

1 MEOHSYNGAS1.0 Mechanism

REACTIONS CONSIDERED				(k = A T**b exp(-E/RT))		
				A	b	E
1. H2+M=2H+M				4.58E+19	-1.4	104400.0
H2	Enhanced by	2.500E+00				
H2O	Enhanced by	1.200E+01				
CO	Enhanced by	1.900E+00				
CO2	Enhanced by	3.800E+00				
CH4	Enhanced by	2.000E+00				
2. H2+O=H+OH				5.08E+04	2.7	6292.0
3. H2+OH=H+H2O				4.38E+13	0.0	6990.0
4. 2O+M=O2+M				6.16E+15	-0.5	0.0
H2	Enhanced by	2.500E+00				
H2O	Enhanced by	1.200E+01				
AR	Enhanced by	8.300E-01				
CO	Enhanced by	1.900E+00				
CO2	Enhanced by	3.800E+00				
CH4	Enhanced by	2.000E+00				
5. O2+H=O+OH				1.04E+14	0.0	15286.0
6. H+OH+M=H2O+M				3.50E+22	-2.0	0.0
H2	Enhanced by	7.300E-01				
H2O	Enhanced by	3.650E+00				
CH4	Enhanced by	2.000E+00				
AR	Enhanced by	3.800E-01				
7. O+H2O=2OH				6.70E+07	1.7	14986.8
8. O+H+M=OH+M				4.71E+18	-1.0	0.0
H2	Enhanced by	2.500E+00				
H2O	Enhanced by	1.200E+01				
AR	Enhanced by	7.500E-01				
CO	Enhanced by	1.500E+00				
CO2	Enhanced by	2.000E+00				
CH4	Enhanced by	2.000E+00				
9. H2O2(+M)=2OH(+M)				2.00E+12	0.9	48749.0
H2O	Enhanced by	7.650E+00				
CO2	Enhanced by	1.600E+00				
N2	Enhanced by	1.500E+00				
O2	Enhanced by	1.200E+00				
H2O2	Enhanced by	7.700E+00				
H2	Enhanced by	3.700E+00				
CO	Enhanced by	2.800E+00				
Low pressure limit:	0.24900E+25	-0.23000E+01	0.48749E+05			

TROE centering:		0.43000E+00	0.10000E-29	0.10000E+31		
10.	H2O2+H=H2O+OH			2.41E+13	0.0	3970.0
11.	H2O2+H=H2+HO2			2.15E+10	1.0	6000.0
12.	H2O2+O=OH+HO2			9.55E+06	2.0	3970.0
13.	H2O2+OH=H2O+HO2			1.74E+12	0.0	318.0
Declared duplicate reaction...						
14.	H2O2+OH=H2O+HO2			7.59E+13	0.0	7269.0
Declared duplicate reaction...						
15.	HO2+H=2OH			7.08E+13	0.0	295.0
16.	HO2+H=H2+O2			1.14E+10	1.1	553.8
17.	HO2+O=OH+O2			3.25E+13	0.0	0.0
18.	OH+HO2=H2O+O2			7.00E+12	0.0	-1093.0
Declared duplicate reaction...						
19.	OH+HO2=H2O+O2			4.50E+14	0.0	10929.6
Declared duplicate reaction...						
20.	2HO2=H2O2+O2			1.00E+14	0.0	11040.9
Declared duplicate reaction...						
21.	2HO2=H2O2+O2			1.90E+11	0.0	-1408.9
Declared duplicate reaction...						
22.	H+O2(+M)=HO2(+M)			4.65E+12	0.4	0.0
	H2	Enhanced by	1.300E+00			
	CO	Enhanced by	1.900E+00			
	CO2	Enhanced by	3.800E+00			
	H2O	Enhanced by	1.000E+01			
	AR	Enhanced by	5.000E-01			
	CH4	Enhanced by	2.000E+00			
Low pressure limit:		0.17370E+20	-0.12300E+01	0.00000E+00		
TROE centering:		0.67000E+00	0.10000E-29	0.10000E+31	0.10000E+31	
23.	CO+O(+M)=CO2(+M)			1.36E+10	0.0	2384.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	1.200E+01			
	CO	Enhanced by	1.750E+00			
	CO2	Enhanced by	3.600E+00			
	AR	Enhanced by	7.000E-01			
Low pressure limit:		0.11730E+25	-0.27900E+01	0.41910E+04		
24.	CO+OH=CO2+H			7.02E+04	2.1	-355.7
Declared duplicate reaction...						
25.	CO+OH=CO2+H			5.76E+12	-0.7	331.8
Declared duplicate reaction...						
26.	CO+HO2=CO2+OH			1.57E+05	2.2	17940.0
27.	CO+O2=CO2+O			1.12E+12	0.0	47700.0
28.	H+CO2=OCHO			7.50E+13	0.0	29000.0
29.	CH3+H(+M)=CH4(+M)			1.27E+16	-0.6	383.0
	H2	Enhanced by	2.000E+00			

H2O	Enhanced by	6.000E+00		
AR	Enhanced by	7.000E-01		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
CH4	Enhanced by	2.000E+00		
Low pressure limit: 0.24770E+34 -0.47600E+01 0.24400E+04				
TROE centering: 0.78300E+00 0.74000E+02 0.29410E+04 0.69640E+04				
30. CH4+H=CH3+H2			6.14E+05	2.5 9587.0
31. CH4+O=CH3+OH			1.02E+09	1.5 8600.0
32. CH4+OH=CH3+H2O			5.83E+04	2.6 2190.0
33. CH4+HO2=CH3+H2O2			1.69E+01	3.7 21010.0
34. CH4+CH3O2=CH3+CH3O2H			9.60E-01	3.8 17810.0
35. CH3+HO2=CH4+O2			1.16E+05	2.2 -3022.0
36. CH4+CH2=2CH3			2.46E+06	2.0 8270.0
37. CH2(S)+N2=CH2+N2			1.50E+13	0.0 600.0
38. CH2(S)+AR=CH2+AR			9.00E+12	0.0 600.0
39. CH2(S)+H2O=CH2+H2O			3.00E+13	0.0 0.0
40. CH2(S)+CO=CH2+CO			9.00E+12	0.0 0.0
41. CH2(S)+CO2=CH2+CO2			7.00E+12	0.0 0.0
42. CH2(S)+O2=>H+OH+CO			2.80E+13	0.0 0.0
43. CH2(S)+O2=CO+H2O			1.20E+13	0.0 0.0
44. CH2(S)+O=CO+H2			1.50E+13	0.0 0.0
45. CH2(S)+O=HCO+H			1.50E+13	0.0 0.0
46. CH2(S)+H2=CH3+H			7.00E+13	0.0 0.0
47. CH2(S)+OH=CH2O+H			3.00E+13	0.0 0.0
48. CH2(S)+CO2=CH2O+CO			1.40E+13	0.0 0.0
49. CH2+H(+M)=CH3(+M)			2.50E+16	-0.8 0.0
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
AR	Enhanced by	7.000E-01		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
CH4	Enhanced by	2.000E+00		
Low pressure limit: 0.32000E+28 -0.31400E+01 0.12300E+04				
TROE centering: 0.68000E+00 0.78000E+02 0.19950E+04 0.55900E+04				
50. CH2+O2=HCO+OH			1.06E+13	0.0 1500.0
51. CH2+O2=>CO2+2H			2.64E+12	0.0 1500.0
52. CH2+O=>CO+2H			5.00E+13	0.0 0.0
53. CH3+O2(+M)=CH3O2(+M)			7.81E+09	0.9 0.0
Low pressure limit: 0.68500E+25 -0.30000E+01 0.00000E+00				
TROE centering: 0.60000E+00 0.10000E+04 0.70000E+02 0.17000E+04				
54. CH3+O2=CH3O+O			7.55E+12	0.0 28320.0
55. CH3+O2=CH2O+OH			2.64E+00	3.3 8105.0
56. CH3+O=CH2O+H			5.54E+13	0.1 -136.0

57. CH ₃ +OH=CH ₂ (S)+H ₂ O	4.94E+14	-0.7	-445.8
Rate coefficients at P=1.00E-02(atm)	4.936E+14	-0.7	-445.8
Rate coefficients at P=1.00E-01(atm)	1.207E+15	-0.8	-175.6
Rate coefficients at P=1.00E+00(atm)	5.282E+17	-1.5	1772.0
Rate coefficients at P=1.00E+01(atm)	4.788E+23	-3.2	7003.0
Rate coefficients at P=1.00E+02(atm)	8.433E+19	-2.0	8244.0
58. CH ₃ +OH=CH ₂ O+H ₂	3.50E+05	1.4	-3244.0
Rate coefficients at P=1.00E-02(atm)	3.502E+05	1.4	-3244.0
Rate coefficients at P=1.00E-01(atm)	8.854E+05	1.3	-2975.0
Rate coefficients at P=1.00E+00(atm)	1.650E+07	1.0	-2010.0
Rate coefficients at P=1.00E+01(atm)	5.374E+09	0.3	280.0
Rate coefficients at P=1.00E+02(atm)	9.494E+18	-2.2	9769.0
59. CH ₃ +OH=CH ₂ OH+H	1.62E+10	1.0	3210.0
Rate coefficients at P=1.00E-02(atm)	1.621E+10	1.0	3214.0
Rate coefficients at P=1.00E-01(atm)	1.807E+10	0.9	3247.0
Rate coefficients at P=1.00E+00(atm)	4.686E+10	0.8	3566.0
Rate coefficients at P=1.00E+01(atm)	1.525E+13	0.1	5641.0
Rate coefficients at P=1.00E+02(atm)	3.590E+14	-0.2	8601.0
60. CH ₃ +OH=H+CH ₃ O	1.19E+09	1.0	11940.0
Rate coefficients at P=1.00E-02(atm)	1.186E+09	1.0	11940.0
Rate coefficients at P=1.00E-01(atm)	1.188E+09	1.0	11940.0
Rate coefficients at P=1.00E+00(atm)	1.230E+09	1.0	11950.0
Rate coefficients at P=1.00E+01(atm)	1.798E+09	1.0	12060.0
Rate coefficients at P=1.00E+02(atm)	5.242E+10	0.6	13070.0
61. CH ₃ +OH=CH ₂ +H ₂ O	4.29E+04	2.6	3997.8
62. CH ₃ +HO ₂ =CH ₃ O+OH	1.00E+12	0.3	-687.5
63. CH ₃ O ₂ +O=CH ₃ O+O ₂	3.60E+13	0.0	0.0
64. CH ₃ O ₂ +H=CH ₃ O+OH	9.60E+13	0.0	0.0
65. CH ₃ O ₂ +OH=CH ₃ OH+O ₂	6.00E+13	0.0	0.0
66. CH ₃ O ₂ +HO ₂ =CH ₃ O ₂ H+O ₂	2.47E+11	0.0	-1570.0
67. CH ₃ O ₂ +H ₂ O ₂ =CH ₃ O ₂ H+HO ₂	2.41E+12	0.0	9936.0
68. CH ₃ O ₂ +CH ₃ =2CH ₃ O	5.08E+12	0.0	-1411.0
69. 2CH ₃ O ₂ =>CH ₂ O+CH ₃ OH+O ₂	3.11E+14	-1.6	-1051.0
70. 2CH ₃ O ₂ =>O ₂ +2CH ₃ O	1.40E+16	-1.6	1860.0
71. H ₂ +CH ₃ O ₂ =H+CH ₃ O ₂ H	1.50E+14	0.0	26030.0
72. CH ₃ O ₂ H=CH ₃ O+OH	6.31E+14	0.0	42300.0
73. CH ₃ OH(+M)=CH ₃ +OH(+M)	2.08E+18	-0.6	92540.6
Low pressure limit:	0.15000E+44	-0.69950E+01	0.97992E+05
TROE centering:	-0.47480E+00	0.35580E+05	0.11160E+04 0.90230E+04
74. CH ₃ OH(+M)=CH ₂ (S)+H ₂ O(+M)	3.12E+18	-1.0	91712.0
Low pressure limit:	0.14300E+48	-0.82270E+01	0.99417E+05
TROE centering:	0.25450E+01	0.32900E+04	0.47320E+05 0.47110E+05
75. CH ₃ OH(+M)=CH ₂ OH+H(+M)	7.90E-03	5.0	84467.4
Low pressure limit:	0.33900E+43	-0.72440E+01	0.10523E+06

TROE centering: -0.73910E+02 0.37050E+05 0.41500E+05 0.52200E+04					
76. CH3OH+H=CH3O+H2	1.99E+05	2.6	10300.0		
77. CH3OH+H=CH2OH+H2	3.07E+05	2.5	5440.0		
78. CH3OH+O=CH3O+OH	3.88E+04	2.5	3080.0		
79. CH3OH+O=CH2OH+OH	3.88E+05	2.5	3080.0		
80. CH3OH+OH=CH3O+H2O	1.50E+02	3.0	-763.0		
81. CH3OH+OH=CH2OH+H2O	3.08E+04	2.6	-806.7		
82. CH3OH+O2=CH3O+HO2	3.58E+04	2.3	42764.5		
83. CH3OH+O2=CH2OH+HO2	3.58E+05	2.3	42764.5		
84. CH3OH+HO2=CH3O+H2O2	1.22E+12	0.0	20070.7		
85. CH3OH+HO2=CH2OH+H2O2	3.26E+13	0.0	18782.2		
86. CH3OH+CH3=CH2OH+CH4	2.13E-01	4.0	7055.1		
87. CH3OH+CH3=CH3O+CH4	3.22E+03	2.4	8579.5		
88. CH3OH+HCO=CH2OH+CH2O	9.63E+03	2.9	13110.0		
89. CH3OH+CH3O=CH2OH+CH3OH	3.00E+11	0.0	4074.0		
90. CH3OH+CH3O2=CH2OH+CH3O2H	1.81E+12	0.0	13710.0		
91. CH2OH+O2=CH2O+HO2	1.51E+15	-1.0	0.0		
Declared duplicate reaction...					
92. CH2OH+O2=CH2O+HO2	2.41E+14	0.0	5017.0		
Declared duplicate reaction...					
93. CH2OH+H=CH2O+H2	6.00E+12	0.0	0.0		
94. CH2OH+HO2=CH2O+H2O2	1.20E+13	0.0	0.0		
95. CH2OH+HCO=2CH2O	1.80E+14	0.0	0.0		
96. CH2OH+HCO=CH3OH+CO	1.00E+13	0.0	0.0		
97. CH2OH+CH3O=CH2O+CH3OH	2.40E+13	0.0	0.0		
98. CH2OH+OH=H2O+CH2O	2.40E+13	0.0	0.0		
99. CH2OH+O=OH+CH2O	4.20E+13	0.0	0.0		
100. 2CH2OH=CH2O+CH3OH	3.00E+12	0.0	0.0		
101. CH2OH+HO2=HOCH2O+OH	1.00E+13	0.0	0.0		
102. CH3O+O2=CH2O+HO2	4.38E-19	9.5	-5501.0		
103. CH3O+H=CH2O+H2	2.00E+13	0.0	0.0		
104. CH3O+HO2=CH2O+H2O2	3.01E+11	0.0	0.0		
105. CH3O+CH3=CH2O+CH4	1.20E+13	0.0	0.0		
106. 2CH3O=CH3OH+CH2O	6.03E+13	0.0	0.0		
107. HCO+H(+M)=CH2O(+M)	1.09E+12	0.5	-260.0		
H2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			
AR	Enhanced by	7.000E-01			
CO	Enhanced by	1.500E+00			
CO2	Enhanced by	2.000E+00			
CH4	Enhanced by	2.000E+00			
Low pressure limit: 0.13500E+25 -0.25700E+01 0.14250E+04					
TROE centering: 0.78240E+00 0.27100E+03 0.27550E+04 0.65700E+04					
108. CO+H2(+M)=CH2O(+M)	4.30E+07	1.5	79600.0		

H2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			
AR	Enhanced by	7.000E-01			
CO	Enhanced by	1.500E+00			
CO2	Enhanced by	2.000E+00			
CH4	Enhanced by	2.000E+00			
Low pressure limit: 0.50700E+28 -0.34200E+01 0.84348E+05					
TROE centering: 0.93200E+00 0.19700E+03 0.15400E+04 0.10300E+05					
109. CH2O+O2=HCO+HO2			8.07E+15	0.0	53420.0
110. CH2O+O=HCO+OH			6.26E+09	1.1	2260.0
111. CH2O+H=HCO+H2			5.74E+07	1.9	2740.0
112. CH2O+OH=HCO+H2O			7.82E+07	1.6	-1055.0
113. CH2O+HO2=HCO+H2O2			1.88E+04	2.7	11520.0
114. CH2O+CH3=HCO+CH4			3.83E+01	3.4	4312.0
115. CH2O+O2CHO=HCO+HO2CHO			1.99E+12	0.0	11660.0
116. CH2O+OCHO=HCO+HOCHO			5.60E+12	0.0	13600.0
117. CH2O+CH3O=HCO+CH3OH			6.62E+11	0.0	2294.0
118. CH2O+CH3O2=HCO+CH3O2H			1.99E+12	0.0	11660.0
119. HCO+M=H+CO+M			5.70E+11	0.7	14870.0
H2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			
CO	Enhanced by	1.500E+00			
CO2	Enhanced by	2.000E+00			
CH4	Enhanced by	2.000E+00			
120. HCO+O2=CO+HO2			7.58E+12	0.0	410.0
121. HCO+O=CO+OH			3.02E+13	0.0	0.0
122. HCO+H=CO+H2			7.34E+13	0.0	0.0
123. HCO+OH=CO+H2O			3.01E+13	0.0	0.0
124. HCO+CH3=CH4+CO			2.65E+13	0.0	0.0
125. 2HCO=CH2O+CO			1.80E+13	0.0	0.0
126. HCO+O=CO2+H			3.00E+13	0.0	0.0
127. HCO+HO2=>CO2+H+OH			3.00E+13	0.0	0.0
128. 2HCO=>H2+2CO			3.00E+12	0.0	0.0
129. CH2O+H(+M)=CH2OH(+M)			5.40E+11	0.5	3600.0
H2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			
CO	Enhanced by	1.500E+00			
CO2	Enhanced by	2.000E+00			
CH4	Enhanced by	2.000E+00			
Low pressure limit: 0.12700E+33 -0.48200E+01 0.65300E+04					
TROE centering: 0.71870E+00 0.10300E+03 0.12910E+04 0.41600E+04					
130. CH3O(+M)=CH2O+H(+M)			6.80E+13	0.0	26170.0
H2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			

CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
CH4	Enhanced by	2.000E+00		
Low pressure limit: 0.18670E+26 -0.30000E+01 0.24307E+05				
TROE centering: 0.90000E+00 0.25000E+04 0.13000E+04 0.10000+100				
131. CH2O+OH=HOCH2O		4.50E+15	-1.1	0.0
132. HOCH2O=HOCHO+H		1.00E+14	0.0	14900.0
133. HCO+O2=O2CHO		1.20E+11	0.0	-1100.0
134. HOCHO=CO+H2O		2.45E+12	0.0	60470.0
135. HOCHO=CO2+H2		2.95E+09	0.0	48520.0
136. OCHO+HO2=HOCHO+O2		3.50E+10	0.0	-3275.0
137. OCHO+H2O2=HOCHO+HO2		2.40E+12	0.0	10000.0
138. HOCHO+H=>H2+CO2+H		4.24E+06	2.1	4868.0
139. HOCHO+H=>H2+CO+OH		6.03E+13	-0.3	2988.0
140. HOCHO+O=>CO+2OH		1.77E+18	-1.9	2975.0
141. HOCHO+OH=>H2O+CO2+H		2.62E+06	2.1	916.0
142. HOCHO+OH=>H2O+CO+OH		1.85E+07	1.5	-962.0
143. HOCHO+CH3=>CH4+CO+OH		3.90E-07	5.8	2200.0
144. HOCHO+HO2=>H2O2+CO+OH		1.00E+12	0.0	11920.0
145. OCHO+OH=HO2CHO		2.00E+13	0.0	0.0
146. CH3O+HCO=CH3OH+CO		9.00E+13	0.0	0.0

UNITS for the preceding reactions (unless otherwise noted):

A units mole-cm-sec-K, E units cal/mole

2 MEOHSYNGAS1.0 Thermodynamic Data

	300.000	1000.000	5000.000						
AR		G-5-97AR	1	G	200.0	6000.0	1000.0	1	
	2.5E0	0.0E0	0.0E0	0.0E0	0.0E0	0.0E0	0.0E0	2	
	-7.45375E2	4.37967491E0	2.5E0	0.0E0	0.0E0	0.0E0	0.0E0	3	
	0.0E0	0.0E0	-7.45375E2	4.37967491E0				4	
N2		G-8-02N	2	G	200.0	6000.0	1000.0	1	
	2.95257637E0	1.3969004E-3	-4.92631603E-7	7.86010195E-11	-4.60755204E-15			2	
	-9.23948688E2	5.87188762E0	3.53100528E0	-1.23660988E-4	-5.02999433E-7			3	
	2.43530612E-9	-1.40881235E-12	-1.04697628E3	2.96747038E0				4	
H2		TPIS78H	2	G	200.0	6000.0	1000.0	1	
	2.93286575E0	8.26608026E-4	-1.46402364E-7	1.54100414E-11	-6.888048E-16			2	
	-8.13065581E2	-1.02432865E0	2.34433112E0	7.98052075E-3	-1.9478151E-5			3	
	2.01572094E-8	-7.37611761E-12	-9.17935173E2	6.83010238E-1				4	
H		L-6-94H	1	G	200.0	6000.0	1000.0	1	
	2.5E0	0.0E0	0.0E0	0.0E0	0.0E0	0.0E0	0.0E0	2	
	2.547366E4	-4.4668285E-1	2.5E0	0.0E0	0.0E0	0.0E0	0.0E0	3	
	0.0E0	0.0E0	2.547366E4	-4.4668285E-1				4	
O2		RUS-89O	2	G	200.0	6000.0	1000.0	1	
	3.66096065E0	6.56365811E-4	-1.41149627E-7	2.05797935E-11	-1.29913436E-15			2	
	-1.21597718E3	3.41536279E0	3.78245636E0	-2.99673416E-3	9.84730201E-6			3	
	-9.68129509E-9	3.24372837E-12	-1.06394356E3	3.65767573E0				4	
O		L-1-90O	1	G	200.0	6000.0	1000.0	1	
	2.54363697E0	-2.73162486E-5	-4.1902952E-9	4.95481845E-12	-4.79553694E-16			2	
	2.9226012E4	4.92229457E0	3.1682671E0	-3.27931884E-3	6.64306396E-6			3	
	-6.12806624E-9	2.11265971E-12	2.91222592E4	2.05193346E0				4	
H2O		L-5-89H	2O 1	G	200.0	6000.0	1000.0	1	
	2.6770389E0	2.9731816E-3	-7.7376889E-7	9.4433514E-11	-4.2689991E-15			2	
	-2.9885894E4	6.88255E0	4.1986352E0	-2.0364017E-3	6.5203416E-6			3	
	-5.4879269E-9	1.771968E-12	-3.0293726E4	-8.4900901E-1				4	
OH		IU3-03H	1O 1	G	200.0	6000.0	1000.0	1	
	2.83853033E0	1.10741289E-3	-2.94000209E-7	4.20698729E-11	-2.4228989E-15			2	
	3.69780808E3	5.84494652E0	3.99198424E0	-2.40106655E-3	4.61664033E-6			3	
	-3.87916306E-9	1.36319502E-12	3.36889836E3	-1.03998477E-1				4	
H2O2		T-8-03H	2O 2	G	200.0	6000.0	1000.0	1	
	4.57977305E0	4.05326003E-3	-1.2984473E-6	1.982114E-10	-1.13968792E-14			2	
	-1.80071775E4	6.64970694E-1	4.31515149E0	-8.47390622E-4	1.76404323E-5			3	
	-2.26762944E-8	9.08950158E-12	-1.77067437E4	3.27373319E0				4	
HO2		T-1-09H	1O 2	G	200.0	5000.0	1000.0	1	
	4.17228741E0	1.88117627E-3	-3.46277286E-7	1.94657549E-11	1.76256905E-16			2	
	3.10206839E1	2.95767672E0	4.30179807E0	-4.74912097E-3	2.11582905E-5			3	
	-2.42763914E-8	9.29225225E-12	2.64018485E2	3.7166622E0				4	

CO	RUS-790	1C	1	G	200.0	6000.0	1000.0	1	
	3.0484859E0	1.3517281E-3	-4.8579405E-7	7.8853644E-11	-4.6980746E-15		2		
	-1.4266117E4	6.0170977E0	3.5795335E0	-6.1035369E-4	1.0168143E-6		3		
	9.0700586E-10	-9.0442449E-13	-1.4344086E4	3.5084093E0			4		
CO2	L-7-88O	2C	1	G	200.0	6000.0	1000.0	1	
	4.6365111E0	2.7414569E-3	-9.9589759E-7	1.6038666E-10	-9.1619857E-15		2		
	-4.9024904E4	-1.9348955E0	2.356813E0	8.9841299E-3	-7.1220632E-6		3		
	2.4573008E-9	-1.4288548E-13	-4.8371971E4	9.9009035E0			4		
CH4	G-8-99H	4C	1	G	200.0	6000.0	1000.0	1	
	1.65326226E0	1.00263099E-2	-3.31661238E-6	5.36483138E-10	-3.14696758E-14		2		
	-1.00095936E4	9.90506283E0	5.14911468E0	-1.36622009E-2	4.91453921E-5		3		
	-4.84246767E-8	1.66603441E-11	-1.02465983E4	-4.63848842E0			4		
CH3	IU0702H	3C	1	G	200.0	6000.0	1000.0	1	
	2.9781206E0	5.797852E-3	-1.97558E-6	3.072979E-10	-1.7917416E-14		2		
	1.6509513E4	4.7224799E0	3.6571797E0	2.1265979E-3	5.4583883E-6		3		
	-6.6181003E-9	2.4657074E-12	1.6422716E4	1.6735354E0			4		
CH2	IU3-03H	2C	1	G	200.0	6000.0	1000.0	1	
	3.14631886E0	3.03671259E-3	-9.96474439E-7	1.5048358E-10	-8.57335515E-15		2		
	4.60412605E4	4.72341711E0	3.71757846E0	1.2739126E-3	2.17347251E-6		3		
	-3.488585E-9	1.65208866E-12	4.58723866E4	1.75297945E0			4		
CH2(S)	IU6-03H	2C	1	G	200.0	6000.0	1000.0	1	
	3.13501686E0	2.89593926E-3	-8.1666809E-7	1.13572697E-10	-6.36262835E-15		2		
	5.05040504E4	4.06030621E0	4.19331325E0	-2.33105184E-3	8.15676451E-6		3		
	-6.62985981E-9	1.93233199E-12	5.03662246E4	-7.4673431E-1			4		
CH3O2H	A-7-05H	4O	2C	1	G	200.0	6000.0	1000.0	1
	7.76538058E0	8.61499712E-3	-2.98006935E-6	4.68638071E-10	-2.75339255E-14		2		
	-1.82979984E4	-1.43992663E1	2.90540897E0	1.74994735E-2	5.2824363E-6		3		
	-2.52827275E-8	1.34368212E-11	-1.68894632E4	1.13741987E1			4		
CH3O2	H	3O	2C	1	G	300.0	5000.0	1374.0	1
	6.47970487E0	7.4440108E-3	-2.52348555E-6	3.89577296E-10	-2.25182399E-14		2		
	-1.56285441E3	-8.19477074E0	1.97339205E0	1.5354234E-2	-6.37314891E-6		3		
	3.19930565E-10	2.82193915E-13	2.54278835E2	1.69194215E1			4		
CH3OH	T06-02H	4O	1C	1	G	200.0	6000.0	1000.0	1
	3.52726795E0	1.03178783E-2	-3.62892944E-6	5.77448016E-10	-3.42182632E-14		2		
	-2.60028834E4	5.16758693E0	5.65851051E0	-1.62983419E-2	6.91938156E-5		3		
	-7.58372926E-8	2.8042755E-11	-2.56119736E4	-8.97330508E-1			4		
CH3O	IU1-03H	3O	1C	1	G	200.0	6000.0	1000.0	1
	4.75779238E0	7.44142474E-3	-2.69705176E-6	4.38090504E-10	-2.63537098E-14		2		
	3.7811194E2	-1.96680028E0	3.71180502E0	-2.80463306E-3	3.76550971E-5		3		
	-4.73072089E-8	1.8658842E-11	1.2956976E3	6.57240864E0			4		
CH2OH	IU2-03H	3O	1C	1	G	200.0	6000.0	1000.0	1
	5.0931437E0	5.9476126E-3	-2.0649746E-6	3.23008173E-10	-1.88125902E-14		2		
	-4.0340964E3	-1.84691493E0	4.47834367E0	-1.3507031E-3	2.7848498E-5		3		
	-3.6486906E-8	1.4790745E-11	-3.5007289E3	3.309135E0			4		

3 Ignition Delay Time Data

Table S1 Ignition delay time of mixture 1

1/T (1/K)	Ignition delay time (μ s)
0.8359	1844.05
0.8230	1438.34
0.8489	1742.67
0.8619	2923.00
0.7217	349.35
0.7718	820.77
0.6726	156.63
0.6604	123.42
0.6970	217.19
0.7973	1080.65

Table S2 Ignition delay time of mixture 2

1/T (1/K)	Ignition delay time (μ s)
0.9195	9292.36
0.8392	2252.49
0.7358	535.82
0.7232	394.31
0.7107	364.78
0.6613	119.85
0.8129	1424.83
0.7741	834.60

Table S3 Ignition delay time of mixture 3

1/T (1/K)	Ignition delay time (μ s)
0.8741	4008.01
0.8076	1339.02
0.8340	2401.44
0.7556	717.93
0.7301	442.41
0.6800	178.81
0.6553	83.30
0.6676	104.34
0.7945	1593.63
0.7174	316.27

Table S4 Ignition delay time of mixture 4

1/T (1/K)	Ignition delay time (μ s)
0.9615	313.86
0.9898	426.13
1.0330	1032.93
0.9329	231.05
0.8914	183.65
1.0324	777.89
0.9470	283.01
0.9756	447.78
1.0184	680.88
0.8780	151.12
0.8372	99.96
0.7963	89.17
0.7188	71.99
0.8640	122.26
0.8232	94.58
0.7575	97.45
0.7446	80.47
0.9051	212.39

Table S5 Ignition delay time of mixture 5

1/T (1/K)	Ignition delay time (μ s)
0.9984	459.68
0.8731	147.46
0.8195	96.03
1.0270	599.69
0.9282	176.47
1.0127	510.47
0.9560	248.33
0.7408	58.50
0.8193	94.19
0.7797	80.05
0.9701	312.93
0.7537	57.55
0.8868	137.47