RATE CONSTANTS FOR THE THERMAL DECOMPOSITION OF ETHANOL AND ITS BIMOLECULAR REACTIONS WITH OH AND D: REFLECTED SHOCK TUBE AND THEORETICAL STUDIES

by

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Supplementary Information

The experimental data are given below in supplementary tables S1-S4.

Table S1: High-T Rate Data: $C_2H_5OH + OH \rightarrow CH_3CHO + H + H_2O$

P_1 / Torr	M_s[a]	ρ_5 / (10^{18} cm^{-3})[b]	T_5 / K[b]	k_{12}[c]	k_{12}[d]	Φ[e]
X_{C2H5OH} = 9.383 x 10^{-5}		$X_{tBH\ Sol`n.}$ = 2.536 x 10^{-5}				
10.89	2.241	1.852	1287	1.620(-11)	1.625(-11)	0.300
10.93	2.251	1.867	1297	1.333(-11)	1.360(-11)	0.310
10.96	2.105	1.728	1150	1.150(-11)	1.100(-11)	0.320
10.92	2.103	1.719	1148	1.103(-11)	1.075(-11)	0.313
10.88	1.970	1.571	1022	1.091(-11)	1.025(-11)	0.310
10.91	2.061	1.674	1108	1.174(-11)	1.070(-11)	0.325
10.86	2.126	1.733	1171	1.244(-11)	1.125(-11)	0.305
10.88	2.059	1.661	1109	1.132(-11)	1.075(-11)	0.310
10.96	1.985	1.599	1036	9.860(-12)	9.850(-12)	0.300
X_{C2H5OH} = 9.383 x 10^{-5}		$X_{tBH\ Sol`n.}$ = 2.536 x 10^{-5}				
15.88	1.999	2.378	1049	1.020(-11)	9.800(-12)	0.318
15.86	1.996	2.370	1045	9.834(-12)	9.800(-12)	0.320
15.97	2.091	2.531	1134	1.056(-11)	1.000(-11)	0.337
15.90	2.126	2.553	1175	1.086(-11)	1.025(-11)	0.335
15.99	2.123	2.562	1172	1.114(-11)	1.030(-11)	0.315
15.92	2.235	2.706	1283	1.118(-11)	1.250(-11)	0.310
15.93	2.183	2.637	1231	1.196(-11)	1.175(-11)	0.300
15.90	2.192	2.644	1240	1.088(-11)	1.075(-11)	0.310
15.92	2.145	2.583	1194	1.180(-11)	1.100(-11)	0.310
15.86	2.105	2.524	1151	1.280(-11)	1.225(-11)	0.308
X_{C2H5OH} = 4.885 x 10^{-5}		$X_{tBH\ Sol`n.}$ = 1.394 x 10^{-5}				
30.98	1.790	3.838	857	9.466(-12)	9.400(-12)	0.325
30.64	1.810	3.889	868	9.843(-12)	9.700(-12)	0.330
30.79	1.849	4.007	907	9.789(-12)	9.650(-12)	0.325
30.67	1.880	4.088	933	9.225(-12)	9.250(-12)	0.320
30.66	1.891	4.120	943	1.080(-11)	1.000(-11)	0.320
30.97	1.901	4.200	951	9.880(-12)	9.850(-12)	0.320

[a]The error in measuring the Mach number, M_s, is typically 0.5-1.0 % at the one standard deviation level. [b]Quantities with the subscript 5 refer to the thermodynamic state of the gas in the reflected shock region. [c]Rate constants: pseudo first order in units cm^3 molecule^{-1} s^{-1}. [d]Rate constants from modeling OH profiles using scheme in Table 4 in units cm^3 molecule^{-1} s^{-1}. [e] $\Phi = X_{tBH} / X_{tBH\ Sol`n}$.

Table S2: High-T Rate Data: D + $C_2H_5OH \rightarrow$ Products

P_1 / Torr	M_s[a]	ρ_5 / (10^{18} cm^{-3})[b]	T_5 / K[b]	k_{13}[c]
X_{C2H5OH} = 8.652 x 10^{-5}		X_{C2D5I} = 5.092 x 10^{-7}		
15.92	2.180	2.615	1236	9.961(-12)
15.92	2.217	2.663	1273	1.162(-11)
15.86	2.300	2.761	1359	1.494(-11)
15.94	2.256	2.719	1314	1.328(-11)
15.88	2.261	2.715	1319	1.370(-11)
15.95	2.174	2.610	1230	9.961(-12)
15.89	2.135	2.545	1192	8.716(-12)
15.88	2.145	2.567	1198	9.131(-12)
15.94	2.105	2.520	1159	8.301(-12)
X_{C2H5OH} = 8.652 x 10^{-5}		X_{C2D5I} = 5.092 x 10^{-7}		
30.78	2.188	4.977	1222	9.546(-12)
30.92	2.154	4.908	1188	7.969(-12)
30.83	2.087	4.710	1124	7.471(-12)
30.83	2.023	4.528	1064	5.728(-12)
30.82	2.052	4.595	1095	7.139(-12)
X_{C2H5OH} = 8.349 x 10^{-5}		X_{C2D5I} = 4.997 x 10^{-7}		
30.90	2.012	4.506	1054	6.641(-12)
30.75	2.123	4.797	1158	8.301(-12)
30.70	2.100	4.726	1136	7.886(-12)

[a]The error in measuring the Mach number, M_s, is typically 0.5-1.0 % at the one standard deviation level. [b]Quantities with the subscript 5 refer to the thermodynamic state of the gas in the reflected shock region. [c]Rate constants from modeling D profiles using scheme in Table 4 in units cm^3 $molecule^{-1}$ s^{-1}.

Table S3: High-T Rate Data: $C_2H_5OH + M \rightarrow C_2H_4 + H + OH + M$

P_1 / Torr	M_s[a]	ρ_5 / (10^{18} cm^{-3})[b]	T_5 / K[b]	k_3[c]
X_{C2H5OH} = 1.155 x 10^{-4}				
10.95	2.340	1.954	1392	5.117(-18)
X_{C2H5OH} = 2.257 x 10^{-4}				
10.89	2.479	2.051	1555	4.875(-17)
X_{C2H5OH} = 3.736x 10^{-4}				
10.89	2.442	2.037	1502	3.683(-17)
10.92	2.582	2.157	1663	1.855(-16)
10.88	2.459	2.049	1521	3.904(-17)
X_{C2H5OH} = 2.341 x 10^{-4}				
15.94	2.391	2.909	1445	1.031(-17)
15.83	2.470	2.981	1530	3.355(-17)
15.88	2.461	2.981	1521	3.355(-17)
15.91	2.402	2.917	1456	1.714(-17)

[a]The error in measuring the Mach number, M_s, is typically 0.5-1.0 % at the one standard deviation level. [b]Quantities with the subscript 5 refer to the thermodynamic state of the gas in the reflected shock region. [c]Rate constants: bimolecular in units cm^{3}molecule^{-1} s^{-1}.

Table S4: High-T Rate Data: $C_2H_5OH \rightarrow C_2H_4 + H_2O$, $C_2H_5OH \rightarrow CH_3 + CH_2O + H$

P_1 / Torr	M_s[a]	ρ_5 / (10^{18} cm^{-3})[b]	T_5 / K[b]	k_1[c]	k_2[c]	$BR_{2,3}$[d]
X_{C2H5OH} = 2.339 x 10^{-6}						
5.94	2.636	1.192	1732	10500	4184	0.300
5.93	2.522	1.142	1597	6750	2178	0.250
5.94	2.507	1.137	1579	4290	1153	0.220
5.92	2.394	1.082	1451	1691	400	0.195
5.94	2.333	1.060	1381	840	157	0.160
5.71	2.403	1.051	1457	3075	665	0.180
5.97	2.418	1.106	1473	2460	527	0.180
X_{C2H5OH} = 1.025 x 10^{-6}						
10.96	2.306	1.917	1361	424	121	0.230
10.87	2.500	2.076	1571	5040	1822	0.280
10.87	2.471	2.052	1538	5181	1331	0.215
10.93	2.483	2.073	1551	3876	1119	0.240
10.98	2.377	1.991	1433	1615	267	0.150
10.89	2.387	1.984	1444	1200	279	0.200
10.90	2.478	2.070	1540	3420	989	0.240
10.89	2.391	1.987	1448	2187	490	0.190
10.94	2.435	2.034	1497	2340	611	0.220
10.94	2.352	1.962	1406	1290	199	0.140
10.90	2.475	2.061	1542	6105	2052	0.260
10.94	2.594	2.164	1681	12420	5068	0.310
X_{C2H5OH} = 2.339 x 10^{-6}						
10.89	2.339	1.947	1386	731	111	0.140
10.9	2.549	2.128	1623	7097	2039	0.245
10.94	2.395	2.000	1452	2053	473	0.195
10.77	2.521	2.074	1596	6503	1808	0.235
10.84	2.458	2.035	1523	3100	829	0.225
10.87	2.371	1.970	1421	1260	226	0.160
10.91	2.367	1.980	1417	850	137	0.150
X_{C2H5OH} = 1.025x 10^{-6}						
15.89	2.420	2.930	1479	1884	455	0.215
15.90	2.414	2.935	1467	1774	326	0.175
15.78	2.328	2.809	1375	1104	86	0.08
15.91	2.348	2.856	1396	792	93	0.12
15.87	2.387	2.897	1438	1408	160	0.12
15.90	2.401	2.919	1453	1868	342	0.17
15.89	2.502	3.033	1563	3850	943	0.23
15.97	2.557	3.109	1626	8195	2343	0.255
X_{C2H5OH} = 6.470x 10^{-7}						
15.89	2.503	3.034	1564	4575	1315	0.250

15.90	2.519	3.054	1583	5325	1906	0.290
15.94	2.541	3.586	1607	8750	3384	0.300
$X_{C2H5OH.}$ = 2.339 x 10^{-6}						
15.99	2.263	2.763	1308	107	11	0.110
15.99	2.368	2.900	1418	1050	128	0.125
15.84	2.371	2.870	1421	860	116	0.140
$X_{C2H5OH.}$ = 6.470 x 10^{-7}						
30.86	2.450	5.663	1486	3488	884	0.225
30.8	2.368	5.463	1398	1485	286	0.175
30.97	2.374	5.507	1404	1733	485	0.230
30.84	2.554	5.885	1601	6900	2450	0.310
30.8	2.387	5.507	1418	1501	358	0.210
30.86	2.291	5.286	1318	595	49	0.085

[a]The error in measuring the Mach number, M_s, is typically 0.5-1.0 % at the one standard deviation level. [b]Quantities with the subscript 5 refer to the thermodynamic state of the gas in the reflected shock region. [c]Rate constants: First order in s^{-1}. [d] $BR_{2,3} = k_2+k_3 / (k_1+k_2+k_3)$.