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异辛烷/正庚烷/乙醇三组分燃料着火的化学动力学模型

郑　东　　钟北京*

(清华大学航天航空学院, 北京 100084)

Chemical Kinetic Model for Ignition of Three-Component Fuel Comprising *iso*-Octane/*n*-Heptane/Ethanol

ZHENG Dong　　ZHONG Bei-Jing*

(*School of Aerospace, Tsinghua University, Beijing 100084, P. R. China*)

*Corresponding author. Email: zhongbj@tsinghua.edu.cn; Tel: +86-10-62772928.

Table S1 Reaction mechanism of three-component fuel Iso-octane/N-heptane/Ethanol

Reactions	Kinetic Parameters			reference
	A	*n*	*E*	
1. $iC_8H_{18}+H=C_8H_{17}+H_2$	4.38×10^{7}	2	7760	12
2. $iC_8H1_8+OH=C_8H1_7+H_2O$	3.47×10^{7}	1.8	278.2	12
3. $iC_8H1_8+HO_2=C_8H1_7+H_2O_2$	2.23×10^{14}	0	18950	12
4. $iC_8H1_8+O_2=C_8H1_7+HO_2$	2.22×10^{15}	0	42904	12
5. $C_8H1_7+O_2=C_8H1_7OO$	1.85×10^{11}	0	0	modified
6. $C_8H1_7OO+O_2=iC_8ket+OH$	8.70×10^{15}	0	21233	12
7. $iC_8ket=CH_2O+C_6H1_3CO+OH$	1.78×10^{14}	0	39100	12
8. $C_6H1_3CO=C_4H_9+C_2H_4+CO$	4.92×10^{16}	0	40200	12
9. $C_4H_9=C_3H_6+CH_3$	4.56×10^{13}	0	36900	12
10. $C_8H1_7=C_3H_7+C_2H_4+C_3H_6$	2.16×10^{16}	0	36600	12
11. $iC_8H1_8+C_7H1_5<=>NC_7H1_6+C_8H1_7$	5.01×10^{10}	0	11200	12
12. $NC_7H1_6+H=C_7H1_5+H_2$	4.38×10^{7}	2	4760	12
13. $NC_7H1_6+OH=C_7H1_5+H_2O$	1.36×10^{10}	1.3	690	12
14. $NC_7H1_6+HO_2=C_7H1_5+H_2O_2$	1.10×10^{14}	0	16950	12
15. $NC_7H1_6+O_2=C_7H1_5+HO_2$	5.00×10^{14}	0	37904	12
16. $C_7H1_5+O_2=C_7H1_5O_2$	2.34×10^{12}	0	0	12
17. $C_7H1_5O_2+O_2=C_7ket+OH$	3.02×10^{14}	0	18232.7	modified
18. $C_7ket=C_5H11CO+CH_2O+OH$	7.00×10^{14}	0	41100	modified
19. $C_5H11CO=C_2H_4+C_3H_7+CO$	9.84×10^{15}	0	40200	12
20. $C_7H1_5=C_2H_5+C_2H_4+C_3H_6$	8.41×10^{14}	0	34600	12
21. $C_3H_7=C_2H_4+CH_3$	9.60×10^{13}	0	30950	12
22. $C_3H_7=C_3H_6+H$	1.25×10^{14}	0	36900	12
23. $C_3H_6+CH_3=C_3H_5+CH_4$	9.00×10^{12}	0	8480	12
24. $C_3H_5+O_2=C_3H_4+HO_2$	6.00×10^{11}	0	10000	12
25. $C_3H_4+OH=C_2H_3+CH_2O$	1.00×10^{12}	0	0	12
26. $C_3H_4+OH=C_2H_4+HCO$	1.00×10^{12}	0	0	12
27. $CH_3+HO_2=CH_3O+OH$	5.00×10^{13}	0	0	12
28. $CH_3+OH=CH_2+H_2O$	7.50×10^{6}	2	5000	12
29. $CH_2+OH=CH_2O+H$	2.50×10^{13}	0	0	12
30. $CH_2+O_2=HCO+OH$	4.30×10^{10}	0	-500	12
31. $CH_2+O_2=CO_2+H_2$	6.90×10^{11}	0	500	12
32. $CH_2+O_2=CO+H_2O$	2.00×10^{10}	0	-1000	12
33. $CH_2+O_2=CH_2O+O$	5.00×10^{13}	0	9000	12
34. $CH_2+O_2=CO_2+H+H$	1.60×10^{12}	0	1000	12
35. $CH_2+O_2=CO+OH+H$	8.60×10^{10}	0	-500	12
36. $CH_3O+CO=CH_3+CO_2$	3.92×10^{13}	0	11800	12
37. $CO+OH=CO_2+H$	1.26×10^{7}	1.3	-758	12

38. $O+CO(+M)<=>CO_2(+M)$	1.80×10^{10}	0	2385	12
39. $O_2+CO<=>O+CO_2$	2.50×10^{12}	0	47800	12
40. $HO_2+CO<=>OH+CO_2$	4.76×10^{13}	0	23600	12
41. $O+OH=O_2+H$	4.00×10^{14}	-0.5	0	12
42. $H+HO_2=OH+OH$	1.70×10^{14}	0	875	12
43. $OH+OH=O+H_2O$	6.00×10^{8}	1.3	0	12
44. $H+O_2(+M)=HO_2(+M)$	1.48×10^{12}	0.6	0	12
45. $OH+OH(+M)=H_2O_2(+M)$	1.24×10^{14}	-0.4	0	12
46. $H_2O_2+H=HO_2+H_2$	1.98×10^{6}	2	2435	12
47. $H_2O_2+H=OH+H_2O$	3.07×10^{13}	0	4217	12
48. $H_2O_2+O=OH+HO_2$	9.55×10^{6}	2	3970	12
49. $H_2O_2+OH=H_2O+HO_2$	2.40×10^{0}	4	-2162	12
50. $H_2+OH=H_2O+H$	1.17×10^{9}	1.3	3626	12
51. $HO_2+HO_2=H_2O_2+O_2$	3.00×10^{12}	0	0	12
52. $CH_2O+OH=HCO+H_2O$	4.86×10^{10}	1.1	-76.5	modified
53. $CH_2O+HO_2=HCO+H_2O_2$	3.00×10^{12}	0	8000	12
54. $HCO+O_2=HO_2+CO$	3.30×10^{13}	-0.4	0	12
55. $HCO+M=H+CO+M$	1.59×10^{18}	0.9	56712.3	12
56. $CH_3+CH_3O=CH_4+CH_2O$	4.30×10^{13}	0	0	12
57. $C_2H_4+OH=CH_2O+CH_3$	1.20×10^{14}	0	960	12
58. $C_2H_4+OH=C_2H_3+H_2O$	8.02×10^{13}	0	5955	12
59. $C_2H_3+O_2=CH_2O+HCO$	4.00×10^{12}	0	-250	12
60. $C_2H_3+HCO=C_2H_4+CO$	6.03×10^{13}	0	0	12
61. $C_2H_5+O_2=C_2H_4+HO_2$	2.00×10^{10}	0	-2200	12
62. $CH_4+O_2=CH_3+HO_2$	7.90×10^{13}	0	56000	12
63. $OH+HO_2=H_2O+O_2$	7.50×10^{12}	0	0	12
64. $CH_3+O_2=CH_2O+OH$	3.80×10^{11}	0	9000	12
65. $CH_4+H=CH_3+H_2$	6.60×10^{8}	1.6	10840	12
66. $CH_4+OH=CH_3+H_2O$	1.60×10^{6}	2.1	2460	12
67. $CH_4+O=CH_3+OH$	1.02×10^{9}	1.5	8604	12
68. $CH_4+HO_2=CH_3+H_2O_2$	9.00×10^{11}	0	18700	12
69. $CH_4+CH_2=CH_3+CH_3$	4.00×10^{12}	0	-570	12
70. $C_3H_6=C_2H_3+CH_3$	3.15×10^{15}	0	85500	12
71. $CH_2+CH_2=C_2H_2+H_2$	1.20×10^{13}	0	800	12
72. $CH_2+CH_2=C_2H_2+H+H$	1.20×10^{14}	0	800	12
73. $C_2H_4+M=C_2H_2+H_2+M$	1.50×10^{15}	0	55800	12
74. $C_2H_2+O_2=HCO+HCO$	4.00×10^{12}	0	28000	12
75. $C_2H_2+O=CH_2+CO$	1.02×10^{7}	2	1900	12
76. $C_2H_2+H+M=C_2H_3+M$	5.54×10^{12}	0	2410	12
77. $C_2H_3+H=C_2H_2+H_2$	4.00×10^{13}	0	0	12

78. $C_2H_3+OH=C_2H_2+H_2O$	3.00×10^{13}	0	0	12
79. $C_2H_3+CH_2=C_2H_2+CH_3$	3.00×10^{13}	0	0	12
80. $C_2H_3+C_2H_3=C_2H_2+C_2H_4$	1.45×10^{13}	0	0	12
81. $C_2H_3+O=C_2H_2+OH$	1.00×10^{13}	0	0	12
82. $C_2H_2+OH=CH_3+CO$	4.83×10^{-4}	4	-2000	12
83. $C_2H_3=C_2H_2+H$	4.60×10^{40}	-8.8	46200	12
84. $C_3H_6+H=C_3H_5+H_2$	5.00×10^{12}	0	1500	12
85. $C_3H_6+O_2=C_3H_5+HO_2$	4.00×10^{12}	0	39900	12
86. $CH_2CHO+H=CH_3+HCO$	2.20×10^{13}	0	0	12
87. $CH_2O+O_2=HCO+HO_2$	6.20×10^{13}	0	39000	12
88. $CH_2O+O=HCO+OH$	4.10×10^{11}	0.6	2760	12
89. $CH_2O+H=HCO+H_2$	2.19×10^{8}	1.8	3000	12
90. $CH_2O+M=CO+H_2+M$	6.25×10^{15}	0	69540	12
91. $CH_2O+M=HCO+H+M$	3.30×10^{16}	0	81000	12
92. $HCO+OH=H_2O+CO$	1.00×10^{14}	0	0	12
93. $HCO+O=OH+CO$	3.00×10^{13}	0	0	12
94. $HCO+O=H+CO_2$	3.00×10^{13}	0	0	12
95. $HCO+HO_2=CO_2+OH+H$	3.00×10^{13}	0	0	12
96. $C_2H_6+CH_3=C_2H_5+CH_4$	1.51×10^{-7}	6	6047	12
Reverse Arrhenius coefficients:	9.65×10^{-10}	6.6	10220	12
97. $C_2H_6+H=C_2H_5+H_2$	5.37×10^{2}	3.5	5200	12
Reverse Arrhenius coefficients:	9.72×10^{2}	3.5	27320	12
98. $C_2H_6+OH=C_2H_5+H_2O$	5.12×10^{6}	2.1	855	12
Reverse Arrhenius coefficients:	1.01×10^{7}	2.1	22980	12
99. $C_2H_6+O=C_2H_5+OH$	1.13×10^{14}	0	7850	12
Reverse Arrhenius coefficients:	2.08×10^{13}	0	12720	12
100. $CH_3+CH_3(+M)=C_2H_6(+M)$	7.37×10^{16}	-1.2	635.8	12
101. $C_2H_6+O_2=C_2H_5+HO_2$	4.00×10^{13}	0	50900	12
Reverse Arrhenius coefficients:	3.00×10^{11}	0	0	12
102. $C_2H_6+HO_2=C_2H_5+H_2O_2$	1.70×10^{13}	0	20460	12
Reverse Arrhenius coefficients:	1.07×10^{11}	0.2	7842	12
103. $C_2H_6+C_2H_4=C_2H_5+C_2H_5$	5.00×10^{11}	0	60000	12
Reverse Arrhenius coefficients:	5.00×10^{11}	0	0	12
104. $C_2H_6+M=C_2H_5+H+M$	8.85×10^{20}	-1.2	102200	12
Reverse Arrhenius coefficients:	1.15×10^{13}	0.3	-1550	12
105. $C_2H_6+CH_2=C_2H_5+CH_3$	2.20×10^{13}	0	8670	12
Reverse Arrhenius coefficients:	2.66×10^{10}	0.6	17060	12
106. $C_2H_6+CH_3O_2=C_2H_5+CH_3O_2H$	1.70×10^{13}	0	20460	12
Reverse Arrhenius coefficients:	7.50×10^{11}	0	1280	12
107. $C_3H_6+C_2H_5=C_3H_5+C_2H_6$	1.00×10^{11}	0	9800	12

Reverse Arrhenius coefficients:	5.37×10^{5}	1.3	16440	12
108. $C_3H_5+C_2H_5=C_2H_6+C_3H_4$	4.00×10^{11}	0	0	12
Reverse Arrhenius coefficients:	1.80×10^{12}	0.1	40330	12
109. $C_2H_4+O=CH_2CHO+H$	3.39×10^{6}	1.9	179	12
110. $C_2H_3+O_2=CH_2CHO+O$	3.50×10^{14}	-0.6	5260	12
111. $CH_2CHO+O_2=CH_2O+CO+OH$	2.00×10^{13}	0	42000	12
112. $C_2H_2+OH=CH_2CO+H$	2.19×10^{-4}	4.5	-1000	12
113. $CH_2CO+H=CH_3+CO$	1.10×10^{13}	0	3400	12
114. $CH_2CO+O=CH_2+CO_2$	1.75×10^{12}	0	1350	12
115. $CH_2CO(+M)=CH_2+CO(+M)$	3.00×10^{14}	0	70980	12
116. $C_3H_6+O=CH_2CO+CH_3+H$	2.50×10^{7}	1.8	76	12
117. $CH_2CHO=CH_2CO+H$	3.09×10^{15}	-0.3	50820	12
118. $CH_3+O_2+M=CH_3O_2+M$	5.44×10^{25}	-3.3	0	12
119. $CH_3O_2+CH_3=CH_3O+CH_3O$	2.41×10^{12}	0	0	12
120. $CH_3O_2+O=CH_3O+O_2$	3.61×10^{13}	0	0	12
121. $CH_3O_2+H=CH_3O+OH$	9.64×10^{13}	0	0	12
122. $CH_3O+H=CH_3+OH$	1.00×10^{14}	0	0	12
123. $CH_3+O=CH_2O+H$	8.00×10^{13}	0	0	12
124. $CH_3+O_2=CH_3O+O$	2.00×10^{18}	-1.6	29210	12
Reverse Arrhenius coefficients:	3.58×10^{18}	-1.6	-1631	12
125. $CH_3+H(+M)=CH_4(+M)$	2.14×10^{15}	-0.4	0	12
126. $CH_3O_2H=CH_3O+OH$	6.31×10^{14}	0	42300	12
127. $CH_3O_2+CH_2O=CH_3O_2H+HCO$	1.99×10^{12}	0	11670	12
128. $C_2H_4+CH_3O_2=C_2H_3+CH_3O_2H$	1.13×10^{13}	0	30430	12
129. $CH_4+CH_3O_2=CH_3+CH_3O_2H$	1.81×10^{11}	0	18480	12
130. $CH_3O_2+HO_2=CH_3O_2H+O_2$	1.75×10^{10}	0	-3275	12
131. $C_2H_5OH(+M)=CH_3+CH_2OH(+M)$	5.94×10^{23}	-1.7	95163	21
132. $C_2H_5OH(+M)=C_2H_5+OH(+M)$	1.25×10^{23}	-1.5	96005	21
133. $C_2H_5OH(+M)=C_2H_4+H_2O(+M)$	9.00×10^{13}	0.1	66136	modified
134. $C_2H_5OH(+M)=CH_3HCO+H_2(+M)$	7.24×10^{11}	0.1	91007	21
135. $C_2H_5OH+OH=C_2H_4OH+H_2O$	1.74×10^{11}	0.3	600	21
136. $C_2H_5OH+OH=CH_3CHOH+H_2O$	4.64×10^{11}	0.1	0	21
137. $C_2H_5OH+OH=CH_3CH_2O+H_2O$	7.46×10^{11}	0.3	1634	21
138. $C_2H_5OH+H=C_2H_4OH+H_2$	1.23×10^{7}	1.8	5098	21
139. $C_2H_5OH+H=CH_3CHOH+H_2$	2.58×10^{7}	1.6	2827	21
140. $C_2H_5OH+H=CH_3CH_2O+H_2$	1.50×10^{7}	1.6	3038	21
141. $C_2H_5OH+O=C_2H_4OH+OH$	9.41×10^{7}	1.7	5459	21
142. $C_2H_5OH+O=CH_3CHOH+OH$	1.88×10^{7}	1.9	1824	21
143. $C_2H_5OH+O=CH_3CH_2O+OH$	1.58×10^{7}	2	4448	21
144. $C_2H_5OH+CH_3=C_2H_4OH+CH_4$	2.19×10^{2}	3.2	9622	21

145. $C_2H_5OH+CH_3=CH_3CHOH+CH_4$	6.28×10^{3}	3	7948	modified
146. $C_2H_5OH+CH_3=CH_3CH_2O+CH_4$	1.45×10^{2}	3	7649	21
147. $C_2H_5OH+HO_2=CH_3CHOH+H_2O_2$	6.50×10^{4}	2.5	10750	modified
148. $C_2H_5OH+HO_2=C_2H_4OH+H_2O_2$	1.23×10^{4}	2.5	15750	21
149. $C_2H_5OH+HO_2=CH_3CH_2O+H_2O_2$	2.50×10^{12}	0	24000	21
150. $C_2H_4+OH=C_2H_4OH$	1.29×10^{12}	0	-817	21
151. $C_2H_4OH+O_2=HOC_2H_4O_2$	1.00×10^{12}	0	-1100	21
152. $HOC_2H_4O_2=CH_2O+CH_2O+OH$	6.00×10^{10}	0	24500	21
153. $CH_3CHOH+O_2=CH_3HCO+HO_2$ DUP	4.82×10^{14}	0	5017	21
154. $CH_3CHOH+O_2=CH_3HCO+HO_2$ DUP	8.43×10^{15}	-1.2	0	21
155. $CH_3CHOH+CH_3=C_3H_6+H_2O$	1.00×10^{13}	0	0	21
156. $CH_3CHOH+O=CH_3HCO+OH$	1.00×10^{14}	0	0	21
157. $CH_3CHOH+H=C_2H_4+H_2O$	3.00×10^{13}	0	0	21
158. $CH_3CHOH+H=CH_3+CH_2OH$	3.00×10^{13}	0	0	21
159. $CH_3CHOH+HO_2=CH_3HCO+OH+OH$	4.00×10^{13}	0	0	21
160. $CH_3CHOH+OH=CH_3HCO+H_2O$	5.00×10^{12}	0	0	21
161. $CH_3CHOH+M=CH_3HCO+H+M$	1.00×10^{14}	0	25000	21
162. $CH_3CH_2O+M=CH_3HCO+H+M$	1.16×10^{35}	-5.9	25274	21
163. $CH_3CH_2O+M=CH_3+CH_2O+M$	1.35×10^{38}	-7	23800	21
164. $CH_3CH_2O+O_2=CH_3HCO+HO_2$	4.00×10^{10}	0	1100	21
165. $CH_3CH_2O+CO=C_2H_5+CO_2$	4.68×10^{2}	3.2	5380	21
166. $CH_3CH_2O+H=CH_3+CH_2OH$	3.00×10^{13}	0	0	21
167. $CH_3CH_2O+H=C_2H_4+H_2O$	3.00×10^{13}	0	0	21
168. $CH_3CH_2O+OH=CH_3HCO+H_2O$	1.00×10^{13}	0	0	21
169. $C_2H_5+HO_2=CH_3CH_2O+OH$	3.00×10^{13}	0	0	21
170. $CH_3HCO=CH_3+HCO$	7.10×10^{15}	0	81280	21
171. $CH_3HCO+H=CH_3CO+H_2$	4.10×10^{9}	1.2	2400	21
172. $CH_3HCO+O=CH_3CO+OH$	5.80×10^{12}	0	1800	21
173. $CH_3HCO+OH=CH_3CO+H_2O$	2.30×10^{10}	0.7	-1110	21
174. $CH_3HCO+O_2=CH_3CO+HO_2$	3.00×10^{13}	0	39000	21
175. $CH_3HCO+CH_3=CH_3CO+CH_4$	2.00×10^{-6}	5.6	2464	21
176. $CH_3HCO+OH=CH_2HCO+H_2O$	1.72×10^{5}	2.4	815	21
177. $CH_3HCO+O=CH_2HCO+OH$	3.72×10^{13}	-0.2	3556	21
178. $CH_3HCO+H=CH_2HCO+H_2$	1.85×10^{12}	0.4	5359	21
179. $CH_3HCO+HO_2=CH_2CHO+H_2O_2$	2.32×10^{11}	0.4	14864	21
180. $CH_3HCO+HO_2=CH_3CO+H_2O_2$	2.40×10^{19}	-2.2	14030	21
181. $CH_2HCO=CH_3+CO$	1.17×10^{43}	-9.8	43756	21
182. $CH_2HCO=CH_2CO+H$	1.81×10^{43}	-9.6	45868	21
183. $CH_3CO(+M)=CH_3+CO(+M)$	2.80×10^{13}	0	17100	21
184. $CH_3CO+H=CH_3+HCO$	2.10×10^{13}	0	0	21

185. $CH_3CO+H=CH_2CO+H_2$	1.20×10^{13}	0	0	21
186. $CH_3CO+O=CH_3+CO_2$	1.50×10^{14}	0	0	21
187. $CH_3CO+O=CH_2CO+OH$	4.00×10^{13}	0	0	21
188. $CH_2OH+O_2=CH_2O+HO_2$ DUP	1.60×10^{15}	-1	0	21
189. $CH_2OH+O_2=CH_2O+HO_2$ DUP	7.20×10^{13}	0	3577	21
190. $CH_2OH+H=CH_3+OH$	1.00×10^{14}	0	0	21
191. $CH_2OH+H=CH_2O+H_2$	2.00×10^{13}	0	0	21
192. $CH_2OH+O=CH_2O+OH$	1.00×10^{13}	0	0	21
193. $CH_2OH+OH=CH_2O+H_2O$	1.00×10^{13}	0	0	21

rate constant $k=AT^n\exp(-E/RT)$, unit of E in $cal\cdot mol^{-1}$