Number		Rea	ction		A	n	E	Ref.	
1f	$\mathrm{H}+\mathrm{O}_2$	$\rightleftharpoons$	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]	
$7 f^a$	$2 O + M^{(3)}$	$\rightleftharpoons$	$O_2 + M^{(3)}$		6.170E+15	-0.50	0	[3]	
$8f^a$	$H + O + M^{(4)}$				4.710E+18	-1.00	0	[3]	
$9f^a$	$O + OH + M^{(4)}$	$\rightleftharpoons$	$\mathrm{HO_2} + \mathrm{M}^{(4)}$		8.000E+15	0.00	0	[3]	
$10\mathbf{f}^{a,b}$	$H + O_2 + M^{(5)}$	$\rightleftharpoons$	$HO_2 + M^{(5)}$	$k_0$	5.750E + 19	-1.40	0	[4, 3]	
				$k_{\infty}$	4.650E+12	0.44	0		
11f	$\mathrm{HO}_2 + \mathrm{H}$	$\rightleftharpoons$	2 OH		7.080E+13	0.00	1.23	[5]	
12f	$\mathrm{HO}_2 + \mathrm{H}$	$\rightleftharpoons$	$H_2 + O_2$		1.660E+13	0.00	3.44	[5]	
13f	$\mathrm{HO}_2 + \mathrm{H}$	$\rightleftharpoons$	$H_2O + O$		3.100E+13	0.00	7.2	[1]	
14f	$HO_2 + O$	$\rightleftharpoons$	$OH + O_2$		2.000E+13	0.00	0	[6]	
15f	$HO_2 + OH$	$\rightleftharpoons$	$H_2O + O_2$		7.000E+12	0.00	-4.58	[7]	$\bigcirc$
				DUPLICATE	4.500E+14	0.00	45.7		
$16f^{a,b}$	$2 \text{ OH} + \text{M}^{(6)}$	$\rightleftharpoons$	$H_2O_2 + M^{(6)}$	$k_0$	2.760E + 25	-3.20	0	[7]	
				$k_{\infty}$	9.550E+13	-0.27	0		
17f	$2 \text{ HO}_2$	$\rightleftharpoons$	$H_2O_2 + O_2$		1.030E+14	0.00	46.2	[2]	
				DUPLICATE	1.940E+11	0.00	-5.89		
18f	$H_2O_2 + H$	$\rightleftharpoons$	$HO_2 + H_2$		2.300E+13	0.00	33.3	[8]	
19f			$H_2O + OH$		1.000E+13	0.00	15	[9]	
20f	$H_2O_2 + OH$	$\rightleftharpoons$	$H_2O + HO_2$		1.740E+12	0.00	6	[2]	$\bigcirc$
				DUPLICATE	7.590E+13	0.00	30.4		
21f			$HO_2 + OH$		9.630E+06	2.00	16.7	[1]	ļ
$a21f^{a,b}$	$CO + O + M^{(11)}$	$\rightleftharpoons$	$CO_2 + M^{(11)}$	$k_0$	1.550E + 24	-2.79	17.5	[8]	
				$k_{\infty}$	1.800E+11	0.00	9.97		
22f	CO + OH				4.400E+06	1.50	-3.1	[1]	
23f			$CO_2 + OH$		2.000E+13	0.00	96	[8]	
24f			$CO_2 + O$	(=)	1.000E+12	0.00	200	[3]	
$25f^a$	$HCO + M^{(7)}$		CO + H + N	$I^{(7)}$	1.860E+17	-1.00	71.1	[10]	<u> </u>
26f	HCO + H	$\rightleftharpoons$	$CO + H_2$		5.000E+13	0.00	0	[11]	
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	[12]	

Number	R	eacti	on	A	n	E	Ref.
30f	$HCO + O_2$	$\rightleftharpoons$	$CO + HO_2$	7.580E+12	0.00	1.72	[11]
31f	$HCO + CH_3$	$\rightleftharpoons$	$CO + CH_4$	5.000E+13	0.00	0	[11]
$32f^{a,b}$	$H + HCO + M^{(8)}$	$\rightleftharpoons$	$CH_2O + M^{(8)} k_0$	1.350E+24	-2.57	1.78	[13]
			$k_{\infty}$	1.090E+12	0.48	-1.09	
33f	$\mathrm{CH_{2}O} + \mathrm{H}$	$\rightleftharpoons$	$HCO + H_2$	5.740E+07	1.90	11.5	[14]
34f	$\mathrm{CH_2O} + \mathrm{O}$	$\rightleftharpoons$	HCO + OH	3.500E+13	0.00	14.7	[1]
35f	$CH_2O + OH$	$\rightleftharpoons$	$HCO + H_2O$	3.900E+10	0.89	1.7	[1]
36f	$CH_2O + O_2$	$\rightleftharpoons$	$HCO + HO_2$	6.000E+13	0.00	170	[15]
37f	$\mathrm{CH_2O} + \mathrm{HO_2}$	$\rightleftharpoons$	$HCO + H_2O_2$	4.110E+04	2.50	42.7	[16]
38f	$CH_4 + H$	$\rightleftharpoons$	$H_2 + CH_3$	1.300E+04	3.00	33.6	[17]
39f	$\mathrm{CH_4} + \mathrm{OH}$	$\rightleftharpoons$	$H_2O + CH_3$	1.600E+07	1.83	11.6	[17]
40f	$CH_4 + O$	$\rightleftharpoons$	$\mathrm{CH}_3 + \mathrm{OH}$	1.900E+09	1.44	36.3	[18]
41f	$CH_4 + O_2$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{HO_2}$	3.980E+13	0.00	238	[10, 19]
42f	$CH_4 + HO_2$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{H_2O_2}$	9.030E+12	0.00	103	[10, 19]
43f	$CH_3 + H$	$\rightleftharpoons$	$T-CH_2 + H_2$	1.800E+14	0.00	63.2	[18]
44f	$CH_3 + H$	$\rightleftharpoons$	$S-CH_2 + H_2$	1.550E+14	0.00	56.4	[18]
45f	$\mathrm{CH_{3}}+\mathrm{OH}$	$\rightleftharpoons$	$S-CH_2 + H_2O$	4.000E+13	0.00	10.5	[20, 11]
46f	$CH_3 + O$	$\rightleftharpoons$	$CH_2O + H$	8.430E+13	0.00	0	[18]
47f	$CH_3 + T-CH_2$	$\rightleftharpoons$	$C_2H_4 + H$	4.220E+13	0.00	0	[15]
48f	$\mathrm{CH_3} + \mathrm{HO_2}$	$\rightleftharpoons$	$CH_3O + OH$	5.000E+12	0.00	0	[15]
49f	$\mathrm{CH_3} + \mathrm{O_2}$	$\rightleftharpoons$	$CH_2O + OH$	3.300E+11	0.00	37.4	[21]
50f	$\mathrm{CH_3} + \mathrm{O_2}$	$\rightleftharpoons$	$CH_3O + O$	1.100E+13	0.00	116	[21]
51f	2 CH <sub>3</sub>	$\rightleftharpoons$	$C_2H_4 + H_2$	1.000E+14	0.00	134	[22]
52f	$2 \text{ CH}_3$	$\rightleftharpoons$	$C_2H_5 + H$	3.160E+13	0.00	61.5	[23]
$53f^{a,b}$	$H + CH_3 + M^{(9)}$	$\rightleftharpoons$	$CH_4 + M^{(9)} \qquad k_0$	2.470E+33	-4.76	10.2	[11]
			$k_{\infty}$	1.270E+16	-0.63	1.6	
$54f^{a,b}$	$2 \text{ CH}_3 + \text{M}^{(8)}$	$\rightleftharpoons$	$C_2H_6 + M^{(8)} k_0$	1.270E+41	-7.00	11.6	[17]
			$k_{\infty}$	1.810E+13	0.00	0	
55f	$S-CH_2 + OH$	$\rightleftharpoons$	$CH_2O + H$	3.000E+13	0.00	0	[18]
56f	$S-CH_2 + O_2$	$\rightleftharpoons$	CO + OH + H	3.130E+13	0.00	0	[18]
57f	$S-CH_2 + CO_2$	$\rightleftharpoons$	$CO + CH_2O$	3.000E+12	0.00	0	[24]
$58f^a$	$S-CH_2 + M^{(10)}$	$\rightleftharpoons$	$T-CH_2 + M^{(10)}$	6.000E+12	0.00	0	[18]
59f	$T-CH_2 + H$	$\rightleftharpoons$	$CH + H_2$	6.020E+12	0.00	-7.48	[15]
60f	$T-CH_2 + OH$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{H}$	2.500E+13	0.00	0	[18]
61f	$T-CH_2 + OH$	$\rightleftharpoons$	$CH + H_2O$	1.130E+07	2.00	12.6	[18]
62f	$T-CH_2 + O$	$\rightleftharpoons$	CO + 2 H	8.000E+13	0.00	0	[25]

Number		Rea	action	A	n	E	Ref.
63f	$T-CH_2 + O$	$\rightleftharpoons$	$CO + H_2$	4.000E+13	0.00	0	[25]
64f	$T-CH_2 + O_2$	$\rightleftharpoons$	$CO_2 + H_2$	2.630E+12	0.00	6.24	[24]
65f	$T-CH_2 + O_2$	$\rightleftharpoons$	CO + OH + H	6.580E+12	0.00	6.24	[24]
66f	2 T-CH <sub>2</sub>	$\rightleftharpoons$	$C_2H_2 + 2 H$	1.000E+14	0.00	0	[18]
67f	CH + O	$\rightleftharpoons$	CO + H	4.000E+13	0.00	0	[26]
68f	$CH + O_2$	$\rightleftharpoons$	HCO + O	1.770E+11	0.76	-2	[27]
69f	$CH + H_2O$	$\rightleftharpoons$	$CH_2O + H$	1.170E+15	-0.75	0	[24]
70f	$CH + CO_2$	$\rightleftharpoons$	HCO + CO	4.800E+01	3.22	-13.5	[27]
71f	$\mathrm{CH_{3}O} + \mathrm{H}$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{H_2}$	2.000E+13	0.00	0	[28]
72f	$\mathrm{CH_{3}O} + \mathrm{H}$	$\rightleftharpoons$	$S-CH_2 + H_2O$	1.600E+13	0.00	0	[28]
73f	$\mathrm{CH_{3}O}+\mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{H_2O}$	5.000E+12	0.00	0	[28]
74f	$CH_3O + O$	$\rightleftharpoons$	$OH + CH_2O$	1.000E+13	0.00	0	[28]
75f	$\mathrm{CH_{3}O}+\mathrm{O_{2}}$	$\rightarrow$	$\mathrm{CH_2O} + \mathrm{HO_2}$	4.280E-13	7.60	-14.8	[28]
$76f^a$	$CH_3O + M^{(9)}$	$\rightleftharpoons$	$CH_2O + H + M^{(9)}$	7.780E+13	0.00	56.5	[11]
77f	$C_2H_6 + H$	$\rightleftharpoons$	$C_2H_5 + H_2$	5.400E+02	3.50	21.8	[18]
78f	$C_2H_6 + O$	$\rightleftharpoons$	$C_2H_5 + OH$	1.400E+00	4.30	11.6	[18]
79f	$C_2H_6 + OH$	$\rightleftharpoons$	$C_2H_5 + H_2O$	2.200E+07	1.90	4.7	[18]
80f	$C_2H_6 + CH_3$	$\rightleftharpoons$	$C_2H_5 + CH_4$	5.500E-01	4.00	34.7	[18]
$81f^{a,b}$	$C_2H_6 + M^{(8)}$	$\rightleftharpoons$	$C_2H_5 + H + M^{(8)}$ $k_0$	4.900E+42	-6.43	448	[17, 13, 11]
			$k_{\infty}$	8.850E+20	-1.23	428	
82f	$C_2H_6 + HO_2$	$\rightleftharpoons$	$\mathrm{C_2H_5} + \mathrm{H_2O_2}$	1.320E+13	0.00	85.6	[15, 11]
83f	$C_2H_5 + H$	$\rightleftharpoons$	$C_2H_4 + H_2$	3.000E+13	0.00	0	[18]
84f	$C_2H_5 + O$	$\rightleftharpoons$	$C_2H_4 + OH$	3.060E+13	0.00	0	[18]
85f	$C_2H_5 + O$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{CH_2O}$	4.240E+13	0.00	0	[18]
86f	$C_2H_5 + O_2$	$\rightleftharpoons$	$C_2H_4 + HO_2$	7.500E+14	-1.00	20.1	[29]
a86f	$C_2H_5 + O_2$	$\rightleftharpoons$	$C_2H_4OOH$	2.000E+12	0.00	0	[29]
b86f	$C_2H_4OOH$	$\rightleftharpoons$	$C_2H_4 + HO_2$	4.000E+34	-7.20	96.2	[29]
c86f	$C_2H_4OOH + O_2$	$\rightleftharpoons$	$OC_2H_3OOH + OH$	7.500E+05	1.30	-24.3	[29]
d86f	$OC_2H_3OOH$	$\rightleftharpoons$	$CH_2O + HCO + OH$	1.000E+15	0.00	180	[29]
$87f^{a,b}$	$C_2H_5 + M^{(9)}$	$\rightleftharpoons$	$C_2H_4 + H + M^{(9)}$ $k_0$	3.990E+33	-4.99	167	[30, 11]
			$k_{\infty}$	1.110E+10	1.04	154	
88f	$C_2H_4 + H$	$\rightleftharpoons$	$C_2H_3 + H_2$	4.490E+07	2.12	55.9	[31]
89f	$C_2H_4 + OH$	$\rightleftharpoons$	$C_2H_3 + H_2O$	5.530E+05	2.31	12.4	[31]
90f	$C_2H_4 + O$	$\rightleftharpoons$	$\mathrm{CH_{3}}+\mathrm{HCO}$	2.250E+06	2.08	0	[15]
91f	$C_2H_4 + O$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{H}$	1.210E+06	2.08	0	[15]
92f	$2 C_2 H_4$	$\rightleftharpoons$	$C_2H_3 + C_2H_5$	5.010E+14	0.00	271	[32]

Number		Re	action	A	n	E	Ref.
93f	$C_2H_4 + O_2$	$\rightleftharpoons$	$C_2H_3 + HO_2$	4.220E+13	0.00	241	[33]
94f	$C_2H_4 + HO_2$	$\rightleftharpoons$	$C_2H_4O + OH$	2.230E+12	0.00	71.9	[15]
95f	$C_2H_4O + HO_2$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{CO} + \mathrm{H_2O_2}$	4.000E+12	0.00	71.2	[15]
96f <sup>a</sup>	$C_2H_4 + M^{(9)}$	$\rightleftharpoons$	$C_2H_3 + H + M^{(9)}$	2.600E+17	0.00	404	[34, 11]
$97f^a$	$C_2H_4 + M^{(9)}$	$\rightleftharpoons$	$C_2H_2 + H_2 + M^{(9)}$	3.500E+16	0.00	299	[34, 11]
98f	$C_2H_3 + H$	$\rightleftharpoons$	$C_2H_2 + H_2$	4.000E+13	0.00	0	[11]
$99f^{a,b}$	$C_2H_3 + M^{(9)}$	$\rightleftharpoons$	$C_2H_2 + H + M^{(9)}$ $k_0$	1.510E+14	0.10	137	[35, 11]
			$k_{\infty}$	6.380E+09	1.00	157	
100f	$C_2H_3 + O_2$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{HCO}$	1.700E+29	-5.31	27.2	[36]
101f	$C_2H_3 + O_2$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{O}$	7.000E+14	-0.61	22	[35, 36]
102f	$C_2H_3 + O_2$	$\rightleftharpoons$	$C_2H_2 + HO_2$	5.190E+15	-1.26	13.9	[35, 36]
103f	$C_2H_2 + O$	$\rightleftharpoons$	HCCO + H	4.000E+14	0.00	44.6	[25]
104f	$C_2H_2 + O$	$\rightleftharpoons$	$T-CH_2 + CO$	1.600E+14	0.00	41.4	[25]
105f	$C_2H_2 + O_2$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{CO}$	4.600E+15	-0.54	188	[37]
106f	$C_2H_2 + OH$	$\rightleftharpoons$	$\mathrm{CH_{2}CO} + \mathrm{H}$	1.900E+07	1.70	4.18	[10, 38]
107f	$C_2H_2 + OH$	$\rightleftharpoons$	$C_2H + H_2O$	3.370E+07	2.00	58.6	[10, 38]
108f	$\mathrm{CH_{2}CO} + \mathrm{H}$	$\rightleftharpoons$	$\mathrm{CH_{3}}+\mathrm{CO}$	1.500E+09	1.43	11.2	[39]
109f	$CH_2CO + O$	$\rightleftharpoons$	$T-CH_2 + CO_2$	2.000E+13	0.00	9.6	[10, 38]
110f	$CH_2CO + O$	$\rightleftharpoons$	HCCO + OH	1.000E+13	0.00	8.37	[10, 38]
111f	$\mathrm{CH_{2}CO} + \mathrm{CH_{3}}$	$\rightleftharpoons$	$C_2H_5 + CO$	9.000E+10	0.00	0	[10, 38]
112f	HCCO + H	$\rightleftharpoons$	$S-CH_2 + CO$	1.500E+14	0.00	0	[25]
113f	HCCO + OH	$\rightleftharpoons$	HCO + CO + H	2.000E+12	0.00	0	[40]
114f	HCCO + O	$\rightleftharpoons$	2  CO + H	9.640E+13	0.00	0	[25]
115f	$HCCO + O_2$	$\rightleftharpoons$	2  CO + OH	2.880E+07	1.70	4.19	[35]
116f	$HCCO + O_2$	$\rightleftharpoons$	$CO_2 + CO + H$	1.400E+07	1.70	4.19	[35]
117f	$C_2H + OH$	$\rightleftharpoons$	HCCO + H	2.000E+13	0.00	0	[18, 38]
118f	$C_2H + O$	$\rightleftharpoons$	CO + CH	1.020E+13	0.00	0	[18, 38]
119f	$C_2H + O_2$	$\rightleftharpoons$	HCCO + O	6.020E+11	0.00	0	[18, 38]
120f	$C_2H + O_2$	$\rightleftharpoons$	$CH + CO_2$	4.500E+15	0.00	105	[18, 38]
121f	$C_2H + O_2$	$\rightleftharpoons$	HCO + CO	2.410E+12	0.00	0	[18, 38]
122f	$CH_2OH + H$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{H_2}$	3.000E+13	0.00	0	[28]
123f	$CH_2OH + H$	$\rightleftharpoons$	$\mathrm{CH_{3}}+\mathrm{OH}$	2.500E+17	-0.93	21.5	[11]
124f	$\mathrm{CH_{2}OH} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{H_2O}$	2.400E+13	0.00	0	[28]
125f	$CH_2OH + O_2$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{HO_2}$	5.000E+12	0.00	0	[28]
$126f^a$	$\mathrm{CH_2OH} + \mathrm{M}^{(9)}$	$\rightleftharpoons$	$CH_2O + H + M^{(9)}$	5.000E+13	0.00	105	[28]
$127f^a$	$CH_3O + M^{(9)}$	$\rightleftharpoons$	$CH_2OH + M^{(9)}$	1.000E+14	0.00	80	[28]

Number		R	Reaction		A	n	E	Ref.
128f	$\mathrm{CH_{2}CO} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_2OH} + \mathrm{CO}$		1.020E+13	0.00	0	[28]
129f	$\mathrm{CH_{3}OH} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_2OH} + \mathrm{H_2O}$		1.440E+06	2.00	-3.51	[28]
130f	$\mathrm{CH_{3}OH} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_3O} + \mathrm{H_2O}$		4.400E+06	2.00	6.3	[11]
131f	$CH_3OH + H$	$\rightleftharpoons$	$\mathrm{CH_2OH} + \mathrm{H_2}$		1.354E+03	3.20	14.6	[41]
132f	$CH_3OH + H$	$\rightleftharpoons$	$\mathrm{CH_3O} + \mathrm{H_2}$		6.830E+01	3.40	30.3	[41]
133f	$CH_3OH + O$	$\rightleftharpoons$	$CH_2OH + OH$		3.880E + 05	2.50	12.9	[42]
134f	$\mathrm{CH_3OH} + \mathrm{HO_2}$	$\rightleftharpoons$	$\mathrm{CH_2OH} + \mathrm{H_2O_2}$		8.000E+13	0.00	81.1	[43, 44]
135f	$CH_3OH + O_2$	$\rightleftharpoons$	$\mathrm{CH_2OH} + \mathrm{HO_2}$		2.000E+13	0.00	188	[28]
$136f^{a,b}$	$\mathrm{CH_3OH} + \mathrm{M}^{(9)}$	$\rightleftharpoons$	$CH_3 + OH + M^{(9)}$	$k_0$	2.950E+44	-7.35	399	[45, 11]
				$k_{\infty}$	1.900E+16	0.00	384	
137f	$\mathrm{CH_{2}CHO}$	$\rightleftharpoons$	$\mathrm{CH_{2}CO} + \mathrm{H}$		1.047E + 37	-7.19	186	[33]
138f	$CH_2CHO + H$	$\rightleftharpoons$	$\mathrm{CH_{3}}+\mathrm{HCO}$		5.000E+13	0.00	0	[14]
139f	$\mathrm{CH_{2}CHO} + \mathrm{H}$	$\rightleftharpoons$	$\mathrm{CH_{2}CO} + \mathrm{H_{2}}$		2.000E+13	0.00	0	[14]
140f	$CH_2CHO + O$	$\rightleftharpoons$	$\mathrm{CH_2O} + \mathrm{HCO}$		1.000E+14	0.00	0	[14]
141f	$\mathrm{CH_{2}CHO} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_{2}CO} + \mathrm{H_{2}O}$		3.000E+13	0.00	0	[14]
142f	$\mathrm{CH_{2}CHO} + \mathrm{O_{2}}$	$\rightleftharpoons$	$CH_2O + CO + OH$		3.000E+10	0.00	0	[14]
143f	$\mathrm{CH_{2}CHO} + \mathrm{CH_{3}}$	$\rightleftharpoons$	$C_2H_5 + CO + H$		4.900E+14	-0.50	0	[14]
144f	$\mathrm{CH_{2}CHO} + \mathrm{HO_{2}}$	$\rightleftharpoons$	$CH_2O + HCO + OH$		7.000E+12	0.00	0	[14]
145f	$\mathrm{CH_{2}CHO} + \mathrm{HO_{2}}$	$\rightleftharpoons$	$CH_3CHO + O_2$		3.000E+12	0.00	0	[14]
146f	$\mathrm{CH_{2}CHO}$	$\rightleftharpoons$	$CH_3 + CO$		1.170E+43	-9.80	183	[14]
147f	$\mathrm{CH_{3}CHO}$	$\rightleftharpoons$	$\mathrm{CH}_3 + \mathrm{HCO}$		7.000E+15	0.00	342	[14]
$148 f^{a,b}$	$\mathrm{CH_3CO} + \mathrm{M}^{(9)}$	$\rightleftharpoons$	$CH_3 + CO + M^{(9)}$	$k_0$	1.200E+15	0.00	52.3	[14]
				$k_{\infty}$	3.000E+12	0.00	69.9	
149f	$\mathrm{CH_{3}CHO} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_{3}CO} + \mathrm{H_{2}O}$		3.370E+12	0.00	-2.59	[14]
150f	$\mathrm{CH_{3}CHO} + \mathrm{OH}$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{H_{2}O}$		3.370E+11	0.00	-2.59	[14]
151f	$CH_3CHO + O$	$\rightleftharpoons$	$\mathrm{CH_{3}CO} + \mathrm{OH}$		1.770E + 18	-1.90	12.5	[14]
152f	$CH_3CHO + O$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{OH}$		3.720E+13	-0.20	14.9	[14]
153f	$CH_3CHO + H$	$\rightleftharpoons$	$\mathrm{CH_{3}CO} + \mathrm{H_{2}}$		4.660E + 13	-0.30	12.5	[14]
154f	$CH_3CHO + H$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{H_{2}}$		1.850E + 12	0.40	22.4	[14]
155f	$\mathrm{CH_{3}CHO} + \mathrm{CH_{3}}$	$\rightleftharpoons$	$\mathrm{CH_{3}CO} + \mathrm{CH_{4}}$		3.900E-07	5.80	9.21	[14]
156f	$\mathrm{CH_3CHO} + \mathrm{CH_3}$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{CH_{4}}$		2.450E+01	3.10	24	[14]
157f	$\mathrm{CH_3CHO} + \mathrm{HO_2}$	$\rightleftharpoons$	$\mathrm{CH_3CO} + \mathrm{H_2O_2}$		3.600E+19	-2.20	58.6	[14]
158f	$\mathrm{CH_3CHO} + \mathrm{HO_2}$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{H_{2}O_{2}}$		2.320E+11	0.40	62.3	[14]
159f	$\mathrm{CH_3CHO} + \mathrm{O_2}$	$\rightleftharpoons$	$\mathrm{CH_{3}CO} + \mathrm{HO_{2}}$		1.000E+14	0.00	177	[14]
$160 f^{a,b}$	$C_2H_5OH + M^{(9)}$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{CH_2OH} + \mathrm{M}^{(9)}$	$k_0$	3.000E+16	0.00	243	[11, 46]
				$k_{\infty}$	5.000E+15	0.00	343	

Number		Rea	action		A	n	E	Ref.
$161 f^{a,b}$	$C_2H_5OH + M^{(9)}$	$\rightleftharpoons$	$C_2H_4 + H_2O + M^{(9)}$	$k_0$	1.000E+17	0.00	226	[11, 46]
			i	$k_{\infty}$	8.000E+13	0.00	272	
162f	$C_2H_5OH + OH$	$\rightleftharpoons$	$\mathrm{CH_{2}CH_{2}OH} + \mathrm{H_{2}O}$		1.810E+11	0.40	3	[14, 46]
163f	$C_2H_5OH + OH$	$\rightleftharpoons$	$\mathrm{CH_{3}CHOH} + \mathrm{H_{2}O}$		3.090E+10	0.50	-1.59	[14, 46]
164f	$C_2H_5OH + OH$	$\rightleftharpoons$	$\mathrm{CH_3CH_2O} + \mathrm{H_2O}$		1.050E+10	0.80	3	[14, 46]
165f	$C_2H_5OH + H$	$\rightleftharpoons$	$\mathrm{CH_{2}CH_{2}OH} + \mathrm{H_{2}}$		1.900E+07	1.80	21.3	[14, 46]
166f	$C_2H_5OH + H$	$\rightleftharpoons$	$CH_3CHOH + H_2$		2.580E+07	1.60	11.8	[14, 46]
167f	$C_2H_5OH + H$	$\rightleftharpoons$	$\mathrm{CH_3CH_2O} + \mathrm{H_2}$		1.500E+07	1.60	12.7	[14, 46]
168f	$C_2H_5OH + O$	$\rightleftharpoons$	$\mathrm{CH_{2}CH_{2}OH} + \mathrm{OH}$		9.410E+07	1.70	22.8	[14, 46]
169f	$C_2H_5OH + O$	$\rightleftharpoons$	$CH_3CHOH + OH$		1.880E+07	1.90	7.62	[14, 46]
170f	$C_2H_5OH + O$	$\rightleftharpoons$	$\mathrm{CH_{3}CH_{2}O} + \mathrm{OH}$		1.580E+07	2.00	18.6	[14, 46]
171f	$C_2H_5OH + CH_3$	$\rightleftharpoons$	$\mathrm{CH_{2}CH_{2}OH} + \mathrm{CH_{4}}$		2.190E+02	3.20	40.2	[14, 46]
172f	$C_2H_5OH + CH_3$	$\rightleftharpoons$	$\mathrm{CH_{3}CHOH} + \mathrm{CH_{4}}$		7.280E+02	3.00	33.3	[14, 46]
173f	$C_2H_5OH + CH_3$	$\rightleftharpoons$	$\mathrm{CH_3CH_2O} + \mathrm{CH_4}$		1.450E+02	3.00	32	[14, 46]
174f	$C_2H_5OH + HO_2$	$\rightleftharpoons$	$\mathrm{CH_3CHOH} + \mathrm{H_2O_2}$		8.200E+03	2.50	45.2	[14, 46]
175f	$C_2H_5OH + HO_2$	$\rightleftharpoons$	$\mathrm{CH_{2}CH_{2}OH} + \mathrm{H_{2}O_{2}}$		2.430E+04	2.50	66.1	[14, 46]
176f	$C_2H_5OH + HO_2$	$\rightleftharpoons$	$\mathrm{CH_3CH_2O} + \mathrm{H_2O_2}$		3.800E+12	0.00	100	[14, 46]
177f	$C_2H_4 + OH$	$\rightleftharpoons$	CH <sub>2</sub> CH <sub>2</sub> OH		2.410E+11	0.00	-9.96	[14, 46]
178f	$C_2H_5 + HO_2$	$\rightleftharpoons$	$\mathrm{CH_3CH_2O} + \mathrm{OH}$		4.000E+13	0.00	0	[14, 46]
$179f^a$	$CH_3CH_2O + M^{(9)}$	$\rightleftharpoons$	$CH_3CHO + H + M^{(9)}$		5.600E+34	-5.90	106	[14, 46]
$180 \mathrm{f}^a$	$\mathrm{CH_3CH_2O} + \mathrm{M}^{(9)}$	$\rightleftharpoons$	$CH_3 + CH_2O + M^{(9)}$		5.350E+37	-7.00	99.6	[14, 46]
181f	$CH_3CH_2O + O_2$	$\rightleftharpoons$	$\mathrm{CH_3CHO} + \mathrm{HO_2}$		4.000E+10	0.00	4.6	[14, 46]
182f	$CH_3CH_2O + CO$	$\rightleftharpoons$	$C_2H_5 + CO_2$		4.680E+02	3.20	22.5	[14, 46]
183f	$CH_3CH_2O + H$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{CH_2OH}$		3.000E+13	0.00	0	[14, 46]
184f	$\mathrm{CH_{3}CH_{2}O} + \mathrm{H}$	$\rightleftharpoons$	$C_2H_4 + H_2O$		3.000E+13	0.00	0	[14, 46]
185f	$CH_3CH_2O + OH$	$\rightleftharpoons$	$\mathrm{CH_{3}CHO} + \mathrm{H_{2}O}$		1.000E+13	0.00	0	[14, 46]
186f	$CH_3CHOH + O_2$	$\rightleftharpoons$	$\mathrm{CH_3CHO} + \mathrm{HO_2}$		4.820E+13	0.00	21	[14, 46]
187f	$CH_3CHOH + O$	$\rightleftharpoons$	$\mathrm{CH_{3}CHO} + \mathrm{OH}$		1.000E+14	0.00	0	[14, 46]
188f	$CH_3CHOH + H$	$\rightleftharpoons$	$C_2H_4 + H_2O$		3.000E+13	0.00	0	[14, 46]
189f	$CH_3CHOH + H$	$\rightleftharpoons$	$\mathrm{CH_3} + \mathrm{CH_2OH}$		3.000E+13	0.00	0	[14, 46]
190f	$\mathrm{CH_3CHOH} + \mathrm{HO_2}$	$\rightleftharpoons$	$CH_3CHO + 2 OH$		4.000E+13	0.00	0	[14, 46]
191f	$CH_3CHOH + OH$	$\rightleftharpoons$	$\mathrm{CH_3CHO} + \mathrm{H_2O}$		5.000E+12	0.00	0	[14, 46]
192f <sup>a</sup>	$\mathrm{CH_3CHOH} + \mathrm{M}^{(9)}$	$\rightleftharpoons$	$CH_3CHO + H + M^{(9)}$		1.000E+14	0.00	105	[14, 46]
193f	$C_3H_4 + O$	$\rightleftharpoons$	$C_2H_4 + CO$		2.000E+07	1.80	4.18	[47]
194f	$CH_3 + C_2H_2$	$\rightleftharpoons$	$C_3H_4 + H$		2.560E+09	1.10	57.1	[47]
195f	$C_3H_4 + O$	$\rightleftharpoons$	$HCCO + CH_3$		7.300E+12	0.00	9.41	[47]

Number	]	Reac	tion		A	n	E	Ref.
196f <sup>a,b</sup>	$C_3H_3 + H + M$	$\rightleftharpoons$	$C_3H_4 + M$	$k_0$	9.000E+15	1.00	0	[39]
				$k_{\infty}$	3.000E+13	0.00	0	
197f	$C_3H_3 + HO_2$	$\rightleftharpoons$	$C_3H_4 + O_2$		2.500E+12	0.00	0	[39]
198f	$C_3H_4 + OH$	$\rightleftharpoons$	$C_3H_3 + H_2O$		5.300E+06	2.00	8.37	[48]
199f	$C_3H_3 + O_2$	$\rightleftharpoons$	$\mathrm{CH_{2}CO} + \mathrm{HCO}$		3.000E+10	0.00	12	[49]
$200f^{a,b}$	$C_3H_4 + H + M$	$\stackrel{\textstyle \smile}{}$	$C_3H_5 + M$	$k_0$	3.000E+24	-2.00	0	[39]
				$k_{\infty}$	4.000E+13	0.00	0	
201f	$C_3H_5 + H$	$\rightleftharpoons$	$C_3H_4 + H_2$		1.800E+13	0.00	0	[50]
202f	$C_3H_5 + O_2$	$\rightleftharpoons$	$C_3H_4 + HO_2$		4.990E+15	-1.40	93.8	[51]
203f	$C_3H_5 + CH_3$	$\rightleftharpoons$	$C_3H_4 + CH_4$		3.000E+12	-0.32	-0.548	[39]
$204f^{a,b}$	$C_2H_2 + CH_3 + M$	$\rightleftharpoons$	$C_3H_5 + M$	$k_0$	2.000E+09	1.00	0	[39]
				$k_{\infty}$	6.000E+08	0.00	0	
205f	$C_3H_5 + OH$	$\rightleftharpoons$	$C_3H_4 + H_2O$		6.000E+12	0.00	0	[39]
206f	$C_3H_3 + HCO$	$\rightleftharpoons$	$C_3H_4 + CO$		2.500E+13	0.00	0	[48]
207f	$C_3H_3 + HO_2$	$\rightleftharpoons$	$OH + CO + C_2H_3$		8.000E+11	0.00	0	[47]
208f	$C_3H_4 + O_2$	$\rightleftharpoons$	$CH_3 + HCO + CO$		4.000E+14	0.00	175	[52]
209f	$C_3H_6 + O$	$\rightleftharpoons$	$C_2H_5 + HCO$		3.500E+07	1.65	-4.07	[50]
210f	$C_3H_6 + OH$	$\rightleftharpoons$	$C_3H_5 + H_2O$		3.100E+06	2.00	-1.25	[50]
211f	$C_3H_6 + O$	$\stackrel{\longleftarrow}{}$	$CH_2CO + CH_3 + H$		1.200E+08	1.65	1.37	[50]
212f			$C_3H_5 + H_2$		1.700E+05	2.50	10.4	[50]
$213f^{a,b}$	$C_3H_5 + H + M^{(8)}$	$\rightleftharpoons$	$C_3H_6 + M^{(8)}$	$k_0$	1.330E+60	-12.00	25	[47]
				$k_{\infty}$	2.000E+14	0.00	0	
214f	$C_3H_5 + HO_2$	$\rightleftharpoons$	$C_3H_6 + O_2$		2.660E+12	0.00	0	[15]
215f			$OH + C_2H_3 + CH_2O$	О	3.000E+12	0.00	0	[15]
$216f^{a,b}$	$C_2H_3 + CH_3 + M^{(8)}$	$\rightleftharpoons$	$C_3H_6 + M^{(8)}$	$k_0$	4.270E + 58	-11.94	40.9	[47]
				$k_{\infty}$	2.500E+13	0.00	0	
217f			$C_2H_4 + CH_3$		1.600E+22	-2.39	46.8	[47]
218f	$CH_3 + C_2H_3$				1.500E+24	-2.83	77.9	[47]
$219f^{a,b}$	$C_3H_8 + M$	$\rightleftharpoons$	$CH_3 + C_2H_5 + M$	$k_0$	7.830E+18	0.00	272	[34]
				$k_{\infty}$	1.100E+17	0.00	353	
220f			$I-C_3H_7 + HO_2$		4.000E+13	0.00	199	[53, 47, 54]
221f			$N-C_3H_7 + HO_2$		4.000E+13	0.00	213	[53, 47, 54]
222f			$I-C_3H_7 + H_2$		1.300E+06	2.40	18.7	[53, 47, 54]
223f			$N-C_3H_7 + H_2$		1.330E+06	2.54	28.3	[54, 55]
224f			$I-C_3H_7 + OH$		4.760E+04	2.71	8.82	[54, 47]
225f	$C_3H_8 + O$	$\rightleftharpoons$	$N-C_3H_7 + OH$		1.900E+05	2.68	15.6	[54, 47]

Number		Re	action		A	n	E	Ref.
226f	$C_3H_8 + OH$	$\rightleftharpoons$	$N-C_3H_7 + H_2O$		1.000E+10	1.00	6.69	[29]
227f	$C_3H_8 + OH$	$\rightleftharpoons$	$I-C_3H_7 + H_2O$		2.000E+07	-1.60	-0.418	[29]
228f	$C_3H_8 + HO_2$	$\rightleftharpoons$	$I-C_3H_7 + H_2O_2$		9.640E+03	2.60	58.2	[54, 55, 47]
229f	$C_3H_8 + HO_2$	$\rightleftharpoons$	$N-C_3H_7 + H_2O_2$		4.760E+04	2.55	69	[54, 55, 47]
230f	$I-C_3H_7 + C_3H_8$	$\rightleftharpoons$	$N-C_3H_7+C_3H_8$		8.400E-03	4.20	36.3	[54, 56]
$231f^{a,b}$	$C_3H_6 + H + M^{(8)}$	$\rightleftharpoons$	$I-C_3H_7 + M^{(8)}$	$k_0$	8.700E+42	-7.50	19.8	[47]
				$k_{\infty}$	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	[54, 47]
$233f^{a,b}$	$N-C_3H_7 + M$	$\rightleftharpoons$	$CH_3 + C_2H_4 + M$	$k_0$	5.490E+49	-10.00	150	[54, 47]
				$k_{\infty}$	1.230E+13	-0.10	126	
$234f^{a,b}$	$H + C_3H_6 + M^{(8)}$	$\rightleftharpoons$	$N-C_3H_7 + M^{(8)}$	$k_0$	6.260E+38	-6.66	29.3	[54, 47]
				$k_{\infty}$	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	[29]
a235f	$N-C_3H_7 + O_2$	$\rightleftharpoons$	$C_3H_6OOH$		2.000E+12	0.00	0	[29]
b235f	$C_3H_6OOH$	$\rightleftharpoons$	$C_3H_6 + HO_2$		2.500E + 35	-8.30	92	[29]
c235f	$C_3H_6OOH + O_2$	$\rightleftharpoons$	$OC_3H_5OOH + OH$		1.500E+08	0.00	-29.3	[29]
d235f	$OC_3H_5OOH$	$\rightleftharpoons$	$\mathrm{CH_{2}CHO} + \mathrm{CH_{2}O}$	+ OH	1.000E+15	0.00	180	[29]

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

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

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<sup>a</sup>Third-body efficiencies are:
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[M1] = 0.5 [AR] + 0.5 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].
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$$[M2] = 0.38 [AR] + 0.38 [HE] + 2.5 [H2] + 12 [H2O] + 1.9 [CO] + 3.8 [CO2] + 1 [other].$$

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

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

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

[M] = 1 [other].

$$[M6] = 0.7 [AR] + 0.4 [HE] + 2.5 [H2] + 6 [H2O] + 6 [H2O2] + 1.5 [CO] + 2 [CO2] + 1 [other].$$

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

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

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

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

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

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

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

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

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

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

 $F_{c,a21f} = 1.$ 

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

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

<sup>&</sup>lt;sup>b</sup>Pressure dependent reactions are described by the TROE-formulation [57]. The centering parameters are given by:

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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}).
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## 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  $H + O_2 (+M) \rightarrow HO_2 (+M)$ . 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<sub>2</sub>/O<sub>2</sub> reaction. *International Journal of Chemical Kinetics*, 31:113–125, 1999.
- [6] J. Warnatz. Combustion Chemistry. Springer-Verlag, Berlin, 1984.
- [7] Z. Hong, K. Lam, R. Sur, S. Wang, D. Davidson, and R. Hanson. On the rate constants of oh+ho2 and ho2+ho2: A comprehensive study of h2o2 thermal decomposition using multi-species laser absorption. *Proceedings of the Combustion Institute*, 34:565–571, 2013.

- [8] P. Saxena and F. A. Williams. Detailed and short mechanisms for syngas combustion. 2011 7th US National Combustion Meeting, 2011.
- [9] 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.
- [10] R. P. Lindstedt and G. Skevis. Chemistry of acetylene flames. Combustion Science and Technology, 125(1–6):73–137, 1997.
- [11] P. Saxena. Numerical and Experimental Studies of Ethanol Flames and Autoignition Theory for Higher Alkanes. PhD thesis, University of California at San Diego, 2007.
- [12] 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.
- [13] Gri-mech 1.2. http://www.me.berkeley.edu/gri\_mech/.
- [14] J. Li. Experimental and Numerical Studies of Ethanol Chemical Kinetics. PhD thesis, Princeton University, 2004.
- [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. Evaluated kinetic data for combustion modeling. Journal of Physical and Chemical Reference Data, 21(3):411-749, 1992.
- [16] 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.
- [17] 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.
- [18] 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.
- [19] 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.
- [20] 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.

- [21] R. Zellner and F. Ewig. Computational study of the  $ch_3 + o_2$  chain branching reaction. Journal of Physical Chemistry, 92:2971–2974, 1988.
- [22] 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.
- [23] K.P. Lim and J.V. Michael. The thermal reactions of CH<sub>3</sub>. Twenty-Fifth Symposium (International) on Combustion, page 713, 1994.
- [24] 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.
- [25] P. Frank, K.A. Bhaskaran, and T. Just. Acetylene oxidation: The reaction C<sub>2</sub>H<sub>2</sub> + O at high temperatures. In Twenty-First Symposium (International) on Combustion, page 885, Pittsburgh, Pennsylvania, 1986. The Combustion Institute.
- [26] 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.
- [27] M.W. Markus, P. Roth, and T. Just. A shock tube study of the reactions of ch with CO<sub>2</sub> and O<sub>2</sub>. *International Journal of Chemical Kinetics*, 28:171, 1996.
- [28] S.C. Li and Williams F.A. Formation of NO<sub>x</sub>, CH<sub>4</sub>, and C<sub>2</sub> species in laminar methanol flames. *Proceedings of the Combustion Institute*, 27:485–493, 1998.
- [29] 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.
- [30] 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.
- [31] 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.
- [32] 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.
- [33] 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.

- [34] 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.
- [35] 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.
- [36] 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.
- [37] 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.
- [38] 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.
- [39] M. Petrova and F. A. Williams. A small detailed chemical-kinetic mechanism for hydrocarbon combustion. *Combustion and Flame*, 144:526–544, 2006.
- [40] C.K. Westbrook and F.L. Dryer. Chemical kinetic modeling of hydrocarbon combustion. Progress in Energy and Combustion Science, 10:1–57, 1984.
- [41] 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.
- [42] H. S. T. Driver, R. J. Hutcheon, R. D. Lockett, G. N. Robertson, H. H. Grotheer, and Kelm. Elementary reactions in the methanol oxidation system. part ii: Measurement and modeling of autoignition in a methanol-fuelled otto engine. *Berichte der Bunsen-Gesellschaft – Physical Chemistry Chemical Physics*, 96:1376–1387, 1992.
- [43] T. S. Norton and F. L. Dryer. Toward a comprehensive mechanism for methanol pyrolysis. *Journal of Chemical Kinetics*, 22:219–241, 1990.
- [44] R. Seiser, K. Seshadri, and F. A. Williams. Detailed and reduced chemistry for methanol ignition. *Combustion and Flame*, 2011.
- [45] T. Held and F. L. Dryer. A comprehensive mechanism for methanol oxidation. *International Journal of Chemical Kinetics*, 30:805–830, 1998.

- [46] P. Saxena and F. A. Williams. Numerical and experimental studies of ethanol flames. *Proceedings of the Combustion Institute*, 31(1):1149–1156, 2007.
- [47] 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.
- [48] 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.
- [49] 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.
- [50] W. Tsang. Journal of Physical and Chemical Reference Data, 20, 1991.
- [51] 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.
- [52] 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.
- [53] B. Varatharajan and F. A. Williams. Ignition times in the theory of branched-chain thermal explosions. *Combustion and Flame*, 121:551–554, 2000.
- [54] W. Tsang. Chemical kinetic data base for combustion chemistry. part 3. propane. Journal of Physical and Chemical Reference Data, 17(2):887–951, 1988.
- [55] 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.
- [56] Z. Qin. Shock Tube Modeling Study of Propane Ignition. PhD thesis, University of Texas at Austin, 1998.
- [57] 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.