Table 5.4 Complex natural gas (methane) combustion mechanism (GRI Mech 3.0) [23]

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
C–H–O Reactions				
1	$O + O + M \rightarrow O_2 + M$	1.20E + 17	−1.0	0.0
2	$O + H + M \rightarrow OH + M$	5.00E + 17	−1.0	0.0
3	$O + H_2 \rightarrow H + OH$	3.87E + 04	2.7	6,260
4	$O + HO_2 \rightarrow OH + O_2$	2.00E + 13	0.0	0.0
5	$O + H_2O_2 \rightarrow OH + HO_2$	9.63E + 06	2.0	4,000
6	$O + CH \rightarrow H + CO$	5.70E + 13	0.0	0.0
7	$O + CH_2 \rightarrow H + HCO$	8.00E + 13	0.0	0.0
8[b]	$O + CH_2(S) \rightarrow H_2 + CO$	1.50E + 13	0.0	0.0
9[b]	$O + CH_2(S) \rightarrow H + HCO$	1.50E + 13	0.0	0.0
10	$O + CH_3 \rightarrow H + CH_2O$	5.06E + 13	0.0	0.0
11	$O + CH_4 \rightarrow OH + CH_3$	1.02E + 09	1.5	8,600
12	$O + CO + M \rightarrow CO_2 + M$	1.8E + 10	0.0	2,385
13	$O + HCO \rightarrow OH + CO$	3.00E + 13	0.0	0.0
14	$O + HCO \rightarrow H + CO_2$	3.00E + 13	0.0	0.0
15	$O + CH_2O \rightarrow OH + HCO$	3.90E + 13	0.0	3,540
16	$O + CH_2OH \rightarrow OH + CH_2O$	1.00E + 13	0.0	0.0
17	$O + CH_3O \rightarrow OH + CH_2O$	1.00E + 13	0.0	0.0
18	$O + CH_3OH \rightarrow OH + CH_2OH$	3.88E + 05	2.5	3,100
19	$O + CH_3OH \rightarrow OH + CH_3O$	1.30E + 05	2.5	5,000
20	$O + C_2H \rightarrow CH + CO$	5.00E + 13	0.0	0.0
21	$O + C_2H_2 \rightarrow H + HCCO$	1.35E + 07	2.0	1,900
22	$O + C_2H_2 \rightarrow OH + C_2H$	4.60E + 19	−1.4	28,950
23	$O + C_2H_2 \rightarrow CO + CH_2$	9.64E + 06	2.0	1,900
24	$O + C_2H_3 \rightarrow H + CH_2CO$	3.00E + 13	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
	C–H–O Reactions (continued)			
25	$O + C_2H_4 \rightarrow CH_3 + HCO$	1.25E + 07	1.83	220
26	$O + C_2H_5 \rightarrow CH_3 + CH_2O$	2.24E + 13	0.0	0.0
27	$O + C_2H_6 \rightarrow OH + C_2H_5$	8.98E + 07	1.9	5,690
28	$O + HCCO \rightarrow H + CO + CO$	1.00E + 14	0.0	0.0
29	$O + CH_2CO \rightarrow OH + HCCO$	1.00E + 13	0.0	8,000
30	$O + CH_2CO \rightarrow CH_2 + CO_2$	1.75E + 12	0.0	1,350
31	$O_2 + CO \rightarrow O + CO_2$	2.50E + 12	0.0	47,800
32	$O_2 + CH_2O \rightarrow HO_2 + HCO$	1.00E + 14	0.0	40,000
33	$H + O_2 + M \rightarrow HO_2 + M$	2.80E + 18	−0.9	0.0
34	$H + O_2 + O_2 \rightarrow HO_2 + O_2$	2.08E + 19	−1.2	0.0
35	$H + O_2 + H_2O \rightarrow HO_2 + H_2O$	1.13E + 19	−0.8	0.0
36	$H + O_2 + N_2 \rightarrow HO_2 + N_2$	2.60E + 19	−1.2	0.0
37	$H + O_2 + Ar \rightarrow HO_2 + Ar$	7.00E + 17	−0.8	0.0
38	$H + O_2 \rightarrow O + OH$	2.65E + 16	−0.7	17,041
39	$H + H + M \rightarrow H_2 + M$	1.00E + 18	−1.0	0.0
40	$H + H + H_2 \rightarrow H_2 + H_2$	9.00E + 16	−0.6	0.0
41	$H + H + H_2O \rightarrow H_2 + H_2O$	6.00E + 19	−1.2	0.0
42	$H + H + CO_2 \rightarrow H_2 + CO_2$	5.50E + 20	−2.0	0.0
43	$H + OH + M \rightarrow H_2O + M$	2.20E + 22	−2.0	0.0
44	$H + HO_2 \rightarrow O + H_2O$	3.97E + 12	0.0	671
45	$H + HO_2 \rightarrow O_2 + H_2$	4.48E + 13	0.0	1,068
46	$H + HO_2 \rightarrow OH + OH$	8.4E + 13	0.0	635
47	$H + H_2O_2 \rightarrow HO_2 + H_2$	1.21E + 07	2.0	5,200
48	$H + H_2O_2 \rightarrow OH + H_2O$	1.00E + 13	0.0	3,600
49	$H + CH \rightarrow C + H_2$	1.65E + 14	0.0	0.0
50	$H + CH_2 (+ M) \rightarrow CH_3 (+ M)$		pressure dependent	
51[b]	$H + CH_2(S) \rightarrow CH + H_2$	3.00E + 13	0.0	0.0
52	$H + CH_3 (+ M) \rightarrow CH_4 (+ M)$		pressure dependent	
53	$H + CH_4 \rightarrow CH_3 + H_2$	6.60E + 08	1.6	10,840
54	$H + HCO (+ M) \rightarrow CH_2O (+ M)$		pressure dependent	
55	$H + HCO \rightarrow H_2 + CO$	7.34E + 13	0.0	0.0
56	$H + CH_2O (+ M) \rightarrow CH_2OH (+ M)$		pressure dependent	
57	$H + CH_2O (+ M) \rightarrow CH_3O (+ M)$		pressure dependent	
58	$H + CH_2O \rightarrow HCO + H_2$	5.74E + 07	1.9	2,742
59	$H + CH_2OH (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
60	$H + CH_2OH \rightarrow H_2 + CH_2O$	2.00E + 13	0.0	0.0
61	$H + CH_2OH \rightarrow OH + CH_3$	1.65E + 11	0.7	−284
62[b]	$H + CH_2OH \rightarrow CH_2(S) + H_2O$	3.28E + 13	−0.1	610
63	$H + CH_3O (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
64[b]	$H + CH_2OH \rightarrow CH_2(S) + H_2O$	4.15E + 07	1.6	1,924
65	$H + CH_3O \rightarrow H_2 + CH_2O$	2.00E + 13	0.0	0.0
66	$H + CH_3O \rightarrow OH + CH_3$	1.50E + 12	0.5	−110
67[b]	$H + CH_3O \rightarrow CH_2(S) + H_2O$	2.62E + 14	−0.2	1,070
68	$H + CH_3OH \rightarrow CH_2OH + H_2$	1.70E + 07	2.1	4,870
69	$H + CH_3OH \rightarrow CH_3O + H_2$	4.20E + 06	2.1	4,870
70	$H + C_2H (+ M) \rightarrow C_2H_2 (+ M)$		pressure dependent	

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
C–H–O Reactions (continued)				
71	$H + C_2H_2 (+ M) \rightarrow C_2H_3 (+ M)$		pressure dependent	
72	$H + C_2H_3 (+ M) \rightarrow C_2H_4 (+ M)$		pressure dependent	
73	$H + C_2H_3 \rightarrow H_2 + C_2H_2$	3.00E + 13	0.0	0.0
74	$H + C_2H_4 (+ M) \rightarrow C_2H_5 (+ M)$		pressure dependent	
75	$H + C_2H_4 \rightarrow C_2H_3 + H_2$	1.32E + 06	2.5	12,240
76	$H + C_2H_5 (+ M) \rightarrow C_2H_6 (+ M)$		pressure dependent	
77	$H + C_2H_5 \rightarrow C_2H_4 + H_2$	2.00E + 12	0.0	0.0
78	$H + C_2H_6 \rightarrow C_2H_5 + H_2$	1.15E + 08	1.9	7,530
79[b]	$H + HCCO \rightarrow CH_2(S) + CO$	1.00E + 14	0.0	0.0
80	$H + CH_2CO \rightarrow HCCO + H_2$	5.00E + 13	0.0	8,000
81	$H + CH_2CO \rightarrow CH_3 + CO$	1.13E + 13	0.0	3,428
82	$H + HCCOH \rightarrow H + CH_2CO$	1.00E + 13	0.0	0.0
83	$H_2 + CO (+ M) \rightarrow CH_2O (+ M)$		pressure dependent	
84	$OH + H_2 \rightarrow H + H_2O$	2.16E + 08	1.5	3,430
85	$OH + OH (+ M) \rightarrow H_2O_2 (+ M)$		pressure dependent	
86	$OH + OH \rightarrow O + H_2O$	3.57E + 04	2.4	−2,110
87	$OH + HO_2 \rightarrow O_2 + H_2O$	1.45E + 13	0.0	−500
88	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2.00E + 12	0.0	427
89	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	1.70E + 18	0.0	29,410
90	$OH + C \rightarrow H + CO$	5.00E + 13	0.0	0.0
91	$OH + CH \rightarrow H + HCO$	3.00E + 13	0.0	0.0
92	$OH + CH_2 \rightarrow H + CH_2O$	2.00E + 13	0.0	0.0
93	$OH + CH_2 \rightarrow CH + H_2O$	1.13E + 07	2.0	3,000
94[b]	$OH + CH_2(S) \rightarrow H + CH_2O$	3.00E + 13	0.0	0.0
95	$OH + CH_3 (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
96	$OH + CH_3 \rightarrow CH_2 + H_2O$	5.60E + 07	1.6	5,420
97[b]	$OH + CH_3 \rightarrow CH_2(S) + H_2O$	6.44E + 17	−1.3	1,417
98	$OH + CH_4 \rightarrow CH_3 + H_2O$	1.00E + 08	1.6	3,120
99	$OH + CO \rightarrow H + CO_2$	4.76E + 07	1.2	70
100	$OH + HCO \rightarrow H_2O + CO$	5.00E + 13	0.0	0.0
101	$OH + CH_2O \rightarrow HCO + H_2O$	3.43E + 09	1.2	−447
102	$OH + CH_2OH \rightarrow H_2O + CH_2O$	5.00E + 12	0.0	0.0
103	$OH + CH_3O \rightarrow H_2O + CH_2O$	5.00E + 12	0.0	0.0
104	$OH + CH_3OH \rightarrow CH_2OH + H_2O$	1.44E + 06	2.0	−840
105	$OH + CH_3OH \rightarrow CH_3O + H_2O$	6.30E + 06	2.0	1,500
106	$OH + C_2H \rightarrow H + HCCO$	2.00E + 13	0.0	0.0
107	$OH + C_2H_2 \rightarrow H + CH_2CO$	2.18E − 04	4.5	−1,000
108	$OH + C_2H_2 \rightarrow H + HCCOH$	5.04E + 05	2.3	13,500
109	$OH + C_2H_2 \rightarrow C_2H + H_2O$	3.37E + 07	2.0	14,000
110	$OH + C_2H_2 \rightarrow CH_3 + CO$	4.83E − 04	4.0	−2,000
111	$OH + C_2H_3 \rightarrow H_2O + C_2H_2$	5.00E + 12	0.0	0.0
112	$OH + C_2H_4 \rightarrow C_2H_3 + H_2O$	3.60E + 06	2.0	2,500
113	$OH + C_2H_6 \rightarrow C_2H_5 + H_2O$	3.54E + 06	2.1	870
114	$OH + CH_2CO \rightarrow HCCO + H_2O$	7.50E + 12	0.0	2,000
115	$HO_2 + HO_2 \rightarrow O_2 + H_2O_2$	1.30E + 11	0.0	−1,630
116	$HO_2 + HO_2 \rightarrow O_2 + H_2O_2$	4.20E + 14	0.0	12,000

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
C–H–O Reactions (continued)				
117	$HO_2 + CH_2 \rightarrow OH + CH_2O$	2.00E + 13	0.0	0.0
118	$HO_2 + CH_3 \rightarrow O_2 + CH_4$	1.00E + 12	0.0	0.0
119	$HO_2 + CH_3 \rightarrow OH + CH_3O$	3.78E + 13	0.0	0.0
120	$HO_2 + CO \rightarrow OH + CO_2$	1.50E + 14	0.0	23,600
121	$HO_2 + CH_2O \rightarrow HCO + H_2O_2$	5.60E + 06	2.0	12,000
122	$C + O_2 \rightarrow O + CO$	5.80E + 13	0.0	576
123	$C + CH_2 \rightarrow H + C_2H$	5.00E + 13	0.0	0.0
124	$C + CH_3 \rightarrow H + C_2H_2$	5.00E + 13	0.0	0.0
125	$CH + O_2 \rightarrow O + HCO$	6.71E + 13	0.0	0.0
126	$CH + H_2 \rightarrow H + CH_2$	1.08E + 14	0.0	3,110
127	$CH + H_2O \rightarrow H + CH_2O$	5.71E + 12	0.0	−755
128	$CH + CH_2 \rightarrow H + C_2H_2$	4.00E + 13	0.0	0.0
129	$CH + CH_3 \rightarrow H + C_2H_3$	3.00E + 13	0.0	0.0
130	$CH + CH_4 \rightarrow H + C_2H_4$	6.00E + 13	0.0	0.0
131	$CH + CO (+ M) \rightarrow HCCO (+ M)$		pressure dependent	
132	$CH + CO_2 \rightarrow HCO + CO$	1.90E + 14	0.0	15,792
133	$CH + CH_2O \rightarrow H + CH_2CO$	9.46E + 13	0.0	−515
134	$CH + HCCO \rightarrow CO + C_2H_2$	5.00E + 13	0.0	0.0
135	$CH_2 + O_2 \rightarrow OH + HCO$	5.00E + 12	0.0	1,500
136	$CH_2 + H_2 \rightarrow H + CH_3$	5.00E + 05	2.0	7,230
137	$CH_2 + CH_2 \rightarrow H_2 + C_2H_2$	1.60E + 15	0.0	11,944
138	$CH_2 + CH_3 \rightarrow H + C_2H_4$	4.00E + 13	0.0	0.0
139	$CH_2 + CH_4 \rightarrow CH_3 + CH_3$	2.46E + 06	2.0	8,270
140	$CH_2 + CO (+ M) \rightarrow CH_2CO (+ M)$		pressure dependent	
141	$CH_2 + HCCO \rightarrow C_2H_3 + CO$	3.00E + 13	0.0	0.0
142[b]	$CH_2(S) + N_2 \rightarrow CH_2 + N_2$	1.50E + 13	0.0	600
143[b]	$CH_2(S) + Ar \rightarrow CH_2 + Ar$	9.00E + 12	0.0	600
144[b]	$CH_2(S) + O_2 \rightarrow H + OH + CO$	2.80E + 13	0.0	0.0
145[b]	$CH_2(S) + O_2 \rightarrow CO + H_2O$	1.20E + 13	0.0	0.0
146[b]	$CH_2(S) + H_2 \rightarrow CH_3 + H$	7.00E + 13	0.0	0.0
147[b]	$CH_2(S) + H_2O (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
148[b]	$CH_2(S) + H_2O \rightarrow CH_2 + H_2O$	3.00E + 13	0.0	0.0
149[b]	$CH_2(S) + CH_3 \rightarrow H + C_2H_4$	1.20E + 13	0.0	−570
150[b]	$CH_2(S) + CH_4 \rightarrow CH_3 + CH_3$	1.60E + 13	0.0	−570
151[b]	$CH_2(S) + CO \rightarrow CH_2 + CO$	9.00E + 12	0.0	0.0
152[b]	$CH_2(S) + CO_2 \rightarrow CH_2 + CO_2$	7.00E + 12	0.0	0.0
153[b]	$CH_2(S) + CO_2 \rightarrow CO + CH_2O$	1.40E + 13	0.0	0.0
154[b]	$CH_2(S) + C_2H_6 \rightarrow CH_3 + C_2H_5$	4.00E + 13	0.0	−550
155	$CH_3 + O_2 \rightarrow O + CH_3O$	3.56E + 13	0.0	30,480
156	$CH_3 + O_2 \rightarrow OH + CH_2O$	2.31E + 12	0.0	20,315
157	$CH_3 + H_2O_2 \rightarrow HO_2 + CH_4$	2.45E + 04	2.47	5,180
158	$CH_3 + CH_3 (+ M) \rightarrow C_2H_6 (+ M)$		pressure dependent	
159	$CH_3 + CH_3 \rightarrow H + C_2H_5$	6.48E + 12	0.1	10,600
160	$CH_3 + HCO \rightarrow CH_4 + CO$	2.65E + 13	0.0	0.0
161	$CH_3 + CH_2O \rightarrow HCO + CH_4$	3.32E + 03	2.8	5,860

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a] A	b	E
C–H–O Reactions (continued)				
162	$CH_3 + CH_3OH \rightarrow CH_2OH + CH_4$	3.00E + 07	1.5	9,940
163	$CH_3 + CH_3OH \rightarrow CH_3O + CH_4$	1.00E + 07	1.5	9,940
164	$CH_3 + C_2H_4 \rightarrow C_2H_3 + CH_4$	2.27E + 05	2.0	9,200
165	$CH_3 + C_2H_6 \rightarrow C_2H_5 + CH_4$	6.14E + 06	1.7	10,450
166	$HCO + H_2O \rightarrow H + CO + H_2O$	1.55E + 18	−1.0	17,000
167	$HCO + M \rightarrow H + CO + M$	1.87E + 17	−1.0	17,000
168	$HCO + O_2 \rightarrow HO_2 + CO$	1.35E + 13	0.0	400
169	$CH_2OH + O_2 \rightarrow HO_2 + CH_2O$	1.80E + 13	0.0	900
170	$CH_3O + O_2 \rightarrow HO_2 + CH_2O$	4.28E − 13	7.6	−3,530
171	$C_2H + O_2 \rightarrow HCO + CO$	1.00E + 13	0.0	−755
172	$C_2H + H_2 \rightarrow H + C_2H_2$	5.68E + 10	0.9	1,993
173	$C_2H_3 + O_2 \rightarrow HCO + CH_2O$	4.58E + 16	−1.4	1,015
174	$C_2H_4 (+ M) \rightarrow H_2 + C_2H_2 (+ M)$		pressure dependent	
175	$C_2H_5 + O_2 \rightarrow HO_2 + C_2H_4$	8.40E + 11	0.0	3,875
176	$HCCO + O_2 \rightarrow OH + CO + CO$	3.20E + 12	0.0	854
177	$HCCO + HCCO \rightarrow CO + CO + C_2H_2$	1.00E + 13	0.0	0.0
N-Containing Reactions				
178	$N + NO \rightarrow N_2 + O$	2.70E + 13	0.0	355
179	$N + O_2 \rightarrow NO + O$	9.00E + 09	1.0	6,500
180	$N + OH \rightarrow NO + H$	3.36E + 13	0.0	385
181	$N_2O + O \rightarrow N_2 + O_2$	1.40E + 12	0.0	10,810
182	$N_2O + O \rightarrow NO + NO$	2.90E + 13	0.0	23,150
183	$N_2O + H \rightarrow N_2 + OH$	3.87E + 14	0.0	18,880
184	$N_2O + OH \rightarrow N_2 + HO_2$	2.00E + 12	0.0	21,060
185	$N_2O (+ M) \rightarrow N_2 + O (+ M)$		pressure dependent	
186	$HO_2 + NO \rightarrow NO_2 + OH$	2.11E + 12	0.0	−480
187	$NO + O + M \rightarrow NO_2 + M$	1.06E + 20	−1.4	0.0
188	$NO_2 + O \rightarrow NO + O_2$	3.90E + 12	0.0	−240
189	$NO_2 + H \rightarrow NO + OH$	1.32E + 14	0.0	360
190	$NH + O \rightarrow NO + H$	4.00E + 13	0.0	0.0
191	$NH + H \rightarrow N + H_2$	3.20E + 13	0.0	330
192	$NH + OH \rightarrow HNO + H$	2.00E + 13	0.0	0.0
193	$NH + OH \rightarrow N + H_2O$	2.00E + 09	1.2	0.0
194	$NH + O_2 \rightarrow HNO + O$	4.61E + 05	2.0	6,500
195	$NH + O_2 \rightarrow NO + OH$	1.28E + 06	1.5	100
196	$NH + N \rightarrow N_2 + H$	1.50E + 13	0.0	0.0
197	$NH + H_2O \rightarrow HNO + H_2$	2.00E + 13	0.0	13,850
198	$NH + NO \rightarrow N_2 + OH$	2.16E + 13	−0.2	0.0
199	$NH + NO \rightarrow N_2O + H$	3.65E + 14	−0.5	0.0
200	$NH_2 + O \rightarrow OH + NH$	3.00E + 12	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
N-Containing Reactions (continued)				
201	$NH_2 + O \rightarrow H + HNO$	3.9E + 13	0.0	0.0
202	$NH_2 + H \rightarrow NH + H_2$	4.00E + 13	0.0	3,650
203	$NH_2 + OH \rightarrow NH + H_2O$	9.00E + 07	1.5	−460
204	$NNH \rightarrow N_2 + H$	3.30E + 08	0.0	0.0
205	$NNH + M \rightarrow N_2 + H + M$	1.30E + 14	−0.1	4,980
206	$NNH + O_2 \rightarrow HO_2 + N_2$	5.00E + 12	0.0	0.0
207	$NNH + O \rightarrow OH + N_2$	2.50E + 13	0.0	0.0
208	$NNH + O \rightarrow NH + NO$	7.00E + 13	0.0	0.0
209	$NNH + H \rightarrow H_2 + N_2$	5.00E + 13	0.0	0.0
210	$NNH + OH \rightarrow H_2O + N_2$	2.00E + 13	0.0	0.0
211	$NNH + CH_3 \rightarrow CH_4 + N_2$	2.50E + 13	0.0	0.0
212	$H + NO + M \rightarrow HNO + M$	4.48E + 19	−1.3	740
213	$HNO + O \rightarrow NO + OH$	2.50E + 13	0.0	0.0
214	$HNO + H \rightarrow H_2 + NO$	9.00E + 11	0.7	660
215	$HNO + OH \rightarrow NO + H_2O$	1.30E + 07	1.9	−950
216	$HNO + O_2 \rightarrow HO_2 + NO$	1.00E + 13	0.0	13,000
217	$CN + O \rightarrow CO + N$	7.70E + 13	0.0	0.0
218	$CN + OH \rightarrow NCO + H$	4.00E + 13	0.0	0.0
219	$CN + H_2O \rightarrow HCN + OH$	8.00E + 12	0.0	7,460
220	$CN + O_2 \rightarrow NCO + O$	6.14E + 12	0.0	−440
221	$CN + H_2 \rightarrow HCN + H$	2.95E + 05	2.5	2,240
222	$NCO + O \rightarrow NO + CO$	2.35E + 13	0.0	0.0
223	$NCO + H \rightarrow NH + CO$	5.40E + 13	0.0	0.0
224	$NCO + OH \rightarrow NO + H + CO$	2.50E + 12	0.0	0.0
225	$NCO + N \rightarrow N_2 + CO$	2.00E + 13	0.0	0.0
226	$NCO + O_2 \rightarrow NO + CO_2$	2.00E + 12	0.0	20,000
227	$NCO + M \rightarrow N + CO + M$	3.10E + 14	0.0	54,050
228	$NCO + NO \rightarrow N_2O + CO$	1.90E + 17	−1.5	740
229	$NCO + NO \rightarrow N_2 + CO_2$	3.80E + 18	−2.0	800
230	$HCN + M \rightarrow H + CN + M$	1.04E + 29	−3.3	126,600
231	$HCN + O \rightarrow NCO + H$	2.03E + 04	2.6	4,980
232	$HCN + O \rightarrow NH + CO$	5.07E + 03	2.6	4,980
233	$HCN + O \rightarrow CN + OH$	3.91E + 09	1.6	26,600
234	$HCN + OH \rightarrow HOCN + H$	1.10E + 06	2.0	13,370
235	$HCN + OH \rightarrow HNCO + H$	4.40E + 03	2.3	6,400
236	$HCN + OH \rightarrow NH_2 + CO$	1.60E + 02	2.6	9,000
237	$H + HCN + M \rightarrow H_2CN + M$		pressure dependent	
238	$H_2CN + N \rightarrow N_2 + CH_2$	6.00E + 13	0.0	400
239	$C + N_2 \rightarrow CN + N$	6.30E + 13	0.0	46,020
240	$CH + N_2 \rightarrow HCN + N$	3.12E + 09	0.9	20,130
241	$CH + N_2 (+ M) \rightarrow HCNN (+ M)$		pressure dependent	
242	$CH_2 + N_2 \rightarrow HCN + NH$	1.00E + 13	0.0	74,000
243[b]	$CH_2(S) + N_2 \rightarrow NH + HCN$	1.00E + 11	0.0	65,000

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a] A	b	E
N-Containing Reactions (continued)				
244	$C + NO \rightarrow CN + O$	1.90E + 13	0.0	0.0
245	$C + NO \rightarrow CO + N$	2.90E + 13	0.0	0.0
246	$CH + NO \rightarrow HCN + O$	4.10E + 13	0.0	0.0
247	$CH + NO \rightarrow H + NCO$	1.62E + 13	0.0	0.0
248	$CH + NO \rightarrow N + HCO$	2.46E + 13	0.0	0.0
249	$CH_2 + NO \rightarrow H + HNCO$	3.10E + 17	−1.4	1,270
250	$CH_2 + NO \rightarrow OH + HCN$	2.90E + 14	−0.7	760
251	$CH_2 + NO \rightarrow H + HCNO$	3.80E + 13	−0.4	580
252[b]	$CH_2(S) + NO \rightarrow H + HNCO$	3.10E + 17	−1.4	1,270
253[b]	$CH_2(S) + NO \rightarrow OH + HCN$	2.90E + 14	−0.7	760
254[b]	$CH_2(S) + NO \rightarrow H + HCNO$	3.80E + 13	−0.4	580
255	$CH_3 + NO \rightarrow HCN + H_2O$	9.60E + 13	0.0	28,800
256	$CH_3 + NO \rightarrow H_2CN + OH$	1.00E + 12	0.0	21,750
257	$HCNN + O \rightarrow CO + H + N_2$	2.20E + 13	0.0	0.0
258	$HCNN + O \rightarrow HCN + NO$	2.00E + 12	0.0	0.0
259	$HCNN + O_2 \rightarrow O + HCO + N_2$	1.20E + 13	0.0	0.0
260	$HCNN + OH \rightarrow H + HCO + N_2$	1.20E + 13	0.0	0.0
261	$HCNN + H \rightarrow CH_2 + N_2$	1.00E + 14	0.0	0.0
262	$HNCO + O \rightarrow NH + CO_2$	9.80E + 07	1.4	8,500
263	$HNCO + O \rightarrow HNO + CO$	1.50E + 08	1.6	44,000
264	$HNCO + O \rightarrow NCO + OH$	2.20E + 06	2.1	11,400
265	$HNCO + H \rightarrow NH_2 + CO$	2.25E + 07	1.7	3,800
266	$HNCO + H \rightarrow H_2 + NCO$	1.05E + 05	2.5	13,300
267	$HNCO + OH \rightarrow NCO + H_2O$	3.30E + 07	1.5	3,600
268	$HNCO + OH \rightarrow NH_2 + CO_2$	3.30E + 06	1.5	3,600
269	$HNCO + M \rightarrow NH + CO + M$	1.18E + 16	0.0	84,720
270	$HCNO + H \rightarrow H + HNCO$	2.10E + 15	−0.7	2,850
271	$HCNO + H \rightarrow OH + HCN$	2.70E + 11	0.2	2,120
272	$HCNO + H \rightarrow NH_2 + CO$	1.70E + 14	−0.8	2,890
273	$HOCN + H \rightarrow H + HNCO$	2.00E + 07	2.0	2,000
274	$HCCO + NO \rightarrow HCNO + CO$	9.00E + 12	0.0	0.0
275	$CH_3 + N \rightarrow H_2CN + H$	6.10E + 14	−0.3	290
276	$CH_3 + N \rightarrow HCN + H_2$	3.70E + 12	0.1	−90
277	$NH_3 + H \rightarrow NH_2 + H_2$	5.40E + 05	2.4	9,915
278	$NH_3 + OH \rightarrow NH_2 + H_2O$	5.00E + 07	1.6	955
279	$NH_3 + O \rightarrow NH_2 + OH$	9.40E + 06	1.9	6,460
Reactions Added in Update from Version 2.11 to Version 3.0				
280	$NH + CO_2 \rightarrow HNO + CO$	1.00E + 13	0.0	14,350
281	$CN + NO_2 \rightarrow NCO + NO$	6.16E + 15	−0.8	345
282	$NCO + NO_2 \rightarrow N_2O + CO_2$	3.25E + 12	0.0	−705
283	$N + CO_2 \rightarrow NO + CO$	3.00E + 12	0.0	11,300
284	$O + CH_3 \rightarrow H + H_2 + CO$	3.37E + 13	0.0	0.0
285	$O + C_2H_4 \rightarrow CH_2CHO$	6.70E + 06	1.8	220
286	$O + C_2H_5 \rightarrow H + CH_3CHO$	1.10E + 14	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient[a]		
		A	*b*	*E*
Reactions Added in Update from Version 2.11 to Version 3.0 (continued)				
287	$OH + HO_2 \rightarrow O_2 + H_2O$	5.00E + 15	0.0	17,330
288	$OH + CH_3 \rightarrow H_2 + CH_2O$	8.00E + 09	0.5	−1,755
289	$CH + H_2 + M \rightarrow CH_3 + M$		pressure dependent	
290	$CH_2 + O_2 \rightarrow H + H + CO_2$	5.80E + 12	0.0	1,500
291	$CH_2 + O_2 \rightarrow O + CH_2O$	2.40E + 12	0.0	1,500
292	$CH_2 + CH_2 \rightarrow H + H + C_2H_2$	2.00E + 14	0.0	10,989
293[b]	$CH_2(S) + H_2O \rightarrow H_2 + CH_2O$	6.82E + 10	0.2	−935
294	$C_2H_3 + O_2 \rightarrow O + CH_2CHO$	3.03E + 11	0.3	11
295	$C_2H_3 + O_2 \rightarrow HO_2 + C_2H_2$	1.34E + 06	1.6	−384
296	$O + CH_3CHO \rightarrow OH + CH_2CHO$	2.92E + 12	0.0	1,808
297	$O + CH_3CHO \rightarrow OH + CH_3 + CO$	2.92E + 12	0.0	1,808
298	$O_2 + CH_3CHO \rightarrow HO_2 + CH_3 + CO$	3.01E + 13	0.0	39,150
299	$H + CH_3CHO \rightarrow CH_2CHO + H_2$	2.05E + 09	1.2	2,405
300	$H + CH_3CHO \rightarrow CH_3 + H_2 + CO$	2.05E + 09	1.2	2,405
301	$OH + CH_3CHO \rightarrow CH_3 + H_2O + CO$	2.34E + 10	0.7	−1,113
302	$HO_2 + CH_3CHO \rightarrow CH_3 + H_2O_2 + CO$	3.01E + 12	0.0	11,923
303	$CH_3 + CH_3CHO \rightarrow CH_3 + CH_4 + CO$	2.72E + 06	1.8	5,920
304	$H + CH_2CO + M \rightarrow CH_2CHO + M$		pressure dependent	
305	$O + CH_2CHO \rightarrow H + CH_2 + CO_2$	1.50E + 14	0.0	0.0
306	$O_2 + CH_2CHO \rightarrow OH + CO + CH_2O$	1.81E + 10	0.0	0.0
307	$O_2 + CH_2CHO \rightarrow OH + HCO + HCO$	2.35E + 10	0.0	0.0
308	$H + CH_2CHO \rightarrow CH_3 + HCO$	2.20E + 13	0.0	0.0
309	$H + CH_2CHO \rightarrow CH_2CO + H_2$	1.10E + 13	0.0	0.0
310	$OH + CH_2CHO \rightarrow H_2O + CH_2CO$	1.20E + 13	0.0	0.0
311	$OH + CH_2CHO \rightarrow HCO + CH_2OH$	3.01E + 13	0.0	0.0
312	$CH_3 + C_2H_5 + M \rightarrow C_3H_8 + M$		pressure dependent	
313	$O + C_3H_8 \rightarrow OH + C_3H_7$	1.93E + 05	2.7	3,716
314	$H + C_3H_8 \rightarrow C_3H_7 + H_2$	1.32E + 06	2.5	6,756
315	$OH + C_3H_8 \rightarrow C_3H_7 + H_2O$	3.16E + 07	1.8	934
316	$C_3H_7 + H_2O_2 \rightarrow HO_2 + C_3H_8$	3.78E + 02	2.7	1,500
317	$CH_3 + C_3H_8 \rightarrow C_3H_7 + CH_4$	9.03E − 01	3.6	7,154
318	$CH_3 + C_2H_4 + M \rightarrow C_3H_7 + M$		pressure dependent	
319	$O + C_3H_7 \rightarrow C_2H_5 + CH_2O$	9.64E + 13	0.0	0.0
320	$H + C_3H_7 + M \rightarrow C_3H_8 + M$		pressure dependent	
321	$H + C_3H_7 \rightarrow CH_3 + C_2H_5$	4.06E + 06	2.2	890
322	$OH + C_3H_7 \rightarrow C_2H_5 + CH_2OH$	2.41E + 13	0.0	0.0
323	$HO_2 + C_3H_7 \rightarrow O_2 + C_3H_8$	2.55E + 10	0.3	−943
324	$HO_2 + C_3H_7 \rightarrow OH + C_2H_5 + CH_2O$	2.41E + 13	0.0	0.0
325	$CH_3 + C_3H_7 \rightarrow C_2H_5 + C_2H_5$	1.93E + 13	−0.3	0.0

[a]The forward rate coefficient $k = AT^b \exp(-E/RT)$. R is the universal gas constant, T is the temperature in K. The units of A involve gmol/cm^3 and s, and those of E, cal/gmol.

[b]$CH_2(S)$ designates the singlet state of CH_2.

Smith, G. P., Golden, D. M., Frenklach, M., Moriarity, N. M., Eiteneer, B., Goldenberg, M., Bowman, C. T., Hanson, R. K., Song, S., Gardiner, W. C., Jr., Lissianski, V. V., and Qin, Z., GRI-Mech Home Page, http://www.me.berkeley.edu/gri_mech/.