

Reaction of HO with Hydroxyacetone (HOCH₂C(O)CH₃): Rate Coefficients (233 - 363 K) and Mechanism.

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SUPPORTING INFORMATION

CH₃COCH₂OH

E(RB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -268.475447936

E(CCSD(T)/6-311G(d,p)) (Hartree): -267.78101793

E(MP2/6-311G(d,p)) (Hartree): -267.71563195

E(MP3/6-311G(d,p)) (Hartree): -267.73768696

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.473655	0.159849	-0.014378
O	0.291462	1.357891	-0.012129
C	1.846228	-0.457933	0.013848
C	-0.723048	-0.773656	-0.028584
H	2.079510	-0.751899	1.040316
H	1.895396	-1.357436	-0.600360
H	2.588243	0.264844	-0.315496
H	-0.666868	-1.380720	-0.942452
H	-0.636075	-1.470725	0.814482
O	-1.933702	-0.075404	0.031869
H	-1.703290	0.866484	0.020272

Rotational constants (GHz): 10.1531600 3.8097200 2.8693700

Vibrational harmonic frequencies (cm⁻¹):

47.1168	131.0513	276.8287
407.6845	419.7609	493.7989
619.0672	807.6016	859.8321
978.0131	1095.1176	1115.1782
1204.8168	1257.1477	1303.8703
1393.8135	1436.1016	1465.3171
1478.7075	1482.8819	1776.9162
2980.7721	3002.4320	3037.0122
3094.8983	3142.1786	3694.6213

Zero-point correction (Hartree): 0.088854

OH

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E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -75.7655727121

E(UHF/6-311G(d,p)) (Hartree): -75.4102023317

E(CCSD(T)/6-311G(d,p)) (Hartree): -75.58917125

E(MP2/6-311G(d,p)) (Hartree): -75.57283875

E(MP3/6-311G(d,p)) (Hartree): -75.58383839

E(PMP2/6-311G(d,p)) (Hartree): -75.57434902

E(PMP3/6-311G(d,p)) (Hartree): -75.58468278

E(PUHF/6-311G(d,p)) (Hartree): -75.41283215

Point group : C₂V

Cartesian coordinates (Angs):

O	0.000000	0.000000	0.108289
H	0.000000	0.000000	-0.866311

Rotational constants (GHz): 0.0000000 561.1982077 561.1982077

Vibrational harmonic frequencies (cm-1):
3710.8220 (SG)
Zero-point correction (Hartree): 0.008454

CH3COCH2OH..OH.a

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.249776442
E(UHF/6-311G(d,p)) (Hartree): -342.298250260
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.37533667
E(MP2/6-311G(d,p)) (Hartree): -343.29332205
E(MP3/6-311G(d,p)) (Hartree): -343.32585508
E(PMP2/6-311G(d,p)) (Hartree): -343.29477124
E(PMP3/6-311G(d,p)) (Hartree): -343.32665888
E(PUHF/6-311G(d,p)) (Hartree): -342.30082860

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.849937	-0.247319	-0.030715
O	0.081168	-1.158633	-0.265175
C	2.333182	-0.481944	0.093907
C	0.379687	1.183925	0.171705
H	2.802002	-0.246035	-0.865043
H	2.784303	0.169320	0.842968
H	2.531009	-1.524435	0.328820
H	0.521386	1.394762	1.245645
H	1.067088	1.851131	-0.354702
O	-0.910006	1.478372	-0.267737
H	-1.553311	0.838206	0.075864
H	-1.753446	-1.160514	-0.064667
O	-2.643145	-0.826039	0.205630

Rotational constants (GHz): 4.8476100 2.1397700 1.5449900

Vibrational harmonic frequencies (cm-1):

57.9880	94.8549	118.2573
140.0415	178.9313	272.6751
383.2354	399.6478	409.1257
474.7712	621.6156	713.2113
804.6023	848.1774	977.2495
1076.6327	1127.1569	1201.3342
1246.5944	1366.7245	1391.7581
1419.6737	1461.3325	1467.0368
1480.2066	1765.1318	2930.8791
3035.8850	3054.7040	3094.9199
3143.9236	3457.0628	3664.7221

Zero-point correction (Hartree): 0.099966

CH3COCH2OH..OH.b

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -344.104582591
E(UHF/6-311G(d,p)) (Hartree): -342.300758672
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.37534907
E(MP2/6-311G(d,p)) (Hartree): -343.29352831
E(MP3/6-311G(d,p)) (Hartree): -343.32627248
E(PMP2/6-311G(d,p)) (Hartree): -343.29495869
E(PMP3/6-311G(d,p)) (Hartree): -343.32705402
E(PUHF/6-311G(d,p)) (Hartree): -342.30332042

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.336004	-0.610976	-0.006502
O	-0.620771	-1.369399	-0.077297
C	0.104103	0.901497	0.065406

C	1.756339	-1.113576	0.045081	
H	-0.403797	1.096286	1.017609	
O	1.281300	1.682903	0.040116	
H	-0.616941	1.173477	-0.719437	
H	2.318095	-0.749280	-0.822707	
H	2.265492	-0.710680	0.926470	
H	1.762240	-2.203713	0.058035	
H	-2.307019	-0.493431	-0.005502	
O	-2.877905	0.312426	0.012251	
H	1.542265	1.818240	-0.878933	
Rotational constants (GHz):	4.1417900	2.2024800	1.4719500	
Vibrational harmonic frequencies (cm-1):				
37.6426	66.4279		126.7850	
136.0002	180.1835		265.9217	
293.4908	458.0191		482.8975	
511.8255	521.9931		727.2554	
792.3303	837.8083		994.7686	
1066.4049	1117.3212		1216.2190	
1253.8052	1385.2075		1399.1829	
1428.1903	1463.0591		1479.5520	
1504.7260	1793.5656		3046.4920	
3056.0505	3105.0759		3117.9211	
3176.4923	3545.0560		3834.4035	
Zero-point correction (Hartree):	0.101201			

CH3COCH2OH..OH.c

E(UB+HF-LYP/6-31G(d,p)) (Hartree): -344.106550564
E(UHF/6-311G(d,p)) (Hartree): -342.300650366
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.37536171
E(MP2/6-311G(d,p)) (Hartree): -343.29353889
E(MP3/6-311G(d,p)) (Hartree): -343.32624180
E(PMP2/6-311G(d,p)) (Hartree): -343.29497045
E(PMP3/6-311G(d,p)) (Hartree): -343.32702445
E(PUHF/6-311G(d,p)) (Hartree): -342.30321285
Electronic state : 2-A
Cartesian coordinates (Angs):

C	0.334612	-0.599406	0.086680	
O	-0.674243	-1.292324	0.115096	
C	0.239060	0.906242	0.339325	
C	1.701671	-1.188222	-0.152078	
H	2.129278	-0.778401	-1.073489	
H	2.385713	-0.897213	0.652051	
H	1.630220	-2.273805	-0.223969	
H	0.174082	1.029150	1.429489	
H	-0.712218	1.265710	-0.072938	
O	1.369570	1.643202	-0.088826	
H	1.257146	1.851783	-1.024350	
O	-2.971939	0.332639	-0.190682	
H	-2.303385	-0.377050	-0.015066	
Rotational constants (GHz):	4.1121500	2.0780100	1.4386800	
Vibrational harmonic frequencies (cm-1):				
56.7382	86.0602		112.4927	
123.1835	190.0850		259.8651	
300.0050	447.3194		498.5578	
519.2809	544.2303		684.4257	
773.5788	852.8253		999.8660	
1064.4497	1105.4007		1210.8965	
1263.2162	1387.8832		1393.1668	

1405.1829	1462.7860	1476.6350
1483.3371	1788.3975	3032.8431
3058.9943	3082.8343	3119.0463
3175.6281	3491.4506	3832.7616

Zero-point correction (Hartree): 0.100885

CH3COCH2OH..OH.d

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.250828073
E(UHF/6-311G(d,p)) (Hartree): -342.305938793
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.38205792
E(MP2/6-311G(d,p)) (Hartree): -343.30081483
E(MP3/6-311G(d,p)) (Hartree): -343.33304383
E(PMP2/6-311G(d,p)) (Hartree): -343.30226582
E(PMP3/6-311G(d,p)) (Hartree): -343.33384248
E(PUHF/6-311G(d,p)) (Hartree): -342.30852393

Electronic state : 2-A

Cartesian coordinates (Angs):

C	1.265251	0.101858	-0.041760
O	1.310847	1.286597	-0.291599
C	2.433494	-0.825050	-0.226407
C	-0.036527	-0.488180	0.472711
H	2.521682	-1.523949	0.606127
H	2.277339	-1.418630	-1.130650
H	3.350893	-0.253253	-0.336918
H	-0.338548	-1.322182	-0.169682
H	0.139448	-0.900353	1.473325
O	-1.047853	0.489598	0.514306
H	-0.628312	1.324005	0.243748
H	-2.747302	0.016425	-0.086405
O	-3.581558	-0.357924	-0.451058

Rotational constants (GHz): 7.4223800 1.3031100 1.1933400

Vibrational harmonic frequencies (cm-1):

14.6883	40.1374	54.3235
125.9459	175.6499	289.7040
415.4349	426.9264	458.4395
526.1797	619.9198	650.8425
811.4262	864.4741	976.6768
1097.7816	1106.3765	1209.5197
1257.8556	1299.3792	1394.9257
1437.1670	1464.4242	1477.6171
1485.9475	1778.9384	3003.9255
3032.5854	3038.2488	3094.7727
3146.0265	3518.6187	3653.3910

Zero-point correction (Hartree): 0.100122

CH3COCH2OH..OH.e

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.249601000
E(UHF/6-311G(d,p)) (Hartree): -342.305743235
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.38058369
E(MP2/6-311G(d,p)) (Hartree): -343.29902448
E(MP3/6-311G(d,p)) (Hartree): -343.33159375
E(PMP2/6-311G(d,p)) (Hartree): -343.30049593
E(PMP3/6-311G(d,p)) (Hartree): -343.33241322
E(PUHF/6-311G(d,p)) (Hartree): -342.30834421

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.258183	0.349525	-0.012754
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O	-0.406845	-0.669448	-0.000223
C	-0.353135	1.721454	0.017001
C	1.765106	0.242428	-0.038793
H	-0.571809	1.975683	1.057229
H	0.321375	2.479127	-0.378694
H	-1.292791	1.729105	-0.531243
H	2.112821	0.728085	-0.961548
H	2.168547	0.835933	0.791696
O	2.216590	-1.077415	0.033455
H	1.432098	-1.644953	0.021060
H	-2.317899	-0.771897	0.008851
O	-3.293904	-0.654579	-0.008242
Rotational constants (GHz): 5.5607300 1.5971600 1.2603500			
Vibrational harmonic frequencies (cm-1):			
32.5174	38.8844	66.8767	
139.2162	142.8714	288.1649	
381.4854	409.1436	456.0978	
480.8371	576.8796	622.7873	
820.0247	854.1660	995.0657	
1091.7730	1117.5759	1206.4528	
1259.2267	1306.2561	1395.5645	
1432.0847	1467.3957	1475.5187	
1483.4613	1758.3748	2978.1243	
3002.3347	3040.2216	3103.4681	
3139.0741	3545.8344	3720.8790	

Zero-point correction (Hartree): 0.099849

TS_Habs.a.2

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.241989469

E(UHF/6-311G(d,p)) (Hartree): -342.276366061

E(CCS(D)/6-311G(d,p)) (Hartree): -343.36532202

E(MP2/6-311G(d,p)) (Hartree): -343.28055556

E(MP3/6-311G(d,p)) (Hartree): -343.31164044

E(PMP2/6-311G(d,p)) (Hartree): -343.28335984

E(PMP3/6-311G(d,p)) (Hartree): -343.31339053

E(PUHF/6-311G(d,p)) (Hartree): -342.28065188

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.579012	-0.559952	0.115775
O	0.044048	-1.641773	0.201466
C	-0.219347	0.697921	0.459251
C	2.019892	-0.391425	-0.290134
H	2.075261	0.104979	-1.261841
H	2.544857	0.253777	0.415170
H	2.497401	-1.364860	-0.354732
H	-0.297870	0.769970	1.546191
H	-1.291319	0.490653	0.087078
O	0.278830	1.914729	-0.008065
H	0.197313	1.958780	-0.965997
O	-2.548822	-0.219986	-0.318400
H	-2.195430	-1.116334	-0.175225

Rotational constants (GHz): 3.7973400 2.6091100 1.6604900

Vibrational harmonic frequencies (cm-1):

-217.9093	49.0024	127.7519
132.1831	144.1763	256.0052
349.9615	388.8425	477.9245
509.2667	545.2784	673.7475
765.8888	860.4329	991.7951

1059.2112	1122.1480	1197.0933
1235.4418	1316.0953	1333.7106
1388.5411	1399.8038	1459.0625
1470.7823	1760.9755	1948.9591
3039.5958	3069.8477	3094.8408
3151.8497	3699.2372	3820.6240

Zero-point correction (Hartree): 0.097597

TS_Habs.d.2

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.697994	0.542394	-0.018485
O	-1.643977	0.474576	-0.773508
C	-0.049039	1.835308	0.383667
C	-0.125010	-0.747773	0.549807
H	-0.179417	1.995869	1.456266
H	1.024193	1.791194	0.193241
H	-0.494709	2.662527	-0.161899
H	0.922072	-0.815762	0.216349
H	-0.085785	-0.688947	1.643341
O	-0.855879	-1.863641	0.144354
H	-1.519905	-1.535445	-0.484042
H	3.059624	-0.919580	-0.844816
O	2.813129	-0.144614	-0.309393

Rotational constants (GHz): 3.3349400 2.2550800 1.5294700

Vibrational harmonic frequencies (cm-1):

-68.8533	34.7608	56.9144
67.8898	96.4856	136.7321
279.6469	333.5815	408.2498
432.6347	506.6600	622.3895
803.1430	853.4938	973.9210
1091.0646	1122.5408	1204.0343
1222.8611	1295.3375	1396.3890
1415.3111	1447.6655	1469.9547
1478.2081	1774.3999	2875.5241
3017.8611	3039.3351	3097.2554
3146.3950	3667.1322	3719.5477

Zero-point correction (Hartree): 0.098160

TS_Habs.e.1

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.240680528

E(UHF/6-311G(d,p)) (Hartree): -342.268981047

E(CCSD(T)/6-311G(d,p)) (Hartree): -343.36080028

E(MP2/6-311G(d,p)) (Hartree): -343.27653944

E(MP3/6-311G(d,p)) (Hartree): -343.30691455

E(PMP2/6-311G(d,p)) (Hartree): -343.28040091

E(PMP3/6-311G(d,p)) (Hartree): -343.30936393

E(PUHF/6-311G(d,p)) (Hartree): -342.27449763

Electronic state : 2-A

Cartesian coordinates (Angs):

C	-0.241376	0.476916	0.172907
O	-0.569043	1.315424	-0.641044
C	1.057857	0.544919	0.908206
C	-1.151658	-0.701765	0.450006
H	1.464095	1.551518	0.936383
H	1.049363	0.069493	1.887615
H	1.818028	-0.110085	0.294083

H	-0.580637	-1.621658	0.268049
H	-1.406678	-0.697268	1.518030
O	-2.308928	-0.668766	-0.333913
H	2.836484	-0.140667	-1.245498
O	2.763475	-0.784773	-0.521327
H	-2.253625	0.133168	-0.875106
Rotational constants (GHz):	5.2078300	1.6881600	1.5445000
Vibrational harmonic frequencies (cm-1):			
-433.1239	29.8438		63.7769
139.6501	154.0276		269.5966
333.9008	398.7629		410.8956
496.8314	617.8095		772.9560
815.6770	868.0879		982.2773
1059.8007	1116.4534		1197.2941
1206.8557	1253.1652		1301.6693
1354.1133	1432.1152		1439.2362
1478.9330	1485.8249		1754.3945
2984.3560	3002.6688		3085.2300
3167.5620	3706.5231		3738.0010
Zero-point correction (Hartree):	0.095953		

TS_introt.a.c

E(UB+HF-LYP/6-311++G(2df,2pd)) (Hartree): -344.243284240
E(UHF/6-311G(d,p)) (Hartree): -342.299048052
E(CCSD(T)/6-311G(d,p)) (Hartree): -343.37438341
E(MP2/6-311G(d,p)) (Hartree): -343.29243989
E(MP3/6-311G(d,p)) (Hartree): -343.32522982
E(PMP2/6-311G(d,p)) (Hartree): -343.29387670
E(PMP3/6-311G(d,p)) (Hartree): -343.32601893
E(PUHF/6-311G(d,p)) (Hartree): -342.30161386

Electronic state : 2-A

Cartesian coordinates (Angs):

C	0.519294	-0.552827	0.148750
O	-0.418883	-1.323325	0.084551
C	0.323863	0.882034	0.642443
C	1.911351	-0.952845	-0.251134
H	2.362677	-0.182875	-0.876308
H	2.528026	-1.032902	0.648466
H	1.900176	-1.910608	-0.763538
O	0.698433	1.820974	-0.357343
H	-0.711337	1.013681	0.958521
H	0.979088	1.058296	1.498188
H	-0.031043	1.915530	-0.977568
O	-2.952277	-0.056719	-0.185391
H	-2.172826	-0.646724	-0.062649
Rotational constants (GHz):	3.8741000	2.1517600	1.5034700
Vibrational harmonic frequencies (cm-1):			
-51.3186	38.3310		66.2311
115.7398	171.2810		247.8971
320.5090	400.4905		440.2262
521.9513	593.9020		616.3803
787.9861	875.4106		1019.9597
1057.8756	1067.1973		1182.8835
1264.9020	1376.9280		1388.4019
1392.0041	1463.1029		1475.4041
1485.6323	1761.1133		3034.4606
3040.5896	3093.0024		3099.1676
3151.2498	3503.0170		3826.0851

Zero-point correction (Hartree): 0.099964