Supplementary Information

Reaction Kinetics of 1,4-Cyclohexadienes with OH radicals: Part I. An Experimental and Theoretical Study

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Table S1: Optimized geometries, rotational constants (GHz), 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 M06-2X/aug-cc-pVTZ level of theory for the title reaction.

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
OH ($C_{\infty v}$)	8	0.000000000	0.000000000	0.107999000	564.211029	-75.733789	0.008530	3742.0378 (3737.8)[1]		
	1	0.000000000	0.000000000	-0.863995000						
H_2O (C_{2v})	8	0.000000000	0.000000000	0.116332000	834.47311	-76.4300922	0.021565	1615.7190	3873.1681	3977.2474
	1	0.000000000	0.762680000	-0.465326000	431.04032			(1595.0; 3657.0[2]; 3756.0[1])		
	1	0.000000000	-0.762680000	-0.465326000	284.22579					
H ($D_{\infty h}$)	1	1.216198000	-1.008264000	0.000000000	/	-0.498207	0.00000	/		
14CHD (D_{2h})	6	0.662714000	1.248273000	0.000039000	5.19892	-233.391815	0.123092	120.2293	389.9917	415.4630
	6	-0.662714000	1.248273000	-0.000016000	4.94389			541.8477	579.8579	635.9665
	6	-1.493271000	0.000000000	-0.000061000	2.61366			731.4655	873.8115	905.1970
	6	-0.662714000	-1.248273000	-0.000040000				961.1601	967.1537	974.9870
	6	0.662714000	-1.248273000	0.000015000				992.8766	1021.5142	1039.9698
	6	1.493271000	0.000000000	0.000063000				1051.2751	1176.4052	1227.2242
	1	-2.161712000	-0.000008000	0.867632000				1230.6402	1230.8702	1366.3316
	1	-1.194524000	2.192590000	-0.000031000				1392.9875	1417.6612	1441.6111
	1	1.194524000	2.192590000	0.000070000				1474.0635	1477.1235	1734.1692
	1	-1.194524000	-2.192590000	-0.000073000				1780.3398	3029.4932	3031.3341
	1	1.194524000	-2.192590000	0.000027000				3043.7916	3045.1906	3171.0332
	1	2.161640000	-0.000008000	0.867812000				3171.3025	3192.5942	3194.3053
	1	2.161716000	0.000008000	-0.867627000						
	1	-2.161644000	0.000008000	-0.867807000						
RC (C_s)	6	-0.636695000	0.664414000	-1.036871000	2.89060	-309.135752	0.134257	78.7539	78.9420	138.1434
	6	-0.636650000	-0.664486000	-1.036856000	2.51017			145.8412	336.0845	386.9745
	6	0.380957000	-1.494025000	-0.313428000	2.24494			415.2247	513.1466	542.1583
	6	1.324438000	-0.663910000	0.506443000				580.2514	646.3938	741.8548
	6	1.324392000	0.664006000	0.506428000				872.9647	905.7025	954.0078
	6	0.380854000	1.494039000	-0.313461000				957.9271	983.9148	993.5833
	1	-0.130841000	-2.218237000	0.328460000				1022.1280	1044.1668	1050.3100
	1	-1.413770000	-1.196407000	-1.571543000				1177.4284	1227.4712	1227.7715
	1	-1.413853000	1.196270000	-1.571568000				1228.5405	1365.9759	1389.9499
	1	2.040658000	-1.195646000	1.121900000				1417.1172	1443.0305	1469.4024
	1	2.040577000	1.195805000	1.121872000				1472.5426	1717.3631	1767.5658

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	-0.130993000	2.218230000	0.328411000				3031.8906	3034.1166	3051.1187
	1	0.948504000	2.098863000	-1.028775000				3052.5664	3172.3936	3180.6209
	1	0.948647000	-2.098828000	-1.028727000				3193.6316	3201.0956	3722.0672
	8	-1.851692000	-0.000031000	1.358111000						
	1	-0.899170000	-0.000035000	1.561549000						
I1	6	0.126683000	-1.239431000	-0.624268000	3.77907	-309.178190	0.137374	113.9622	139.8964	323.6166
(C_1)	6	1.131570000	-0.170195000	-0.358615000	2.89003			340.6083	387.2436	398.4954
	6	0.524325000	1.210111000	-0.601837000	2.15267			531.7447	553.1161	605.1359
	6	-0.816273000	1.336293000	0.070732000				679.9324	828.5189	882.7320
	6	-1.586878000	0.291258000	0.350018000				917.1201	921.7145	926.0921
	6	-1.221512000	-1.124492000	0.000206000				975.1250	1022.5165	1046.4665
	1	1.213288000	1.967560000	-0.225601000				1063.6413	1122.7672	1177.6640
	1	0.451768000	-2.197453000	-1.003292000				1188.7670	1206.4658	1261.1318
	1	-1.157683000	2.330851000	0.331650000				1330.6251	1353.4568	1386.6947
	1	-2.540668000	0.443852000	0.840991000				1394.8447	1418.3153	1431.1656
	1	-1.283426000	-1.746835000	0.905344000				1458.1022	1471.2195	1741.3703
	1	-1.984936000	-1.541006000	-0.665658000				2976.6315	3037.1971	3051.4494
	1	0.417876000	1.380792000	-1.676998000				3100.0480	3116.1772	3175.0784
	1	2.011035000	-0.306973000	-0.984624000				3196.6149	3207.9340	3838.8114
	8	1.628244000	-0.261759000	0.985031000						
	1	0.899306000	-0.057979000	1.580521000						
TS1	6	0.413681000	-1.058210000	-0.696044000	3.43546	-309.132935	0.134443	-294.0800	89.1048	113.7140
(C_1)	6	0.918253000	0.186824000	-0.807958000	2.61607			197.4673	286.3076	359.7016
	6	0.130067000	1.417721000	-0.483160000	2.07407			409.9393	541.6616	579.0386
	6	-1.134702000	1.110426000	0.262129000				661.1916	723.5485	762.7477
	6	-1.600857000	-0.118647000	0.439774000				874.0541	907.6573	936.7455
	6	-0.920472000	-1.347073000	-0.088351000				957.5901	981.5821	988.5633
	1	0.756562000	2.099196000	0.096211000				1005.7771	1033.9926	1051.9605
	1	1.017399000	-1.901684000	-1.003499000				1174.6681	1218.3837	1222.4236
	1	-1.685702000	1.952071000	0.664305000				1224.8567	1364.9569	1390.1698
	1	-2.524897000	-0.266082000	0.985746000				1418.9421	1442.6822	1464.3155
	1	-0.802330000	-2.086126000	0.711290000				1467.3640	1642.9573	1757.7024
	1	-1.563254000	-1.839261000	-0.827517000				3025.3079	3031.8410	3043.7158
	1	-0.107822000	1.951075000	-1.410456000				3079.9361	3176.3729	3197.5956
	1	1.879990000	0.326530000	-1.280633000				3200.8819	3222.3278	3783.6919
	8	1.890118000	-0.157968000	1.087261000						
	1	1.073287000	-0.118220000	1.608135000						

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
TS2	6	-0.259301000	-1.212262000	-0.119152000	4.77804	-309.120049	0.130046	-1006.1226	132.6895	213.7824
(C_1)	6	-0.952586000	-0.061583000	0.042997000	2.44084			370.1151	393.2425	398.9723
	6	-0.327888000	1.296610000	-0.088501000	1.68804			461.6678	546.2519	550.8392
	6	1.166645000	1.237978000	-0.012941000				571.0416	616.8243	685.4050
	6	1.855414000	0.106714000	0.021967000				776.9111	812.5900	911.9624
	6	1.230648000	-1.255230000	-0.023765000				944.8863	968.3843	978.3687
	1	-0.650495000	1.717067000	-1.047078000				987.4424	1030.9468	1072.8412
	1	-0.799535000	-2.151445000	-0.167721000				1188.8636	1198.2477	1219.1229
	1	1.690517000	2.185320000	0.014566000				1222.5396	1248.3862	1352.5532
	1	2.936321000	0.143267000	0.083693000				1380.7895	1426.3611	1454.1705
	1	1.645064000	-1.820027000	-0.865114000				1469.2029	1477.2337	1657.7741
	1	1.528222000	-1.817442000	0.870450000				1760.7001	3011.4363	3041.1153
	1	-0.732775000	1.954948000	0.682117000				3043.1342	3088.6156	3171.9951
	1	-0.707438000	-0.100623000	1.806346000				3180.4043	3202.0873	3863.6675
	8	-2.312353000	0.011050000	-0.038587000						
	1	-2.688645000	-0.872825000	0.007807000						
TS3	6	-0.141046000	-1.311090000	0.314730000	3.99166	-309.113312	0.129465	-844.6039	122.8731	180.5938
(C_1)	6	-1.095176000	-0.150833000	0.402454000	2.76508			320.5837	360.2265	370.3849
	6	-0.350001000	1.154330000	0.673580000	2.07499			384.2721	428.6019	520.8403
	6	0.882842000	1.298889000	-0.167600000				578.1326	634.0774	746.9246
	6	1.594466000	0.220176000	-0.487526000				805.4053	834.7763	896.6461
	6	1.139628000	-1.114363000	-0.064589000				957.2742	967.3781	979.9992
	1	-1.036159000	1.988744000	0.534272000				1013.6014	1035.4361	1078.0978
	1	-0.520690000	-2.306500000	0.501567000				1106.1672	1166.5252	1193.2699
	1	1.209802000	2.286448000	-0.465076000				1211.5598	1276.0494	1337.5329
	1	2.518013000	0.297825000	-1.044952000				1358.0556	1409.1403	1421.4775
	1	1.779767000	-1.963610000	-0.264337000				1441.1280	1455.0713	1615.0540
	1	2.058214000	-0.999686000	1.594815000				1715.5218	3015.9924	3105.5192
	1	-0.043509000	1.156233000	1.727853000				3118.0221	3190.2038	3198.5721
	1	-1.817634000	-0.314916000	1.200665000				3211.9475	3219.1521	3846.3048
	8	-1.881448000	-0.083033000	-0.784372000						
	1	-1.280494000	-0.062929000	-1.536131000						
TS4	6	-1.099759000	1.225165000	-0.181433000	3.74372	-309.126889	0.130724	-716.3404	40.8116	51.7741
(C_1)	6	0.047214000	1.208290000	0.487807000	1.86428			129.8218	173.4216	378.9077
	6	0.733240000	-0.049993000	0.894338000	1.55641			389.9807	542.0323	579.9945
	6	-0.025673000	-1.285000000	0.556777000				602.3382	706.0015	743.9677
	6	-1.174709000	-1.270505000	-0.108875000				878.2306	911.8644	934.1135
	6	-1.843532000	-0.014092000	-0.575215000				961.3892	976.7192	979.8550

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	1.744570000	-0.094147000	0.370010000				1019.8906	1040.8668	1049.1216
	1	0.532643000	2.141072000	0.747970000				1158.1881	1179.0271	1224.1264
	1	-1.543746000	2.174670000	-0.456064000				1224.8181	1358.9956	1388.7746
	1	0.403463000	-2.229603000	0.867057000				1418.5207	1422.3059	1443.3252
	1	-1.675233000	-2.205683000	-0.329753000				1468.1093	1711.6879	1728.8356
	1	-1.967357000	-0.042320000	-1.663783000				1901.8339	3028.3702	3042.8238
	1	-2.865278000	0.028671000	-0.182615000				3061.8548	3177.2376	3179.4419
	1	1.029971000	-0.027459000	1.946684000				3198.4031	3201.5673	3771.7810
	8	2.795390000	0.086257000	-0.795744000						
	1	2.115246000	0.353030000	-1.435808000						
TS5	6	0.128921000	-1.169246000	-0.087660000	4.87793	-309.119713	0.129002	-853.0439	69.3051	77.7894
(C_1)	6	0.719789000	0.007686000	-0.137986000	1.63390			147.1211	170.4055	348.8020
	6	0.053614000	1.339914000	-0.075094000	1.25179			405.4758	476.2843	541.4253
	6	-1.437915000	1.189022000	0.052026000				598.5933	682.0886	821.6555
	6	-2.060718000	0.019854000	0.088537000				852.1169	903.7732	925.1182
	6	-1.365608000	-1.307097000	0.011450000				961.2399	967.5303	988.0400
	1	0.447529000	1.917836000	0.766373000				996.2013	1030.9452	1042.4844
	1	1.895894000	0.028047000	-0.245051000				1123.7716	1200.9921	1214.6922
	1	0.719962000	-2.076757000	-0.128253000				1221.7978	1301.9718	1360.7983
	1	-2.014172000	2.104731000	0.113311000				1378.9959	1388.1803	1420.9828
	1	-3.140393000	-0.001042000	0.179197000				1472.2390	1476.9240	1739.4215
	1	-1.619563000	-1.912318000	0.887707000				1774.3334	3035.6639	3043.7182
	1	-1.740864000	-1.875355000	-0.845731000				3053.0511	3062.4498	3172.6422
	1	0.298701000	1.924509000	-0.966656000				3184.0300	3194.4791	3797.8762
	8	3.220805000	-0.036293000	0.022306000						
	1	3.157966000	-0.300112000	0.953014000						
PC1	6	0.352638000	1.247641000	0.725267000	2.72699	-309.2008493	0.132895	55.4810	76.6007	85.8495
(C_1)	6	0.771447000	1.222599000	-0.564865000	2.20254			135.2806	175.1516	178.3854
	6	0.987578000	0.001212000	-1.247045000	2.18784			302.7127	391.7633	529.9695
	6	0.772365000	-1.221321000	-0.566655000				562.2415	589.6042	647.1311
	6	0.353581000	-1.248558000	0.723438000				756.2443	799.4243	886.4499
	6	0.094497000	-0.001132000	1.505046000				941.1908	980.8251	990.8196
	1	-1.863498000	-0.756520000	-0.624544000				996.9878	999.8306	1004.0398
	1	0.946072000	2.154664000	-1.086813000				1098.7071	1166.8974	1197.8941
	1	0.196540000	2.194144000	1.225988000				1199.8520	1312.9177	1368.3029
	1	0.947730000	-2.152492000	-1.089951000				1423.5324	1430.7578	1458.6433
	1	0.198241000	-2.195904000	1.222802000				1564.8146	1627.3862	1631.3179
	1	-0.942874000	-0.001800000	1.870064000				2981.3618	2984.2644	3190.5730

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	1	0.698611000	-0.001569000	2.423588000				3191.7441	3208.3353	3209.0010
	1	1.319258000	0.002095000	-2.274054000				3236.3974	3843.6050	3922.0697
	8	-2.454048000	0.000042000	-0.562099000						
	1	-1.860330000	0.754404000	-0.621410000						
PC2	6	0.393040000	-0.845609000	0.000103000	4.85236	-309.1460101	0.133341	19.6452	56.9493	71.4658
(C_1)	6	0.509734000	0.457039000	0.000112000	1.37389			115.3761	130.7628	187.0332
	6	-0.523416000	1.510193000	0.000040000	1.09019			303.2638	379.0524	405.6544
	6	-1.889113000	0.858961000	-0.000060000				526.1507	576.3028	665.8073
	6	-2.079371000	-0.453033000	-0.000073000				784.5717	871.2722	921.3028
	6	-0.981982000	-1.477327000	0.000008000				924.7396	953.6637	967.2631
	1	-0.418041000	2.160127000	0.873113000				989.8267	1029.2506	1042.7027
	1	3.056271000	0.212948000	-0.755233000				1187.1785	1210.7599	1213.6924
	1	1.259225000	-1.499029000	0.000166000				1270.6710	1339.5927	1361.4736
	1	-2.742571000	1.526827000	-0.000122000				1411.7155	1471.8734	1474.4634
	1	-3.094063000	-0.833817000	-0.000146000				1625.1114	1738.2153	1772.0602
	1	-1.086039000	-2.132658000	0.870251000				3038.0609	3045.7021	3058.3879
	1	-1.085916000	-2.132665000	-0.870243000				3067.9973	3165.6511	3171.3175
	1	-0.417915000	2.160133000	-0.873013000				3193.1681	3851.9264	3938.7155
	8	3.612420000	0.002949000	-0.000078000						
	1	3.056341000	0.213196000	0.755061000						
P1	6	-0.277205000	-1.207823000	0.000000000	4.97278	-308.628811	0.127873	117.5750	250.3592	403.0228
(C_s)	6	-0.963313000	-0.071684000	0.000000000	2.48575			405.4914	414.0186	490.9710
	6	-0.345960000	1.287841000	0.000000000	1.69111			494.2340	568.4200	687.3755
	6	1.151438000	1.236245000	0.000000000				786.7911	822.3224	914.1331
	6	1.845663000	0.107867000	0.000000000				946.4181	977.1814	980.3807
	6	1.221554000	-1.254295000	0.000000000				985.4776	1032.9024	1073.2938
	1	-0.714489000	1.840405000	-0.870040000				1189.1257	1201.2903	1221.9194
	1	-0.812591000	-2.151767000	0.000000000				1227.8828	1249.7061	1352.4082
	1	1.671725000	2.186313000	-0.000001000				1382.3106	1427.3704	1457.2025
	1	2.928422000	0.149418000	-0.000001000				1476.4676	1482.1263	1746.6012
	1	1.582064000	-1.815609000	-0.868774000				1792.0985	3027.2432	3039.8463
	1	1.582064000	-1.815608000	0.868775000				3041.0150	3060.9644	3166.1934
	1	-0.714488000	1.840404000	0.870042000				3176.3917	3198.6173	3862.7573
	8	-2.327005000	0.007116000	0.000000000						
	1	-2.699729000	-0.879386000	0.000000000						
P2	6	-0.232097000	1.282079000	-0.441925000	4.11758	-308.620543	0.128084	125.6604	243.6844	310.4134
(C_1)	6	-1.085653000	0.040158000	-0.384644000	2.88515			370.6471	406.5724	526.5106
	6	-0.250208000	-1.221343000	-0.590234000	2.11699			574.6578	628.8995	727.7822

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\,K}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm^{-1})		
	6	1.061963000	-1.181274000	0.134086000				807.2136	834.4487	902.6028
	6	1.667968000	-0.016676000	0.366564000				956.2380	977.8928	983.3483
	6	1.042862000	1.240409000	-0.051426000				1016.0390	1025.0994	1079.1969
	1	-0.845345000	-2.083904000	-0.290040000				1108.6206	1169.7765	1200.6063
	1	-0.708070000	2.217781000	-0.704108000				1214.9097	1278.0798	1344.2357
	1	1.528521000	-2.113675000	0.424679000				1361.0997	1409.5683	1425.0225
	1	2.634198000	0.019104000	0.851646000				1444.4834	1455.9879	1671.9528
	1	1.633105000	2.146992000	-0.013468000				1733.1617	3027.5568	3107.0441
	1	-0.045648000	-1.332724000	-1.662009000				3109.9988	3188.6080	3195.1505
	1	-1.860352000	0.076249000	-1.148795000				3210.8045	3218.0908	3850.6383
	8	-1.799993000	0.008970000	0.848397000						
	1	-1.165463000	0.138305000	1.560388000						
P3 (C_{2v})	6	-0.619666000	-1.248242000	-0.000001000	5.39110	-232.762553	0.109461	166.8983	388.5388	528.8322
	6	0.735115000	-1.221179000	-0.000002000	5.30371			562.4582	589.7407	643.6157
	6	1.449138000	0.000000000	-0.000001000	2.71671			745.4125	796.8784	887.9329
	6	0.735115000	1.221179000	-0.000002000				941.7741	982.1833	992.1747
	6	-0.619666000	1.248242000	-0.000001000				994.0679	997.0331	997.2256
	6	-1.441322000	0.000000000	0.000005000				1098.4352	1165.6252	1193.4141
	1	1.285917000	-2.152897000	-0.000004000				1199.0590	1312.8759	1367.3338
	1	-1.143252000	-2.195184000	-0.000003000				1422.0177	1439.3877	1458.0230
	1	1.285916000	2.152897000	-0.000004000				1567.3665	1634.0315	2971.3039
	1	-1.143252000	2.195184000	-0.000003000				2974.3542	3189.7098	3191.0994
	1	-2.123086000	0.000000000	0.863375000				3207.7366	3208.9364	3232.4877
	1	-2.123100000	0.000000000	-0.863353000						
	1	2.528574000	0.000000000	-0.000001000						
P4 (C_s)	6	-0.997902000	-1.073726000	0.000081000	5.64548	-232.710242	0.110038	132.9465	375.2349	407.0468
	6	0.272212000	-1.381213000	0.000046000	4.90099			526.7509	574.1574	657.4017
	6	1.460667000	-0.506747000	-0.000033000	2.70962			760.2409	870.3280	917.9842
	6	1.015072000	0.938614000	-0.000077000				924.2706	954.2668	967.9275
	6	-0.255808000	1.316482000	-0.000045000				984.5466	1025.6333	1041.6262
	6	-1.427283000	0.377528000	0.000039000				1184.8744	1211.8155	1214.4063
	1	2.089384000	-0.704713000	0.872735000				1260.1228	1340.8327	1361.7246
	1	-1.771506000	-1.833678000	0.000141000				1411.1038	1473.8815	1475.5225
	1	1.798425000	1.687786000	-0.000139000				1737.6573	1775.0378	3036.3050
	1	-0.486372000	2.375629000	-0.000081000				3045.3635	3055.4217	3066.6907
	1	-2.060468000	0.577102000	0.870346000				3168.9712	3169.7628	3191.3434
	1	-2.060535000	0.577031000	-0.870236000						
	1	2.089322000	-0.704786000	-0.872830000						

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

Table S2: Calculated overall rate constants, k_{tot}, of the 14CHD + OH → products over the range of temperature 200 – 2000 K at P = 760 Torr, including the HIR treatments, Eckart quantum tunneling effects and those collected from the literatures.

This work (Calc.)		**This work (Expt.)**		**Lui *et al.* (2020)**[3]		**Ohta *et al.* (1983)**[4]		**Atkinson *et al.* (1983)**[5]		**Grosjean *et al.* (1992)**[6]	
***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)	***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)	***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)	***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)	***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)	***T* (K)**	***k_tot*** (× 10^{11}) ($cm^3 \cdot molecule^{-1} \cdot s^{-1}$)
200	23.1	**295.15**	**9.73**	921	3.11	**297**	**9.86**	**298**	**9.48**	**298**	**7.21**
250	17.2	322.15	9.1	923	3.11						
300	**11.9**	372.15	7.74	941	3.16						
400	5.39	399.15	7.36	956	4.10						
500	2.63	438.15	6.32	991	3.49						
600	1.57			1014	3.65						
700	1.22			1027	3.77						
800	1.22			1040	3.74						
900	1.42			1046	4.27						
1000	1.77			1089	4.27						
1100	2.23										
1200	2.80										
1300	3.48										
1400	4.27										
1500	5.17										
1600	6.18										
1700	7.30										
1800	8.53										
1900	9.89										
2000	11.3										

Table S3: Calculated overall rate constants, k_{tot}, of the 14CHD + OH → products over the range of temperature 200 – 2000 K at different pressures e.g., P = 0.76 – 7600 Torr, including the HIR treatments, 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	2.29E-10	2.29E-10	2.29E-10	2.31E-10	2.48E-10
250	1.70E-10	1.70E-10	1.71E-10	1.72E-10	1.81E-10
300	1.19E-10	1.19E-10	1.19E-10	1.19E-10	1.24E-10
400	5.35E-11	5.37E-11	5.37E-11	5.39E-11	5.46E-11
500	2.57E-11	2.62E-11	2.62E-11	2.63E-11	2.64E-11
600	1.50E-11	1.56E-11	1.57E-11	1.57E-11	1.57E-11
700	1.14E-11	1.21E-11	1.22E-11	1.22E-11	1.23E-11
800	1.15E-11	1.20E-11	1.22E-11	1.22E-11	1.22E-11
900	1.37E-11	1.40E-11	1.42E-11	1.42E-11	1.42E-11
1000	1.74E-11	1.75E-11	1.76E-11	1.77E-11	1.77E-11
1100	2.21E-11	2.22E-11	2.22E-11	2.23E-11	2.23E-11
1200	2.79E-11	2.79E-11	2.80E-11	2.80E-11	2.80E-11
1300	3.48E-11	3.48E-11	3.49E-11	3.48E-11	3.48E-11
1400	4.27E-11	4.27E-11	4.27E-11	4.27E-11	4.27E-11
1500	5.17E-11	5.17E-11	5.17E-11	5.17E-11	5.17E-11
1600	6.18E-11	6.17E-11	6.18E-11	6.18E-11	6.18E-11
1700	7.30E-11	7.29E-11	7.30E-11	7.30E-11	7.30E-11
1800	8.53E-11	8.53E-11	8.53E-11	8.53E-11	8.54E-11
1900	9.88E-11	9.88E-11	9.88E-11	9.89E-11	9.90E-11
2000	1.14E-10	1.14E-10	1.14E-10	1.13E-10	1.13E-10

- $k(T) = 3.58\times10^{5}\times T^{-5.67}\times\exp[-986.0\ \text{K}/T] + 3.35\times10^{-18}\times T^{2.33}\times\exp[-705.2\ \text{K}/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 0.76 Torr**; error = 0.4 %).
- $k(T) = 2.93\times10^{5}\times T^{-5.64}\times\exp[-977.2\ \text{K}/T] + 2.77\times10^{-19}\times T^{2.63}\times\exp[-254.8\ \text{K}/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 7.6 Torr**; error = 0.3 %).
- $k(T) = 3.52\times10^{5}\times T^{-5.67}\times\exp[-983.8\ \text{K}/T] + 1.71\times10^{-19}\times T^{2.68}\times\exp[-155.6\ \text{K}/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 76 Torr**; error = 0.2 %).
- $k(T) = 2.73\times10^{5}\times T^{-5.63}\times\exp[-971.4\ \text{K}/T] + 3.68\times10^{-19}\times T^{2.59}\times\exp[-267.4\ \text{K}/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 760 Torr**; error = 0.2 %).
- $k(T) = 4.59\times10^{8}\times T^{-5.72}\times\exp[-971.6\ \text{K}/T] + 1.41\times10^{-19}\times T^{2.70}\times\exp[-92.1\ \text{K}/T]$ (cm^3/molecule/s) (T = 200 – 2000 K & ***P* = 7600 Torr**; error = 0.3 %).

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

T (K)	via TS1	via TS2	via TS3	via TS4	via TS5
200	1.21	13.40	5.18	3.05	3.89
250	1.13	4.70	2.76	2.01	2.46
300	1.09	2.82	2.00	1.62	1.90
400	1.05	1.76	1.47	1.31	1.46
500	1.03	1.44	1.28	1.19	1.29
600	1.02	1.29	1.19	1.13	1.20
700	1.02	1.21	1.14	1.09	1.15
800	1.01	1.16	1.10	1.07	1.12
900	1.01	1.12	1.08	1.06	1.09
1000	1.01	1.10	1.07	1.05	1.08
1100	1.01	1.08	1.06	1.04	1.06
1200	1.01	1.07	1.05	1.03	1.06
1300	1.01	1.06	1.04	1.03	1.05
1400	1.00	1.05	1.03	1.02	1.04
1500	1.00	1.04	1.03	1.02	1.04
1600	1.00	1.04	1.03	1.02	1.03
1700	1.00	1.04	1.02	1.02	1.03
1800	1.00	1.03	1.02	1.01	1.03
1900	1.00	1.03	1.02	1.01	1.03
2000	1.00	1.03	1.02	1.01	1.02

Table S5: Individual rate constants for 14CHD + OH → Products (cm^3/molecule/s) at different pressures (0.76, 7.6, 76, 760, and 7600 Torr). ("Unc." stands for the uncertainty). Units are in cm^3/molecule/s.

P = 0.76 Torr												
T (K)	**RC**	**unc.(%)**	**I1**	**unc.(%)**	**P1 + H**	**unc.(%)**	**P2 + H**	**unc.(%)**	**P3 + H_2O**	**unc.(%)**	**P4 + H_2O**	**unc.(%)**
200	1.20E-17	1.00E+02	1.50E-10	8.00E-06	1.20E-17	1.00E+02	1.20E-17	1.00E+02	7.87E-11	1.50E-05	1.05E-13	1.10E-02
250	1.20E-17	1.00E+02	1.09E-10	1.10E-05	2.40E-17	5.00E+01	1.20E-17	1.00E+02	6.08E-11	2.00E-05	2.18E-13	5.50E-03
300	1.20E-17	1.00E+02	7.40E-11	1.60E-05	1.32E-16	9.10E+00	1.20E-17	1.00E+02	4.44E-11	2.70E-05	3.94E-13	3.10E-03
400	1.20E-17	1.00E+02	2.99E-11	4.00E-05	6.50E-16	1.90E+00	1.20E-17	1.00E+02	2.26E-11	5.30E-05	9.97E-13	1.20E-03
500	1.21E-17	1.00E+02	1.13E-11	1.10E-04	1.58E-15	7.60E-01	1.21E-17	1.00E+02	1.24E-11	9.70E-05	2.01E-12	6.00E-04
600	1.21E-17	1.00E+02	3.89E-12	3.10E-04	2.39E-15	5.10E-01	3.63E-17	3.30E+01	7.58E-12	1.60E-04	3.50E-12	3.50E-04
700	1.22E-17	1.00E+02	1.08E-12	1.10E-03	3.07E-15	4.00E-01	4.87E-17	2.50E+01	4.78E-12	2.50E-04	5.56E-12	2.20E-04
800	1.23E-17	1.00E+02	2.04E-13	6.00E-03	2.76E-15	4.40E-01	7.35E-17	1.70E+01	3.02E-12	4.10E-04	8.30E-12	1.50E-04
900	1.24E-17	1.00E+02	2.20E-14	5.60E-02	2.30E-15	5.40E-01	6.18E-17	2.00E+01	1.93E-12	6.40E-04	1.18E-11	1.00E-04
1000	1.25E-17	1.00E+02	1.30E-15	9.60E-01	2.06E-15	6.10E-01	9.99E-17	1.20E+01	1.29E-12	9.70E-04	1.61E-11	7.80E-05
1100	1.26E-17	1.00E+02	5.05E-17	2.50E+01	1.57E-15	8.10E-01	1.14E-16	1.10E+01	8.90E-13	1.40E-03	2.12E-11	6.00E-05
1200	1.28E-17	1.00E+02	1.28E-17	1.00E+02	1.54E-15	8.30E-01	1.67E-16	7.70E+00	6.38E-13	2.00E-03	2.73E-11	4.70E-05
1300	1.30E-17	1.00E+02	1.30E-17	1.00E+02	1.23E-15	1.10E+00	1.95E-16	6.70E+00	4.72E-13	2.80E-03	3.43E-11	3.80E-05
1400	1.33E-17	1.00E+02	1.33E-17	1.00E+02	1.15E-15	1.10E+00	1.73E-16	7.70E+00	3.62E-13	3.70E-03	4.23E-11	3.10E-05
1500	1.35E-17	1.00E+02	1.35E-17	1.00E+02	1.04E-15	1.30E+00	2.03E-16	6.70E+00	2.80E-13	4.80E-03	5.14E-11	2.60E-05
1600	1.38E-17	1.00E+02	1.38E-17	1.00E+02	7.34E-16	1.90E+00	1.66E-16	8.30E+00	2.25E-13	6.10E-03	6.15E-11	2.20E-05
1700	1.42E-17	1.00E+02	1.42E-17	1.00E+02	9.36E-16	1.50E+00	3.12E-16	4.50E+00	1.82E-13	7.80E-03	7.28E-11	1.90E-05
1800	1.46E-17	1.00E+02	1.46E-17	1.00E+02	7.86E-16	1.90E+00	2.91E-16	5.00E+00	1.51E-13	9.70E-03	8.52E-11	1.70E-05
1900	1.50E-17	1.00E+02	1.50E-17	1.00E+02	8.38E-16	1.80E+00	2.39E-16	6.20E+00	1.31E-13	1.10E-02	9.87E-11	1.50E-05
2000	1.54E-17	1.00E+02	1.54E-17	1.00E+02	8.47E-16	1.80E+00	2.77E-16	5.60E+00	1.20E-13	1.30E-02	1.13E-10	1.40E-05
P = 7.6 Torr												
T (K)	**RC**	**unc.(%)**	**I1**	**unc.(%)**	**P1 + H**	**unc.(%)**	**P2 + H**	**unc.(%)**	**P3 + H_2O**	**unc.(%)**	**P4 + H_2O**	**unc.(%)**
200	1.20E-17	1.00E+02	1.50E-10	8.00E-06	1.20E-17	1.00E+02	1.20E-17	1.00E+02	7.87E-11	1.50E-05	1.06E-13	1.10E-02
250	1.20E-17	1.00E+02	1.10E-10	1.10E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	6.07E-11	2.00E-05	2.20E-13	5.50E-03
300	1.20E-17	1.00E+02	7.43E-11	1.60E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	4.42E-11	2.70E-05	3.92E-13	3.10E-03
400	1.20E-17	1.00E+02	3.06E-11	3.90E-05	8.42E-17	1.40E+01	1.20E-17	1.00E+02	2.22E-11	5.40E-05	9.98E-13	1.20E-03

500	1.21E-17	1.00E+02	1.25E-11	9.60E-05	4.70E-16	2.60E+00	1.21E-17	1.00E+02	1.17E-11	1.00E-04	1.99E-12	6.00E-04
600	1.21E-17	1.00E+02	5.29E-12	2.30E-04	1.28E-15	9.40E-01	7.26E-17	1.70E+01	6.81E-12	1.80E-04	3.48E-12	3.50E-04
700	1.22E-17	1.00E+02	2.13E-12	5.70E-04	2.28E-15	5.30E-01	1.34E-16	9.10E+00	4.38E-12	2.80E-04	5.56E-12	2.20E-04
800	1.23E-17	1.00E+02	7.05E-13	1.70E-03	3.08E-15	4.00E-01	1.59E-16	7.70E+00	2.97E-12	4.10E-04	8.29E-12	1.50E-04
900	1.24E-17	1.00E+02	1.64E-13	7.50E-03	3.40E-15	3.60E-01	2.35E-16	5.30E+00	2.03E-12	6.10E-04	1.18E-11	1.00E-04
1000	1.25E-17	1.00E+02	2.22E-14	5.60E-02	2.92E-15	4.30E-01	1.50E-16	8.30E+00	1.37E-12	9.10E-04	1.61E-11	7.80E-05
1100	1.26E-17	1.00E+02	1.83E-15	6.90E-01	2.11E-15	6.00E-01	2.15E-16	5.90E+00	9.27E-13	1.40E-03	2.12E-11	6.00E-05
1200	1.28E-17	1.00E+02	1.03E-16	1.20E+01	1.68E-15	7.60E-01	1.67E-16	7.70E+00	6.54E-13	2.00E-03	2.73E-11	4.70E-05
1300	1.30E-17	1.00E+02	1.30E-17	1.00E+02	1.42E-15	9.20E-01	1.69E-16	7.70E+00	4.81E-13	2.70E-03	3.43E-11	3.80E-05
1400	1.33E-17	1.00E+02	1.33E-17	1.00E+02	1.19E-15	1.10E+00	1.86E-16	7.10E+00	3.66E-13	3.60E-03	4.23E-11	3.10E-05
1500	1.35E-17	1.00E+02	1.35E-17	1.00E+02	9.07E-16	1.50E+00	2.44E-16	5.60E+00	2.84E-13	4.80E-03	5.14E-11	2.60E-05
1600	1.39E-17	1.00E+02	1.39E-17	1.00E+02	9.55E-16	1.40E+00	1.80E-16	7.70E+00	2.27E-13	6.10E-03	6.15E-11	2.30E-05
1700	1.42E-17	1.00E+02	1.42E-17	1.00E+02	7.52E-16	1.90E+00	2.55E-16	5.60E+00	1.83E-13	7.70E-03	7.27E-11	1.90E-05
1800	1.46E-17	1.00E+02	1.46E-17	1.00E+02	7.57E-16	1.90E+00	3.20E-16	4.50E+00	1.49E-13	9.80E-03	8.52E-11	1.70E-05
1900	1.50E-17	1.00E+02	1.50E-17	1.00E+02	6.73E-16	2.20E+00	1.95E-16	7.70E+00	1.37E-13	1.10E-02	9.87E-11	1.50E-05
2000	1.54E-17	1.00E+02	1.54E-17	1.00E+02	7.70E-16	2.00E+00	2.93E-16	5.30E+00	1.22E-13	1.30E-02	1.13E-10	1.40E-05
P = 76 Torr												
T (K)	**RC**	**unc.(%)**	**I1**	**unc.(%)**	**P1 + H**	**unc.(%)**	**P2 + H**	**unc.(%)**	**P3 + H_2O**	**unc.(%)**	**P4 + H_2O**	**unc.(%)**
200	1.08E-16	1.10E+01	1.51E-10	8.00E-06	1.20E-17	1.00E+02	1.20E-17	1.00E+02	7.88E-11	1.50E-05	1.05E-13	1.10E-02
250	1.08E-16	1.10E+01	1.10E-10	1.10E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	6.08E-11	2.00E-05	2.19E-13	5.50E-03
300	3.60E-17	3.30E+01	7.43E-11	1.60E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	4.42E-11	2.70E-05	3.98E-13	3.00E-03
400	2.41E-17	5.00E+01	3.07E-11	3.90E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	2.21E-11	5.50E-05	9.94E-13	1.20E-03
500	1.21E-17	1.00E+02	1.28E-11	9.40E-05	9.65E-17	1.20E+01	1.21E-17	1.00E+02	1.15E-11	1.10E-04	1.99E-12	6.10E-04
600	1.21E-17	1.00E+02	5.70E-12	2.10E-04	3.75E-16	3.20E+00	2.42E-17	5.00E+01	6.48E-12	1.90E-04	3.49E-12	3.50E-04
700	1.22E-17	1.00E+02	2.68E-12	4.50E-04	1.07E-15	1.10E+00	1.70E-16	7.10E+00	3.97E-12	3.10E-04	5.57E-12	2.20E-04
800	1.23E-17	1.00E+02	1.23E-12	1.00E-03	2.01E-15	6.10E-01	1.96E-16	6.20E+00	2.65E-12	4.60E-04	8.31E-12	1.50E-04
900	1.24E-17	1.00E+02	4.88E-13	2.50E-03	3.03E-15	4.10E-01	4.57E-16	2.70E+00	1.91E-12	6.50E-04	1.18E-11	1.00E-04
1000	1.25E-17	1.00E+02	1.48E-13	8.40E-03	3.33E-15	3.70E-01	4.12E-16	3.00E+00	1.39E-12	9.00E-04	1.61E-11	7.80E-05
1100	1.26E-17	1.00E+02	2.98E-14	4.20E-02	3.01E-15	4.20E-01	4.68E-16	2.70E+00	9.97E-13	1.30E-03	2.12E-11	6.00E-05
1200	1.28E-17	1.00E+02	3.68E-15	3.50E-01	2.85E-15	4.50E-01	5.13E-16	2.50E+00	7.13E-13	1.80E-03	2.73E-11	4.70E-05
1300	1.30E-17	1.00E+02	2.48E-16	5.30E+00	2.09E-15	6.20E-01	3.26E-16	4.00E+00	5.16E-13	2.50E-03	3.43E-11	3.80E-05

1400	1.33E-17	1.00E+02	1.33E-17	1.00E+02	1.37E-15	9.70E-01	1.86E-16	7.10E+00	3.78E-13	3.50E-03	4.23E-11	3.10E-05
1500	1.36E-17	1.00E+02	1.36E-17	1.00E+02	1.29E-15	1.10E+00	2.57E-16	5.30E+00	2.95E-13	4.60E-03	5.14E-11	2.60E-05
1600	1.39E-17	1.00E+02	1.39E-17	1.00E+02	1.09E-15	1.30E+00	2.49E-16	5.60E+00	2.28E-13	6.10E-03	6.16E-11	2.20E-05
1700	1.42E-17	1.00E+02	1.42E-17	1.00E+02	8.37E-16	1.70E+00	2.27E-16	6.20E+00	1.87E-13	7.60E-03	7.28E-11	1.90E-05
1800	1.46E-17	1.00E+02	1.46E-17	1.00E+02	7.57E-16	1.90E+00	2.33E-16	6.20E+00	1.54E-13	9.50E-03	8.52E-11	1.70E-05
1900	1.50E-17	1.00E+02	1.50E-17	1.00E+02	6.28E-16	2.40E+00	2.99E-16	5.00E+00	1.33E-13	1.10E-02	9.87E-11	1.50E-05
2000	1.54E-17	1.00E+02	1.54E-17	1.00E+02	7.55E-16	2.00E+00	3.24E-16	4.80E+00	1.20E-13	1.30E-02	1.13E-10	1.40E-05
P = 760 Torr												
T (K)	**RC**	**unc.(%)**	**I1**	**unc.(%)**	**P1 + H**	**unc.(%)**	**P2 + H**	**unc.(%)**	**P3 + H_2O**	**unc.(%)**	**P4 + H_2O**	**unc.(%)**
200	3.78E-15	3.20E-01	1.52E-10	7.90E-06	1.20E-17	1.00E+02	1.20E-17	1.00E+02	7.91E-11	1.50E-05	1.04E-13	1.20E-02
250	1.47E-15	8.20E-01	1.10E-10	1.10E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	6.09E-11	2.00E-05	2.19E-13	5.50E-03
300	6.25E-16	1.90E+00	7.46E-11	1.60E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	4.43E-11	2.70E-05	3.94E-13	3.10E-03
400	1.93E-16	6.20E+00	3.08E-11	3.90E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	2.21E-11	5.40E-05	9.92E-13	1.20E-03
500	4.82E-17	2.50E+01	1.28E-11	9.40E-05	1.21E-17	1.00E+02	1.21E-17	1.00E+02	1.15E-11	1.00E-04	2.00E-12	6.00E-04
600	1.21E-17	1.00E+02	5.77E-12	2.10E-04	4.84E-17	2.50E+01	1.21E-17	1.00E+02	6.41E-12	1.90E-04	3.49E-12	3.50E-04
700	1.22E-17	1.00E+02	2.85E-12	4.30E-04	2.31E-16	5.30E+00	3.65E-17	3.30E+01	3.84E-12	3.20E-04	5.55E-12	2.20E-04
800	1.23E-17	1.00E+02	1.48E-12	8.30E-04	5.76E-16	2.10E+00	2.33E-16	5.30E+00	2.44E-12	5.00E-04	8.28E-12	1.50E-04
900	1.24E-17	1.00E+02	7.65E-13	1.60E-03	1.48E-15	8.30E-01	2.72E-16	4.50E+00	1.68E-12	7.30E-04	1.18E-11	1.00E-04
1000	1.25E-17	1.00E+02	3.62E-13	3.40E-03	2.71E-15	4.60E-01	5.62E-16	2.20E+00	1.24E-12	1.00E-03	1.61E-11	7.80E-05
1100	1.26E-17	1.00E+02	1.43E-13	8.80E-03	3.01E-15	4.20E-01	8.72E-16	1.40E+00	9.35E-13	1.40E-03	2.12E-11	6.00E-05
1200	1.28E-17	1.00E+02	4.44E-14	2.90E-02	3.35E-15	3.80E-01	1.03E-15	1.20E+00	7.13E-13	1.80E-03	2.72E-11	4.70E-05
1300	1.30E-17	1.00E+02	9.42E-15	1.40E-01	3.18E-15	4.10E-01	1.00E-15	1.30E+00	5.40E-13	2.40E-03	3.43E-11	3.80E-05
1400	1.33E-17	1.00E+02	1.35E-15	9.80E-01	2.42E-15	5.50E-01	7.96E-16	1.70E+00	4.13E-13	3.20E-03	4.23E-11	3.10E-05
1500	1.35E-17	1.00E+02	1.63E-16	8.30E+00	1.80E-15	7.50E-01	6.09E-16	2.20E+00	3.16E-13	4.30E-03	5.14E-11	2.60E-05
1600	1.39E-17	1.00E+02	1.39E-17	1.00E+02	1.88E-15	7.40E-01	4.43E-16	3.10E+00	2.43E-13	5.70E-03	6.16E-11	2.20E-05
1700	1.42E-17	1.00E+02	1.42E-17	1.00E+02	1.21E-15	1.20E+00	3.12E-16	4.50E+00	1.97E-13	7.20E-03	7.28E-11	1.90E-05
1800	1.46E-17	1.00E+02	1.46E-17	1.00E+02	9.46E-16	1.50E+00	4.22E-16	3.40E+00	1.64E-13	8.90E-03	8.52E-11	1.70E-05
1900	1.50E-17	1.00E+02	1.50E-17	1.00E+02	1.00E-15	1.50E+00	3.74E-16	4.00E+00	1.41E-13	1.10E-02	9.87E-11	1.50E-05
2000	1.54E-17	1.00E+02	1.54E-17	1.00E+02	8.47E-16	1.80E+00	5.24E-16	2.90E+00	1.25E-13	1.20E-02	1.13E-10	1.40E-05
P = 7600 Torr												
T (K)	**RC**	**unc.(%)**	**I1**	**unc.(%)**	**P1 + H**	**unc.(%)**	**P2 + H**	**unc.(%)**	**P3 + H_2O**	**unc.(%)**	**P4 + H_2O**	**unc.(%)**

200	4.57E-13	2.60E-03	1.66E-10	7.20E-06	1.20E-17	1.00E+02	1.20E-17	1.00E+02	8.14E-11	1.50E-05	1.06E-13	1.10E-02
250	7.32E-14	1.60E-02	1.18E-10	1.00E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	6.28E-11	1.90E-05	2.18E-13	5.50E-03
300	1.98E-14	6.10E-02	7.80E-11	1.50E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	4.53E-11	2.70E-05	3.97E-13	3.00E-03
400	2.66E-15	4.50E-01	3.13E-11	3.80E-05	1.20E-17	1.00E+02	1.20E-17	1.00E+02	2.23E-11	5.40E-05	9.94E-13	1.20E-03
500	4.22E-16	2.90E+00	1.29E-11	9.30E-05	1.21E-17	1.00E+02	1.21E-17	1.00E+02	1.15E-11	1.00E-04	2.01E-12	6.00E-04
600	3.63E-17	3.30E+01	5.82E-12	2.10E-04	1.21E-17	1.00E+02	1.21E-17	1.00E+02	6.43E-12	1.90E-04	3.49E-12	3.50E-04
700	1.22E-17	1.00E+02	2.87E-12	4.20E-04	3.65E-17	3.30E+01	1.22E-17	1.00E+02	3.82E-12	3.20E-04	5.57E-12	2.20E-04
800	1.23E-17	1.00E+02	1.53E-12	8.00E-04	1.23E-16	1.00E+01	2.45E-17	5.00E+01	2.40E-12	5.10E-04	8.31E-12	1.50E-04
900	1.24E-17	1.00E+02	8.67E-13	1.40E-03	2.97E-16	4.20E+00	4.94E-17	2.50E+01	1.59E-12	7.80E-04	1.18E-11	1.00E-04
1000	1.25E-17	1.00E+02	5.07E-13	2.50E-03	7.49E-16	1.70E+00	2.25E-16	5.60E+00	1.12E-12	1.10E-03	1.61E-11	7.80E-05
1100	1.26E-17	1.00E+02	2.79E-13	4.50E-03	1.66E-15	7.60E-01	4.93E-16	2.60E+00	8.09E-13	1.60E-03	2.12E-11	6.00E-05
1200	1.28E-17	1.00E+02	1.46E-13	8.80E-03	1.97E-15	6.50E-01	1.00E-15	1.30E+00	6.24E-13	2.10E-03	2.72E-11	4.70E-05
1300	1.30E-17	1.00E+02	6.51E-14	2.00E-02	2.91E-15	4.50E-01	1.17E-15	1.10E+00	4.99E-13	2.60E-03	3.43E-11	3.80E-05
1400	1.33E-17	1.00E+02	2.46E-14	5.40E-02	2.87E-15	4.60E-01	1.35E-15	9.80E-01	4.00E-13	3.30E-03	4.23E-11	3.10E-05
1500	1.35E-17	1.00E+02	7.57E-15	1.80E-01	2.90E-15	4.70E-01	1.30E-15	1.00E+00	3.19E-13	4.30E-03	5.14E-11	2.60E-05
1600	1.39E-17	1.00E+02	1.66E-15	8.30E-01	2.52E-15	5.50E-01	1.11E-15	1.20E+00	2.53E-13	5.50E-03	6.15E-11	2.30E-05
1700	1.42E-17	1.00E+02	2.84E-16	5.00E+00	2.18E-15	6.50E-01	1.04E-15	1.40E+00	2.04E-13	7.00E-03	7.28E-11	1.90E-05
1800	1.46E-17	1.00E+02	7.28E-17	2.00E+01	1.54E-15	9.40E-01	8.73E-16	1.70E+00	1.72E-13	8.50E-03	8.52E-11	1.70E-05
1900	1.50E-17	1.00E+02	1.50E-17	1.00E+02	1.54E-15	9.70E-01	7.63E-16	2.00E+00	1.48E-13	1.00E-02	9.88E-11	1.50E-05
2000	1.54E-17	1.00E+02	1.54E-17	1.00E+02	1.28E-15	1.20E+00	8.93E-16	1.70E+00	1.32E-13	1.20E-02	1.13E-10	1.40E-05

Table S6: Calculated branching ratios (%) for each species of 14CHD + OH → products reactions at P = 760 Torr.

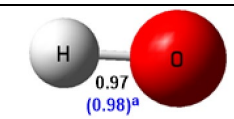
T (K)	RC	I1	P1 + H	P2 + H	P3 + H_2O	P4 + H_2O
200	0.00	65.77	0.00	0.00	34.19	0.04
250	0.00	64.36	0.00	0.00	35.51	0.13
300	0.00	62.52	0.00	0.00	37.15	0.33
400	0.00	57.12	0.00	0.00	41.04	1.84
500	0.00	48.63	0.00	0.00	43.76	7.60
600	0.00	36.84	0.00	0.00	40.90	22.26
700	0.00	23.26	0.00	0.00	31.36	45.38
800	0.00	12.10	0.00	0.00	19.98	67.91
900	0.00	5.37	0.01	0.00	11.81	82.81
1000	0.00	2.05	0.02	0.00	7.04	90.89
1100	0.00	0.64	0.01	0.00	4.19	95.15
1200	0.00	0.16	0.01	0.00	2.55	97.28
1300	0.00	0.03	0.01	0.00	1.55	98.41
1400	0.00	0.00	0.01	0.00	0.97	99.02
1500	0.00	0.00	0.00	0.00	0.61	99.38
1600	0.00	0.00	0.00	0.00	0.39	99.60
1700	0.00	0.00	0.00	0.00	0.27	99.73
1800	0.00	0.00	0.00	0.00	0.19	99.81
1900	0.00	0.00	0.00	0.00	0.14	99.86
2000	0.00	0.00	0.00	0.00	0.11	99.89

Table S7: Relative energies to that of the reactants (14CHD + OH) of main TSs (**TS1**, **TS4** and **TS5**), calculated at M06-2X/aug-cc-pVTZ and CCSD(T)/CBS//M06-2X/aug-cc-pVTZ. Units are in kcal/mol.

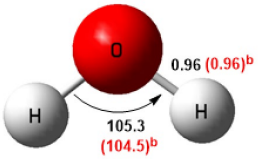
Species	CCSD(T)/CBS//M06-2X/aug-cc-pVTZ	M06-2X/aug-cc-pVTZ
TS1	-2.6	-2.9
TS4	-0.9	-1.4
TS5	2.8	2.1

Table S8: Ratios of $k_{TST}(T)/k_{VTST}(T)$ for the reaction channels of **RC** → [**TS1**]‡ → **IM1** and **RC** → [**TS4**]‡ → **P3** + H_2O. The constant rate calculations were carried out with the minimum energy paths (MEPs), together with its properties (i.e., Hessian and Gradient), obtained at the M06-2X/aug-cc-pVTZ level.

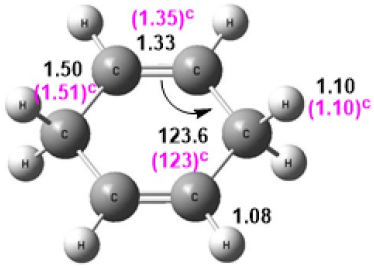
T (K)	$k_{TST}(T)/k_{VTST}(T)$ ($P \sim \infty$)	
	RC → [**TS1**]‡ → **IM1**	**RC** → [**TS4**]‡ → **P3** + H_2O
200	1.00	1.00
250	1.00	1.00
300	1.00	1.31
400	1.00	1.87
500	1.00	1.58
600	1.00	1.42
700	1.00	1.32
800	1.00	1.26
900	1.00	1.22
1000	1.00	1.18
1100	1.00	1.16
1200	1.00	1.14
1300	1.00	1.13
1400	1.00	1.12
1500	1.00	1.11
1600	1.06	1.11
1700	1.21	1.10
1800	1.38	1.10
1900	1.56	1.09
2000	1.75	1.09



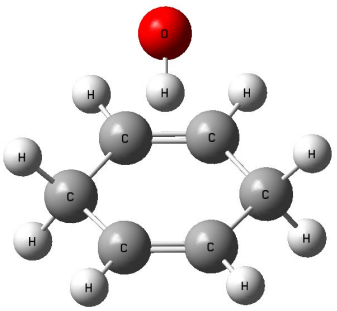
OH



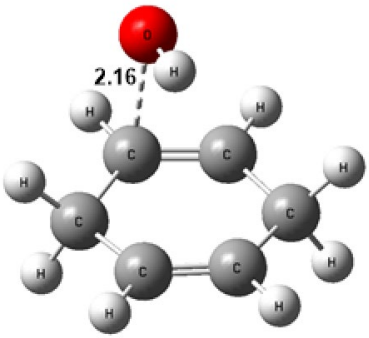
H_2O



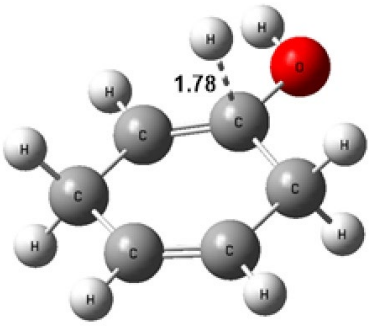
14CHD



RC



TS1



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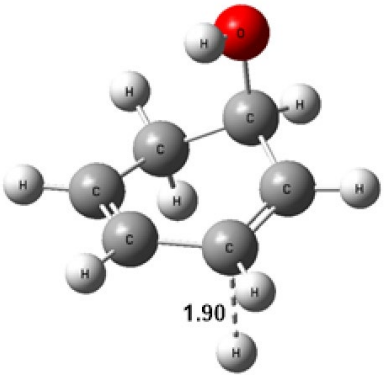
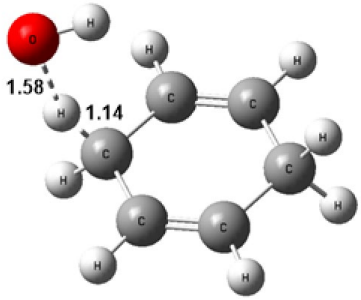


TS3



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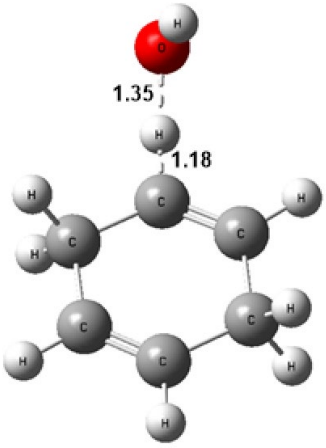

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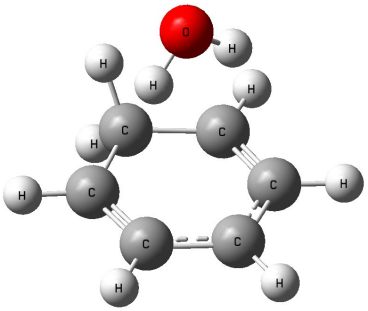

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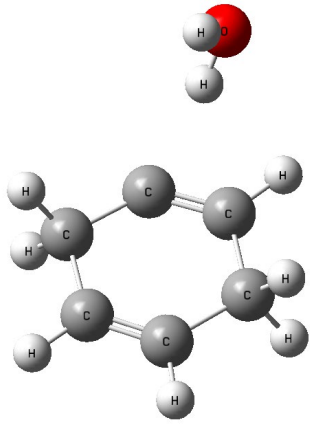

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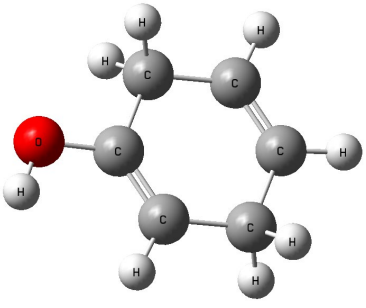

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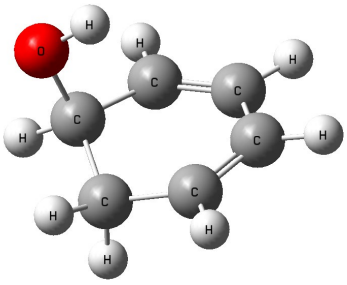

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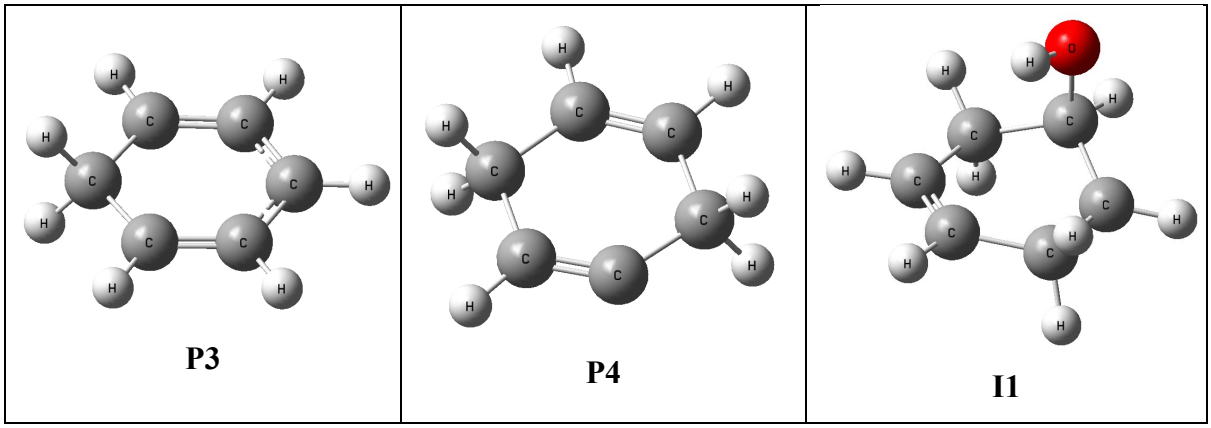


Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the 14CHD + OH reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree (°), respectively. [a, b, c] obtained from Huber *et al.*[1], Hoy *et al.*[7], and Hellwege *et al.*[8], respectively.

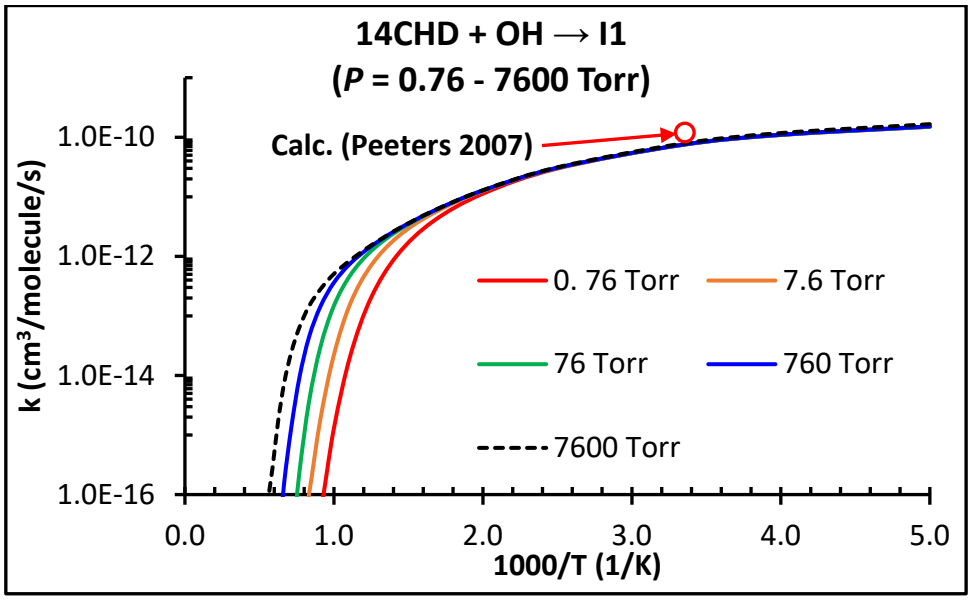


Figure S2: Predicted rate coefficients, $k(T, P)$, for the 14CHD + OH → **I1** as functions of temperature at different pressures (e.g., 0.76, 7.6, 76, 760, and 7600 Torr). Literature data is from Peeters *et al.*[9] ("Calc. (Peeters 2007)").

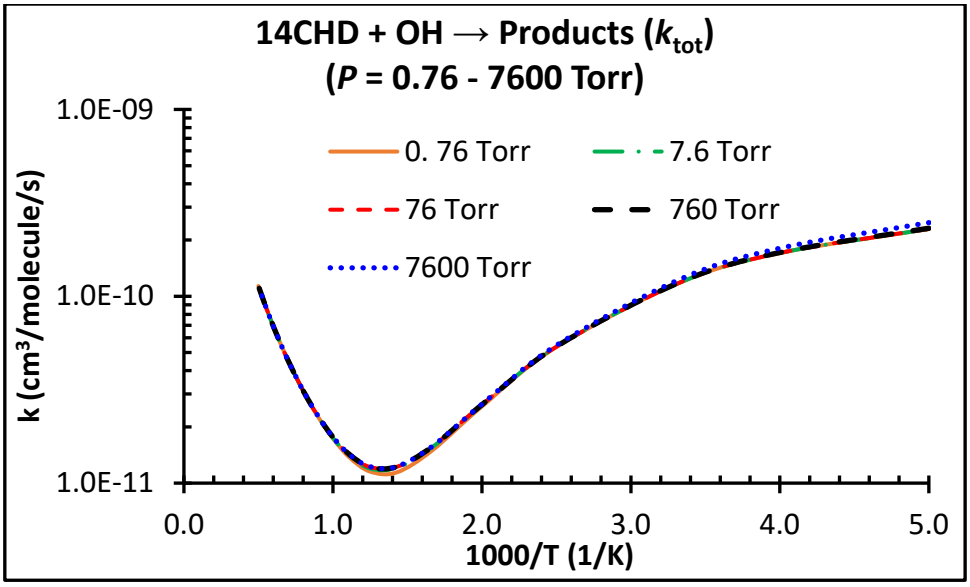


Figure S3: Calculated overall rate coefficients, $k_{tot}(T, P)$, for the 14CHD + OH → Products as functions of temperature at different pressures (e.g., 0.76, 7.6, 76, 760, and 7600 Torr).

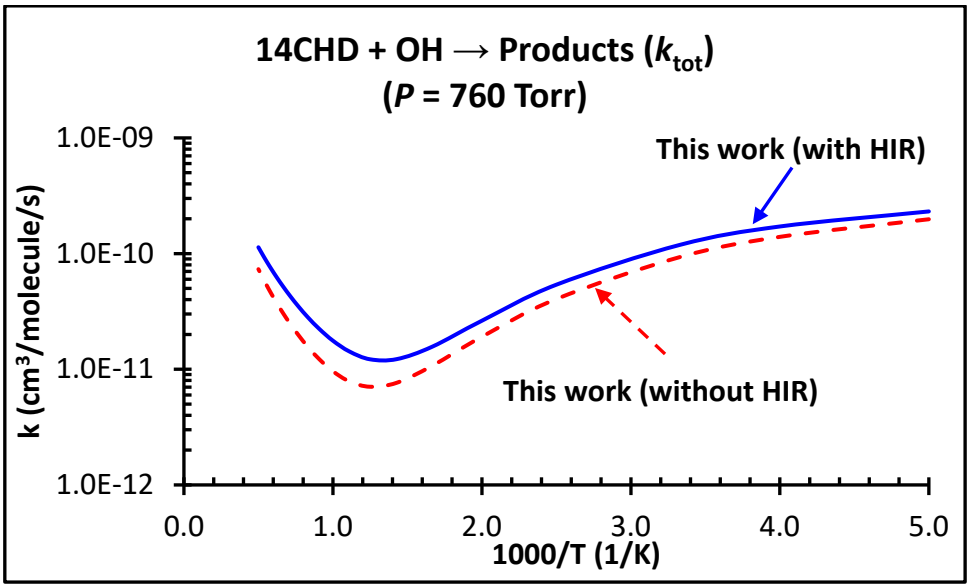
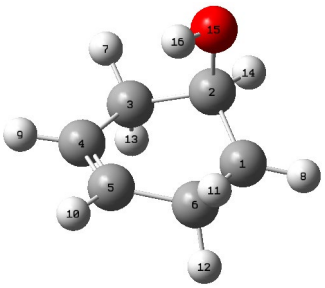
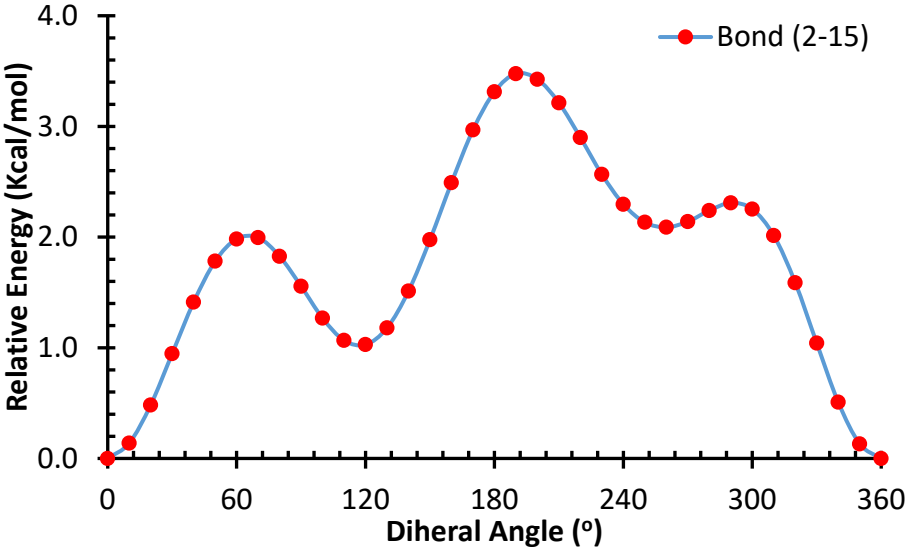
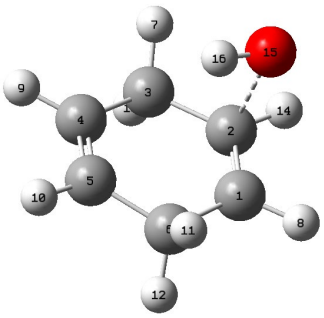
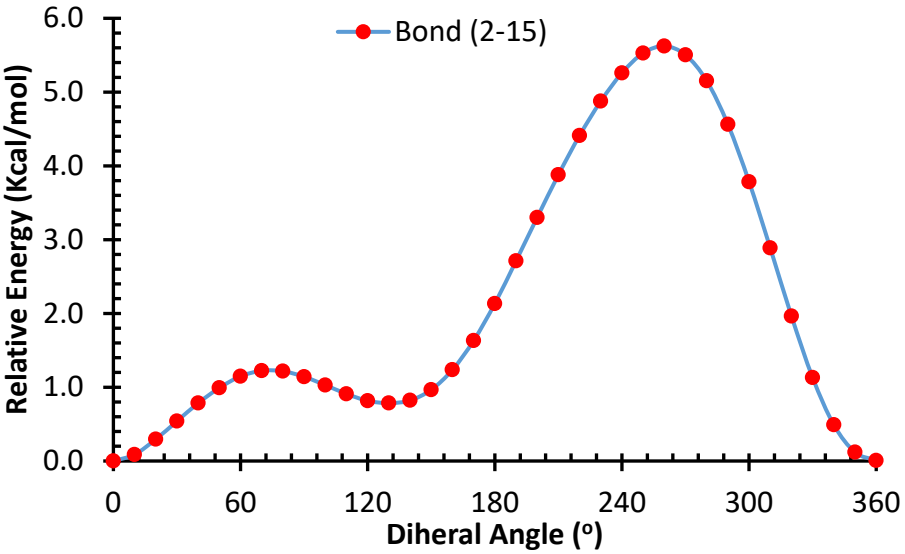
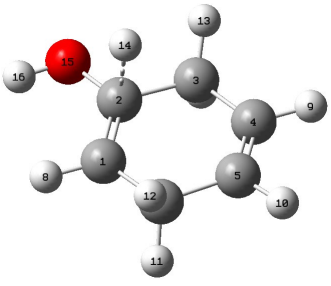
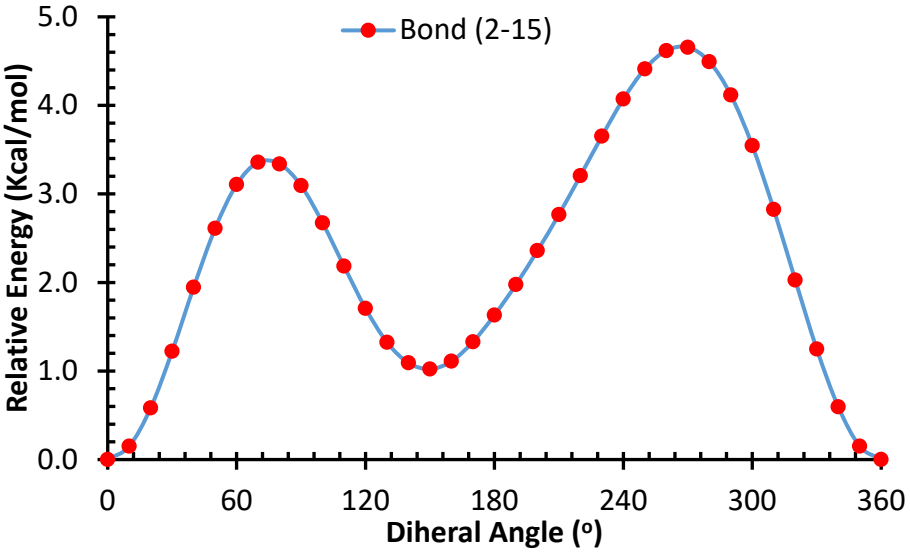
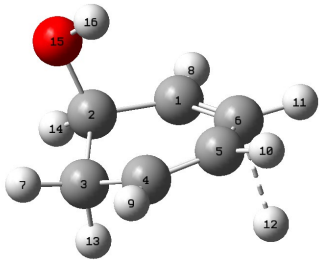
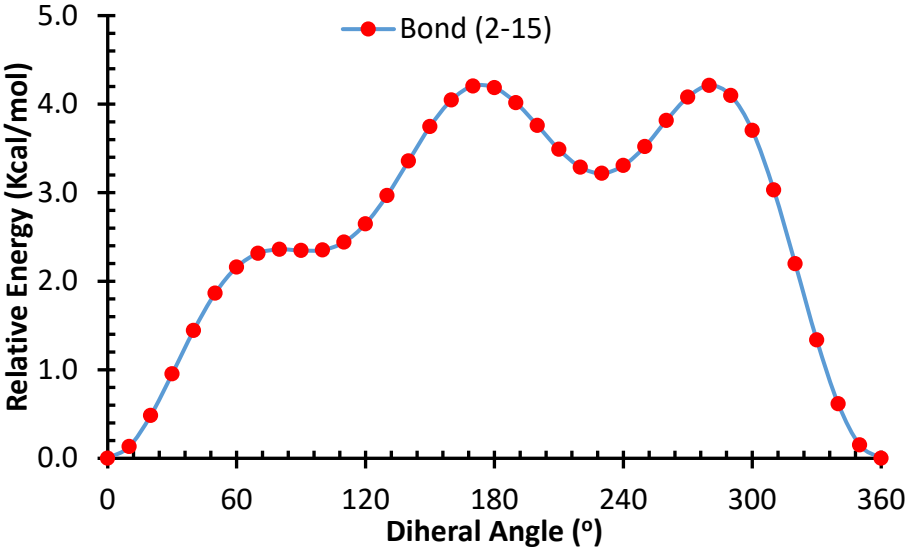
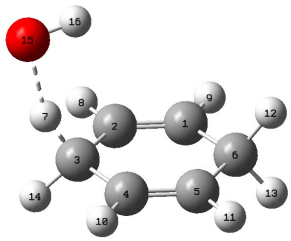
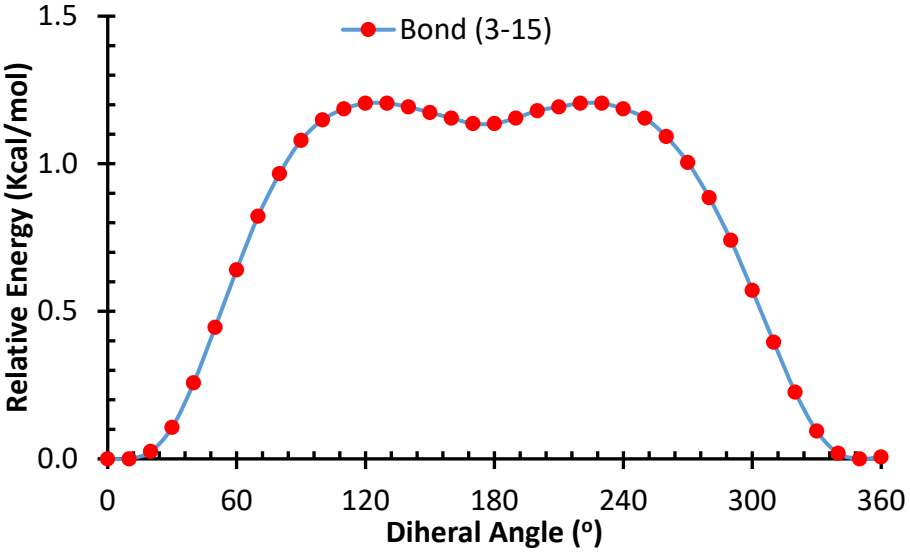
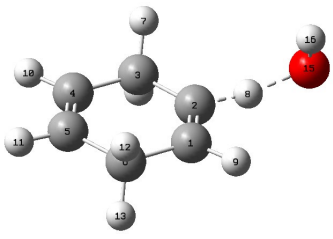
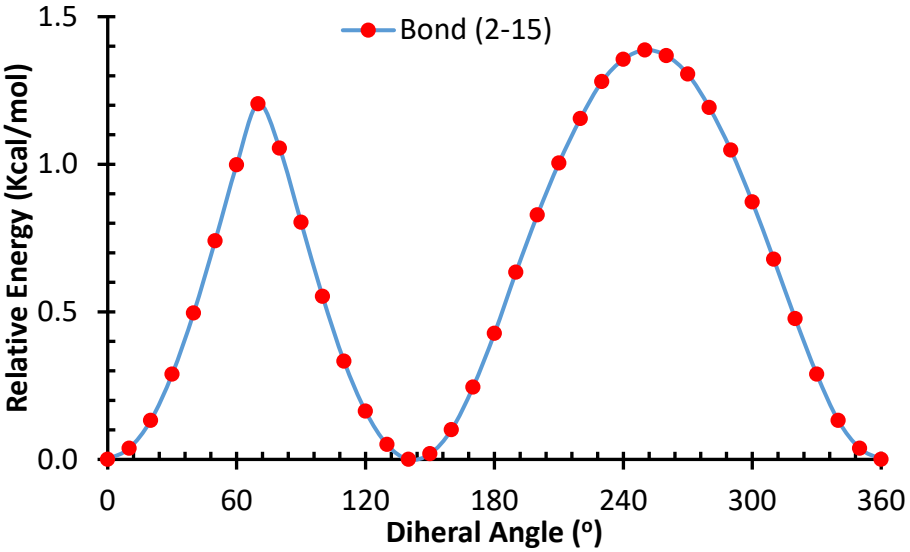


Figure S4: Calculated overall rate constant, k_{tot}, for the *14CHD + OH → products* reaction at P = 760 Torr as a function of temperature with (solid line) and without (dashed line) HIR treatment.

Species	Potential energy surfaces for the internal rotations
 I1	
 TS1	
 TS2	

Species	Potential energy surfaces for the internal rotations
 TS3	
 TS4	
 TS5	

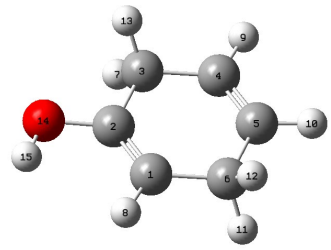
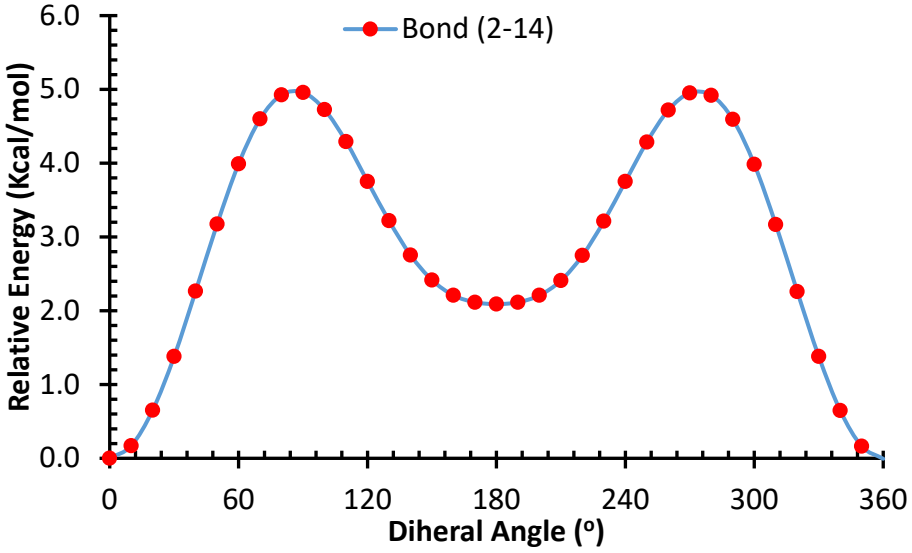
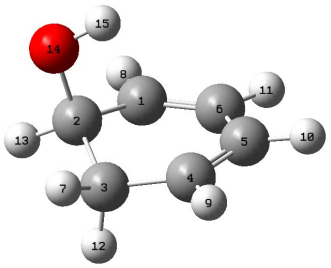
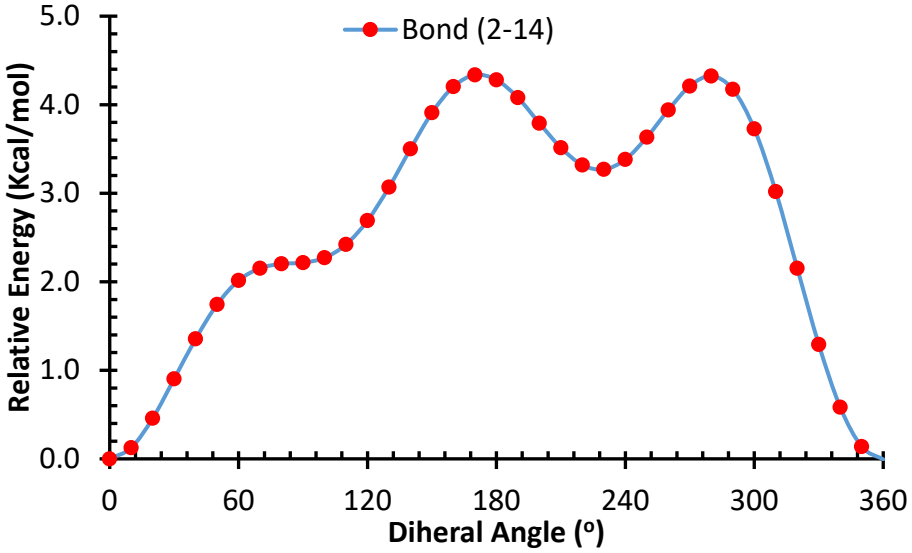
Species	Potential energy surfaces for the internal rotations
 P1	
 P2	

Figure S5: Hindrance potentials for the species involved in the 14CHD + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

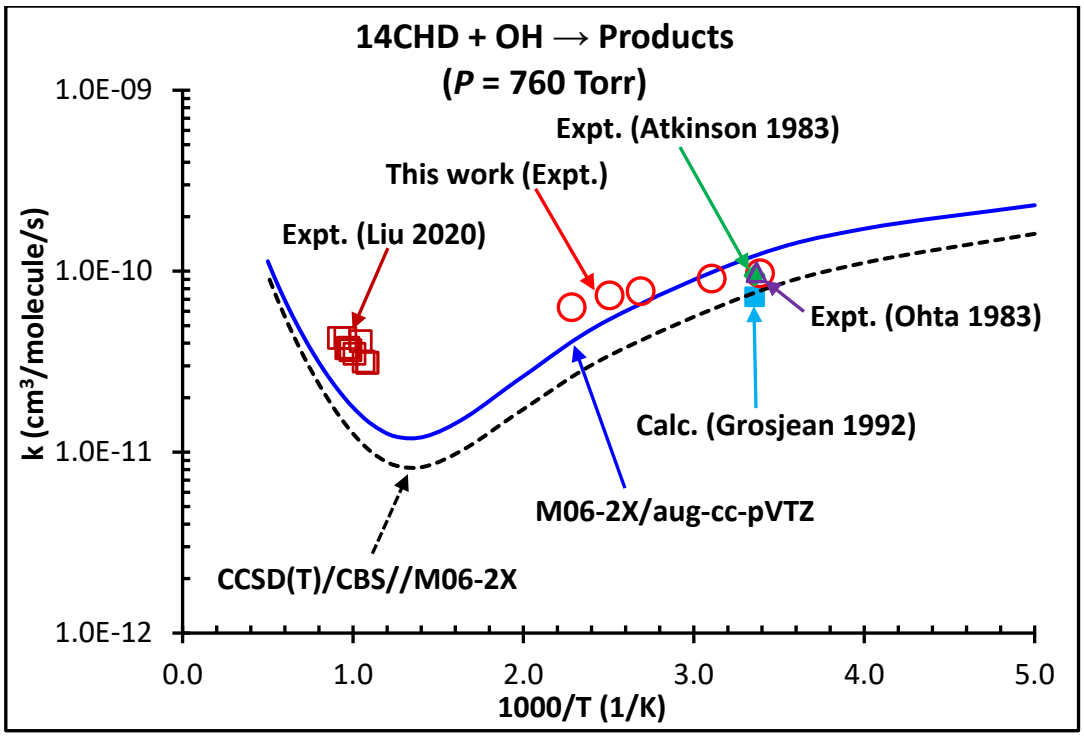


Figure S6: Comparison between the calculated and experimental global rate coefficients, $k(T, P)$, for 14CHD + OH → Products. Note that there is no energetic adjustment used in the calculations.

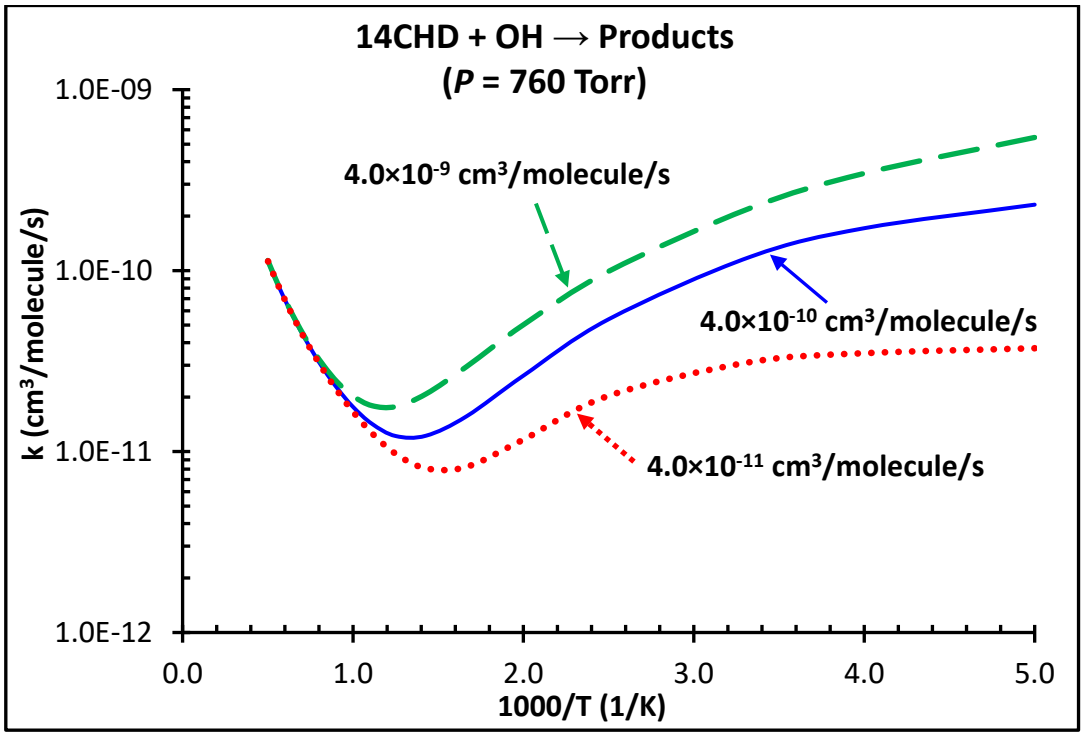


Figure S7: Comparison of the computed global rate constant, k_{tot}, for 14CHD + OH → Products reaction by using the $k^{\infty}(T)$ of 4.0×10^{-10} (solid line), 4.0×10^{-9} (dashed line) and 4.0×10^{-11} (dotted line) cm^3/molecule/s, at T = 200 – 2000 K & P = 760 Torr.

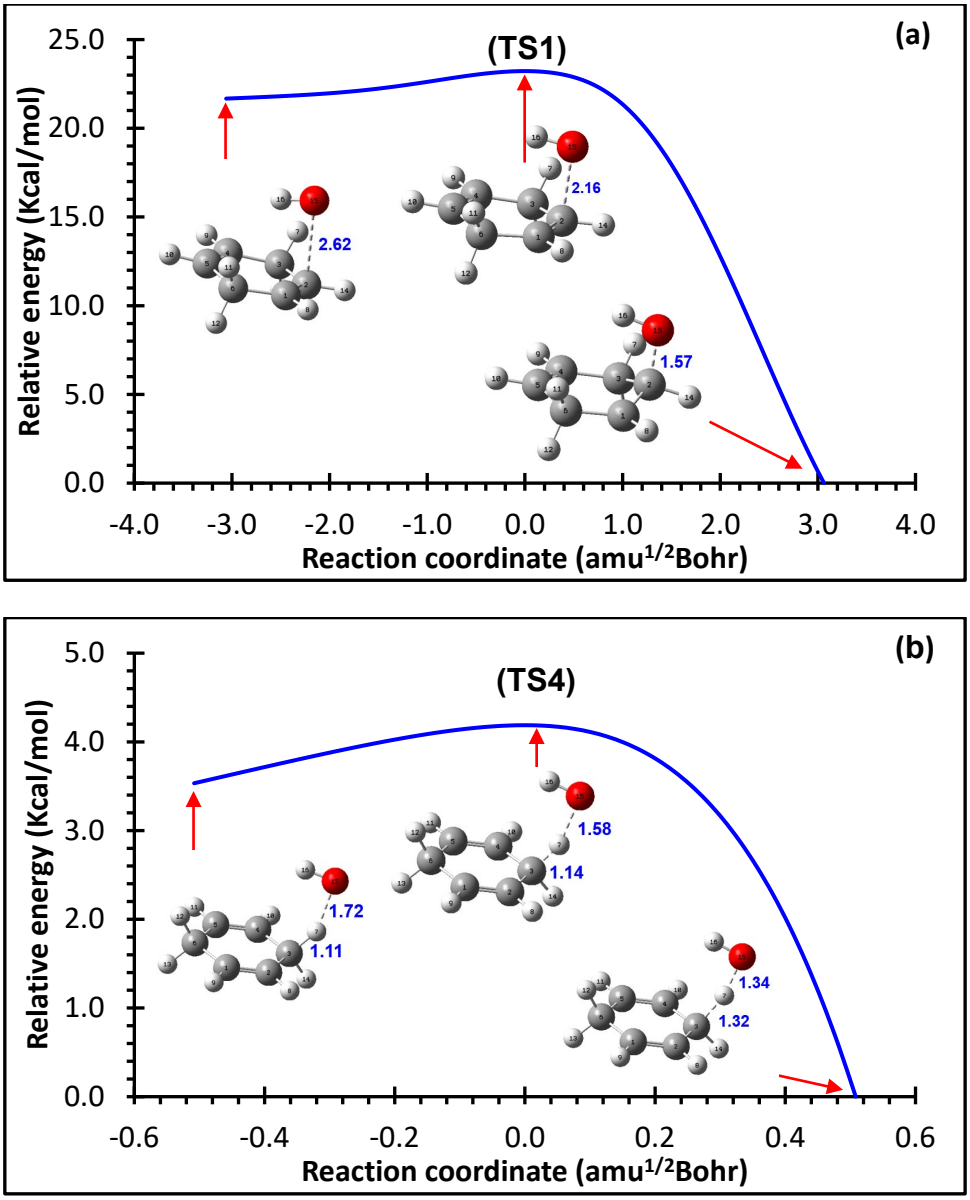


Figure S8: IRC data for **TS1** (a) and **TS4** (b) calculated at M06-2X/aug-cc-pVTZ level of theory. Distances are in Å.

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