Number	Reaction		A	n	E	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	$H_2O + O \rightleftharpoons 2\ OH$		7.600E+00	3.84	53.5	[1]
a5f[a]	$H + O + M^{(2)} \rightleftharpoons OH + M^{(2)}$		6.200E+16	-0.60	0	[2, 3]
a6f	$H_2 + O_2 \rightleftharpoons 2\ OH$		1.700E+13	0.00	200	[4, 3]
5f[a]	$2\ H + M^{(1)} \rightleftharpoons H_2 + M^{(1)}$		7.200E+17	-1.00	0	[1]
6f[a]	$H + OH + M^{(2)} \rightleftharpoons H_2O + M^{(2)}$		3.800E+22	-2.00	0	[5]
7f[a]	$2\ O + M^{(2)} \rightleftharpoons O_2 + M^{(2)}$		6.170E+15	-0.50	0	[1]
8f[a,b]	$H + O_2 + M^{(6)} \rightleftharpoons HO_2 + M^{(6)}$	k_0	2.600E+19	-1.20	0	[6]
		k_∞	4.650E+12	0.44	0	
a11f[a]	$O + OH + M \rightleftharpoons HO_2 + M$		1.000E+16	0.00	0	[4, 3]
9f	$HO_2 + H \rightleftharpoons 2\ OH$		7.080E+13	0.00	1.25	[5]
10f	$HO_2 + H \rightleftharpoons H_2 + O_2$		4.280E+13	0.00	5.9	[1]
11f	$HO_2 + H \rightleftharpoons H_2O + O$		3.100E+13	0.00	7.2	[1]
12f	$HO_2 + O \rightleftharpoons OH + O_2$		2.000E+13	0.00	0	[1]
13f	$HO_2 + OH \rightleftharpoons H_2O + O_2$		2.890E+13	0.00	-2.08	[1]
14f[a,b]	$2\ OH + M^{(7)} \rightleftharpoons H_2O_2 + M^{(7)}$	k_0	1.340E+17	-0.58	-9.6	[1]
		k_∞	7.400E+13	-0.37	0	
15f	$2\ HO_2 \rightleftharpoons H_2O_2 + O_2$		3.020E+12	0.00	5.8	[1]
16f	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$		4.790E+13	0.00	33.3	[1]
17f	$H_2O_2 + H \rightleftharpoons H_2O + OH$		1.000E+13	0.00	15	[1]
18f	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$		7.080E+12	0.00	6	[1]
19f	$H_2O_2 + O \rightleftharpoons HO_2 + OH$		9.630E+06	2.00	16.7	[1]
20f	$CO + OH \rightleftharpoons CO_2 + H$		4.400E+06	1.50	-3.1	[1]
21f	$CO + HO_2 \rightleftharpoons CO_2 + OH$		6.030E+13	0.00	96	[1]
22f[a]	$HCO + M^{(4)} \rightleftharpoons CO + H + M^{(4)}$		1.860E+17	-1.00	71.1	[7]
23f	$HCO + H \rightleftharpoons CO + H_2$		1.000E+14	0.00	0	[1]
24f	$HCO + O \rightleftharpoons CO + OH$		3.000E+13	0.00	0	[1]
25f	$HCO + O \rightleftharpoons CO_2 + H$		3.000E+13	0.00	0	[1]
26f	$HCO + OH \rightleftharpoons CO + H_2O$		5.020E+13	0.00	0	[1]
27f	$HCO + O_2 \rightleftharpoons CO + HO_2$		3.000E+12	0.00	0	[1]
28f[a]	$CH_2O + M^{(1)} \rightleftharpoons HCO + H + M^{(1)}$		6.260E+16	0.00	326	[1]
29f	$CH_2O + H \rightleftharpoons HCO + H_2$		1.260E+08	1.62	9.06	[1]
30f	$CH_2O + O \rightleftharpoons HCO + OH$		3.500E+13	0.00	14.7	[1]
31f	$CH_2O + OH \rightleftharpoons HCO + H_2O$		3.900E+10	0.89	1.7	[1]

Number	Reaction		A	n	E	Ref.
32f	$CH_4 + H \rightleftharpoons H_2 + CH_3$		1.300E+04	3.00	33.6	[8]
33f	$CH_4 + OH \rightleftharpoons H_2O + CH_3$		1.600E+07	1.83	11.6	[8]
34f	$CH_4 + O \rightleftharpoons CH_3 + OH$		1.900E+09	1.44	36.3	[9]
35f	$CH_4 + O_2 \rightleftharpoons CH_3 + HO_2$		3.980E+13	0.00	238	[7, 10]
36f	$CH_4 + HO_2 \rightleftharpoons CH_3 + H_2O_2$		9.030E+12	0.00	103	[7, 10]
37f	$CH_3 + H \rightleftharpoons T\text{-}CH_2 + H_2$		1.800E+14	0.00	63.2	[9]
38f	$CH_3 + H \rightleftharpoons S\text{-}CH_2 + H_2$		1.550E+14	0.00	56.4	[9]
39f	$CH_3 + OH \rightleftharpoons S\text{-}CH_2 + H_2O$		1.000E+13	0.00	10.5	[11]
40f	$CH_3 + O \rightleftharpoons CH_2O + H$		8.430E+13	0.00	0	[9]
41f	$CH_3 + T\text{-}CH_2 \rightleftharpoons C_2H_4 + H$		4.220E+13	0.00	0	[12]
42f	$CH_3 + HO_2 \rightleftharpoons CH_3O + OH$		5.000E+12	0.00	0	[12]
43f	$CH_3 + O_2 \rightleftharpoons CH_2O + OH$		3.300E+11	0.00	37.4	[12]
44f	$CH_3 + O_2 \rightleftharpoons CH_3O + O$		1.330E+14	0.00	131	[12]
45f	$2\ CH_3 \rightleftharpoons C_2H_4 + H_2$		1.000E+14	0.00	134	[13]
46f	$2\ CH_3 \rightleftharpoons C_2H_5 + H$		3.160E+13	0.00	61.5	[14]
47f[a,b]	$CH_3 + H + M \rightleftharpoons CH_4 + M$	k_0	6.260E+23	-1.80	0	[15]
		k_∞	2.110E+14	0.00	0	
48f[a,b]	$2\ CH_3 + M \rightleftharpoons C_2H_6 + M$	k_0	1.270E+41	-7.00	11.6	[8]
		k_∞	1.810E+13	0.00	0	
49f	$S\text{-}CH_2 + OH \rightleftharpoons CH_2O + H$		3.000E+13	0.00	0	[9]
50f	$S\text{-}CH_2 + O_2 \rightleftharpoons CO + OH + H$		3.130E+13	0.00	0	[9]
51f	$S\text{-}CH_2 + CO_2 \rightleftharpoons CO + CH_2O$		3.000E+12	0.00	0	[16]
52f[a]	$S\text{-}CH_2 + M^{(5)} \rightleftharpoons T\text{-}CH_2 + M^{(5)}$		6.000E+12	0.00	0	[9]
53f	$T\text{-}CH_2 + H \rightleftharpoons CH + H_2$		6.020E+12	0.00	-7.48	[12]
54f	$T\text{-}CH_2 + OH \rightleftharpoons CH_2O + H$		2.500E+13	0.00	0	[9]
55f	$T\text{-}CH_2 + OH \rightleftharpoons CH + H_2O$		1.130E+07	2.00	12.6	[9]
56f	$T\text{-}CH_2 + O \rightleftharpoons CO + 2\ H$		8.000E+13	0.00	0	[17]
57f	$T\text{-}CH_2 + O \rightleftharpoons CO + H_2$		4.000E+13	0.00	0	[17]
58f	$T\text{-}CH_2 + O_2 \rightleftharpoons CO_2 + H_2$		2.630E+12	0.00	6.24	[16]
59f	$T\text{-}CH_2 + O_2 \rightleftharpoons CO + OH + H$		6.580E+12	0.00	6.24	[16]
60f	$2\ T\text{-}CH_2 \rightleftharpoons C_2H_2 + 2\ H$		1.000E+14	0.00	0	[9]
61f	$CH + O \rightleftharpoons CO + H$		4.000E+13	0.00	0	[18]
62f	$CH + O_2 \rightleftharpoons HCO + O$		1.770E+11	0.76	-2	[19]
63f	$CH + H_2O \rightleftharpoons CH_2O + H$		1.170E+15	-0.75	0	[16]
64f	$CH + CO_2 \rightleftharpoons HCO + CO$		4.800E+01	3.22	-13.5	[19]
70f	$CH_3O + H \rightleftharpoons CH_2O + H_2$		2.000E+13	0.00	0	[20]

Number	Reaction		A	n	E	Ref.
71f	$CH_3O + H \rightleftharpoons S\text{-}CH_2 + H_2O$		1.600E+13	0.00	0	[20]
72f	$CH_3O + OH \rightleftharpoons CH_2O + H_2O$		5.000E+12	0.00	0	[20]
73f	$CH_3O + O \rightleftharpoons OH + CH_2O$		1.000E+13	0.00	0	[20]
74f	$CH_3O + O_2 \rightarrow CH_2O + HO_2$		4.280E-13	7.60	-14.8	[20]
75f[a]	$CH_3O + M \rightleftharpoons CH_2O + H + M$		1.000E+13	0.00	56.5	[20]
77f	$C_2H_6 + H \rightleftharpoons C_2H_5 + H_2$		5.400E+02	3.50	21.8	[9]
78f	$C_2H_6 + O \rightleftharpoons C_2H_5 + OH$		1.400E+00	4.30	11.6	[9]
79f	$C_2H_6 + OH \rightleftharpoons C_2H_5 + H_2O$		2.200E+07	1.90	4.7	[9]
80f	$C_2H_6 + CH_3 \rightleftharpoons C_2H_5 + CH_4$		5.500E-01	4.00	34.7	[9]
81f[a,b]	$C_2H_6 + M \rightleftharpoons C_2H_5 + H + M$	k_0	4.900E+42	-6.43	448	[8]
		k_∞	8.850E+20	-1.23	428	
82f	$C_2H_5 + H \rightleftharpoons C_2H_4 + H_2$		3.000E+13	0.00	0	[9]
83f	$C_2H_5 + O \rightleftharpoons C_2H_4 + OH$		3.060E+13	0.00	0	[9]
84f	$C_2H_5 + O \rightleftharpoons CH_3 + CH_2O$		4.240E+13	0.00	0	[9]
85f	$C_2H_5 + O_2 \rightleftharpoons C_2H_4 + HO_2$		2.000E+12	0.00	20.9	[9]
86f	$C_2H_5 \rightleftharpoons C_2H_4 + H$	k_0	3.990E+33	-4.99	167	[21]
		k_∞	1.110E+10	1.04	154	
87f	$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$		4.490E+07	2.12	55.9	[22]
88f	$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$		5.530E+05	2.31	12.4	[22]
89f	$C_2H_4 + O \rightleftharpoons CH_3 + HCO$		2.250E+06	2.08	0	[12]
90f	$C_2H_4 + O \rightleftharpoons CH_2CHO + H$		1.210E+06	2.08	0	[12]
91f	$2\ C_2H_4 \rightleftharpoons C_2H_3 + C_2H_5$		5.010E+14	0.00	271	[23]
92f	$C_2H_4 + O_2 \rightleftharpoons C_2H_3 + HO_2$		4.220E+13	0.00	241	[24]
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[a]	$C_2H_4 + M \rightleftharpoons C_2H_3 + H + M$		2.600E+17	0.00	404	[15]
95f[a]	$C_2H_4 + M \rightleftharpoons C_2H_2 + H_2 + M$		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[a,b]	$C_2H_3 + M \rightleftharpoons C_2H_2 + H + M$	k_0	1.510E+14	0.10	137	[25]
		k_∞	6.380E+09	1.00	157	
98f	$C_2H_3 + O_2 \rightleftharpoons CH_2O + HCO$		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	[17]
103f	$C_2H_2 + O \rightleftharpoons T\text{-}CH_2 + CO$		1.600E+14	0.00	41.4	[17]

Number	Reaction	A	n	E	Ref.
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	$CH_2CO + H \rightleftharpoons CH_3 + CO$	1.500E+09	1.43	11.2	[7, 28]
108f	$CH_2CO + O \rightleftharpoons T\text{-}CH_2 + CO_2$	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]
111f	$CH_2CO + CH_3 \rightleftharpoons C_2H_5 + CO$	9.000E+10	0.00	0	[7, 28]
112f	$HCCO + H \rightleftharpoons S\text{-}CH_2 + CO$	1.500E+14	0.00	0	[17]
113f	$HCCO + OH \rightleftharpoons HCO + CO + H$	2.000E+12	0.00	0	[29]
114f	$HCCO + O \rightleftharpoons 2\ CO + H$	9.640E+13	0.00	0	[17]
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	$C_2H + O_2 \rightleftharpoons HCO + CO$	2.410E+12	0.00	0	[9, 28]
65f	$CH_2OH + H \rightleftharpoons CH_2O + H_2$	3.000E+13	0.00	0	[20]
66f	$CH_2OH + H \rightleftharpoons CH_3 + OH$	1.750E+14	0.00	11.7	[20]
67f	$CH_2OH + OH \rightleftharpoons CH_2O + H_2O$	2.400E+13	0.00	0	[20]
68f	$CH_2OH + O_2 \rightleftharpoons CH_2O + HO_2$	5.000E+12	0.00	0	[20]
69f[a]	$CH_2OH + M^{(5)} \rightleftharpoons CH_2O + H + M^{(5)}$	5.000E+13	0.00	105	[20]
76f[a]	$CH_3O + M^{(2)} \rightleftharpoons CH_2OH + M^{(2)}$	1.000E+14	0.00	80	[20]
110f	$CH_2CO + OH \rightleftharpoons CH_2OH + CO$	1.020E+13	0.00	0	[20]
m1f	$CH_3OH + OH \rightleftharpoons CH_2OH + H_2O$	1.440E+06	2.00	-3.51	[20]
m2f	$CH_3OH + OH \rightleftharpoons CH_3O + H_2O$	6.300E+06	2.00	6.3	[20]
m3f	$CH_3OH + H \rightleftharpoons CH_2OH + H_2$	1.640E+07	2.00	18.9	[20]
m4f	$CH_3OH + H \rightleftharpoons CH_3O + H_2$	3.830E+07	2.00	24.5	[20]
m5f	$CH_3OH + O \rightleftharpoons CH_2OH + OH$	1.000E+13	0.00	19.6	[20]
m6f	$CH_3OH + HO_2 \rightleftharpoons CH_2OH + H_2O_2$	6.200E+12	0.00	81.1	[20]
m7f	$CH_3OH + O_2 \rightleftharpoons CH_2OH + HO_2$	2.000E+13	0.00	188	[20]
c1f	$C_3H_4 + O \rightleftharpoons C_2H_4 + CO$	2.000E+07	1.80	4.18	[35]
c2f	$CH_3 + C_2H_2 \rightleftharpoons C_3H_4 + H$	2.560E+09	1.10	57.1	[35]
c3f	$C_3H_4 + O \rightleftharpoons HCCO + CH_3$	7.300E+12	0.00	9.41	[35]
c6f	$C_3H_3 + H \rightleftharpoons C_3H_4 \quad k_0$	9.000E+15	1.00	0	[30]
	k_∞	3.000E+13	0.00	0	

Number	Reaction		A	n	E	Ref.
c8f	$C_3H_3 + HO_2 \rightleftharpoons C_3H_4 + O_2$		2.500E+12	0.00	0	[30]
c9f	$C_3H_4 + OH \rightleftharpoons C_3H_3 + H_2O$		5.300E+06	2.00	8.37	[31]
c10f	$C_3H_3 + O_2 \rightleftharpoons CH_2CO + HCO$		3.000E+10	0.00	12	[32]
c11f[a,b]	$C_3H_4 + H + M \rightleftharpoons C_3H_5 + M$	k_0	3.000E+24	-2.00	0	[30]
		k_∞	4.000E+13	0.00	0	
c12f	$C_3H_5 + H \rightleftharpoons C_3H_4 + H_2$		1.800E+13	0.00	0	[33]
c13f	$C_3H_5 + O_2 \rightleftharpoons C_3H_4 + HO_2$		4.990E+15	-1.40	93.8	[34]
c14f	$C_3H_5 + CH_3 \rightleftharpoons C_3H_4 + CH_4$		3.000E+12	-0.32	-0.548	[30]
c15f[a,b]	$C_2H_2 + CH_3 + M \rightleftharpoons C_3H_5 + M$	k_0	2.000E+09	1.00	0	[30]
		k_∞	6.000E+08	0.00	0	
c16f	$C_3H_5 + OH \rightleftharpoons C_3H_4 + H_2O$		6.000E+12	0.00	0	[30]
c18f	$C_3H_3 + HCO \rightleftharpoons C_3H_4 + CO$		2.500E+13	0.00	0	[31]
c20f	$C_3H_3 + HO_2 \rightleftharpoons OH + CO + C_2H_3$		8.000E+11	0.00	0	[35]
c21f	$C_3H_4 + O_2 \rightleftharpoons CH_3 + HCO + CO$		4.000E+14	0.00	175	[36]
140f	$C_3H_6 + O \rightleftharpoons C_2H_5 + HCO$		3.500E+07	1.65	-4.07	[33]
142f	$C_3H_6 + OH \rightleftharpoons C_3H_5 + H_2O$		3.100E+06	2.00	-1.25	[33]
e3f	$C_3H_6 + O \rightleftharpoons CH_2CO + CH_3 + H$		1.200E+08	1.65	1.37	[33]
138f	$C_3H_6 + H \rightleftharpoons C_3H_5 + H_2$		1.700E+05	2.50	10.4	[33]
136f[a,b]	$C_3H_5 + H + M^{(7)} \rightleftharpoons C_3H_6 + M^{(7)}$	k_0	1.330E+60	-12.00	25	[35]
		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	[12]
e2f	$C_3H_5 + HO_2 \rightleftharpoons OH + C_2H_3 + CH_2O$		3.000E+12	0.00	0	[12]
137f[a,b]	$C_2H_3 + CH_3 + M^{(7)} \rightleftharpoons C_3H_6 + M^{(7)}$	k_0	4.270E+58	-11.94	40.9	[35]
		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	[35]
e5f	$CH_3 + C_2H_3 \rightleftharpoons C_3H_5 + H$		1.500E+24	-2.83	77.9	[35]
p1f[a,b]	$C_3H_8 + M \rightleftharpoons CH_3 + C_2H_5 + M$	k_0	7.830E+18	0.00	272	[15]
		k_∞	1.100E+17	0.00	353	
p2f	$C_3H_8 + O_2 \rightleftharpoons I\text{-}C_3H_7 + HO_2$		4.000E+13	0.00	199	[37, 35, 38]
p3f	$C_3H_8 + O_2 \rightleftharpoons N\text{-}C_3H_7 + HO_2$		4.000E+13	0.00	213	[37, 35, 38]
p4f	$C_3H_8 + H \rightleftharpoons I\text{-}C_3H_7 + H_2$		1.300E+06	2.40	18.7	[37, 35, 38]
p5f	$C_3H_8 + H \rightleftharpoons N\text{-}C_3H_7 + H_2$		1.330E+06	2.54	28.3	[38, 39]
p6f	$C_3H_8 + O \rightleftharpoons I\text{-}C_3H_7 + OH$		4.760E+04	2.71	8.82	[38, 35]
p7f	$C_3H_8 + O \rightleftharpoons N\text{-}C_3H_7 + OH$		1.900E+05	2.68	15.6	[38, 35]
p8f	$C_3H_8 + OH \rightleftharpoons N\text{-}C_3H_7 + H_2O$		1.400E+03	2.66	2.21	[35]
p9f	$C_3H_8 + OH \rightleftharpoons I\text{-}C_3H_7 + H_2O$		2.700E+04	2.39	1.65	[35]

Number	Reaction		A	n	E	Ref.
p10f	$C_3H_8 + HO_2 \rightleftharpoons I\text{-}C_3H_7 + H_2O_2$		9.640E+03	2.60	58.2	[38, 39, 35]
p11f	$C_3H_8 + HO_2 \rightleftharpoons N\text{-}C_3H_7 + H_2O_2$		4.760E+04	2.55	69	[38, 39, 35]
p12f	$I\text{-}C_3H_7 + C_3H_8 \rightleftharpoons N\text{-}C_3H_7 + C_3H_8$		8.400E-03	4.20	36.3	[38, 40]
p13f[a,b]	$C_3H_6 + H + M^{(7)} \rightleftharpoons I\text{-}C_3H_7 + M^{(7)}$	k_0	8.700E+42	-7.50	19.8	[35]
		k_∞	1.330E+13	0.00	6.53	
p14f	$I\text{-}C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$		1.300E+11	0.00	0	[38, 35]
p15f[a,b]	$N\text{-}C_3H_7 + M \rightleftharpoons CH_3 + C_2H_4 + M$	k_0	5.490E+49	-10.00	150	[38, 35]
		k_∞	1.230E+13	-0.10	126	
p16f[a,b]	$H + C_3H_6 + M^{(7)} \rightleftharpoons N\text{-}C_3H_7 + M^{(7)}$	k_0	6.260E+38	-6.66	29.3	[38, 35]
		k_∞	1.330E+13	0.00	13.6	
p17f	$N\text{-}C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$		9.000E+10	0.00	0	[38, 35]

Units are mol, cm^3, kJ, K.

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

[a]Third-body efficiencies are:

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

[M1] = 2.5 [H2] + 16.3 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].

[M6] = 0.5 [AR] + 0.3 [O2] + 7 [H2O] + 0.75 [CO] + 1.5 [CO2] + 1.5 [C2H6] + 1 [other].

[M] = 1 [other].

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

[M4] = 1.9 [H2] + 12 [H2O] + 2.5 [CO] + 2.5 [CO2] + 1 [other].

[M5] = 2.4 [H2] + 15.4 [H2O] + 1.8 [CO] + 3.6 [CO2] + 1 [other].

[b]Pressure dependent reactions are described by the TROE-formulation [41]. The centering parameters are given by:

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

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

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

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

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

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

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

$F_{c,c6f}$ = 0.5.

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

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

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

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

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

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

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

$F_{c,p16f}$ = exp(-T/1310 K) + exp(-48097 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] M. D. Smooke. In *Reduced Kinetic Mechanisms and Approximations for Methane-Air Flames*. Springer-Verlag, New York, 1991.

[5] A. Kazakov J. Li, Z. Zhao and F. Dryer. An updated comprehensive kinetic model of hydrogen combustion. *International Journal of Chemical Kinetics*, 36:566–575, 2004.

[6] E. L. Petersen and R. K. Hanson. Reduced kinetics mechanisms for ram accelerator combustion. *Journal of Propulsion and Power*, 15(4):591–600, 1999.

[7] R. P. Lindstedt and G. Skevis. Chemistry of acetylene flames. *Combustion Science and Technology*, 125(1–6):73–137, 1997.

[8] 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.

[9] 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.

[10] S. C. Li and F. A. Williams. Reaction mechanisms for methane ignition. *Journal of Engineering for Gas Turbines and Power*, 2001, to appear. ASME Paper No. 2000-GT-0145.

[11] S. C. Li and F. A. Williams. Nox formation in two-stage methane-air flames. *Combustion and Flame*, 118(3):399–414, 1999.

[12] 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.

[13] 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.

[14] K.P. Lim and J.V. Michael. The thermal reactions of CH_3. *Twenty-Fifth Symposium (International) on Combustion*, page 713, 1994.

[15] 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.

[16] 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.

[17] 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.

[18] 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.

[19] 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.

[20] 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.

[21] Y. Feng, J. T. Niiranen, A. Bencsura, V. D. Knyazev, and D. Gutman. Weak collision effects in the reaction c2h5 = c2h4 + h. *Journal of Physical Chemistry*, 97(4):871–880, 1993.

[22] 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.

[23] 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.

[24] 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.

[25] 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.

[26] 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.

[27] 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.

[28] 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.

[29] C.K. Westbrook and F.L. Dryer. Chemical kinetic modeling of hydrocarbon combustion. *Progress in Energy and Combustion Science*, 10:1–57, 1984.

[30] M. Petrova and F. Williams. A small detailed chemical-kinetic mechanism for hydrocarbon combustion. *submitted for publication*, 2005.

[31] 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.

[32] 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.

[33] W. Tsang. *Journal of Physical and Chemical Reference Data*, 20, 1991.

[34] 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.

[35] 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.

[36] 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.

[37] B. Varatharajan and F. A. Williams. Ignition times in the theory of branched-chain thermal explosions. *Combustion and Flame*, 121:551–554, 2000.

[38] W. Tsang. Chemical kinetic data base for combustion chemistry. part 3. propane. *Journal of Physical and Chemical Reference Data*, 17(2):887–951, 1988.

[39] 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.

[40] W. Qin. *Detailed Studies on the Combustion of Landfill Gases*. PhD thesis, Department of Aerospace and Mechanical Engineering, University of Southern California, 2000.

[41] 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.