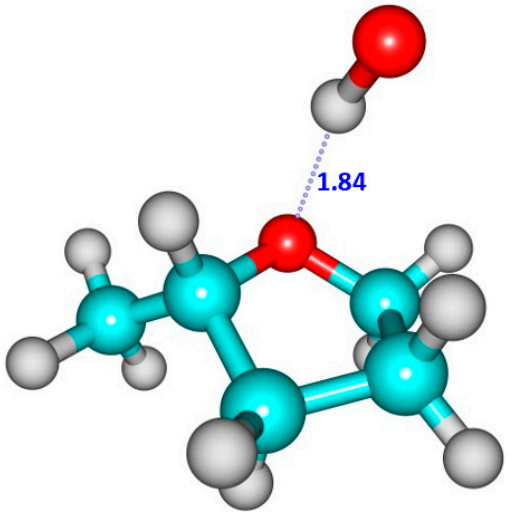
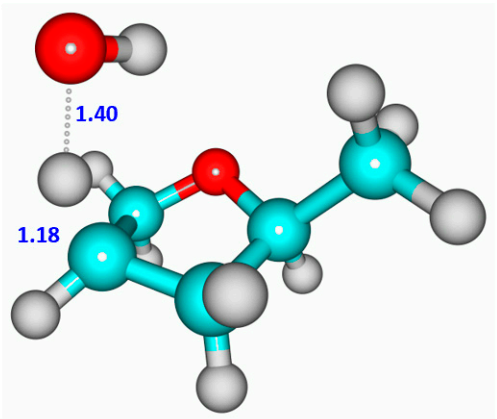
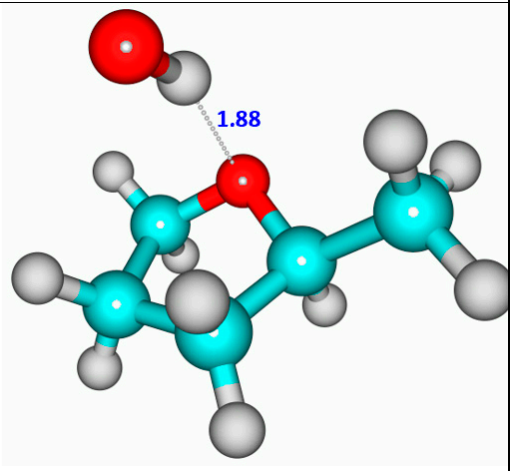
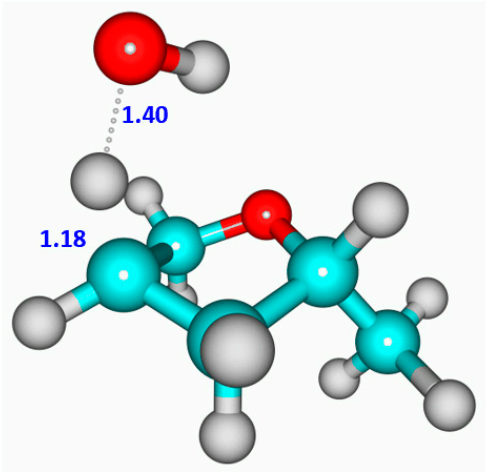
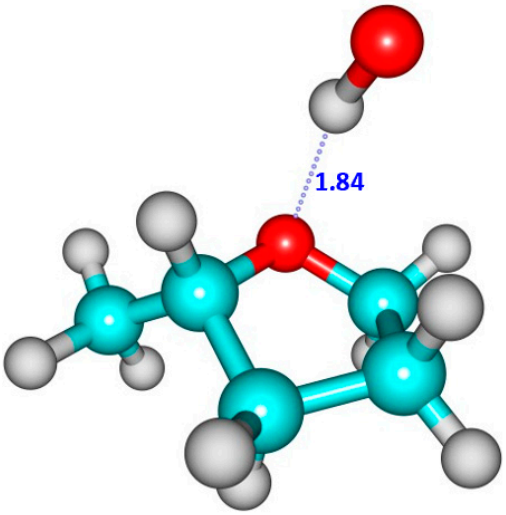
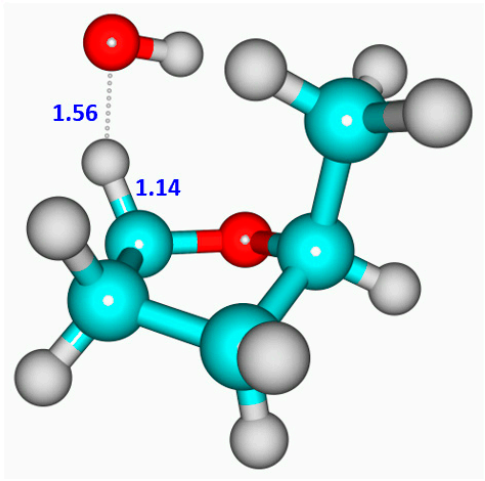
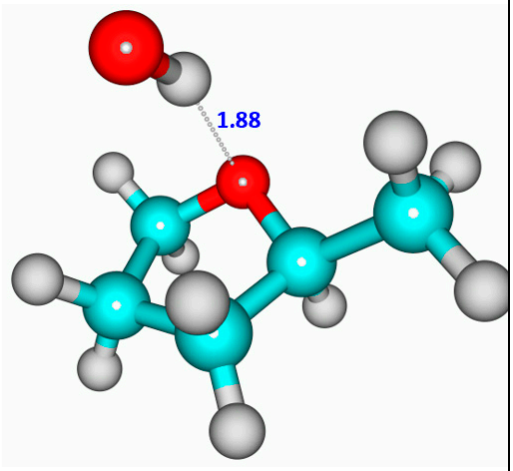
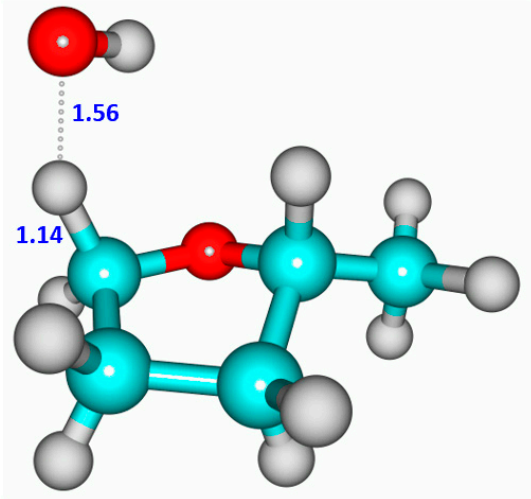
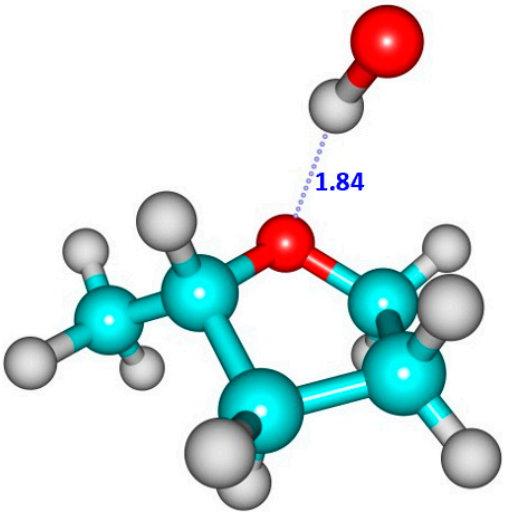


Figure S3: Effects of updated rate coefficients for OH/HO_2 + 2MTHF → products on the prediction of the ignition delay times of 2MTHF/air mixtures at 20 bar and ϕ = 0.5. The experimental data are taken from Tripathi et al. [4]. The comparison of the various scenarios for the performance of the kinetic model is shown. The red line shows the performance of the updated kinetic model from this work with the rate coefficients for OH + 2MTHF → products (this work) and HO_2 + 2MTHF → products (Chakravarty and Fernandes [5]).



 TS2a	IRC →	 RC[2a,3a,4a,5]
 TS2b	IRC →	 RC[1,2b,3b,4b]
 TS3a	IRC →	 RC[2a,3a,4a,5]

 TS3b	IRC →	 RC[1,2b,3b,4b]
 TS4a	IRC →	 RC[2a,3a,4a,5]
 TS4b	IRC →	 RC[1,2b,3b,4b]

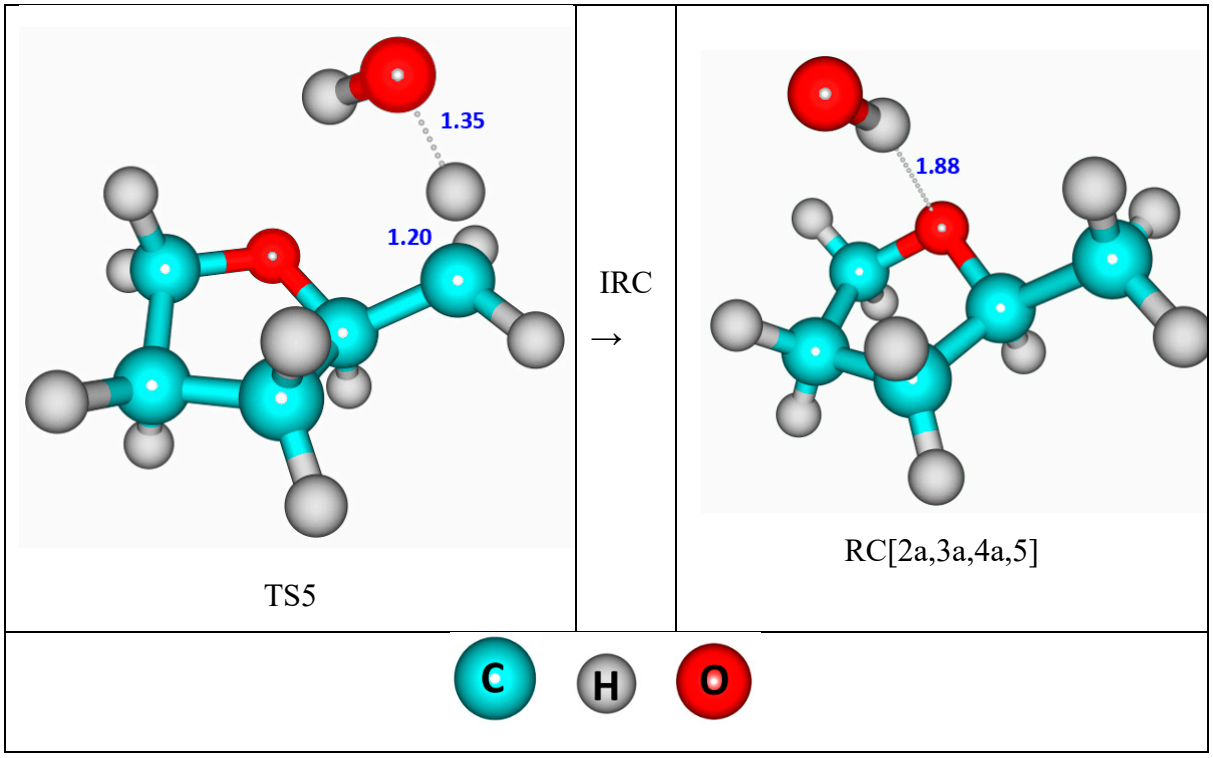


Figure S4: Optimized TSs and corresponding RCs obtained at M06-2X/aug-cc-pVTZ level.

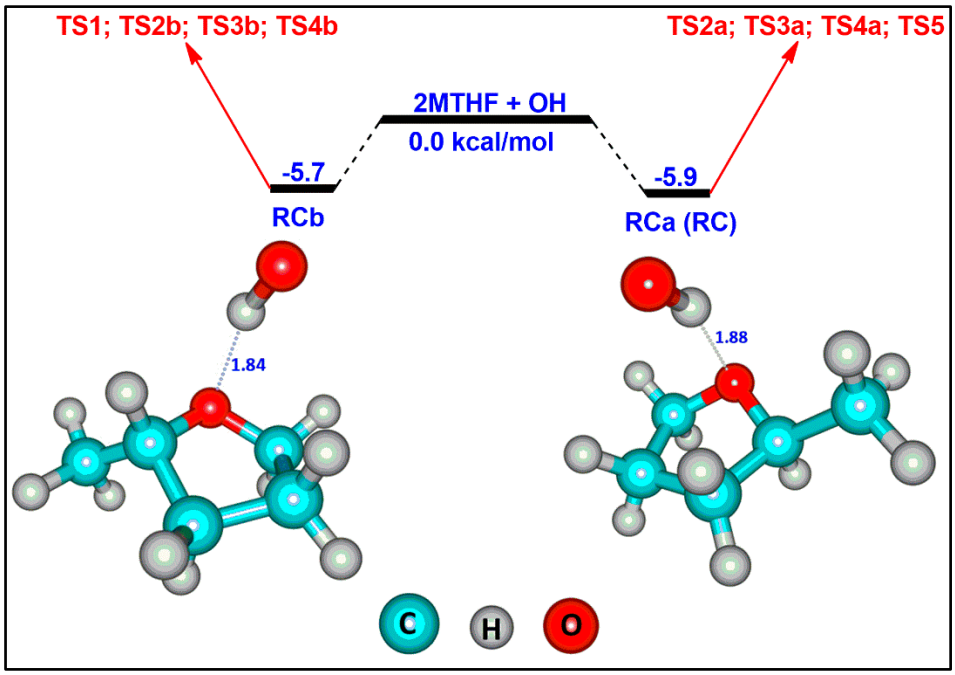


Figure S5: Simplified PES for the formation of RCs from 2MTHF and OH radical (+ZPE, 0 K) calculated at CCSD(T)/cc-pVTZ//M06-2X/aug-cc-pVTZ.

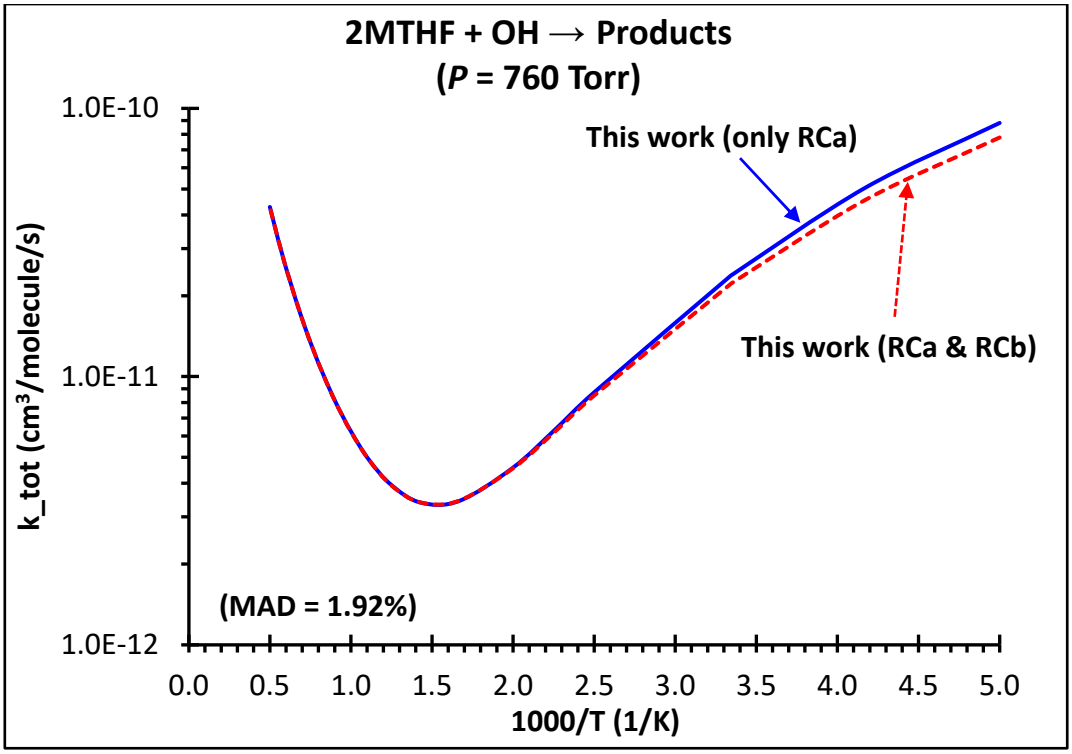


Figure S6: Comparison of the computed global rate constants (2MTHF + OH → products) using one-RC (**RCa**) and two-RC models (**RCa** & **RCb**) at *P* = 760 Torr.

References:

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