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适用于 HCCI 燃烧研究的甲苯参比燃料化学动力学简化模型

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Reduced Chemical Kinetic Model of Toluene Reference Fuels for HCCI Combustion

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Table S1 Reduced mechanism in CHEMKIN format

Species				
C_8H_{18}	C_8H_{17}	$C_8H_{17}OO$	$C_8H_{16}OOH$	$OOC_8H_{16}OOH$
$OC_8H_{15}OOH$	C_8H_{16}	$C_6H_{13}CO$	C_6H_{13}	C_7H_{16}
C_7H_{15}	$C_7H_{15}OO$	$C_7H_{14}OOH$	$OOC_7H_{14}OOH$	$OC_7H_{13}OOH$
C_7H_{14}	$C_5H_{11}CO$	C_5H_{11}	$C_6H_5CH_3$	$C_6H_5CH_2$
C_6H_5CHO	C_6H_5CO	$C_6H_5CH_2O$	$C_6H_5CH_2OH$	C_6H_6
C_6H_5	C_6H_5O	C_6H_5OH	$OC_6H_4CH_3$	$HOC_6H_4CH_3$
C_5H_6	C_5H_5	C_5H_5O	C_5H_4O	C_5H_4OH
$C_6H_5CH_2OO$	$1,3C_4H_6$	nC_4H_5	iC_4H_5	C_4H_4
C_4H_3	C_3H_3	C_2H_2	CH_2CO	CH_2OH
HCCOH	HCCO	C_3H_7	C_3H_6	C_3H_5
C_3H_4	C_2H_5	C_2H_4	C_2H_3	CH_4
CH_3	CH_2	CH_3O	CH_2O	CO_2
CO	HCO	H_2O_2	HO_2	H_2O
H	H_2	O	O_2	OH

No.	**Reactions**	**A**	**b**	**E**	**Ref.**
	***iso*-octane oxidation branch**				
1	$C_8H_{18}+O_2=C_8H_{17}+HO_2$	1.000E+16	0.0	46000.0	3
	Reverse Arrhenius coefficients:	1.000E+12	0.0	0.0	3
2	$C_8H_{18}+O_2=C_8H_{17}OO$	1.000E+12	0.0	0.0	3
	Reverse Arrhenius coefficients:	2.510E+13	0.0	27400.0	3
3	$C_8H_{17}OO=C_8H_{16}OOH$	1.510E+11	0.0	21800.0	14
	Reverse Arrhenius coefficients:	1.000E+11	0.0	11000.0	14
4	$C_8H_{16}OOH+O_2=OOC_8H_{16}OOH$	3.160E+11	0.0	0.0	3
	Reverse Arrhenius coefficients:	2.510E+13	0.0	27400.0	3
5	$OOC_8H_{16}OOH=>OC_8H_{15}OOH+OH$	8.910E+10	0.0	17000.0	3
6	$OC_8H_{15}OOH=>C_6H_{13}CO+CH_2O+OH$	3.980E+15	0.0	43000.0	14
7	$C_6H_{13}CO+O_2=>C_3H_6+C_3H_6+CO+HO_2$	3.160E+13	0.0	10000.0	14
8	$C_8H_{18}+OH=>C_8H_{17}+H_2O$	6.000E+13	0.0	3000.0	14
9	$C_8H_{17}+O_2=C_8H_{16}+HO_2$	3.160E+11	0.0	6000.0	3
	Reverse Arrhenius coefficients:	3.160E+11	0.0	19500.0	3
10	$C_8H_{16}+O_2=>C_6H_{13}+CH_2O+HCO$	3.160E+13	0.0	10000.0	14
11	$C_8H_{18}+HO_2=C_8H_{17}+H_2O_2$	1.000E+13	0.0	16950.0	14
12	$C_8H_{17}=>C_6H_{13}+C_2H_4$	3.617E+17	-1.27	29700.0	14
13	$C_6H_{13}=C_3H_7+C_3H_6$	7.204E+13	-0.03	27900.0	14
	***n*-heptane oxidation branch**				
14	$C_7H_{16}+O_2=C_7H_{15}+HO_2$	1.000E+16	0.0	46000.0	3
	Reverse Arrhenius coefficients:	1.000E+12	0.0	0.0	3
15	$C_7H_{15}+O_2=C_7H_{15}OO$	1.000E+12	0.0	0.0	3
	Reverse Arrhenius coefficients:	2.510E+13	0.0	27400.0	3
16	$C_7H_{15}OO=C_7H_{14}OOH$	1.150E+11	0.0	19000.0	3

Reverse Arrhenius coefficients:		1.000E+11	0.0	11000.0	3
17	$C_7H_{14}OOH+O_2=OOC_7H_{14}OOH$	3.160E+11	0.0	0.0	3
Reverse Arrhenius coefficients:		2.510E+13	0.0	27400.0	3
18	$OOC_7H_{14}OOH=>OC_7H_{13}OOH+OH$	8.910E+10	0.0	17000.0	3
19	$OC_7H_{13}OOH=>C_5H_{11}CO+CH_2O+OH$	3.980E+15	0.0	43000.0	14
20	$C_5H_{11}+O_2=>C_3H_6+C_2H_4+CO+HO_2$	3.160E+13	0.0	10000.0	14
21	$C_7H_{16}+OH=>C_7H_{15}+H_2O$	6.000E+14	0.0	3000.0	14
22	$C_7H_{15}+O_2=C_7H_{14}+HO_2$	3.160E+11	0.0	6000.0	14
Reverse Arrhenius coefficients:		3.160E+11	0.0	19500.0	14
23	$C_7H_{14}+O_2=>C_5H_{11}+CH_2O+HCO$	3.16E+13	0.0	10000.0	14
24	$C_7H_{16}+HO_2=C_7H_{15}+H_2O_2$	1.000E+13	0.0	16950.0	14
25	$C_7H_{15}=>C_5H_{11}+C_2H_4$	2.500E+13	0.0	28810.0	14
26	$C_5H_{11}=C_3H_7+C_2H_4$	1.138E+15	-0.42	27010.0	14
toluene oxidation branch					
27	$C_6H_5CH_3=C_6H_5CH_2+H$	2.090E+15	0.0	87510.0	17
28	$C_6H_5CH_3=C_6H_5+CH_3$	2.660E+16	0.0	97880.0	17
29	$C_6H_5CH_3+H=C_6H_5CH_2+H_2$	1.330E+15	0.0	14880.0	18
30	$C_6H_5CH_3+O_2=C_6H_5CH_2+HO_2$	2.180E+09	2.5	6045.0	19,modified
31	$C_6H_5CH_3+OH=C_6H_5CH_2+H2O$	8.900E-11	0.0	4690.0	20
32	$C_6H_5CH_3+O=C_6H_5CH_2+OH$	6.300E+11	0.0	0.0	10
33	$C_6H_5CH_3+HO_2=C_6H_5CH_2+H_2O_2$	1.300E+11	0.0	14070.0	10
34	$C_6H_5CH_3+CH_3=CH_4+C_6H_5CH_2$	3.160E+09	0.0	15000.0	This work
35	$C_6H_5CH_3+O=OC_6H_4CH_3+H$	1.630E+13	0.0	3418.0	4
36	$C_6H_5CH_3+H=C_6H_6+CH_3$	1.200E+13	0.0	5148.0	4
37	$C_6H_5CH_3+C_6H_5=C_6H_6+C_6H_5CH_2$	7.940E+13	0.0	11935.0	4
38	$C_6H_5CH_2+HO_2=C_6H_5CHO+H+OH$	3.670E+14	0.0	0.0	23
39	$C_6H_5CH_2+HO_2=C_6H_5+CH_2O+OH$	1.170E+14	0.0	0.0	23
40	$C_6H_5CH_2+O=C_6H_5CHO+H$	2.500E+14	0.0	0.0	4
41	$C_6H_5CH_2+O_2=C_6H_5O+CH_2O$	5.300E+13	-1.07	10840.0	12
42	$C_6H_5CH_2+O_2=C_6H_5CH_2O+CH_2O$	6.320E+12	0.0	42920.0	12
43	$C_6H_5CH_2+HO_2=C_6H_5CH_2O+OH$	1.600E+21	0.0	0.0	This work
44	$C_6H_5CH_2O=C_6H_5CHO+H$	2.000E+13	0.0	27500.0	10
45	$C_6H_5CH_2=C_6H_5+CH_2O$	2.000E+13	0.0	27500.0	10
46	$C_6H_5CH_2+O_2=C_6H_5+CH_2O+O$	6.320E+11	0.0	14500.0	10
47	$C_6H_5CH_2+O_2=C_6H_5CH_2OO$	4.600E+11	0.0	-380.0	10
Reverse Arrhenius coefficients:		4.380E+13	0.0	20217.0	10
48	$C_6H_5CH_2OO=C_6H_5CHO+OH$	3.000E+09	1.1	29500.0	10
49	$C_6H_5CH_2=C_4H_4+C_3H_3$	2.000E+14	0.0	83600.0	10
50	$C_6H_5CH_2=C_5H_5+C_2H_2$	6.000E+13	0.0	70000.0	10
51	$C_6H_5CH_2+O=C_6H_5+CH_2O$	8.000E+13	0.0	0.0	4
52	$C_6H_5CH_2+OH=C_6H_5CH_2OH$	6.000E+13	0.0	0.0	4
53	$C_6H_5CHO+O_2=C_6H_5CO+HO_2$	1.020E+13	0.0	38950.0	4
54	$C_6H_5CHO+OH=C_6H_5CO+H_2O$	1.710E+09	1.2	-447.0	4

55	$C_6H_5CHO+H=C_6H_5CO+H_2$	5.000E+13	0.0	4928.0	4
56	$C_6H_5CHO+H=C_6H_6+HCO$	1.200E+13	0.0	5148.0	4
57	$C_6H_5CHO+O=C_6H_5CO+OH$	9.040E+12	0.0	3080.0	4
58	$C_6H_5CH_2+C_6H_5CHO=C_6H_5CH_3+C_6H_5CO$	2.770E+03	2.8	5773.0	4
59	$CH_3+C_6H_5CHO=CH_4+C_6H_5CO$	2.770E+03	2.8	5773.0	4
60	$C_6H_5+C_6H_5CHO=C_6H_6+C_6H_5CO$	7.010E+11	0.0	4400.0	4
61	$C_6H_5CO=C_6H_5+CO$	3.980E+14	0.0	29400.0	4
62	$C_6H_5CH_2OH+O_2=C_6H_5CHO+HO_2+H$	2.000E+14	0.0	41400.0	4
63	$C_6H_5CH_2OH+OH=C_6H_5CHO+H_2O+H$	8.430E+14	0.0	2583.0	4
64	$C_6H_5CH_2OH+H=C_6H_5CHO+H_2+H$	8.000E+13	0.0	8235.0	4
65	$C_6H_5CH_2OH+H=C_6H_6+CH_2OH$	1.200E+13	0.0	5148.0	4
66	$C_6H_5CH_2OH+C_6H_5CH_2=C_6H_5CHO+C_6H_5CH_3+H$	2.110E+11	0.0	9500.0	4
67	$C_6H_5CH_2OH+C_6H_5=C_6H_5CHO+C_6H_6+H$	1.400E+12	0.0	4400.0	4
68	$OC_6H_4CH_3+H=HOC_6H_4CH_3$	2.500E+14	0.0	0.0	4
69	$OC_6H_4CH_3=C_6H_6+H+CO$	2.510E+11	0.0	43900.0	4
70	$HOC_6H_4CH_3+OH=OC_6H_4CH_3+H_2O$	6.000E+12	0.0	0.0	4
71	$HOC_6H_4CH_3+H=OC_6H_4CH_3+H_2$	1.150E+14	0.0	12400.0	4
72	$HOC_6H_4CH_3+H=C_6H_5CH_3+OH$	2.210E+13	0.0	7910.0	4
73	$HOC_6H_4CH_3+H=C_6H_5OH+CH_3$	1.200E+13	0.0	5148.0	4
74	$HOC_6H_4CH_3+C_6H_5CH_2=OC_6H_4CH_3+C_6H_5CH_3$	1.050E+11	0.0	9500.0	4
75	$C_6H_5+H=C_6H_6$	2.200E+14	0.0	0.0	9
76	$C_6H_6+O_2=C_6H_5+HO_2$	6.300E+13	0.0	60000.0	9
77	$C_6H_6+OH=C_6H_5+H_2O$	2.110E+13	0.0	4570.0	9
78	$C_6H_6+H=C_6H_5+H_2$	2.500E+14	0.0	16000.0	9
79	$C_6H_6+O=C_6H_5O+O$	2.780E+13	0.0	4910.0	9
80	$C_6H_5+O_2=C_6H_5O+O$	2.600E+13	0.0	6120.0	9
81	$C_6H_5O+H=C_6H_5OH$	2.500E+14	0.0	0.0	9
82	$C_6H_5OH+OH=C_6H_5O+H_2O$	6.000E+12	0.0	0.0	9
83	$C_6H_5OH+H=C_6H_6+OH$	2.210E+13	0.0	7910.0	9
84	$C_6H_5OH+H=C_6H_5O+H_2$	1.150E+14	0.0	12400.0	9
85	$C_6H_5OH+O=C_6H_5O+OH$	2.810E+13	0.0	7352.0	9
86	$C_6H_5OH+O_2=C_6H_5O+HO_2$	1.000E+13	0.0	38000.0	15
87	$C_6H_5OH+HO_2=C_6H_5O+H_2O_2$	1.000E+12	0.0	1000.0	15
88	$C_2H_3+C_6H_5OH=C_2H_4+C_6H_5O$	6.000E+12	0.0	0.0	9
89	$nC_4H_5+C_6H_5OH=1,3C_4H_6+C_6H_5O$	6.000E+12	0.0	0.0	9
90	$C_6H_5+C_6H_5OH=C_6H_5O+C_6H_6$	4.910E+12	0.0	4400.0	9
91	$C_6H_5OH+C_6H_5CH_2=C_6H_5O+C_6H_5CH_3$	1.050E+11	0.0	9500.0	9
92	$C_6H_5O=C_5H_5+CO$	7.400E+15	0.0	13900.0	This work
93	$C_5H_5+H=C_5H_6$	1.500E+14	0.0	0.0	15
94	$C_5H_6+O_2=C_5H_5+HO_2$	4.000E+13	0.0	37150.0	15
95	$C_5H_6+HO_2=C_5H_5+H_2O_2$	1.990E+12	0.0	11660.0	9
96	$C_5H_6+OH=C_5H_5+H_2O$	3.430E+09	1.2	-447.0	9
97	$C_5H_6+H=C_5H_5+H_2$	2.190E+08	1.8	3000.0	9

98	$C_5H_6+O=C_5H_5+OH$	1.810E+13	0.0	3080.0	9
99	$C_5H_6+C_2H_3=C_5H_5+C_2H_4$	6.000E+12	0.0	0.0	9
100	$C_5H_6+nC_4H_5=C_5H_5+1,3C_4H_6$	6.000E+12	0.0	0.0	9
101	$C_5H_6+C_6H_5O=C_5H_5+C_6H_5OH$	3.160E+11	0.0	8000.0	9
102	$C_3H_3+C_3H_3=C_6H_6$	7.500E+12	0.0	0.0	9
103	$C_4H_3+C_2H_3=C_6H_6$	2.870E+14	0.0	817.0	9
104	$C_6H_5=C_4H_3+C_2H_2$	1.580E+15	0.0	82000.0	9
105	$C_5H_5=C_2H_2+C_3H_3$	3.000E+15	0.0	71000.0	9
106	$C_5H_5+O=nC_4H_5+CO$	1.000E+14	0.0	0.0	9
107	$C_5H_5+HO_2=C_5H_5O+OH$	3.000E+13	0.0	0.0	9
108	$C_5H_5+OH=C_5H_4OH+H$	3.000E+13	0.0	0.0	9
109	$C_5H_5O=nC_4H_5+CO$	2.510E+11	0.0	43900.0	9
110	$C_4H_5=C_2H_3+C_2H_2$	3.980E+11	0.7	42260.0	9
111	$C_5H_4OH=C_5H_4O+H$	2.100E+13	0.0	48000.0	9
112	$C_5H_4O=CO+C_2H_2+C_2H_2$	1.000E+15	0.0	78000.0	9
113	$C_5H_5+O=C_5H_4O+H$	5.800E+13	0.0	0.0	15
114	$iC_4H_5=nC_4H_5$	2.000E+13	0.0	53500.0	9
115	$C_5H_6+iC_4H_5=C_5H_5+1,3C_4H_6$	6.000E+12	0.0	0.0	9
116	$iC_4H_5+C_6H_5CH_3=1,3C_4H_6+C_6H_5CH_2$	6.000E+12	0.0	0.0	9
117	$1,3C_4H_6+OH= nC_4H_5+H_2O$	2.000E+07	2.0	5000.0	9
118	$1,3C_4H_6+OH= iC_4H_5+H_2O$	2.000E+07	2.0	2000.0	9
119	$1,3C_4H_6+H= nC_4H_5+H_2$	3.000E+07	2.0	13000.0	9
120	$1,3C_4H_6+H= iC_4H_5+H_2$	3.000E+07	2.0	6000.0	9
121	$iC_4H_5+H=CH_3+C_3H_3$	1.000E+14	0.0	0.0	9
122	$nC_4H_5+H= iC_4H_5+H$	1.000E+14	0.0	0.0	9
123	$nC_4H_5+OH=C_4H_4+H_2O$	2.000E+07	2.0	1000.0	9
124	$nC_4H_5+H=C_4H_4+H_2$	3.000E+07	2.0	1000.0	9
125	$nC_4H_5+O_2=C_4H_4+HO_2$	1.000E+07	2.0	1000.0	9
transition reactions					
126	$CH_2+C_2H_2=C_3H_3+H$	1.200E+13	0.0	6600.0	9
127	$C_2H_2+OH=HCCOH+H$	5.040E+05	2.3	13500.0	9
128	$HCCOH+H=CH_2CO+H$	1.000E+13	0.0	0.0	9
129	$HCCO+C_2H_2=C_3H_3+CO$	1.000E+11	0.0	3000.0	9
130	$HCCO+O_2=HCO+CO+O$	9.780E+11	0.0	850.0	4
131	$HCCO+O_2=HCO+CO_2$	6.520E+11	0.0	850.0	4
132	$C_4H_4+OH=C_4H_3+H_2O$	7.500E+06	2.0	5000.0	9
133	$C_4H_4+H=C_4H_3+H_2$	2.000E+07	2.0	15000.0	9
134	$CH_2OH+H=CH_2O+H_2$	3.000E+13	0.0	0.0	16
135	$CH_2OH+H=CH_3+OH$	2.500E+17	-0.93	5126.8	16
136	$CH_2OH+OH=CH_2O+H_2O$	2.400E+13	0.0	0.0	16
137	$CH_2OH+O_2=CH_2O+HO_2$	5.000E+12	0.0	0.0	16
138	$CH_2CO+H=CH_3+CO$	1.500E+09	1.43	2688.81	16
139	$CH_2CO+O=HCCO+OH$	1.000E+13	0.0	2000.48	16

140	$CH_2CO+CH_3=C_2H_5+CO$	9.000E+10	0.0	0.0	16
141	$CH_3+C_2H_2=C_3H_4+H$	2.560E+09	1.1	13643.88	16
142	$C_3H_4+O=HCCO+CH_3$	7.300E+12	0.0	2250.0	16
143	$C_3H_3+HO_2=C_3H_4+O_2$	2.500E+12	0.0	0.0	16
144	$C_3H_4+OH=C_3H_3+H_2O$	5.300E+06	2.0	2000.0	16
145	$C_3H_3+O_2=CH_2CO+HCO$	3.000E+10	0.0	2868.07	16
146	$C_4H_3+H=C_2H_2+C_2H_2$	2.000E+11	0.0	0.0	16
cooxidation reaction					
147	$C_8H_{18}+C_7H_{15}=C_7H_{16}+C_8H_{17}$	9.000E+11	0.0	14500.0	10
148	$C_8H_{17}+C_6H_5CH_3=C_6H_5CH_2+C_8H_{18}$	1.000E+11	0.0	12000.0	10
149	$C_7H_{15}+C_6H_5CH_3=C_6H_5CH_2+C_7H_{16}$	1.000E+11	0.0	12000.0	10
150	$C_6H_5+C_8H_{18}=C_8H_{17}+C_6H_6$	9.000E+11	0.0	15500.0	10
151	$C_6H_5+C_7H_{16}=C_7H_{15}+C_6H_6$	2.000E+11	0.0	12500.0	10
little molecule branch					
152	$C_3H_7=C_2H_4+CH_3$	9.600E+13	0.0	35900.0	24
153	$C_3H_7=C_3H_6+H$	1.250E+14	0.0	36900.0	24
154	$C_3H_6+CH_3=C_3H_5+CH_4$	9.000E+12	0.0	8480.0	24
155	$C_3H_5+O_2=C_3H_4+HO_2$	6.000E+11	0.0	10000.0	24
156	$C_3H_4+OH=C_2H_3+CH_2O$	1.000E+12	0.0	0.0	24
157	$C_3H_4+OH=C_2H_4+HCO$	1.000E+12	0.0	0.0	24
158	$CH_3+HO_2=CH_3O+OH$	5.000E+13	0.0	0.0	24
159	$CH_3+OH=CH_2+H_2O$	7.500E+06	2.0	5000.0	24
160	$CH_2+OH=CH_2O+H$	2.500E+13	0.0	0.0	24
161	$CH_2+O_2=HCO+OH$	4.300E+10	0.0	-500.0	24
162	$CH_2+O_2=CO_2+H_2$	6.900E+11	0.0	500.0	24
163	$CH_2+O_2=CO+H_2O$	2.000E+10	0.0	-1000.0	24
164	$CH_2+O_2=CH_2O+O$	5.000E+13	0.0	9000.0	24
165	$CH_2+O_2=CO_2+H+H$	1.600E+12	0.0	1000.0	24
166	$CH_2+O_2=CO+OH+H$	8.600E+10	0.0	-500.0	24
167	$CO+OH=CO_2+H$	5.990E+07	1.3	5232.9	24
168	$OH+CH_3O=H_2O+CH_2O$	5.000E+12	0.0	0.0	24
169	$O+CH_3O=OH+CH_2O$	1.000E+13	0.0	0.0	24
170	$O+OH=O_2+H$	4.000E+14	-0.5	0.0	24
171	$H+HO_2=OH+OH$	1.700E+14	0.0	875.0	24
172	$OH+OH=O+H_2O$	6.000E+08	1.3	0.0	24
173	$H_2O_2+M=OH+OH+M$	1.200E+15	0.0	46000.0	24,modified
	H_2O/21.0/ CO_2/5.0/ H_2/3.3/ CO/2.0/				
174	$H+O_2+M=O+OH+M$	2.800E+18	-0.9	0.0	This work
175	$H+O_2+M=O+OH+M$	2.800E+18	-0.7		24
	H_2O/21.0/ CO_2/5.0/ H_2/3.3/ CO/2.0/				
176	$H_2+OH=H_2O+H$	1.170E+09	1.3	3626.0	24
177	$HO_2+HO_2=H_2O_2+O_2$	3.000E+12	0.0	0.0	24
178	$CH_2O+OH=HCO+H_2O$	5.560E+10	1.1	-76.5	24

179	$CH_2O+HO_2=HCO+H_2O_2$	3.000E+12	0.0	8000.0	24
180	$HCO+O_2=HO_2+CO$	3.300E+13	-0.4	0.0	24
181	HCO+M=H+CO+M	1.590E+18	0.9	56712.3	24
182	$CH_3+CH_3O=CH_4+CH_2O$	4.300E+14	0.0	0.0	24
183	$C_2H_4+OH=CH_2O+CH_3$	6.000E+13	0.0	960.0	24
184	$C_2H_4+OH=C_2H_3+H_2O$	8.020E+13	0.0	5955.0	24
185	$C_2H_3+O_2=CH_2O+HCO$	4.000E+12	0.0	-250.0	24
186	$C_2H_3+HCO=C_2H_4+CO$	6.030E+13	0.0	0.0	24
187	$C_2H_5+O_2=C_2H_4+HO_2$	2.000E+10	0.0	-2200.0	24
188	$CH_4+O_2=CH_3+HO_2$	7.900E+13	0.0	56000.0	24
189	$OH+HO_2=H_2O+O_2$	7.500E+12	0.0	0.0	24
190	$CH_3+O_2=CH_2O+OH$	3.800E+11	0.0	9000.0	24
191	$CH_4+H=CH_3+H_2$	6.600E+08	1.6	10840.0	24
192	$CH_4+OH=CH_3+H_2O$	1.600E+06	2.1	2460.0	24
193	$CH_4+O=CH_3+OH$	1.020E+09	1.5	86040.0	24
194	$CH_4+HO_2=CH_3+H_2O_2$	9.000E+11	0.0	18700.0	24
195	$CH_4+CH_2=CH_3+CH_3$	4.000E+12	0.0	-570.0	24
196	$C_3H_6=C_2H_3+CH_3$	3.150E+15	0.0	85500.0	24

k=ATbexp(-E/RT): rate constant (Units: mol, s, cm^3, and cal)**