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适用于 HCCI 燃烧的汽油替代燃料化学动力学简化模型

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Reduced Chemical Kinetic Model of a Gasoline Surrogate Fuel for HCCI Combustion

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Appendix A Supplementary material

Species					
NC_7H_{16}	C_7H_{15}-1	C_7H_{15}-2	$C_7H_{15}O$	$C_7H_{15}OO$	$C_7H_{14}OOH$
$OC_7H_{13}O$	$HO_2C_7H_{13}O_2H$	C_5H_{11}	PC_4H_9	IC_3H_7	C_3H_6
IC_8H_{18}	$AC_8H_{16}OOH$	$AC_8H_{17}O2$	$AC_8H_{17}O$	JC_8H_{16}	AC_8H_{17}
$OC_8H_{15}O$	$AOOC_8H_{16}OOH$	$OC_8H_{15}OOH$	IC_4H_8	C_3H_5	$C_6H_5CH_3$
JC_8H_{15}-B	$DMPD_{13}HO$	JC_8H_{15}-D	DMPD13	DMPD13-E	DMPD13O
JC_8H_{15}-A	$DMPD_{13}CO$	DMBD13-D	MP1CO-C	MP1OCO	$C(CO)_2$
$C(CO)_2$-A	$CH2CCH_2OH$	IC_4H_7	IC_4H_7O	IC_4H_6OH	TC_4H_9
CH_2OH	IC_3H_5CHO	IC_3H_5CO	C_3H_5-T	C_4H_5	C_6H_5
C_6H_5CH2	C_6H_5CH2OO	C_6H_5CO	$C_6H_5CH_2O$	C_6H_5CHO	$C_6H_4CH_3$
C_6H_5O	$HOC_6H_4CH_3$	C_6H_4O2	C_6H_5OH	$OC_6H_4CH_3$	C_3H_4
C_5H_4O	CH_3COCH_2	C_4H_4	C_4H_3	C_3H_3	C_2H_2
C_2H_5	C_2H_5O	C_2H_5O2	C_2H_4	C_2H_3	CH_3OH
CH_3CHO	CH_3CO	HCCO	CH_4	CH_3O_2	CH_2CO
CH_3O	CH_3	CH_2	CH_2O	CH_2CHO	N
CH	C_2H	HCO	CO	CO_2	HO_2
NO	N_2	NO_2	HONO	OH	O_2
H	H_2	$H2O_2$	H_2O	O	

No.	Reactions	*A*	*b*	*E*a	Ref.
	$k = AT^{b} \exp\left(-E_a / RT\right)$				
1	$NC_7H_{16}=PC_4H_9+IC_3H_7$	3.16×10^{18}	0	81020	6
2	$NC_7H_{16}+O_2=C_7H_{15}$-1$+HO_2$	6.00×10^{13}	0	52820	6
3	$NC_7H_{16}+O_2=C_7H_{15}$-2$+HO_2$	4.00×10^{13}	0	50190	6
4	$NC_7H_{16}+HO_2=C_7H_{15}-1+H_2O_2$	5.00×10^{13}	0	20430	6
5	$NC_7H_{16}+HO_2=C_7H_{15}-2+H_2O_2$	3.36×10^{13}	0	17690	6
6	$NC_7H_{16}+OH=C_7H_{15}$-1$+H_2O$	1.05×10^{10}	1	1590	6
7	$NC_7H_{16}+OH=C_7H_{15}$-2$+H_2O$	9.40×10^{7}	1.6	-35	6
8	C_7H_{15}-1$=C_7H_{15}$-2	2.00×10^{11}	0	18120	6
9	C_7H_{15}-2$=C_7H_{15}$-1	2.00×10^{11}	0	18120	6
10	C_7H_{15}-1$+O_2=C_7H_{15}OO$	2.50×10^{12}	0	0	6
11	$C_7H_{15}OO=C_7H_{15}$-1$+O_2$	2.20×10^{15}	0	27960	6
12	C_7H_{15}-2$+O_2=C_7H_{15}OO$	2.50×10^{12}	0	0	6
13	$C_7H_{15}OO=C7H_{15}$-2$+O_2$	2.20×10^{15}	0	26960	6
14	$C_7H_{15}OO=C_7H_{14}OOH$	2.00×10^{11}	0	17010	6
15	$C_7H_{14}OOH+O_2=OOC_7H_{14}OOH$	5.60×10^{12}	0	0	6
16	$OOC_7H_{14}OOH=HO_2C_7H_{13}O_2H$	2.00×10^{11}	0	17010	6
17	$HO_2C_7H_{13}O_2H=OC_7H_{13}OOH+OH$	1.00×10^{9}	0	7500	6
18	$OC_7H_{13}OOH=OC_7H_{13}O+OH$	8.40×10^{14}	0	43020	6
19	$OC_7H_{13}O=CH_2O+C_5H_{11}+CO$	2.00×10^{13}	0	15000	6
20	C_7H_{15}-1$=C_5H_{11}+C_2H_4$	2.50×10^{13}	0	28920	6
21	C_7H_{15}-2$=PC_4H_9+C_3H_6$	1.20×10^{13}	0	28203	6

22	$C_5H_{11}=C_2H_4+IC_3H_7$	7.97×10^{17}	-1.4	29876	6
23	$NC_7H_{16}+H=C_7H_{15}\text{-}1+H_2$	1.88×10^{05}	2.8	6286	6
24	$NC_7H_{16}+H=C7H_{15}\text{-}2+H_2$	2.60×10^{06}	2.4	4469	6
25	$IC_3H_7+O_2=C_3H_6+HO_2$	6.10×10^{20}	-2.9	7910	6
26	$C_3H_6+H(+M)=IC_3H_7(+M)$	5.70×10^{09}	1.2	874	6
	Low pressure limit:	0.164×10^{55}	-11.1	9364	
	TROE centering:	0.1×10^{03}	260	3000	
	H_2O Enhanced by	5.00			
	H_2 Enhanced by	2.00			
	CO_2 Enhanced by	3.00			
	CO Enhanced by	2.00			
27	$IC_3H_7+H=C_2H_5+CH_3$	5.00×10^{13}	0	0	6
28	$PC_4H_9(+M)=C_2H_5+C_2H_4(+M)$	1.06×10^{13}	0	27828	6
	Low pressure limit: 0.18970×1056	-11.9		32263	
	H_2O Enhanced by	5.00			
	H_2 Enhanced by	2.00			
	CO_2 Enhanced by	3.00			
	CO Enhanced by	2.00			
29	$PC_4H_9=C_2H_5+C_2H_4$	2.50×10^{13}	0	28800	6
30	$IC_8H_{18}+O_2=AC_8H_{17}+HO_2$	1.00×10^{16}	0	49000	11
	Reverse Arrhenius coefficients	1.00×10^{12}	0	0	6
31	$IC_8H_{18}+HO_2=AC_8H_{17}+H_2O_2$	3.02×10^{12}	0	14700	11
32	$AC_8H_{17}+O_2=AC_8H_{17}O_2$	1.00×10^{12}	0	0	6
	Reverse Arrhenius coefficients	2.51×10^{13}	0	27400	6
33	$AC_8H_{17}O_2=AC_8H_{16}OOH$	1.14×10^{11}	0	22400	6
	Reverse Arrhenius coefficients	1.00×10^{11}	0	11000	6
34	$AC_8H_{16}OOH+O_2=AOOC_8H_{16}OOH$	3.16×10^{11}	0	0	6
	Reverse Arrhenius coefficients	2.51×10^{13}	0	27400	6
35	$AOOC_8H_{16}OOH=OC_8H_{15}OOH+OH$	8.91×10^{10}	0	17000	6
36	$IC_8H_{18}+OH=AC_8H_{17}+H_2O$	3.00×10^{13}	0	3000	11
37	$OC_8H_{15}OOH=OC_8H_{15}O+OH$	3.98×10^{15}	0	43000	6
38	$AC_8H_{17}+O_2=JC_8H_{16}+HO_2$	3.16×10^{11}	0	6300	11
	Reverse Arrhenius coefficients	3.16×10^{11}	0	19500	6
39	$OC_8H_{15}O+O_2=C_2H_3+2CH_2O+C_3H4+CH_3+HO_2$	2.45×10^{13}	0	32000	6
40	$AC_8H_{17}=IC_4H_8+C_3H_6+CH_3$	1.28×10^{12}	0	49000	6
41	$JC_8H_{16}=IC_4H_8+C_3H_5+CH_3$	1.92×10^{12}	0	49000	11
42	$IC_4H_8+O_2=C_2H_3+C_2H_4+HO_2$	2.00×10^{14}	0	35900	6
43	$IC_4H_8=C_3H_5+CH_3$	1.92×10^{66}	-14	128100	6
	Reverse Arrhenius coefficients	2.09×10^{59}	-13	29530	
44	$C_6H_5CH_3+O_2=C_6H_5CH_2+HO_2$	1.81×10^{12}	0	39717	11
45	$C_6H_5CH_3+OH=C_6H_5CH_2+H_2O$	6.70×10^{09}	1	870	11
46	$C_6H_5CH_3+O=C_6H_5CH_2+OH$	6.30×10^{11}	0	0	11
47	$C_6H_5CH_3+H=C_6H_5CH_2+H_2$	6.00×10^{13}	0	8235	11

48	$C_6H_5CH_2+O=C_6H_5CHO+H$	2.50×10^{14}	0	0	11
49	$C_6H_5CH_2+O=C_6H_5+CH_2O$	8.00×10^{13}	0	0	11
50	$C_6H_5CH_2+HO_2=C_6H_5CHO+H+OH$	2.60×10^{13}	0	0	11
51	$C_6H_5CH_2+HO_2=C_6H_5CHO+H_2O$	7.50×10^{12}	0	0	11
52	$C_6H_5CH_2+HO_2=C_6H_5+CH_2O+OH$	6.00×10^{12}	0	0	11
53	$C_6H_5CH_2+H=C_6H_5CH_3$	1.80×10^{14}	0	0	11
54	$C_6H_5CHO+OH=C_6H_5CO+H_2O$	1.71×10^{09}	1.2	-447	11
55	$C_6H_5CHO+H=C_6H_5CO+H_2$	5.00×10^{13}	0	4928	11
56	$C_6H_5CHO+O=C_6H_5CO+OH$	9.04×10^{12}	0	3080	11
57	$C_6H_5CH_2+C_6H_5CHO=C_6H_5CH_3+C_6H_5CO$	2.77×10^{03}	2.8	5773	11
58	$C_6H_5CO=C_6H_5+CO$	3.98×10^{14}	0	29400	11
59	$C_6H_5+O_2=CH_2CO+CH_2CO+C_2H$	7.80×10^{16}	-1.8	0	11
60	$C_6H_5+O_2=C_6H_5O+O$	2.60×10^{13}	0	6100	11
61	$C_6H_5+OH=C_6H_5O+H$	5.00×10^{13}	0	0	11
62	$C_6H_5OH+OH=C_6H_5O+H_2O$	3.00×10^{06}	2	-1310	11
63	$C_6H_5CH_2+C_6H_5OH=C_6H_5CH_3+C_6H_5O$	1.05×10^{12}	0	9500	11
64	$C_6H_5+O_2=C_6H_4O_2+H$	3.00×10^{13}	0	8980	11
65	$C_6H_5O+O=C_6H_4O_2+H$	5.00×10^{13}	0	0	11
66	$C_6H_5O+HO_2=C_6H_4O_2+H_2O$	1.00×10^{13}	0	0	11
67	$C_6H_4O_2+O=2CO+C_2H_2+CH_2CO$	3.00×10^{13}	0	5000	11
68	$C_6H_5CH_3+OH=C_6H_4CH_3+H_2O$	3.40×10^{08}	1.4	1450	11
69	$C_6H_4CH_3+O_2=OC_6H_4CH_3+O$	2.60×10^{13}	0	6100	11
70	$HOC_6H_4CH_3+H=C_6H_5CH_3+OH$	2.21×10^{13}	0	7910	11
71	$OC_6H_4CH_3+H=HOC_6H_4CH_3$	2.50×10^{14}	0	0	11
72	$HOC_6H_4CH_3+OH=OC_6H_4CH_3+H2O$	6.00×10^{12}	0	0	11
73	$C_5H_4O+O=C_4H_4+CO_2$	1.00×10^{13}	0	2000	11
74	$C_4H_5+O_2=C_4H_4+HO_2$	1.00×10^{08}	2	10000	11
75	$C_4H_4+OH=C_4H_3+H2O$	7.50×10^{06}	2	5000	11
76	$C_4H_4+O=C_3H_3+HCO$	8.10×10^{06}	1.9	180	11
77	$C_4H_3+O_2=C_2H_2+CO+HCO$	3.00×10^{12}	0	0	11
78	$C_7H_{15}\text{-}1+C_6H_5CH_3=C_6H_5CH_2+NC_7H_{16}$	1.00×10^{11}	0	12000	11
79	$C_7H_{15}\text{-}2+C_6H_5CH_3=C_6H_5CH_2+NC7H_{16}$	1.00×10^{11}	0	12000	11
80	$AC_8H_{17}+C_6H_5CH_3=C_6H_5CH_2+IC_8H_{18}$	1.00×10^{11}	0	12000	11
81	$IC_8H_{18}+C_7H_{15}\text{-}1=NC_7H_{16}+AC_8H_{17}$	9.00×10^{11}	0	13500	11
82	$IC_8H_{18}+C_7H_{15}\text{-}2=NC_7H_{16}+AC_8H_{17}$	9.00×10^{11}	0	14500	11
83	$C_3H_6+H=C_2H_4+CH_3$	7.20×10^{12}	0	1300	11
84	$C_3H_6+O=C_3H_5+OH$	5.20×10^{11}	0.7	5884	11
85	$C_3H_6+OH=C_3H_5+H_2O$	3.10×10^{06}	2	1451	11
86	$C_3H_6+OH=C_2H_5+CH_2O$	7.90×10^{12}	0	0	11
87	$C_3H_6+O_2=C_3H_5+HO_2$	2.00×10^{13}	0	47600	11
88	$C_3H_5+O_2=CH_2CHO+CH_2O$	1.10×10^{10}	0.3	12840	11
89	$C_3H_5+O_2=C_3H_4+HO_2$	5.00×10^{15}	-1.4	22430	11
90	$C_3H_5+OH=C_3H_4+H_2O$	2.00×10^{13}	0	0	11

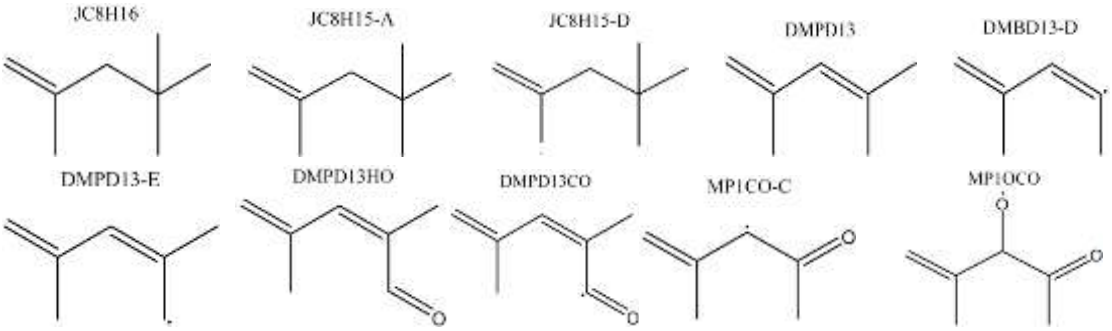
91	$C_3H_4+OH=C_2H_3+CH_2O$	1.00×10^{12}	0	0	11
92	$C_3H_4+OH=C_2H_4+HCO$	1.00×10^{12}	0	0	11
93	$C_2H_5+O=CH_3CHO+H$	5.30×10^{13}	0	0	11
94	$C_2H_5+OH=C_2H_4+H_2O$	2.40×10^{13}	0	0	11
95	$C_2H_5+O_2=C_2H_4+HO_2$	1.00×10^{10}	0	-2190	11
96	$C_2H_4+H=C_2H_3+H_2$	5.40×10^{14}	0	14900	11
97	$C_2H_4+H(+M)=C_2H_5(+M)$	1.10×10^{12}	0.5	1822	11
	Low pressure limit:	1.112×10^{03}	-5	4448	
	TROE centering:	5×10^{02}	95.00	2000	
	H_2O Enhanced by	5.00			
98	$C_2H_4+OH=C_2H_3+H_2O$	8.02×10^{13}	0	5955	11
99	$C_2H_3+O_2=CH_2O+HCO$	1.10×10^{23}	-3.3	3890	11
100	$C_2H_3+O_2=CH_2CHO+O$	2.50×10^{15}	-0.8	3135	11
101	$C_2H_2+O_2=HCCO+OH$	2.00×10^{08}	1.5	30100	11
102	$C_2H_2+OH=CH_3+CO$	2.00×10^{07}	2	3214.3	11
103	$C_2H_2+O=HCCO+H$	1.40×10^{07}	2	1900	11
104	$C_2H_2+O=CH_2+CO$	6.10×10^{06}	2	1900	11
105	$C_2H+O_2=CO+CO+H$	2.50×10^{13}	0	0	11
106	$HCCO+O_2=HCO+CO+O$	9.78×10^{11}	0	850	11
107	$HCCO+O_2=HCO+CO_2$	6.52×10^{11}	0	850	11
108	$HCCO+O_2=CO+CO+OH$	2.90×10^{07}	1.7	1000	11
109	$CH_3CHO+OH=CH_3CO+H_2O$	2.30×10^{10}	0.7	-1110	11
110	$CH_3CO(+M)=CH_3+CO(+M)$	2.80×10^{13}	0	17100	11
	Low pressure limit:	2.1×10^{15}	0	14000	
	TROE centering:	5×10^{02}	0	0.1E31	
	H_2 Enhanced by	2.00			
	CO Enhanced by	2.00			
	CO_2 Enhanced by	3.00			
	H_2O Enhanced by	5.00			
111	$CH_2CHO+O_2=CH_2O+CO+OH$	2.20×10^{11}	0	1500	11
112	$CH_2CO+OH=HCCO+H2O$	1.00×10^{07}	2	3000	11
113	$CH_3+O=CH_2O+H$	8.40×10^{13}	0	0	11
114	$CH_3+O_2=CH_2O+OH$	1.90×10^{12}	0	20315	11
115	$CH_3+HO_2=CH_3O+OH$	8.00×10^{12}	0	0	11
116	$CH_3+H(+M)=CH_4(+M)$	1.30×10^{16}	-0.6	383	11
	Low pressure limit:	1.75×10^{03}	-4.67	2440	
	TROE centering:	7.83×10^{02}	74	6964	
	H_2O Enhanced by	8.57			
	N_2 Enhanced by	1.43			
117	$CH_3+CH_2O=CH_4+HCO$	7.80×10^{-08}	6.1	1967	11
118	$CH_2O+H(+M)=CH_3O(+M)$	5.40×10^{11}	0.5	2600	11
	Low pressure limit:	1.54×10^{02}	-4.8	5560	
	TROE centering:	7.58×10^{02}	94	4200	

	N_2 Enhanced by	1.43			
	H_2O Enhanced by	8.58			
119	$CH_2O+OH=HCO+H_2O$	3.40×10^{09}	1.2	-447	11
120	$CH_2O+O_2+M=H+CO+M+HO_2$	6.20×10^{16}	0	36939.9	11
121	$CH_2O+HO_2=HCO+H_2O_2$	2.17×10^{11}	0	7987	11
122	$CH_2+OH=CH+H_2O$	1.13×10^{07}	2	3000	11
123	$CH_2+O_2=CO+H_2O$	2.20×10^{22}	-3.3	2867	11
124	$CH_2+H=CH+H_2$	1.00×10^{18}	-1.6	0	11
125	$CH_2+O2=CO+OH+H$	1.60×10^{21}	-3.3	2867	11
126	$CH_2+H_2=H+CH_3$	5.00×10^{05}	2	7230	11
127	$CH_2+CO_2=CH_2O+CO$	1.10×10^{12}	0	1000	11
128	$HCO+O_2=HO_2+CO$	7.60×10^{12}	0	406	11
129	$HCO+M=H+CO+M$	1.90×10^{17}	-1	17000	11
	H_2O Enhanced by	5.00			
130	$HCO+H=CO+H_2$	1.20×10^{13}	0.2	0	11
131	$HCO+OH=H_2O+CO$	1.00×10^{14}	0	0	11
132	$CO+HO_2=CO_2+OH$	1.51×10^{14}	0	23611.6	11
133	$CO+O=CO_2$	1.80×10^{10}	0	2434	11
134	$CO+O+M=CO_2+M$	5.89×10^{15}	0	4093.3	11
135	$CO+OH=CO_2+H$	3.09×10^{11}	0	733.8	11
136	$CO_2+O=CO+O_2$	2.75×10^{12}	0	43758.8	11
	Reverse Arrhenius coefficients	3.25×10^{11}	0	36610.4	
137	$CH_3OH+OH=CH_3O+H_2O$	1.00×10^{06}	2.1	496.7	11
	Reverse Arrhenius coefficients	8.98×10^{06}	2.1	17380	
138	$O+OH=O_2+H$	2.00×10^{14}	-0.4	0	11
139	$O+H_2=OH+H$	5.00×10^{04}	2.7	6290	11
140	$OH+H_2=H_2O+H$	2.10×10^{08}	1.5	3450	11
141	$2OH=O+H_2O$	4.30×10^{03}	2.7	-2486	11
142	$H+H+M=H_2+M$	1.00×10^{18}	-1	0	11
	H_2O Enhanced by	0.00			
143	$H+H+H_2O=H_2+H_2O$	6.00×10^{19}	-1.2	0	11
144	$H+O+M=OH+M$	6.20×10^{16}	-0.6	0	11
	H_2O Enhanced by	5.00			
145	$H+OH+M=H_2O+M$	1.60×10^{21}	-2	0	11
	H_2O Enhanced by	5.00			
146	$O+O+M=O_2+M$	1.90×10^{13}	0	-1788	11
	H_2O Enhanced by	5.00			
147	$H+O_2+M=HO_2+M$	2.10×10^{18}	-1	0	11
	H_2O Enhanced by	10.00			
	N_2 Enhanced by	0.00			
148	$H+O_2+N_2=HO_2+N_2$	6.70×10^{19}	-1.4	0	11
149	$H+HO_2=H_2+O_2$	4.30×10^{13}	0	1411	11
150	$H+HO_2=2OH$	1.70×10^{14}	0	874	11

151	$H+HO_2=O+H_2O$	3.00×10^{13}	0	1721	11
152	$O+HO_2=O_2+OH$	3.30×10^{13}	0	0	11
153	$OH+HO_2=H_2O+O_2$	8.90×10^{16}	-1	0	11
154	$HO_2+HO_2=H_2O_2+O_2$	4.20×10^{14}	0	11982	11
	Declared duplicate reaction...				
155	$HO_2+HO_2=H_2O_2+O_2$	1.30×10^{11}	0	-1629	11
	Declared duplicate reaction...				
156	$H_2O_2+M=OH+OH+M$	1.80×10^{17}	0	45500	11
	H_2O Enhanced by	5.00			
157	$H_2O_2+H=HO_2+H_2$	1.70×10^{12}	0	3755	11
158	$H_2O_2+H=OH+H_2O$	1.00×10^{13}	0	3576	11
159	$H_2O_2+O=OH+HO_2$	6.60×10^{11}	0	3974	11
160	$H_2O_2+OH=H_2O+HO_2$	7.80×10^{12}	0	1330	11
	Declared duplicate reaction...				
161	$H_2O_2+OH=H_2O+HO_2$	5.80×10^{14}	0	9560	11
	Declared duplicate reaction...				
162	$JC_8H_{16}=TC_4H_9+IC_4H_7$	9.18×10^{72}	-16.4	99576	24
163	$JC_8H_{16}+OH=JC_8H_{15}\text{-}A+H_2O$	2.63×10^{07}	1.8	278.2	24
164	$JC_8H_{16}+OH=JC_8H_{15}\text{-}B+H_2O$	3.17×10^{06}	2	-1434	24
165	$JC_8H_{16}+O2=JC_8H1_5\text{-}B+HO_2$	6.20×10^{08}	1.3	38339	24
166	$JC_8H_{16}+HO_2=JC_8H_{15}\text{-}B+H_2O_2$	6.80×10^{03}	2.5	10113.8	24
167	$JC_8H_{16}+OH=JC_8H_{15}\text{-}D+H_2O$	3.00×10^{06}	2	-239	24
168	$JC_8H_{15}\text{-}A=JC_8H_{15}\text{-}D$	1.10×10^{13}	-0.6	7500	24
169	$IC_4H_8+IC_4H_7=JC_8H_{15}\text{-}A$	2.92×10^{03}	2.4	11860	24
170	$DMPD13+CH_3=JC_8H_{15}\text{-}B$	2.92×10^{03}	2.4	8360	24
171	$DMPD13+OH=DMPD13+H_2O$	6.00×10^{06}	2	-239	24
172	$DMPD13+HO_2=DMPD13O+OH$	7.00×10^{12}	0	-1000	24
173	$DMPD13O=DMPD13HO+H$	4.63×10^{15}	-0.8	21016.4	24
174	$DMPD13HO+OH=DMPD13CO+H_2O$	2.69×10^{10}	0.8	-340	24
175	$DMBD13\text{-}D+CO=DMPD13CO$	1.51×10^{11}	0	4810	24
176	$DMBD13\text{-}D+O_2=MP1CO\text{-}C+O$	3.81×10^{17}	-1.4	5580	24
177	$MP1CO\text{-}C+HO_2=MP1OCO+OH$	7.00×10^{12}	0	-1000	24
178	$DMBD13\text{-}D+O_2=IC_3H_5CHO+CH_3CO$	3.71×10^{25}	-4	7043	24
179	$IC_3H_5CHO+CH_3CO=MP1OCO$	1.00×10^{11}	0	9200	24
180	$C(CO)_2+C_3H_5\text{-}T=MP1OCO$	1.00×10^{11}	0	9200	24
181	$C(CO)_2+OH=C(CO)_2\text{-}A+H_2O$	2.69×10^{10}	0.8	-340	24
182	$CO+CH_3CO=C(CO)_2\text{-}A$	1.51×10^{11}	0	4810	24
183	$TC_4H_9=H+IC_4H_8$	4.65×10^{46}	-9.8	55080	24
	Reverse Arrhenius coefficients	5.89×10^{44}	-9.4	16980	
184	$IC_4H_8+OH=IC_4H_7+H_2O$	5.20×10^{06}	2	-298	24
	Reverse Arrhenius coefficients	5.16×10^{06}	1.9	29880	
185	$IC_4H_8+O=CH_2CO+CH_3+CH_3$	3.33×10^{07}	1.8	76	24
186	$IC_4H_8=IC_4H_7+H$	3.07×10^{55}	-11.5	114300	24

	Reverse Arrhenius coefficients	7.17×10^{54}	-11.7	26010	
187	$IC_4H_7+HO_2=IC_4H_7O+OH$	7.00×10^{12}	0	-1000	24
	Reverse Arrhenius coefficients	3.42×10^{12}	0.1	11230	
188	$IC_4H_7O=IC_4H_6OH$	1.39×10^{11}	0	15600	24
	Reverse Arrhenius coefficients	4.23×10^{11}	-0.2	31670	
189	$IC_4H_7O=IC_3H_5CHO+H$	5.00×10^{13}	0	29100	24
	Reverse Arrhenius coefficients	6.67×10^{13}	-0.1	18410	
190	$IC_3H_5CHO+OH=IC_3H_5CO+H_2O$	2.69×10^{10}	0.8	-340	24
	Reverse Arrhenius coefficients	4.40×10^{10}	0.8	36080	
191	$IC_3H_5CHO+O=IC_3H_5CO+OH$	7.18×10^{12}	0	1389	24
	Reverse Arrhenius coefficients	1.19×10^{12}	0	20560	
192	$IC_3H_5CO=C_3H_5\text{-}T+CO$	1.28×10^{20}	-1.9	34460	24
	Reverse Arrhenius coefficients	1.51×10^{11}	0	4809	
193	$C_3H_5\text{-}T+O_2=CH_3COCH_2+O$	3.81×10^{17}	-1.4	5580	24
	Reverse Arrhenius coefficients	2.00×10^{11}	0	17500	
194	$C_3H_5\text{-}T+O_2=CH_2O+CH_3CO$	3.71×10^{25}	-4	7043	24
	Reverse Arrhenius coefficients	1.87×10^{27}	-4.4	101200	
195	$CH_3COCH_2=CH_2CO+CH_3$	1.00×10^{14}	0	31000	24
	Reverse Arrhenius coefficients	1.00×10^{11}	0	6000	
196	$IC_4H_6OH+HO_2=CH_2CCH_2OH+CH_2O+OH$	1.45×10^{13}	0	0	24
197	$CH_2CCH_2OH+O_2=CH_2OH+CO+CH_2O$	4.34×10^{12}	0	0	24
198	$CH_2CO+OH=CH_2OH+CO$	3.73×10^{12}	0	-1013	24
	Reverse Arrhenius coefficients	9.43×10^{06}	1.7	27490	
199	$CH_2OH+O_2=CH_2O+HO_2$	3.81×10^{06}	2	1641	24
	Reverse Arrhenius coefficients	1.77×10^{11}	0.7	24180	

Appendix B Species glossary for di-isobutylene mechanism (see notes on naming conventions below)



Appendix C Reactions in figure

Reactions in Fig.1	
JC_8H_{16}	R3596:$JC_8H_{16}=TC_4H_9+IC_4H_7$, R3606:$JC_8H_{16}+OH=JC_8H_{15}\text{-}A+H_2O$ R3607:$JC_8H_{16}+OH=JC_8H_{15}\text{-}B+H_2O$, R3608:$JC_8H16+OH=JC_8H_{15}\text{-}D+H_2O$
JC_8H_{15}-A	R3641:$JC_8H_{16}+C_2H_5=JC_8H_{15}\text{-}A+C_2H_6$, R3648:$IC_4H_8+IC_4H_7=JC_8H_{15}\text{-}A$
JC_8H_{15}-B	R3649:$DMPD13+CH_3=JC_8H_{15}\text{-}B$, R3654:$JC_8H_{15}\text{-}B+HO_2=JC_8H_{15}O\text{-}B+OH$

	R3655:JC_8H_{15}-B+HO_2=$IC_8H_{15}O$-D+OH
JC_8H_{15}-D	R3633:JC_8H_{16}+CH_3O=JC_8H_{15}-D+CH_3OH,R3650:$NEOC_5H_{11}$+C_3H_4-A=JC_8H_{15}-D R3652:JC_8H_{15}-A=JC_8H_{15}-D, R3656:JC_8H_{15}-D+HO_2=$JC_8H_{15}O$-D+OH
DMPD13	R3665:DMPD13+H=YC_7H_{13}-Y2, R3669:DMPD13+OH=DMPD13-E+H_2O R3670:DMPD13+H=DMPD13-B+H
DMPD13-E	R3675:DMPD13+CH_3=DMPD13-E+CH_4,R3679:MPT124+CH_3=DMPD13-E R3722:DMPD13-E+HO_2=DMPD13O+OH, R3724:DMPD13-E+O=DMPD13HO+H
DMPD13O	R3733:DMPD13O=DMPD13HO+H, R3734:DMPD13O+O2=DMPD13HO+HO_2
DMPD13HO	R3736:DMPD13O+CH_3=DMPD13HO+CH_4, R3740:DMPD13HO+OH=DMPD13CO+H_2O R3741:DMPD13HO+HO_2=DMPD13CO+H_2O_2
DMPD13CO	R3746:DMBD13-D+CO=DMPD13CO
Reactions in Fig.2	
DMBD13-D	R3747:DMBD13-D=C_3H_5-T+C_3H_4-P, R3771:DMBD13-D+O2=IC_3H_5CHO+CH_3CO R3772:DMBD13-D+O_2=MPT124+HO_2, R3773:DMBD13-D+O_2=MP1CO-C+O
MP1CO-C	R3774:MP1CO-C+HO_2=MP1OCO+OH
MP1OCO	R3775:IC_3H_5CHO+CH_3CO=MP1OCO, R3776:$C(CO)_2$+C_3H_5-T=MP1OCO
IC_3H_5CHO	R190:IC_3H_5CHO+OH=IC_3H_5CO+H_2O, R191:IC_3H_5CHO+HO_2=IC_3H_5CO+H_2O_2 R192:IC_3H_5CHO+CH_3=IC_3H_5CO+CH_4, R193:IC_3H_5CHO+O=IC_3H_5CO+OH
IC_3H_5CO	R196:IC_3H_5CO=C_3H_5-T+CO, R1806:$IC_3H_5COC_2H_4$=C_2H_4+IC_3H_5CO
C_3H_5-T	R1423:C_3H_5-T+O_2=CH_3COCH_2+O, R1435:C_3H_5-T=C_3H_4-A+H R1449:C_3H_5-T=C_3H_4-P+H
CH_3COCH_2	R396:CH_3COCH_2=CH_2CO+CH_3, R397:CH_3COCH_3+O_2=CH_3COCH_2+HO_2 R398:CH_3COCH_3+HO_2=CH_3COCH_2+H_2O_2
Reactions in Fig.3	
TC_4H_9	R342:TC_4H_9=H+IC_4H_8, R1467:TC_4H_9+HO_2=TC_4H_9O+OH R359:IC_4H_{10}+HO_2=TC_4H_9+H_2O_2, R1468:CH_3O_2+TC_4H_9=CH_3O+TC_4H_9O
IC_4H_8	R154:IC_4H_8+O=IC_3H_6CO+H+H, R163:IC_4H_8+OH=IC_4H_7+H_2O R164:IC_4H_8+O=IC_3H_7+HCO
IC_4H_7	R172:CH_3O_2+IC_4H_7=CH_3O+IC_4H_7O, R173:IC_4H_7+HO_2=IC_4H_7O+OH R206:IC_4H_7OH=IC_4H_7+OH
IC_4H_7O	R175:IC_4H_7O=IC_4H_6OH, R176:IC_4H_7O=IC_3H_5CHO+H R184:IC_4H_7O+O_2=IC_3H_5CHO+HO_2
IC_4H_6OH	R178:IC_4H_6OH+HO_2=IC_4H_7OH+O_2, R179:IC_4H_6OH+CH_2O=IC_4H_7OH+HCO R180:IC_4H_6OH+IC_4H_8=IC_4H_7OH+IC_4H_7,R233:IC_4H_6OH+HO_2=CH_2CCH_2OH+CH_2O+OH
CH_2CCH_2OH	R236:C_3H_5OH+OH=CH_2CCH_2OH+H_2O, R237:C_3H_5OH+H=CH_2CCH_2OH+H_2 R242:CH_2CCH_2OH+O_2=CH_2OH+CO+CH_2O
IC_4H_7OH	R177:IC_4H_6OH+H_2=IC_4H_7OH+H, R178:IC_4H_6OH+HO_2=IC_4H_7OH+O_2 R3518:IC_4H_6OH+H_2O=IC_4H_7OH+OH
C_2H_3	R456:C_2H_4+H=C_2H_3+H_2, R460:C_2H_4+OH=C_2H_3+H_2O R468:C_2H_3+O_2=CH_2O+HCO, R469:C_2H_3+O_2=CH_2CHO+O
Reactions in Fig.5	

CH_3CO	R136:$CH_3CO(+M)=CH_3+CO(+M)$, R138:$CH_3CHO+O_2=CH_3CO+HO_2$ R1532:$C_3H_5\text{-}T+O_{2=}CH_2O+CH_3CO$
CH_2OH	R83:$CH_2OH+O_2=CH_2O+HO_2$, R84:$CH_2OH(+M)=CH_2O+H(+M)$
CH_2CO	R90:$CH_2CO+O=CH_2+CO_2$,R93:$CH_2CO+O=HCCO+OH$ R95:$CH_2CO+H=HCCO+H_2$, R1529:$CH_2CO+OH=CH_2OH+CO$
CH_3	R16:$CH_3OH(+M)=CH_3+OH(+M)$, R24:$CH_3+CH_3(+M)=C_2H_6(+M)$ R36:$CH_3+O=CH_2O+H$, R_4:$CH3+HO_2=CH_4+O_2$