

Table S1: TDRF-NO simplified mechanism

Species				
AC ₈ H ₁₆ OOH	C ₄ H ₅	CH ₃	H ₂ CNO ₂	MPT124
AC ₈ H ₁₇	C ₅ H ₁₁	CH ₃ CHO	H ₂ O	MPT124J
AC ₈ H ₁₇ O	C ₅ H ₄ O	CH ₃ CO	H ₂ O ₂	N
AC ₈ H ₁₇ O ₂	C ₆ H ₄ CH ₃	CH ₃ COCH ₂	HCCO	N ₂
AOC ₈ H ₁₆ OOH	C ₆ H ₄ O ₂	CH ₃ NO ₂	HCN	NC ₇ H ₁₆
AR	C ₆ H ₅	CH ₃ O	HCO	NCO
MP1OCO	C ₆ H ₅ CH ₂	CH ₃ O ₂	HO ₂	NO
MP1CO-C	C ₆ H ₅ CH ₂ O	CH ₃ O ₂ H	H	NO ₂
C ₆ H ₅ CH ₂ OO	C ₂ H	CH ₃ OH	HOC ₆ H ₄ CH ₃	O
HO ₂ C ₇ H ₁₃ O ₂ H	C ₆ H ₅ CH ₃	CH ₄	HONO	O ₂
C ₂ H ₃	C ₆ H ₅ CHO	CO	IC ₃ H ₅ CHO	OC ₆ H ₄ CH ₃
C ₂ H ₄	C ₆ H ₅ CO	CO ₂	IC ₃ H ₅ CO	OC ₇ H ₁₃ O
C ₂ H ₅	C ₆ H ₅ O	DMPD13-D	IC ₃ H ₇	OC ₇ H ₁₃ OOH
C ₂ H ₅ O	C ₆ H ₅ OH	DMPD13	IC ₄ H ₇	OC ₈ H ₁₅ O
C ₂ H ₅ O ₂	C ₇ H ₁₄ OOH	DMPD13-B	IC ₄ H ₇ O	OC ₈ H ₁₅ OOH
C ₂ H ₆	C ₇ H ₁₅ -1	DMPD13CO	IC ₄ H ₈	OH
C ₃ H ₃	C ₇ H ₁₅ -2	DMPD13-E	IC ₈ H ₁₅ -A	OOC ₇ H ₁₄ OOH
C ₃ H ₄	C ₇ H ₁₅ O	DMPD13HO	IC ₈ H ₁₆	PC ₄ H ₉
C ₃ H ₄ -A	C ₇ H ₁₅ OO	DMPD13O	IC ₈ H ₁₈	PD12CO
C ₃ H ₄ -P	CH	DMPD13OHE	JC ₈ H ₁₅ -B	PD12CO-E
C ₃ H ₅	CH ₂	DMPDBCO	JC ₈ H ₁₆	TC ₄ H ₉
C ₃ H ₅ -T	CH ₂ CHO	DMPDBHO	M4PD12-D	YC ₇ H ₁₃ -Y2
C ₃ H ₆	CH ₂ CO	DMPDBO	M4PD12O	C ₄ H ₄
C ₄ H ₃	CH ₂ O	H ₂	CH ₂ OH	

No.	Reactions	A	b	E _a
$k = AT^b \exp(-E_a/RT)$				
2	NC ₇ H ₁₆ + O ₂ => C ₇ H ₁₅ -1+ HO ₂	6.00E+13	0	52820
3	NC ₇ H ₁₆ + O ₂ => C ₇ H ₁₅ -2+ HO ₂	4.00E+13	0	50190
4	NC ₇ H ₁₆ + HO ₂ => C ₇ H ₁₅ -1+ H ₂ O ₂	5.00E+13	0	20430
5	NC ₇ H ₁₆ + HO ₂ => C ₇ H ₁₅ -2+ H ₂ O ₂	3.36E+13	0	17690
6	NC ₇ H ₁₆ +OH=> C ₇ H ₁₅ -1+ H ₂ O	1.05E+10	1	1590
7	NC ₇ H ₁₆ +OH=> C ₇ H ₁₅ -2+ H ₂ O	9.40E+07	1.6	-35
8	C ₇ H ₁₅ -1=> C ₇ H ₁₅ -2	2.00E+11	0	18120
9	C ₇ H ₁₅ -2=> C ₇ H ₁₅ -1	2.00E+11	0	18120
10	C ₇ H ₁₅ -1+ O ₂ => C ₇ H ₁₅ OO	2.50E+12	0	0
11	C ₇ H ₁₅ OO=> C ₇ H ₁₅ -1+ O ₂	2.20E+15	0	27960

12	$C_7H_{15-2} + O_2 \Rightarrow C_7H_{15}OO$	2.50E+12	0	0
13	$C_7H_{15}OO \Rightarrow C_7H_{15-2} + O_2$	2.20E+15	0	26960
14	$C_7H_{15}OO \Rightarrow C_7H_{14}OOH$	2.00E+11	0	17010
15	$C_7H_{14}OOH + O_2 \Rightarrow OO C_7H_{14}OOH$	5.60E+12	0	0
16	$OO C_7H_{14}OOH \Rightarrow HO_2C_7H_{13}O_2H$	2.00E+11	0	17010
17	$HO_2C_7H_{13}O_2H \Rightarrow OC_7H_{13}OOH + OH$	1.00E+09	0	7500
18	$OC_7H_{13}OOH \Rightarrow OC_7H_{13}O + OH$	8.40E+14	0	43020
19	$OC_7H_{13}O \Rightarrow C H_2O + C_5H_{11} + CO$	2.00E+13	0	15000
20	$C_7H_{15-1} \Rightarrow C_5H_{11} + C_2H_4$	2.50E+13	0	28920
21	$C_7H_{15-2} \Rightarrow PC_4H_9 + C_3H_6$	1.20E+13	0	28203
22	$C_5H_{11} \Rightarrow C_2H_4 + IC_3H_7$	7.97E+17	-1.4	29876
23	$NC_7H_{16} + H \Rightarrow C_7H_{15-1} + H_2$	1.88E+05	2.8	6286
24	$NC_7H_{16} + H \Rightarrow C_7H_{15-2} + H_2$	2.60E+06	2.4	4469
25	$IC_3H_7 + O_2 = C_3H_6 + HO_2$	6.10E+20	-2.9	7910
26	$C_3H_6 + H(+M) = IC_3H_7(+M)$	5.70E+09	1.2	874
Low pressure limit: 1.64E+54 -1.11E+01 9.36E+03				
TROE centering: 1.00E+00 1.00E-15 2.60E+02 3.00E+03				
H ₂ O	Enhanced by 5.00E+00			
H ₂	Enhanced by 2.00E+00			
CO ₂	Enhanced by 3.00E+00			
CO	Enhanced by 2.00E+00			
27	$IC_3H_7 + H = C_2H_5 + CH_3$	5.00E+13	0	0
28	$PC_4H_9(+M) = C_2H_5 + C_2H_4(+M)$	1.06E+13	0	27828
Low pressure limit: 1.90E+55 -1.19E+01 3.23E+04				
H ₂ O	Enhanced by		5.00E+00	
H ₂	Enhanced by		2.00E+00	
CO ₂	Enhanced by		3.00E+00	
CO	Enhanced by		2.00E+00	
29	$PC_4H_9 = C_2H_5 + C_2H_4$	2.50E+13	0	28800
30	$IC_8H_{18} + O_2 = AC_8H_{17} + HO_2$	1.00E+16	0	49000
Reverse Arrhenius coefficients:				
31	$IC_8H_{18} + HO_2 = AC_8H_{17} + H_2O_2$	3.02E+12	0	14700
32	$AC_8H_{17} + O_2 = AC_8H_{17}O_2$	1.00E+12	0	0
Reverse Arrhenius coefficients:				
33	$AC_8H_{17}O_2 = AC_8H_{16}OOH$	1.14E+11	0	22400
Reverse Arrhenius coefficients:				
34	$AC_8H_{16}OOH + O_2 = AOOC_8H_{16}OOH$	3.16E+11	0	0
Reverse Arrhenius coefficients:				
35	$AOOC_8H_{16}OOH \Rightarrow OC_8H_{15}OOH + OH$	8.91E+10	0	17000
36	$IC_8H_{18} + OH \Rightarrow AC_8H_{17} + H_2O$	3.00E+13	0	3000
37	$OC_8H_{15}OOH \Rightarrow OC_8H_{15}O + OH$	3.98E+15	0	43000
38	$AC_8H_{17} + O_2 = JC_8H_{16} + HO_2$	3.16E+11	0	6300
Reverse Arrhenius coefficients:				
		3.16E+11	0	19500

39	$\text{OC}_8\text{H}_{15}\text{O} + \text{O}_2 \Rightarrow$ $\text{C}_2\text{H}_3 + 2\text{CH}_2\text{O} + \text{C}_3\text{H}_4 + \text{CH}_3 + \text{HO}_2$	2.45E+13	0	32000
40	$\text{AC}_8\text{H}_{17} \Rightarrow \text{IC}_4\text{H}_8 + \text{C}_3\text{H}_6 + \text{CH}_3$	1.28E+12	0	49000
41	$\text{JC}_8\text{H}_{16} \Rightarrow \text{IC}_4\text{H}_8 + \text{C}_3\text{H}_5 + \text{CH}_3$	1.92E+12	0	49000
42	$\text{IC}_4\text{H}_8 + \text{O}_2 \Rightarrow \text{C}_2\text{H}_3 + \text{C}_2\text{H}_4 + \text{HO}_2$	2.00E+14	0	35900
43	$\text{IC}_4\text{H}_8 = \text{C}_3\text{H}_5 + \text{CH}_3$	1.92E+66	-14.2	128100
Reverse Arrhenius coefficients:		2.09E+59	-13.2	29530
44	$\text{C}_6\text{H}_5\text{CH}_3 + \text{O}_2 = \text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2$	1.81E+12	0	39717
45	$\text{C}_6\text{H}_5\text{CH}_3 + \text{OH} = \text{C}_6\text{H}_5\text{CH}_2 + \text{H}_2\text{O}$	6.70E+09	1	870
46	$\text{C}_6\text{H}_5\text{CH}_3 + \text{O} = \text{C}_6\text{H}_5\text{CH}_2 + \text{OH}$	6.30E+11	0	0
47	$\text{C}_6\text{H}_5\text{CH}_3 + \text{H} = \text{C}_6\text{H}_5\text{CH}_2 + \text{H}_2$	6.00E+13	0	8235
48	$\text{C}_6\text{H}_5\text{CH}_2 + \text{O} = \text{C}_6\text{H}_5\text{CHO} + \text{H}$	2.50E+14	0	0
49	$\text{C}_6\text{H}_5\text{CH}_2 + \text{O} = \text{C}_6\text{H}_5 + \text{CH}_2\text{O}$	8.00E+13	0	0
50	$\text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2 = \text{C}_6\text{H}_5\text{CHO} + \text{H} + \text{OH}$	2.60E+13	0	0
51	$\text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2 = \text{C}_6\text{H}_5\text{CHO} + \text{H}_2\text{O}$	7.50E+12	0	0
52	$\text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2 = \text{C}_6\text{H}_5 + \text{CH}_2\text{O} + \text{OH}$	6.00E+12	0	0
53	$\text{C}_6\text{H}_5\text{CH}_2 + \text{H} = \text{C}_6\text{H}_5\text{CH}_3$	1.80E+14	0	0
54	$\text{C}_6\text{H}_5\text{CHO} + \text{OH} = \text{C}_6\text{H}_5\text{CO} + \text{H}_2\text{O}$	1.71E+09	1.2	-447
55	$\text{C}_6\text{H}_5\text{CHO} + \text{H} = \text{C}_6\text{H}_5\text{CO} + \text{H}_2$	5.00E+13	0	4928
56	$\text{C}_6\text{H}_5\text{CHO} + \text{O} = \text{C}_6\text{H}_5\text{CO} + \text{OH}$	9.04E+12	0	3080
57	$\text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_5\text{CHO} = \text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{CO}$	2.77E+03	2.8	5773
58	$\text{C}_6\text{H}_5\text{CO} = \text{C}_6\text{H}_5 + \text{CO}$	3.98E+14	0	29400
59	$\text{C}_6\text{H}_5 + \text{O}_2 = \text{C}_6\text{H}_5\text{O} + \text{O}$	2.60E+13	0	6100
60	$\text{C}_6\text{H}_5 + \text{O}_2 = \text{C}_6\text{H}_5\text{O} + \text{O}$	2.60E+13	0	6100
61	$\text{C}_6\text{H}_5 + \text{OH} = \text{C}_6\text{H}_5\text{O} + \text{H}$	5.00E+13	0	0
62	$\text{C}_6\text{H}_5\text{OH} + \text{OH} = \text{C}_6\text{H}_5\text{O} + \text{H}_2\text{O}$	3.00E+06	2	-1310
63	$\text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_5\text{OH} = \text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{O}$	1.05E+12	0	9500
64	$\text{C}_6\text{H}_5 + \text{O}_2 = \text{C}_6\text{H}_4\text{O}_2 + \text{H}$	3.00E+13	0	8980
65	$\text{C}_6\text{H}_5\text{O} + \text{O} = \text{C}_6\text{H}_4\text{O}_2 + \text{H}$	5.00E+13	0	0
66	$\text{C}_6\text{H}_5\text{O} + \text{HO}_2 = \text{C}_6\text{H}_4\text{O}_2 + \text{H}_2\text{O}$	1.00E+13	0	0
67	$\text{C}_6\text{H}_4\text{O}_2 + \text{O} \Rightarrow 2\text{CO} + \text{C}_2\text{H}_2 + \text{CH}_2\text{CO}$	3.00E+13	0	5000
68	$\text{C}_6\text{H}_5\text{CH}_3 + \text{OH} = \text{C}_6\text{H}_4\text{CH}_3 + \text{H}_2\text{O}$	3.40E+08	1.4	1450
69	$\text{C}_6\text{H}_4\text{CH}_3 + \text{O}_2 = \text{O} + \text{C}_6\text{H}_4\text{CH}_3 + \text{O}$	2.60E+13	0	6100
70	$\text{HO} + \text{C}_6\text{H}_4\text{CH}_3 + \text{H} = \text{C}_6\text{H}_5\text{CH}_3 + \text{OH}$	2.21E+13	0	7910
71	$\text{O} + \text{C}_6\text{H}_4\text{CH}_3 + \text{H} = \text{HOC}_6\text{H}_4\text{CH}_3$	2.50E+14	0	0
72	$\text{HO} + \text{C}_6\text{H}_4\text{CH}_3 + \text{OH} = \text{OC}_6\text{H}_4\text{CH}_3 + \text{H}_2\text{O}$	6.00E+12	0	0
73	$\text{C}_5\text{H}_4\text{O} + \text{O} = \text{C}_4\text{H}_4 + \text{CO}_2$	1.00E+13	0	2000
74	$\text{C}_4\text{H}_5 + \text{O}_2 \Rightarrow \text{C}_4\text{H}_4 + \text{HO}_2$	1.00E+08	2	10000
75	$\text{C}_4\text{H}_4 + \text{OH} = \text{C}_4\text{H}_3 + \text{H}_2\text{O}$	7.50E+06	2	5000
76	$\text{C}_4\text{H}_4 + \text{O} = \text{C}_3\text{H}_3 + \text{HCO}$	8.10E+06	1.9	180
77	$\text{C}_4\text{H}_3 + \text{O}_2 = \text{C}_2\text{H}_2 + \text{CO} + \text{HCO}$	3.00E+12	0	0
78	$\text{C}_7\text{H}_{15-1} + \text{C}_6\text{H}_5\text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2 + \text{NC}_7\text{H}_{16}$	1.00E+11	0	12000
79	$\text{C}_7\text{H}_{15-2} + \text{C}_6\text{H}_5\text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2 + \text{NC}_7\text{H}_{16}$	1.00E+11	0	12000
80	$\text{AC}_8\text{H}_{17} + \text{C}_6\text{H}_5\text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2 + \text{IC}_8\text{H}_{18}$	1.00E+11	0	12000

81	$\text{IC}_8\text{H}_{18} + \text{C}_7\text{H}_{15} - 1 = \text{NC}_7\text{H}_{16} + \text{AC}_8\text{H}_{17}$	9.00E+11	0	13500
82	$\text{IC}_8\text{H}_{18} + \text{C}_7\text{H}_{15} - 2 = \text{NC}_7\text{H}_{16} + \text{AC}_8\text{H}_{17}$	9.00E+11	0	14500
83	$\text{C}_3\text{H}_6 + \text{H} = \text{C}_2\text{H}_4 + \text{CH}_3$	7.20E+12	0	1300
84	$\text{C}_3\text{H}_6 + \text{O} = \text{C}_3\text{H}_5 + \text{OH}$	5.20E+11	0.7	5884
85	$\text{C}_3\text{H}_6 + \text{OH} = \text{C}_3\text{H}_5 + \text{H}_2\text{O}$	3.10E+06	2	1451
86	$\text{C}_3\text{H}_6 + \text{OH} \Rightarrow \text{C}_2\text{H}_5 + \text{C H}_2\text{O}$	7.90E+12	0	0
87	$\text{C}_3\text{H}_6 + \text{O}_2 = \text{C}_3\text{H}_5 + \text{HO}_2$	2.00E+13	0	47600
88	$\text{C}_3\text{H}_5 + \text{O}_2 = \text{CH}_2\text{CHO} + \text{CH}_2\text{O}$	1.10E+10	0.3	12840
89	$\text{C}_3\text{H}_5 + \text{O}_2 = \text{C}_3\text{H}_4 + \text{HO}_2$	5.00E+15	-1.4	22430
90	$\text{C}_3\text{H}_5 + \text{OH} = \text{C}_3\text{H}_4 + \text{H}_2\text{O}$	2.00E+13	0	0
91	$\text{C}_3\text{H}_4 + \text{OH} = \text{C}_2\text{H}_3 + \text{C H}_2\text{O}$	1.00E+12	0	0
92	$\text{C}_3\text{H}_4 + \text{OH} = \text{C}_2\text{H}_4 + \text{HCO}$	1.00E+12	0	0
93	$\text{C}_2\text{H}_5 + \text{O} = \text{CH}_3\text{CHO} + \text{H}$	5.30E+13	0	0
94	$\text{C}_2\text{H}_5 + \text{OH} = \text{C}_2\text{H}_4 + \text{H}_2\text{O}$	2.40E+13	0	0
95	$\text{C}_2\text{H}_5 + \text{O}_2 \Rightarrow \text{C}_2\text{H}_4 + \text{HO}_2$	1.00E+10	0	-2190
96	$\text{C}_2\text{H}_4 + \text{H} = \text{C}_2\text{H}_3 + \text{H}_2$	5.40E+14	0	14900
97	$\text{C}_2\text{H}_4 + \text{H} (+\text{M}) = \text{C}_2\text{H}_5 (+\text{M})$	1.10E+12	0.5	1822
Low pressure limit: 1.11E+34 -5.00E+00 4.45E+03				
TROE centering: 5.00E-01 9.50E+01 9.50E+01 2.00E+02				
H_2O	Enhanced	by	5.00E+0	
98	$\text{C}_2\text{H}_4 + \text{OH} \Rightarrow \text{C}_2\text{H}_3 + \text{H}_2\text{O}$	8.02E+13	0	5955
99	$\text{C}_2\text{H}_3 + \text{O}_2 = \text{C H}_2\text{O} + \text{HCO}$	1.10E+23	-3.3	3890
100	$\text{C}_2\text{H}_3 + \text{O}_2 = \text{C H}_2\text{CHO} + \text{O}$	2.50E+15	-0.8	3135
101	$\text{C}_2\text{H}_2 + \text{O}_2 \Rightarrow \text{HCCO} + \text{OH}$	2.00E+08	1.5	30100
102	$\text{C}_2\text{H}_2 + \text{OH} \Rightarrow \text{CH}_3 + \text{CO}$	2.00E+07	2	3214.3
103	$\text{C}_2\text{H}_2 + \text{O} = \text{HCCO} + \text{H}$	1.40E+07	2	1900
104	$\text{C}_2\text{H}_2 + \text{O} = \text{CH}_2 + \text{CO}$	6.10E+06	2	1900
105	$\text{C}_2\text{H} + \text{O}_2 = \text{CO} + \text{CO} + \text{H}$	2.50E+13	0	0
106	$\text{HCCO} + \text{O}_2 \Rightarrow \text{HCO} + \text{CO} + \text{O}$	9.78E+11	0	850
107	$\text{HCCO} + \text{O}_2 \Rightarrow \text{HCO} + \text{CO}_2$	6.52E+11	0	850
108	$\text{HCCO} + \text{O}_2 = \text{CO} + \text{CO} + \text{OH}$	2.90E+07	1.7	1000
109	$\text{CH}_3\text{CHO} + \text{OH} = \text{CH}_3\text{CO} + \text{H}_2\text{O}$	2.30E+10	0.7	-1110
110	$\text{CH}_3\text{CO} (+\text{M}) = \text{CH}_3 + \text{CO} (+\text{M})$	2.80E+13	0	17100
Low pressure limit: 2.10E+15 0.00E+00 1.40E+04				
TROE centering: 5.00E-01 1.00E-30 1.00E+30				
H_2	Enhanced	by	2.00E+00	
CO	Enhanced	by	2.00E+00	
CO_2	Enhanced	by	3.00E+00	
H_2O	Enhanced	by	5.00E+00	
111	$\text{CH}_2\text{CHO} + \text{O}_2 = \text{CH}_2\text{O} + \text{CO} + \text{OH}$	2.20E+11	0	1500
112	$\text{CH}_2\text{CO} + \text{OH} = \text{HCCO} + \text{H}_2\text{O}$	1.00E+07	2	3000
113	$\text{CH}_3 + \text{O} = \text{C H}_2\text{O} + \text{H}$	8.40E+13	0	0
114	$\text{CH}_3 + \text{O}_2 = \text{C H}_2\text{O} + \text{OH}$	1.90E+12	0	20315
115	$\text{CH}_3 + \text{HO}_2 = \text{CH}_3\text{O} + \text{OH}$	8.00E+12	0	0

	116	$\text{CH}_3+\text{H}(+\text{M})=\text{CH}_4(+\text{M})$	1.30E+16	-0.6	383
Low pressure limit: 1.75E+33 -4.76E+00 2.44E+03					
TROE centering: 7.83E-01 7.40E+01 2.94E+03 6.96E+03					
H ₂ O		Enhanced		by	8.57E+00
N ₂		Enhanced		by	1.43E+00
	117	$\text{CH}_3+\text{CH}_2\text{O}=\text{CH}_4+\text{HCO}$	7.80E-08	6.1	1967
	118	$\text{CH}_2\text{O}+\text{H}(+\text{M})=\text{CH}_3\text{O}(+\text{M})$	5.40E+11	0.5	2600
Low pressure limit: 1.54E+30 -4.80E+00 5.56E+03					
TROE centering: 7.58E-01 9.40E+01 1.56E+03 4.20E+03					
N ₂		Enhanced		by	1.43E+00
H ₂ O		Enhanced		by	8.58E+00
	119	$\text{CH}_2\text{O}+\text{OH}=\text{HCO}+\text{H}_2\text{O}$	3.40E+09	1.2	-447
	120	$\text{CH}_2\text{O}+\text{O}_2+\text{M}=\text{H}+\text{CO}+\text{M}+\text{HO}_2$	6.20E+16	0	36939.9
	121	$\text{CH}_2\text{O}+\text{HO}_2=\text{HCO}+\text{H}_2\text{O}_2$	2.17E+11	0	7987
	122	$\text{CH}_2+\text{OH}=\text{CH}+\text{H}_2\text{O}$	1.13E+07	2	3000
	123	$\text{CH}_2+\text{O}_2=\text{CO}+\text{H}_2\text{O}$	2.20E+22	-3.3	2867
	124	$\text{CH}_2+\text{H}=\text{CH}+\text{H}_2$	1.00E+18	-1.6	0
	125	$\text{CH}_2+\text{O}_2=\text{CO}+\text{OH}+\text{H}$	1.60E+21	-3.3	2867
	126	$\text{CH}_2+\text{H}_2=\text{H}+\text{CH}_3$	5.00E+05	2	7230
	127	$\text{CH}_2+\text{CO}_2=\text{C}+\text{H}_2\text{O}+\text{CO}$	1.10E+12	0	1000
	128	$\text{HCO}+\text{O}_2=\text{HO}_2+\text{CO}$	7.60E+12	0	406
	129	$\text{HCO}+\text{M}=\text{H}+\text{CO}+\text{M}$	1.90E+17	-1	17000
H ₂ O		Enhanced		by	5.00E+00
	130	$\text{HCO}+\text{H}=\text{CO}+\text{H}_2$	1.20E+13	0.2	0
	131	$\text{HCO}+\text{OH}=\text{H}_2\text{O}+\text{CO}$	1.00E+14	0	0
	132	$\text{CO}+\text{HO}_2=\text{CO}_2+\text{OH}$	1.51E+14	0	23611.6
	133	$\text{CO}+\text{O}=\text{CO}_2$	1.80E+10	0	2434
	134	$\text{CO}+\text{O}+\text{M}=\text{CO}_2+\text{M}$	5.89E+15	0	4093.3
	135	$\text{CO}+\text{OH}=\text{CO}_2+\text{H}$	3.09E+11	0	733.8
	136	$\text{CO}_2+\text{O}=\text{CO}+\text{O}_2$	2.75E+12	0	43758.8
Reverse Arrhenius coefficients:			3.25E+11	0	36610.4
	137	$\text{CH}_3\text{OH}+\text{OH}=\text{CH}_3\text{O}+\text{H}_2\text{O}$	1.00E+06	2.1	496.7
Reverse Arrhenius coefficients:			8.98E+06	2.1	17380
	138	$\text{O}+\text{OH}=\text{O}_2+\text{H}$	2.00E+14	-0.4	0
	139	$\text{O}+\text{H}_2=\text{OH}+\text{H}$	5.00E+04	2.7	6290
	140	$\text{OH}+\text{H}_2=\text{H}_2\text{O}+\text{H}$	2.10E+08	1.5	3450
	141	$2\text{OH}=\text{O}+\text{H}_2\text{O}$	4.30E+03	2.7	-2486
	142	$\text{H}+\text{H}+\text{M}=\text{H}_2+\text{M}$	1.00E+18	-1	0
H ₂ O		Enhanced		by	0.00E+00
	143	$\text{H}+\text{H}+\text{H}_2\text{O}=\text{H}_2+\text{H}_2\text{O}$	6.00E+19	-1.2	0
	144	$\text{H}+\text{O}+\text{M}=\text{OH}+\text{M}$	6.20E+16	-0.6	0
H ₂ O		Enhanced		by	5.00E+00
	145	$\text{H}+\text{OH}+\text{M}=\text{H}_2\text{O}+\text{M}$	1.60E+21	-2	0
H ₂ O		Enhanced		by	5.00E+00

	146	$O+O+M=O_2+M$	1.90E+13	0	-1788
H ₂ O		Enhanced	by		5.00E+00
	147	$H+O_2+M=HO_2+M$	2.10E+18	-1	0
H ₂ O		Enhanced	by		1.00E+01
N ₂		Enhanced	by		0.00E+00
	148	$H+O_2+N_2=HO_2+N_2$	6.70E+19	-1.4	0
	149	$H+HO_2=H_2+O_2$	4.30E+13	0	1411
	150	$H+HO_2=2OH$	1.70E+14	0	874
	151	$H+HO_2=O+H_2O$	3.00E+13	0	1721
	152	$O+HO_2=O_2+OH$	3.30E+13	0	0
	153	$OH+HO_2=H_2O+O_2$	8.90E+16	-1	0
	154	$HO_2+HO_2=H_2O_2+O_2$	4.20E+14	0	11982
Declared duplicate reaction...					
	155	$HO_2+HO_2=H_2O_2+O_2$	1.30E+11	0	-1629
Declared duplicate reaction...					
	156	$H_2O_2+M=OH+OH+M$	1.80E+17	0	45500
H ₂ O		Enhanced	by		5.00E+00
	157	$H_2O_2+H=HO_2+H_2$	1.70E+12	0	3755
	158	$H_2O_2+H=OH+H_2O$	1.00E+13	0	3576
	159	$H_2O_2+O=OH+HO_2$	6.60E+11	0	3974
	160	$H_2O_2+OH=H_2O+HO_2$	7.80E+12	0	1330
Declared duplicate reaction...					
	161	$H_2O_2+OH=H_2O+HO_2$	5.80E+14	0	9560
Declared duplicate reaction...					
	162	$IC_8H_{16}=YC_7H_{13}-Y_2+CH_3$	7.05E+66	-14.8	100101
	163	$IC_8H_{16}+OH=IC_8H_{15}-A+H_2O$	2.63E+07	1.8	278.2
	164	$IC_8H_{16}+OH=JC_8H_{15}-B+H_2O$	6.00E+06	2	-239
	165	$DMPD13+H=YC_7H_{13}-Y_2$	1.06E+12	0.5	1230
	166	$DMPD13+CH_3=JC_8H_{15}-B$	2.92E+03	2.4	8360
	167	$DMPD13+CH_3=IC_8H_{15}-A$	2.92E+03	2.4	8360
	168	$DMPD13+OH=DMPD13-E+H_2O$	6.00E+06	2	-239
	169	$DMPD13-E+HO_2=DMPD13O+OH$	7.00E+12	0	-1000
	170	$DMPD13O=DMBD13-D+C H_2O$	9.37E+18	-1.7	23116
	171	$DMPD13O=DMPD13HO+H$	4.63E+15	-0.8	21016.4
	172	$DMBD13-D=C_3H_5-T+C_3H_4-P$	9.60E+39	-8.2	42030
	173	$DMBD13-D+CO=DMPD13CO$	1.51E+11	0	4810
	174	$DMPD13HO+O=DMPD13CO+OH$	7.18E+12	0	1389
	175	$DMPD13HO+OH=DMPD13CO+H_2O$	2.69E+10	0.8	-340
	176	$C_3H_3+O_2=CH_2CO+HCO$	3.01E+10	0	2870
Reverse Arrhenius coefficients:			4.88E+11	0	
59470					
	177	$JC_8H_{16}=IC_4H_8+IC_4H_8$	3.96E+27	-5	224293.2
	178	$JC_8H_{16}=TC_4H_9+IC_4H_7$	1.13E+92	-22	459246.3
	179	$TC_4H_9=H+IC_4H_8$	4.65E+46	-9.8	230344.6

Reverse Arrhenius coefficients:	5.89E+44	-9.4	71010.4
180 $\text{IC}_4\text{H}_8+\text{H}=\text{IC}_4\text{H}_7+\text{H}_2$	3.40E+05	2.5	10421.5
Reverse Arrhenius coefficients:	3.17E+04	2.5	74314.1
181 $\text{IC}_4\text{H}_8+\text{OH}=\text{IC}_4\text{H}_7+\text{H}_2\text{O}$	5.20E+06	2	-1246.2
Reverse Arrhenius coefficients:	5.16E+06	1.9	124958.2
182 $\text{IC}_4\text{H}_8=\text{IC}_4\text{H}_7+\text{H}$	3.07E+55	-11.5	478002.6
Reverse Arrhenius coefficients:	7.17E+54	-11.7	108773.8
183 $\text{IC}_4\text{H}_7+\text{HO}_2=\text{IC}_4\text{H}_7\text{O}+\text{OH}$	7.00E+12	0	-4182
Reverse Arrhenius coefficients:	3.42E+12	0.1	46963.9
184 $\text{IC}_4\text{H}_7\text{O}=\text{IC}_3\text{H}_5\text{CHO}+\text{H}$	5.00E+13	0	121696.2
Reverse Arrhenius coefficients:	6.67E+13	-0.1	76990.6
185 $\text{IC}_4\text{H}_7+\text{O}=\text{IC}_3\text{H}_5\text{CHO}+\text{H}$	6.03E+13	0	0
Reverse Arrhenius coefficients:	2.88E+16	-0.5	280779.5
186 $\text{IC}_4\text{H}_8+\text{O}=\text{C H}_2\text{CO}+\text{CH}_3+\text{CH}_3$	3.33E+07	1.8	317.8
187 $\text{IC}_4\text{H}_8+\text{H}=\text{C}_3\text{H}_6+\text{CH}_3$	5.68E+33	-5.7	83640
Reverse Arrhenius coefficients:	3.06E+26	-4.2	113792.2
188 $\text{IC}_4\text{H}_7=\text{C}_3\text{H}_4\text{-A}+\text{CH}_3$	1.23E+47	-9.7	310555.3
Reverse Arrhenius coefficients:	1.13E+38	-7.8	99615.2
189 $\text{IC}_4\text{H}_7\text{O}=\text{C}_3\text{H}_5\text{-T}+\text{C H}_2\text{O}$	2.92E+21	-2.4	147917.3
Reverse Arrhenius coefficients:	1.00E+11	0	52693.2
190 $\text{IC}_3\text{H}_5\text{CHO}+\text{OH}=\text{IC}_3\text{H}_5\text{CO}+\text{H}_2\text{O}$	2.69E+10	0.8	-1421.9
Reverse Arrhenius coefficients:	4.40E+10	0.8	150886.6
191 $\text{IC}_3\text{H}_5\text{CHO}+\text{CH}_3=\text{IC}_3\text{H}_5\text{CO}+\text{CH}_4$	3.98E+12	0	36383.4
Reverse Arrhenius coefficients:	3.93E+13	0	127341.9
192 $\text{IC}_3\text{H}_5\text{CHO}+\text{O}=\text{IC}_3\text{H}_5\text{CO}+\text{OH}$	7.18E+12	0	5808.8
Reverse Arrhenius coefficients:	1.19E+12	0	85981.9
193 $\text{IC}_3\text{H}_5\text{CHO}+\text{H}=\text{IC}_3\text{H}_5\text{CO}+\text{H}_2$	2.60E+12	0	10873.2
Reverse Arrhenius coefficients:	9.82E+11	0	99824.3
194 $\text{IC}_3\text{H}_5\text{CO}=\text{C}_3\text{H}_5\text{-T}+\text{CO}$	1.28E+20	-1.9	144111.7
Reverse Arrhenius coefficients:	1.51E+11	0	20111.2
195 $\text{C}_3\text{H}_5\text{-T}=\text{C}_3\text{H}_4\text{-A}+\text{H}$	3.51E+14	-0.4	171002
Reverse Arrhenius coefficients:	8.50E+12	0	8364
196 $\text{C}_3\text{H}_5\text{-T}=\text{C}_3\text{H}_4\text{-P}+\text{H}$	1.08E+15	-0.6	160965.2
Reverse Arrhenius coefficients:	6.50E+12	0	8364
197 $\text{C}_3\text{H}_5\text{-T}+\text{O}_2=\text{CH}_3\text{COCH}_2+\text{O}$	3.81E+17	-1.4	23335.6
Reverse Arrhenius coefficients:	2.00E+11	0	73185
198 $\text{C}_3\text{H}_5\text{-T}+\text{O}_2=\text{C H}_2\text{O}+\text{CH}_3\text{CO}$	3.71E+25	-4	29453.8
Reverse Arrhenius coefficients:	1.87E+27	-4.4	423218.4
199 $\text{C}_2\text{H}_2+\text{CH}_3=\text{C}_3\text{H}_4\text{-P}+\text{H}$	1.21E+17	-1.2	69755.8
Reverse Arrhenius coefficients:	1.00E+14	0	16728
200 $\text{C}_3\text{H}_4\text{-P}+\text{OH}=\text{C}_3\text{H}_3+\text{H}_2\text{O}$	1.00E+07	2	4182
Reverse Arrhenius coefficients:	2.80E+07	1.8	134325.8
201 $\text{C}_3\text{H}_4\text{-P}+\text{H}=\text{C}_3\text{H}_3+\text{H}_2$	2.00E+07	2	20910
Reverse Arrhenius coefficients:	1.30E+07	1.8	87654.7

202	$\text{CH}_3\text{COC H}_2=\text{C H}_2\text{CO}+\text{CH}_3$	1.00E+14	0	129642
Reverse Arrhenius coefficients: 1.00E+11 0 25092				
203	$\text{C}_3\text{H}_4\text{-A}+\text{OH}=\text{C}_3\text{H}_3+\text{H}_2\text{O}$	1.00E+07	2	4182
Reverse Arrhenius coefficients: 7.00E+06 2 144362.6				
204	$\text{C}_3\text{H}_4\text{-A}+\text{H}=\text{C}_3\text{H}_3+\text{H}_2$	2.00E+07	2	20910
Reverse Arrhenius coefficients: 3.24E+06 2 97691.5				
205	$\text{CH}_3+\text{HO}_2=\text{CH}_4+\text{O}_2$	3.60E+12	0	0
Reverse Arrhenius coefficients: 5.18E+15 -0.3 57960				
206	$\text{CH}_4+\text{OH}=\text{CH}_3+\text{H}_2\text{O}$	1.93E+05	2.4	2106
Reverse Arrhenius coefficients: 4.82E+02 2.9 14860				
207	$\text{CH}_3\text{O}_2\text{H}=\text{CH}_3\text{O}+\text{OH}$	6.31E+14	0	42300
208	$\text{CH}_2\text{OH}+\text{O}_2=\text{CH}_2\text{O}+\text{HO}_2$	3.81E+06	2	1641
Reverse Arrhenius coefficients: 1.77E+11 0.7 24180				
209	$\text{CH}_3\text{O}_2+\text{M}=\text{CH}_3+\text{O}_2+\text{M}$	4.34E+27	-3.4	30470
Reverse Arrhenius coefficients: 5.44E+25 -3.3 0				
210	$\text{CH}_3\text{O}_2+\text{C H}_2\text{O}=\text{CH}_3\text{O}_2\text{H}+\text{HCO}$	1.99E+12	0	11670
Reverse Arrhenius coefficients: 8.50E+12 -0.5 7009				
211	$\text{IC}_8\text{H}_{16}+\text{CH}_3\text{O}_2=\text{JC}_8\text{H}_{15}\text{-B}+\text{CH}_3\text{O}_2\text{H}$	2.04E+04	2.5	12339.3
212	$\text{IC}_8\text{H}_{16}+\text{HO}_2=\text{JC}_8\text{H}_{15}\text{-B}+\text{H}_2\text{O}_2$	2.04E+04	2.5	12339.3
213	$\text{IC}_8\text{H}_{16}+\text{CH}_3\text{O}_2=\text{IC}_8\text{H}_{15}\text{-A}+\text{CH}_3\text{O}_2\text{H}$	8.10E+04	2.5	16690.8
214	$\text{DMPD13}+\text{OH}=\text{DMPD13-B}+\text{H}_2\text{O}$	3.00E+06	2	-239
215	$\text{DMPD13-B}+\text{HO}_2=\text{DMPDBO}+\text{OH}$	7.00E+12	0	-1000
216	$\text{DMPDBO}=\text{M4PD12-D}+\text{CH}_2\text{O}$	9.37E+18	-1.7	23116
217	$\text{DMPDBO}=\text{DMPDBHO}+\text{H}$	4.63E+15	-0.8	21016.4
218	$\text{M4PD12-D}+\text{HO}_2=\text{M4PD12O}+\text{OH}$	7.00E+12	0	-1000
219	$\text{DMPDBHO}+\text{OH}=\text{DMPDBCO}+\text{H}_2\text{O}$	2.69E+10	0.8	-340
220	$\text{M4PD12-D}+\text{CO}=\text{DMPDBCO}$	1.51E+11	0	4810
221	$\text{M4PD12O}=\text{PD12CO}+\text{CH}_3$	4.86E+14	-0.2	15240
222	$\text{PD12CO}+\text{OH}=\text{PD12CO-E}+\text{H}_2\text{O}$	9.79E+00	3.6	-1128
223	$\text{PD12CO-E}=\text{C}_3\text{H}_3+\text{CH}_2\text{CO}$	1.00E+14	0	31000
224	$\text{MPT124}+\text{OH}=\text{MPT124J}+\text{H}_2\text{O}$	3.00E+06	2	-239
225	$\text{MPT124}+\text{CH}_3=\text{DMPD13-E}$	1.50E+11	0	4970
226	$\text{C}_3\text{H}_3+\text{C}_3\text{H}_4\text{-A}=\text{MPT124J}$	8.50E+10	0	11300
227	$\text{DMPD13O}=\text{DMPD13OHE}$	1.39E+11	0	15600
228	$\text{DMPD13OHE}=\text{MPT124}+\text{CH}_2\text{OH}$	1.06E+20	-1.9	56180
229	$\text{DMBD13-D}+\text{O}_2=\text{MP1CO-C}+\text{O}$	3.81E+17	-1.4	5580
230	$\text{MP1CO-C}+\text{HO}_2=\text{MP1OCO}+\text{OH}$	7.00E+12	0	-1000
231	$\text{DMBD13-D}+\text{O}_2=\text{IC}_3\text{H}_5\text{CHO}+\text{CH}_3\text{CO}$	3.71E+25	-4	7043
232	$\text{IC}_3\text{H}_5\text{CHO}+\text{CH}_3\text{CO}=\text{MP1OCO}$	1.00E+11	0	9200
233	$\text{IC}_8\text{H}_{16}+\text{H}=\text{JC}_8\text{H}_{15}\text{-B}+\text{H}_2$	3.79E+05	2.5	2390.1
234	$\text{N}+\text{NO}=\text{N}_2+\text{O}$	2.70E+13	0	355
235	$\text{N}+\text{O}_2=\text{NO}+\text{O}$	9.00E+09	1	6500
236	$\text{N}+\text{OH}=\text{NO}+\text{H}$	3.36E+13	0	385
237	$\text{NO}_2+\text{HO}_2=\text{HONO}+\text{O}_2$	3.65E+08	1.2	4993

238	$\text{CH}_3 + \text{NO}_2 = \text{CH}_3\text{O} + \text{NO}$	1.36E+13	0	0		
239	$\text{CH}_3\text{O} + \text{NO}_2 = \text{C}_2\text{H}_2\text{O} + \text{HONO}$	6.02E+12	0	2281		
240	$\text{CH}_3\text{O}_2 + \text{NO} = \text{CH}_3\text{O} + \text{NO}_2$	3.00E+12	0	-358		
241	$\text{C}_2\text{H}_5 + \text{NO}_2 = \text{C}_2\text{H}_5\text{O} + \text{NO}$	1.36E+13	0	0		
242	$\text{C}_2\text{H}_5\text{O} + \text{NO}_2 = \text{CH}_3\text{CHO} + \text{HONO}$	4.00E+11	0	0		
243	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} = \text{C}_2\text{H}_5\text{O} + \text{NO}_2$	3.00E+12	0	-358		
244	$\text{C}_7\text{H}_{15}\text{OO} + \text{NO} = \text{C}_7\text{H}_{15}\text{O} + \text{NO}_2$	4.00E+12	0	-358		
245	$\text{C}_7\text{H}_{15-2} + \text{NO}_2 = \text{C}_7\text{H}_{15}\text{O} + \text{NO}$	4.00E+13	-0.2	0		
246	$\text{C}_7\text{H}_{15-1} + \text{NO}_2 = \text{C}_7\text{H}_{15}\text{O} + \text{NO}$	4.00E+13	-0.2	0		
247	$\text{AC}_8\text{H}_{17}\text{O}_2 + \text{NO} = \text{AC}_8\text{H}_{17}\text{O} + \text{NO}_2$	1.00E+10	0	0		
248	$\text{AC}_8\text{H}_{17} + \text{NO}_2 = \text{AC}_8\text{H}_{17}\text{O} + \text{NO}$	1.00E+12	-0.2	0		
249	$\text{C}_6\text{H}_5\text{CH}_2\text{OO} + \text{NO} = \text{C}_6\text{H}_5\text{CH}_2\text{O} + \text{NO}_2$	1.03E+14	0	-714		
250	$\text{C}_6\text{H}_5\text{CH}_2 + \text{NO}_2 = \text{C}_6\text{H}_5\text{CH}_2\text{O} + \text{NO}$	1.51E+13	-0.2	0		
251	$\text{HO}_2 + \text{NO} = \text{NO}_2 + \text{OH}$	2.11E+12	0	-479		
252	$\text{NO} + \text{OH} (+\text{M}) = \text{HONO} (+\text{M})$	1.10E+14	-0.3	0		
Low pressure limit:		2.35E+23	-2.40E+00	0.00E+00		
SRI centering:		1.00E+00	0.00E+00	1.00E-18	8.10E-01	0.00E+00
253	$\text{HONO} + \text{OH} = \text{H}_2\text{O} + \text{NO}_2$	1.26E+10	1	135		
254	$\text{NO}_2 + \text{H} = \text{NO} + \text{OH}$	1.30E+14	0	360		
255	$\text{C}_2\text{H}_2\text{O} + \text{NO}_2 = \text{HCO} + \text{HONO}$	8.00E-11	6.7	8300		
256	$\text{C}_6\text{H}_5\text{CHO} + \text{NO}_2 = \text{C}_6\text{H}_5\text{CO} + \text{HONO}$	8.35E-10	6.7	8300		
257	$\text{C}_3\text{H}_3 + \text{N} = \text{HCN} + \text{C}_2\text{H}_2$	1.00E+13	0	0		
258	$\text{CH}_3 + \text{HONO} = \text{CH}_4 + \text{NO}_2$	8.10E+05	1.9	5504		
259	$\text{H}_2\text{CNO}_2 + \text{OH} = \text{C}_2\text{H}_2\text{OH} + \text{NO}_2$	1.00E+13	0	0		
260	$\text{CH}_3\text{NO}_2 + \text{OH} = \text{H}_2\text{CNO}_2 + \text{H}_2\text{O}$	1.49E+13	0	5740		
261	$\text{H}_2\text{CNO}_2 = \text{CH}_2\text{O} + \text{NO}$	1.00E+13	0	36000		
262	$\text{CH}_3\text{NO}_2 (+\text{M}) = \text{CH}_3 + \text{NO}_2 (+\text{M})$	1.80E+16	0	58500		
Low pressure limit:		1.30E+17	0.00E+00	4.20E+04		
TROE centering:		1.83E-01	1.00E-30	1.00E+30		
263	$\text{HCCO} + \text{NO} = \text{HCN} + \text{CO}_2$	1.64E+13	-0.3	-707		
264	$\text{HCN} + \text{O} = \text{NCO} + \text{H}$	1.38E+04	2.6	4980		
265	$\text{NCO} + \text{O} = \text{NO} + \text{CO}$	2.00E+13	0	0		
266	$\text{NCO} + \text{M} = \text{N} + \text{CO} + \text{M}$	3.10E+16	-0.5	48000		
H ₂ O	Enhanced	by	1.63E+01			
CO	Enhanced	by	1.88E+00			
CO ₂	Enhanced	by	3.75E+00			
CH ₄	Enhanced	by	1.63E+01			
C ₂ H ₆	Enhanced	by	1.63E+01			