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RP-3 航空煤油替代燃料及其化学反应动力学模型

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RP-3 Aviation Kerosene Surrogate Fuel and the Chemical Reaction Kinetic Model

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(A) Sub-mechanisms of *n*-decane and *n*-dodecane				
No.	reaction	*A*	*n*	*E*
1	*px*$C_{12}H_{25}$+H(+M)=*n*$C_{12}H_{26}$(+M)	3.60×10^{13}	0	0.0
2	C_7H_{14}+*px*C_5H_{11}=*s5x*$C_{12}H_{25}$	3.00×10^{11}	0	7300.0
3	C_8H_{16}+*p*C_4H_9=*s5x*$C_{12}H_{25}$	3.00×10^{11}	0	7300.0
4	C_2H_4+*px*$C_{10}H_{21}$=*px*$C_{12}H_{25}$	3.00×10^{09}	0	7300.0
5	*px*$C_{12}H_{25}$=*s5x*$C_{12}H_{25}$	2.80×10^{10}	0	18400.0
6	*px*$C_{10}H_{21}$+C_2H_5=*n*$C_{12}H_{26}$	1.88×10^{14}	-0.5	0.0
7	*px*C_9H_{19}+*n*C_3H_7=*n*$C_{12}H_{26}$	1.88×10^{14}	-0.5	0.0
8	*px*C_8H_{17}+*p*C_4H_9=*n*$C_{12}H_{26}$	1.88×10^{14}	-0.5	0.0
9	*px*C_7H_{15}+*px*C_5H_{11}=*n*$C_{12}H_{26}$	1.88×10^{14}	-0.5	0.0
10	*px*C_6H_{13}+*px*C_6H_{13}=*n*$C_{12}H_{26}$	1.88×10^{14}	-0.5	0.0
11	*n*$C_{12}H_{26}$+O=*px*$C_{12}H_{25}$+OH	1.90×10^{05}	2.7	3716.0
12	*n*$C_{12}H_{26}$+O=*s5x*$C_{12}H_{25}$+OH	1.90×10^{05}	2.7	3716.0
13	*n*$C_{12}H_{26}$+HO_2=*px*$C_{12}H_{25}$+H_2O_2	4.76×10^{04}	2.5	16490.0
14	*n*$C_{12}H_{26}$+HO_2=*s5x*$C_{12}H_{25}$+H_2O_2	4.76×10^{04}	2.5	16490.0
15	*n*$C_{12}H_{26}$+CH_3=*px*$C_{12}H_{25}$+CH_4	1.81×10^{00}	3.6	7153.0
16	*n*$C_{12}H_{26}$+CH_3=*s5x*$C_{12}H_{25}$+CH_4	1.81×10^{00}	3.6	7153.0
17	*n*$C_{12}H_{26}$+O_2<=>*px*$C_{12}H_{25}$+HO_2	7.00×10^{12}	0	27800.0
	Reverse arrhenius coefficients:	1.00×10^{12}	0	0.0
18	*n*$C_{12}H_{26}$+O_2<=>*s5x*$C_{12}H_{25}$+HO_2	7.00×10^{12}	0	27800.0
	Reverse arrhenius coefficients:	1.00×10^{12}	0	0.0
19	*n*$C_{12}H_{26}$+OH<=>*px*$C_{12}H_{25}$+H_2O	5.00×10^{07}	1.9	58.5
	Reverse arrhenius coefficients:	6.15×10^{08}	1.9	21910.0
20	*n*$C_{12}H_{26}$+OH<=>*s5x*$C_{12}H_{25}$+H_2O	5.00×10^{07}	1.9	58.5
	Reverse arrhenius coefficients:	6.15×10^{08}	1.9	21910.0
21	*n*$C_{12}H_{26}$+H=>*px*$C_{12}H_{25}$+H_2	1.00×10^{08}	2	2500.0
22	*n*$C_{12}H_{26}$+H=>*s5x*$C_{12}H_{25}$+H_2	1.00×10^{08}	2	2500.0
23	*px*$C_{12}H_{25}$+O_2<=>$C_{12}H_{25}OO$	3.00×10^{12}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
24	*s5x*$C_{12}H_{25}$+O_2<=>$C_{12}H_{25}OO$	3.00×10^{12}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
25	$C_{12}H_{25}OO$<=>$C_{12}H_{24}OOH$	1.51×10^{11}	0	19000.0
	Reverse arrhenius coefficients:	1.00×10^{11}	0	11000.0
26	$C_{12}H_{24}OOH$+O_2<=>$OOC_{12}H_{24}OOH$	3.56×10^{10}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
27	$OOC_{12}H_{24}OOH$<=>$OC_{12}H_{23}OOH$+OH	8.91×10^{10}	0	17000.0
28	$OC_{12}H_{23}OOH$=>CH_2O+C_2H_4+$C_5H_{11}CO$+OH+C_3H_6	1.98×10^{15}	0	43000.0
29	$C_5H_{11}CO$+O_2=>*n*C_3H_7+C_2H_3+CO+HO_2	3.16×10^{13}	0	10000.0
30	$C_5H_{11}CO$+O_2=>*n*C_3H_7+C_2H_3+CO+HO_2	3.16×10^{13}	0	10000.0
31	*px*C_9H_{19}+CH_3=*n*$C_{10}H_{22}$	1.93×10^{14}	-0.3	0.0

32	*px*C_8H_{17}+C_2H_5=*n*$C_{10}H_{22}$	1.88×10^{14}	-0.5	0.0
33	*px*C_7H_{15}+*n*C_3H_7=*n*$C_{10}H_{22}$	1.88×10^{14}	-0.5	0.0
34	*px*C_6H_{13}+*p*C_4H_9=*n*$C_{10}H_{22}$	1.88×10^{14}	-0.5	0.0
35	*px*C_5H_{11}+*px*C_5H_{11}=*n*$C_{10}H_{22}$	1.88×10^{14}	-0.5	0.0
36	*n*$C_{10}H_{22}$+O=*px*$C_{10}H_{21}$+OH	1.90×10^{05}	2.7	3716.0
37	*n*$C_{10}H_{22}$+O=*s4x*$C_{10}H_{21}$+OH	9.52×10^{04}	2.7	2106.0
38	*n*$C_{10}H_{22}$+HO_2=*px*$C_{10}H_{21}$+H_2O_2	4.76×10^{04}	2.5	16490.0
39	*n*$C_{10}H_{22}$+HO_2=*s4x*$C_{10}H_{21}$+H_2O_2	1.90×10^{04}	2.6	13910.0
40	*n*$C_{10}H_{22}$+CH_3=*px*$C_{10}H_{21}$+CH_4	9.03×10^{-1}	3.6	7153.0
41	*n*$C_{10}H_{22}$+CH_3=*s4x*$C_{10}H_{21}$+CH_4	3.00×10^{00}	3.5	5480.0
42	*n*$C_{10}H_{22}$+O_2=*px*$C_{10}H_{21}$+HO_2	3.00×10^{12}	0	27800.0
	Reverse arrhenius coefficients:	1.00×10^{12}	0	0.0
43	*n*$C_{10}H_{22}$+O_2=*s4x*$C_{10}H_{21}$+HO_2	3.00×10^{12}	0	27800.0
	Reverse arrhenius coefficients:	1.00×10^{12}	0	0.0
44	*n*$C_{10}H_{22}$+OH=*px*$C_{10}H_{21}$+H_2O	5.00×10^{07}	1.9	58.5
	Reverse arrhenius coefficients:	6.15×10^{08}	1.9	21910.0
45	*n*$C_{10}H_{22}$+OH=*s4x*$C_{10}H_{21}$+H_2O	5.00×10^{07}	1.9	58.5
	Reverse arrhenius coefficients:	6.15×10^{08}	1.9	21910.0
46	*n*$C_{10}H_{22}$+H=*px*$C_{10}H_{21}$+H_2	1.00×10^{08}	2	2500.0
47	*n*$C_{10}H_{22}$+H=*s4x*$C_{10}H_{21}$+H_2	1.00×10^{08}	2	2500.0
48	*px*$C_{10}H_{21}$+O_2<=>$C_{10}H_{21}OO$	3.00×10^{12}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
49	*s4x*$C_{10}H_{21}$+O_2<=>$C_{10}H_{21}OO$	3.00×10^{12}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
50	$C_{10}H_{21}OO$<=>$C_{10}H_{20}OOH$	1.51×10^{11}	0	19000.0
	Reverse arrhenius coefficients:	1.00×10^{11}	0	11000.0
51	$C_{10}H_{20}OOH$+O_2<=>$OOC_{10}H_{20}OOH$	3.56×10^{11}	0	0.0
	Reverse arrhenius coefficients:	2.51×10^{13}	0	27400.0
52	$OOC_{10}H_{20}OOH$<=>$OC_{10}H_{19}OOH$+OH	4.10×10^{11}	0	17000.0
53	$OC_{10}H_{19}OOH$=>CH_2O+$C_5H_{11}CO$+OH+C_3H_6	9.98×10^{13}	0	43000.0
54	C_5H_9+H(+M)=C_5H_{10}(+M)	3.60×10^{13}	0	0.0
55	C_5H_9+H=CH_3+C_4H_7	2.00×10^{21}	-2	11000.0
56	C_5H_9+HO_2=CH_2O+OH+C_4H_7	2.40×10^{13}	0	0.0
57	C_5H_9+HCO=C_5H_{10}+CO	6.00×10^{13}	0	0.0
58	C_5H_{10}+H(+M)=*px*C_5H_{11}(+M)	1.33×10^{13}	0	3260.7
59	C_5H_{10}+H=C_2H_4+*n*C_3H_7	8.00×10^{21}	-2.4	11180.0
60	C_5H_{10}+H=C_3H_6+C_2H_5	1.60×10^{22}	-2.4	11180.0
61	C_5H_{10}+H=C_5H_9+H_2	6.50×10^{05}	2.5	6756.0
62	C_5H_{10}+O=*p*C_4H_9+HCO	3.30×10^{08}	1.4	-402.0
63	C_5H_{10}+O=C_5H_9+OH	1.50×10^{13}	0	5760.0
	dup			
64	C_5H_{10}+O=C_5H_9+OH	2.60×10^{13}	0	4470.0

	dup			
65	$C_5H_{10}+OH=C_5H_9+H_2O$	7.00×10^{02}	2.7	527.0
66	$C_5H_{10}+O_2=C_5H_9+HO_2$	2.00×10^{13}	0	50930.0
67	$C_5H_{10}+HO_2=C_5H_9+H_2O_2$	1.00×10^{12}	0	14340.0
68	$C_5H_{10}+CH_3=C_5H_9+CH_4$	4.50×10^{-1}	3.6	7153.0
69	$C_2H_4+nC_3H_7=pxC_5H_{11}$	3.00×10^{11}	0	7300.0
70	$pxC_5H_{11}+H=nC_3H_7+C_2H_5$	3.70×10^{24}	-2.9	12505.0
71	$pxC_5H_{11}+H=C_5H_{10}+H_2$	1.80×10^{12}	0	0.0
72	$pxC_5H_{11}+O=pC_4H_9+CH_2O$	9.60×10^{13}	0	0.0
73	$pxC_5H_{11}+OH=C_5H_{10}+H_2O$	2.40×10^{13}	0	0.0
74	$pxC_5H_{11}+O_2=C_5H_{10}+HO_2$	9.00×10^{10}	0	0.0
75	$pxC_5H_{11}+HO_2=pC_4H_9+OH+CH_2O$	2.40×10^{13}	0	0.0
76	$pxC_5H_{11}+CH_3=C_5H_{10}+CH_4$	1.10×10^{13}	0	0.0
77	$C_6H_{11}+H(+M)=C_6H_{12}(+M)$	3.60×10^{13}	0	0.0
78	$C_6H_{11}+H=CH_3+C_5H_9$	2.00×10^{21}	-2	11000.0
79	$C_6H_{11}+HO_2=CH_2O+OH+C_5H_9$	2.40×10^{13}	0	0.0
80	$C_6H_{11}+HCO=C_6H_{12}+CO$	6.00×10^{13}	0	0.0
81	$C_2H_4+aC_3H_5=C_5H_9$	3.00×10^{11}	0	7300.0
82	$C_6H_{12}+H(+M)=pxC_6H_{13}(+M)$	1.33×10^{13}	0	3260.7
83	$C_6H_{12}+H=C_2H_4+pC_4H_9$	8.00×10^{21}	-2.4	11180.0
84	$C_6H_{12}+H=C_3H_6+nC_3H_7$	1.60×10^{22}	-2.4	11180.0
85	$C_6H_{12}+H=C_6H_{11}+H_2$	6.50×10^{05}	2.5	6756.0
86	$C_6H_{12}+O=pxC_5H_{11}+HCO$	3.30×10^{08}	1.4	-402.0
87	$C_6H_{12}+O=C_6H_{11}+OH$	1.50×10^{13}	0	5760.0
	dup			
88	$C_6H_{12}+O=C_6H_{11}+OH$	2.60×10^{13}	0	4470.0
	dup			
89	$C_6H_{12}+OH=C_6H_{11}+H_2O$	7.00×10^{02}	2.7	527.0
90	$C_6H_{12}+O_2=C_6H_{11}+HO_2$	2.00×10^{13}	0	50930.0
91	$C_6H_{12}+HO_2=C_6H_{11}+H_2O_2$	1.00×10^{12}	0	14340.0
92	$C_6H_{12}+CH_3=C_6H_{11}+CH_4$	4.50×10^{-1}	3.6	7153.0
93	$C_2H_4+pC_4H_9=pxC_6H_{13}$	3.00×10^{11}	0	7300.0
94	$pxC_6H_{13}+H=pC_4H_9+C_2H_5$	3.70×10^{24}	-2.9	12505.0
95	$pxC_6H_{13}+H=C_6H_{12}+H_2$	1.80×10^{12}	0	0.0
96	$pxC_6H_{13}+O=pxC_5H_{11}+CH_2O$	9.60×10^{13}	0	0.0
97	$pxC_6H_{13}+OH=C_6H_{12}+H_2O$	2.40×10^{13}	0	0.0
98	$pxC_6H_{13}+O_2=C_6H_{12}+HO_2$	9.00×10^{10}	0	0.0
99	$pxC_6H_{13}+HO_2=pxC_5H_{11}+OH+CH_2O$	2.40×10^{13}	0	0.0
100	$pxC_6H_{13}+CH_3=C_6H_{12}+CH_4$	1.10×10^{13}	0	0.0
101	$C_7H_{13}+H(+M)=C_7H_{14}(+M)$	3.60×10^{13}	0	0.0
102	$C_7H_{13}+H=CH_3+C_6H_{11}$	2.00×10^{21}	-2	11000.0
103	$C_7H_{13}+HO_2=CH_2O+OH+C_6H_{11}$	2.40×10^{13}	0	0.0

104	$C_7H_{13}+HCO=C_7H_{14}+CO$	6.00×10^{13}	0	0.0
105	$C_2H_4+C_5H_9=C_7H_{13}$	3.00×10^{11}	0	7300.0
106	$C_7H_{14}+H(+M)=pxC_7H_{15}(+M)$	1.33×10^{13}	0	3260.7
107	$C_7H_{14}+H=C_2H_4+pxC_5H_{11}$	8.00×10^{21}	-2.4	11180.0
108	$C_7H_{14}+H=C_3H_6+pC_4H_9$	1.60×10^{22}	-2.4	11180.0
109	$C_7H_{14}+H=C_7H_{13}+H_2$	6.50×10^{05}	2.5	6756.0
110	$C_7H_{14}+O=pxC_6H_{13}+HCO$	3.30×10^{08}	1.4	-402.0
111	$C_7H_{14}+O=C_7H_{13}+OH$	1.50×10^{13}	0	5760.0
	dup			
112	$C_7H_{14}+O=C_7H_{13}+OH$	2.60×10^{13}	0	4470.0
	dup			
113	$C_7H_{14}+OH=C_7H_{13}+H_2O$	7.00×10^{02}	2.7	527.0
114	$C_7H_{14}+O_2=C_7H_{13}+HO_2$	2.00×10^{13}	0	50930.0
115	$C_7H_{14}+HO_2=C_7H_{13}+H_2O_2$	1.00×10^{12}	0	14340.0
116	$C_7H_{14}+CH_3=C_7H_{13}+CH_4$	4.50×10^{-1}	3.6	7153.0
117	$C_2H_4+pxC_5H_{11}=pxC_7H_{15}$	3.00×10^{11}	0	7300.0
118	$pxC_7H_{15}+H=pxC_5H_{11}+C_2H_5$	3.70×10^{24}	-2.9	12505.0
119	$pxC_7H_{15}+H=C_7H_{14}+H_2$	1.80×10^{12}	0	0.0
120	$pxC_7H_{15}+O=pxC_6H_{13}+CH_2O$	9.60×10^{13}	0	0.0
121	$pxC_7H_{15}+OH=C_7H_{14}+H_2O$	2.40×10^{13}	0	0.0
122	$pxC_7H_{15}+O_2=C_7H_{14}+HO_2$	9.00×10^{10}	0	0.0
123	$pxC_7H_{15}+HO_2=pxC_6H_{13}+OH+CH_2O$	2.40×10^{13}	0	0.0
124	$pxC_7H_{15}+CH_3=C_7H_{14}+CH_4$	1.10×10^{13}	0	0.0
125	$C_8H_{15}+H(+M)=C_8H_{16}(+M)$	3.60×10^{13}	0	0.0
126	$C_8H_{15}+H=CH_3+C_7H_{13}$	2.00×10^{21}	-2	11000.0
127	$C_8H_{15}+HO_2=CH_2O+OH+C_7H_{13}$	2.40×10^{13}	0	0.0
128	$C_8H_{15}+HCO=C_8H_{16}+CO$	6.00×10^{13}	0	0.0
129	$C_2H_4+C_6H_{11}=C_8H_{15}$	3.00×10^{11}	0	7300.0
130	$C_8H_{16}+H(+M)=pxC_8H_{17}(+M)$	1.33×10^{13}	0	3260.7
131	$C_8H_{16}+H=C_2H_4+pxC_6H_{13}$	8.00×10^{21}	-2.4	11180.0
132	$C_8H_{16}+H=C_3H_6+pxC_5H_{11}$	1.60×10^{22}	-2.4	11180.0
133	$C_8H_{16}+H=C_8H_{15}+H_2$	6.50×10^{05}	2.5	6756.0
134	$C_8H_{16}+O=pxC_7H_{15}+HCO$	3.30×10^{08}	1.4	-402.0
135	$C_8H_{16}+O=C_8H_{15}+OH$	1.50×10^{13}	0	5760.0
	dup			
136	$C_8H_{16}+O=C_8H_{15}+OH$	2.60×10^{13}	0	4470.0
	dup			
137	$C_8H_{16}+OH=C_8H_{15}+H_2O$	7.00×10^{02}	2.7	527.0
138	$C_8H_{16}+O_2=C_8H_{15}+HO_2$	2.00×10^{13}	0	50930.0
139	$C_8H_{16}+HO_2=C_8H_{15}+H_2O_2$	1.00×10^{12}	0	14340.0
140	$C_8H_{16}+CH_3=C_8H_{15}+CH_4$	4.50×10^{-1}	3.6	7153.0
141	$C_2H_4+pxC_6H_{13}=pxC_8H_{17}$	3.00×10^{11}	0	7300.0

142	*px*C_8H_{17}+H=*px*C_6H_{13}+C_2H_5	3.70×10^{24}	-2.9	12505.0
143	*px*C_8H_{17}+H=C_8H_{16}+H_2	1.80×10^{12}	0	0.0
144	*px*C_8H_{17}+O=*px*C_7H_{15}+CH_2O	9.60×10^{13}	0	0.0
145	*px*C_8H_{17}+OH=C_8H_{16}+H_2O	2.40×10^{13}	0	0.0
146	*px*C_8H_{17}+O_2=C_8H_{16}+HO_2	9.00×10^{10}	0	0.0
147	*px*C_8H_{17}+HO_2=*px*C_7H_{15}+OH+CH_2O	2.40×10^{13}	0	0.0
148	*px*C_8H_{17}+CH_3=C_8H_{16}+CH_4	1.10×10^{13}	0	0.0
149	C_9H_{18}+H(+M)=*px*C_9H_{19}(+M)	1.33×10^{13}	0	3260.7
150	C_9H_{18}+H=C_2H_4+*px*C_7H_{15}	8.00×10^{21}	-2.4	11180.0
151	C_9H_{18}+H=C_3H_6+*px*C_6H_{13}	1.60×10^{22}	-2.4	11180.0
152	C_9H_{18}+O=*px*C_8H_{17}+HCO	3.30×10^{08}	1.4	-402.0
153	C_2H_4+*px*C_7H_{15}=*px*C_9H_{19}	3.00×10^{11}	0	7300.0
154	*px*C_9H_{19}+H=*px*C_7H_{15}+C_2H_5	3.70×10^{24}	-2.9	12505.0
155	*px*C_9H_{19}+H=C_9H_{18}+H_2	1.80×10^{12}	0	0.0
156	*px*C_9H_{19}+O=*px*C_8H_{17}+CH_2O	9.60×10^{13}	0	0.0
157	*px*C_9H_{19}+OH=C_9H_{18}+H_2O	2.40×10^{13}	0	0.0
158	*px*C_9H_{19}+O_2=C_9H_{18}+HO_2	9.00×10^{10}	0	0.0
159	*px*C_9H_{19}+HO_2=*px*C_8H_{17}+OH+CH_2O	2.40×10^{13}	0	0.0
160	*px*C_9H_{19}+CH_3=C_9H_{18}+CH_4	1.10×10^{13}	0	0.0
161	C_2H_4+*px*C_8H_{17}=*px*$C_{10}H_{21}$	3.00×10^{11}	0	7300.0
162	*px*$C_{10}H_{21}$+H=*px*C_8H_{17}+C_2H_5	3.70×10^{24}	-2.9	12505.0
163	*px*$C_{10}H_{21}$+O=*px*C_9H_{19}+CH_2O	9.60×10^{13}	0	0.0
164	*px*$C_{10}H_{21}$+HO_2=*px*C_9H_{19}+OH+CH_2O	2.40×10^{13}	0	0.0
165	*p*C_4H_9+C_6H_{12}=*s4x*$C_{10}H_{21}$	3.00×10^{11}	0	7300.0
166	C_7H_{14}+*n*C_3H_7=*s4x*$C_{10}H_{21}$	3.00×10^{11}	0	7300.0
167	*px*$C_{10}H_{21}$=*s4x*$C_{10}H_{21}$	3.67×10^{12}	-0.6	14400.0
(B) Sub-mechanisms of ethycyclohexane				
No.	reaction	*A*	*n*	*E*
1	*c*C_6H_{11}+C_2H_5=C_2H_5*c*C_6H_{11}	1.95×10^{14}	-0.3	0.0
2	C_2H_5*c*C_6H_{11}=C_8H_{16}	1.67×10^{16}	0	87232.0
3	C_2H_5*c*C_6H_{11}+H=*sx*C_2H_4*c*C_6H_{11}+H_2	1.30×10^{06}	2.4	4471.0
4	C_2H_5*c*C_6H_{11}+H=C_2H_5*s3xc*C_6H_{10}+H_2	2.60×10^{06}	2.4	4471.0
5	C_2H_5*c*C_6H_{11}+O=*sx*C_2H_4*c*C_6H_{11}+OH	3.10×10^{05}	2.5	2225.0
6	C_2H_5*c*C_6H_{11}+O=C_2H_5*s3xc*C_6H_{10}+OH	9.52×10^{04}	2.7	2106.0
7	C_2H_5*c*C_6H_{11}+O=C_2H_5*s4xc*C_6H_{10}+OH	4.76×10^{04}	2.7	2106.0
8	C_2H_5*c*C_6H_{11}+OH=*sx*C_2H_4*c*C_6H_{11}+H_2O	7.05×10^{09}	0.9	504.7
9	C_2H_5*c*C_6H_{11}+OH=C_2H_5*s3xc*C_6H_{10}+H_2O	1.94×10^{05}	2.5	1164.4
10	C_2H_5*c*C_6H_{11}+OH=C_2H_5*s4xc*C_6H_{10}+H_2O	9.71×10^{04}	2.5	1164.4
11	C_2H_5*c*C_6H_{11}+O_2=*sx*C_2H_4*c*C_6H_{11}+HO_2	4.00×10^{13}	0	47590.0
12	C_2H_5*c*C_6H_{11}+O_2=C_2H_5*s3xc*C_6H_{10}+HO_2	8.00×10^{13}	0	47590.0
13	C_2H_5*c*C_6H_{11}+O_2=C_2H_5*s4xc*C_6H_{10}+HO_2	4.00×10^{13}	0	47590.0
14	C_2H_5*c*C_6H_{11}+HO_2=*sx*C_2H_4*c*C_6H_{11}+H_2O_2	9.64×10^{05}	2.6	13910.0

15	$C_2H_5cC_6H_{11}+HO_2=C_2H_5s3xcC_6H_{10}+H_2O_2$	1.93×10^{03}	2.6	13910.0
16	$C_2H_5cC_6H_{11}+HO_2=C_2H_5s4xcC_6H_{10}+H_2O_2$	9.64×10^{05}	2.6	13910.0
17	$C_2H_5cC_6H_{11}+CH_3=sxC_2H_4cC_6H_{11}+CH_4$	1.51×10^{00}	3.5	5480.0
18	$C_2H_5cC_6H_{11}+CH_3=C_2H_5s3xcC_6H_{10}+CH_4$	3.00×10^{00}	3.5	5480.0
19	$C_2H_5cC_6H_{11}+CH_3=C_2H_5s4xcC_6H_{10}+CH_4$	1.50×10^{00}	3.5	5480.0
20	$sxC_2H_4cC_6H_{11}+H(+M)=C_2H_5cC_6H_{11}(+M)$	4.80×10^{13}	0	0.0
21	$C_2H_5s3xcC_6H_{10}+H(+M)=C_2H_5cC_6H_{11}(+M)$	4.80×10^{13}	0	0.0
22	$C_2H_5s4xcC_6H_{10}+H(+M)=C_2H_5cC_6H_{11}(+M)$	4.80×10^{13}	0	0.0
23	$C_2H_5cC_6H_{11}+H=C_2H_5s4xcC_6H_{10}+H_2$	1.30×10^{06}	2.4	4471.0
24	$C_2H_5s4xcC_6H_{10}(+M)=pxCH_2C_7H_{13}(+M)$	6.03×10^{12}	0.1	27982.9
25	$sxC_2H_4cC_6H_{11}=C_2H_5s4xcC_6H_{10}$	1.19×10^{09}	0.9	22700.0
26	$C_2H_5s4xcC_6H_{10}+H=cC_6H_{11}+C_2H_5$	2.80×10^{28}	-3.9	15916.0
27	$C_2H_5s3xcC_6H_{10}(+M)=pxC_2H_4C_6H_{11}(+M)$	3.01×10^{12}	0.1	27982.9
28	$sxC_2H_4cC_6H_{11}=C_2H_5s3xcC_6H_{10}$	4.65×10^{08}	1	28687.0
29	$C_2H_5s3xcC_6H_{10}+H=cC_6H_{11}+C_2H_5$	2.80×10^{28}	-3.9	15916.0
30	$pxCH_2C_7H_{13}(+M)=C_4H_7+C_4H_{81}(+M)$	1.76×10^{11}	0.6	28791.6
31	$pxCH_2C_7H_{13}(+M)=C_6H_{10}+C_2H_5(+M)$	1.76×10^{11}	0.6	28791.6
32	$pxCH_2C_7H_{13}(+M)=CH_3saxC_7H_{12}(+M)$	1.55×10^{02}	2.8	15566.2
33	$C_6H_{10}+H=C_4H_7+C_2H_4$	1.60×10^{22}	-2.4	11180.0
34	$aC_3H_5+aC_3H_5=C_6H_{10}$	1.02×10^{13}	0	262.0
35	$C_6H_{10}+H=saxC_6H_9+H_2$	3.30×10^{05}	2.5	2490.0
36	$C_6H_{10}+OH=saxC_6H_9+H_2O$	4.14×10^{06}	2	-298.0
37	$C_6H_{10}+CH_3=saxC_6H_9+CH_4$	2.94×10^{00}	3.5	5675.0
38	$C_4H_6+C_2H_3=saxC_6H_9$	4.20×10^{13}	0	1300.0
39	$CH_3sax_1C_7H_{12}(+M)=C_4H_6+sC_4H_9(+M)$	3.39×10^{11}	0.7	31262.9
40	$sxC_2H_4cC_6H_{11}(+M)=pxC_8H_{15}(+M)$	6.03×10^{12}	0.1	26982.9
41	$sxC_2H_4cC_6H_{11}+H=cC_6H_{11}+C_2H_5$	2.80×10^{28}	-3.9	15916.0
42	$pxC_8H_{15}(+M)=saxC_8H_{15}(+M)$	1.46×10^{11}	0	10516.8
43	$pxC_8H_{15}(+M)=pxC_6H_{11}+C_2H_4(+M)$	9.12×10^{11}	0.3	27237.8
44	$saxC_8H_{15}(+M)=C_5H_8+nC_3H_7(+M)$	3.39×10^{11}	0.7	32262.9
45	$C_5H_8+H=C_2H_4+CH_3CHCH$	1.46×10^{30}	-4.3	21647.0
46	$C_5H_8+H=C_4H_6+CH_3$	2.00×10^{12}	0	7000.0
47	$C_5H_8+H=C_4H_6+CH_3$	2.00×10^{12}	0	7000.0
48	$C_5H_8+H=lC_5H_7+H_2$	1.73×10^{05}	2.5	2490.0
49	$C_5H_8+OH=lC_5H_7+H_2O$	3.10×10^{06}	2	-298.0
50	$C_5H_8+CH_3=lC_5H_7+CH_4$	2.20×10^{00}	3.5	5675.0
51	$nC_4H_5+CH_3=C_5H_8$	7.23×10^{13}	0	0.0
52	$pxC_6H_{11}(+M)=saxC_4H_7+C_2H_4(+M)$	1.04×10^{12}	-0.4	25124.2
53	$saxC_4H_7(+M)=C_4H_6+H(+M)$	4.70×10^{08}	1.3	44697.6
54	$saxC_4H_7+H(+M)=C_4H_{81}(+M)$	2.00×10^{14}	0	0.0
55	$C_4H_{81}+H=saxC_4H_7+H_2$	5.40×10^{04}	2.5	-1900.0
56	$C_4H_{81}+OH=saxC_4H_7+H_2O$	3.00×10^{06}	2	-1520.0

57	$C_4H_{81}+CH_3=saxC_4H_7+CH_4$	1.00×10^{11}	0	7300.0
58	$cC_6H_{12}+H=cC_6H_{11}+H_2$	7.80×10^{06}	2.4	4471.0
59	$cC_6H_{12}+O=cC_6H_{11}+OH$	2.86×10^{05}	2.7	2106.0
60	$cC_6H_{12}+OH=cC_6H_{11}+H_2O$	5.83×10^{05}	2.5	1164.4
61	$cC_6H_{12}+O_2=cC_6H_{11}+HO_2$	2.40×10^{14}	0	47590.0
62	$cC_6H_{12}+HO_2=cC_6H_{11}+H_2O_2$	5.78×10^{04}	2.6	13910.0
63	$cC_6H_{11}+H(+M)=cC_6H_{12}(+M)$	4.80×10^{13}	0	0.0
64	$cC_6H_{11}+H=C_6H_{12}$	2.80×10^{28}	-3.9	15916.0
65	$cC_6H_{12}=C_6H_{12}$	5.01×10^{16}	0	88232.0
66	$cC_6H_{12}+CH_3=cC_6H_{11}+CH_4$	9.00×10^{00}	3.5	5480.0
67	$C_6H_{12}=aC_3H_5+nC_3H_7$	1.07×10^{23}	-2	74958.0
68	$C_6H_{12}=C_3H_6+C_3H_6$	7.08×10^{06}	1.6	53752.0
69	$C_6H_{12}+H=s2xC_6H_{11}+H_2$	1.30×10^{06}	2.4	4471.0
70	$C_8H_{16}=pxC_5H_{11}+aC_3H_5$	1.07×10^{23}	-2	74958.0
71	$pxC_5H_{11}(+M)=C_2H_4+nC_3H_7(+M)$	1.00×10^{13}	0	28366.4
72	$pxC_2H_4C_6H_{11}(+M)=s2xC_6H_{11}+C_2H_4(+M)$	9.12×10^{11}	0.3	27237.8
73	$pxC_2H_4C_6H_{11}(+M)=C_2H_5saxC_6H_{10}(+M)$	1.55×10^{02}	2.8	15566.2
74	$s2xC_6H_{11}(+M)=pxCH_2C_5H_9(+M)$	7.59×10^{06}	1.8	6447.8
75	$pxCH_2C_5H_9(+M)=C_4H_6+C_2H_5(+M)$	4.90×10^{12}	0.1	11139.1
76	$CH_3saxC_6H_{10}(+M)=C_4H_6+iC_3H_7(+M)$	3.39×10^{11}	0.7	31262.9
(C) Sub-mechanisms of *p*-xylene				
No.	reaction	*A*	*n*	*E*
1	$pC_6H_4(CH_3)_2+H=C_6H_5CH_3+CH_3$	1.80×10^{16}	0	8090.0
2	$pC_6H_4(CH_3)_2=C_6H_4CH_3+CH_3$	5.80×10^{15}	0	90951.0
3	$pC_6H_4(CH_3)_2=pC_8H_9+H$	2.57×10^{17}	0	83360.0
4	$pC_6H_4(CH_3)_2+H=pC_8H_9+H_2$	4.00×10^{14}	0	8370.0
5	$pC_6H_4(CH_3)_2+O=pC_8H_9+OH$	2.60×10^{13}	0	3062.0
6	$pC_6H_4(CH_3)_2+OH=pC_8H_9+H_2O$	2.00×10^{13}	0	2180.0
7	$pC_6H_4(CH_3)_2+HO_2=pC_8H_9+H_2O_2$	7.94×10^{12}	0	14069.0
8	$pC_6H_4(CH_3)_2+CH_3=pC_8H_9+CH_4$	1.77×10^{12}	0	8754.0
9	$pC_6H_4(CH_3)_2+O_2=pC_8H_9+HO_2$	3.00×10^{14}	0	43062.0
10	$pC_6H_4(CH_3)_2+aC_3H_5=pC_8H_9+C_3H_6$	5.00×10^{12}	0	14019.0
11	$pC_6H_4(CH_3)_2+C_2H_5=pC_8H_9+C_2H_6$	1.01×10^{11}	0	9514.0
12	$pC_6H_4(CH_3)_2+C_6H_5=pC_8H_9+C_6H_6$	1.00×10^{13}	0	4400.0
13	$pC_6H_4(CH_3)_2+C_6H_4CH_3=pC_8H_9+C_6H_5CH_3$	2.10×10^{12}	0	4400.0
14	$pC_6H_4(CH_3)_2+nC_4H_5=pC_8H_9+C_4H_6$	6.00×10^{12}	0	7500.0
15	$pC_6H_4(CH_3)_2+C_2H_3=pC_8H_9+C_2H_4$	4.00×10^{12}	0	7500.0
16	$pC_8H_9=C_5H_6+C_3H_3$	1.00×10^{14}	0	71000.0
17	$pC_8H_9+O=C_6H_4CH_3+CH_2O$	1.00×10^{13}	0	0.0
18	$pC_8H_9+H=C_6H_4C_2H_4+H_2$	1.00×10^{16}	0	8365.0
19	$pC_8H_9=C_6H_4C_2H_4+H$	1.00×10^{13}	0	86124.0
20	$pC_8H_9=C_6H_3+CH_3+CH_3$	1.00×10^{12}	0	76200.0

21	$pC_8H_9=C_5H_4CH_3+C_2H_2$	1.00×10^{14}	0	70000.0
22	$pC_8H_9=C_6H_5C_2H_3+H$	1.00×10^{13}	0	61500.0
23	$pC_8H_9+C_6H_5OH=pC_6H_4(CH_3)_2+C_6H_5O$	2.05×10^{11}	0	9500.0
24	$pC_8H_9+OH+H=C_6H_5CH_3+CH_2OH$	6.00×10^{12}	0	5155.5
25	$pC_8H_9+O_2=C_6H_4C_2H_4+HO_2$	3.00×10^{15}	0	43062.0
26	$pC_8H_9+HO_2=C_6H_4C_2H_4+H_2O_2$	1.00×10^{14}	0	7895.0
27	$C_6H_4C_2H_4=oC_6H_4+C_2H_4$	2.00×10^{14}	0	83000.0
28	$C_5H_4CH_3=C_6H_6+H$	6.02×10^{12}	0	0.0
29	$C_6H_4CH_3+H=C_6H_5CH_3$	7.80×10^{13}	0	0.0
30	$C_6H_4CH_3+C_2H_4=C_6H_5CH_3+C_2H_3$	1.00×10^{12}	0	6206.0
31	$C_6H_6+C_2H_3=C_6H_5C_2H_3+H$	3.60×10^{12}	0	6400.0
32	$C_6H_5+C_2H_4=C_6H_5C_2H_3+H$	5.10×10^{12}	0	6190.0
33	$C_6H_5+C_2H_3=C_6H_5C_2H_3$	1.90×10^{48}	-10.5	17489.0
34	$C_6H_5C_2H_3=C_6H_5CCH_2+H$	6.00×10^{46}	-9.1	118323.0
35	$C_6H_5C_2H_3+H=C_6H_5CCH_2+H_2$	3.33×10^{05}	2.5	9240.0
36	$C_6H_5C_2H_3+OH=C_6H_5CCH_2+H_2O$	1.55×10^{06}	2	430.0
37	$C_6H_5C_2H_3=C_6H_5CHCH+H$	9.50×10^{54}	-11.4	130224.0
38	$C_6H_5C_2H_3+H=C_6H_5CHCH+H_2$	6.65×10^{05}	2.5	12240.0
39	$C_6H_5C_2H_3+OH=C_6H_5CHCH+H_2O$	3.10×10^{06}	2	3430.0
40	$C_6H_5+C_2H_3=C_6H_5CCH_2+H$	1.80×10^{31}	-4.6	31652.0
41	$C_6H_5CCH_2+O_2=C_6H_5CO+CH_2O$	4.60×10^{16}	-1.4	1010.0
42	$C_6H_5CHCH+H=C_6H_5CCH_2+H$	2.30×10^{37}	-6	35164.0
43	$C_6H_5CCH_2+OH=C_6H_5CHO+CH_2$	4.00×10^{07}	1.8	220.0
44	$C_6H_5C_2H+H=C_6H_5CCH_2$	5.00×10^{54}	-12.8	17185.0
45	$C_6H_5CCH_2+H=C_6H_5C_2H+H_2$	3.00×10^{13}	0	0.0
46	$C_6H_5CCH_2+OH=C_6H_5C_2H+H_2O$	5.00×10^{12}	0	0.0
47	$C_6H_5CCH_2+O=CH_2CO+C_6H_5$	4.80×10^{13}	0	0.0
48	$C_6H_5+C_2H_3=C_6H_5CHCH+H$	1.50×10^{32}	-4.9	35504.0
49	$C_6H_5+C_2H_2=C_6H_5CHCH$	7.70×10^{40}	-9.2	13400.0
50	$C_6H_5CHCH+O_2=C_6H_5CHO+HCO$	4.60×10^{16}	-1.4	1010.0
51	$C_6H_5C_2H+H=C_6H_5CHCH$	5.00×10^{54}	-12.8	17185.0
52	$C_6H_5CHCH+H=C_6H_5C_2H+H_2$	3.00×10^{13}	0	0.0
53	$C_6H_5CHCH+OH=C_6H_5C_2H+H_2O$	2.50×10^{12}	0	0.0
54	$C_5H_5+C_3H_3=C_6H_5C_2H_3$	1.64×10^{66}	-15.9	27529.0
55	$C_6H_5C_2H_3+O=C_6H_5CCH_2+OH$	1.51×10^{07}	1.9	3740.0
56	$C_6H_5C_2H_3+O=C_6H_5CHCH+OH$	1.51×10^{07}	1.9	3740.0
57	$C_6H_5C_2H_3+O=C_6H_5CH_2+HCO$	1.92×10^{07}	1.8	220.0
58	$C_6H_5C_2H_3+O=C_6H_5CO+CH_3$	1.92×10^{07}	1.8	220.0
59	$C_6H_5C_2H_3+O=C_6H_5CHO+CH_2$	3.84×10^{05}	1.8	220.0
60	$C_6H_5+C_2H_2=C_6H_5C_2H+H$	7.50×10^{26}	-4	17100.0
61	$nC_4H_5+C_4H_2=C_6H_5C_2H+H$	3.16×10^{11}	0	1800.0
62	$C_6H_5C_2H+OH=CH_2CO+C_6H_5$	1.10×10^{13}	0	7170.0

63	$C_6H_5C_2H+O=HCCO+C_6H_5$	1.63×10^{07}	2	1900.0
$k_f = AT^n \exp(-E/RT)$ *A* unit: mol, cm, s; *E* unit: cal/mol.				