

Mechanismus: Methanol

Number	Reaction	A	n	E
1f	$\text{O}_2 + \text{H} \rightarrow \text{OH} + \text{O}$	2.000E+14	0.00	70.3
1b	$\text{OH} + \text{O} \rightarrow \text{O}_2 + \text{H}$	1.568E+13	0.00	3.52
2f	$\text{H}_2 + \text{O} \rightarrow \text{OH} + \text{H}$	5.060E+04	2.67	26.3
2b	$\text{OH} + \text{H} \rightarrow \text{H}_2 + \text{O}$	2.222E+04	2.67	18.3
3f	$\text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}$	1.000E+08	1.60	13.8
3b	$\text{H}_2\text{O} + \text{H} \rightarrow \text{H}_2 + \text{OH}$	4.312E+08	1.60	76.5
4f	$2\text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	1.500E+09	1.14	0.42
4b	$\text{H}_2\text{O} + \text{O} \rightarrow 2\text{OH}$	1.473E+10	1.14	71.1
5f	$\text{O}_2 + \text{H} + \text{M}' \rightarrow \text{HO}_2 + \text{M}'$	2.300E+18	-0.80	0
5b	$\text{HO}_2 + \text{M}' \rightarrow \text{O}_2 + \text{H} + \text{M}'$	3.190E+18	-0.80	195
6	$\text{HO}_2 + \text{H} \rightarrow 2\text{OH}$	1.500E+14	0.00	4.2
7	$\text{HO}_2 + \text{H} \rightarrow \text{H}_2 + \text{O}_2$	2.500E+13	0.00	2.9
8	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	6.000E+13	0.00	0
9	$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O}$	3.000E+13	0.00	7.2
10	$\text{HO}_2 + \text{O} \rightarrow \text{OH} + \text{O}_2$	1.800E+13	0.00	-1.7
11	$2\text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	2.500E+11	0.00	-5.2
12f	$2\text{OH} + \text{M}' \rightarrow \text{H}_2\text{O}_2 + \text{M}'$	3.250E+22	-2.00	0
12b	$\text{H}_2\text{O}_2 + \text{M}' \rightarrow 2\text{OH} + \text{M}'$	1.692E+24	-2.00	202
13	$\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{OH}$	1.000E+13	0.00	15
14f	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	5.400E+12	0.00	4.2
14b	$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{OH}$	1.802E+13	0.00	135
15	$2\text{H} + \text{M}' \rightarrow \text{H}_2 + \text{M}'$	1.800E+18	-1.00	0
16	$\text{OH} + \text{H} + \text{M}' \rightarrow \text{H}_2\text{O} + \text{M}'$	2.200E+22	-2.00	0
17	$2\text{O} + \text{M}' \rightarrow \text{O}_2 + \text{M}'$	2.900E+17	-1.00	0
18f	$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	4.400E+06	1.50	-3.1
18b	$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$	4.956E+08	1.50	89.8
19	$\text{CH} + \text{O}_2 \rightarrow \text{CHO} + \text{O}$	3.000E+13	0.00	0
20	$\text{CO}_2 + \text{CH} \rightarrow \text{CHO} + \text{CO}$	3.400E+12	0.00	2.9
21	$\text{CHO} + \text{H} \rightarrow \text{CO} + \text{H}_2$	2.000E+14	0.00	0
22	$\text{CHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	1.000E+14	0.00	0
23	$\text{CHO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	3.000E+12	0.00	0
24f	$\text{CHO} + \text{M}' \rightarrow \text{CO} + \text{H} + \text{M}'$	7.100E+14	0.00	70.3
24b	$\text{CO} + \text{H} + \text{M}' \rightarrow \text{CHO} + \text{M}'$	1.136E+15	0.00	9.97

Number	Reaction	A	n	E
25f	$\text{CH}_2 + \text{H} \rightarrow \text{CH} + \text{H}_2$	8.400E+09	1.50	1.4
25b	$\text{CH} + \text{H}_2 \rightarrow \text{CH}_2 + \text{H}$	5.830E+09	1.50	13.1
26	$\text{CH}_2 + \text{O} \rightarrow \text{CO} + 2\text{H}$	8.000E+13	0.00	0
27	$\text{CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$	6.500E+12	0.00	6.3
28	$\text{CH}_2 + \text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}$	6.500E+12	0.00	6.3
29	$\text{CH}_2\text{O} + \text{H} \rightarrow \text{CHO} + \text{H}_2$	2.500E+13	0.00	16.7
30	$\text{CH}_2\text{O} + \text{O} \rightarrow \text{CHO} + \text{OH}$	3.500E+13	0.00	14.6
31	$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{CHO} + \text{H}_2\text{O}$	3.000E+13	0.00	5
32	$\text{CH}_2\text{O} + \text{M}' \rightarrow \text{CHO} + \text{H} + \text{M}'$	1.400E+17	0.00	320
33f	$\text{CH}_3 + \text{H} \rightarrow \text{CH}_2 + \text{H}_2$	1.800E+14	0.00	63
33b	$\text{CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$	3.680E+13	0.00	44.3
34	$\text{CH}_3 + \text{H} \rightarrow \text{CH}_4$	k_0 2.108E+14	-1.80 0.00	0 0
35	$\text{CH}_3 + \text{O} \rightarrow \text{CH}_2\text{O} + \text{H}$	7.000E+13	0.00	0
36	$2\text{CH}_3 \rightarrow \text{C}_2\text{H}_6$	k_0 3.613E+13	-7.00 0.00	11.6 0
37	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$	3.400E+11	0.00	37.4
38f	$\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$	2.200E+04	3.00	36.6
38b	$\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \text{H}$	8.391E+02	3.00	34.6
39	$\text{CH}_4 + \text{O} \rightarrow \text{CH}_3 + \text{OH}$	1.200E+07	2.10	31.9
40f	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	1.600E+06	2.10	10.3
40b	$\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{OH}$	2.631E+05	2.10	70.9
41f	$\text{C}_2\text{H} + \text{H}_2 \rightarrow \text{C}_2\text{H}_2 + \text{H}$	1.100E+13	0.00	12
41b	$\text{C}_2\text{H}_2 + \text{H} \rightarrow \text{C}_2\text{H} + \text{H}_2$	5.270E+13	0.00	120
42	$\text{C}_2\text{H} + \text{O}_2 \rightarrow \text{CHCO} + \text{O}$	5.000E+13	0.00	6.3
43f	$\text{CHCO} + \text{H} \rightarrow \text{CH}_2 + \text{CO}$	3.000E+13	0.00	0
43b	$\text{CH}_2 + \text{CO} \rightarrow \text{CHCO} + \text{H}$	2.361E+12	0.00	-29.4
44	$\text{CHCO} + \text{O} \rightarrow 2\text{CO} + \text{H}$	1.000E+14	0.00	0
45	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{CH}_2 + \text{CO}$	4.100E+08	1.50	7.1
46	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{CHCO} + \text{H}$	4.300E+14	0.00	50.7
47f	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{C}_2\text{H} + \text{H}_2\text{O}$	1.000E+13	0.00	29.3
47b	$\text{C}_2\text{H} + \text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_2 + \text{OH}$	9.000E+12	0.00	-16
48	$\text{C}_2\text{H}_2 + \text{CH} \rightarrow \text{C}_3\text{H}_3$	3.000E+13	0.00	0
49	$\text{C}_2\text{H}_3 + \text{H} \rightarrow \text{C}_2\text{H}_2 + \text{H}_2$	3.000E+13	0.00	0
50	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{C}_2\text{H}_2 + \text{HO}_2$	5.400E+11	0.00	0

Number	Reaction	A	n	E	
51f	$C_2H_3 \rightarrow C_2H_2 + H$	k_0	1.187E+42	-7.50	190
		k_∞	2.000E+14	0.00	166
51b	$C_2H_2 + H \rightarrow C_2H_3$	k_0	6.245E+41	-7.50	27.5
		k_∞	1.053E+14	0.00	3.39
52f	$C_2H_4 + H \rightarrow C_2H_3 + H_2$		1.500E+14	0.00	42.7
52b	$C_2H_3 + H_2 \rightarrow C_2H_4 + H$		9.605E+12	0.00	32.6
53	$C_2H_4 + O \rightarrow CH_3 + CO + H$		1.600E+09	1.20	3.1
54f	$C_2H_4 + OH \rightarrow C_2H_3 + H_2O$		3.000E+13	0.00	12.6
54b	$C_2H_3 + H_2O \rightarrow C_2H_4 + OH$		8.283E+12	0.00	65.2
55	$C_2H_4 + M' \rightarrow C_2H_2 + H_2 + M'$		2.500E+17	0.00	320
56f	$C_2H_5 + H \rightarrow 2CH_3$		3.000E+13	0.00	0
56b	$2CH_3 \rightarrow C_2H_5 + H$		3.457E+12	0.00	49.7
57	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$		2.000E+12	0.00	20.9
58f	$C_2H_5 \rightarrow C_2H_4 + H$	k_0	1.000E+16	0.00	126
		k_∞	1.300E+13	0.00	167
58b	$C_2H_4 + H \rightarrow C_2H_5$	k_0	1.595E+16	0.00	-27.4
		k_∞	2.073E+13	0.00	13.6
59	$C_2H_6 + H \rightarrow C_2H_5 + H_2$		5.400E+02	3.50	21.8
60	$C_2H_6 + O \rightarrow C_2H_5 + OH$		3.000E+07	2.00	21.4
61	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$		6.300E+06	2.00	2.7
62	$C_3H_3 + O_2 \rightarrow CHCO + CH_2O$		6.000E+12	0.00	0
63	$C_3H_3 + O \rightarrow C_2H_3 + CO$		3.800E+13	0.00	0
64f	$C_3H_4 \rightarrow C_3H_3 + H$		5.000E+14	0.00	370
64b	$C_3H_3 + H \rightarrow C_3H_4$		1.700E+13	0.00	19.9
65	$C_3H_4 + O \rightarrow C_2H_2 + CH_2O$		1.000E+12	0.00	0
66	$C_3H_4 + O \rightarrow C_2H_3 + CHO$		1.000E+12	0.00	0
67	$C_3H_4 + OH \rightarrow C_2H_3 + CH_2O$		1.000E+12	0.00	0
68	$C_3H_4 + OH \rightarrow C_2H_4 + CHO$		1.000E+12	0.00	0
69f	$C_3H_5 \rightarrow C_3H_4 + H$		3.980E+13	0.00	293
69b	$C_3H_4 + H \rightarrow C_3H_5$		1.267E+13	0.00	32.5
70	$C_3H_5 + H \rightarrow C_3H_4 + H_2$		1.000E+13	0.00	0
71f	$C_3H_6 \rightarrow C_2H_3 + CH_3$		3.150E+15	0.00	359
71b	$C_2H_3 + CH_3 \rightarrow C_3H_6$		2.511E+12	0.00	-34.7
72	$C_3H_6 + H \rightarrow C_3H_5 + H_2$		5.000E+12	0.00	6.3
73	$N-C_3H_7 \rightarrow C_2H_4 + CH_3$		9.600E+13	0.00	130
74f	$N-C_3H_7 \rightarrow C_3H_6 + H$		1.250E+14	0.00	155
74b	$C_3H_6 + H \rightarrow N-C_3H_7$		4.609E+14	0.00	21.5

Number	Reaction	A	n	E
75	$\text{I-C}_3\text{H}_7 \rightarrow \text{C}_2\text{H}_4 + \text{CH}_3$	6.300E+13	0.00	154
76	$\text{I-C}_3\text{H}_7 + \text{O}_2 \rightarrow \text{C}_3\text{H}_6 + \text{HO}_2$	1.000E+12	0.00	20.9
77	$\text{C}_3\text{H}_8 + \text{H} \rightarrow \text{N-C}_3\text{H}_7 + \text{H}_2$	1.300E+14	0.00	40.6
78	$\text{C}_3\text{H}_8 + \text{H} \rightarrow \text{I-C}_3\text{H}_7 + \text{H}_2$	1.000E+14	0.00	34.9
79	$\text{C}_3\text{H}_8 + \text{O} \rightarrow \text{N-C}_3\text{H}_7 + \text{OH}$	3.000E+13	0.00	24.1
80	$\text{C}_3\text{H}_8 + \text{O} \rightarrow \text{I-C}_3\text{H}_7 + \text{OH}$	2.600E+13	0.00	18.7
81	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{N-C}_3\text{H}_7 + \text{H}_2\text{O}$	3.700E+12	0.00	6.9
82	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{I-C}_3\text{H}_7 + \text{H}_2\text{O}$	2.800E+12	0.00	3.6
83	$\text{CH}_2\text{OH} + \text{H} \rightarrow \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0
84	$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	1.000E+13	0.00	30.1
85	$\text{CH}_2\text{OH} + \text{M}' \rightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105
86	$\text{CH}_3\text{OH} + \text{M}' \rightarrow \text{CH}_3 + \text{OH} + \text{M}'$	3.160E+18	0.00	336
87	$\text{CH}_3\text{OH} + \text{H} \rightarrow \text{CH}_2\text{OH} + \text{H}_2$	4.000E+13	0.00	25.5
88	$\text{CH}_3\text{OH} + \text{O} \rightarrow \text{CH}_2\text{OH} + \text{OH}$	1.000E+13	0.00	19.6
89	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{CH}_2\text{OH} + \text{H}_2\text{O}$	1.000E+13	0.00	7.1
90f	$\text{CH}_3\text{OH} + \text{HO}_2 \rightarrow \text{CH}_2\text{OH} + \text{H}_2\text{O}_2$	6.200E+12	0.00	81.1
90b	$\text{CH}_2\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{CH}_3\text{OH} + \text{HO}_2$	1.000E+07	1.70	47.9

Mechanismus: *n*-Heptan

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>
01. H2-O2 React. (no HO2, H2O2)				
1f	$\text{O}_2 + \text{H} \rightarrow \text{OH} + \text{O}$	2.000E+14	0.00	70.3
1b	$\text{O} + \text{OH} \rightarrow \text{H} + \text{O}_2$	1.157E+13	0.00	0.622
2f	$\text{H}_2 + \text{O} \rightarrow \text{OH} + \text{H}$	5.060E+04	2.67	26.3
2b	$\text{H} + \text{OH} \rightarrow \text{O} + \text{H}_2$	2.275E+04	2.67	18.5
3f	$\text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}$	1.000E+08	1.60	13.8
3b	$\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$	4.652E+08	1.60	77.3
4f	$2\text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	1.500E+09	1.14	0.42
4b	$\text{O} + \text{H}_2\text{O} \rightarrow 2\text{OH}$	1.552E+10	1.14	71.7
02. Recombination Reactions				
5f	$2\text{H} + \text{M}' \rightarrow \text{H}_2 + \text{M}'$	1.800E+18	-1.00	0
5b	$\text{H}_2 + \text{M}' \rightarrow 2\text{H} + \text{M}'$	5.862E+18	-1.00	435
6f	$2\text{O} + \text{M}' \rightarrow \text{O}_2 + \text{M}'$	2.900E+17	-1.00	0
6b	$\text{O}_2 + \text{M}' \rightarrow 2\text{O} + \text{M}'$	7.341E+18	-1.00	497
7f	$\text{H} + \text{OH} + \text{M}' \rightarrow \text{H}_2\text{O} + \text{M}'$	2.200E+22	-2.00	0
7b	$\text{H}_2\text{O} + \text{M}' \rightarrow \text{OH} + \text{H} + \text{M}'$	3.333E+23	-2.00	498
03. HO2 Formation/Consumption				
8f	$\text{H} + \text{O}_2 + \text{M}' \rightarrow \text{HO}_2 + \text{M}'$	2.300E+18	-0.80	0
8b	$\text{HO}_2 + \text{M}' \rightarrow \text{O}_2 + \text{H} + \text{M}'$	3.287E+18	-0.80	196
9	$\text{HO}_2 + \text{H} \rightarrow 2\text{OH}$	1.500E+14	0.00	4.2
10	$\text{HO}_2 + \text{H} \rightarrow \text{H}_2 + \text{O}_2$	2.500E+13	0.00	2.9
11	$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O}$	3.000E+13	0.00	7.2
12	$\text{HO}_2 + \text{O} \rightarrow \text{OH} + \text{O}_2$	1.800E+13	0.00	-1.7
13f	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	6.000E+13	0.00	0
13b	$\text{O}_2 + \text{H}_2\text{O} \rightarrow \text{OH} + \text{HO}_2$	6.361E+14	0.00	303
04. H2O2 Formation/Consumption				
14	$2\text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	2.500E+11	0.00	-5.2
15f	$2\text{OH} + \text{M}' \rightarrow \text{H}_2\text{O}_2 + \text{M}'$	3.250E+22	-2.00	0
15b	$\text{H}_2\text{O}_2 + \text{M}' \rightarrow 2\text{OH} + \text{M}'$	4.145E+24	-2.00	211
17	$\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{OH}$	1.000E+13	0.00	15
18f	$\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{OH} + \text{HO}_2$	2.803E+13	0.00	26.8
18b	$\text{HO}_2 + \text{OH} \rightarrow \text{O} + \text{H}_2\text{O}_2$	5.429E+12	0.00	81.4
19f	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	5.400E+12	0.00	4.2
19b	$\text{HO}_2 + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2\text{O}_2$	1.082E+13	0.00	130
05. CO REACTIONS				
20f	$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	6.000E+06	1.50	-3.1
20b	$\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$	1.739E+09	1.50	98.7
21	$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1.500E+14	0.00	98.7

Number	Reaction	A	n	E	
22	$\text{CO} + \text{O} + \text{M}' \rightarrow \text{CO}_2 + \text{M}'$	7.100E+13	0.00	-19	
10. CH Reactions					
24	$\text{CH} + \text{O} \rightarrow \text{CO} + \text{H}$	4.000E+13	0.00	0	
25	$\text{CH} + \text{O}_2 \rightarrow \text{CHO} + \text{O}$	6.000E+13	0.00	0	
26	$\text{CH} + \text{CO}_2 \rightarrow \text{CHO} + \text{CO}$	3.400E+12	0.00	2.9	
27f	$\text{CH} + \text{H}_2\text{O} \rightarrow \text{CH}_2\text{OH}$	5.700E+12	0.00	-3.2	
27b	$\text{CH}_2\text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}$	4.449E+14	0.00	363	
11. CHO REACTIONS					
28f	$\text{CHO} + \text{M}' \rightarrow \text{CO} + \text{H} + \text{M}'$	7.100E+14	0.00	70.3	
28b	$\text{H} + \text{CO} + \text{M}' \rightarrow \text{CHO} + \text{M}'$	9.294E+14	0.00	8.03	
29	$\text{CHO} + \text{H} \rightarrow \text{CO} + \text{H}_2$	9.000E+13	0.00	0	
32	$\text{CHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	1.000E+14	0.00	0	
33	$\text{CHO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	3.000E+12	0.00	0	
12. CH2 Reactions					
35f	${}_3\text{-CH}_2 + \text{H} \rightarrow \text{CH} + \text{H}_2$	6.000E+12	0.00	-7.5	
35b	$\text{H}_2 + \text{CH} \rightarrow \text{H} + {}_3\text{-CH}_2$	3.763E+12	0.00	3.16	
38	${}_2{}_3\text{-CH}_2 \rightarrow \text{C}_2\text{H}_2 + 2\text{H}$	1.100E+14	0.00	3.4	
39	${}_3\text{-CH}_2 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_4 + \text{H}$	4.200E+13	0.00	0	
40	${}_3\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$	1.300E+13	0.00	6.2	
41	${}_3\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2$	1.200E+13	0.00	6.2	
42f	${}_1\text{-CH}_2 + \text{M}' \rightarrow {}_3\text{-CH}_2 + \text{M}'$	1.200E+13	0.00	0	
42b	${}_3\text{-CH}_2 + \text{M}' \rightarrow {}_1\text{-CH}_2 + \text{M}'$	4.892E+12	0.00	37.5	
43	${}_1\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$	3.100E+13	0.00	0	
44f	${}_1\text{-CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$	7.200E+13	0.00	0	
44b	$\text{H} + \text{CH}_3 \rightarrow \text{H}_2 + {}_1\text{-CH}_2$	2.246E+14	0.00	60.5	
13. CH2O Reactions					
45	$\text{CH}_2\text{O} + \text{M}' \rightarrow \text{CHO} + \text{H} + \text{M}'$	5.000E+16	0.00	320	
46	$\text{CH}_2\text{O} + \text{H} \rightarrow \text{CHO} + \text{H}_2$	2.300E+10	1.05	13.7	
47	$\text{CH}_2\text{O} + \text{O} \rightarrow \text{CHO} + \text{OH}$	4.150E+11	0.57	11.6	
48	$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{CHO} + \text{H}_2\text{O}$	3.400E+09	1.20	-1.9	
49	$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{CHO} + \text{H}_2\text{O}_2$	3.000E+12	0.00	54.7	
14. CH3 Reactions					
53	$\text{CH}_3 + \text{O} \rightarrow \text{CH}_2\text{O} + \text{H}$	8.430E+13	0.00	0	
34f	$\text{CH}_3 + \text{H} \rightarrow \text{CH}_4$	k_0	6.257E+23	-1.80	0
		k_∞	2.108E+14	0.00	0
34b	$\text{CH}_4 \rightarrow \text{H} + \text{CH}_3$	k_0	6.561E+25	-1.80	439
		k_∞	2.211E+16	0.00	439
55	$\text{CH}_3 + \text{OH} \rightarrow \text{CH}_2\text{OH} + \text{H}$	2.260E+14	0.00	64.8	
57	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4	
145	$\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_2\text{OH} + \text{OH}$	1.800E+13	0.00	0	

Number	Reaction	A	n	E	
59	$\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_4 + \text{O}_2$	3.600E+12	0.00	0	
36f	$2\text{CH}_3 \rightarrow \text{C}_2\text{H}_6$	k_0	1.272E+41	-7.00	11.6
		k_∞	1.813E+13	0.00	0
36b	$\text{C}_2\text{H}_6 \rightarrow 2\text{CH}_3$	k_0	5.014E+44	-7.00	385
		k_∞	7.146E+16	0.00	373
15a. CH3O Reactions					
62	$\text{CH}_2\text{OH} + \text{M}' \rightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105	
63	$\text{CH}_2\text{OH} + \text{H} \rightarrow \text{CH}_2\text{O} + \text{H}_2$	1.800E+13	0.00	0	
64	$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	4.000E+10	0.00	8.9	
67	$\text{CH}_2\text{OH} + \text{O} \rightarrow \text{O}_2 + \text{CH}_3$	1.100E+13	0.00	0	
15b. CH2OH Reactions					
69	$\text{CH}_2\text{OH} + \text{M}' \rightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105	
70	$\text{CH}_2\text{OH} + \text{H} \rightarrow \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0	
71	$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	1.000E+13	0.00	30	
17. CH4 Reactions					
84f	$\text{CH}_4 + \text{H} \rightarrow \text{H}_2 + \text{CH}_3$	1.300E+04	3.00	33.6	
84b	$\text{CH}_3 + \text{H}_2 \rightarrow \text{H} + \text{CH}_4$	4.038E+02	3.00	29.3	
85	$\text{CH}_4 + \text{O} \rightarrow \text{OH} + \text{CH}_3$	6.923E+08	1.56	35.5	
86f	$\text{CH}_4 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6	
86b	$\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{OH} + \text{CH}_4$	2.312E+06	1.83	70.8	
18. CH3OH Reactions					
90f	$\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{OH}$	k_0	1.596E+44	-8.20	0
		k_∞	6.022E+13	0.00	0
90b	$\text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{OH}$	k_0	6.633E+46	-8.20	385
		k_∞	2.503E+16	0.00	385
91	$\text{CH}_3\text{OH} + \text{H} \rightarrow \text{CH}_2\text{OH} + \text{H}_2$	4.000E+13	0.00	25.5	
92	$\text{CH}_3\text{OH} + \text{O} \rightarrow \text{CH}_2\text{OH} + \text{OH}$	1.000E+13	0.00	19.6	
93	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{CH}_2\text{OH} + \text{H}_2\text{O}$	1.000E+13	0.00	7.1	
96	$\text{CH}_3\text{OH} + \text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{OH}$	9.000E+12	0.00	41.1	
97	$+ \text{M} \rightarrow + \text{M}$	2.000E+11	0.00	29.3	
20. C2H REACTIONS					
103	$\text{C}_2\text{H} + \text{O} \rightarrow \text{CO} + \text{CH}$	1.000E+13	0.00	0	
104	$\text{C}_2\text{H} + \text{O}_2 \rightarrow \text{HCCO} + \text{O}$	3.000E+12	0.00	0	
20A. HCCO REACTIONS					
105f	$\text{HCCO} + \text{H} \rightarrow \text{}_3\text{-CH}_2 + \text{CO}$	1.500E+14	0.00	0	
105b	$\text{CO} + \text{}_3\text{-CH}_2 \rightarrow \text{H} + \text{HCCO}$	3.483E+13	0.00	124	
106	$\text{HCCO} + \text{O} \rightarrow 2\text{CO} + \text{H}$	9.600E+13	0.00	0	
21. C2H2 REACTIONS					
109	$\text{C}_2\text{H}_2 + \text{O}_2 \rightarrow \text{HCCO} + \text{OH}$	2.000E+08	1.50	126	
110f	$\text{C}_2\text{H}_2 + \text{H} \rightarrow \text{C}_2\text{H} + \text{H}_2$	1.500E+14	0.00	79.6	
110b	$\text{H}_2 + \text{C}_2\text{H} \rightarrow \text{H} + \text{C}_2\text{H}_2$	1.563E+13	0.00	-34.9	
111	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{}_3\text{-CH}_2 + \text{CO}$	1.720E+04	2.80	2.1	
112	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{HCCO} + \text{H}$	1.720E+04	2.80	2.1	
113f	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}$	6.000E+13	0.00	54.2	

Number	Reaction	A	n	E	
113b	$C_2H + H_2O \rightarrow OH + C_2H_2$	2.908E+13	0.00	3.16	
25. C2H3 REACTIONS					
51f	$C_2H_3 \rightarrow C_2H_2 + H$	k_0	1.187E+42	-7.50	190
		k_∞	2.000E+14	0.00	166
51b	$C_2H_2 + H \rightarrow C_2H_3$	k_0	6.245E+41	-7.50	27.5
		k_∞	1.053E+14	0.00	3.39
120	$C_2H_3 + OH \rightarrow C_2H_2 + H_2O$	5.000E+13	0.00	0	
121	$C_2H_3 + H \rightarrow C_2H_2 + H_2$	1.200E+13	0.00	0	
125	$C_2H_3 + O_2 \rightarrow C_2H_2 + HO_2$	1.210E+11	0.00	0	
a125	$C_2H_3 + O_2 \rightarrow CH_2O + CHO$	5.420E+12	0.00	0	
23. C2H4 REACTIONS					
129f	$C_2H_4 + M' \rightarrow C_2H_2 + H_2 + M'$	2.500E+17	0.00	320	
129b	$H_2 + C_2H_2 + M' \rightarrow C_2H_4 + M'$	6.928E+15	0.00	145	
131f	$C_2H_4 + H \rightarrow C_2H_3 + H_2$	1.700E+15	0.00	62.9	
131b	$H_2 + C_2H_3 \rightarrow H + C_2H_4$	6.285E+13	0.00	47.5	
133	$C_2H_4 + O \rightarrow CHO + CH_3$	1.210E+06	2.08	0	
134f	$C_2H_4 + OH \rightarrow C_2H_3 + H_2O$	6.500E+13	0.00	24.9	
134b	$H_2O + C_2H_3 \rightarrow OH + C_2H_4$	1.118E+13	0.00	73	
24. C2H5 REACTIONS					
58f	$C_2H_5 \rightarrow C_2H_4 + H$	k_0	1.000E+16	0.00	126
		k_∞	1.300E+13	0.00	167
58b	$C_2H_4 + H \rightarrow C_2H_5$	k_0	1.595E+16	0.00	-27.4
		k_∞	2.073E+13	0.00	13.6
146	$C_2H_5 + H \rightarrow 2CH_3$	3.000E+13	0.00	0	
149	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	1.100E+10	0.00	-6.3	
150	$C_2H_5 + CH_3 \rightarrow C_2H_4 + CH_4$	1.140E+12	0.00	0	
25. C2H6 REACTIONS					
164f	$C_2H_6 + H \rightarrow C_2H_5 + H_2$	1.400E+09	1.50	31.1	
164b	$H_2 + C_2H_5 \rightarrow H + C_2H_6$	1.812E+07	1.50	49	
165	$C_2H_6 + O \rightarrow C_2H_5 + OH$	1.000E+09	1.50	24.4	
166	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$	7.200E+06	2.00	3.6	
168f	$C_2H_6 + O_2 \rightarrow C_2H_5 + HO_2$	6.000E+13	0.00	217	
168b	$HO_2 + C_2H_5 \rightarrow O_2 + C_2H_6$	3.407E+11	0.00	-4.16	
170f	$C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$	1.500E-07	6.00	25.4	
170b	$CH_4 + C_2H_5 \rightarrow CH_3 + C_2H_6$	6.250E-08	6.00	47.6	
32. C3H4 Reactions					
187	$C_3H_4 + O \rightarrow CH_2O + C_2H_2$	1.000E+12	0.00	0	
188	$C_3H_4 + O \rightarrow CHO + C_2H_3$	1.000E+12	0.00	0	
189	$C_3H_4 + OH \rightarrow CH_2O + C_2H_3$	1.000E+12	0.00	0	
190	$C_3H_4 + OH \rightarrow CHO + C_2H_4$	1.000E+12	0.00	0	
33. C3H5 Reactions					
191f	$C_3H_5 \rightarrow C_3H_4 + H$	3.980E+13	0.00	293	
191b	$H + C_3H_4 \rightarrow C_3H_5$	6.394E+12	0.00	25.9	

Number	Reaction	A	n	E
192	$\text{C}_3\text{H}_5 + \text{H} \rightarrow \text{C}_3\text{H}_4 + \text{H}_2$	1.000E+13	0.00	0
193	$\text{C}_3\text{H}_5 + \text{O}_2 \rightarrow \text{C}_3\text{H}_4 + \text{HO}_2$	6.000E+11	0.00	41.9
34. C3H6 Reactions				
195f	$\text{C}_3\text{H}_6 \rightarrow \text{C}_2\text{H}_3 + \text{CH}_3$	3.150E+15	0.00	359
195b	$\text{CH}_3 + \text{C}_2\text{H}_3 \rightarrow \text{C}_3\text{H}_6$	6.426E+11	0.00	-47.9
196f	$\text{H} + \text{C}_3\text{H}_6 \rightarrow \text{C}_3\text{H}_5 + \text{H}_2$	5.000E+12	0.00	6.3
196b	$\text{H}_2 + \text{C}_3\text{H}_5 \rightarrow \text{C}_3\text{H}_6 + \text{H}$	4.818E+11	0.00	109
197	$\text{C}_3\text{H}_6 + \text{O} \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{O}$	5.900E+13	0.00	21
198	$\text{C}_3\text{H}_6 + \text{O} \rightarrow \text{C}_2\text{H}_5 + \text{CHO}$	3.600E+12	0.00	0
200	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5 + \text{CH}_2\text{O}$	7.900E+12	0.00	0
202	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{C}_3\text{H}_5 + \text{H}_2\text{O}$	4.000E+12	0.00	0
203	$\text{CH}_3 + \text{C}_3\text{H}_6 \rightarrow \text{CH}_4 + \text{C}_3\text{H}_5$	8.960E+12	0.00	35.6
35a. n-C3H7 Reactions				
205f	$\text{N-C}_3\text{H}_7 \rightarrow \text{CH}_3 + \text{C}_2\text{H}_4$	9.600E+13	0.00	130
205b	$\text{C}_2\text{H}_4 + \text{CH}_3 \rightarrow \text{N-C}_3\text{H}_7$	5.125E+11	0.00	32.2
206f	$\text{N-C}_3\text{H}_7 \rightarrow \text{H} + \text{C}_3\text{H}_6$	1.250E+14	0.00	155
206b	$\text{C}_3\text{H}_6 + \text{H} \rightarrow \text{N-C}_3\text{H}_7$	3.713E+13	0.00	14
207	$\text{N-C}_3\text{H}_7 + \text{O}_2 \rightarrow \text{C}_3\text{H}_6 + \text{HO}_2$	1.000E+12	0.00	20.9
40. C4H6 Reactions				
234	$\text{C}_4\text{H}_6 \rightarrow 2\text{C}_2\text{H}_3$	4.030E+19	-1.00	411
235f	$\text{C}_2\text{H}_3 + \text{C}_2\text{H}_4 \rightarrow \text{C}_4\text{H}_6 + \text{H}$	1.000E+11	0.00	30.5
235b	$\text{H} + \text{C}_4\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{C}_2\text{H}_3$	8.397E+12	0.00	-0.244
239	$\text{C}_4\text{H}_6 + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{C}_3\text{H}_5$	2.000E+12	0.00	0
41. C4H7 Reactions				
241f	$\text{C}_4\text{H}_7 \rightarrow \text{C}_4\text{H}_6 + \text{H}$	1.200E+14	0.00	206
241b	$\text{H} + \text{C}_4\text{H}_6 \rightarrow \text{C}_4\text{H}_7$	1.343E+14	0.00	30.3
242	$\text{C}_4\text{H}_7 \rightarrow \text{C}_2\text{H}_4 + \text{C}_2\text{H}_3$	1.000E+11	0.00	155
257	$\text{C}_4\text{H}_7 + \text{H} \rightarrow \text{1-C}_4\text{H}_8$	4.397E+17	-1.00	4.52
244	$\text{C}_4\text{H}_7 + \text{O}_2 \rightarrow \text{C}_4\text{H}_6 + \text{HO}_2$	1.000E+11	0.00	0
246	$\text{C}_4\text{H}_7 + \text{CH}_3 \rightarrow \text{C}_4\text{H}_6 + \text{CH}_4$	1.000E+13	0.00	0
252f	$\text{C}_4\text{H}_7 + \text{C}_3\text{H}_5 \rightarrow \text{C}_4\text{H}_6 + \text{C}_3\text{H}_6$	4.000E+13	0.00	0
252b	$\text{C}_3\text{H}_6 + \text{C}_4\text{H}_6 \rightarrow \text{C}_3\text{H}_5 + \text{C}_4\text{H}_7$	1.513E+15	0.00	156
42. 1-C4H8 Reactions				
255f	$\text{1-C}_4\text{H}_8 \rightarrow \text{C}_3\text{H}_5 + \text{CH}_3$	8.000E+16	0.00	307
255b	$\text{CH}_3 + \text{C}_3\text{H}_5 \rightarrow \text{1-C}_4\text{H}_8$	2.070E+14	0.00	30.2
258	$\text{1-C}_4\text{H}_8 + \text{H} \rightarrow \text{C}_4\text{H}_7 + \text{H}_2$	5.000E+13	0.00	16.3
265	$\text{1-C}_4\text{H}_8 + \text{OH} \rightarrow \text{N-C}_3\text{H}_7 + \text{CH}_2\text{O}$	6.500E+12	0.00	0
279	$\text{1-C}_4\text{H}_8 + \text{OH} \rightarrow \text{C}_4\text{H}_7 + \text{H}_2\text{O}$	2.265E+14	0.00	12.8

Number	Reaction	A	n	E
43. P-C4H9 REACTIONS				
292	P-C ₄ H ₉ → C ₂ H ₅ + C ₂ H ₄	2.500E+13	0.00	121
294	P-C ₄ H ₉ + O ₂ → 1-C ₄ H ₈ + HO ₂	1.000E+12	0.00	8.4
50. 1-C5H9 Reactions				
a327	C ₅ H ₉ → C ₃ H ₅ + C ₂ H ₄	2.500E+13	0.00	126
a328	C ₃ H ₅ + C ₂ H ₄ → C ₅ H ₉	1.500E+10	0.00	31
a329	C ₅ H ₉ → C ₂ H ₃ + C ₃ H ₆	2.500E+13	0.00	126
51. 1-C5H10 Reactions				
a331f	1-C ₅ H ₁₀ → C ₂ H ₅ + C ₃ H ₅	1.000E+16	0.00	299
a331b	C ₃ H ₅ + C ₂ H ₅ → 1-C ₅ H ₁₀	8.947E+12	0.00	33.4
333	1-C ₅ H ₁₀ + H → C ₅ H ₉ + H ₂	2.800E+13	0.00	16.8
335	1-C ₅ H ₁₀ + O → C ₅ H ₉ + OH	2.540E+05	2.60	-4.7
341	1-C ₅ H ₁₀ + OH → C ₅ H ₉ + H ₂ O	6.800E+13	0.00	12.8
347	1-C ₅ H ₁₀ + CH ₃ → C ₅ H ₉ + CH ₄	1.000E+11	0.00	30.6
52. 1-C5H11 Reactions				
349	1-C ₅ H ₁₁ → C ₂ H ₄ + N-C ₃ H ₇	3.200E+13	0.00	119
352	H + 1-C ₅ H ₁₀ → 1-C ₅ H ₁₁	7.900E+12	0.00	12.1
61. 1-C6H12 Reactions				
355	1-C ₆ H ₁₂ → N-C ₃ H ₇ + C ₃ H ₅	2.500E+16	0.00	298
356	N-C ₃ H ₇ + C ₃ H ₅ → 1-C ₆ H ₁₂	1.000E+13	0.00	0
359	1-C ₆ H ₁₂ + H → C ₄ H ₇ + C ₂ H ₄ + H ₂	2.800E+07	2.00	32.2
361	1-C ₆ H ₁₂ + H → C ₃ H ₅ + C ₃ H ₆ + H ₂	8.000E+06	2.00	20.9
363	1-C ₆ H ₁₂ + H → 1-C ₄ H ₈ + C ₂ H ₃ + H ₂	8.000E+06	2.00	20.9
369	1-C ₆ H ₁₂ + O → C ₄ H ₇ + C ₂ H ₄ + OH	5.000E+13	0.00	32.9
371	1-C ₆ H ₁₂ + O → C ₃ H ₅ + C ₃ H ₆ + OH	2.800E+13	0.00	21.8
373	1-C ₆ H ₁₂ + O → 1-C ₄ H ₈ + C ₂ H ₃ + OH	2.800E+13	0.00	21.8
379	1-C ₆ H ₁₂ + OH → C ₄ H ₇ + C ₂ H ₄ + H ₂ O	4.300E+09	1.10	7.6
381	1-C ₆ H ₁₂ + OH → C ₃ H ₅ + C ₃ H ₆ + H ₂ O	1.300E+09	1.30	2.9
383	1-C ₆ H ₁₂ + OH → 1-C ₄ H ₈ + C ₂ H ₃ + H ₂ O	1.300E+09	1.30	2.9
71. 1-C7H14 Reactions				
395	1-C ₇ H ₁₄ → P-C ₄ H ₉ + C ₃ H ₅	2.500E+16	0.00	298
396	P-C ₄ H ₉ + C ₃ H ₅ → 1-C ₇ H ₁₄	1.000E+13	0.00	0
16. C7H15 REACTIONS				
441	1-C ₇ H ₁₅ → 1-C ₅ H ₁₁ + C ₂ H ₄	2.500E+13	0.00	121
443	2-C ₇ H ₁₅ → 1-C ₇ H ₁₄ + H	2.000E+13	0.00	169
445	2-C ₇ H ₁₅ → P-C ₄ H ₉ + C ₃ H ₆	1.600E+13	0.00	118
447	3-C ₇ H ₁₅ → 1-C ₆ H ₁₂ + CH ₃	8.000E+13	0.00	138
449	3-C ₇ H ₁₅ → 1-C ₄ H ₈ + N-C ₃ H ₇	5.000E+12	0.00	122
451	4-C ₇ H ₁₅ → C ₂ H ₅ + 1-C ₅ H ₁₀	1.000E+13	0.00	117
453	4-C ₇ H ₁₅ → 1-C ₇ H ₁₄ + H	1.000E+13	0.00	159

Number	Reaction	A	n	E
471	$1\text{-C}_7\text{H}_{15} \rightarrow 3\text{-C}_7\text{H}_{15}$	2.000E+11	0.00	46.5
472	$3\text{-C}_7\text{H}_{15} \rightarrow 1\text{-C}_7\text{H}_{15}$	3.000E+11	0.00	59
473	$1\text{-C}_7\text{H}_{15} \rightarrow 4\text{-C}_7\text{H}_{15}$	2.000E+11	0.00	75.8
474	$4\text{-C}_7\text{H}_{15} \rightarrow 1\text{-C}_7\text{H}_{15}$	6.000E+11	0.00	88.4
475	$2\text{-C}_7\text{H}_{15} \rightarrow 3\text{-C}_7\text{H}_{15}$	2.000E+11	0.00	75.8
476	$3\text{-C}_7\text{H}_{15} \rightarrow 2\text{-C}_7\text{H}_{15}$	2.000E+11	0.00	75.8
477	$1\text{-C}_7\text{H}_{15} \rightarrow 2\text{-C}_7\text{H}_{15}$	2.000E+11	0.00	75.8
478	$2\text{-C}_7\text{H}_{15} \rightarrow 1\text{-C}_7\text{H}_{15}$	3.000E+11	0.00	88.4
455	$1\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow 1\text{-C}_7\text{H}_{14} + \text{HO}_2$	1.000E+10	0.00	8.4
457	$2\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow 1\text{-C}_7\text{H}_{14} + \text{HO}_2$	1.000E+10	0.00	8.4
459	$3\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow 1\text{-C}_7\text{H}_{14} + \text{HO}_2$	1.000E+10	0.00	8.4
461	$4\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow 1\text{-C}_7\text{H}_{14} + \text{HO}_2$	1.000E+10	0.00	8.4
78. N-C7H16 REACTIONS				
659	$\text{N-C}_7\text{H}_{16} \rightarrow \text{P-C}_4\text{H}_9 + \text{N-C}_3\text{H}_7$	3.160E+16	0.00	339
669	$\text{N-C}_7\text{H}_{16} + \text{H} \rightarrow 1\text{-C}_7\text{H}_{15} + \text{H}_2$	5.600E+07	2.00	32.2
671	$\text{N-C}_7\text{H}_{16} + \text{H} \rightarrow 2\text{-C}_7\text{H}_{15} + \text{H}_2$	1.750E+07	2.00	20.9
673	$\text{N-C}_7\text{H}_{16} + \text{H} \rightarrow 3\text{-C}_7\text{H}_{15} + \text{H}_2$	1.750E+07	2.00	20.9
675	$\text{N-C}_7\text{H}_{16} + \text{H} \rightarrow 4\text{-C}_7\text{H}_{15} + \text{H}_2$	8.780E+06	2.00	20.9
677	$\text{N-C}_7\text{H}_{16} + \text{O} \rightarrow 1\text{-C}_7\text{H}_{15} + \text{OH}$	1.000E+14	0.00	32.9
679	$\text{N-C}_7\text{H}_{16} + \text{O} \rightarrow 2\text{-C}_7\text{H}_{15} + \text{OH}$	5.600E+13	0.00	21.8
681	$\text{N-C}_7\text{H}_{16} + \text{O} \rightarrow 3\text{-C}_7\text{H}_{15} + \text{OH}$	5.600E+13	0.00	21.8
683	$\text{N-C}_7\text{H}_{16} + \text{O} \rightarrow 4\text{-C}_7\text{H}_{15} + \text{OH}$	2.800E+13	0.00	21.8
685	$\text{N-C}_7\text{H}_{16} + \text{OH} \rightarrow 1\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}$	8.610E+09	1.10	7.6
687	$\text{N-C}_7\text{H}_{16} + \text{OH} \rightarrow 2\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}$	2.600E+09	1.30	2.9
689	$\text{N-C}_7\text{H}_{16} + \text{OH} \rightarrow 3\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}$	2.600E+09	1.30	2.9
691	$\text{N-C}_7\text{H}_{16} + \text{OH} \rightarrow 4\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}$	1.300E+09	1.30	2.9
693	$\text{N-C}_7\text{H}_{16} + \text{HO}_2 \rightarrow 1\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}_2$	1.120E+13	0.00	81.2
695	$\text{N-C}_7\text{H}_{16} + \text{HO}_2 \rightarrow 2\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}_2$	6.700E+12	0.00	71.2
697	$\text{N-C}_7\text{H}_{16} + \text{HO}_2 \rightarrow 3\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}_2$	6.700E+12	0.00	71.2
699	$\text{N-C}_7\text{H}_{16} + \text{HO}_2 \rightarrow 4\text{-C}_7\text{H}_{15} + \text{H}_2\text{O}_2$	3.350E+12	0.00	71.2
701	$\text{N-C}_7\text{H}_{16} + \text{CH}_3 \rightarrow 1\text{-C}_7\text{H}_{15} + \text{CH}_4$	1.300E+12	0.00	48.6
703	$\text{N-C}_7\text{H}_{16} + \text{CH}_3 \rightarrow 2\text{-C}_7\text{H}_{15} + \text{CH}_4$	8.000E+11	0.00	39.8
705	$\text{N-C}_7\text{H}_{16} + \text{CH}_3 \rightarrow 3\text{-C}_7\text{H}_{15} + \text{CH}_4$	8.000E+11	0.00	39.8
707	$\text{N-C}_7\text{H}_{16} + \text{CH}_3 \rightarrow 4\text{-C}_7\text{H}_{15} + \text{CH}_4$	4.000E+11	0.00	39.8

Number	Reaction	A	n	E
709	$\text{N-C}_7\text{H}_{16} + \text{O}_2 \rightarrow \text{}_1\text{-C}_7\text{H}_{15} + \text{HO}_2$	2.500E+13	0.00	205
711	$\text{N-C}_7\text{H}_{16} + \text{O}_2 \rightarrow \text{}_2\text{-C}_7\text{H}_{15} + \text{HO}_2$	4.000E+13	0.00	199
713	$\text{N-C}_7\text{H}_{16} + \text{O}_2 \rightarrow \text{}_3\text{-C}_7\text{H}_{15} + \text{HO}_2$	4.000E+13	0.00	199
715	$\text{N-C}_7\text{H}_{16} + \text{O}_2 \rightarrow \text{}_4\text{-C}_7\text{H}_{15} + \text{HO}_2$	2.000E+13	0.00	199
8. Low Temperature branch				
121f	$\text{}_1\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow \text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2$	2.000E+12	0.00	0
121b	$\text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_1\text{-C}_7\text{H}_{15} + \text{O}_2$	3.000E+14	0.00	117
122f	$\text{}_2\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow \text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2$	2.000E+12	0.00	0
122b	$\text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_2\text{-C}_7\text{H}_{15} + \text{O}_2$	6.600E+14	0.00	117
123f	$\text{}_3\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow \text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2$	2.000E+12	0.00	0
123b	$\text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_3\text{-C}_7\text{H}_{15} + \text{O}_2$	6.900E+14	0.00	117
124f	$\text{}_4\text{-C}_7\text{H}_{15} + \text{O}_2 \rightarrow \text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2$	2.000E+12	0.00	0
124b	$\text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_4\text{-C}_7\text{H}_{15} + \text{O}_2$	3.500E+14	0.00	117
125f	$\text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_1\text{HEOOH-2-C}_7\text{H}_{15}\text{O}_2$	2.000E+11	0.00	71.2
125b	$\text{}_1\text{HEOOH-2-C}_7\text{H}_{15}\text{O}_2 \rightarrow \text{}_1\text{C}_7\text{H}_{15}\text{O}_2\text{-C}_7\text{H}_{15}\text{O}_2$	1.000E+11	0.00	52.3
129	$\text{}_1\text{HEOOH-2-C}_7\text{H}_{15}\text{O}_2 + \text{O}_2 \rightarrow \text{OOC}_7\text{OOH-O}_2\text{C}_7\text{H}_{14}\text{OOH}$	5.000E+11	0.00	0
133	$\text{OOC}_7\text{OOH-O}_2\text{C}_7\text{H}_{14}\text{OOH} \rightarrow \text{HOOC}_7\text{OOH-HOOC}_7\text{H}_{13}\text{OOH}$	2.000E+11	0.00	71.2
134	$\text{HOOC}_7\text{OOH-HOOC}_7\text{H}_{13}\text{OOH} \rightarrow \text{OC}_7\text{OOH-OC}_7\text{H}_{13}\text{OOH} + \text{OH}$	1.000E+09	0.00	31.4
135	$\text{OC}_7\text{OOH-OC}_7\text{H}_{13}\text{OOH} \rightarrow \text{OC}_7\text{H}_{13}\text{O} + \text{OH}$	8.400E+14	0.00	180
136	$\text{OC}_7\text{H}_{13}\text{O} \rightarrow \text{CH}_2\text{O} + \text{}_1\text{-C}_5\text{H}_{11} + \text{CO}$	2.000E+13	0.00	62.8

Mechanismus: *i*-Oktan

Number	Reaction	A	n	E
1f	$O_2 + H \rightarrow OH + O$	2.000E+14	0.00	70.3
1b	$O + OH \rightarrow H + O_2$	1.157E+13	0.00	0.622
2f	$H_2 + O \rightarrow OH + H$	5.060E+04	2.67	26.3
2b	$H + OH \rightarrow O + H_2$	2.275E+04	2.67	18.5
3f	$H_2 + OH \rightarrow H_2O + H$	1.000E+08	1.60	13.8
3b	$H + H_2O \rightarrow OH + H_2$	4.652E+08	1.60	77.3
4f	$2OH \rightarrow H_2O + O$	1.500E+09	1.14	0.42
4b	$O + H_2O \rightarrow 2OH$	1.552E+10	1.14	71.7
5f	$2H + M' \rightarrow H_2 + M'$	1.800E+18	-1.00	0
5b	$H_2 + M' \rightarrow 2H + M'$	5.862E+18	-1.00	435
6f	$2O + M' \rightarrow O_2 + M'$	2.900E+17	-1.00	0
6b	$O_2 + M' \rightarrow 2O + M'$	7.341E+18	-1.00	497
7f	$H + OH + M' \rightarrow H_2O + M'$	2.200E+22	-2.00	0
7b	$H_2O + M' \rightarrow OH + H + M'$	3.333E+23	-2.00	498
8f	$H + O_2 + M' \rightarrow HO_2 + M'$	2.300E+18	-0.80	0
8b	$HO_2 + M' \rightarrow O_2 + H + M'$	3.287E+18	-0.80	196
9f	$HO_2 + H \rightarrow 2OH$	1.500E+14	0.00	4.2
9b	$2OH \rightarrow H + HO_2$	8.891E+12	0.00	166
10f	$HO_2 + H \rightarrow H_2 + O_2$	2.500E+13	0.00	2.9
10b	$O_2 + H_2 \rightarrow H + HO_2$	5.698E+13	0.00	242
11f	$HO_2 + H \rightarrow H_2O + O$	3.000E+13	0.00	7.2
11b	$O + H_2O \rightarrow H + HO_2$	1.840E+13	0.00	240
12f	$HO_2 + O \rightarrow OH + O_2$	1.800E+13	0.00	-1.7
12b	$O_2 + OH \rightarrow O + HO_2$	1.844E+13	0.00	230
13f	$HO_2 + OH \rightarrow H_2O + O_2$	6.000E+13	0.00	0
13b	$O_2 + H_2O \rightarrow OH + HO_2$	6.361E+14	0.00	303
14	$2HO_2 \rightarrow H_2O_2 + O_2$	2.500E+11	0.00	-5.2
15f	$2OH + M' \rightarrow H_2O_2 + M'$	3.250E+22	-2.00	0
15b	$H_2O_2 + M' \rightarrow 2OH + M'$	4.145E+24	-2.00	211
17	$H_2O_2 + H \rightarrow H_2O + OH$	1.000E+13	0.00	15
18f	$H_2O_2 + O \rightarrow OH + HO_2$	2.803E+13	0.00	26.8
18b	$HO_2 + OH \rightarrow O + H_2O_2$	5.429E+12	0.00	81.4
19f	$H_2O_2 + OH \rightarrow H_2O + HO_2$	5.400E+12	0.00	4.2

Number	Reaction	A	n	E	
19b	$\text{HO}_2 + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2\text{O}_2$	1.082E+13	0.00	130	
20f	$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$	6.000E+06	1.50	-3.1	
20b	$\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$	1.739E+09	1.50	98.7	
21	$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$	1.500E+14	0.00	98.7	
25	$\text{CH} + \text{O}_2 \rightarrow \text{CHO} + \text{O}$	6.000E+13	0.00	0	
26	$\text{CH} + \text{CO}_2 \rightarrow \text{CHO} + \text{CO}$	3.400E+12	0.00	2.9	
27	$\text{CH} + \text{H}_2\text{O} \rightarrow \text{}_3\text{-CH}_2 + \text{OH}$	5.700E+12	0.00	-3.2	
28f	$\text{CHO} + \text{M}' \rightarrow \text{CO} + \text{H} + \text{M}'$	1.566E+14	0.00	65.9	
28b	$\text{H} + \text{CO} + \text{M}' \rightarrow \text{CHO} + \text{M}'$	2.050E+14	0.00	3.66	
29	$\text{CHO} + \text{H} \rightarrow \text{CO} + \text{H}_2$	1.800E+14	0.00	0	
32	$\text{CHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O}$	1.000E+14	0.00	0	
35f	$\text{}_3\text{-CH}_2 + \text{H} \rightarrow \text{CH} + \text{H}_2$	6.000E+12	0.00	-7.5	
35b	$\text{H}_2 + \text{CH} \rightarrow \text{H} + \text{}_3\text{-CH}_2$	3.763E+12	0.00	3.16	
38	$\text{}_2\text{-CH}_2 \rightarrow \text{C}_2\text{H}_2 + 2\text{H}$	1.100E+14	0.00	3.4	
39	$\text{}_3\text{-CH}_2 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_4 + \text{H}$	4.200E+13	0.00	0	
40	$\text{}_3\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$	1.300E+13	0.00	6.2	
41	$\text{}_3\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2$	1.200E+13	0.00	6.2	
42f	$\text{}_1\text{-CH}_2 + \text{M}' \rightarrow \text{}_3\text{-CH}_2 + \text{M}'$	1.200E+13	0.00	0	
42b	$\text{}_3\text{-CH}_2 + \text{M}' \rightarrow \text{}_1\text{-CH}_2 + \text{M}'$	4.892E+12	0.00	37.5	
43	$\text{}_1\text{-CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{OH} + \text{H}$	3.100E+13	0.00	0	
44f	$\text{}_1\text{-CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$	7.200E+13	0.00	0	
44b	$\text{H} + \text{CH}_3 \rightarrow \text{H}_2 + \text{}_1\text{-CH}_2$	2.246E+14	0.00	60.5	
45	$\text{CH}_2\text{O} + \text{M}' \rightarrow \text{CHO} + \text{H} + \text{M}'$	5.000E+16	0.00	320	
46	$\text{CH}_2\text{O} + \text{H} \rightarrow \text{CHO} + \text{H}_2$	2.300E+10	1.05	13.7	
47	$\text{CH}_2\text{O} + \text{O} \rightarrow \text{CHO} + \text{OH}$	4.150E+11	0.57	11.6	
48	$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{CHO} + \text{H}_2\text{O}$	3.400E+09	1.20	-1.9	
49	$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{CHO} + \text{H}_2\text{O}_2$	3.000E+12	0.00	54.7	
53	$\text{CH}_3 + \text{O} \rightarrow \text{CH}_2\text{O} + \text{H}$	5.319E+13	0.00	0	
34f	$\text{CH}_3 + \text{H} \rightarrow \text{CH}_4$	k_0	1.251E+24	-1.80	0
		k_∞	2.108E+14	0.00	0
34b	$\text{CH}_4 \rightarrow \text{H} + \text{CH}_3$	k_0	1.312E+26	-1.80	439
		k_∞	2.211E+16	0.00	439
55	$\text{CH}_3 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{H}$	2.260E+14	0.00	64.8	
56	$\text{CH}_3\text{O} + \text{H} \rightarrow \text{CH}_3 + \text{OH}$	4.750E+16	-0.13	88	
57	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$	3.300E+11	0.00	37.4	

Number	Reaction	A	n	E	
145	$\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{O} + \text{OH}$	9.000E+13	0.00	0	
59	$\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_4 + \text{O}_2$	3.600E+12	0.00	0	
36f	$2\text{CH}_3 \rightarrow \text{C}_2\text{H}_6$	k_0	1.272E+41	-7.00	11.6
		k_∞	1.813E+13	0.00	0
36b	$\text{C}_2\text{H}_6 \rightarrow 2\text{CH}_3$	k_0	5.014E+44	-7.00	385
		k_∞	7.146E+16	0.00	373
62	$\text{CH}_3\text{O} + \text{M}' \rightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105	
63	$\text{CH}_3\text{O} + \text{H} \rightarrow \text{CH}_2\text{O} + \text{H}_2$	1.800E+13	0.00	0	
64	$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	4.000E+10	0.00	8.9	
69	$\text{CH}_3\text{O} + \text{M}' \rightarrow \text{CH}_2\text{O} + \text{H} + \text{M}'$	5.000E+13	0.00	105	
70	$\text{CH}_3\text{O} + \text{H} \rightarrow \text{CH}_2\text{O} + \text{H}_2$	3.000E+13	0.00	0	
71	$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	1.000E+13	0.00	30	
72	$\text{CH}_3\text{O}_2 + \text{M}' \rightarrow \text{CH}_3 + \text{O}_2 + \text{M}'$	7.240E+16	0.00	111	
73	$\text{CH}_3 + \text{O}_2 + \text{M}' \rightarrow \text{CH}_3\text{O}_2 + \text{M}'$	1.410E+16	0.00	-4.6	
84f	$\text{CH}_4 + \text{H} \rightarrow \text{H}_2 + \text{CH}_3$	1.300E+04	3.00	33.6	
84b	$\text{CH}_3 + \text{H}_2 \rightarrow \text{H} + \text{CH}_4$	4.038E+02	3.00	29.3	
85	$\text{CH}_4 + \text{O} \rightarrow \text{OH} + \text{CH}_3$	6.923E+08	1.56	35.5	
86f	$\text{CH}_4 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_3$	1.600E+07	1.83	11.6	
86b	$\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{OH} + \text{CH}_4$	2.312E+06	1.83	70.8	
90f	$\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{OH}$	k_0	1.596E+44	-8.20	0
		k_∞	6.022E+13	0.00	0
90b	$\text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{OH}$	k_0	6.633E+46	-8.20	385
		k_∞	2.503E+16	0.00	385
91	$\text{CH}_3\text{OH} + \text{H} \rightarrow \text{CH}_3\text{O} + \text{H}_2$	4.000E+13	0.00	25.5	
92	$\text{CH}_3\text{OH} + \text{O} \rightarrow \text{CH}_3\text{O} + \text{OH}$	1.000E+13	0.00	19.6	
93	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{H}_2\text{O}$	1.000E+13	0.00	7.1	
96	$\text{CH}_3\text{OH} + \text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{O}$	9.000E+12	0.00	41.1	
100	$2\text{CH}_3\text{O} \rightarrow \text{CH}_3\text{OH} + \text{CH}_2\text{O}$	3.000E+13	0.00	0	
105f	$\text{HCCO} + \text{H} \rightarrow \text{}_3\text{-CH}_2 + \text{CO}$	1.500E+14	0.00	0	
105b	$\text{CO} + \text{}_3\text{-CH}_2 \rightarrow \text{H} + \text{HCCO}$	3.483E+13	0.00	124	
106	$\text{HCCO} + \text{O} \rightarrow 2\text{CO} + \text{H}$	9.600E+13	0.00	0	
109	$\text{C}_2\text{H}_2 + \text{O}_2 \rightarrow \text{HCCO} + \text{OH}$	2.000E+08	1.50	126	
110f	$\text{C}_2\text{H}_2 + \text{H} \rightarrow \text{C}_2\text{H} + \text{H}_2$	1.500E+14	0.00	79.6	
110b	$\text{H}_2 + \text{C}_2\text{H} \rightarrow \text{H} + \text{C}_2\text{H}_2$	1.563E+13	0.00	-34.9	
111	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{}_3\text{-CH}_2 + \text{CO}$	1.720E+04	2.80	2.1	
112	$\text{C}_2\text{H}_2 + \text{O} \rightarrow \text{HCCO} + \text{H}$	1.720E+04	2.80	2.1	
113f	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}$	6.000E+13	0.00	54.2	

Number	Reaction	A	n	E
113b	$\text{C}_2\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{C}_2\text{H}_2$	2.908E+13	0.00	3.16
51f	$\text{C}_2\text{H}_3 \rightarrow \text{C}_2\text{H}_2 + \text{H}$	k_0	1.187E+42	-7.50
		k_∞	2.000E+14	0.00
51b	$\text{C}_2\text{H}_2 + \text{H} \rightarrow \text{C}_2\text{H}_3$	k_0	6.245E+41	-7.50
		k_∞	1.053E+14	0.00
120	$\text{C}_2\text{H}_3 + \text{OH} \rightarrow \text{C}_2\text{H}_2 + \text{H}_2\text{O}$	5.000E+13	0.00	0
125	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{C}_2\text{H}_2 + \text{HO}_2$	1.210E+11	0.00	0
a125	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{CHO}$	5.420E+12	0.00	0
129	$\text{C}_2\text{H}_4 + \text{M}' \rightarrow \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}'$	2.500E+17	0.00	320
131f	$\text{C}_2\text{H}_4 + \text{H} \rightarrow \text{C}_2\text{H}_3 + \text{H}_2$	1.700E+15	0.00	62.9
131b	$\text{H}_2 + \text{C}_2\text{H}_3 \rightarrow \text{H} + \text{C}_2\text{H}_4$	6.285E+13	0.00	47.5
133	$\text{C}_2\text{H}_4 + \text{O} \rightarrow \text{CHO} + \text{CH}_3$	1.210E+06	2.08	0
134f	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{C}_2\text{H}_3 + \text{H}_2\text{O}$	6.500E+13	0.00	24.9
134b	$\text{H}_2\text{O} + \text{C}_2\text{H}_3 \rightarrow \text{OH} + \text{C}_2\text{H}_4$	1.118E+13	0.00	73
58f	$\text{C}_2\text{H}_5 \rightarrow \text{C}_2\text{H}_4 + \text{H}$	k_0	1.000E+16	0.00
		k_∞	1.300E+13	0.00
58b	$\text{C}_2\text{H}_4 + \text{H} \rightarrow \text{C}_2\text{H}_5$	k_0	1.595E+16	0.00
		k_∞	2.073E+13	0.00
146f	$\text{C}_2\text{H}_5 + \text{H} \rightarrow 2\text{CH}_3$	3.000E+13	0.00	0
146b	$2\text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_5$	1.916E+12	0.00	43.6
149	$\text{C}_2\text{H}_5 + \text{O}_2 \rightarrow \text{C}_2\text{H}_4 + \text{HO}_2$	1.100E+10	0.00	-6.3
164f	$\text{C}_2\text{H}_6 + \text{H} \rightarrow \text{C}_2\text{H}_5 + \text{H}_2$	1.400E+09	1.50	31.1
164b	$\text{H}_2 + \text{C}_2\text{H}_5 \rightarrow \text{H} + \text{C}_2\text{H}_6$	1.812E+07	1.50	49
165	$\text{C}_2\text{H}_6 + \text{O} \rightarrow \text{C}_2\text{H}_5 + \text{OH}$	1.000E+09	1.50	24.4
166	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5 + \text{H}_2\text{O}$	7.200E+06	2.00	3.6
170	$\text{C}_2\text{H}_6 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_5 + \text{CH}_4$	1.500E-07	6.00	25.4
187	$\text{C}_3\text{H}_4 + \text{O} \rightarrow \text{CH}_2\text{O} + \text{C}_2\text{H}_2$	1.000E+12	0.00	0
188	$\text{C}_3\text{H}_4 + \text{O} \rightarrow \text{CHO} + \text{C}_2\text{H}_3$	1.000E+12	0.00	0
189	$\text{C}_3\text{H}_4 + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{C}_2\text{H}_3$	1.000E+12	0.00	0
190	$\text{C}_3\text{H}_4 + \text{OH} \rightarrow \text{CHO} + \text{C}_2\text{H}_4$	1.000E+12	0.00	0
191f	$\text{C}_3\text{H}_5 \rightarrow \text{C}_3\text{H}_4 + \text{H}$	3.000E+11	0.84	250
191b	$\text{H} + \text{C}_3\text{H}_4 \rightarrow \text{C}_3\text{H}_5$	4.820E+10	0.84	-17.2
a192f	$\text{C}_3\text{H}_5 + \text{OH} \rightarrow \text{C}_3\text{H}_4 + \text{H}_2\text{O}$	6.000E+12	0.00	0
a192b	$\text{H}_2\text{O} + \text{C}_3\text{H}_4 \rightarrow \text{OH} + \text{C}_3\text{H}_5$	1.460E+13	0.00	231
192	$\text{C}_3\text{H}_5 + \text{H} \rightarrow \text{C}_3\text{H}_4 + \text{H}_2$	1.000E+13	0.00	0
193	$\text{C}_3\text{H}_5 + \text{O}_2 \rightarrow \text{C}_3\text{H}_4 + \text{HO}_2$	6.000E+11	0.00	41.9
195	$\text{C}_3\text{H}_6 \rightarrow \text{C}_2\text{H}_3 + \text{CH}_3$	3.150E+15	0.00	359

Number	Reaction	A	n	E
196	$\text{H} + \text{C}_3\text{H}_6 \rightarrow \text{C}_3\text{H}_5 + \text{H}_2$	5.000E+12	0.00	6.3
197	$\text{C}_3\text{H}_6 + \text{O} \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{O}$	5.900E+13	0.00	21
198	$\text{C}_3\text{H}_6 + \text{O} \rightarrow \text{C}_2\text{H}_5 + \text{CHO}$	3.600E+12	0.00	0
200	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5 + \text{CH}_2\text{O}$	7.900E+12	0.00	0
202	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{C}_3\text{H}_5 + \text{H}_2\text{O}$	4.000E+12	0.00	0
203	$\text{CH}_3 + \text{C}_3\text{H}_6 \rightarrow \text{CH}_4 + \text{C}_3\text{H}_5$	8.960E+12	0.00	35.6
205f	$\text{N-C}_3\text{H}_7 \rightarrow \text{CH}_3 + \text{C}_2\text{H}_4$	9.600E+13	0.00	130
205b	$\text{C}_2\text{H}_4 + \text{CH}_3 \rightarrow \text{N-C}_3\text{H}_7$	5.125E+11	0.00	32.2
206f	$\text{N-C}_3\text{H}_7 \rightarrow \text{H} + \text{C}_3\text{H}_6$	1.250E+14	0.00	155
206b	$\text{C}_3\text{H}_6 + \text{H} \rightarrow \text{N-C}_3\text{H}_7$	3.713E+13	0.00	14
208f	$\text{I-C}_3\text{H}_7 \rightarrow \text{H} + \text{C}_3\text{H}_6$	6.300E+13	0.00	154
208b	$\text{C}_3\text{H}_6 + \text{H} \rightarrow \text{I-C}_3\text{H}_7$	2.499E+12	0.00	-4.74
234	$\text{C}_4\text{H}_6 \rightarrow 2\text{C}_2\text{H}_3$	4.030E+19	-1.00	411
235f	$\text{C}_2\text{H}_3 + \text{C}_2\text{H}_4 \rightarrow \text{C}_4\text{H}_6 + \text{H}$	1.000E+11	0.00	30.5
235b	$\text{C}_4\text{H}_6 + \text{H} \rightarrow \text{C}_2\text{H}_3 + \text{C}_2\text{H}_4$	9.111E+12	0.00	0.0225
239	$\text{C}_4\text{H}_6 + \text{OH} \rightarrow \text{CH}_2\text{O} + \text{C}_3\text{H}_5$	2.000E+12	0.00	0
241f	$\text{C}_4\text{H}_7 \rightarrow \text{C}_4\text{H}_6 + \text{H}$	1.200E+14	0.00	206
241b	$\text{H} + \text{C}_4\text{H}_6 \rightarrow \text{C}_4\text{H}_7$	1.343E+14	0.00	30.3
244	$\text{C}_4\text{H}_7 + \text{O}_2 \rightarrow \text{C}_4\text{H}_6 + \text{HO}_2$	1.000E+11	0.00	0
255f	$1\text{-C}_4\text{H}_8 \rightarrow \text{C}_3\text{H}_5 + \text{CH}_3$	8.000E+16	0.00	307
255b	$\text{CH}_3 + \text{C}_3\text{H}_5 \rightarrow 1\text{-C}_4\text{H}_8$	2.070E+14	0.00	30.2
257f	$1\text{-C}_4\text{H}_8 \rightarrow \text{H} + \text{C}_4\text{H}_7$	4.110E+18	-1.00	408
257b	$\text{C}_4\text{H}_7 + \text{H} \rightarrow 1\text{-C}_4\text{H}_8$	1.494E+17	-1.00	4.53
258	$1\text{-C}_4\text{H}_8 + \text{H} \rightarrow \text{C}_4\text{H}_7 + \text{H}_2$	5.000E+13	0.00	16.3
265	$1\text{-C}_4\text{H}_8 + \text{OH} \rightarrow \text{N-C}_3\text{H}_7 + \text{CH}_2\text{O}$	6.500E+12	0.00	0
266	$1\text{-C}_4\text{H}_8 + \text{OH} \rightarrow \text{C}_4\text{H}_7 + \text{H}_2\text{O}$	1.750E+13	0.00	29.1
353	$\text{C}_6\text{H}_{11} \rightarrow \text{C}_3\text{H}_5 + \text{C}_3\text{H}_6$	2.500E+13	0.00	126
393	$\text{C}_7\text{H}_{13} \rightarrow \text{C}_3\text{H}_5 + 1\text{-C}_4\text{H}_8$	2.500E+13	0.00	126
751	$\text{I-C}_4\text{H}_7 \rightarrow \text{C}_3\text{H}_4 + \text{CH}_3$	1.000E+13	0.00	214
752	$\text{C}_3\text{H}_4 + \text{CH}_3 \rightarrow \text{I-C}_4\text{H}_7$	2.000E+11	0.00	31.4
753	$\text{I-C}_4\text{H}_8 \rightarrow \text{C}_3\text{H}_5 + \text{CH}_3$	5.000E+18	-1.00	307
754	$\text{C}_3\text{H}_5 + \text{CH}_3 \rightarrow \text{I-C}_4\text{H}_8$	2.000E+13	0.00	0
755	$\text{I-C}_4\text{H}_8 \rightarrow \text{I-C}_4\text{H}_7 + \text{H}$	1.000E+17	0.00	368

Number	Reaction	A	n	E
756	$\text{I-C}_4\text{H}_7 + \text{H} \rightarrow \text{I-C}_4\text{H}_8$	2.000E+13	0.00	0
757	$\text{I-C}_4\text{H}_8 + \text{H} \rightarrow \text{I-C}_4\text{H}_7 + \text{H}_2$	1.000E+13	0.00	15.9
758	$\text{I-C}_4\text{H}_7 + \text{H}_2 \rightarrow \text{I-C}_4\text{H}_8 + \text{H}$	3.000E+13	0.00	105
759	$\text{I-C}_4\text{H}_8 + \text{O} \rightarrow \text{I-C}_4\text{H}_7 + \text{OH}$	2.500E+05	2.60	-4.7
761	$\text{I-C}_4\text{H}_8 + \text{O} \rightarrow \text{I-C}_3\text{H}_7 + \text{CHO}$	7.230E+05	2.30	-4.4
763	$\text{I-C}_4\text{H}_8 + \text{OH} \rightarrow \text{I-C}_4\text{H}_7 + \text{H}_2\text{O}$	9.600E+12	0.00	5.2
765	$\text{I-C}_4\text{H}_8 + \text{OH} \rightarrow \text{I-C}_3\text{H}_7 + \text{CH}_2\text{O}$	1.500E+12	0.00	0
769	$\text{I-C}_4\text{H}_9 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_3$	1.000E+14	0.00	137
771	$\text{I-C}_4\text{H}_9 \rightarrow \text{I-C}_4\text{H}_8 + \text{H}$	2.000E+13	0.00	151
772	$\text{I-C}_4\text{H}_8 + \text{H} \rightarrow \text{I-C}_4\text{H}_9$	1.000E+13	0.00	5
773	$\text{I-C}_4\text{H}_9 + \text{O}_2 \rightarrow \text{I-C}_4\text{H}_8 + \text{HO}_2$	2.340E+10	0.00	0
775	$\text{T-C}_4\text{H}_9 \rightarrow \text{H} + \text{I-C}_4\text{H}_8$	3.160E+15	0.00	183
776	$\text{H} + \text{I-C}_4\text{H}_8 \rightarrow \text{T-C}_4\text{H}_9$	3.100E+13	0.00	6.3
777	$\text{T-C}_4\text{H}_9 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_3$	1.585E+15	0.00	194
779	$\text{T-C}_4\text{H}_9 + \text{O}_2 \rightarrow \text{I-C}_4\text{H}_8 + \text{HO}_2$	1.170E+11	0.00	0
811	$\text{NEOC}_5\text{H}_{11}\text{-C}_5\text{H}_{11} \rightarrow \text{I-C}_4\text{H}_8 + \text{CH}_3$	1.000E+11	0.00	109
815	$\text{C}_6\text{H}_{10} \rightarrow 2\text{C}_3\text{H}_5$	2.512E+14	0.00	249
816	$2\text{C}_3\text{H}_5 \rightarrow \text{C}_6\text{H}_{10}$	1.020E+13	0.00	-1.1
817	$\text{I-C}_6\text{H}_{13} \rightarrow \text{I-C}_3\text{H}_7 + \text{C}_3\text{H}_6$	2.512E+13	0.00	118
819	$\text{I-C}_6\text{H}_{13} \rightarrow \text{T-C}_4\text{H}_9 + \text{C}_2\text{H}_4$	2.512E+13	0.00	121
821	$\text{I-C}_6\text{H}_{13} \rightarrow \text{I-C}_4\text{H}_9 + \text{C}_2\text{H}_4$	2.512E+13	0.00	121
823	$\text{I-C}_7\text{H}_{13} \rightarrow \text{I-C}_4\text{H}_8 + \text{C}_3\text{H}_5$	2.500E+13	0.00	25.6
825	$\text{I-C}_7\text{H}_{13} \rightarrow \text{C}_3\text{H}_6 + \text{I-C}_4\text{H}_7$	2.500E+13	0.00	25.6
827	$\text{I-C}_7\text{H}_{13} \rightarrow \text{C}_6\text{H}_{10} + \text{CH}_3$	1.000E+14	0.00	37.4
828	$\text{C}_6\text{H}_{10} + \text{CH}_3 \rightarrow \text{I-C}_7\text{H}_{13}$	3.200E+11	0.00	38.1
829	$\text{A-C}_7\text{H}_{14} \rightarrow \text{I-C}_4\text{H}_7 + \text{I-C}_3\text{H}_7$	2.500E+16	0.00	297
831	$\text{A-C}_7\text{H}_{14} \rightarrow \text{C}_3\text{H}_5 + \text{T-C}_4\text{H}_9$	2.500E+16	0.00	297
835	$\text{A-C}_7\text{H}_{14} + \text{O} \rightarrow \text{I-C}_7\text{H}_{13} + \text{OH}$	2.540E+05	2.60	-4.6
839	$\text{A-C}_7\text{H}_{14} + \text{OH} \rightarrow \text{I-C}_7\text{H}_{13} + \text{H}_2\text{O}$	6.800E+13	0.00	13
843	$\text{C-C}_7\text{H}_{14} \rightarrow \text{C}_6\text{H}_{11} + \text{CH}_3$	2.500E+16	0.00	297
845	$\text{C-C}_7\text{H}_{14} + \text{H} \rightarrow \text{I-C}_7\text{H}_{13} + \text{H}_2$	2.800E+13	0.00	16.8
847	$\text{C-C}_7\text{H}_{14} + \text{O} \rightarrow \text{I-C}_7\text{H}_{13} + \text{OH}$	2.540E+05	2.60	-4.6
851	$\text{C-C}_7\text{H}_{14} + \text{OH} \rightarrow \text{I-C}_7\text{H}_{13} + \text{H}_2\text{O}$	6.800E+13	0.00	13

Number	Reaction	<i>A</i>	<i>n</i>	<i>E</i>
855	$\text{I-C}_7\text{H}_{15} \rightarrow \text{I-C}_4\text{H}_8 + \text{I-C}_3\text{H}_7$	2.500E+13	0.00	117
858	$\text{A-C}_7\text{H}_{14} + \text{H} \rightarrow \text{I-C}_7\text{H}_{15}$	8.000E+12	0.00	5
860	$\text{C-C}_7\text{H}_{14} + \text{H} \rightarrow \text{I-C}_7\text{H}_{15}$	8.000E+12	0.00	5
861	$\text{I-C}_7\text{H}_{15} \rightarrow \text{C}_3\text{H}_6 + \text{T-C}_4\text{H}_9$	2.512E+13	0.00	118
863	$\text{I-C}_8\text{H}_{16} \rightarrow \text{I-C}_4\text{H}_7 + \text{T-C}_4\text{H}_9$	2.500E+16	0.00	297
865	$\text{I-C}_8\text{H}_{16} \rightarrow \text{C}_7\text{H}_{13} + \text{CH}_3$	2.500E+16	0.00	297
873	$\text{I-C}_8\text{H}_{16} + \text{OH} \rightarrow \text{I-C}_4\text{H}_8 + \text{I-C}_4\text{H}_7 + \text{H}_2\text{O}$	1.300E+09	1.30	2.9
886	$\text{A-C}_8\text{H}_{17} \rightarrow \text{D-C}_8\text{H}_{17}$	6.000E+11	0.00	59
887	$\text{D-C}_8\text{H}_{17} \rightarrow \text{A-C}_8\text{H}_{17}$	9.000E+11	0.00	59
888	$\text{A-C}_8\text{H}_{17} \rightarrow \text{C-C}_8\text{H}_{17}$	1.000E+11	0.00	67.4
889	$\text{C-C}_8\text{H}_{17} \rightarrow \text{A-C}_8\text{H}_{17}$	9.000E+11	0.00	88.4
882	$\text{A-C}_8\text{H}_{17} \rightarrow \text{A-C}_7\text{H}_{14} + \text{CH}_3$	1.000E+11	0.00	109
884	$\text{A-C}_8\text{H}_{17} \rightarrow \text{I-C}_4\text{H}_8 + \text{I-C}_4\text{H}_9$	1.300E+13	0.00	124
890	$\text{B-C}_8\text{H}_{17} \rightarrow \text{C-C}_7\text{H}_{14} + \text{CH}_3$	1.000E+13	0.00	109
894	$\text{C-C}_8\text{H}_{17} \rightarrow \text{I-C}_4\text{H}_8 + \text{T-C}_4\text{H}_9$	5.000E+12	0.00	121
900	$\text{D-C}_8\text{H}_{17} \rightarrow \text{A-C}_7\text{H}_{14} + \text{CH}_3$	1.250E+13	0.00	137
902	$\text{D-C}_8\text{H}_{17} \rightarrow \text{C}_3\text{H}_6 + \text{NEOC}_5\text{H}_{11}\text{-C}_5\text{H}_{11}$	1.300E+13	0.00	124
904	$\text{D-C}_8\text{H}_{17} \rightarrow \text{I-C}_8\text{H}_{16} + \text{H}$	3.300E+14	0.00	151
1064	$\text{I-C}_8\text{H}_{18} \rightarrow \text{T-C}_4\text{H}_9 + \text{I-C}_4\text{H}_9$	2.000E+16	0.00	327
1066	$\text{I-C}_8\text{H}_{18} \rightarrow \text{NEOC}_5\text{H}_{11}\text{-C}_5\text{H}_{11} + \text{I-C}_3\text{H}_7$	2.000E+16	0.00	327
1068	$\text{I-C}_8\text{H}_{18} + \text{H} \rightarrow \text{A-C}_8\text{H}_{17} + \text{H}_2$	8.440E+07	2.00	32.2
1070	$\text{I-C}_8\text{H}_{18} + \text{H} \rightarrow \text{B-C}_8\text{H}_{17} + \text{H}_2$	9.000E+06	2.00	20.9
1072	$\text{I-C}_8\text{H}_{18} + \text{H} \rightarrow \text{C-C}_8\text{H}_{17} + \text{H}_2$	1.260E+14	0.00	30.6
1074	$\text{I-C}_8\text{H}_{18} + \text{H} \rightarrow \text{D-C}_8\text{H}_{17} + \text{H}_2$	5.628E+07	2.00	32.2
1076	$\text{I-C}_8\text{H}_{18} + \text{O} \rightarrow \text{A-C}_8\text{H}_{17} + \text{OH}$	1.500E+14	0.00	32.9
1078	$\text{I-C}_8\text{H}_{18} + \text{O} \rightarrow \text{B-C}_8\text{H}_{17} + \text{OH}$	2.800E+13	0.00	21.8
1080	$\text{I-C}_8\text{H}_{18} + \text{O} \rightarrow \text{C-C}_8\text{H}_{17} + \text{OH}$	1.000E+13	0.00	13.7
1082	$\text{I-C}_8\text{H}_{18} + \text{O} \rightarrow \text{D-C}_8\text{H}_{17} + \text{OH}$	1.000E+14	0.00	32.9
1084	$\text{I-C}_8\text{H}_{18} + \text{OH} \rightarrow \text{A-C}_8\text{H}_{17} + \text{H}_2\text{O}$	1.290E+10	1.10	7.6
1086	$\text{I-C}_8\text{H}_{18} + \text{OH} \rightarrow \text{B-C}_8\text{H}_{17} + \text{H}_2\text{O}$	1.300E+09	1.30	2.9
1088	$\text{I-C}_8\text{H}_{18} + \text{OH} \rightarrow \text{C-C}_8\text{H}_{17} + \text{H}_2\text{O}$	1.960E+12	0.00	1.9
1090	$\text{I-C}_8\text{H}_{18} + \text{OH} \rightarrow \text{D-C}_8\text{H}_{17} + \text{H}_2\text{O}$	8.610E+09	1.10	7.6
1092	$\text{I-C}_8\text{H}_{18} + \text{HO}_2 \rightarrow \text{A-C}_8\text{H}_{17} + \text{H}_2\text{O}_2$	1.680E+13	0.00	81.2

Number	Reaction	A	n	E
1094	$\text{I-C}_8\text{H}_{18} + \text{HO}_2 \rightarrow \text{B-C}_8\text{H}_{17} + \text{H}_2\text{O}_2$	3.350E+12	0.00	71.2
1096	$\text{I-C}_8\text{H}_{18} + \text{HO}_2 \rightarrow \text{C-C}_8\text{H}_{17} + \text{H}_2\text{O}_2$	3.000E+12	0.00	60.3
1098	$\text{I-C}_8\text{H}_{18} + \text{HO}_2 \rightarrow \text{D-C}_8\text{H}_{17} + \text{H}_2\text{O}_2$	1.120E+13	0.00	81.2
1100	$\text{I-C}_8\text{H}_{18} + \text{CH}_3 \rightarrow \text{A-C}_8\text{H}_{17} + \text{CH}_4$	5.850E+12	0.00	48.6
1102	$\text{I-C}_8\text{H}_{18} + \text{CH}_3 \rightarrow \text{B-C}_8\text{H}_{17} + \text{CH}_4$	1.200E+12	0.00	39.8
1104	$\text{I-C}_8\text{H}_{18} + \text{CH}_3 \rightarrow \text{C-C}_8\text{H}_{17} + \text{CH}_4$	1.000E+11	0.00	33.1
1106	$\text{I-C}_8\text{H}_{18} + \text{CH}_3 \rightarrow \text{D-C}_8\text{H}_{17} + \text{CH}_4$	3.900E+12	0.00	48.6
1116	$\text{I-C}_8\text{H}_{18} + \text{O}_2 \rightarrow \text{A-C}_8\text{H}_{17} + \text{HO}_2$	3.750E+13	0.00	205
1118	$\text{I-C}_8\text{H}_{18} + \text{O}_2 \rightarrow \text{B-C}_8\text{H}_{17} + \text{HO}_2$	2.000E+13	0.00	201
1120	$\text{I-C}_8\text{H}_{18} + \text{O}_2 \rightarrow \text{C-C}_8\text{H}_{17} + \text{HO}_2$	2.000E+12	0.00	193
1122	$\text{I-C}_8\text{H}_{18} + \text{O}_2 \rightarrow \text{D-C}_8\text{H}_{17} + \text{HO}_2$	2.500E+13	0.00	205
11f	$\text{A-C}_8\text{H}_{17} + \text{O}_2 \rightarrow \text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2$	2.000E+12	0.00	0
11b	$\text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2 \rightarrow \text{A-C}_8\text{H}_{17} + \text{O}_2$	5.850E+14	0.00	100
127f	$\text{B-C}_8\text{H}_{17} + \text{O}_2 \rightarrow \text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2$	2.000E+12	0.00	0
127b	$\text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2 \rightarrow \text{B-C}_8\text{H}_{17} + \text{O}_2$	1.850E+14	0.00	100
153f	$\text{C-C}_8\text{H}_{17} + \text{O}_2 \rightarrow \text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2$	2.000E+12	0.00	0
153b	$\text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2 \rightarrow \text{C-C}_8\text{H}_{17} + \text{O}_2$	8.450E+14	0.00	100
179f	$\text{D-C}_8\text{H}_{17} + \text{O}_2 \rightarrow \text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2$	2.000E+12	0.00	0
179b	$\text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2 \rightarrow \text{D-C}_8\text{H}_{17} + \text{O}_2$	3.850E+14	0.00	100
123f	$\text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2 \rightarrow \text{AOEOOH-2-C}_8\text{H}_{16}\text{OOH}$	3.000E+12	0.00	61.1
123b	$\text{AOEOOH-2-C}_8\text{H}_{16}\text{OOH} \rightarrow \text{AC}_8\text{H}_{17}\text{O}_2\text{-C}_8\text{H}_{17}\text{O}_2$	1.000E+11	0.00	27.6
1112	$\text{AOEOOH-2-C}_8\text{H}_{16}\text{OOH} + \text{O}_2 \rightarrow \text{OCTO}_4\text{H-O}_2\text{C}_8\text{H}_{16}\text{OOH}$	5.000E+11	0.00	0
1247	$\text{OCTO}_4\text{H-O}_2\text{C}_8\text{H}_{16}\text{OOH} \rightarrow \text{HOCTO}_4\text{H-HOOC}_8\text{H}_{15}\text{OOH}$	6.000E+11	0.00	61.1
1248	$\text{HOCTO}_4\text{H-HOOC}_8\text{H}_{15}\text{OOH} \rightarrow \text{OCTO}_3\text{H-OC}_8\text{H}_{15}\text{OOH} + \text{OH}$	1.000E+09	0.00	31.2
1249	$\text{OCTO}_3\text{H-OC}_8\text{H}_{15}\text{OOH} \rightarrow \text{OC}_8\text{H}_{15}\text{O} + \text{OH}$	2.000E+14	0.00	180
1250	$\text{OC}_8\text{H}_{15}\text{O} \rightarrow \text{I-C}_6\text{H}_{13} + \text{CH}_2\text{O} + \text{CO}$	2.000E+13	0.00	62.8