

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>	Ref.	
1f	$H + O_2 \rightleftharpoons OH + O$	3.520E+16	-0.70	71.4	[1]	
2f	$H_2 + O \rightleftharpoons OH + H$	5.060E+04	2.67	26.3	[1]	
3f	$H_2 + OH \rightleftharpoons H_2O + H$	1.170E+09	1.30	15.2	[1]	
4f	$H_2O + O \rightleftharpoons 2 OH$	7.000E+05	2.33	60.9	[2]	
5f ^a	$2 H + M^{(1)} \rightleftharpoons H_2 + M^{(1)}$	1.300E+18	-1.00	0	[3]	
6f ^a	$H + OH + M^{(2)} \rightleftharpoons H_2O + M^{(2)}$	4.000E+22	-2.00	0	[3]	
7f ^a	$2 O + M^{(3)} \rightleftharpoons O_2 + M^{(3)}$	6.170E+15	-0.50	0	[3]	
8f ^a	$H + O + M^{(4)} \rightleftharpoons OH + M^{(4)}$	4.710E+18	-1.00	0	[3]	
9f ^a	$O + OH + M^{(4)} \rightleftharpoons HO_2 + M^{(4)}$	8.000E+15	0.00	0	[3]	
10f ^{a,b}	$H + O_2 + M^{(5)} \rightleftharpoons HO_2 + M^{(5)}$	k_0	5.750E+19	-1.40	0	[4, 3]
		k_∞	4.650E+12	0.44	0	
11f	$HO_2 + H \rightleftharpoons 2 OH$	7.080E+13	0.00	1.23	[5]	
12f	$HO_2 + H \rightleftharpoons H_2 + O_2$	1.660E+13	0.00	3.44	[5]	
13f	$HO_2 + H \rightleftharpoons H_2O + O$	3.100E+13	0.00	7.2	[1]	
14f	$HO_2 + O \rightleftharpoons OH + O_2$	2.000E+13	0.00	0	[6]	
15f ^{a,b}	$HO_2 + OH + M \rightleftharpoons H_2O + O_2 + M$	k_0	2.890E+13	0.00	-2.08	[2]
		k_∞	4.500E+14	0.00	45.7	
16f ^{a,b}	$2 OH + M^{(6)} \rightleftharpoons H_2O_2 + M^{(6)}$	k_0	2.760E+25	-3.20	0	[2]
		k_∞	9.550E+13	-0.27	0	
17f ^{a,b}	$2 HO_2 + M \rightleftharpoons H_2O_2 + O_2 + M$	k_0	1.030E+14	0.00	46.2	[2]
		k_∞	1.940E+11	0.00	-5.89	
18f	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	2.300E+13	0.00	33.3	[7]	
19f	$H_2O_2 + H \rightleftharpoons H_2O + OH$	1.000E+13	0.00	15	[8]	
20f ^{a,b}	$H_2O_2 + OH + M \rightleftharpoons H_2O + HO_2 + M$	k_0	1.740E+12	0.00	6	[2]
		k_∞	7.590E+13	0.00	30.4	
21f	$H_2O_2 + O \rightleftharpoons HO_2 + OH$	9.630E+06	2.00	16.7	[1]	
a21f ^{a,b}	$CO + O + M^{(11)} \rightleftharpoons CO_2 + M^{(11)}$	k_0	1.550E+24	-2.79	17.5	[7]
		k_∞	1.800E+11	0.00	9.97	
22f	$CO + OH \rightleftharpoons CO_2 + H$	4.400E+06	1.50	-3.1	[1]	
23f	$CO + HO_2 \rightleftharpoons CO_2 + OH$	2.000E+13	0.00	96	[7]	
24f	$CO + O_2 \rightleftharpoons CO_2 + O$	1.000E+12	0.00	200	[3]	
25f ^a	$HCO + M^{(7)} \rightleftharpoons CO + H + M^{(7)}$	1.860E+17	-1.00	71.1	[9]	
26f	$HCO + H \rightleftharpoons CO + H_2$	5.000E+13	0.00	0	[10]	
27f	$HCO + O \rightleftharpoons CO + OH$	3.000E+13	0.00	0	[1]	
28f	$HCO + O \rightleftharpoons CO_2 + H$	3.000E+13	0.00	0	[1]	
29f	$HCO + OH \rightleftharpoons CO + H_2O$	3.000E+13	0.00	0	[11]	

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30f	$\text{HCO} + \text{O}_2 \rightleftharpoons \text{CO} + \text{HO}_2$	7.580E+12	0.00	1.72	[10]	
31f	$\text{HCO} + \text{CH}_3 \rightleftharpoons \text{CO} + \text{CH}_4$	5.000E+13	0.00	0	[10]	
32f ^{a,b}	$\text{H} + \text{HCO} + \text{M}^{(8)} \rightleftharpoons \text{CH}_2\text{O} + \text{M}^{(8)}$	k_0 k_∞	1.350E+24 1.090E+12	-2.57 0.48	1.78 -1.09	[12]
33f	$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{HCO} + \text{H}_2$	5.740E+07	1.90	11.5	[13]	
34f	$\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{HCO} + \text{OH}$	3.500E+13	0.00	14.7	[1]	
35f	$\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{HCO} + \text{H}_2\text{O}$	3.900E+10	0.89	1.7	[1]	
36f	$\text{CH}_2\text{O} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{HO}_2$	6.000E+13	0.00	170	[14]	
37f	$\text{CH}_2\text{O} + \text{HO}_2 \rightleftharpoons \text{HCO} + \text{H}_2\text{O}_2$	4.110E+04	2.50	42.7	[15]	
38f	$\text{CH}_4 + \text{H} \rightleftharpoons \text{H}_2 + \text{CH}_3$	1.300E+04	3.00	33.6	[16]	
39f	$\text{CH}_4 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6	[16]	
40f	$\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$	1.900E+09	1.44	36.3	[17]	
41f	$\text{CH}_4 + \text{O}_2 \rightleftharpoons \text{CH}_3 + \text{HO}_2$	3.980E+13	0.00	238	[9, 18]	
42f	$\text{CH}_4 + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}_2$	9.030E+12	0.00	103	[9, 18]	
43f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{T-CH}_2 + \text{H}_2$	1.800E+14	0.00	63.2	[17]	
44f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{H}_2$	1.550E+14	0.00	56.4	[17]	
45f	$\text{CH}_3 + \text{OH} \rightleftharpoons \text{S-CH}_2 + \text{H}_2\text{O}$	4.000E+13	0.00	10.5	[19, 10]	
46f	$\text{CH}_3 + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	8.430E+13	0.00	0	[17]	
47f	$\text{CH}_3 + \text{T-CH}_2 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}$	4.220E+13	0.00	0	[14]	
48f	$\text{CH}_3 + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{OH}$	5.000E+12	0.00	0	[14]	
49f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4	[20]	
50f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{O}$	1.100E+13	0.00	116	[20]	
51f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}_2$	1.000E+14	0.00	134	[21]	
52f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}$	3.160E+13	0.00	61.5	[22]	
53f ^{a,b}	$\text{H} + \text{CH}_3 + \text{M}^{(9)} \rightleftharpoons \text{CH}_4 + \text{M}^{(9)}$	k_0 k_∞	2.470E+33 1.270E+16	-4.76 -0.63	10.2 1.6	[10]
54f ^{a,b}	$2 \text{CH}_3 + \text{M}^{(8)} \rightleftharpoons \text{C}_2\text{H}_6 + \text{M}^{(8)}$	k_0 k_∞	1.270E+41 1.810E+13	-7.00 0.00	11.6 0	[16]
55f	$\text{S-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	3.000E+13	0.00	0	[17]	
56f	$\text{S-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH} + \text{H}$	3.130E+13	0.00	0	[17]	
57f	$\text{S-CH}_2 + \text{CO}_2 \rightleftharpoons \text{CO} + \text{CH}_2\text{O}$	3.000E+12	0.00	0	[23]	
58f ^a	$\text{S-CH}_2 + \text{M}^{(10)} \rightleftharpoons \text{T-CH}_2 + \text{M}^{(10)}$	6.000E+12	0.00	0	[17]	
59f	$\text{T-CH}_2 + \text{H} \rightleftharpoons \text{CH} + \text{H}_2$	6.020E+12	0.00	-7.48	[14]	
60f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	2.500E+13	0.00	0	[17]	
61f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH} + \text{H}_2\text{O}$	1.130E+07	2.00	12.6	[17]	
62f	$\text{T-CH}_2 + \text{O} \rightleftharpoons \text{CO} + 2 \text{H}$	8.000E+13	0.00	0	[24]	

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63f	T-CH ₂ + O \rightleftharpoons CO + H ₂	4.000E+13	0.00	0	[24]
64f	T-CH ₂ + O ₂ \rightleftharpoons CO ₂ + H ₂	2.630E+12	0.00	6.24	[23]
65f	T-CH ₂ + O ₂ \rightleftharpoons CO + OH + H	6.580E+12	0.00	6.24	[23]
66f	2 T-CH ₂ \rightleftharpoons C ₂ H ₂ + 2 H	1.000E+14	0.00	0	[17]
67f	CH + O \rightleftharpoons CO + H	4.000E+13	0.00	0	[25]
68f	CH + O ₂ \rightleftharpoons HCO + O	1.770E+11	0.76	-2	[26]
69f	CH + H ₂ O \rightleftharpoons CH ₂ O + H	1.170E+15	-0.75	0	[23]
70f	CH + CO ₂ \rightleftharpoons HCO + CO	4.800E+01	3.22	-13.5	[26]
71f	CH ₃ O + H \rightleftharpoons CH ₂ O + H ₂	2.000E+13	0.00	0	[27]
72f	CH ₃ O + H \rightleftharpoons S-CH ₂ + H ₂ O	1.600E+13	0.00	0	[27]
73f	CH ₃ O + OH \rightleftharpoons CH ₂ O + H ₂ O	5.000E+12	0.00	0	[27]
74f	CH ₃ O + O \rightleftharpoons OH + CH ₂ O	1.000E+13	0.00	0	[27]
75f	CH ₃ O + O ₂ \rightarrow CH ₂ O + HO ₂	4.280E-13	7.60	-14.8	[27]
76f ^a	CH ₃ O + M ⁽⁹⁾ \rightleftharpoons CH ₂ O + H + M ⁽⁹⁾	7.780E+13	0.00	56.5	[10]
77f	C ₂ H ₆ + H \rightleftharpoons C ₂ H ₅ + H ₂	5.400E+02	3.50	21.8	[17]
78f	C ₂ H ₆ + O \rightleftharpoons C ₂ H ₅ + OH	1.400E+00	4.30	11.6	[17]
79f	C ₂ H ₆ + OH \rightleftharpoons C ₂ H ₅ + H ₂ O	2.200E+07	1.90	4.7	[17]
80f	C ₂ H ₆ + CH ₃ \rightleftharpoons C ₂ H ₅ + CH ₄	5.500E-01	4.00	34.7	[17]
81f ^{a,b}	C ₂ H ₆ + M ⁽⁸⁾ \rightleftharpoons C ₂ H ₅ + H + M ⁽⁸⁾	4.900E+42 k ₀	-6.43	448	[16, 12, 10]
		k _∞	-1.23	428	
82f	C ₂ H ₆ + HO ₂ \rightleftharpoons C ₂ H ₅ + H ₂ O ₂	1.320E+13	0.00	85.6	[14, 10]
83f	C ₂ H ₅ + H \rightleftharpoons C ₂ H ₄ + H ₂	3.000E+13	0.00	0	[17]
84f	C ₂ H ₅ + O \rightleftharpoons C ₂ H ₄ + OH	3.060E+13	0.00	0	[17]
85f	C ₂ H ₅ + O \rightleftharpoons CH ₃ + CH ₂ O	4.240E+13	0.00	0	[17]
86f	C ₂ H ₅ + O ₂ \rightleftharpoons C ₂ H ₄ + HO ₂	7.500E+14	-1.00	20.1	[28]
a86f	C ₂ H ₅ + O ₂ \rightleftharpoons C ₂ H ₄ OOH	2.000E+12	0.00	0	[28]
b86f	C ₂ H ₄ OOH \rightleftharpoons C ₂ H ₄ + HO ₂	4.000E+34	-7.20	96.2	[28]
c86f	C ₂ H ₄ OOH + O ₂ \rightleftharpoons OC ₂ H ₃ OOH + OH	7.500E+05	1.30	-24.3	[28]
d86f	OC ₂ H ₃ OOH \rightleftharpoons CH ₂ O + HCO + OH	1.000E+15	0.00	180	[28]
87f ^{a,b}	C ₂ H ₅ + M ⁽⁹⁾ \rightleftharpoons C ₂ H ₄ + H + M ⁽⁹⁾	3.990E+33 k ₀	-4.99	167	[29, 10]
		k _∞	1.110E+10	1.04	154
88f	C ₂ H ₄ + H \rightleftharpoons C ₂ H ₃ + H ₂	4.490E+07	2.12	55.9	[30]
89f	C ₂ H ₄ + OH \rightleftharpoons C ₂ H ₃ + H ₂ O	5.530E+05	2.31	12.4	[30]
90f	C ₂ H ₄ + O \rightleftharpoons CH ₃ + HCO	2.250E+06	2.08	0	[14]
91f	C ₂ H ₄ + O \rightleftharpoons CH ₂ CHO + H	1.210E+06	2.08	0	[14]
92f	2 C ₂ H ₄ \rightleftharpoons C ₂ H ₃ + C ₂ H ₅	5.010E+14	0.00	271	[31]

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93f	$\text{C}_2\text{H}_4 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_3 + \text{HO}_2$	4.220E+13	0.00	241	[32]
94f	$\text{C}_2\text{H}_4 + \text{HO}_2 \rightleftharpoons \text{C}_2\text{H}_4\text{O} + \text{OH}$	2.230E+12	0.00	71.9	[14]
95f	$\text{C}_2\text{H}_4\text{O} + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{CO} + \text{H}_2\text{O}_2$	4.000E+12	0.00	71.2	[14]
96f ^a	$\text{C}_2\text{H}_4 + \text{M}^{(9)} \rightleftharpoons \text{C}_2\text{H}_3 + \text{H} + \text{M}^{(9)}$	2.600E+17	0.00	404	[33, 10]
97f ^a	$\text{C}_2\text{H}_4 + \text{M}^{(9)} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}^{(9)}$	3.500E+16	0.00	299	[33, 10]
98f	$\text{C}_2\text{H}_3 + \text{H} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H}_2$	4.000E+13	0.00	0	[10]
99f ^{a,b}	$\text{C}_2\text{H}_3 + \text{M}^{(9)} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H} + \text{M}^{(9)}$	k_0	1.510E+14	0.10	137
		k_∞	6.380E+09	1.00	157
100f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HCO}$	1.700E+29	-5.31	27.2	[35]
101f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{CHO} + \text{O}$	7.000E+14	-0.61	22	[34, 35]
102f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_2 + \text{HO}_2$	5.190E+15	-1.26	13.9	[34, 35]
103f	$\text{C}_2\text{H}_2 + \text{O} \rightleftharpoons \text{HCCO} + \text{H}$	4.000E+14	0.00	44.6	[24]
104f	$\text{C}_2\text{H}_2 + \text{O} \rightleftharpoons \text{T-CH}_2 + \text{CO}$	1.600E+14	0.00	41.4	[24]
105f	$\text{C}_2\text{H}_2 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{CO}$	4.600E+15	-0.54	188	[36]
106f	$\text{C}_2\text{H}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}$	1.900E+07	1.70	4.18	[9, 37]
107f	$\text{C}_2\text{H}_2 + \text{OH} \rightleftharpoons \text{C}_2\text{H} + \text{H}_2\text{O}$	3.370E+07	2.00	58.6	[9, 37]
108f	$\text{CH}_2\text{CO} + \text{H} \rightleftharpoons \text{CH}_3 + \text{CO}$	1.500E+09	1.43	11.2	[38]
109f	$\text{CH}_2\text{CO} + \text{O} \rightleftharpoons \text{T-CH}_2 + \text{CO}_2$	2.000E+13	0.00	9.6	[9, 37]
110f	$\text{CH}_2\text{CO} + \text{O} \rightleftharpoons \text{HCCO} + \text{OH}$	1.000E+13	0.00	8.37	[9, 37]
111f	$\text{CH}_2\text{CO} + \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{CO}$	9.000E+10	0.00	0	[9, 37]
112f	$\text{HCCO} + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{CO}$	1.500E+14	0.00	0	[24]
113f	$\text{HCCO} + \text{OH} \rightleftharpoons \text{HCO} + \text{CO} + \text{H}$	2.000E+12	0.00	0	[39]
114f	$\text{HCCO} + \text{O} \rightleftharpoons 2 \text{ CO} + \text{H}$	9.640E+13	0.00	0	[24]
115f	$\text{HCCO} + \text{O}_2 \rightleftharpoons 2 \text{ CO} + \text{OH}$	2.880E+07	1.70	4.19	[34]
116f	$\text{HCCO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{CO} + \text{H}$	1.400E+07	1.70	4.19	[34]
117f	$\text{C}_2\text{H} + \text{OH} \rightleftharpoons \text{HCCO} + \text{H}$	2.000E+13	0.00	0	[17, 37]
118f	$\text{C}_2\text{H} + \text{O} \rightleftharpoons \text{CO} + \text{CH}$	1.020E+13	0.00	0	[17, 37]
119f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{HCCO} + \text{O}$	6.020E+11	0.00	0	[17, 37]
120f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{CH} + \text{CO}_2$	4.500E+15	0.00	105	[17, 37]
121f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{CO}$	2.410E+12	0.00	0	[17, 37]
122f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0	[27]
123f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_3 + \text{OH}$	2.500E+17	-0.93	21.5	[10]
124f	$\text{CH}_2\text{OH} + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2\text{O}$	2.400E+13	0.00	0	[27]
125f	$\text{CH}_2\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HO}_2$	5.000E+12	0.00	0	[27]
126f ^a	$\text{CH}_2\text{OH} + \text{M}^{(9)} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}^{(9)}$	5.000E+13	0.00	105	[27]
127f ^a	$\text{CH}_3\text{O} + \text{M}^{(9)} \rightleftharpoons \text{CH}_2\text{OH} + \text{M}^{(9)}$	1.000E+14	0.00	80	[27]

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128f	$\text{CH}_2\text{CO} + \text{OH} \rightleftharpoons \text{CH}_2\text{OH} + \text{CO}$	1.020E+13	0.00	0	[27]	
129f	$\text{CH}_3\text{OH} + \text{OH} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2\text{O}$	1.440E+06	2.00	-3.51	[27]	
130f	$\text{CH}_3\text{OH} + \text{OH} \rightleftharpoons \text{CH}_3\text{O} + \text{H}_2\text{O}$	4.400E+06	2.00	6.3	[10]	
131f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2$	1.354E+03	3.20	14.6	[40]	
132f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_3\text{O} + \text{H}_2$	6.830E+01	3.40	30.3	[40]	
133f	$\text{CH}_3\text{OH} + \text{O} \rightleftharpoons \text{CH}_2\text{OH} + \text{OH}$	1.000E+13	0.00	19.6	[27]	
134f	$\text{CH}_3\text{OH} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$	8.000E+13	0.00	81.1	[41, 42]	
135f	$\text{CH}_3\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{OH} + \text{HO}_2$	2.000E+13	0.00	188	[27]	
136f ^{a,b}	$\text{CH}_3\text{OH} + \text{M}^{(9)} \rightleftharpoons \text{CH}_3 + \text{OH} + \text{M}^{(9)}$	<i>k</i> ₀	2.950E+44	-7.35	399	[43, 10]
		<i>k</i> _∞	1.900E+16	0.00	384	
137f	$\text{CH}_2\text{CHO} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}$	1.047E+37	-7.19	186	[32]	
138f	$\text{CH}_2\text{CHO} + \text{H} \rightleftharpoons \text{CH}_3 + \text{HCO}$	5.000E+13	0.00	0	[13]	
139f	$\text{CH}_2\text{CHO} + \text{H} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}_2$	2.000E+13	0.00	0	[13]	
140f	$\text{CH}_2\text{CHO} + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{HCO}$	1.000E+14	0.00	0	[13]	
141f	$\text{CH}_2\text{CHO} + \text{OH} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}_2\text{O}$	3.000E+13	0.00	0	[13]	
142f	$\text{CH}_2\text{CHO} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{CO} + \text{OH}$	3.000E+10	0.00	0	[13]	
143f	$\text{CH}_2\text{CHO} + \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{CO} + \text{H}$	4.900E+14	-0.50	0	[13]	
144f	$\text{CH}_2\text{CHO} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HCO} + \text{OH}$	7.000E+12	0.00	0	[13]	
145f	$\text{CH}_2\text{CHO} + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{CHO} + \text{O}_2$	3.000E+12	0.00	0	[13]	
146f	$\text{CH}_2\text{CHO} \rightleftharpoons \text{CH}_3 + \text{CO}$	1.170E+43	-9.80	183	[13]	
147f	$\text{CH}_3\text{CHO} \rightleftharpoons \text{CH}_3 + \text{HCO}$	7.000E+15	0.00	342	[13]	
148f ^{a,b}	$\text{CH}_3\text{CO} + \text{M}^{(9)} \rightleftharpoons \text{CH}_3 + \text{CO} + \text{M}^{(9)}$	<i>k</i> ₀	1.200E+15	0.00	52.3	[13]
		<i>k</i> _∞	3.000E+12	0.00	69.9	
149f	$\text{CH}_3\text{CHO} + \text{OH} \rightleftharpoons \text{CH}_3\text{CO} + \text{H}_2\text{O}$	3.370E+12	0.00	-2.59	[13]	
150f	$\text{CH}_3\text{CHO} + \text{OH} \rightleftharpoons \text{CH}_2\text{CHO} + \text{H}_2\text{O}$	3.370E+11	0.00	-2.59	[13]	
151f	$\text{CH}_3\text{CHO} + \text{O} \rightleftharpoons \text{CH}_3\text{CO} + \text{OH}$	1.770E+18	-1.90	12.5	[13]	
152f	$\text{CH}_3\text{CHO} + \text{O} \rightleftharpoons \text{CH}_2\text{CHO} + \text{OH}$	3.720E+13	-0.20	14.9	[13]	
153f	$\text{CH}_3\text{CHO} + \text{H} \rightleftharpoons \text{CH}_3\text{CO} + \text{H}_2$	4.660E+13	-0.30	12.5	[13]	
154f	$\text{CH}_3\text{CHO} + \text{H} \rightleftharpoons \text{CH}_2\text{CHO} + \text{H}_2$	1.850E+12	0.40	22.4	[13]	
155f	$\text{CH}_3\text{CHO} + \text{CH}_3 \rightarrow \text{CH}_3\text{CO} + \text{CH}_4$	3.900E-07	5.80	9.21	[13]	
156f	$\text{CH}_3\text{CHO} + \text{CH}_3 \rightleftharpoons \text{CH}_2\text{CHO} + \text{CH}_4$	2.450E+01	3.10	24	[13]	
157f	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{CO} + \text{H}_2\text{O}_2$	3.600E+19	-2.20	58.6	[13]	
158f	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{CHO} + \text{H}_2\text{O}_2$	2.320E+11	0.40	62.3	[13]	
159f	$\text{CH}_3\text{CHO} + \text{O}_2 \rightleftharpoons \text{CH}_3\text{CO} + \text{HO}_2$	1.000E+14	0.00	177	[13]	
160f ^{a,b}	$\text{C}_2\text{H}_5\text{OH} + \text{M}^{(9)} \rightleftharpoons \text{CH}_3 + \text{CH}_2\text{OH} + \text{M}^{(9)}$	<i>k</i> ₀	3.000E+16	0.00	243	[10, 44]
		<i>k</i> _∞	5.000E+15	0.00	343	

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>	Ref.	
161f ^{a,b}	$C_2H_5OH + M^{(9)} \rightleftharpoons C_2H_4 + H_2O + M^{(9)}$	k_0	1.000E+17	0.00	226	[10, 44]
		k_∞	8.000E+13	0.00	272	
162f	$C_2H_5OH + OH \rightleftharpoons CH_2CH_2OH + H_2O$	1.810E+11	0.40	3	[13, 44]	
163f	$C_2H_5OH + OH \rightleftharpoons CH_3CHOH + H_2O$	3.090E+10	0.50	-1.59	[13, 44]	
164f	$C_2H_5OH + OH \rightleftharpoons CH_3CH_2O + H_2O$	1.050E+10	0.80	3	[13, 44]	
165f	$C_2H_5OH + H \rightleftharpoons CH_2CH_2OH + H_2$	1.900E+07	1.80	21.3	[13, 44]	
166f	$C_2H_5OH + H \rightleftharpoons CH_3CHOH + H_2$	2.580E+07	1.60	11.8	[13, 44]	
167f	$C_2H_5OH + H \rightleftharpoons CH_3CH_2O + H_2$	1.500E+07	1.60	12.7	[13, 44]	
168f	$C_2H_5OH + O \rightleftharpoons CH_2CH_2OH + OH$	9.410E+07	1.70	22.8	[13, 44]	
169f	$C_2H_5OH + O \rightleftharpoons CH_3CHOH + OH$	1.880E+07	1.90	7.62	[13, 44]	
170f	$C_2H_5OH + O \rightleftharpoons CH_3CH_2O + OH$	1.580E+07	2.00	18.6	[13, 44]	
171f	$C_2H_5OH + CH_3 \rightleftharpoons CH_2CH_2OH + CH_4$	2.190E+02	3.20	40.2	[13, 44]	
172f	$C_2H_5OH + CH_3 \rightleftharpoons CH_3CHOH + CH_4$	7.280E+02	3.00	33.3	[13, 44]	
173f	$C_2H_5OH + CH_3 \rightleftharpoons CH_3CH_2O + CH_4$	1.450E+02	3.00	32	[13, 44]	
174f	$C_2H_5OH + HO_2 \rightleftharpoons CH_3CHOH + H_2O_2$	8.200E+03	2.50	45.2	[13, 44]	
175f	$C_2H_5OH + HO_2 \rightleftharpoons CH_2CH_2OH + H_2O_2$	2.430E+04	2.50	66.1	[13, 44]	
176f	$C_2H_5OH + HO_2 \rightleftharpoons CH_3CH_2O + H_2O_2$	3.800E+12	0.00	100	[13, 44]	
177f	$C_2H_4 + OH \rightleftharpoons CH_2CH_2OH$	2.410E+11	0.00	-9.96	[13, 44]	
178f	$C_2H_5 + HO_2 \rightleftharpoons CH_3CH_2O + OH$	4.000E+13	0.00	0	[13, 44]	
179f ^a	$CH_3CH_2O + M^{(9)} \rightleftharpoons CH_3CHO + H + M^{(9)}$	5.600E+34	-5.90	106	[13, 44]	
180f ^a	$CH_3CH_2O + M^{(9)} \rightleftharpoons CH_3 + CH_2O + M^{(9)}$	5.350E+37	-7.00	99.6	[13, 44]	
181f	$CH_3CH_2O + O_2 \rightleftharpoons CH_3CHO + HO_2$	4.000E+10	0.00	4.6	[13, 44]	
182f	$CH_3CH_2O + CO \rightleftharpoons C_2H_5 + CO_2$	4.680E+02	3.20	22.5	[13, 44]	
183f	$CH_3CH_2O + H \rightleftharpoons CH_3 + CH_2OH$	3.000E+13	0.00	0	[13, 44]	
184f	$CH_3CH_2O + H \rightleftharpoons C_2H_4 + H_2O$	3.000E+13	0.00	0	[13, 44]	
185f	$CH_3CH_2O + OH \rightleftharpoons CH_3CHO + H_2O$	1.000E+13	0.00	0	[13, 44]	
186f	$CH_3CHOH + O_2 \rightleftharpoons CH_3CHO + HO_2$	4.820E+13	0.00	21	[13, 44]	
187f	$CH_3CHOH + O \rightleftharpoons CH_3CHO + OH$	1.000E+14	0.00	0	[13, 44]	
188f	$CH_3CHOH + H \rightleftharpoons C_2H_4 + H_2O$	3.000E+13	0.00	0	[13, 44]	
189f	$CH_3CHOH + H \rightleftharpoons CH_3 + CH_2OH$	3.000E+13	0.00	0	[13, 44]	
190f	$CH_3CHOH + HO_2 \rightleftharpoons CH_3CHO + 2 OH$	4.000E+13	0.00	0	[13, 44]	
191f	$CH_3CHOH + OH \rightleftharpoons CH_3CHO + H_2O$	5.000E+12	0.00	0	[13, 44]	
192f ^a	$CH_3CHOH + M^{(9)} \rightleftharpoons CH_3CHO + H + M^{(9)}$	1.000E+14	0.00	105	[13, 44]	
193f	$C_3H_4 + O \rightleftharpoons C_2H_4 + CO$	2.000E+07	1.80	4.18	[45]	
194f	$CH_3 + C_2H_2 \rightleftharpoons C_3H_4 + H$	2.560E+09	1.10	57.1	[45]	
195f	$C_3H_4 + O \rightleftharpoons HCCO + CH_3$	7.300E+12	0.00	9.41	[45]	

Number	Reaction		A	n	E	Ref.
196f ^{a,b}	$C_3H_3 + H + M \rightleftharpoons C_3H_4 + M$	k_0	9.000E+15	1.00	0	[38]
		k_∞	3.000E+13	0.00	0	
197f	$C_3H_3 + HO_2 \rightleftharpoons C_3H_4 + O_2$		2.500E+12	0.00	0	[38]
198f	$C_3H_4 + OH \rightleftharpoons C_3H_3 + H_2O$		5.300E+06	2.00	8.37	[46]
199f	$C_3H_3 + O_2 \rightleftharpoons CH_2CO + HCO$		3.000E+10	0.00	12	[47]
200f ^{a,b}	$C_3H_4 + H + M \rightleftharpoons C_3H_5 + M$	k_0	3.000E+24	-2.00	0	[38]
		k_∞	4.000E+13	0.00	0	
201f	$C_3H_5 + H \rightleftharpoons C_3H_4 + H_2$		1.800E+13	0.00	0	[48]
202f	$C_3H_5 + O_2 \rightleftharpoons C_3H_4 + HO_2$		4.990E+15	-1.40	93.8	[49]
203f	$C_3H_5 + CH_3 \rightleftharpoons C_3H_4 + CH_4$		3.000E+12	-0.32	-0.548	[38]
204f ^{a,b}	$C_2H_2 + CH_3 + M \rightleftharpoons C_3H_5 + M$	k_0	2.000E+09	1.00	0	[38]
		k_∞	6.000E+08	0.00	0	
205f	$C_3H_5 + OH \rightleftharpoons C_3H_4 + H_2O$		6.000E+12	0.00	0	[38]
206f	$C_3H_3 + HCO \rightleftharpoons C_3H_4 + CO$		2.500E+13	0.00	0	[46]
207f	$C_3H_3 + HO_2 \rightleftharpoons OH + CO + C_2H_3$		8.000E+11	0.00	0	[45]
208f	$C_3H_4 + O_2 \rightleftharpoons CH_3 + HCO + CO$		4.000E+14	0.00	175	[50]
209f	$C_3H_6 + O \rightleftharpoons C_2H_5 + HCO$		3.500E+07	1.65	-4.07	[48]
210f	$C_3H_6 + OH \rightleftharpoons C_3H_5 + H_2O$		3.100E+06	2.00	-1.25	[48]
211f	$C_3H_6 + O \rightleftharpoons CH_2CO + CH_3 + H$		1.200E+08	1.65	1.37	[48]
212f	$C_3H_6 + H \rightleftharpoons C_3H_5 + H_2$		1.700E+05	2.50	10.4	[48]
213f ^{a,b}	$C_3H_5 + H + M^{(8)} \rightleftharpoons C_3H_6 + M^{(8)}$	k_0	1.330E+60	-12.00	25	[45]
		k_∞	2.000E+14	0.00	0	
214f	$C_3H_5 + HO_2 \rightleftharpoons C_3H_6 + O_2$		2.660E+12	0.00	0	[14]
215f	$C_3H_5 + HO_2 \rightleftharpoons OH + C_2H_3 + CH_2O$		3.000E+12	0.00	0	[14]
216f ^{a,b}	$C_2H_3 + CH_3 + M^{(8)} \rightleftharpoons C_3H_6 + M^{(8)}$	k_0	4.270E+58	-11.94	40.9	[45]
		k_∞	2.500E+13	0.00	0	
217f	$C_3H_6 + H \rightleftharpoons C_2H_4 + CH_3$		1.600E+22	-2.39	46.8	[45]
218f	$CH_3 + C_2H_3 \rightleftharpoons C_3H_5 + H$		1.500E+24	-2.83	77.9	[45]
219f ^{a,b}	$C_3H_8 + M \rightleftharpoons CH_3 + C_2H_5 + M$	k_0	7.830E+18	0.00	272	[33]
		k_∞	1.100E+17	0.00	353	
220f	$C_3H_8 + O_2 \rightleftharpoons I-C_3H_7 + HO_2$		4.000E+13	0.00	199	[51, 45, 52]
221f	$C_3H_8 + O_2 \rightleftharpoons N-C_3H_7 + HO_2$		4.000E+13	0.00	213	[51, 45, 52]
222f	$C_3H_8 + H \rightleftharpoons I-C_3H_7 + H_2$		1.300E+06	2.40	18.7	[51, 45, 52]
223f	$C_3H_8 + H \rightleftharpoons N-C_3H_7 + H_2$		1.330E+06	2.54	28.3	[52, 53]
224f	$C_3H_8 + O \rightleftharpoons I-C_3H_7 + OH$		4.760E+04	2.71	8.82	[52, 45]
225f	$C_3H_8 + O \rightleftharpoons N-C_3H_7 + OH$		1.900E+05	2.68	15.6	[52, 45]

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>	Ref.
226f	$C_3H_8 + OH \rightleftharpoons N-C_3H_7 + H_2O$	1.000E+10	1.00	6.69	[28]
227f	$C_3H_8 + OH \rightleftharpoons I-C_3H_7 + H_2O$	2.000E+07	-1.60	-0.418	[28]
228f	$C_3H_8 + HO_2 \rightleftharpoons I-C_3H_7 + H_2O_2$	9.640E+03	2.60	58.2	[52, 53, 45]
229f	$C_3H_8 + HO_2 \rightleftharpoons N-C_3H_7 + H_2O_2$	4.760E+04	2.55	69	[52, 53, 45]
230f	$I-C_3H_7 + C_3H_8 \rightleftharpoons N-C_3H_7 + C_3H_8$	8.400E-03	4.20	36.3	[52, 54]
231 ^{a,b}	$C_3H_6 + H + M^{(8)} \rightleftharpoons I-C_3H_7 + M^{(8)}$	k_0	8.700E+42	-7.50	19.8
		k_∞	1.330E+13	0.00	6.53
232f	$I-C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.300E+11	0.00	0	[52, 45]
233 ^{a,b}	$N-C_3H_7 + M \rightleftharpoons CH_3 + C_2H_4 + M$	k_0	5.490E+49	-10.00	150
		k_∞	1.230E+13	-0.10	126
234 ^{a,b}	$H + C_3H_6 + M^{(8)} \rightleftharpoons N-C_3H_7 + M^{(8)}$	k_0	6.260E+38	-6.66	29.3
		k_∞	1.330E+13	0.00	13.6
235f	$N-C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	3.500E+16	-1.60	14.6	[28]
a235f	$N-C_3H_7 + O_2 \rightleftharpoons C_3H_6OOH$	2.000E+12	0.00	0	[28]
b235f	$C_3H_6OOH \rightleftharpoons C_3H_6 + HO_2$	2.500E+35	-8.30	92	[28]
c235f	$C_3H_6OOH + O_2 \rightleftharpoons OC_3H_5OOH + OH$	1.500E+08	0.00	-29.3	[28]
d235f	$OC_3H_5OOH \rightleftharpoons CH_2CHO + CH_2O + OH$	1.000E+15	0.00	180	[28]

Units are mol, cm³, kJ, K.

The backward rates for all reversible reactions can be calculated from thermodynamic data.

^aThird-body efficiencies are:

$$[M] = 1 \text{ [other].}$$

$$[M1] = 0.5 [AR] + 0.5 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 \text{ [other].}$$

$$[M2] = 0.38 [AR] + 0.38 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 \text{ [other].}$$

$$[M3] = 0.2 [AR] + 0.2 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 \text{ [other].}$$

$$[M4] = 0.75 [AR] + 0.75 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 \text{ [other].}$$

$$[M5] = 0.7 [AR] + 0.7 [HE] + 2.5 [H2] + 16 [H2O] + 1.2 [CO] + 2.4 [CO2] + 1.5 [C2H6] + 1 \text{ [other].}$$

$$[M6] = 0.7 [AR] + 0.4 [HE] + 2.5 [H2] + 6 [H2O] + 1.5 [CO] + 2 [CO2] + 1 \text{ [other].}$$

$$[M7] = 1.9 [H2] + 12 [H2O] + 2.5 [CO] + 2.5 [CO2] + 1 \text{ [other].}$$

$$[M8] = 0.7 [AR] + 2 [H2] + 6 [H2O] + 1.5 [CO] + 2 [CO2] + 2 [CH4] + 3 [C2H6] + 1 \text{ [other].}$$

$$[M9] = 0.7 [AR] + 2 [H2] + 6 [H2O] + 1.5 [CO] + 2 [CO2] + 2 [CH4] + 1 \text{ [other].}$$

$$[M10] = 2.4 [H2] + 15.4 [H2O] + 1.8 [CO] + 3.6 [CO2] + 1 \text{ [other].}$$

$$[M11] = 0.7 [AR] + 0.7 [HE] + 2.5 [H2] + 12 [H2O] + 2 [CO] + 4 [CO2] + 1 \text{ [other].}$$

^bPressure dependent reactions are described by the TROE-formulation [55]. The centering parameters are given by:

$$F_{c,10f} = 0.5.$$

$$F_{c,15f} = 1.$$

$$F_{c,16f} = 0.43.$$

$$F_{c,17f} = 1.$$

$$F_{c,20f} = 1.$$

$$F_{c,a21f} = 1.$$

$$F_{c,32f} = 0.2176 \exp(-T/271 \text{ K}) + 0.7824 \exp(-T/2755 \text{ K}) + \exp(-6570 \text{ K}/T).$$

$$F_{c,53f} = 0.217 \exp(-T/74 \text{ K}) + 0.783 \exp(-T/2941 \text{ K}) + \exp(-6964 \text{ K}/T).$$

$$F_{c,54f} = 0.38 \exp(-T/73 \text{ K}) + 0.62 \exp(-T/1180 \text{ K}).$$

$$F_{c,81f} = 0.16 \exp(-T/125 \text{ K}) + 0.84 \exp(-T/2219 \text{ K}) + \exp(-6882 \text{ K}/T).$$

$$F_{c,87f} = 0.832 \exp(-T/1203 \text{ K}).$$

$$F_{c,99f} = 0.7.$$

$$F_{c,136f} = 0.586 \exp(-T/279 \text{ K}) + 0.414 \exp(-T/5459 \text{ K}).$$

$$F_{c,148f} = 1.$$

$$F_{c,160f} = 0.5.$$

$$F_{c,161f} = 0.5.$$

$$F_{c,196f} = 0.5.$$

$$F_{c,200f} = 0.2.$$

$$F_{c,204f} = 0.5.$$

$$F_{c,213f} = 0.98 \exp(-T/1097 \text{ K}) + 0.02 \exp(-T/1097 \text{ K}) + \exp(-6860 \text{ K}/T).$$

$$F_{c,216f} = 0.825 \exp(-T/1341 \text{ K}) + 0.175 \exp(-T/60000 \text{ K}) + \exp(-10140 \text{ K}/T).$$

$$F_{c,219f} = 0.24 \exp(-T/1946 \text{ K}) + 0.76 \exp(-T/38 \text{ K}).$$

$$F_{c,231f} = \exp(-T/645.4 \text{ K}) + \exp(-6844 \text{ K}/T).$$

$$F_{c,233f} = 2.17 \exp(-T/251 \text{ K}) + \exp(-1185 \text{ K}/T).$$

$$F_{c,234f} = \exp(-T/1310 \text{ K}) + \exp(-48100 \text{ K}/T).$$

References

- [1] M.L. Rightley and F.A. Williams. Structures of co diffusion flames near extinction. *Combustion Science and Technology*, 125:181, 1997.
- [2] A. L. Sanchez and F. A. Williams. Recent advances in understanding of flammability characteristics of hydrogen. *Progress in Energy and Combustion Science*, pages 1–55, 2013.
- [3] P. Saxena and F. A. Williams. Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide. *Combustion and Flame*, In Press, 2006.
- [4] J. Troe. Detailed modeling of the temperature and pressure dependence of the reaction $\text{H} + \text{O}_2 (+\text{M}) \rightarrow \text{HO}_2 (+\text{M})$. *Proceedings of the Combustion Institute*, 28:1463–1469, 2000.
- [5] M. Mueller, T. Kim, R. Yetter, and F. Dryer. Flow reactor studies and kinetic modeling of the H_2/O_2 reaction. *International Journal of Chemical Kinetics*, 31:113–125, 1999.
- [6] J. Warnatz. *Combustion Chemistry*. Springer-Verlag, Berlin, 1984.
- [7] P. Saxena and F. A. Williams. Detailed and short mechanisms for syngas combustion. *2011 7th US National Combustion Meeting*, 2011.

- [8] R. A. Yetter, F. L. Dryer, and H. Rabitz. A comprehensive reaction mechanism for carbon monoxide/hydrogen/oxygen kinetics. *Combustion Science and Technology*, 79:97–128, 1991.
- [9] R. P. Lindstedt and G. Skevis. Chemistry of acetylene flames. *Combustion Science and Technology*, 125(1–6):73–137, 1997.
- [10] P. Saxena. *Numerical and Experimental Studies of Ethanol Flames and Autoignition Theory for Higher Alkanes*. PhD thesis, University of California at San Diego, 2007.
- [11] W. Tsang and R. F. Hampson. Chemical kinetic data base for combustion chemistry. part 1. methane and related compounds. *Journal of Physical and Chemical Reference Data*, 15:1087–1276, 1986.
- [12] Gri-mech 1.2. http://www.me.berkeley.edu/gri_mech/.
- [13] J. Li. *Experimental and Numerical Studies of Ethanol Chemical Kinetics*. PhD thesis, Princeton University, 2004.
- [14] D.L. Baulch, C.J. Cobos, R.A. Cox, C. Esser, P. Frank, T. Just, J.A. Kerr, M.J. Pilling, J. Troe, R.W. Walker, and J. Warnatz. Evaluated kinetic data for combustion modeling. *Journal of Physical and Chemical Reference Data*, 21(3):411–749, 1992.
- [15] B. Eiteneer, C. L. Yu, M. Goldenberg, and M. Frenklach. Determination of rate coefficients for reactions of formaldehyde pyrolysis and oxidation in the gas phase. *Journal of Physical Chemistry A*, 102:5196–5205, 1998.
- [16] J.C. Hewson and F.A. Williams. Rate-ratio asymptotic analysis of methane-air diffusion flame structure for predicting production of oxides of nitrogen. *Combustion and Flame*, 117(3):441–476, 1999.
- [17] M. Frenklach, H. Wang, and M. Rabinowitz. Optimization and analysis of large chemical kinetic mechanisms using the solution mapping method - combustion of methane. *Progress in Energy and Combustion Science*, 18(1):47–73, 1992.
- [18] S. C. Li and F. A. Williams. Reaction mechanisms for methane ignition. *Journal of Engineering for Gas Turbines and Power*, 124:471–480, 2002. ASME Paper No. 2000-GT-0145.
- [19] H. H. Grotheer, Kelm, Siegfried, H. S. T. Driver, R. J. Hutcheon, R. D. Lockett, and G. N. Robertson. Elementary reactions in the methanol oxidation system. part i: Establishment of the mechanism and modeling of laminar burning velocities. *Berichte der Bunsen-Gesellschaft – Physical Chemistry Chemical Physics*, 96:1360–1373, 1992.

- [20] R. Zellner and F. Ewig. Computational study of the $ch_3 + o_2$ chain branching reaction. *Journal of Physical Chemistry*, 92:2971–2974, 1988.
- [21] Y. Hidaka, T. Nakamura, H. Tanaka, K. Inami, and H. Kawano. High-temperature pyrolysis of methane in shock-waves - rates for dissociative recombination reactions of methyl radicals and for propyne formation reaction. *International Journal of Chemical Kinetics*, 22:701–709, 1990.
- [22] K.P. Lim and J.V. Michael. The thermal reactions of CH_3 . *Twenty-Fifth Symposium (International) on Combustion*, page 713, 1994.
- [23] K.M. Leung and R.P. Lindstedt. Detailed kinetic modeling of $C_1 - C_3$ alkane diffusion flames. *Combustion and Flame*, 102:129–160, 1995.
- [24] P. Frank, K.A. Bhaskaran, and T. Just. Acetylene oxidation: The reaction $C_2H_2 + O$ at high temperatures. In *Twenty-First Symposium (International) on Combustion*, page 885, Pittsburgh, Pennsylvania, 1986. The Combustion Institute.
- [25] N. Peters. Flame calculations with reduced mechanisms - an outline. In N. Peters and B. Rogg, editors, *Reduced Kinetic Mechanisms for Applications in Combustion Systems*, volume **m 15** of *Lecture Notes in Physics*, chapter 1, pages 3–14. Springer-Verlag Berlin, 1993.
- [26] M.W. Markus, P. Roth, and T. Just. A shock tube study of the reactions of ch with CO_2 and O_2 . *International Journal of Chemical Kinetics*, 28:171, 1996.
- [27] S.C. Li and Williams F.A. Formation of NO_x , CH_4 , and C_2 species in laminar methanol flames. *Proceedings of the Combustion Institute*, 27:485–493, 1998.
- [28] J. C. Prince and F. A. Williams. Short chemical-kinetic mechanisms for low-temperature ignition of propane and ethane. *Combustion and Flame*, 159:2236–2344, 2012.
- [29] Y. Feng, J. T. Niiranen, A. Bencsura, V. D. Knyazev, and D. Gutman. Weak collision effects in the reaction $C_2H_5 = C_2H_4 + H$. *Journal of Physical Chemistry*, 97(4):871–880, 1993.
- [30] A. Bhargava and P. R. Westmoreland. Measured flame structure and kinetics in a fuel-rich ethylene flame. *Combustion and Flame*, 113(3):333–347, 1998.
- [31] Y. Hidaka, T. Nishimori, K. Sato, Y. Henmi, R. Okuda, and K. Inami. Shock-tube and modeling study of ethylene pyrolysis and oxidation. *Combustion and Flame*, 117(4):755–776, 1999.
- [32] N. M. Marinov and P. C. Malte. Ethylene oxidation in a well-stirred reactor-stirred reactor. *International Journal of Chemical Kinetics*, 27(10):957–986, 1995.

- [33] D.L. Baulch, C.J. Cobos, R.A. Cox, C. Esser, P. Frank, T. Just, J.A. Kerr, M.J. Pilling, J. Troe, R.W. Walker, and J. Warnatz. Summary table of evaluated kinetic data for combustion modeling: Supplement 1. *Combustion and Flame*, 98:59–79, 1994.
- [34] B. Varatharajan and F. A. Williams. Chemical-kinetic descriptions of high-temperature ignition and detonation of acetylene-oxygen-diluent systems. *Combustion and Flame*, 124(4):624–645, 2001.
- [35] N. M. Marinov, W. J. Pitz, C. K. Westbrook, A. M. Vincitroe, M. J. Castaldi, S. M. Senkan, and C. F. Melius. Aromatic and polycyclic aromatic hydrocarbon formation in a laminar premixed n-butane flame. *Combustion and Flame*, 114:192–213, 1998.
- [36] A. Laskin and H. Wang. On initiation reactions of acetylene oxidation in shock tubes - a quantum mechanical and kinetic modeling study. *Chemical Physics Letters*, 303:43–49, 1999.
- [37] M. M. Y. Waly, S. M. A. Ibrahim, S. C. Li, and F. A. Williams. Structure of two-stage flames of natural gas with air. *Combustion and Flame*, 125(3):1217–1221, 2001.
- [38] M. Petrova and F. A. Williams. A small detailed chemical-kinetic mechanism for hydrocarbon combustion. *Combustion and Flame*, 144:526–544, 2006.
- [39] C.K. Westbrook and F.L. Dryer. Chemical kinetic modeling of hydrocarbon combustion. *Progress in Energy and Combustion Science*, 10:1–57, 1984.
- [40] J. T. Jodkowski, M. T. Rayez, J. C. Rayez, T. Berces, and S. Dobe. Theoretical study of the kinetics of the hydrogen abstraction from methanol. 3. reaction of methanol with hydrogen atom, methyl, and hydroxyl radicals. *Journal of Physical Chemistry A*, 103:3750–3765, 1999.
- [41] T. S. Norton and F. L. Dryer. Toward a comprehensive mechanism for methanol pyrolysis. *Journal of Chemical Kinetics*, 22:219–241, 1990.
- [42] R. Seiser, K. Seshadri, and F. A. Williams. Detailed and reduced chemistry for methanol ignition. *Combustion and Flame*, 2011.
- [43] T. Held and F. L. Dryer. A comprehensive mechanism for methanol oxidation. *International Journal of Chemical Kinetics*, 30:805–830, 1998.
- [44] P. Saxena and F. A. Williams. Numerical and experimental studies of ethanol flames. *Proceedings of the Combustion Institute*, 31(1):1149–1156, 2007.
- [45] S. G. Davis, C. K. Law, and H. Wang. Propene pyrolysis and oxidation kinetics in flow reactor and in laminar premixed flames. *Combustion and Flame*, 119:375–399, 1999.

- [46] H. Wang and M. Frenklach. A detailed kinetic modeling study of aromatics formation in laminar premixed acetylene and ethylene flames. *Combustion and Flame*, 110(1-2):173–221, 1997.
- [47] I. Slagle and D. Gutman. Kinetics of the reaction of c_3h_3 with molecular oxygen from 293-900 k . In *Twenty-First Symposium (International) on Combustion*, pages 875–883, Pittsburgh, Pennsylvania, 1986. The Combustion Institute.
- [48] W. Tsang. *Journal of Physical and Chemical Reference Data*, 20, 1991.
- [49] J. Bozelli and A. Dean. Hydrocarbon radical reactions with oxygen: Comparison of allyl, formyl, and vinyl to ethyl. *Journal of Physical Chemistry*, 97:4427–4441, 1993.
- [50] H. Wang. A new mechanism for initiation of free-radical chain reactions during high-temperature, homogeneous oxidation of unsaturated hydrocarbons: Ethylene, propyne and allene. *International Journal of Chemical Kinetics*, 33:698–706, 2001.
- [51] B. Varatharajan and F. A. Williams. Ignition times in the theory of branched-chain thermal explosions. *Combustion and Flame*, 121:551–554, 2000.
- [52] W. Tsang. Chemical kinetic data base for combustion chemistry. part 3. propane. *Journal of Physical and Chemical Reference Data*, 17(2):887–951, 1988.
- [53] N. M. Marinov, W. J. Pitz, C. K. Westbrook, M. J. Castald, and S. M. Senkan. Modeling of aromatic and polycyclic aromatic hydrocarbon formation in premixed methane and ethane flames. *Combustion Science and Technology*, 116–117:211–287, 1996.
- [54] Z. Qin. *Shock Tube Modeling Study of Propane Ignition*. PhD thesis, University of Texas at Austin, 1998.
- [55] R. G. Gilbert, K. Luther, and J. Troe. Theory of thermal unimolecular reactions in the fall-off range. ii. weak collision rate constants. *Ber. Bunsenges. Phys. Chem.*, 87:169–177, 1983.