

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 <sup>a</sup>	$\text{H} + \text{O} + \text{M}^{(2)} \rightleftharpoons \text{OH} + \text{M}^{(2)}$	6.200E+16	-0.60	0	[2, 3]	
a6f	$\text{H}_2 + \text{O}_2 \rightleftharpoons 2 \text{OH}$	1.700E+13	0.00	200	[4, 3]	
5f <sup>a</sup>	$2 \text{H} + \text{M}^{(1)} \rightleftharpoons \text{H}_2 + \text{M}^{(1)}$	7.200E+17	-1.00	0	[1]	
6f <sup>a</sup>	$\text{H} + \text{OH} + \text{M}^{(2)} \rightleftharpoons \text{H}_2\text{O} + \text{M}^{(2)}$	2.200E+22	-2.00	0	[1]	
7f <sup>a</sup>	$2 \text{O} + \text{M}^{(2)} \rightleftharpoons \text{O}_2 + \text{M}^{(2)}$	6.170E+15	-0.50	0	[1]	
8f <sup>a,b</sup>	$\text{H} + \text{O}_2 + \text{M}^{(6)} \rightleftharpoons \text{HO}_2 + \text{M}^{(6)}$	$k_0$	2.600E+19	-1.20	0	[5, 6]
		$k_\infty$	4.650E+12	0.44	0	
a11f <sup>a</sup>	$\text{O} + \text{OH} + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$	1.000E+16	0.00	0	[4, 3]	
9f	$\text{HO}_2 + \text{H} \rightleftharpoons 2 \text{OH}$	1.700E+14	0.00	3.66	[1]	
10f	$\text{HO}_2 + \text{H} \rightleftharpoons \text{H}_2 + \text{O}_2$	4.280E+13	0.00	5.9	[1]	
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	[1]	
13f	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$	2.890E+13	0.00	-2.08	[1]	
14f <sup>a,b</sup>	$2 \text{OH} + \text{M}^{(7)} \rightleftharpoons \text{H}_2\text{O}_2 + \text{M}^{(7)}$	$k_0$	2.300E+18	-0.90	-7.12	[5]
		$k_\infty$	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	[1]	
17f	$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	1.000E+13	0.00	15	[1]	
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	$\text{H}_2\text{O}_2 + \text{O} \rightleftharpoons \text{HO}_2 + \text{OH}$	9.630E+06	2.00	16.7	[1]	
20f	$\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$	4.400E+06	1.50	-3.1	[1]	
21f	$\text{CO} + \text{HO}_2 \rightleftharpoons \text{CO}_2 + \text{OH}$	6.030E+13	0.00	96	[1]	
22f <sup>a</sup>	$\text{CHO} + \text{M}^{(4)} \rightleftharpoons \text{CO} + \text{H} + \text{M}^{(4)}$	1.860E+17	-1.00	71.1	[7]	
23f	$\text{CHO} + \text{H} \rightleftharpoons \text{CO} + \text{H}_2$	1.000E+14	0.00	0	[1]	
24f	$\text{CHO} + \text{O} \rightleftharpoons \text{CO} + \text{OH}$	3.000E+13	0.00	0	[1]	
25f	$\text{CHO} + \text{O} \rightleftharpoons \text{CO}_2 + \text{H}$	3.000E+13	0.00	0	[1]	
26f	$\text{CHO} + \text{OH} \rightleftharpoons \text{CO} + \text{H}_2\text{O}$	5.020E+13	0.00	0	[1]	
27f	$\text{CHO} + \text{O}_2 \rightleftharpoons \text{CO} + \text{HO}_2$	3.000E+12	0.00	0	[1]	
28f <sup>a</sup>	$\text{CH}_2\text{O} + \text{M}^{(1)} \rightleftharpoons \text{CHO} + \text{H} + \text{M}^{(1)}$	6.260E+16	0.00	326	[1]	
29f	$\text{CH}_2\text{O} + \text{H} \rightleftharpoons \text{CHO} + \text{H}_2$	1.260E+08	1.62	9.06	[1]	
30f	$\text{CH}_2\text{O} + \text{O} \rightleftharpoons \text{CHO} + \text{OH}$	3.500E+13	0.00	14.7	[1]	
31f	$\text{CH}_2\text{O} + \text{OH} \rightleftharpoons \text{CHO} + \text{H}_2\text{O}$	3.900E+10	0.89	1.7	[1]	

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32f	$\text{CH}_4 + \text{H} \rightleftharpoons \text{H}_2 + \text{CH}_3$	1.300E+04	3.00	33.6	[8]
33f	$\text{CH}_4 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6	[8]
34f	$\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$	1.900E+09	1.44	36.3	[9]
35f	$\text{CH}_4 + \text{O}_2 \rightleftharpoons \text{CH}_3 + \text{HO}_2$	3.980E+13	0.00	238	[7, 10]
36f	$\text{CH}_4 + \text{HO}_2 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}_2$	9.030E+12	0.00	103	[7, 10]
37f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{T-CH}_2 + \text{H}_2$	1.800E+14	0.00	63.2	[9]
38f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{H}_2$	1.550E+14	0.00	56.4	[9]
39f	$\text{CH}_3 + \text{OH} \rightleftharpoons \text{S-CH}_2 + \text{H}_2\text{O}$	1.000E+13	0.00	10.5	[11]
40f	$\text{CH}_3 + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	8.430E+13	0.00	0	[9]
41f	$\text{CH}_3 + \text{T-CH}_2 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}$	4.220E+13	0.00	0	[12]
42f	$\text{CH}_3 + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{OH}$	2.000E+13	0.00	0	[9]
43f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4	[12]
44f	$\text{CH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_3\text{O} + \text{O}$	1.330E+14	0.00	131	[12]
45f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}_2$	1.000E+14	0.00	134	[13]
46f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}$	3.160E+13	0.00	61.5	[14]
47f	$\text{CH}_3 + \text{H} \rightleftharpoons \text{CH}_4$	$k_0$ 6.260E+23 $k_\infty$ 2.110E+14	-1.80 0.00	0 0	[15]
48f	$2 \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_6$	$k_0$ 1.270E+41 $k_\infty$ 1.810E+13	-7.00 0.00	11.6 0	[8]
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	[16]
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	[16]
m3f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{OH} + \text{H}_2$	1.640E+07	2.00	18.9	[16]
m4f	$\text{CH}_3\text{OH} + \text{H} \rightleftharpoons \text{CH}_3\text{O} + \text{H}_2$	3.830E+07	2.00	24.5	[16]
m5f	$\text{CH}_3\text{OH} + \text{O} \rightleftharpoons \text{CH}_2\text{OH} + \text{OH}$	1.000E+13	0.00	19.6	[16]
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	[16]
m7f	$\text{CH}_3\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{OH} + \text{HO}_2$	2.000E+13	0.00	188	[16]
49f	$\text{S-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	3.000E+13	0.00	0	[9]
50f	$\text{S-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH} + \text{H}$	3.130E+13	0.00	0	[9]
51f	$\text{S-CH}_2 + \text{CO}_2 \rightleftharpoons \text{CO} + \text{CH}_2\text{O}$	3.000E+12	0.00	0	[17]
52f <sup>a</sup>	$\text{S-CH}_2 + \text{M}^{(5)} \rightleftharpoons \text{T-CH}_2 + \text{M}^{(5)}$	6.000E+12	0.00	0	[9]
53f	$\text{T-CH}_2 + \text{H} \rightleftharpoons \text{CH} + \text{H}_2$	6.020E+12	0.00	-7.48	[12]
54f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	2.500E+13	0.00	0	[9]
55f	$\text{T-CH}_2 + \text{OH} \rightleftharpoons \text{CH} + \text{H}_2\text{O}$	1.130E+07	2.00	12.6	[9]
56f	$\text{T-CH}_2 + \text{O} \rightleftharpoons \text{CO} + 2 \text{H}$	8.000E+13	0.00	0	[18]
57f	$\text{T-CH}_2 + \text{O} \rightleftharpoons \text{CO} + \text{H}_2$	4.000E+13	0.00	0	[18]
58f	$\text{T-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO}_2 + \text{H}_2$	2.630E+13	0.00	6.24	[17]

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59f	$\text{T-CH}_2 + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH} + \text{H}$	6.580E+13	0.00	6.24	[17]
60f	$2 \text{T-CH}_2 \rightleftharpoons \text{C}_2\text{H}_2 + 2 \text{H}$	1.000E+14	0.00	0	[9]
61f	$\text{CH} + \text{O} \rightleftharpoons \text{CO} + \text{H}$	4.000E+13	0.00	0	[19]
62f	$\text{CH} + \text{O}_2 \rightleftharpoons \text{CHO} + \text{O}$	1.770E+11	0.76	-2	[20]
63f	$\text{CH} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$	1.170E+15	-0.75	0	[17]
64f	$\text{CH} + \text{CO}_2 \rightleftharpoons \text{CHO} + \text{CO}$	4.800E+01	3.22	-13.5	[20]
65f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0	[16]
66f	$\text{CH}_2\text{OH} + \text{H} \rightleftharpoons \text{CH}_3 + \text{OH}$	1.750E+14	0.00	11.7	[16]
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	[16]
68f	$\text{CH}_2\text{OH} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{O} + \text{HO}_2$	5.000E+12	0.00	0	[16]
69f <sup>a</sup>	$\text{CH}_2\text{OH} + \text{M}^{(5)} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}^{(5)}$	5.000E+13	0.00	105	[16]
70f	$\text{CH}_3\text{O} + \text{H} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$	2.000E+13	0.00	0	[16]
71f	$\text{CH}_3\text{O} + \text{H} \rightleftharpoons \text{S-CH}_2 + \text{H}_2\text{O}$	1.600E+13	0.00	0	[16]
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	[16]
73f	$\text{CH}_3\text{O} + \text{O} \rightleftharpoons \text{OH} + \text{CH}_2\text{O}$	1.000E+13	0.00	0	[16]
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	[16]
75f <sup>a</sup>	$\text{CH}_3\text{O} + \text{M} \rightleftharpoons \text{CH}_2\text{O} + \text{H} + \text{M}$	1.000E+13	0.00	56.5	[16]
76f <sup>a</sup>	$\text{CH}_3\text{O} + \text{M}^{(2)} \rightleftharpoons \text{CH}_2\text{OH} + \text{M}^{(2)}$	1.000E+14	0.00	80	[16]
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	[9]
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	[9]
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	[9]
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	[9]
81f	$\text{C}_2\text{H}_6 \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}$	$k_0$ 8.850E+20	-6.43 -1.23	448 428	[8]
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	[9]
83f	$\text{C}_2\text{H}_5 + \text{O} \rightleftharpoons \text{C}_2\text{H}_4 + \text{OH}$	3.060E+13	0.00	0	[9]
84f	$\text{C}_2\text{H}_5 + \text{O} \rightleftharpoons \text{CH}_3 + \text{CH}_2\text{O}$	4.240E+13	0.00	0	[9]
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	[9]
86f	$\text{C}_2\text{H}_5 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}$	$k_0$ 1.110E+10	-4.99 1.04	167 154	[21]
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	[22]
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	[22]
89f	$\text{C}_2\text{H}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{CHO}$	2.250E+06	2.08	0	[12]
90f	$\text{C}_2\text{H}_4 + \text{O} \rightleftharpoons \text{CH}_2\text{CHO} + \text{H}$	1.210E+06	2.08	0	[12]
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	[23]
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	[24]

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93f	$C_2H_4 + HO_2 \rightleftharpoons C_2H_4O + OH$	2.230E+12	0.00	71.9	[12]	
s93f	$C_2H_4O + HO_2 \rightleftharpoons CH_3 + CO + H_2O_2$	4.000E+12	0.00	71.2	[12]	
94f <sup>a</sup>	$C_2H_4 + M \rightleftharpoons C_2H_3 + H + M$	2.600E+17	0.00	404	[15]	
95f <sup>a</sup>	$C_2H_4 + M \rightleftharpoons C_2H_2 + H_2 + M$	3.500E+16	0.00	299	[15]	
96f	$C_2H_3 + H \rightleftharpoons C_2H_2 + H_2$	1.210E+13	0.00	0	[15]	
97f <sup>a,b</sup>	$C_2H_3 + M \rightleftharpoons C_2H_2 + H + M$	$k_0$	1.510E+14	0.10	137	[25]
		$k_\infty$	6.380E+09	1.00	157	
98f	$C_2H_3 + O_2 \rightleftharpoons CH_2O + CHO$	1.700E+29	-5.31	27.2	[26]	
99f	$C_2H_3 + O_2 \rightleftharpoons CH_2CHO + O$	7.000E+14	-0.61	22	[25, 26]	
100f	$C_2H_3 + O_2 \rightleftharpoons C_2H_2 + HO_2$	5.190E+15	-1.26	13.9	[25, 26]	
101f	$CH_2CHO \rightleftharpoons CH_2CO + H$	1.047E+37	-7.19	186	[24]	
102f	$C_2H_2 + O \rightleftharpoons HCCO + H$	4.000E+14	0.00	44.6	[18]	
103f	$C_2H_2 + O \rightleftharpoons T-CH_2 + CO$	1.600E+14	0.00	41.4	[18]	
104f	$C_2H_2 + O_2 \rightleftharpoons CH_2O + CO$	4.600E+15	-0.54	188	[27]	
105f	$C_2H_2 + OH \rightleftharpoons CH_2CO + H$	1.900E+07	1.70	4.18	[7, 28]	
106f	$C_2H_2 + OH \rightleftharpoons C_2H + H_2O$	3.370E+07	2.00	58.6	[7, 28]	
107f	$CH_2CO + H \rightleftharpoons CH_3 + CO$	1.110E+07	2.00	8.37	[7, 28]	
108f	$CH_2CO + O \rightleftharpoons T-CH_2 + CO_2$	2.000E+13	0.00	9.6	[7, 28]	
109f	$CH_2CO + O \rightleftharpoons HCCO + OH$	1.000E+13	0.00	8.37	[7, 28]	
110f	$CH_2CO + OH \rightleftharpoons CH_2OH + CO$	1.020E+13	0.00	0	[7, 28]	
111f	$CH_2CO + CH_3 \rightleftharpoons C_2H_5 + CO$	9.000E+10	0.00	0	[7, 28]	
112f	$HCCO + H \rightleftharpoons S-CH_2 + CO$	1.500E+14	0.00	0	[18]	
113f	$HCCO + OH \rightleftharpoons CHO + CO + H$	2.000E+12	0.00	0	[29]	
114f	$HCCO + O \rightleftharpoons 2 CO + H$	9.640E+13	0.00	0	[18]	
115f	$HCCO + O_2 \rightleftharpoons 2 CO + OH$	2.880E+07	1.70	4.19	[25]	
116f	$HCCO + O_2 \rightleftharpoons CO_2 + CO + H$	1.400E+07	1.70	4.19	[25]	
117f	$C_2H + OH \rightleftharpoons HCCO + H$	2.000E+13	0.00	0	[9, 28]	
118f	$C_2H + O \rightleftharpoons CO + CH$	1.020E+13	0.00	0	[9, 28]	
119f	$C_2H + O_2 \rightleftharpoons HCCO + O$	6.020E+11	0.00	0	[9, 28]	
120f	$C_2H + O_2 \rightleftharpoons CH + CO_2$	4.500E+15	0.00	105	[9, 28]	
121f	$C_2H + O_2 \rightleftharpoons CHO + CO$	2.410E+12	0.00	0	[9, 28]	
122f	$C_2H_2 + S-CH_2 \rightleftharpoons C_3H_3 + H$	8.000E+13	0.00	0	[17]	
123f	$C_2H_2 + S-CH_2 \rightleftharpoons C_3H_4$	8.000E+13	0.00	0	[17]	
124f	$C_2H_2 + T-CH_2 \rightleftharpoons C_3H_4$	1.200E+13	0.00	27.7	[17]	
125f	$C_2H_2 + CH_3 \rightleftharpoons C_3H_4 + H$	6.740E+19	-2.10	132	[17]	
126f	$C_3H_4 + O \rightleftharpoons CH_2O + C_2H_2$	1.000E+12	0.00	0	[29]	

Number	Reaction		$A$	$n$	$E$	Ref.
127f	$C_3H_4 + O \rightleftharpoons CHO + C_2H_3$		1.000E+12	0.00	0	[29]
128f	$C_3H_4 + OH \rightleftharpoons CH_2O + C_2H_3$		1.000E+12	0.00	0	[29]
129f	$C_3H_4 + OH \rightleftharpoons CHO + C_2H_4$		1.000E+12	0.00	0	[29]
130f	$C_3H_4 \rightleftharpoons C_3H_3 + H$		5.000E+14	0.00	370	[19]
131f	$C_3H_5 \rightleftharpoons C_3H_4 + H$		3.980E+13	0.00	293	[29]
132f	$C_3H_5 + H \rightleftharpoons C_3H_4 + H_2$		1.000E+13	0.00	0	[29]
133f	$C_3H_5 + O_2 \rightleftharpoons C_3H_4 + HO_2$		6.000E+11	0.00	41.9	[29]
134f	$C_2H_4 + S-CH_2 \rightleftharpoons C_3H_6$		6.600E+13	0.00	0	[29]
135f	$C_2H_4 + T-CH_2 \rightleftharpoons C_3H_6$		1.800E+10	0.00	0	[29]
136f	$C_3H_5 + H \rightleftharpoons C_3H_6$	$k_0$	1.330E+60	-12.00	25	[30]
		$k_\infty$	2.000E+14	0.00	0	
137f	$C_2H_3 + CH_3 \rightleftharpoons C_3H_6$	$k_0$	4.270E+58	-11.94	40.9	[30]
		$k_\infty$	2.500E+13	0.00	0	
a137f	$C_3H_6 \rightleftharpoons C_2H_2 + CH_4$		3.500E+12	0.00	293	[29]
138f	$H + C_3H_6 \rightleftharpoons C_3H_5 + H_2$		5.000E+12	0.00	6.3	[29]
139f	$C_3H_6 + O \rightleftharpoons C_2H_4 + CH_2O$		5.900E+13	0.00	21	[29]
140f	$C_3H_6 + O \rightleftharpoons C_2H_5 + CHO$		3.600E+12	0.00	0	[29]
141f	$C_3H_6 + OH \rightleftharpoons C_2H_5 + CH_2O$		7.900E+12	0.00	0	[29]
142f	$C_3H_6 + OH \rightleftharpoons C_3H_5 + H_2O$		4.000E+12	0.00	0	[29]
143f	$CH_3 + C_3H_6 \rightleftharpoons CH_4 + C_3H_5$		8.960E+12	0.00	35.6	[29]
144f	$C_3H_6 + C_2H_5 \rightleftharpoons C_3H_5 + C_2H_6$		1.000E+11	0.00	38.5	[29]
145f	$N-C_3H_7 \rightleftharpoons CH_3 + C_2H_4$	$k_0$	5.490E+49	-10.00	150	[31]
		$k_\infty$	1.230E+13	-0.10	126	
146f	$N-C_3H_7 \rightleftharpoons H + C_3H_6$	$k_0$	7.881E+39	-6.66	178	[30]
		$k_\infty$	1.674E+14	0.00	162	
147f	$N-C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$		9.000E+10	0.00	0	[32, 30]
p1f	$C_3H_8 \rightleftharpoons CH_3 + C_2H_5$	$k_0$	7.830E+18	0.00	272	[15]
		$k_\infty$	1.100E+17	0.00	353	
p4f	$C_3H_8 + O_2 \rightleftharpoons I-C_3H_7 + HO_2$		4.000E+13	0.00	199	[33]
p5f	$C_3H_8 + O_2 \rightleftharpoons N-C_3H_7 + HO_2$		4.000E+13	0.00	199	[33]
p6f	$C_3H_8 + H \rightleftharpoons I-C_3H_7 + H_2$		1.300E+06	2.40	18.7	[33]
p7f	$C_3H_8 + H \rightleftharpoons N-C_3H_7 + H_2$		1.330E+06	2.54	28.3	[32, 31]
p8f	$C_3H_8 + O \rightleftharpoons I-C_3H_7 + OH$		4.760E+04	2.71	8.82	[32, 30]
p9f	$C_3H_8 + O \rightleftharpoons N-C_3H_7 + OH$		1.900E+05	2.68	15.6	[32, 30]
p10f	$C_3H_8 + OH \rightleftharpoons I-C_3H_7 + H_2O$		4.670E+07	1.61	-0.146	[33]
p11f	$C_3H_8 + OH \rightleftharpoons N-C_3H_7 + H_2O$		1.054E+10	0.97	6.64	[33]

Number	Reaction	$A$	$n$	$E$	Ref.	
p12f	$\text{C}_3\text{H}_8 + \text{HO}_2 \rightleftharpoons \text{I-C}_3\text{H}_7 + \text{H}_2\text{O}_2$	9.640E+03	2.60	58.2	[32, 31, 30]	
p13f	$\text{C}_3\text{H}_8 + \text{HO}_2 \rightleftharpoons \text{N-C}_3\text{H}_7 + \text{H}_2\text{O}_2$	4.760E+04	2.55	69	[32, 31, 30]	
p196f	$\text{I-C}_3\text{H}_7 + \text{C}_3\text{H}_8 \rightleftharpoons \text{N-C}_3\text{H}_7 + \text{C}_3\text{H}_8$	8.400E-03	4.20	36.3	[32, 34]	
p17f	$\text{I-C}_3\text{H}_7 \rightleftharpoons \text{C}_3\text{H}_6 + \text{H}$	$k_0$	2.167E+17	0.00	118	[15, 31]
		$k_\infty$	8.760E+07	1.76	149	
p19f	$\text{I-C}_3\text{H}_7 + \text{O}_2 \rightleftharpoons \text{C}_3\text{H}_6 + \text{HO}_2$	1.300E+11	0.00	0	[32, 30]	

Units are mol, cm<sup>3</sup>, kJ, K.

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

<sup>a</sup>Third-body efficiencies are:

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

$$[\text{M1}] = 2.5 [\text{H2}] + 16.3 [\text{H2O}] + 1.9 [\text{CO}] + 3.8 [\text{CO2}] + 1 [\text{other}].$$

$$[\text{M6}] = 0.5 [\text{AR}] + 0.3 [\text{O2}] + 12 [\text{H2O}] + 0.75 [\text{CO}] + 1.5 [\text{CO2}] + 1.5 [\text{C2H6}] + 1 [\text{other}].$$

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

$$[\text{M7}] = 0.7 [\text{AR}] + 2 [\text{H2}] + 6 [\text{H2O}] + 1.5 [\text{CO}] + 2 [\text{CO2}] + 2 [\text{CH4}] + 3 [\text{C2H6}] + 1 [\text{other}].$$

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

$$[\text{M5}] = 2.4 [\text{H2}] + 15.4 [\text{H2O}] + 1.8 [\text{CO}] + 3.6 [\text{CO2}] + 1 [\text{other}].$$

The third-body efficiency for H<sub>2</sub>O in M6 is taken from [35].

<sup>b</sup>Pressure dependent reactions are described by the TROE-formulation [36]. The centering parameters are given by:

$$F_{c,8f} = \exp(-T/345 \text{ K}) + \exp(-345 \text{ K}/T).$$

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

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

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

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

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

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

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

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

$$F_{c,145f} = 2.17 \exp(-T/251 \text{ K}) + \exp(-1185 \text{ K}/T).$$

$$F_{c,146f} = \exp(-T/1310 \text{ K}) + \exp(-48097 \text{ K}/T).$$

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

$$F_{c,p17f} = \exp(-T/260 \text{ K}) + \exp(-3000 \text{ K}/T).$$

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