

Number	Reaction	A	n	E	Ref.	
1f	$\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$	3.520E+16	-0.70	71.4	[1]	
2f	$\text{H}_2 + \text{O} \rightleftharpoons \text{OH} + \text{H}$	5.060E+04	2.67	26.3	[1]	
3f	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}$	1.170E+09	1.30	15.2	[1]	
4f	$\text{H}_2\text{O} + \text{O} \rightleftharpoons 2 \text{OH}$	7.600E+00	3.84	53.5	[1]	
a5f ^a	$\text{H} + \text{O} + \text{M}^{(1)} \rightleftharpoons \text{OH} + \text{M}^{(1)}$	4.710E+18	-1.00	0	[2, 3]	
5f ^a	$2 \text{H} + \text{M}^{(2)} \rightleftharpoons \text{H}_2 + \text{M}^{(2)}$	1.300E+18	-1.00	0	[4]	
6f ^a	$\text{H} + \text{OH} + \text{M}^{(3)} \rightleftharpoons \text{H}_2\text{O} + \text{M}^{(3)}$	4.000E+22	-2.00	0	[4]	
7f ^a	$2 \text{O} + \text{M}^{(4)} \rightleftharpoons \text{O}_2 + \text{M}^{(4)}$	6.170E+15	-0.50	0	[1]	
8f ^{a,b}	$\text{H} + \text{O}_2 + \text{M}^{(5)} \rightleftharpoons \text{HO}_2 + \text{M}^{(5)}$	k_0	5.750E+19	-1.40	0	[5]
		k_∞	4.650E+12	0.44	0	
a11f ^a	$\text{O} + \text{OH} + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$	1.000E+16	0.00	0	[6]	
9f	$\text{HO}_2 + \text{H} \rightleftharpoons 2 \text{OH}$	7.080E+13	0.00	1.23	[7]	
10f	$\text{HO}_2 + \text{H} \rightleftharpoons \text{H}_2 + \text{O}_2$	1.660E+13	0.00	3.44	[7]	
11f	$\text{HO}_2 + \text{H} \rightleftharpoons \text{H}_2\text{O} + \text{O}$	3.100E+13	0.00	7.2	[1]	
12f	$\text{HO}_2 + \text{O} \rightleftharpoons \text{OH} + \text{O}_2$	2.000E+13	0.00	0	[8]	
13f	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$	2.890E+13	0.00	-2.08	[1]	
14f ^{a,b}	$2 \text{OH} + \text{M}^{(6)} \rightleftharpoons \text{H}_2\text{O}_2 + \text{M}^{(6)}$	k_0	2.300E+18	-0.90	-7.12	[1]
		k_∞	7.400E+13	-0.37	0	
15f	$2 \text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$	3.020E+12	0.00	5.8	[1]	
16f	$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{HO}_2 + \text{H}_2$	4.790E+13	0.00	33.3	[2]	
17f	$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	1.000E+13	0.00	15	[2]	
18f	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$	7.080E+12	0.00	6	[1]	
19f	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$	9.550E+06	2.00	16.6	[1]	
s19f	$\text{CO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{O}$	1.000E+12	0.00	200	[4]	
20f	$\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$	4.400E+06	1.50	-3.1	[1]	
21f	$\text{CO} + \text{HO}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$	6.000E+13	0.00	96.2	[1]	
22f ^a	$\text{HCO} + \text{M}^{(7)} \rightleftharpoons \text{CO} + \text{H} + \text{M}^{(7)}$	1.860E+17	-1.00	71.1	[9]	
23f	$\text{HCO} + \text{H} \rightleftharpoons \text{CO} + \text{H}_2$	1.000E+14	0.00	0	[1]	
24f	$\text{HCO} + \text{O} \rightleftharpoons \text{CO} + \text{OH}$	3.000E+13	0.00	0	[1]	
25f	$\text{HCO} + \text{O} \rightleftharpoons \text{CO}_2 + \text{H}$	3.000E+13	0.00	0	[1]	
26f	$\text{HCO} + \text{OH} \rightleftharpoons \text{CO} + \text{H}_2\text{O}$	5.020E+13	0.00	0	[1]	
27f	$\text{HCO} + \text{O}_2 \rightleftharpoons \text{CO} + \text{HO}_2$	3.000E+12	0.00	0	[1]	
28f ^a	$\text{CH}_2\text{O} + \text{M}^{(8)} \rightleftharpoons \text{HCO} + \text{H} + \text{M}^{(8)}$	6.260E+16	0.00	326	[1]	
29f	$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{HCO} + \text{H}_2$	1.260E+08	1.62	9.06	[1]	
30f	$\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{HCO} + \text{OH}$	3.500E+13	0.00	14.7	[1]	
31f	$\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{HCO} + \text{H}_2\text{O}$	3.900E+10	0.89	1.7	[1]	

Number	Reaction	A	n	E	Ref.	
32f	$\text{CH}_4 + \text{H} \rightleftharpoons \text{H}_2 + \text{CH}_3$	1.300E+04	3.00	33.6	[10]	
33f	$\text{CH}_4 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6	[10]	
34f	$\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$	1.900E+09	1.44	36.3	[11]	
35f	$\text{CH}_4 + \text{O}_2 \rightleftharpoons \text{CH}_3 + \text{HO}_2$	3.980E+13	0.00	238	[9, 12]	
36f	$\text{CH}_4 + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}_2$	9.030E+12	0.00	103	[9, 12]	
37f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{T-CH}_2 + \text{H}_2$	1.800E+14	0.00	63.2	[11]	
38f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{H}_2$	1.550E+14	0.00	56.4	[11]	
39f	$\text{CH}_3 + \text{OH} \rightleftharpoons \text{S-CH}_2 + \text{H}_2\text{O}$	1.000E+13	0.00	10.5	[13]	
40f	$\text{CH}_3 + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	8.430E+13	0.00	0	[11]	
41f	$\text{CH}_3 + \text{T-CH}_2 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}$	4.220E+13	0.00	0	[14]	
42f	$\text{CH}_3 + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{OH}$	5.000E+12	0.00	0	[14]	
43f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4	[14]	
44f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{O}$	1.330E+14	0.00	131	[14]	
45f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}_2$	1.000E+14	0.00	134	[15]	
46f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}$	3.160E+13	0.00	61.5	[16]	
47f ^{a,b}	$\text{CH}_3 + \text{H} + \text{M} \rightleftharpoons \text{CH}_4 + \text{M}$	k_0	6.260E+23	-1.80	0	[17]
		k_∞	2.110E+14	0.00	0	
48f ^{a,b}	$2 \text{CH}_3 + \text{M} \rightleftharpoons \text{C}_2\text{H}_6 + \text{M}$	k_0	1.270E+41	-7.00	11.6	[10]
		k_∞	1.810E+13	0.00	0	
49f	$\text{S-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	3.000E+13	0.00	0	[11]	
50f	$\text{S-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH} + \text{H}$	3.130E+13	0.00	0	[11]	
51f	$\text{S-CH}_2 + \text{CO}_2 \rightleftharpoons \text{CO} + \text{CH}_2\text{O}$	3.000E+12	0.00	0	[18]	
52f ^a	$\text{S-CH}_2 + \text{M}^{(5)} \rightleftharpoons \text{T-CH}_2 + \text{M}^{(5)}$	6.000E+12	0.00	0	[11]	
53f	$\text{T-CH}_2 + \text{H} \rightleftharpoons \text{CH} + \text{H}_2$	6.020E+12	0.00	-7.48	[14]	
54f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	2.500E+13	0.00	0	[11]	
55f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH} + \text{H}_2\text{O}$	1.130E+07	2.00	12.6	[11]	
56f	$\text{T-CH}_2 + \text{O} \rightleftharpoons \text{CO} + 2 \text{H}$	8.000E+13	0.00	0	[19]	
57f	$\text{T-CH}_2 + \text{O} \rightleftharpoons \text{CO} + \text{H}_2$	4.000E+13	0.00	0	[19]	
58f	$\text{T-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{H}_2$	2.630E+12	0.00	6.24	[18]	
59f	$\text{T-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH} + \text{H}$	6.580E+12	0.00	6.24	[18]	
60f	$2 \text{T-CH}_2 \rightleftharpoons \text{C}_2\text{H}_2 + 2 \text{H}$	1.000E+14	0.00	0	[11]	
61f	$\text{CH} + \text{O} \rightleftharpoons \text{CO} + \text{H}$	4.000E+13	0.00	0	[20]	
62f	$\text{CH} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{O}$	1.770E+11	0.76	-2	[21]	
63f	$\text{CH} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	1.170E+15	-0.75	0	[18]	
64f	$\text{CH} + \text{CO}_2 \rightleftharpoons \text{HCO} + \text{CO}$	4.800E+01	3.22	-13.5	[21]	
70f	$\text{CH}_3\text{O} + \text{H} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$	2.000E+13	0.00	0	[22]	

Number	Reaction	A	n	E	Ref.	
71f	$\text{CH}_3\text{O} + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{H}_2\text{O}$	1.600E+13	0.00	0	[22]	
72f	$\text{CH}_3\text{O} + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2\text{O}$	5.000E+12	0.00	0	[22]	
73f	$\text{CH}_3\text{O} + \text{O} \rightleftharpoons \text{OH} + \text{CH}_2\text{O}$	1.000E+13	0.00	0	[22]	
74f	$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	4.280E-13	7.60	-14.8	[22]	
75f ^a	$\text{CH}_3\text{O} + \text{M} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}$	1.000E+13	0.00	56.5	[22]	
77f	$\text{C}_2\text{H}_6 + \text{H} \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}_2$	5.400E+02	3.50	21.8	[11]	
78f	$\text{C}_2\text{H}_6 + \text{O} \rightleftharpoons \text{C}_2\text{H}_5 + \text{OH}$	1.400E+00	4.30	11.6	[11]	
79f	$\text{C}_2\text{H}_6 + \text{OH} \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}_2\text{O}$	2.200E+07	1.90	4.7	[11]	
80f	$\text{C}_2\text{H}_6 + \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_4$	5.500E-01	4.00	34.7	[11]	
81f ^{a,b}	$\text{C}_2\text{H}_6 + \text{M} \rightleftharpoons \text{C}_2\text{H}_5 + \text{H} + \text{M}$	k_0	4.900E+42	-6.43	448	[10]
		k_∞	8.850E+20	-1.23	428	
82f	$\text{C}_2\text{H}_5 + \text{H} \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}_2$	3.000E+13	0.00	0	[11]	
83f	$\text{C}_2\text{H}_5 + \text{O} \rightleftharpoons \text{C}_2\text{H}_4 + \text{OH}$	3.060E+13	0.00	0	[11]	
84f	$\text{C}_2\text{H}_5 + \text{O} \rightleftharpoons \text{CH}_3 + \text{CH}_2\text{O}$	4.240E+13	0.00	0	[11]	
85f	$\text{C}_2\text{H}_5 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_4 + \text{HO}_2$	2.000E+12	0.00	20.9	[11]	
86f	$\text{C}_2\text{H}_5 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}$	k_0	3.990E+33	-4.99	167	[23]
		k_∞	1.110E+10	1.04	154	
87f	$\text{C}_2\text{H}_4 + \text{H} \rightleftharpoons \text{C}_2\text{H}_3 + \text{H}_2$	4.490E+07	2.12	55.9	[24]	
88f	$\text{C}_2\text{H}_4 + \text{OH} \rightleftharpoons \text{C}_2\text{H}_3 + \text{H}_2\text{O}$	5.530E+05	2.31	12.4	[24]	
89f	$\text{C}_2\text{H}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{HCO}$	2.250E+06	2.08	0	[14]	
90f	$\text{C}_2\text{H}_4 + \text{O} \rightleftharpoons \text{CH}_2\text{CHO} + \text{H}$	1.210E+06	2.08	0	[14]	
91f	$2 \text{C}_2\text{H}_4 \rightleftharpoons \text{C}_2\text{H}_3 + \text{C}_2\text{H}_5$	5.010E+14	0.00	271	[25]	
92f	$\text{C}_2\text{H}_4 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_3 + \text{HO}_2$	4.220E+13	0.00	241	[26]	
93f	$\text{C}_2\text{H}_4 + \text{HO}_2 \rightleftharpoons \text{C}_2\text{H}_4\text{O} + \text{OH}$	2.230E+12	0.00	71.9	[14]	
s93f	$\text{C}_2\text{H}_4\text{O} + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{CO} + \text{H}_2\text{O}_2$	4.000E+12	0.00	71.2	[14]	
94f ^a	$\text{C}_2\text{H}_4 + \text{M} \rightleftharpoons \text{C}_2\text{H}_3 + \text{H} + \text{M}$	2.600E+17	0.00	404	[17]	
95f ^a	$\text{C}_2\text{H}_4 + \text{M} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}$	3.500E+16	0.00	299	[17]	
96f	$\text{C}_2\text{H}_3 + \text{H} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H}_2$	1.210E+13	0.00	0	[17]	
97f ^{a,b}	$\text{C}_2\text{H}_3 + \text{M} \rightleftharpoons \text{C}_2\text{H}_2 + \text{H} + \text{M}$	k_0	1.510E+14	0.10	137	[27]
		k_∞	6.380E+09	1.00	157	
98f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HCO}$	1.700E+29	-5.31	27.2	[28]	
99f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{CHO} + \text{O}$	7.000E+14	-0.61	22	[27, 28]	
100f	$\text{C}_2\text{H}_3 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_2 + \text{HO}_2$	5.190E+15	-1.26	13.9	[27, 28]	
101f	$\text{CH}_2\text{CHO} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}$	1.047E+37	-7.19	186	[26]	
102f	$\text{C}_2\text{H}_2 + \text{O} \rightleftharpoons \text{HCCO} + \text{H}$	4.000E+14	0.00	44.6	[19]	
103f	$\text{C}_2\text{H}_2 + \text{O} \rightleftharpoons \text{T-CH}_2 + \text{CO}$	1.600E+14	0.00	41.4	[19]	

Number	Reaction	A	n	E	Ref.
104f	$\text{C}_2\text{H}_2 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{CO}$	4.600E+15	-0.54	188	[29]
105f	$\text{C}_2\text{H}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{CO} + \text{H}$	1.900E+07	1.70	4.18	[9, 30]
106f	$\text{C}_2\text{H}_2 + \text{OH} \rightleftharpoons \text{C}_2\text{H} + \text{H}_2\text{O}$	3.370E+07	2.00	58.6	[9, 30]
107f	$\text{CH}_2\text{CO} + \text{H} \rightleftharpoons \text{CH}_3 + \text{CO}$	1.500E+09	1.43	11.2	[9, 30]
108f	$\text{CH}_2\text{CO} + \text{O} \rightleftharpoons \text{T-CH}_2 + \text{CO}_2$	2.000E+13	0.00	9.6	[9, 30]
109f	$\text{CH}_2\text{CO} + \text{O} \rightleftharpoons \text{HCCO} + \text{OH}$	1.000E+13	0.00	8.37	[9, 30]
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, 30]
112f	$\text{HCCO} + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{CO}$	1.500E+14	0.00	0	[19]
113f	$\text{HCCO} + \text{OH} \rightleftharpoons \text{HCO} + \text{CO} + \text{H}$	2.000E+12	0.00	0	[31]
114f	$\text{HCCO} + \text{O} \rightleftharpoons 2 \text{CO} + \text{H}$	9.640E+13	0.00	0	[19]
115f	$\text{HCCO} + \text{O}_2 \rightleftharpoons 2 \text{CO} + \text{OH}$	2.880E+07	1.70	4.19	[27]
116f	$\text{HCCO} + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{CO} + \text{H}$	1.400E+07	1.70	4.19	[27]
117f	$\text{C}_2\text{H} + \text{OH} \rightleftharpoons \text{HCCO} + \text{H}$	2.000E+13	0.00	0	[11, 30]
118f	$\text{C}_2\text{H} + \text{O} \rightleftharpoons \text{CO} + \text{CH}$	1.020E+13	0.00	0	[11, 30]
119f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{HCCO} + \text{O}$	6.020E+11	0.00	0	[11, 30]
120f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{CH} + \text{CO}_2$	4.500E+15	0.00	105	[11, 30]
121f	$\text{C}_2\text{H} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{CO}$	2.410E+12	0.00	0	[11, 30]
65f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0	[22]
66f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_3 + \text{OH}$	1.750E+14	0.00	11.7	[22]
67f	$\text{CH}_2\text{OH} + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2\text{O}$	2.400E+13	0.00	0	[22]
68f	$\text{CH}_2\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HO}_2$	5.000E+12	0.00	0	[22]
69f ^a	$\text{CH}_2\text{OH} + \text{M}^{(5)} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}^{(5)}$	5.000E+13	0.00	105	[22]
76f ^a	$\text{CH}_3\text{O} + \text{M}^{(9)} \rightleftharpoons \text{CH}_2\text{OH} + \text{M}^{(9)}$	1.000E+14	0.00	80	[22]
110f	$\text{CH}_2\text{CO} + \text{OH} \rightleftharpoons \text{CH}_2\text{OH} + \text{CO}$	1.020E+13	0.00	0	[22]
m1f	$\text{CH}_3\text{OH} + \text{OH} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2\text{O}$	1.440E+06	2.00	-3.51	[22]
m2f	$\text{CH}_3\text{OH} + \text{OH} \rightleftharpoons \text{CH}_3\text{O} + \text{H}_2\text{O}$	6.300E+06	2.00	6.3	[22]
m3f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2$	1.640E+07	2.00	18.9	[22]
m4f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_3\text{O} + \text{H}_2$	3.830E+07	2.00	24.5	[22]
m5f	$\text{CH}_3\text{OH} + \text{O} \rightleftharpoons \text{CH}_2\text{OH} + \text{OH}$	1.000E+13	0.00	19.6	[22]
m6f	$\text{CH}_3\text{OH} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$	6.200E+12	0.00	81.1	[22]
m7f	$\text{CH}_3\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{OH} + \text{HO}_2$	2.000E+13	0.00	188	[22]
c1f	$\text{C}_3\text{H}_4 + \text{O} \rightleftharpoons \text{C}_2\text{H}_4 + \text{CO}$	2.000E+07	1.80	4.18	[32]
c2f	$\text{CH}_3 + \text{C}_2\text{H}_2 \rightleftharpoons \text{C}_3\text{H}_4 + \text{H}$	2.560E+09	1.10	57.1	[32]
c3f	$\text{C}_3\text{H}_4 + \text{O} \rightleftharpoons \text{HCCO} + \text{CH}_3$	7.300E+12	0.00	9.41	[32]
c6f	$\text{C}_3\text{H}_3 + \text{H} \rightleftharpoons \text{C}_3\text{H}_4$	k_0 k_∞	1.00 0.00	0 0	[33]

Number	Reaction		A	n	E	Ref.
c8f	$C_3H_3 + HO_2 \rightleftharpoons C_3H_4 + O_2$		2.500E+12	0.00	0	[33]
c9f	$C_3H_4 + OH \rightleftharpoons C_3H_3 + H_2O$		5.300E+06	2.00	8.37	[34]
c10f	$C_3H_3 + O_2 \rightleftharpoons CH_2CO + HCO$		3.000E+10	0.00	12	[35]
c11f ^{a,b}	$C_3H_4 + H + M \rightleftharpoons C_3H_5 + M$	k_0	3.000E+24	-2.00	0	[33]
		k_∞	4.000E+13	0.00	0	
c12f	$C_3H_5 + H \rightleftharpoons C_3H_4 + H_2$		1.800E+13	0.00	0	[36]
c13f	$C_3H_5 + O_2 \rightleftharpoons C_3H_4 + HO_2$		4.990E+15	-1.40	93.8	[37]
c14f	$C_3H_5 + CH_3 \rightleftharpoons C_3H_4 + CH_4$		3.000E+12	-0.32	-0.548	[33]
c15f ^{a,b}	$C_2H_2 + CH_3 + M \rightleftharpoons C_3H_5 + M$	k_0	2.000E+09	1.00	0	[33]
		k_∞	6.000E+08	0.00	0	
c16f	$C_3H_5 + OH \rightleftharpoons C_3H_4 + H_2O$		6.000E+12	0.00	0	[33]
c18f	$C_3H_3 + HCO \rightleftharpoons C_3H_4 + CO$		2.500E+13	0.00	0	[34]
c20f	$C_3H_3 + HO_2 \rightleftharpoons OH + CO + C_2H_3$		8.000E+11	0.00	0	[32]
c21f	$C_3H_4 + O_2 \rightleftharpoons CH_3 + HCO + CO$		4.000E+14	0.00	175	[38]
140f	$C_3H_6 + O \rightleftharpoons C_2H_5 + HCO$		3.500E+07	1.65	-4.07	[36]
142f	$C_3H_6 + OH \rightleftharpoons C_3H_5 + H_2O$		3.100E+06	2.00	-1.25	[36]
e3f	$C_3H_6 + O \rightleftharpoons CH_2CO + CH_3 + H$		1.200E+08	1.65	1.37	[36]
138f	$C_3H_6 + H \rightleftharpoons C_3H_5 + H_2$		1.700E+05	2.50	10.4	[36]
136f ^{a,b}	$C_3H_5 + H + M^{(10)} \rightleftharpoons C_3H_6 + M^{(10)}$	k_0	1.330E+60	-12.00	25	[32]
		k_∞	2.000E+14	0.00	0	
e1f	$C_3H_5 + HO_2 \rightleftharpoons C_3H_6 + O_2$		2.660E+12	0.00	0	[14]
e2f	$C_3H_5 + HO_2 \rightleftharpoons OH + C_2H_3 + CH_2O$		3.000E+12	0.00	0	[14]
137f ^{a,b}	$C_2H_3 + CH_3 + M^{(10)} \rightleftharpoons C_3H_6 + M^{(10)}$	k_0	4.270E+58	-11.94	40.9	[32]
		k_∞	2.500E+13	0.00	0	
e4f	$C_3H_6 + H \rightleftharpoons C_2H_4 + CH_3$		1.600E+22	-2.39	46.8	[32]
e5f	$CH_3 + C_2H_3 \rightleftharpoons C_3H_5 + H$		1.500E+24	-2.83	77.9	[32]
p1f ^{a,b}	$C_3H_8 + M \rightleftharpoons CH_3 + C_2H_5 + M$	k_0	7.830E+18	0.00	272	[17]
		k_∞	1.100E+17	0.00	353	
p2f	$C_3H_8 + O_2 \rightleftharpoons I-C_3H_7 + HO_2$		4.000E+13	0.00	199	[39, 32, 40]
p3f	$C_3H_8 + O_2 \rightleftharpoons N-C_3H_7 + HO_2$		4.000E+13	0.00	213	[39, 32, 40]
p4f	$C_3H_8 + H \rightleftharpoons I-C_3H_7 + H_2$		1.300E+06	2.40	18.7	[39, 32, 40]
p5f	$C_3H_8 + H \rightleftharpoons N-C_3H_7 + H_2$		1.330E+06	2.54	28.3	[40, 41]
p6f	$C_3H_8 + O \rightleftharpoons I-C_3H_7 + OH$		4.760E+04	2.71	8.82	[40, 32]
p7f	$C_3H_8 + O \rightleftharpoons N-C_3H_7 + OH$		1.900E+05	2.68	15.6	[40, 32]
p8f	$C_3H_8 + OH \rightleftharpoons N-C_3H_7 + H_2O$		1.400E+03	2.66	2.21	[32]
p9f	$C_3H_8 + OH \rightleftharpoons I-C_3H_7 + H_2O$		2.700E+04	2.39	1.65	[32]

Number	Reaction	A	n	E	Ref.	
p10f	$C_3H_8 + HO_2 \rightleftharpoons I-C_3H_7 + H_2O_2$	9.640E+03	2.60	58.2	[40, 41, 32]	
p11f	$C_3H_8 + HO_2 \rightleftharpoons N-C_3H_7 + H_2O_2$	4.760E+04	2.55	69	[40, 41, 32]	
p12f	$I-C_3H_7 + C_3H_8 \rightleftharpoons N-C_3H_7 + C_3H_8$	8.400E-03	4.20	36.3	[40, 42]	
p13f ^{a,b}	$C_3H_6 + H + M^{(10)} \rightleftharpoons I-C_3H_7 + M^{(10)}$	k_0	8.700E+42	-7.50	19.8	[32]
		k_∞	1.330E+13	0.00	6.53	
p14f	$I-C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.300E+11	0.00	0	[40, 32]	
p15f ^{a,b}	$N-C_3H_7 + M \rightleftharpoons CH_3 + C_2H_4 + M$	k_0	5.490E+49	-10.00	150	[40, 32]
		k_∞	1.230E+13	-0.10	126	
p16f ^{a,b}	$H + C_3H_6 + M^{(10)} \rightleftharpoons N-C_3H_7 + M^{(10)}$	k_0	6.260E+38	-6.66	29.3	[40, 32]
		k_∞	1.330E+13	0.00	13.6	
p17f	$N-C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	9.000E+10	0.00	0	[40, 32]	

Units are mol, cm³, kJ, K.

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

^aThird-body efficiencies are:

$$[M1] = 0.75 [AR] + 0.75 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

$$[M2] = 0.5 [AR] + 0.5 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

$$[M3] = 0.38 [AR] + 0.38 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

$$[M4] = 0.2 [AR] + 0.2 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

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

$$[M] = 1 [other].$$

$$[M6] = 0.7 [AR] + 0.7 [HE] + 2 [H2] + 6 [H2O] + 1.5 [CO] + 2 [CO2] + 2 [CH4] + 3 [C2H6] + 1 [other].$$

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

$$[M8] = 2.5 [H2] + 16.3 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

$$[M9] = 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

$$[M10] = 0.7 [AR] + 2 [H2] + 6 [H2O] + 1.5 [CO] + 2 [CO2] + 2 [CH4] + 3 [C2H6] + 1 [other].$$

^bPressure dependent reactions are described by the TROE-formulation [43]. The centering parameters are given by:

$$F_{c,8f} = 0.5.$$

$$F_{c,14f} = 0.265 \exp(-T/94 \text{ K}) + 0.735 \exp(-T/1756 \text{ K}) + \exp(-5182 \text{ K}/T).$$

$$F_{c,47f} = 0.63 \exp(-T/3315 \text{ K}) + 0.37 \exp(-T/61 \text{ K}).$$

$$F_{c,48f} = 0.38 \exp(-T/73 \text{ K}) + 0.62 \exp(-T/1180 \text{ K}).$$

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

$$F_{c,86f} = 0.832 \exp(-T/1203 \text{ K}).$$

$$F_{c,97f} = 0.7.$$

$$F_{c,c6f} = 0.5.$$

$$F_{c,c11f} = 0.2 \exp(-T/1e+15 \text{ K}).$$

$$F_{c,c15f} = 0.5 \exp(-T/1e+15 \text{ K}).$$

$$F_{c,136f} = 0.98 \exp(-T/1097 \text{ K}) + 0.02 \exp(-T/1097 \text{ K}) + \exp(-6860 \text{ K}/T).$$

$$F_{c,137f} = 0.825 \exp(-T/1341 \text{ K}) + 0.175 \exp(-T/60000 \text{ K}) + \exp(-10140 \text{ K}/T).$$

$$F_{c,p1f} = 0.24 \exp(-T/1946 \text{ K}) + 0.76 \exp(-T/38 \text{ K}).$$

$$F_{c,p13f} = \exp(-T/645.4 \text{ K}) + \exp(-6844.3 \text{ K}/T).$$

$$F_{c,p15f} = 2.17 \exp(-T/251 \text{ K}) + \exp(-1185 \text{ K}/T).$$

$$F_{c,p16f} = \exp(-T/1310 \text{ K}) + \exp(-48097 \text{ K}/T).$$

References

- [1] M.L. Rightley and F.A. Williams. Structures of co diffusion flames near extinction. *Combustion Science and Technology*, 125:181, 1997.
- [2] 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.
- [3] G. Balakrishnan and F. A. Williams. Turbulent combustion regimes for hypersonic propulsion employing hydrogen-air diffusion flames. *Journal of Propulsion and Power*, 10(3):434–437, 1994.
- [4] P. Saxena and F. A. Williams. Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide. *submitted for publication*, 2005.
- [5] 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.
- [6] E. Gutheil, G. Balakrishnan, and F. A. Williams. Structure and extinction of hydrogen-air diffusion flames. In N. Peters and B. Rogg, editors, *Reduced Kinetic Mechanisms for Applications in Combustion Systems*, chapter 11. Springer-Verlag Berlin, 1993.
- [7] 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.
- [8] J. Warnatz. *Combustion Chemistry*. Springer-Verlag, Berlin, 1984.
- [9] R. P. Lindstedt and G. Skevis. Chemistry of acetylene flames. *Combustion Science and Technology*, 125(1–6):73–137, 1997.
- [10] 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.
- [11] 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.
- [12] 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.
- [13] S. C. Li and F. A. Williams. Nox formation in two-stage methane-air flames. *Combustion and Flame*, 118(3):399–414, 1999.

- [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] 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.
- [16] K.P. Lim and J.V. Michael. The thermal reactions of CH_3 . *Twenty-Fifth Symposium (International) on Combustion*, page 713, 1994.
- [17] 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.
- [18] K.M. Leung and R.P. Lindstedt. Detailed kinetic modeling of $\text{C}_1 - \text{C}_3$ alkane diffusion flames. *Combustion and Flame*, 102:129–160, 1995.
- [19] P. Frank, K.A. Bhaskaran, and T. Just. Acetylene oxidation: The reaction $\text{C}_2\text{H}_2 + \text{O}$ at high temperatures. In *Twenty-First Symposium (International) on Combustion*, page 885, Pittsburgh, Pennsylvania, 1986. The Combustion Institute.
- [20] 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.
- [21] 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.
- [22] 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.
- [23] Y. Feng, J. T. Niiranen, A. Bencsura, V. D. Knyazev, and D. Gutman. Weak collision effects in the reaction $\text{C}_2\text{H}_5 = \text{C}_2\text{H}_4 + \text{H}$. *Journal of Physical Chemistry*, 97(4):871–880, 1993.
- [24] 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.
- [25] 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.

- [26] 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.
- [27] 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.
- [28] 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.
- [29] 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.
- [30] 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.
- [31] C.K. Westbrook and F.L. Dryer. Chemical kinetic modeling of hydrocarbon combustion. *Progress in Energy and Combustion Science*, 10:1–57, 1984.
- [32] 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.
- [33] M. Petrova and F. A. Williams. A small detailed chemical-kinetic mechanism for hydrocarbon combustion. *submitted for publication*, 2005.
- [34] 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.
- [35] 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.
- [36] W. Tsang. *Journal of Physical and Chemical Reference Data*, 20, 1991.
- [37] 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.
- [38] 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.
- [39] B. Varatharajan and F. A. Williams. Ignition times in the theory of branched-chain thermal explosions. *Combustion and Flame*, 121:551–554, 2000.

- [40] W. Tsang. Chemical kinetic data base for combustion chemistry. part 3. propane. *Journal of Physical and Chemical Reference Data*, 17(2):887–951, 1988.
- [41] 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.
- [42] Z. W. Qin. *Shock Tube Modeling Study of Propane Ignition*. PhD thesis, University of Texas, 1998.
- [43] 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.