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正癸烷着火及燃烧的化学动力学模型

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Chemical Kinetic Model for Auto-Ignition and Combustion of *n*-Decane

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表 S1　正癸烷着火及燃烧反应机理

Table S1　Reaction mechanism for ignition and combustion of n-decane

No.	Reactions	*A*	*b*	*E*	Ref.
1.	$H+O_2=OH+O$	9.76×10^{13}	0.0	14842.3	18,19
2.	$O+H_2=OH+H$	5.12×10^{04}	2.7	6285.9	18,19
3.	$OH+H_2=H_2O+H$	1.02×10^{08}	1.6	3298.3	18,19
4.	$2OH=H_2O+O$	1.51×10^{09}	1.1	100.4	18,19
5.	$H+O_2+M=HO_2+M$	3.535×10^{18}	-0.8	0.0	18,19
		1.04×10^{18}	-0.8	0.0	This work
6.	$HO_2+H=2OH$	1.69×10^{14}	0.0	874.8	18,19
7.	$HO_2+H=H_2+O_2$	4.28×10^{13}	0.0	1410.1	18,19
8.	$HO_2+OH=H_2O+O_2$	2.89×10^{13}	0.0	-501.9	18,19
9.	$HO_2+H=H_2O+O$	3.01×10^{13}	0.0	1720.8	18,19
10.	$HO_2+O=OH+O_2$	3.19×10^{13}	0.0	0.0	18,19
11.	$2HO_2=H_2O_2+O_2$	5.20×10^{12}	0.0	1539.2	18,19
12.	$H_2O_2+H=H_2O+OH$	1.02×10^{13}	0.0	3585.1	18,19
13.	$H_2O_2+H=HO_2+H_2$	1.69×10^{12}	0.0	3752.4	18,19
14.	$H_2O_2+O=OH+HO_2$	6.62×10^{11}	0.0	3967.5	18,19
15.	$H_2O_2+OH=H_2O+HO_2$	3.94×10^{12}	0.0	1331.3	18,19
16.	$H_2O_2(+M)=2OH(+M)$	2.49×10^{20}	-1.7	52376.8	18,19
17.	$2H+M=H_2+M$	1.86×10^{18}	-1.0	0.0	18,19
18.	$H+OH+M=H_2O+M$	2.21×10^{22}	-2.0	0.0	18,19
19.	$2O+M=O_2+M$	2.86×10^{17}	-1.0	0.0	18,19
20.	$CO+OH=CO_2+H$	8.97×10^{06}	1.5	-740.9	18,19
21.	$CO+HO_2=CO_2+OH$	1.51×10^{14}	0.0	23637.7	18,19
22.	$CO+O(+M)=CO_2(+M)$	1.80×10^{10}	0.0	2380.5	18,19
23.	$CO+O_2=CO_2+O$	2.51×10^{12}	0.0	47801.2	18,19
24.	$HCO+M=CO+H+M$	7.00×10^{14}	0.0	16802.1	18,19
		7.35×10^{14}	0.0	16802.1	This work
25.	$HCO+H=CO+H_2$	9.03×10^{13}	0.0	0.0	18,19
26.	$HCO+O=CO+OH$	3.01×10^{13}	0.0	0.0	18,19
27.	$HCO+O=CO_2+H$	3.01×10^{13}	0.0	0.0	18,19
28.	$HCO+OH=CO+H_2O$	1.02×10^{15}	0.0	0.0	18,19
29.	$HCO+O_2=CO+HO_2$	3.01×10^{12}	0.0	0.0	18,19
30.	$2HCO=CH_2O+CO$	3.01×10^{13}	0.0	0.0	18,19
31.	$CH_2O+H\rightarrow HCO+H_2$	1.26×10^{08}	1.6	2165.4	18,19
32.	$CH_2O+OH\rightarrow HCO+H_2O$	3.43×10^{09}	1.2	-454.1	18,19
33.	$CH_2O+M\rightarrow HCO+H+M$	1.62×10^{36}	-5.5	96696.9	18,19
34.	$CH_2O+O_2=HCO+HO_2$	6.02×10^{13}	0.0	40631.0	18,19
35.	$2CH_3=C_2H_5+H$	5.65×10^{13}	0.0	14675.0	18,19

		5.65×10^{11}	0.0	14675.0	This work
36.	$2CH_3\rightarrow C_2H_4+H_2$	1.00×10^{14}	0.0	32026.8	18,19
37.	$CH_3+O=CH_2O+H$	8.43×10^{13}	0.0	0.0	18,19
38.	$CH_3+OH=CH_2OH+H$	2.64×10^{19}	-1.8	8068.8	18,19
39.	$CH_3+OH=CH_3O+H$	5.74×10^{12}	-0.2	13929.2	18,19
40.	$CH_3+HO_2=CH_3O+OH$	3.78×10^{13}	0.0	0.0	18,19
41.	$CH_3+HO_2=CH_4+O_2$	1.00×10^{12}	0.0	0.0	18,19
42.	$CH_3+O_2=CH_2O+OH$	3.30×10^{11}	0.0	8938.8	18,19
43.	$CH_3+H(+M)=CH_4(+M)$	2.11×10^{14}	0.0	0.0	18,19
44.	$CH_3O+M\rightarrow CH_2O+H+M$	5.42×10^{13}	0.0	13503.8	18,19
45.	$CH_3O+H=CH_2O+H_2$	1.80×10^{13}	0.0	0.0	18,19
46.	$CH_3O+O_2=CH_2O+HO_2$	2.17×10^{10}	0.0	1744.7	18,19
47.	$CH_3O+O=CH_3+O_2$	1.50×10^{13}	0.0	0.0	18,19
48.	$CH_3O+O=CH_2O+OH$	1.40×10^{12}	0.0	0.0	18,19
49.	$CH_2OH+M\rightarrow CH_2O+H+M$	5.00×10^{13}	0.0	25095.6	18,19
50.	$CH_2OH+H\rightarrow CH_2O+H_2$	3.00×10^{13}	0.0	0.0	18,19
51.	$CH_2OH+O_2=CH_2O+HO_2$	1.00×10^{13}	0.0	7170.2	18,19
52.	$CH_4+H=CH_3+H_2$	1.30×10^{04}	3.0	8030.6	18,19
53.	$CH_4+O=CH_3+OH$	7.23×10^{08}	1.6	8484.7	18,19
54.	$CH_4+OH=CH_3+H_2O$	1.56×10^{07}	1.8	2772.5	18,19
55.	$CH_4+HO_2=CH_3+H_2O_2$	9.03×10^{12}	0.0	24639.1	18,19
56.	$OH+CH_3(+M)=CH_3OH(+M)$	6.02×10^{13}	0.0	0.0	18,19
57.	$CH_3OH+H=CH_2OH+H_2$	4.00×10^{13}	0.0	6094.6	18,19
58.	$CH_3OH+H=CH_3O+H_2$	4.00×10^{12}	0.0	6094.6	18,19
59.	$CH_3OH+O=CH_2OH+OH$	1.00×10^{13}	0.0	4684.5	18,19
60.	$CH_3OH+OH=CH_2OH+H_2O$	3.55×10^{04}	2.6	-884.3	18,19
61.	$CH_3OH+CH_3=CH_4+CH_2OH$	9.00×10^{12}	0.0	9823.1	18,19
62.	$CH_3OH+HO_2\rightarrow CH_2OH+H_2O_2$	6.20×10^{12}	0.0	19383.4	18,19
63.	$CH_2OH+H_2O_2\rightarrow CH_3OH+HO_2$	1.00×10^{07}	1.7	11448.4	18,19
64.	$HCCO+O\rightarrow 2CO+H$	1.00×10^{14}	0.0	0.0	18,19
65.	$HCCO+O_2=HCO+CO_2$	8.13×10^{11}	0.0	855.6	18,19
66.	$HCCO+O_2=2CO+OH$	8.13×10^{11}	0.0	855.6	18,19
67.	$C_2H_2+O_2=HCCO+OH$	2.00×10^{08}	1.5	30114.7	18,19
68.	$C_2H_2+O=HCCO+H$	5.06×10^{06}	2.1	1570.3	18,19
69.	$C_2H_3(+M)=C_2H_2+H(+M)$	2.00×10^{14}	0.0	39744.3	18,19
70.	$C_2H_3+H=C_2H_2+H_2$	1.20×10^{13}	0.0	0.0	18,19
71.	$C_2H_3+O=C_2H_2+OH$	1.00×10^{13}	0.0	0.0	18,19
72.	$C_2H_3+OH=C_2H_2+H_2O$	2.00×10^{13}	0.0	0.0	18,19
73.	$C_2H_3+O=CH_3+CO$	1.00×10^{13}	0.0	0.0	18,19
74.	$C_2H_3+O_2=CH_2O+HCO$	1.70×10^{29}	-5.3	6493.8	18,19

75.	$C_2H_3+O_2=CH_2CHO+O$	3.50×10^{14}	-0.6	5258.1	18,19
76.	$C_2H_3+O_2=C_2H_2+HO_2$	5.19×10^{15}	-1.3	3307.8	18,19
77.	$C_2H_3+O_2=C_2H_2+HO_2$	2.12×10^{-06}	6.0	9474.2	18,19
78.	$CH_3CHO+M\rightarrow CH_3+HCO+M$	7.00×10^{15}	0.0	81931.2	18,19
79.	$CH_3CHO+H=CH_2CHO+H_2$	2.00×10^{09}	1.2	2414.0	18,19
80.	$CH_3CHO+O=CH_2CHO+OH$	8.00×10^{11}	0.0	1816.4	18,19
81.	$C_2H_4+M=C_2H_2+H_2+M$	3.50×10^{16}	0.0	71462.7	18,19
82.	$C_2H_4+M\rightarrow C_2H_3+H+M$	7.30×10^{17}	0.0	96558.3	18,19
83.	$C_2H_4+H=C_2H_3+H_2$	5.40×10^{14}	0.0	14914.0	18,19
84.	$C_2H_4+OH=C_2H_3+H_2O$	3.00×10^{13}	0.0	3011.5	18,19
85.	$C_2H_4+O=CH_3+HCO$	1.36×10^{07}	1.9	178.8	18,19
86.	$C_2H_5(+M)\rightarrow C_2H_4+H(+M)$	8.20×10^{13}	0.0	39914.0	18,19
87.	$C_2H_4+H(+M)\rightarrow C_2H_5(+M)$	3.98×10^{09}	1.3	1290.6	18,19
88.	$C_2H_5+CH_3=C_2H_4+CH_4$	1.14×10^{12}	0.0	0.0	18,19
89.	$C_2H_5+O_2=C_2H_4+HO_2$	1.02×10^{10}	0.0	-2186.9	18,19
90.	$C_2H_5+O=CH_2O+CH_3$	6.62×10^{13}	0.0	0.0	18,19
91.	$C_2H_2+HCCO=C_3H_3+CO$	1.00×10^{11}	0.0	2987.6	18,19
92.	$C_3H_3+O=C_2H_2+CO+H$	1.40×10^{14}	0.0	0.0	18,19
93.	$C_3H_3+O=C_2H_3+CO$	3.80×10^{13}	0.0	0.0	18,19
94.	$C_3H_4+M\rightarrow C_3H_3+H+M$	2.00×10^{18}	0.0	79923.5	18,19
95.	$C_3H_4+H=C_3H_3+H_2$	2.00×10^{07}	2.0	4995.2	18,19
96.	$C_3H_4+CH_3=C_3H_3+CH_4$	2.00×10^{11}	0.0	7696.0	18,19
97.	$C_3H_4+OH=C_3H_3+H_2O$	2.00×10^{07}	2.0	999.0	18,19
98.	$C_3H_4+H=C_3H_5$	2.00×10^{12}	0.0	2700.8	18,19
99.	$C_3H_5+H=C_3H_4+H_2$	3.33×10^{12}	0.0	0.0	18,19
100.	$C_3H_5+O_2=C_3H_4+HO_2$	6.00×10^{11}	0.0	10014.3	18,19
101.	$C_3H_6\rightarrow C_2H_3+CH_3$	3.15×10^{15}	0.0	85803.1	18,19
102.	$C_3H_6+H=C_3H_5+H_2$	5.00×10^{12}	0.0	1505.7	18,19
103.	$C_3H_6+OH=C_3H_5+H_2O$	4.00×10^{12}	0.0	0.0	18,19
104.	$C_3H_6+CH_3=C_3H_5+CH_4$	8.96×10^{12}	0.0	8508.6	18,19
105.	$C_3H_6+O=C_2H_4+CH_2O$	5.90×10^{13}	0.0	5019.1	18,19
106.	$C_3H_6+O=C_2H_5+HCO$	3.60×10^{12}	0.0	0.0	18,19
107.	$C_3H_6+OH=C_2H_5+CH_2O$	7.90×10^{12}	0.0	0.0	18,19
108.	$n\text{-}C_3H_7=CH_3+C_2H_4$	9.60×10^{13}	0.0	31022.9	18,19
109.	$n\text{-}C_3H_7=H+C_3H_6$	1.25×10^{14}	0.0	37022.0	18,19
110.	$n\text{-}C_3H_7+O_2=C_3H_6+HO_2$	1.00×10^{12}	0.0	4995.2	18,19
111.	$i\text{-}C_3H_7=C_3H_6+H$	6.30×10^{13}	0.0	36926.4	18,19
112.	$i\text{-}C_3H_7=C_2H_4+CH_3$	2.00×10^{10}	0.0	29517.2	18,19
113.	$i\text{-}C_3H_7+O_2=C_3H_6+HO_2$	1.00×10^{12}	0.0	4995.2	18,19
114.	$C_3H_5+CH_3=p\text{-}C_4H_8$	1.00×10^{13}	0.0	0.0	18,19

115.	p-$C_4H_8 \rightarrow C_2H_3+C_2H_5$	2.00×10^{18}	-1.0	96845.1	18,19
116.	p-$C_4H_8+O=CH_3CHO+C_2H_4$	2.50×10^{12}	0.0	0.0	18,19
117.	p-$C_4H_8+O=CH_3+C_2H_5+CO$	1.62×10^{13}	0.0	860.4	18,19
118.	p-$C_4H_8+O=C_3H_6+CH_2O$	7.23×10^{05}	2.3	-1051.6	18,19
119.	p-$C_4H_8+OH=CH_3CHO+C_2H_5$	1.00×10^{11}	0.0	0.0	18,19
120.	p-$C_4H_8+OH=n$-$C_3H_7+CH_2O$	6.50×10^{12}	0.0	0.0	18,19
121.	p-$C_4H_9=C_2H_5+C_2H_4$	2.50×10^{13}	0.0	28824.1	18,19
122.	p-$C_4H_9=p$-C_4H_8+H	1.26×10^{13}	0.0	38623.3	18,19
123.	p-$C_4H_9+O_2=p$-$C_4H_8+HO_2$	1.00×10^{12}	0.0	2007.7	18,19
124.	$C_5H_9 \rightarrow C_3H_5+C_2H_4$	2.50×10^{13}	0.0	30019.1	18,19
125.	$C_5H_9 \rightarrow C_2H_3+C_3H_6$	2.50×10^{13}	0.0	30019.1	18,19
126.	p-$C_5H_{10}=C_2H_5+C_3H_5$	3.16×10^{16}	0.0	80927.3	18,19
127.	p-$C_5H_{10}+H \rightarrow C_5H_9+H_2$	2.80×10^{13}	0.0	4015.3	18,19
128.	p-$C_5H_{10}+O \rightarrow C_5H_9+OH$	2.54×10^{05}	2.6	-1123.3	18,19
129.	p-$C_5H_{10}+OH \rightarrow C_5H_9+H_2O$	6.80×10^{13}	0.0	3059.3	18,19
130.	p-$C_5H_{10}+CH_3 \rightarrow C_5H_9+CH_4$	1.00×10^{11}	0.0	7313.6	18,19
131.	p-$C_6H_{13} \rightarrow p$-$C_4H_9+C_2H_4$	2.50×10^{13}	0.0	28776.3	18,19
132.	p-$C_7H_{14} \rightarrow p$-$C_4H_9+C_3H_5$	3.16×10^{16}	0.0	80927.3	18,19
133.	p-$C_7H_{14}+H \rightarrow 3C_2H_4+CH_3$	7.20×10^{12}	2.0	2896.8	18,19
134.	p-$C_7H_{14}+H \rightarrow C_3H_6+C_2H_5+C_2H_4$	7.20×10^{12}	1.3	1298.8	18,19
135.	p-$C_7H_{15}+O_2 \rightarrow p$-$C_7H_{14}+HO_2$	3.20×10^{12}	0.0	4995.2	18,19
136.	p-$C_7H_{15} \rightarrow p$-$C_5H_{10}+C_2H_5$	4.00×10^{13}	0.0	28776.3	18,19
137.	p-$C_7H_{15} \rightarrow p$-C_4H_8+n-C_3H_7	2.00×10^{13}	0.0	28776.3	18,19
138.	p-$C_7H_{15} \rightarrow p$-$C_4H_9+C_3H_6$	2.00×10^{13}	0.0	28776.3	18,19
139.	2-$C_{10}H_{21} \rightarrow p$-$C_7H_{15}+C_3H_6$	1.50×10^{13}	0.0	28274.4	18,19
140.	3-$C_{10}H_{21} \rightarrow p$-$C_6H_{13}+p$-$C_4H_8$	1.50×10^{13}	0.0	28274.4	18,19
141.	n-$C_{10}H_{22} \rightarrow p$-$C_4H_9+p$-$C_6H_{13}$	5.10×10^{16}	0.0	84335.6	18,19
142.	n-$C_{10}H_{22} \rightarrow n$-$C_3H_7+p$-$C_7H_{15}$	5.10×10^{16}	0.0	84335.6	18,19
143.	n-$C_{10}H_{22}+O_2 \rightarrow$ 3-$C_{10}H_{21}+HO_2$	3.00×10^{14}	0.0	47562.1	18,19
144.	n-$C_{10}H_{22}+O_2 \rightarrow$ 2-$C_{10}H_{21}+HO_2$	3.00×10^{14}	0.0	47562.1	18,19
145.	n-$C_{10}H_{22}+OH \rightarrow$ 3-$C_{10}H_{21}+H_2O$	1.30×10^{07}	2.0	-764.8	18,19
146.	n-$C_{10}H_{22}+OH \rightarrow$ 2-$C_{10}H_{21}+H_2O$	1.30×10^{07}	2.0	-764.8	18,19
147.	n-$C_{10}H_{22}+HO_2 \rightarrow$ 3-$C_{10}H_{21}+H_2O_2$	4.00×10^{13}	0.0	17017.2	18,19
148.	n-$C_{10}H_{22}+HO_2 \rightarrow$ 2-$C_{10}H_{21}+H_2O_2$	4.00×10^{13}	0.0	17017.2	18,19
149.	n-$C_{10}H_{22}+CH_3 \rightarrow$ 3-$C_{10}H_{21}+CH_4$	1.00×10^{12}	0.0	9591.3	18,19
150.	n-$C_{10}H_{22}+CH_3 \rightarrow$ 2-$C_{10}H_{21}+CH_4$	1.00×10^{12}	0.0	9591.3	18,19
151.	n-$C_{10}H_{22}+H \rightarrow$ 3-$C_{10}H_{21}+H_2$	4.50×10^{07}	2.0	4995.2	18,19
152.	n-$C_{10}H_{22}+H \rightarrow$ 2-$C_{10}H_{21}+H_2$	4.50×10^{07}	2.0	4995.2	18,19
153.	n-$C_{10}H_{22}+O \rightarrow$ 3-$C_{10}H_{21}+OH$	3.25×10^{13}	0.0	5210.3	18,19
154.	n-$C_{10}H_{22}+O \rightarrow$ 2-$C_{10}H_{21}+OH$	3.25×10^{13}	0.0	5210.3	18,19
155.	2-$C_{10}H_{21} \rightarrow$ 3-$C_{10}H_{21}$	2.00×10^{11}	0.0	18116.6	18,19
156.	3-$C_{10}H_{21} \rightarrow$ 2-$C_{10}H_{21}$	2.00×10^{11}	0.0	18116.6	18,19
157.	2-$C_{10}H_{21}+O_2 \rightarrow C_{10}H_{21}O_2$	4.00×10^{12}	0.0	0.0	18,19

158.	$C_{10}H_{21}O_2 \rightarrow 2\text{-}C_{10}H_{21}+O_2$	3.75×10^{21}	-1.7	35659.7	18,19
159.	$3\text{-}C_{10}H_{21}+O_2 \rightarrow C_{10}H_{21}O_2$	4.00×10^{12}	0.0	0.0	18,19
160.	$C_{10}H_{21}O_2 \rightarrow 3\text{-}C_{10}H_{21}+O_2$	3.75×10^{21}	-1.7	35659.7	18,19
161.	$C_{10}H_{21}O_2 \rightarrow C_{10}H_{20}O_2H$	2.00×10^{11}	0.0	17017.2	18,19
162.	$C_{10}H_{20}O_2H \rightarrow C_{10}H_{21}O_2$	1.00×10^{11}	0.0	12500.0	18,19
163.	$C_{10}H_{20}O_2H = p\text{-}C_{10}H_{20}+HO_2$	8.50×10^{12}	0.0	25621.4	18,19
164.	$p\text{-}C_{10}H_{20} = p\text{-}C_7H_{15}+C_3H_5$	3.50×10^{16}	0.0	70936.9	18,19
165.	$C_{10}H_{20}O_2H+O_2 = O_2C_{10}H_{20}O_2H$	2.50×10^{11}	0.0	0.0	18,19
166.	$O_2C_{10}H_{20}O_2H = OC_{10}H_{19}O_2H+OH$	3.50×10^{13}	0.0	24976.1	18,19
167.	$OC_{10}H_{19}O_2H \rightarrow CH_2O+CO+3C_2H_4+C_2H_5+OH$	7.00×10^{15}	0.0	41945.5	18,19
		7.20×10^{14}	0.0	42065.0	This work

a) Rate constants are written as $AT^n\exp(-E/RT)$, A units mole-cm-sec-K, E units cal/mole