Supplementary information for

Kinetics of the Tetrahydrofurfuryl Alcohol + •OH Reaction from *Ab Initio* RRKM-Master Equation Calculations

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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 ($C_{\infty v}$)	O	0.000000	0.000000	0.107999	-75.637723	0.008530	3744.2044	
	H	0.000000	0.000000	-0.863995				
H_2O (C_{2v})	O	0.000000	0.000000	0.116363	-76.332140	0.021565	1616.2259	3871.2897	3975.2726
	H	0.000000	0.762747	-0.465451				
	H	0.000000	-0.762747	-0.465451				
THFA (C_1)	C	1.654782	-0.754886	0.172286	-346.429827	0.151797	53.5218	136.5753	247.5977
	O	0.338588	-1.158494	-0.165993			269.8399	343.4932	437.6462
	C	-0.304827	-0.074433	-0.838988			579.4882	633.6844	720.8015
	C	0.477045	1.200722	-0.456415			796.6210	889.1323	901.6419
	C	1.509348	0.707815	0.563990			920.0369	949.9764	1015.0611
	H	2.011147	-1.402099	0.970859			1029.9474	1069.9751	1110.7234
	H	2.316923	-0.864451	-0.694810			1140.1917	1163.1223	1204.6350
	H	-0.264628	-0.248870	-1.919011			1215.3931	1237.6036	1280.2498
	H	0.969518	1.618916	-1.332832			1320.9552	1326.0603	1349.9246
	H	-0.183725	1.957066	-0.038925			1363.6821	1395.4531	1406.0463
	H	2.448509	1.255419	0.524835			1428.6003	1486.7677	1503.0760
	H	1.105853	0.777639	1.573844			1506.4109	1528.2592	3017.3311
	C	-1.751590	-0.073019	-0.387375			3033.8023	3049.1395	3088.6037
	H	-2.223598	-1.014482	-0.684900			3094.1281	3116.6887	3130.5592
	H	-2.287859	0.746713	-0.865195			3139.2978	3151.1479	3848.3879
	O	-1.849433	0.121324	1.007025					
	H	-1.313932	-0.565687	1.416883					
RC (C_1)	C	-1.231122	1.353397	-0.143149	-422.082937	0.163413	36.8458	70.7450	126.1324
	O	-0.166816	0.727672	-0.859019			185.1469	193.7063	258.4646
	C	-0.341218	-0.701452	-0.832579			277.7269	360.5557	423.1626
	C	-1.469833	-0.973109	0.176082			480.2549	562.5939	629.4645
	C	-1.604358	0.349604	0.932937			734.7533	765.1245	797.4920
	H	-0.862867	2.305111	0.237195			877.1650	909.0859	916.6762
	H	-2.067746	1.541999	-0.822606			953.2735	1012.0454	1027.1374
	H	-0.616809	-1.025913	-1.839407			1072.0458	1110.0600	1129.0664
	H	-2.395923	-1.208404	-0.346905			1160.8356	1211.5617	1219.7504
	H	-1.219851	-1.802354	0.833403			1248.1514	1283.5161	1324.4035
	H	-2.600907	0.514421	1.336373			1334.5059	1356.3144	1388.9344
	H	-0.878665	0.390859	1.744060			1397.7641	1415.1853	1427.4717
	C	0.978530	-1.352060	-0.457229			1485.9271	1496.6312	1501.1076
	H	1.761333	-1.000806	-1.137321			1531.4115	3038.7745	3043.9083
	H	0.880391	-2.430558	-0.593722			3060.0604	3092.0413	3094.6820
	O	1.330999	-1.124834	0.887656			3100.1683	3122.6097	3145.3581
	H	1.810594	-0.288813	0.936841			3155.3369	3391.2937	3793.5030
	O	2.187800	1.593042	0.211267					
	H	1.382589	1.379138	-0.323514					

TS1a	C	0.147428	-1.452848	0.132016	-422.070763	0.160918	-758.5280	88.4911	119.0181
(C_1)	O	-0.058953	-0.564335	1.198452			135.0153	186.6125	202.0649
	C	-0.898018	0.518093	0.777285			255.9375	363.8048	397.0902
	C	-1.791753	-0.089119	-0.303618			546.7421	606.5362	665.3616
	C	-0.911728	-1.176050	-0.939257			700.8495	776.5539	811.1950
	H	1.188437	-1.270772	-0.296916			843.4078	894.4904	906.3289
	H	0.163725	-2.471217	0.520658			956.0754	978.3405	1019.6436
	H	-1.460819	0.826860	1.659398			1054.7213	1080.7425	1103.1874
	H	-2.674460	-0.530654	0.155593			1150.9882	1192.1792	1220.1750
	H	-2.110117	0.655644	-1.029316			1242.5616	1250.6984	1305.4709
	H	-1.474006	-2.075697	-1.179455			1320.9174	1343.5386	1370.3804
	H	-0.446133	-0.806651	-1.848954			1388.3234	1412.4774	1438.7489
	C	-0.076409	1.702213	0.291923			1450.9549	1486.6464	1496.5269
	H	0.650899	1.968727	1.066142			1509.6080	2040.2149	3035.0148
	H	-0.747123	2.553157	0.156668			3086.7884	3093.4084	3097.8456
	O	0.554420	1.472353	-0.947404			3100.1287	3109.7796	3144.4948
	H	1.344390	0.934022	-0.800040			3160.9087	3740.3166	3752.5438
	O	2.550955	-0.459520	-0.124057					
	H	2.376716	-0.385134	0.830190					
TS1b	C	1.124602	0.026876	1.034595	-422.067727	0.159412	-743.1273	38.6646	59.5087
(C_1)	O	-0.014220	-0.672547	0.607207			96.4896	143.9906	191.8731
	C	-0.558851	-0.043866	-0.569058			233.9283	269.4121	388.4866
	C	0.296224	1.200645	-0.825969			426.9273	490.6288	593.1005
	C	0.965976	1.446312	0.528843			659.0514	711.2833	825.7289
	H	1.244468	-0.099018	2.109181			853.5234	878.1466	949.6819
	H	2.048602	-0.424238	0.534122			973.3562	1006.6375	1032.2490
	H	-0.504626	-0.765241	-1.386504			1074.3977	1086.0227	1125.9941
	H	1.052013	0.991918	-1.580157			1157.7725	1183.4396	1215.4840
	H	-0.308624	2.042328	-1.160384			1240.3610	1281.8715	1307.9587
	H	1.913817	1.972542	0.448523			1329.6619	1347.2184	1352.0217
	H	0.309999	2.005048	1.198452			1378.7445	1396.0599	1414.1216
	C	-2.010751	0.276667	-0.273787			1443.0825	1483.6866	1500.2890
	H	-2.495065	0.649222	-1.176717			1505.3791	1910.9040	3010.9476
	H	-2.052299	1.065613	0.488433			3076.4978	3077.8597	3095.9807
	O	-2.720954	-0.865858	0.140088			3111.8968	3124.5180	3141.9641
	H	-2.206342	-1.282023	0.839226			3152.6050	3772.3982	3849.4692
	O	2.736157	-1.174071	-0.632399					
	H	2.086995	-1.896155	-0.601079					
TS2a	C	-1.320627	-1.017402	-0.789945	-422.068828	0.159224	-848.4225	73.2434	111.6892
(C_1)	O	0.083880	-1.033663	-0.980146			135.8978	160.0034	249.1438
	C	0.732423	-1.010632	0.291393			260.2893	336.4594	401.4990
	C	-0.314267	-0.514084	1.310935			571.5952	604.3899	651.5308
	C	-1.533070	-0.189745	0.459001			716.5461	761.9078	828.6530
	H	-1.780016	-0.598369	-1.682736			893.3587	909.6821	934.1408
	H	-1.694797	-2.038877	-0.643652			948.7145	1021.8826	1031.2902
	H	1.070973	-2.020260	0.543392			1057.8242	1079.7076	1112.5079
	H	-0.545560	-1.296681	2.033134			1143.4265	1164.7887	1201.0754
	H	0.040872	0.354696	1.863613			1229.5950	1248.4166	1268.6587
	H	-2.495620	-0.321163	0.947193			1316.9479	1323.6612	1342.3526
	H	-1.499084	0.941456	0.157459			1372.5474	1392.8828	1407.8246
	C	1.940103	-0.103607	0.143798			1429.5863	1449.8416	1492.0706
	H	2.652136	-0.553274	-0.553208			1508.4497	1515.6629	3009.2483
	H	2.433077	0.026733	1.106306			3040.5515	3060.7762	3085.4471

	O	1.551786	1.179721	-0.309336			3126.1524	3129.6380	3131.2398
	H	1.104595	1.042559	-1.153332			3142.6287	3686.4902	3818.6446
	O	-1.149934	2.268324	-0.109694					
	H	-0.199807	2.160948	0.084145					
TS2b	C	0.766121	-0.122479	1.365705	-422.064675	0.158786	-985.6943	49.3465	109.7587
(C_1)	O	-0.078553	-0.836885	0.473033			116.8124	152.6643	226.9412
	C	-0.552030	0.084136	-0.526884			299.7770	374.1333	399.7624
	C	0.413560	1.282493	-0.511862			421.9042	494.9213	526.4895
	C	1.496015	0.841733	0.460232			696.2344	805.4865	839.4505
	H	0.174215	0.415566	2.116503			868.5444	904.3974	943.0375
	H	1.410597	-0.839042	1.870363			958.0051	1013.4723	1033.3068
	H	-0.534227	-0.455047	-1.474414			1061.9437	1095.3054	1116.8149
	H	0.807688	1.506880	-1.499705			1144.4872	1171.6843	1194.9893
	H	-0.093300	2.175766	-0.137000			1218.7391	1245.8592	1273.8464
	H	2.263183	0.186678	-0.149085			1284.9950	1305.4505	1337.6586
	H	2.069249	1.627992	0.944620			1356.7048	1377.8858	1403.0385
	C	-1.979636	0.467237	-0.194617			1438.2410	1488.1168	1502.0304
	H	-2.368834	1.142522	-0.957689			1519.1600	1626.8318	3005.5898
	H	-1.990129	1.000563	0.765309			3017.4923	3057.7158	3092.7606
	O	-2.823355	-0.657986	-0.157698			3108.4864	3134.4610	3143.2086
	H	-2.393725	-1.317607	0.396554			3147.7189	3744.9303	3848.3629
	O	2.643174	-0.917858	-0.905857					
	H	1.860983	-1.461156	-0.706723					
TS3a	C	-2.099588	-0.063643	-0.390500	-422.069292	0.159057	-980.2265	40.6308	115.2854
(C_1)	O	-1.113439	-1.071477	-0.227177			150.8344	216.2932	233.6432
	C	-0.215332	-0.633712	0.788319			283.1717	327.1803	439.8808
	C	-0.256241	0.899564	0.752862			562.8784	587.0792	642.7023
	C	-1.327764	1.247784	-0.276123			673.4973	769.9714	850.2207
	H	-2.581394	-0.216409	-1.353196			883.9151	910.7990	941.5551
	H	-2.850987	-0.148300	0.402327			953.9998	1005.8955	1029.3380
	H	-0.565151	-0.992936	1.763426			1048.1035	1085.4142	1116.1059
	H	-0.413254	1.339269	1.735321			1146.2674	1158.8717	1172.9709
	H	0.779009	1.352236	0.412016			1217.7930	1231.4119	1266.0683
	H	-1.952262	2.086172	0.022470			1305.5441	1318.3305	1339.9772
	H	-0.861651	1.489446	-1.231658			1354.5407	1387.8831	1401.1514
	C	1.130087	-1.271119	0.486934			1432.4144	1443.0372	1491.4835
	H	1.056964	-2.352445	0.626734			1506.6962	1526.3095	3022.0151
	H	1.888700	-0.877531	1.162147			3030.8858	3062.6485	3086.9409
	O	1.546843	-0.973667	-0.832963			3126.1959	3130.8946	3140.2646
	H	0.803295	-1.181981	-1.410071			3150.6287	3669.1590	3829.2409
	O	1.969194	1.735649	-0.146461					
	H	2.088972	0.905198	-0.645664					
TS3b	C	2.317156	-0.227492	0.034443	-422.061016	0.157830	-1149.2913	46.2074	86.9057
(C_1)	O	1.298621	-1.137467	-0.387801			139.5921	152.8027	204.2261
	C	0.030627	-0.494472	-0.367093			225.4923	250.0997	411.4107
	C	0.221505	0.740861	0.490972			435.2745	447.1764	523.5264
	C	1.646904	1.144101	0.166866			626.9014	692.6233	846.2279
	H	2.713539	-0.566245	0.994266			877.0380	897.2369	958.0504
	H	3.122360	-0.236525	-0.699143			993.6674	1000.6451	1019.3571
	H	-0.250187	-0.192812	-1.383222			1072.4875	1099.8679	1127.8599
	H	-0.570691	1.576778	0.173835			1155.7593	1165.7455	1208.6923
	H	0.040556	0.552268	1.550056			1231.8550	1244.2351	1259.6207

	H	1.676870	1.675804	-0.784507			1284.2517	1302.8937	1332.0529
	H	2.109773	1.766665	0.927838			1349.5673	1388.2969	1410.4776
	C	-1.002764	-1.466300	0.155342			1467.1264	1479.3109	1496.1282
	H	-0.734438	-1.763099	1.173578			1529.7604	1537.1187	3025.7780
	H	-1.024144	-2.356094	-0.477444			3044.0728	3056.9050	3084.8362
	O	-2.252278	-0.787338	0.130186			3094.1506	3100.3262	3113.6322
	H	-2.949480	-1.379654	0.416949			3154.7565	3723.6781	3903.7996
	O	-1.695957	2.106841	-0.308457					
	H	-2.217813	1.286436	-0.246809					
TS4	C	1.711790	0.317096	-1.044245	-422.070848	0.159863	-617.2888	36.4753	70.9142
(C_1)	O	0.439138	-0.316488	-1.022165			131.1892	147.2763	206.1447
	C	-0.082757	-0.096696	0.261344			238.9201	348.7678	424.2435
	C	1.096026	-0.168883	1.234730			475.2552	499.9302	565.2659
	C	2.328217	-0.007813	0.318517			639.8761	740.9728	817.9039
	H	2.268389	-0.074979	-1.891094			868.8990	902.3467	939.7855
	H	1.573907	1.395442	-1.169806			976.8506	1018.4972	1052.6931
	H	-0.524823	0.967006	0.292278			1080.8306	1101.3394	1135.8261
	H	1.026488	0.611654	1.988584			1166.9190	1191.1470	1206.9129
	H	1.105374	-1.130925	1.748612			1233.2107	1265.1598	1288.5330
	H	3.003841	0.773968	0.656617			1304.8632	1322.0535	1342.0039
	H	2.887847	-0.939225	0.264158			1368.2464	1395.2539	1428.7969
	C	-1.233965	-1.040870	0.491138			1488.2259	1498.3672	1508.4213
	H	-1.663204	-0.864650	1.476478			1527.9694	1818.5646	3036.3022
	H	-0.867316	-2.072320	0.443729			3045.6952	3080.5715	3102.5718
	O	-2.263938	-0.823880	-0.454681			3129.1560	3134.4587	3147.1547
	H	-1.869847	-0.898211	-1.330356			3157.6151	3717.0080	3846.3330
	O	-1.622447	1.996756	0.234592					
	H	-2.278553	1.364132	-0.110080					
TS5	C	-1.508713	-1.258473	-0.356654	-422.069099	0.159714	-837.6178	52.9383	63.6660
(C_1)	O	-0.129192	-1.012032	-0.118222			125.2972	161.9325	243.4064
	C	-0.006173	0.095782	0.783410			263.1452	303.0954	376.2444
	C	-1.369198	0.818671	0.767774			469.5497	575.5658	629.7501
	C	-2.138013	0.125067	-0.361618			730.3100	746.3600	801.4427
	H	-1.595058	-1.797131	-1.297621			891.3871	919.2556	925.7629
	H	-1.921879	-1.876892	0.447450			949.7382	994.9255	1023.4158
	H	0.236789	-0.280840	1.780417			1058.6757	1105.1127	1132.0907
	H	-1.877206	0.679094	1.720516			1148.4371	1198.8543	1212.6238
	H	-1.250759	1.885684	0.593885			1220.4842	1275.3107	1286.0628
	H	-3.213086	0.104359	-0.197840			1321.9465	1326.2960	1347.0325
	H	-1.939094	0.616600	-1.313664			1359.6946	1393.3090	1398.2186
	C	1.148060	0.936230	0.283436			1430.5018	1487.7856	1502.8774
	H	2.079019	0.241218	0.279248			1530.2593	1722.9393	3033.3961
	H	1.377224	1.760362	0.958176			3059.3879	3090.0022	3096.9533
	O	0.934093	1.451407	-0.991486			3121.2131	3136.0291	3142.5519
	H	0.748497	0.706785	-1.574362			3153.6887	3733.1009	3834.4714
	O	2.774100	-1.038564	0.108273					
	H	1.967765	-1.549388	-0.082803					
TS6	C	-1.492947	1.081305	-0.291329	-422.065863	0.158038	-1729.0808	67.0504	85.4403
(C_1)	O	-0.439433	0.510861	-1.068554			183.8448	212.7424	266.8479
	C	-0.282288	-0.872485	-0.724580			274.7628	370.2750	456.6312
	C	-1.195105	-1.123763	0.485727			543.9403	560.4494	631.5829
	C	-1.490603	0.285455	1.001470			747.2541	796.1337	851.9859

	H	-1.276249	2.140288	-0.161186			873.9865	905.6638	925.8828
	H	-2.441279	0.974735	-0.826934			951.6192	956.0685	1010.9573
	H	-0.578093	-1.475645	-1.586905			1033.0298	1075.6957	1120.9061
	H	-2.114400	-1.614635	0.168283			1128.8401	1153.7135	1209.3966
	H	-0.707380	-1.748164	1.230792			1218.5651	1277.3604	1283.2529
	H	-2.431416	0.355815	1.542636			1323.1017	1331.2495	1356.8191
	H	-0.679082	0.629472	1.641324			1375.0440	1399.4148	1404.7056
	C	1.188399	-1.143866	-0.439512			1456.4483	1488.1271	1501.9357
	H	1.803348	-0.815194	-1.282965			1531.1273	1560.7132	3029.1226
	H	1.322310	-2.225335	-0.325357			3042.4248	3057.6937	3075.4156
	O	1.632191	-0.577908	0.760231			3091.1620	3096.5574	3126.1870
	H	1.948947	0.466717	0.589863			3143.9590	3155.7720	3650.1957
	O	1.772652	1.620473	0.216898					
	H	1.065268	1.524672	-0.448805					
PC1a	C	0.550284	-1.508325	0.073064	-422.116410	0.162810	54.3330	115.2393	151.5722
(C_1)	O	0.077572	-0.757660	-0.972448			160.8381	180.7958	205.6993
	C	0.591623	0.589120	-0.877156			225.2059	259.6441	322.6450
	C	1.841707	0.469973	-0.002485			375.1046	462.0895	516.2332
	C	1.570434	-0.766896	0.870862			558.7026	650.6383	710.2141
	H	-2.871099	-1.526719	0.500599			797.2582	806.4169	861.2897
	H	0.519964	-2.573810	-0.098033			915.0364	961.2018	988.1775
	H	0.822886	0.900434	-1.896311			1029.2993	1052.8564	1081.8341
	H	2.717621	0.306933	-0.627961			1134.4504	1181.2711	1203.2091
	H	1.996803	1.369508	0.588496			1237.8441	1254.6764	1300.7502
	H	2.468892	-1.358312	1.046842			1312.0612	1343.1498	1380.3221
	H	1.169196	-0.464590	1.839837			1400.5905	1419.3024	1444.3243
	C	-0.469414	1.515992	-0.308234			1479.1113	1497.7639	1501.1027
	H	-1.363999	1.471291	-0.936721			1626.3820	3046.0513	3063.4008
	H	-0.082946	2.537005	-0.346591			3089.3052	3094.2847	3098.9586
	O	-0.778255	1.219095	1.032386			3108.4215	3151.7411	3220.9196
	H	-1.479445	0.552589	1.023831			3734.2913	3769.4579	3929.8494
	O	-2.619147	-0.719477	0.047425					
	H	-1.847028	-0.949173	-0.489204					
PC1b	C	0.759967	0.855505	1.197036	-422.110475	0.161488	43.5713	59.6040	98.0629
(C_1)	O	0.111545	-0.311323	0.877638			111.4834	142.0017	160.3714
	C	-0.355069	-0.241015	-0.493014			195.0039	268.2012	281.1915
	C	0.429006	0.906651	-1.121504			388.2257	394.3085	422.1498
	C	0.704054	1.832201	0.073903			483.7862	507.0696	681.1727
	H	0.796514	1.080129	2.251566			748.5391	840.7230	864.2157
	H	3.209114	-1.922694	0.073441			938.5435	968.9865	989.5427
	H	-0.141456	-1.209183	-0.943154			1036.6748	1068.8290	1085.6277
	H	1.364273	0.528319	-1.527755			1126.4775	1176.5558	1199.2752
	H	-0.135076	1.393765	-1.915009			1230.3480	1236.5987	1300.7322
	H	1.630123	2.394516	-0.036154			1322.5990	1336.8068	1350.9219
	H	-0.105130	2.560808	0.203549			1383.9444	1419.6247	1443.7718
	C	-1.851140	0.001012	-0.454176			1482.9919	1498.7296	1506.1397
	H	-2.246422	-0.023477	-1.469833			1622.2611	3007.2030	3017.6313
	H	-2.045506	0.997282	-0.036481			3099.4592	3110.0745	3111.1047
	O	-2.524404	-0.994752	0.278683			3126.7599	3154.2361	3232.3617
	H	-2.068832	-1.090711	1.120958			3812.1674	3851.2893	3947.2518
	O	2.387630	-1.629100	-0.324125					
	H	1.823318	-1.353483	0.407835					

PC2a	C	-1.754471	-0.069809	-0.834435	-422.104186	0.161344	35.4497	97.0337	102.9787
(C_1)	O	-0.524823	-0.754672	-1.015033			131.4470	153.6078	204.9433
	C	-0.056385	-1.214722	0.249674			247.8529	260.8466	289.9675
	C	-0.593313	-0.218847	1.292323			323.5906	364.4960	415.4744
	C	-1.701182	0.454918	0.558934			608.9959	637.8585	672.9617
	H	-1.829501	0.704973	-1.600446			743.4743	848.4181	893.0296
	H	-2.597340	-0.762774	-0.977704			940.1032	955.7674	984.4106
	H	-0.455450	-2.216641	0.444512			1014.8374	1045.4614	1089.7717
	H	-0.929527	-0.728104	2.197929			1120.4431	1158.8020	1182.3503
	H	0.188724	0.485431	1.596341			1211.9594	1252.1184	1282.0196
	H	-2.486523	1.035774	1.014886			1322.0028	1359.4600	1373.5462
	H	-0.157226	2.318971	0.055123			1394.4347	1409.5868	1433.7809
	C	1.456172	-1.281188	0.154393			1477.6191	1506.4806	1507.1798
	H	1.744212	-2.070857	-0.544357			1638.3576	2969.0746	3026.9136
	H	1.881451	-1.511987	1.130509			3032.4843	3059.7392	3075.2645
	O	1.990954	-0.038961	-0.256077			3077.6966	3124.6776	3245.9841
	H	1.577239	0.171508	-1.102003			3797.0471	3821.6849	3898.2559
	O	0.741658	2.629102	-0.086592					
	H	1.296704	1.867842	0.121486					
PC2b	C	0.599995	0.692473	1.307887	-422.104568	0.160866	35.4109	70.9268	101.4270
(C_1)	O	0.125931	-0.517875	0.704099			140.4914	145.0570	153.0285
	C	-0.425199	-0.203749	-0.587447			199.2380	264.6953	290.6530
	C	0.391414	0.985136	-1.097303			337.1283	389.6238	416.0197
	C	0.810986	1.633442	0.175711			518.5067	579.1657	729.2645
	H	-0.135968	1.060201	2.034366			753.5204	839.5213	886.5684
	H	1.517140	0.453980	1.853647			954.1915	969.1765	975.8977
	H	-0.310047	-1.102357	-1.192538			1017.5104	1060.9375	1070.4496
	H	1.254627	0.637739	-1.673658			1108.4872	1134.3415	1201.4170
	H	-0.201077	1.640018	-1.740491			1210.5179	1236.4679	1287.6979
	H	3.048256	-2.089207	-0.209427			1315.3583	1342.5102	1358.6553
	H	1.340096	2.567470	0.259074			1378.2012	1406.8661	1441.7598
	C	-1.897332	0.126340	-0.422775			1472.9426	1504.2072	1515.9183
	H	-2.355109	0.262156	-1.402827			1621.4557	2996.3459	3010.4496
	H	-1.994941	1.070974	0.129085			3036.1344	3056.5711	3079.4502
	O	-2.588684	-0.914692	0.225860			3105.9816	3118.0323	3257.0971
	H	-2.048177	-1.189559	0.973907			3733.3475	3844.0505	3939.1142
	O	2.615609	-1.246814	-0.357766					
	H	1.783177	-1.278213	0.134882					
PC3a	C	1.944570	-0.635110	-0.583055	-422.106658	0.161588	32.6812	94.9825	103.3145
(C_1)	O	1.394584	0.677380	-0.510404			116.1548	183.4929	199.2200
	C	0.639885	0.786845	0.697041			242.8189	274.3093	315.3311
	C	0.302669	-0.619485	1.065707			326.9942	390.1262	464.3176
	C	0.904519	-1.546409	0.070637			627.6451	650.3092	663.2750
	H	2.138818	-0.855322	-1.630113			740.3313	876.3544	880.8501
	H	2.888346	-0.667980	-0.029943			905.8377	955.4880	1007.5309
	H	1.245185	1.282324	1.470922			1019.5378	1040.2472	1086.8228
	H	-0.439341	-0.886478	1.799428			1105.2788	1152.3744	1200.1754
	H	-3.390814	-1.385526	-0.426300			1210.3244	1259.3310	1293.9312
	H	1.348176	-2.438361	0.514161			1303.1178	1338.6101	1340.1398
	H	0.151120	-1.878736	-0.653398			1396.6138	1398.4048	1427.2556
	C	-0.559106	1.675814	0.387827			1480.5057	1507.0599	1526.4989
	H	-0.215316	2.691830	0.177208			1633.9325	2971.2185	3018.0590
	H	-1.234072	1.701939	1.242150			3039.9467	3057.7538	3097.1960

	O	-1.288611	1.166808	-0.714261			3129.5042	3137.8936	3254.7588
	H	-0.640401	0.998296	-1.408805			3698.8316	3819.0001	3933.1864
	O	-2.491691	-1.351984	-0.095285					
	H	-2.161171	-0.469544	-0.324650					
PC3b	C	2.382056	0.081438	0.057030	-422.099027	0.160706	44.8819	62.5064	95.2650
(C_1)	O	1.401257	0.514412	0.992982			133.1562	148.0571	166.7245
	C	0.112342	0.217344	0.475796			196.2697	237.9754	266.1232
	C	0.332180	-0.861059	-0.532724			293.5736	359.5887	436.0657
	C	1.788728	-1.162080	-0.610889			471.5867	508.4847	640.7375
	H	2.565987	0.862823	-0.687531			747.2007	859.9959	887.3331
	H	3.301503	-0.104625	0.606718			957.4629	965.9392	1017.3645
	H	-0.521159	-0.104949	1.309784			1053.6666	1063.5527	1070.4438
	H	-2.126043	-1.946933	0.437345			1108.2033	1156.3906	1203.7513
	H	-0.432777	-1.233732	-1.193916			1220.9676	1244.6190	1256.7556
	H	2.044903	-2.062604	-0.041021			1301.9822	1312.8653	1345.8617
	H	2.148181	-1.306438	-1.629426			1376.2490	1397.7421	1439.2833
	C	-0.512017	1.475736	-0.122763			1474.5513	1522.5366	1528.3042
	H	0.128362	1.854941	-0.924721			1643.2081	3015.3065	3028.4093
	H	-0.597862	2.235307	0.657081			3033.3223	3043.3622	3095.8524
	O	-1.787898	1.104607	-0.625087			3108.9291	3137.1720	3252.6540
	H	-2.269638	1.882383	-0.912206			3779.0820	3901.3336	3929.0785
	O	-2.894953	-1.374252	0.470633					
	H	-2.608443	-0.542589	0.070973					
PC4	C	1.962077	-0.175288	-1.028207	-422.111046	0.162377	36.1189	40.5986	82.0405
(C_1)	O	0.732383	-0.821630	-0.689941			110.5671	177.8647	187.5694
	C	0.107999	-0.058813	0.261823			203.0496	231.1079	247.7931
	C	1.089793	0.851589	0.943896			362.9477	380.7732	425.3401
	C	2.422386	0.464127	0.276872			582.1361	614.5260	685.3976
	H	2.636495	-0.929270	-1.423953			814.2249	881.2781	896.2933
	H	1.766089	0.577131	-1.796541			942.5309	955.4662	1013.6984
	H	-1.775969	1.722955	-0.785375			1055.9857	1078.9621	1091.5259
	H	0.844830	1.902299	0.773619			1166.3365	1196.4822	1216.2233
	H	1.108890	0.701307	2.025640			1260.9163	1276.8830	1287.8748
	H	3.084964	1.310469	0.115182			1334.0678	1346.9556	1352.9834
	H	2.945799	-0.273926	0.882821			1405.1548	1446.6883	1485.7284
	C	-1.022282	-0.750429	0.931057			1492.5048	1502.3425	1526.0308
	H	-1.536359	-0.052966	1.590442			1646.4915	2970.6970	3051.5964
	H	-0.648849	-1.587797	1.540412			3054.4114	3077.9136	3098.0615
	O	-1.986266	-1.233392	0.005251			3126.5632	3149.6218	3157.7524
	H	-1.516343	-1.707585	-0.687899			3780.1637	3854.0808	3914.8410
	O	-2.691129	1.528346	-0.569567					
	H	-2.709287	0.563660	-0.512938					
PC5	C	-1.330798	-1.073786	-0.821181	-422.111029	0.162481	32.8961	59.7595	87.1787
(C_1)	O	-0.005929	-0.600804	-0.548360			115.3213	160.5024	186.0194
	C	-0.005960	0.265407	0.602994			199.3251	276.1905	291.3035
	C	-1.456202	0.753301	0.687976			324.8667	499.5630	548.1309
	C	-2.223557	-0.499785	0.277902			561.8600	601.2783	663.2919
	H	-1.625514	-0.711508	-1.807737			682.2273	845.8792	889.2955
	H	-1.320296	-2.162641	-0.837318			905.6400	947.6845	979.4995
	H	0.250028	-0.314339	1.495680			1022.9575	1054.5711	1105.0601
	H	-1.707082	1.117243	1.681260			1138.2749	1181.0924	1199.4827
	H	-1.607641	1.559547	-0.032030			1215.3066	1267.8767	1301.8010

	H -2.284885 -1.192172 1.117488			1327.2595	1341.3523	1346.4994
	H -3.232750 -0.298963 -0.074247			1389.3059	1399.0338	1459.2464
	C 1.033397 1.302188 0.377530			1488.0111	1503.3768	1539.5128
	H 2.932611 -0.843480 0.439631			1648.0489	3045.6742	3065.4143
	H 1.379182 1.926955 1.186891			3078.2738	3087.0768	3118.4484
	O 1.060152 1.900621 -0.838647			3144.5248	3152.4791	3228.5056
	H 0.748813 1.250811 -1.482725			3794.6110	3799.0117	3915.6375
	O 2.527857 -1.709861 0.348795					
	H 1.709611 -1.535054 -0.132519					
PC6	C 1.044210 -1.425736 -0.322945	-422.094284	0.161073	15.1730	71.9705	97.6470
(C_1)	O 0.194897 -0.524765 -1.031649			133.5906	171.6202	184.3406
	C 0.556783 0.821153 -0.717550			251.9533	268.0713	306.5254
	C 1.540705 0.742707 0.463973			338.1741	472.1512	562.0102
	C 1.373764 -0.693591 0.965734			587.1333	634.4392	749.8539
	H 0.494085 -2.353427 -0.180098			797.0602	898.0458	913.1561
	H 1.944844 -1.624679 -0.912280			936.4986	953.3738	1009.8486
	H 1.021683 1.275468 -1.597191			1042.8559	1075.4655	1114.0531
	H 2.559372 0.909529 0.116695			1137.5030	1193.8533	1207.4026
	H 1.314646 1.483757 1.228203			1214.9615	1281.5482	1322.3553
	H 2.262212 -1.080053 1.459790			1329.5460	1353.1296	1360.4139
	H 0.526538 -0.760557 1.647247			1392.5832	1397.8517	1406.0035
	C -0.717451 1.582897 -0.393118			1486.5947	1501.3662	1528.0901
	H -1.471368 1.431528 -1.181534			1642.1965	2973.2647	2999.2037
	H -0.539323 2.669273 -0.370461			3039.0419	3052.7951	3092.7590
	O -1.296496 1.234431 0.799134			3094.9621	3137.2967	3138.3427
	H -2.350142 -0.861614 0.881354			3154.7345	3764.6850	3915.4020
	O -2.275586 -1.474300 0.145608					
	H -1.533132 -1.136732 -0.373031					
P1	C -1.456844 -0.953089 -0.268620	-345.770116	0.137691	79.6560	141.1014	234.5072
(C_1)	O -0.284481 -1.086219 0.423733			280.4926	319.3811	413.5837
	C 0.245995 0.216567 0.732421			508.3416	597.7934	665.8075
	C -0.568288 1.195166 -0.110611			749.1775	846.6505	868.3115
	C -1.907893 0.467972 -0.272262			918.1762	964.6199	995.4381
	H -2.088508 -1.828012 -0.253106			1012.6812	1059.2927	1086.6122
	H 0.091888 0.391558 1.801453			1135.3943	1174.3792	1210.3191
	H -0.656835 2.165936 0.371292			1236.4163	1242.0229	1298.5639
	H -0.086427 1.320820 -1.079592			1316.5652	1343.4515	1364.8766
	H -2.571186 0.687307 0.574340			1393.5096	1414.6323	1431.0483
	H -2.437490 0.741505 -1.183159			1484.0285	1501.0906	1507.6078
	C 1.731791 0.182582 0.433245			2997.2517	3040.8766	3054.6974
	H 2.216464 -0.533434 1.103866			3096.3604	3114.1384	3116.5431
	H 2.162584 1.167512 0.615185			3152.7483	3226.2076	3845.0972
	O 1.982675 -0.139802 -0.915048					
	H 1.515387 -0.960207 -1.104787					
P2	C -1.704746 -0.821039 -0.112183	-345.762156	0.136346	110.6448	121.9646	174.6688
(C_1)	O -0.334371 -1.068543 0.174330			240.1557	283.8451	317.2617
	C 0.235697 0.122870 0.712002			435.3048	604.8862	668.5215
	C -0.480695 1.270171 -0.010431			740.2060	861.6998	892.0230
	C -1.792718 0.649366 -0.335642			942.5015	955.2329	974.6136
	H -1.985521 -1.421320 -0.981233			1008.3222	1047.6849	1086.6387
	H -2.328744 -1.149886 0.731934			1121.0622	1158.5521	1186.2040

	H	0.031884	0.171387	1.788931			1204.3229	1250.7781	1274.0534
	H	-0.560820	2.161445	0.614131			1323.8951	1355.7000	1363.0941
	H	0.079376	1.545580	-0.911796			1392.4192	1410.3672	1434.2372
	H	-2.667378	1.161609	-0.699156			1474.8543	1507.0812	1507.7509
	C	1.731401	0.042885	0.484925			2972.5445	3013.0870	3022.6692
	H	2.136986	-0.788605	1.069484			3046.5132	3060.2159	3088.2091
	H	2.204038	0.963978	0.826241			3114.0914	3258.5560	3842.6041
	O	2.040444	-0.105343	-0.882155					
	H	1.507968	-0.838613	-1.207958					
P3	C	1.672292	-0.738107	0.161872	-345.761325	0.136658	77.5886	124.3698	231.8574
(C_1)	O	0.331799	-1.117372	-0.117889			254.0735	295.2282	350.8290
	C	-0.301254	-0.045897	-0.818637			415.8454	637.0883	651.9304
	C	0.480198	1.166803	-0.435950			738.1750	876.5874	879.4660
	C	1.614880	0.766378	0.438641			901.7759	953.1732	1003.9482
	H	2.020439	-1.334590	1.001820			1021.9153	1034.6424	1085.1503
	H	2.304882	-0.942169	-0.708277			1112.5851	1160.2851	1201.3249
	H	-0.255238	-0.235418	-1.902199			1212.6093	1260.6652	1292.2941
	H	0.146861	2.175441	-0.616055			1302.8165	1338.2887	1340.4007
	H	2.552294	1.273201	0.206404			1398.7402	1399.4186	1424.9857
	H	1.389765	0.956722	1.494956			1473.1674	1505.1323	1525.7605
	C	-1.764622	-0.031286	-0.396377			2965.9931	3010.6680	3036.5417
	H	-2.237913	-0.959176	-0.733145			3040.8911	3094.9943	3118.2917
	H	-2.273097	0.807261	-0.871540			3136.9863	3253.0332	3846.3591
	O	-1.896613	0.128924	0.996179					
	H	-1.338448	-0.541036	1.404420					
P4	C	-1.590473	-0.929268	0.222803	-345.769834	0.138076	81.1006	95.8244	187.9505
(C_1)	O	-0.290973	-1.050040	-0.368293			232.4892	297.8083	371.8209
	C	0.267703	0.195953	-0.513286			499.8709	626.8352	673.2150
	C	-0.592414	1.219099	0.155041			810.7182	883.2263	906.2530
	C	-1.965151	0.543413	0.090663			917.3941	946.2871	1006.6771
	H	-2.265077	-1.608333	-0.293551			1018.1627	1068.3723	1078.2453
	H	-1.516752	-1.228793	1.270981			1159.2104	1183.6766	1218.0362
	H	-0.279463	1.368518	1.196657			1261.0039	1275.7787	1298.2802
	H	-0.560633	2.186350	-0.343088			1338.0783	1353.2860	1361.0548
	H	-2.649951	0.866607	0.870816			1415.1796	1418.4383	1481.9269
	H	-2.426282	0.727949	-0.878930			1493.1907	1498.7754	1531.3225
	C	1.746954	0.196314	-0.546583			3002.2410	3052.7744	3058.3275
	H	2.110444	1.189768	-0.801884			3092.1573	3121.4113	3134.0746
	H	2.103098	-0.508306	-1.303016			3134.4428	3151.9286	3871.4280
	O	2.323877	-0.118543	0.726049					
	H	2.021675	-0.998163	0.968141					
P5	C	-1.332571	-1.090999	-0.102851	-345.768457	0.138102	67.2098	116.7800	208.1019
(C_1)	O	-0.093677	-0.961361	0.601182			278.5696	388.3998	502.8235
	C	0.294206	0.417442	0.664245			597.5031	605.8756	653.7112
	C	-0.940107	1.217575	0.261684			770.3687	850.6390	880.9810
	C	-1.607750	0.268578	-0.734123			912.0080	945.5431	978.7902
	H	-1.238133	-1.893533	-0.832844			1000.4268	1065.4845	1110.7652
	H	-2.111807	-1.360082	0.614535			1139.7981	1187.8302	1206.0873
	H	0.594007	0.608239	1.701863			1213.7271	1266.8363	1299.6754
	H	-1.581577	1.383251	1.127230			1323.8470	1334.4503	1348.4379
	H	-0.679138	2.181145	-0.172047			1363.0472	1397.6739	1461.4872
	H	-2.670859	0.458021	-0.863362			1486.2538	1498.2746	1535.9816

	H	-1.116600	0.343413	-1.703737			3004.8043	3053.8197	3085.7651
	C	1.438078	0.623994	-0.277176			3092.5037	3117.1342	3139.5091
	H	1.860970	1.608060	-0.424464			3151.4683	3206.5032	3770.9442
	O	2.338439	-0.382889	-0.375343					
	H	1.873904	-1.194059	-0.124564					
P6	C	1.375912	-0.858212	0.292749	-345.748530	0.136528	45.9161	122.2087	168.0174
(C_1)	O	0.411582	-1.039045	-0.748059			258.9275	351.8936	478.1738
	C	-0.352916	0.131504	-0.921535			629.3087	732.6342	804.7839
	C	0.520562	1.268514	-0.395543			839.0881	868.2832	889.9675
	C	1.262290	0.596466	0.761752			922.3740	946.8107	977.9068
	H	1.166584	-1.563281	1.096476			1040.2966	1057.4158	1116.8455
	H	2.359532	-1.078190	-0.125276			1136.1628	1163.6398	1204.4744
	H	-0.578209	0.239074	-1.984469			1220.1908	1247.8229	1267.6782
	H	1.218914	1.572421	-1.175021			1321.1558	1332.0455	1351.0722
	H	-0.056834	2.139587	-0.091123			1380.9926	1407.5096	1424.6120
	H	2.235190	1.044597	0.950354			1489.4238	1504.0114	1533.4208
	H	0.674414	0.655323	1.675444			2945.3841	3018.9351	3066.6192
	C	-1.694947	0.014429	-0.181399			3075.5029	3089.4509	3098.2300
	H	-2.179767	-0.903140	-0.557171			3112.5390	3135.9726	3151.1465
	H	-2.351008	0.864910	-0.411621					
	O	-1.555860	-0.196893	1.158843					

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

No.	Species	T1 diagnostics
1	THFA	0.01044046
2	•OH	0.00704816
3	**RC**	0.01103182
4	**TS1a**	0.01737949
5	**TS1b**	0.01662276
6	**TS2a**	0.01560761
7	**TS2b**	0.01571134
8	**TS3a**	0.01572722
9	**TS3b**	0.01523644
10	**TS4**	0.01647617
11	**TS5**	0.01645527
12	**TS6**	0.02110088
13	**PC1a**	0.01292513
14	**PC1b**	0.01258271
15	**PC2a**	0.01150485
16	**PC2b**	0.01129716
17	**PC3a**	0.01136321
18	**PC3b**	0.01131811
19	**PC4**	0.01305098
20	**PC5**	0.01274914
21	**PC6**	0.01340023
22	**P1**	0.01328370
23	**P2**	0.01166460
24	**P3**	0.01174922
25	**P4**	0.01370887
26	**P5**	0.01327101
27	**P6**	0.01718661
28	H_2O	0.00652040

Table S3: Calculated global rate constants, k_{tot}, of the THFA + •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.

T (K)	0.76 Torr	7.6 Torr	76 Torr	760 Torr	7,600 Torr	76,000 Torr
200	8.77E-11	9.03E-11	9.85E-11	1.52E-10	3.02E-10	3.86E-10
240	5.07E-11	5.35E-11	5.68E-11	7.62E-11	1.74E-10	3.42E-10
298	**2.35E-11**	**2.44E-11**	**2.62E-11**	**3.02E-11**	**4.56E-11**	**1.45E-10**
300	2.29E-11	2.38E-11	2.56E-11	2.93E-11	4.35E-11	1.37E-10
400	7.08E-12	7.25E-12	7.51E-12	8.03E-12	8.84E-12	1.21E-11
440	4.73E-12	4.79E-12	4.92E-12	5.17E-12	5.59E-12	7.47E-12
500	2.75E-12	2.79E-12	2.84E-12	2.92E-12	3.07E-12	3.91E-12
600	1.36E-12	1.36E-12	1.36E-12	1.40E-12	1.43E-12	1.66E-12
700	8.63E-13	8.69E-13	8.69E-13	8.80E-13	8.85E-13	9.69E-13
800	7.22E-13	7.18E-13	7.19E-13	7.27E-13	7.29E-13	7.50E-13
900	7.47E-13	7.40E-13	7.40E-13	7.42E-13	7.34E-13	7.52E-13
1000	8.60E-13	8.57E-13	8.67E-13	8.69E-13	8.65E-13	8.67E-13
1100	1.06E-12	1.06E-12	1.06E-12	1.05E-12	1.06E-12	1.06E-12
1200	1.31E-12	1.32E-12	1.31E-12	1.32E-12	1.32E-12	1.31E-12
1300	1.63E-12	1.64E-12	1.64E-12	1.64E-12	1.64E-12	1.64E-12
1400	2.02E-12	2.01E-12	2.01E-12	2.01E-12	2.01E-12	2.01E-12
1500	2.45E-12	2.46E-12	2.45E-12	2.45E-12	2.45E-12	2.45E-12
1600	2.96E-12	2.97E-12	2.94E-12	2.96E-12	2.96E-12	2.95E-12
1700	3.53E-12	3.52E-12	3.51E-12	3.50E-12	3.53E-12	3.53E-12
1800	4.17E-12	4.15E-12	4.13E-12	4.15E-12	4.16E-12	4.16E-12
1900	4.86E-12	4.87E-12	4.86E-12	4.86E-12	4.87E-12	4.87E-12
2000	5.61E-12	5.63E-12	5.62E-12	5.62E-12	5.64E-12	5.61E-12

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

T (K)	via TS1a	via TS1b	via TS2a	via TS2b	via TS3a	via TS3b	via TS4	via TS5	via TS6
200	4.38	4.24	6.54	2.69	12.30	10.90	2.54	6.24	1330.00
240	2.64	2.57	3.42	2.08	5.17	5.44	1.87	3.31	143.00
298	**1.84**	**1.80**	**2.16**	**1.66**	**2.78**	**3.08**	**1.49**	**2.11**	**23.40**
300	1.82	1.79	2.13	1.65	2.74	3.04	1.48	2.09	22.40
400	1.40	1.38	1.52	1.35	1.75	1.91	1.25	1.50	5.55
440	1.32	1.30	1.42	1.29	1.59	1.72	1.20	1.40	4.12
500	1.24	1.23	1.31	1.22	1.43	1.53	1.15	1.30	3.00
600	1.16	1.16	1.21	1.15	1.29	1.35	1.11	1.20	2.17
700	1.12	1.11	1.15	1.11	1.21	1.26	1.08	1.15	1.79
800	1.09	1.09	1.12	1.08	1.16	1.20	1.06	1.11	1.57
900	1.07	1.07	1.09	1.06	1.13	1.15	1.05	1.09	1.44
1000	1.06	1.06	1.08	1.05	1.10	1.13	1.04	1.07	1.35
1100	1.05	1.05	1.06	1.04	1.09	1.10	1.03	1.06	1.29
1200	1.04	1.04	1.05	1.03	1.07	1.09	1.03	1.05	1.25
1300	1.04	1.03	1.05	1.03	1.06	1.08	1.02	1.04	1.21
1400	1.03	1.03	1.04	1.02	1.05	1.07	1.02	1.04	1.18
1500	1.03	1.03	1.04	1.02	1.05	1.06	1.02	1.03	1.16
1600	1.02	1.02	1.03	1.02	1.04	1.05	1.02	1.03	1.14
1700	1.02	1.02	1.03	1.02	1.04	1.05	1.01	1.03	1.13
1800	1.02	1.02	1.03	1.01	1.03	1.04	1.01	1.02	1.12
1900	1.02	1.02	1.02	1.01	1.03	1.04	1.01	1.02	1.11
2000	1.02	1.02	1.02	1.01	1.03	1.03	1.01	1.02	1.10

Table S5: Calculated overall rate constants, k_{tot}, of the THFA + •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)	THFA + •OH → products (k_tot)		HIR factor
	With HIR	Without HIR	
200	1.52E-10	1.58E-10	0.97
240	7.62E-11	8.27E-11	0.92
298	3.02E-11	3.45E-11	0.88
300	2.93E-11	3.36E-11	0.87
400	8.03E-12	9.83E-12	0.82
440	5.17E-12	6.42E-12	0.81
500	2.92E-12	3.72E-12	0.79
600	1.40E-12	1.88E-12	0.74
700	8.80E-13	1.27E-12	0.69
800	7.27E-13	1.14E-12	0.64
900	7.42E-13	1.22E-12	0.61
1000	8.69E-13	1.46E-12	0.60
1100	1.05E-12	1.84E-12	0.57
1200	1.32E-12	2.30E-12	0.57
1300	1.64E-12	2.86E-12	0.57
1400	2.01E-12	3.53E-12	0.57
1500	2.45E-12	4.31E-12	0.57
1600	2.96E-12	5.19E-12	0.57
1700	3.50E-12	6.22E-12	0.56
1800	4.15E-12	7.36E-12	0.56
1900	4.86E-12	8.65E-12	0.56
2000	5.62E-12	1.01E-11	0.56

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

thfa C 5O 2H 10 G 300.000 2500.000 1500.000 1
1.44199204E+003-2.96098649E+0002.27953884E-003-7.73336656E-0079.75468362E-011 2
-5.59798200E+005-7.77553111E+0032.27636269E+001-6.72883380E-0021.41364688E-004 3
-1.20425233E-0073.53843552E-011-1.29649011E+0041.25759690E+001 4
p1 C 5O 2H 9 G 300.000 2500.000 1500.000 1
9.76336354E+002-1.97303482E+0001.49337881E-003-4.96199789E-0076.11009829E-011 2
-3.79575041E+005-5.24219352E+0031.29651612E+001-1.05110008E-0022.14023222E-005 3
-1.71937639E-0084.69909471E-012-6.86470688E+0034.79093292E+001 4
p2 C 5O 2H 9 G 300.000 2500.000 1500.000 1
4.58337269E+002-8.79559832E-0016.43619042E-004-2.08036706E-0072.50869870E-011 2
-1.86172719E+005-2.41657602E+0031.69126261E+001-3.92445375E-0028.99152215E-005 3
-8.15139153E-0082.50976841E-011-6.75152985E+0033.16654172E+001 4
p3 C 5O 2H 9 G 300.000 2500.000 1500.000 1
1.05087061E+001-4.75154370E-0027.51089246E-005-3.87170602E-0086.53555595E-012 2
2.92713672E+0038.30205727E+0018.83906782E+0001.32182348E-002-2.13620872E-005 3
1.22232083E-008-2.18572969E-012-5.80275788E+0036.62516170E+001 4
p4 C 5O 2H 9 G 300.000 2500.000 1500.000 1
4.07768231E+002-8.18885324E-0016.22518210E-004-2.06801311E-0072.53603892E-011 2
-1.57564323E+005-2.11580696E+0031.29214888E+001-8.93141752E-0031.53177141E-005 3
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p5 C 5O 2H 9 G 300.000 2500.000 1500.000 1
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1.33650537E-008-3.65793656E-012-6.18738122E+0036.65164109E+001 4
p6 C 5O 2H 9 G 300.000 2500.000 1500.000 1
3.52734594E+002-6.66045515E-0014.78394630E-004-1.50174932E-0071.73978299E-011 2
-1.42758161E+005-1.83156433E+0031.32172358E+001-1.19744701E-0022.28259825E-005 3
-1.86970333E-0085.60636335E-012-5.18509133E+0034.98886498E+001 4
h H 1 G 300.000 2500.000 1500.000 1
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6.09430563E+003-7.42447376E-0035.96967320E-0018.73608570E-007-1.71249373E-009 3
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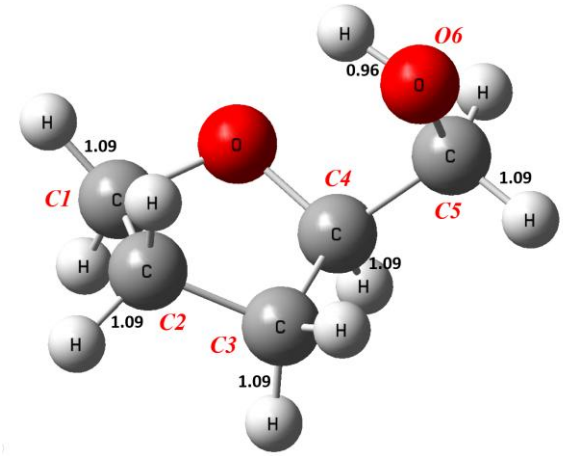
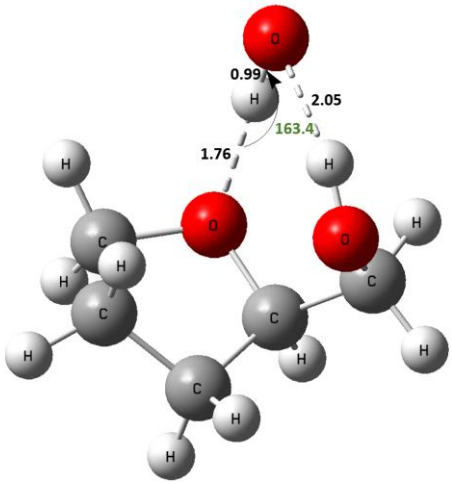
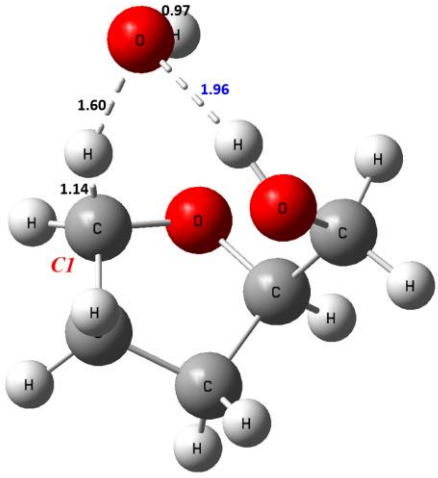
-1.02419927E+003-2.47784756E+0011.10615246E+000-2.24996554E-0045.51410556E-007 3
-5.35349385E-0101.76874109E-0138.13989365E+0021.36953152E+000 4
h2o O 1H 2 G 300.000 2500.000 1500.000 1
-3.38999858E+0017.22984856E-002-5.45933831E-0051.81609996E-008-2.24679443E-012 2
6.59630499E+0031.99083965E+0021.63301321E+0002.91315042E-004-7.69280969E-007 3
8.12651090E-010-2.87529901E-013-7.26567317E+0033.71963447E+000 4



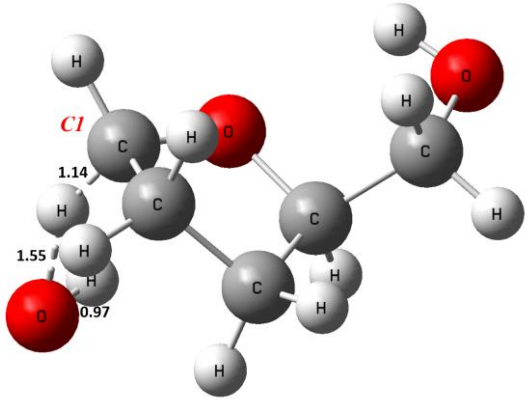
THFA



reactant-complex (RC)



TS1a



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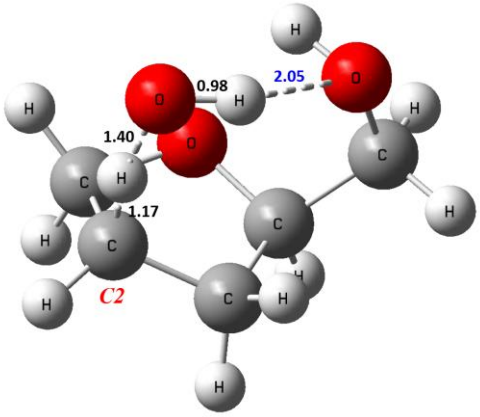
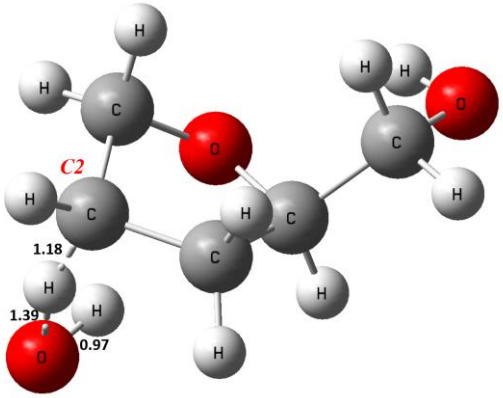


TS2a



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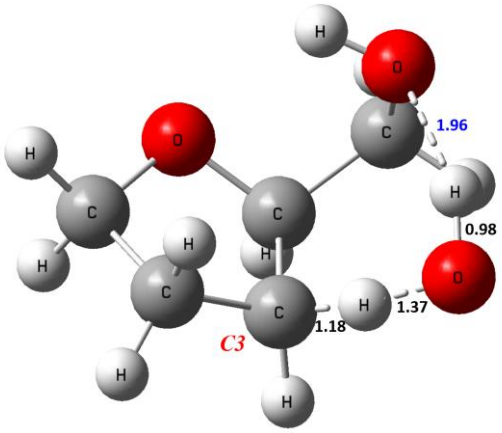

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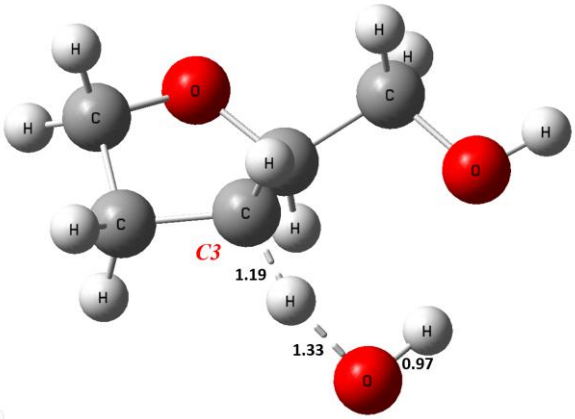

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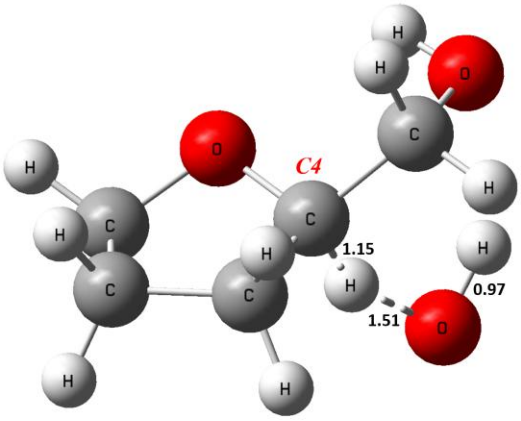

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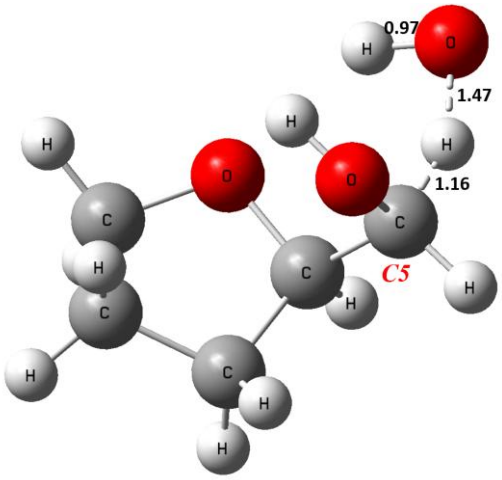

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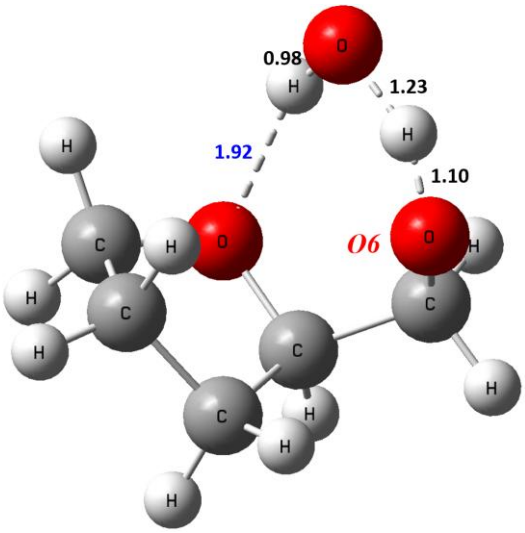

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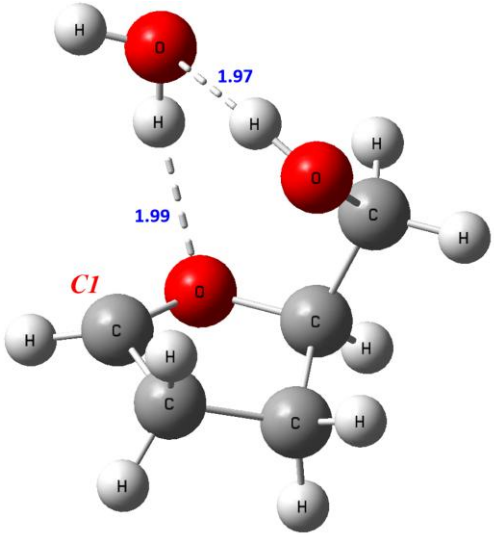

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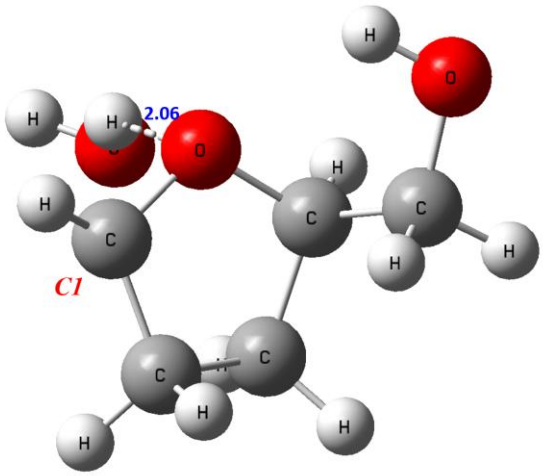

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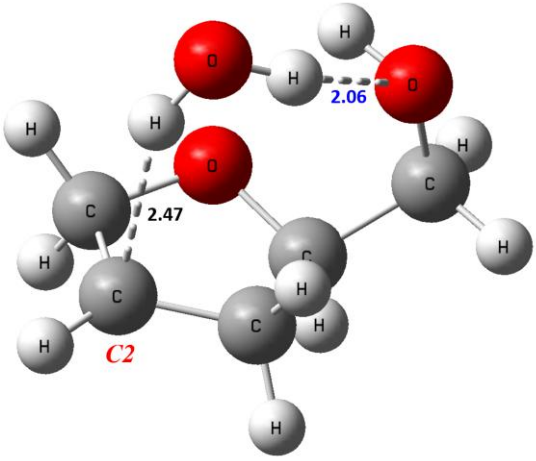

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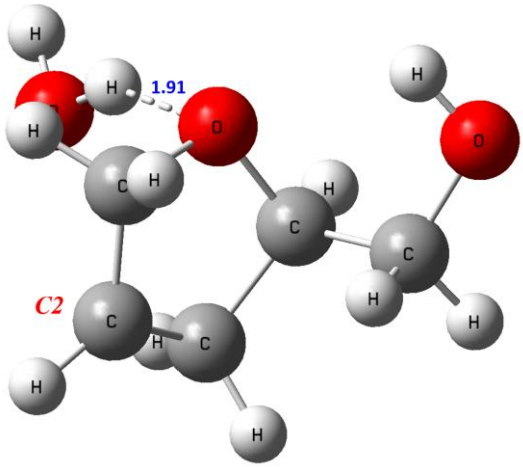

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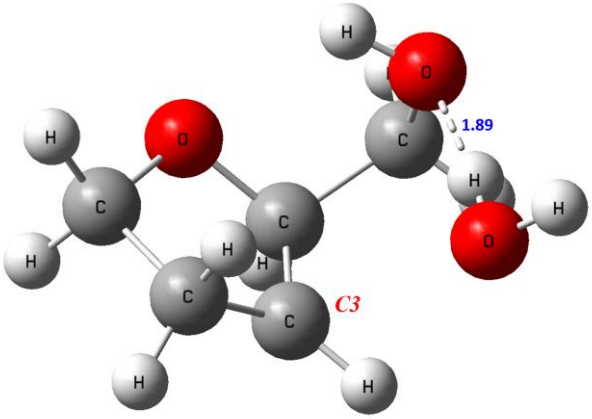

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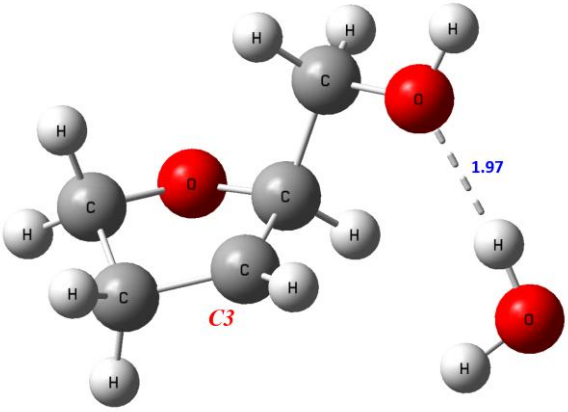

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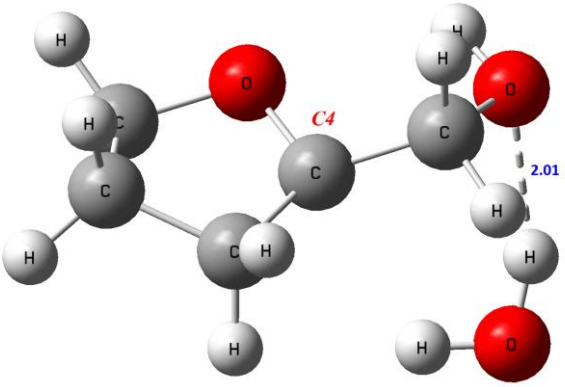

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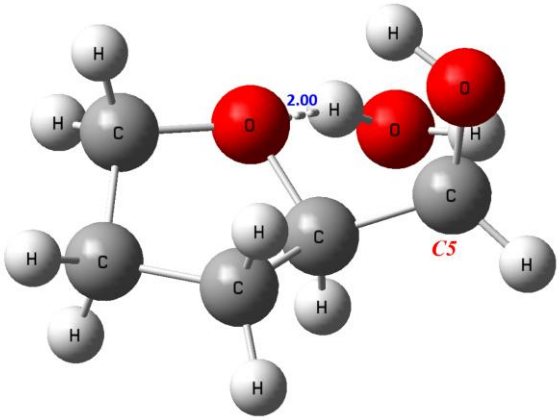

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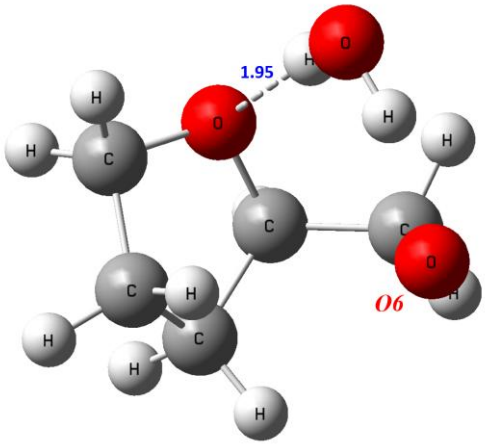

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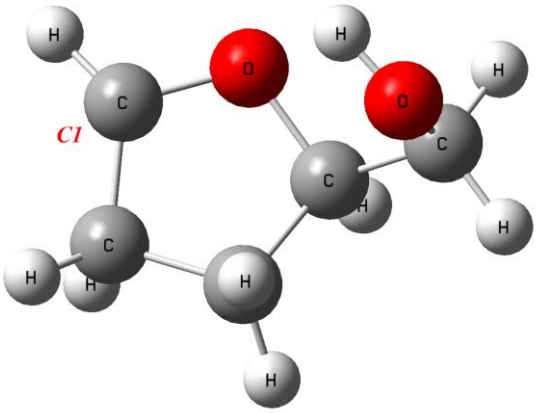

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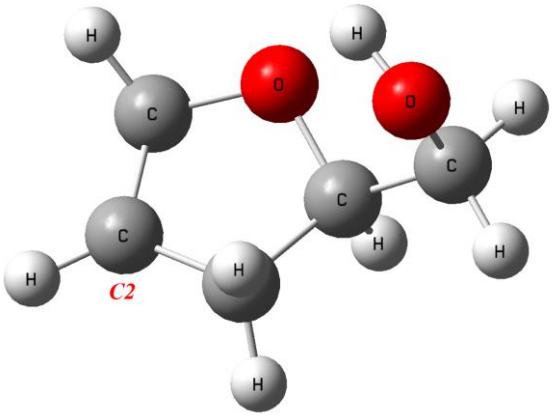

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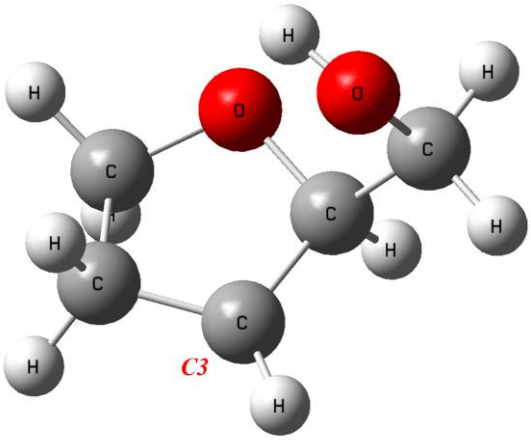

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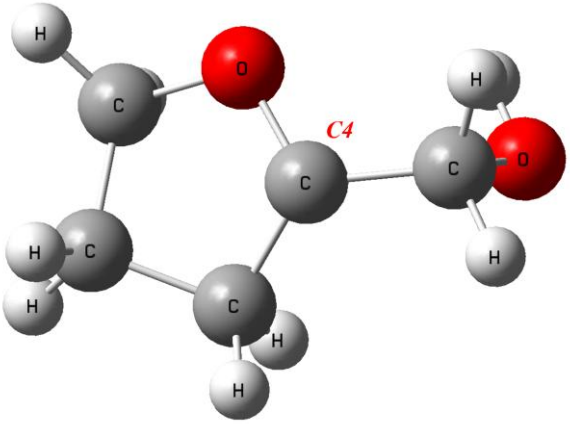

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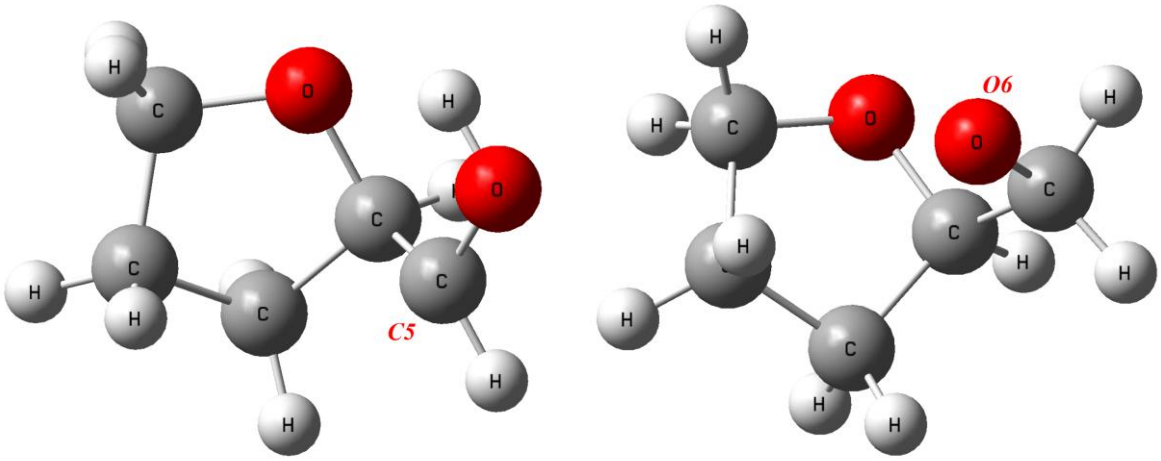
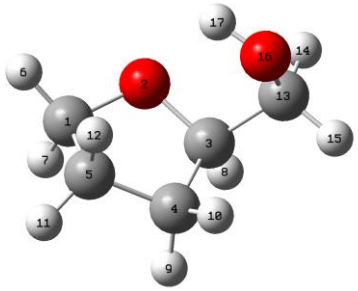
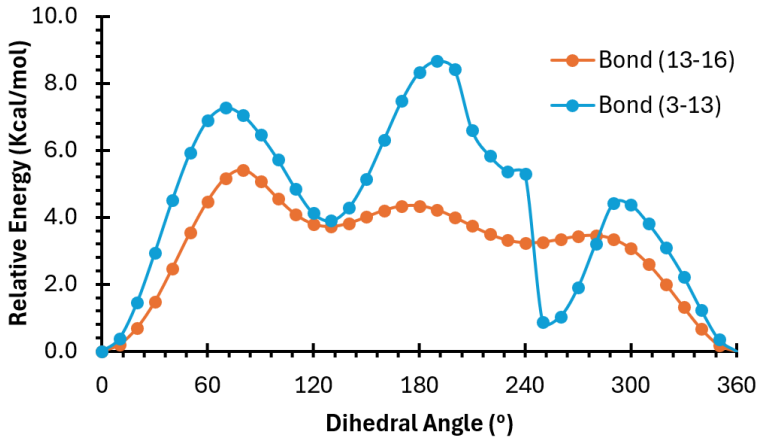
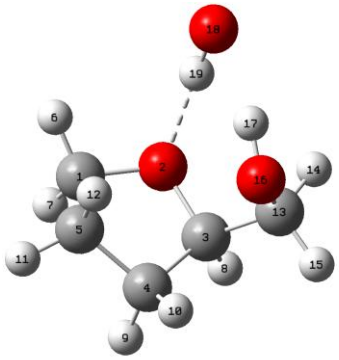
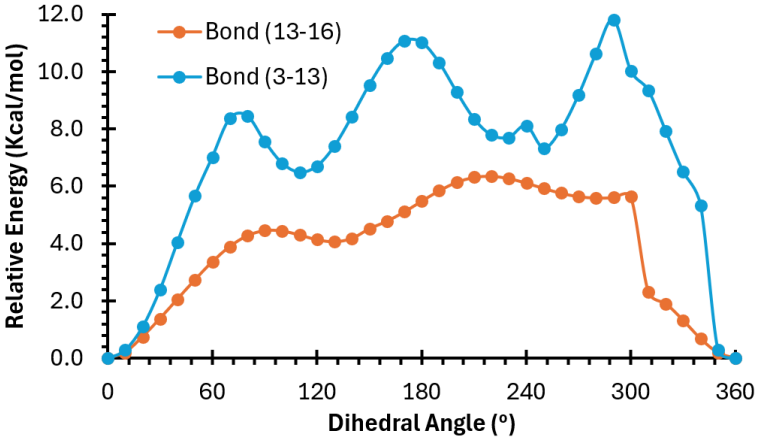
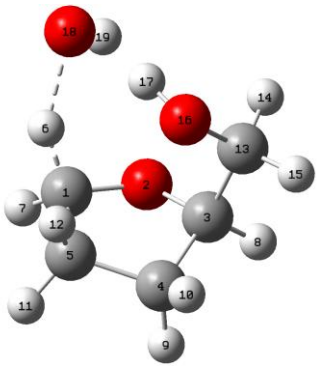
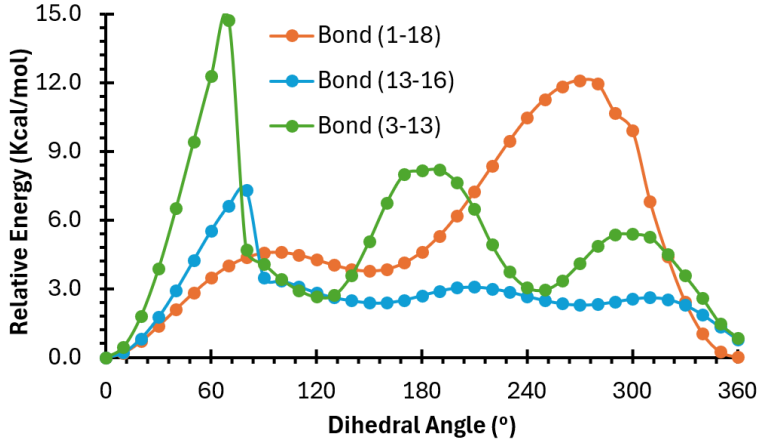
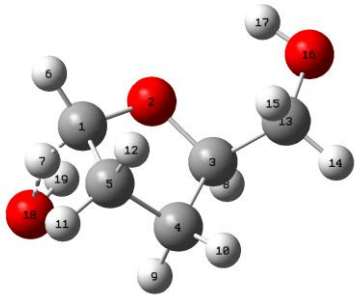


P5 **P6**

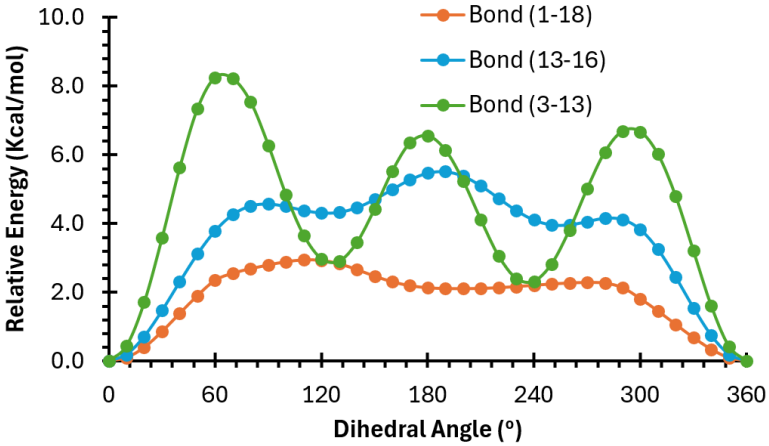
•OH **H_2O**

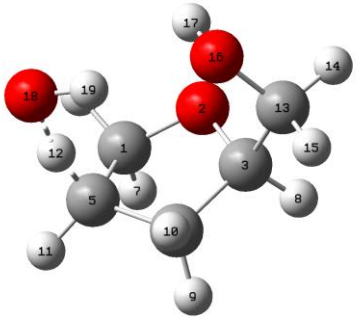
Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the title reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree (°), respectively.

Species	Potential energy surfaces for the internal rotations
 **THFA**	
 **RC**	
 **TS1a**	



TS1b





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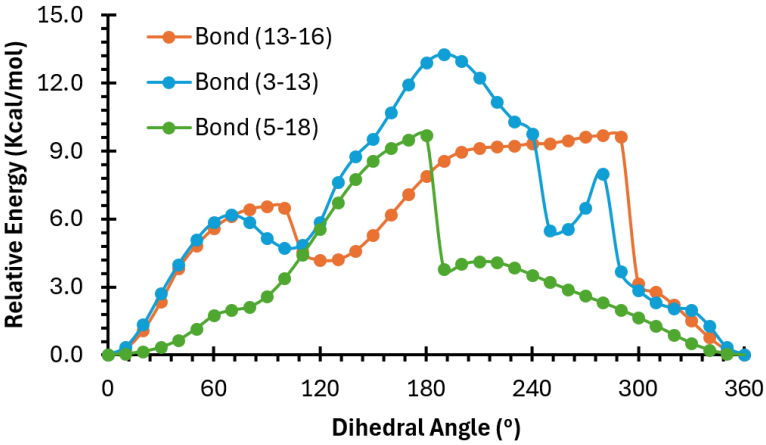

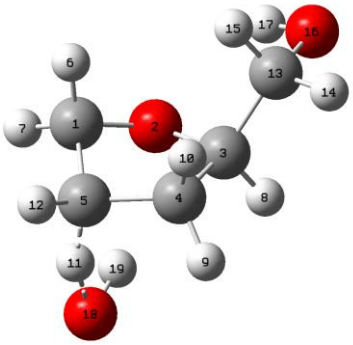

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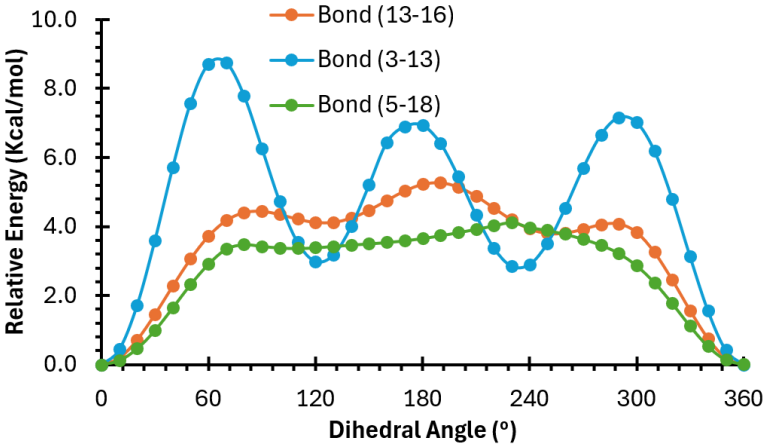

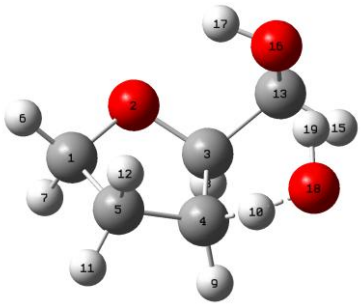

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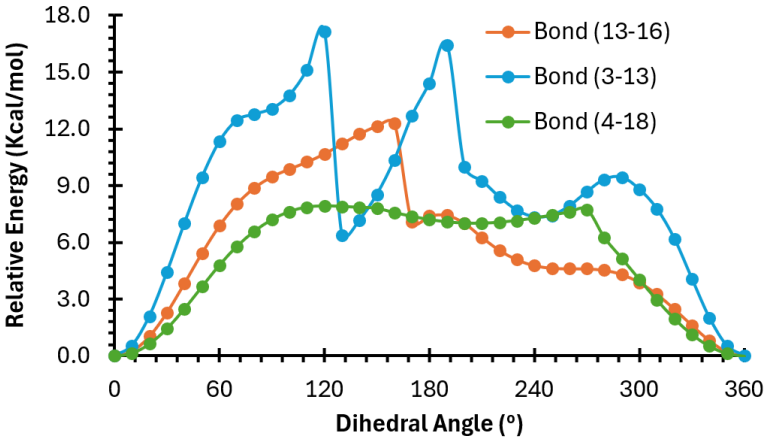

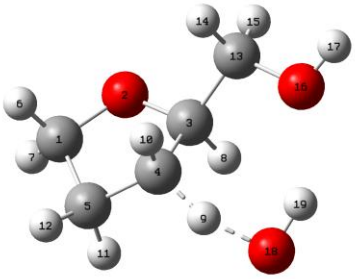

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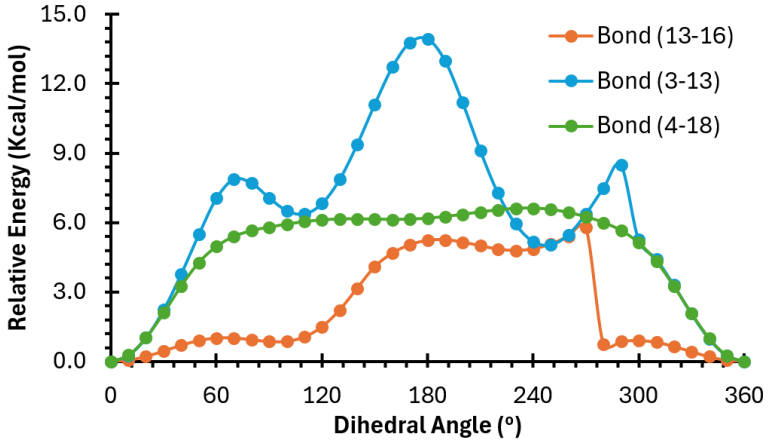

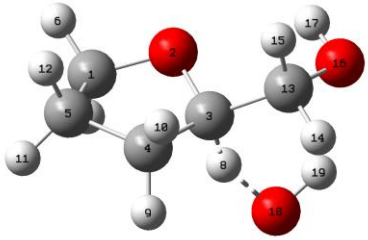

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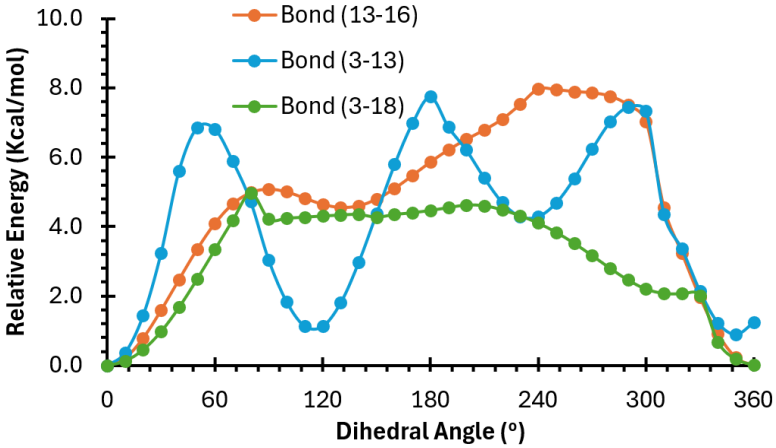

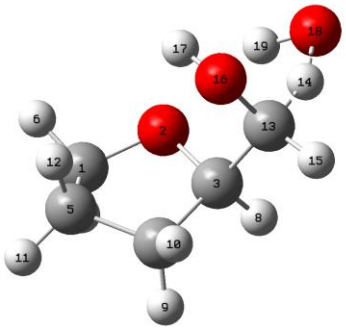

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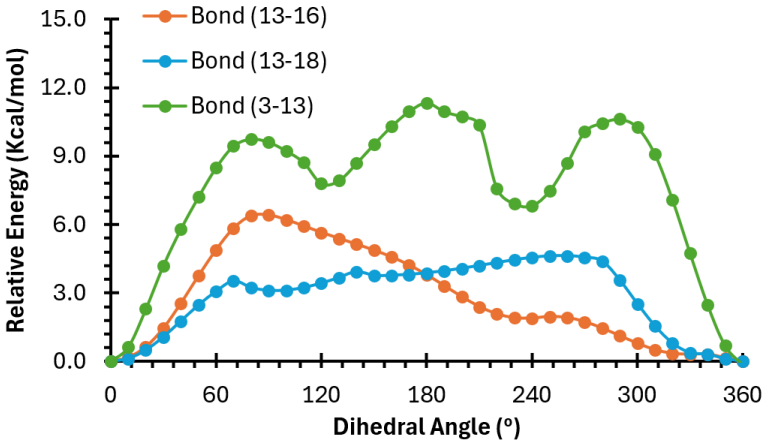
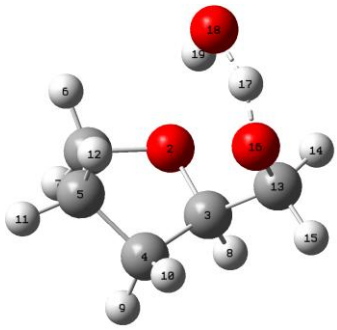
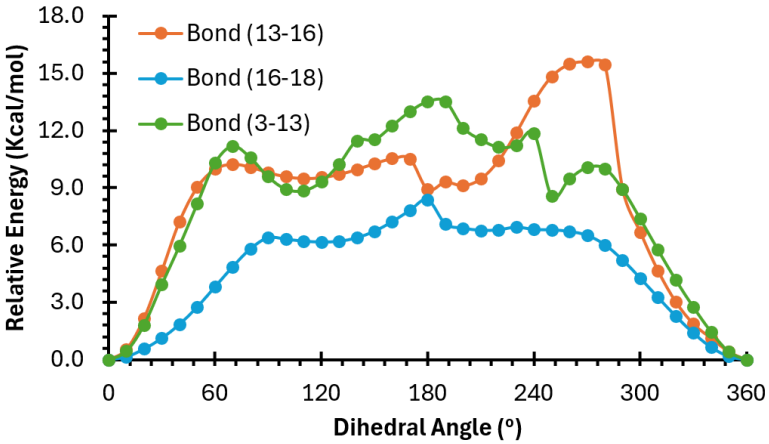
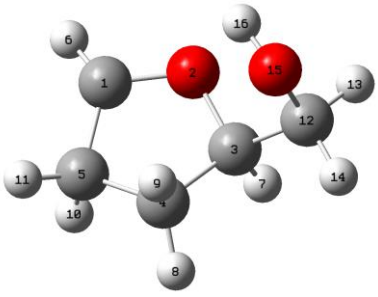

Bond (13-16)
Bond (13-18)
Bond (3-13)
Relative Energy (Kcal/mol)
15.0
12.0
9.0
6.0
3.0
0.0
0
60
120
180
240
300
360
Dihedral Angle (°)

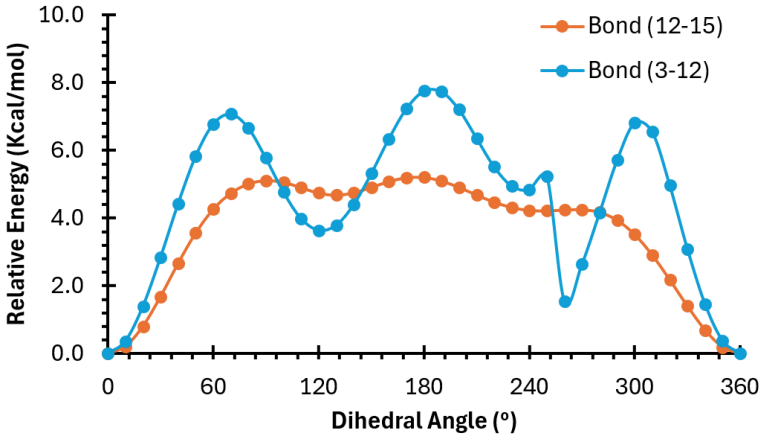


TS6


Bond (13-16)
Bond (16-18)
Bond (3-13)
Relative Energy (Kcal/mol)
18.0
15.0
12.0
9.0
6.0
3.0
0.0
0
60
120
180
240
300
360
Dihedral Angle (°)



P1


Bond (12-15)
Bond (3-12)
Relative Energy (Kcal/mol)
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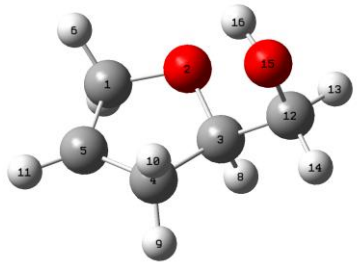
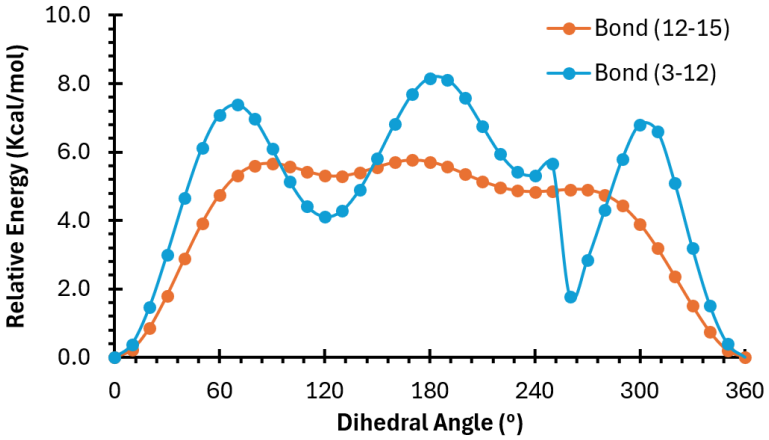
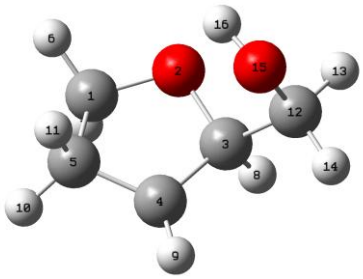
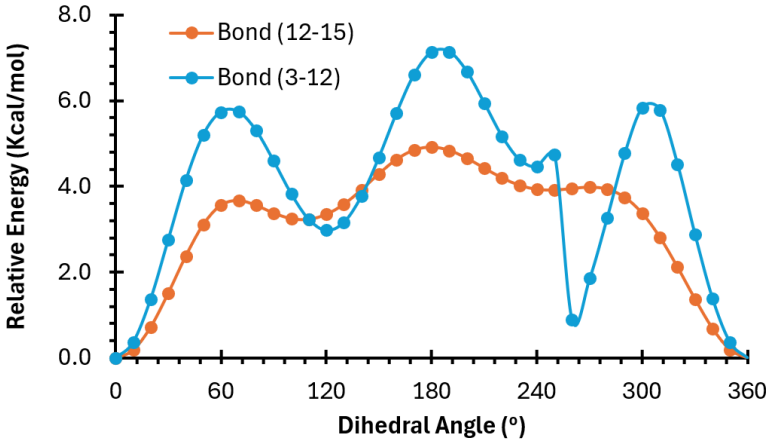
6.0
4.0
2.0
0.0
0
60
120
180
240
300
360
Dihedral Angle (°)




Bond (12-15)
Bond (3-12)
Relative Energy (Kcal/mol)
10.0
8.0
6.0
4.0
2.0
0.0
0
60
120
180
240
300
360
Dihedral Angle (°)

P2




Bond (12-15)
Bond (3-12)
Relative Energy (Kcal/mol)
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6.0
4.0
2.0
0.0
0
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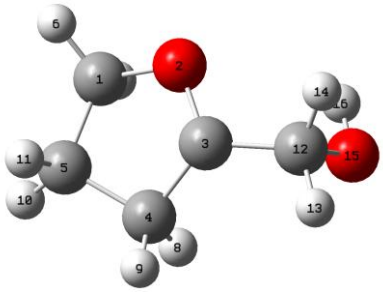
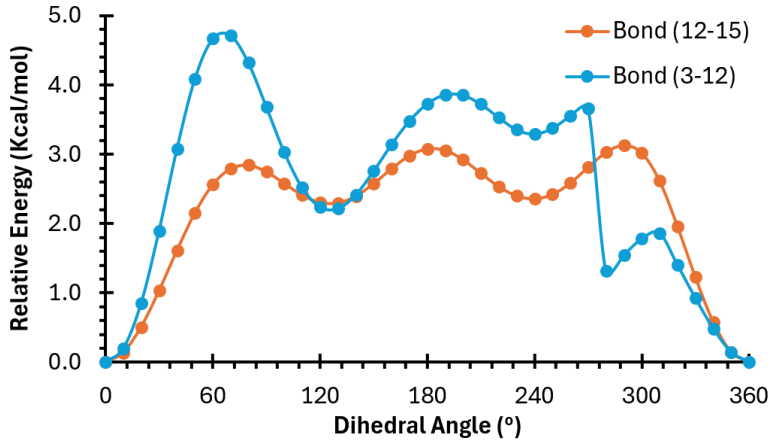
120
180
240
300
360
Dihedral Angle (°)

P3




Bond (12-15)
Bond (3-12)
Relative Energy (Kcal/mol)
5.0
4.0
3.0
2.0
1.0
0.0
0
60
120
180
240
300
360
Dihedral Angle (°)

P4

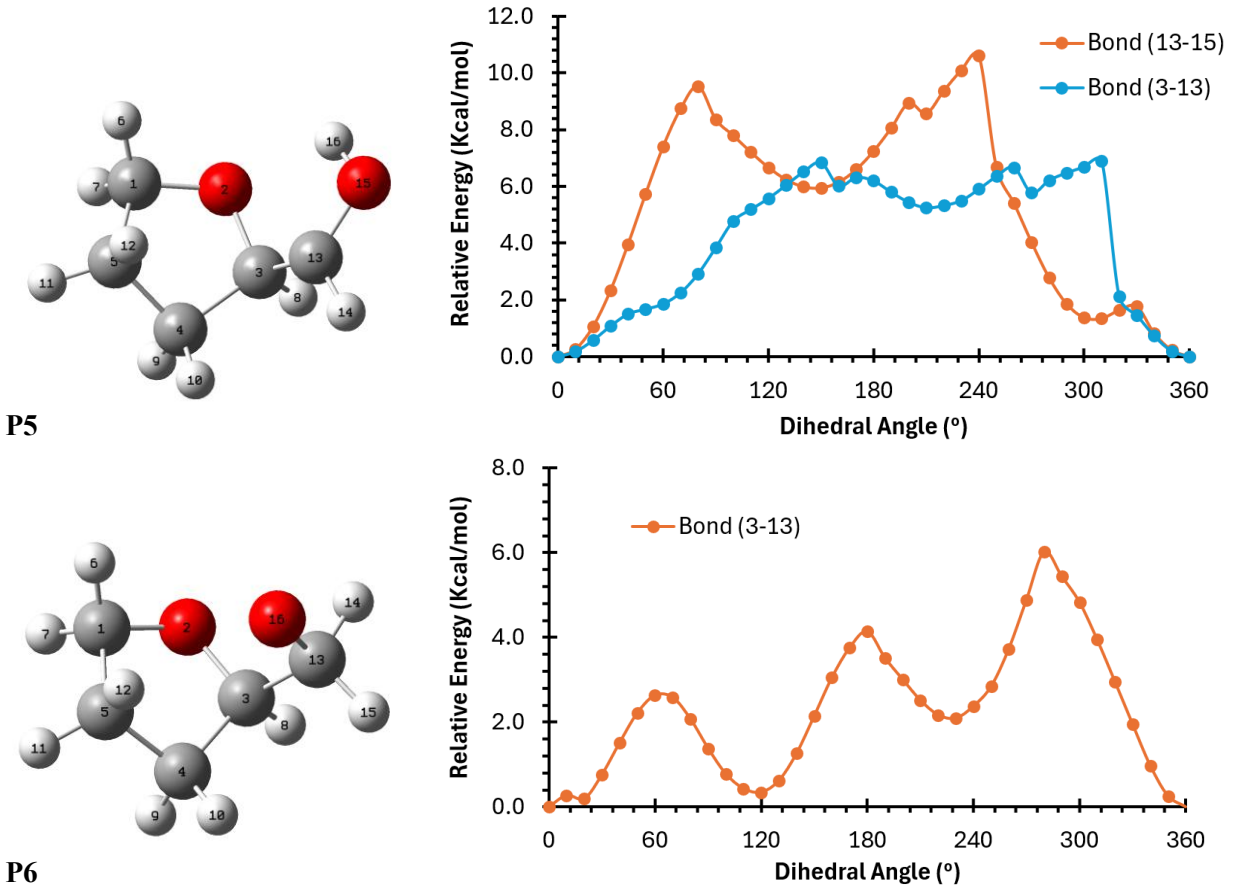


Figure S2: Hindrance potentials for the species involved in the THFA + •OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

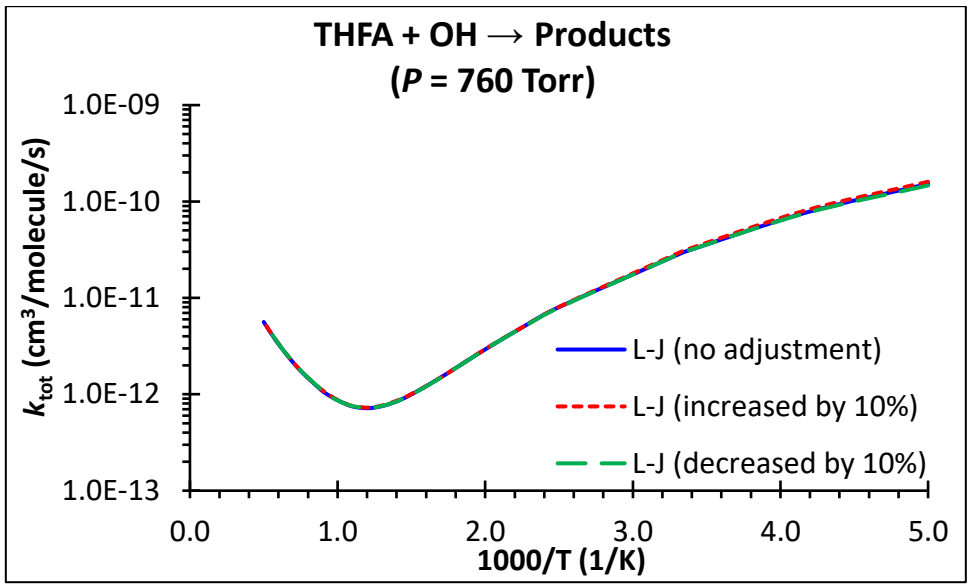


Figure S3: Calculated total rate constants for the reaction between THFA and •OH radicals with and without adjustment of the Lennard-Jones (L-J) parameters at 760 Torr.

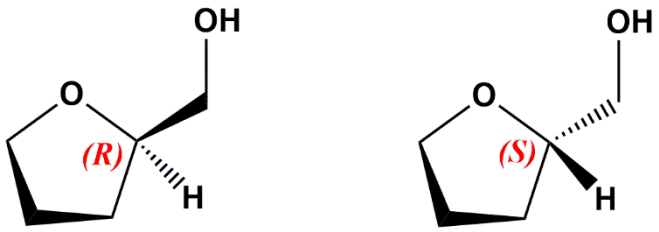


Figure S4: Structures of the two enantiomers of THFA: the (*R*) conformer (a) and the (*S*) conformer (b).

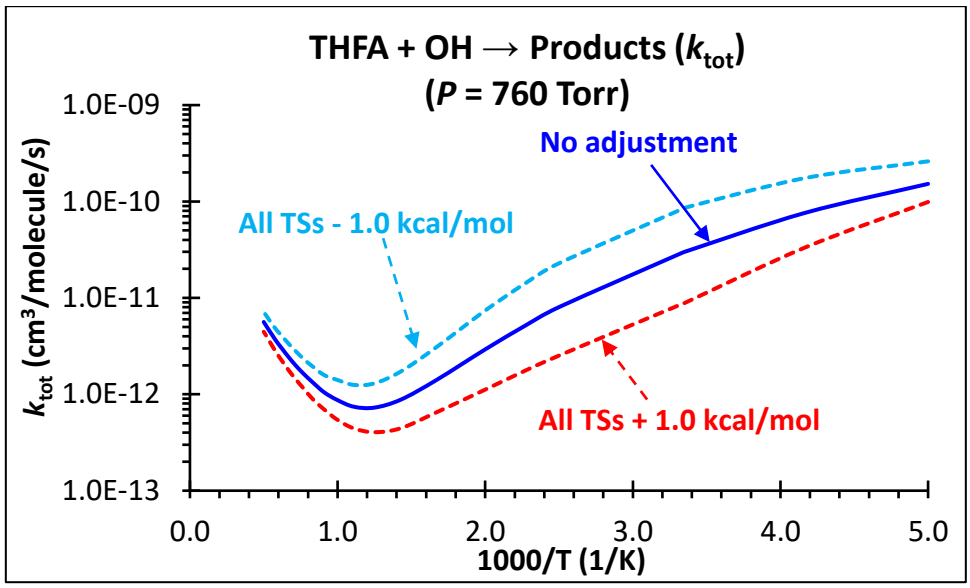


Figure S5: Predicted total rate constant (k_{tot}) for the reaction of THFA with •OH radicals at 760 Torr, calculated without barrier adjustment and with all barrier heights varied by ±1.0 kcal/mol.