Appendix C

CB6r5h Gas-Phase Chemistry

Table C-1. Reactions and rate constant expressions for the CB6r5h mechanism. k_{298} is the rate constant at 298 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. See Table C-2 for species names. See Section 3.1 on temperature and pressure dependencies. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL. See Table C-3 for a listing of photolysis rates by zenith angle.

yellow means different k btwn cb6r2 and this doc

Number	Reactants and Products	Rate Constant Expression	k_{298}
1	NO2 = NO + O	Photolysis	6.30E-3
2	O + O2 + M = O3 + M	k = 6.00E-34 (T/300)^-2.6	6.11E-34
3	O3 + NO = NO2	k = 2.07E-12 exp(-1400/T)	1.89E-14
4	O + NO = NO2	Falloff: F=0.85; n=0.84 k(0) = 1.00E-31 (T/300)^-1.6 k(inf) = 5.00E-11 (T/300)^-0.3	2.26E-12
5	O + NO2 = NO	k = 5.10E-12 exp(198/T)	9.91E-12
6	O + NO2 = NO3	Falloff: F=0.6; n=1.03 k(0) = 1.30E-31 (T/300)^-1.5 k(inf) = 2.30E-11 (T/300)^0.24	2.09E-12
7	O + O3 =	k = 8.00E-12 exp(-2060/T)	7.96E-15
8	O3 = O	Photolysis copy from all rxns file	3.33E-4
9	O3 = O1D	Photolysis	8.78E-6
10	O1D + M = O + M	k = 2.23E-11 exp(115/T)	3.28E-11
11	O1D + H2O = 2 OH	k = 2.14E-10	2.14E-10
12	O3 + OH = HO2	k = 1.70E-12 exp(-940/T)	7.25E-14
13	O3 + HO2 = OH	k = 2.03E-16 (T/300)^4.57 exp(693/T)	2.01E-15
14	OH + O = HO2	k = 2.40E-11 exp(110/T)	3.47E-11
15	HO2 + O = OH	k = 3.00E-11 exp(200/T)	5.87E-11
16	OH + OH = O	k = 6.20E-14 (T/298)^2.6 exp(945/T)	1.48E-12
17	OH + OH = H2O2	Falloff: F=0.42; n=1.23 k(0) = 9.00E-31 (T/300)^-3.2 k(inf) = 3.90E-11 (T/300)^-0.47	6.21E-12
18	OH + HO2 =	k = 4.80E-11 exp(250/T)	1.11E-10
19	HO2 + HO2 = H2O2	k = k1 + k2 [M] k1 = 2.20E-13 exp(600/T) k2 = 1.90E-33 exp(980/T)	2.90E-12
20	HO2 + HO2 + H2O = H2O2	k = k1 + k2 [M] k1 = 3.08E-34 exp(2800/T) k2 = 2.66E-54 exp(3180/T)	6.53E-30
21	H2O2 = 2 OH	Photolysis	3.78E-6
22	H2O2 + OH = HO2	k = 1.80E-12	1.80E-12
23	H2O2 + O = OH + HO2	k = 1.40E-12 exp(-2000/T)	1.70E-15
24	NO + NO + O2 = 2 NO2	k = 4.25E-39 exp(664/T)	3.95E-38
25	HO2 + NO = OH + NO2	k = 3.45E-12 exp(270/T)	8.54E-12
26	NO2 + O3 = NO3	k = 1.40E-13 exp(-2470/T)	3.52E-17
27	NO3 = NO2 + O	Photolysis	1.56E-1
28	NO3 = NO	Photolysis JNO3NO	1.98E-2
29	NO3 + NO = 2 NO2	k = 1.80E-11 exp(110/T)	2.60E-11
30	NO3 + NO2 = NO + NO2	k = 4.50E-14 exp(-1260/T)	6.56E-16

give a name in k file
put the string into the list as 'filename'

Number	Reactants and Products	Rate Constant Expression	k_{298}
31	NO3 + O = NO2	k = 1.70E-11	1.70E-11
32	NO3 + OH = HO2 + NO2	k = 2.00E-11	2.00E-11
33	NO3 + HO2 = OH + NO2	k = 4.00E-12	4.00E-12
34	NO3 + O3 = NO2	k = 1.00E-17	1.00E-17
35	NO3 + NO3 = 2 NO2	k = 8.50E-13 exp(-2450/T)	2.28E-16
36	NO3 + NO2 = N2O5	Falloff: F=0.35; n=1.33 k(0) = 3.60E-30 (T/300)^-4.1 k(inf) = 1.90E-12 (T/300)^0.2	1.24E-12
37	N2O5 = NO3 + NO2	Falloff: F=0.35; n=1.33 k(0) = 1.30E-3 (T/300)^-3.5 exp(-11000/T) k(inf) = 9.70E+14 (T/300)^0.1 exp(-11080/T)	4.46E-2
38	N2O5 = NO2 + NO3	Photolysis	2.52E-5
39	N2O5 + H2O = 2 HNO3	k = 1.00E-22	1.00E-22
40	NO + OH = HONO	Falloff: F=0.81; n=0.87 k(0) = 7.40E-31 (T/300)^-2.4 k(inf) = 3.30E-11 (T/300)^-0.3	9.77E-12
41	NO + NO2 + H2O = 2 HONO	k = 5.00E-40	5.00E-40
42	HONO + HONO = NO + NO2	k = 1.00E-20	1.00E-20
43	HONO = NO + OH	Photolysis	1.04E-3
44	HONO + OH = NO2	k = 2.50E-12 exp(260/T)	5.98E-12
45	NO2 + OH = HNO3	Falloff: F=0.6; n=1 k(0) = 1.80E-30 (T/300)^-3 k(inf) = 2.80E-11	1.06E-11
46	HNO3 + OH = NO3	k = k1 + k3 [M] / (1 + k3 [M]/k2) k1 = 2.40E-14 exp(460/T) k2 = 2.70E-17 exp(2199/T) k3 = 6.50E-34 exp(1335/T)	1.54E-13
47	HNO3 = OH + NO2	Photolysis	2.54E-7
48	HO2 + NO2 = PNA	Falloff: F=0.4; n=1.26 k(0) = 1.40E-31 (T/300)^-3.1 k(inf) = 4.00E-12	7.50E-13
49	PNA = HO2 + NO2	Falloff: F=0.4; n=1.26 k(0) = 4.10E-5 exp(-10650/T) k(inf) = 6.00E+15 exp(-11170/T)	6.20E-2
50	PNA = 0.59 HO2 + 0.59 NO2 + 0.41 OH + 0.41 NO3	Photolysis	2.36E-6
51	PNA + OH = NO2	k = 3.20E-13 exp(690/T)	3.24E-12
52	SO2 + OH = SULF + HO2	Falloff: F=0.53; n=1.1 k(0) = 2.80E-31 (T/300)^-2.6 k(inf) = 2.00E-12	9.35E-13
53	C2O3 + NO = NO2 + MEO2 + RO2	k = 7.50E-12 exp(290/T)	1.98E-11
54	C2O3 + NO2 = PAN	Falloff: F=0.3; n=1.41 k(0) = 3.61E-28 (T/300)^-6.87 k(inf) = 1.24E-11 (T/300)^-1.105	9.86E-12
55	PAN = NO2 + C2O3	Falloff: F=0.3; n=1.41 k(0) = 1.10E-5 exp(-10100/T) k(inf) = 1.90E+17 exp(-14100/T)	4.31E-4

Number	Reactants and Products	Rate Constant Expression	k_{298}
56	PAN = 0.6 NO2 + 0.6 C2O3 + 0.4 NO3 + 0.4 MEO2 + 0.4 RO2	Photolysis	3.47E-7
57	C2O3 + HO2 = 0.37 PACD + 0.13 AACD + 0.13 O3 + 0.5 OH + 0.5 MEO2 + 0.5 RO2	k = 3.14E-12 exp(580/T)	2.20E-11
58	C2O3 + RO2 = MEO2	k = 4.40E-13 exp(1070/T)	1.60E-11
59	C2O3 + C2O3 = 2 MEO2 + 2 RO2	k = 2.90E-12 exp(500/T)	1.55E-11
60	C2O3 + CXO3 = MEO2 + ALD2 + XO2H + 2 RO2	k = k(ref)/K k(ref) = k(59) K = 1.00E+0	1.55E-11
61	CXO3 + NO = NO2 + ALD2 + XO2H + RO2	k = 6.70E-12 exp(340/T)	2.10E-11
62	CXO3 + NO2 = PANX	k = k(ref)/K k(ref) = k(54) K = 1.19E+0	8.28E-12
63	PANX = NO2 + CXO3	k = k(ref)/K k(ref) = k(55) K = 1.19E+0	3.62E-4
64	PANX = 0.6 NO2 + 0.6 CXO3 + 0.4 NO3 + 0.4 ALD2 + 0.4 XO2H + 0.4 RO2	Photolysis	3.47E-7
65	CXO3 + HO2 = 0.37 PACD + 0.13 AACD + 0.13 O3 + 0.5 OH + 0.5 MEO2 + 0.5 RO2	k = k(ref)/K k(ref) = k(57) K = 1.00E+0	2.20E-11
66	CXO3 + RO2 = MEO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
67	CXO3 + CXO3 = 2 MEO2 + 2 RO2	k = k(ref)/K k(ref) = k(59) K = 1.00E+0	1.55E-11
68	RO2 + NO = NO	k = 2.40E-12 exp(360/T)	8.03E-12
69	RO2 + HO2 = HO2	k = 4.80E-13 exp(800/T)	7.03E-12
70	RO2 + RO2 =	k = 6.50E-14 exp(500/T)	3.48E-13
71	MEO2 + NO = FORM + HO2 + NO2	k = 2.30E-12 exp(360/T)	7.70E-12
72	MEO2 + HO2 = 0.9 MEPX + 0.1 FORM	k = 3.80E-13 exp(780/T)	5.21E-12
73	MEO2 + C2O3 = FORM + 0.9 HO2 + 0.9 MEO2 + 0.1 AACD + 0.9 RO2	k = 2.00E-12 exp(500/T)	1.07E-11
74	MEO2 + RO2 = 0.685 FORM + 0.315 MEOH + 0.37 HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
75	XO2H + NO = NO2 + HO2	k = 2.70E-12 exp(360/T)	9.04E-12
76	XO2H + HO2 = ROOH	k = 6.80E-13 exp(800/T)	9.96E-12
77	XO2H + C2O3 = 0.8 HO2 + 0.8 MEO2 + 0.2 AACD + 0.8 RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
78	XO2H + RO2 = 0.6 HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
79	XO2 + NO = NO2	k = k(ref)/K k(ref) = k(75) K = 1.00E+0	9.04E-12

Number	Reactants and Products	Rate Constant Expression	k_{298}
80	XO2 + HO2 = ROOH	k = k(ref)/K k(ref) = k(76) K = 1.00E+0	9.96E-12
81	XO2 + C2O3 = 0.8 MEO2 + 0.2 AACD + 0.8 RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
82	XO2 + RO2 = RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
83	XO2N + NO = 0.5 NTR1 + 0.5 NTR2	k = k(ref)/K k(ref) = k(75) K = 1.00E+0	9.04E-12
84	XO2N + HO2 = ROOH	k = k(ref)/K k(ref) = k(76) K = 1.00E+0	9.96E-12
85	XO2N + C2O3 = 0.8 HO2 + 0.8 MEO2 + 0.2 AACD + 0.8 RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
86	XO2N + RO2 = RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
87	MEPX + OH = 0.6 MEO2 + 0.6 RO2 + 0.4 FORM + 0.4 OH	k = 5.30E-12 exp(190/T)	1.00E-11
88	MEPX = MEO2 + RO2 + OH	Photolysis	2.68E-6
89	ROOH + OH = 0.54 XO2H + 0.06 XO2N + 0.6 RO2 + 0.4 OH	k = 5.30E-12 exp(190/T)	1.00E-11
90	ROOH = HO2 + OH	Photolysis	2.68E-6
91	NTR1 + OH = NTR2	k = 2.00E-12	2.00E-12
92	NTR1 = NO2	Photolysis	1.06E-6
93	FACD + OH = HO2	k = 4.50E-13	4.50E-13
94	AACD + OH = MEO2 + RO2	k = 4.00E-14 exp(850/T)	6.93E-13
95	PACD + OH = C2O3	k = 1.00E-14	1.00E-14
96	FORM + OH = HO2 + CO	k = 5.40E-12 exp(135/T)	8.49E-12
97	FORM = 2 HO2 + CO	Photolysis	1.69E-5
98	FORM = CO + H2	Photolysis	2.69E-5
99	FORM + NO3 = HNO3 + HO2 + CO	k = 5.50E-16	5.50E-16
100	FORM + HO2 = HCO3	k = 9.70E-15 exp(625/T)	7.90E-14
101	HCO3 = FORM + HO2	k = 2.40E+12 exp(-7000/T)	1.51E+2
102	HCO3 + NO = FACD + NO2 + HO2	k = 5.60E-12	5.60E-12
103	HCO3 + HO2 = 0.5 MEPX + 0.5 FACD + 0.2 OH + 0.2 HO2	k = 5.60E-15 exp(2300/T)	1.26E-11
104	ALD2 + OH = C2O3	k = 4.70E-12 exp(345/T)	1.50E-11
105	ALD2 + NO3 = C2O3 + HNO3	k = 1.40E-12 exp(-1860/T)	2.73E-15
106	ALD2 = MEO2 + RO2 + CO + HO2	Photolysis	1.96E-6
107	ALDX + OH = CXO3	k = 4.90E-12 exp(405/T)	1.91E-11
108	ALDX + NO3 = CXO3 + HNO3	k = 6.30E-15	6.30E-15
109	ALDX = ALD2 + XO2H + RO2 + CO + HO2	Photolysis	2.62E-5
110	GLYD + OH = 0.2 GLY + 0.2 HO2 + 0.8 C2O3	k = 8.00E-12	8.00E-12

Number	Reactants and Products	Rate Constant Expression	k_{298}
111	GLYD = 0.74 FORM + 0.89 CO + 1.4 HO2 + 0.15 MEOH + 0.19 OH + 0.11 GLY + 0.11 XO2H + 0.11 RO2	Photolysis	2.76E-6
112	GLYD + NO3 = HNO3 + C2O3	k = k(ref)/K k(ref) = k(105) K = 1.00E+0	2.73E-15
113	GLY + OH = 1.8 CO + 0.2 XO2 + 0.2 RO2 + HO2	k = 3.10E-12 exp(340/T)	9.70E-12
114	GLY = 2 HO2 + 2 CO	Photolysis	7.95E-5
115	GLY + NO3 = HNO3 + 1.5 CO + 0.5 XO2 + 0.5 RO2 + HO2	k = 4.00E-16	4.00E-16
116	MGLY = C2O3 + HO2 + CO	Photolysis	1.46E-4
117	MGLY + NO3 = HNO3 + C2O3 + XO2 + RO2	k = 5.00E-16	5.00E-16
118	MGLY + OH = C2O3 + CO	k = 1.90E-12 exp(575/T)	1.31E-11
119	H2 + OH = HO2	k = 7.70E-12 exp(-2100/T)	6.70E-15
120	CO + OH = HO2	k = k1 + k2 [M] k1 = 1.44E-13 k2 = 3.43E-33	2.28E-13
121	CH4 + OH = MEO2 + RO2	k = 1.85E-12 exp(-1690/T)	6.37E-15
122	ETHA + OH = 0.991 ALD2 + 0.991 XO2H + 0.009 XO2N + RO2	k = 6.90E-12 exp(-1000/T)	2.41E-13
123	MEOH + OH = FORM + HO2	k = 2.85E-12 exp(-345/T)	8.95E-13
124	ETOH + OH = 0.95 ALD2 + 0.9 HO2 + 0.1 XO2H + 0.1 RO2 + 0.078 FORM + 0.011 GLYD	k = 3.00E-12 exp(20/T)	3.21E-12
125	KET = 0.5 ALD2 + 0.5 C2O3 + 0.5 XO2H + 0.5 CXO3 + 0.5 MEO2 + RO2 - 2.5 PAR	Photolysis	2.27E-7
126	ACET = 0.38 CO + 1.38 MEO2 + 1.38 RO2 + 0.62 C2O3	Photolysis	2.08E-7
127	ACET + OH = FORM + C2O3 + XO2 + RO2	k = 1.41E-12 exp(-620.6/T)	1.76E-13
128	PRPA + OH = XPRP	k = 7.60E-12 exp(-585/T)	1.07E-12
129	PAR + OH = XPAR	k = 8.10E-13	8.10E-13
130	ROR = 0.2 KET + 0.42 ACET + 0.74 ALD2 + 0.37 ALDX + 0.04 XO2N + 0.94 XO2H + 0.98 RO2 + 0.02 ROR - 2.7 PAR	k = 5.70E+12 exp(-5780/T)	2.15E+4
131	ROR + O2 = KET + HO2	k = 1.50E-14 exp(-200/T)	7.67E-15
132	ROR + NO2 = NTR1	k = 8.60E-12 exp(400/T)	3.29E-11
133	ETHY + OH = 0.7 GLY + 0.7 OH + 0.3 FACD + 0.3 CO + 0.3 HO2	Falloff: F=0.37; n=1.3 k(0) = 5.00E-30 (T/300)^-1.5 k(inf) = 1.00E-12	7.52E-13
134	ETH + OH = XO2H + RO2 + 1.56 FORM + 0.22 GLYD	Falloff: F=0.48; n=1.15 k(0) = 8.60E-29 (T/300)^-3.1 k(inf) = 9.00E-12 (T/300)^-0.85	7.84E-12
135	ETH + O3 = FORM + 0.35 CO + 0.27 HO2 + 0.17 OH + 0.42 FACD	k = 6.82E-15 exp(-2500/T)	1.55E-18
136	ETH + NO3 = 0.5 NO2 + 0.5 NTR1 + 0.5 XO2H + 0.5 XO2 + RO2 + 1.125 FORM	k = 3.30E-12 exp(-2880/T)	2.10E-16

Number	Reactants and Products	Rate Constant Expression	k_{298}
137	OLE + OH = 0.781 FORM + 0.488 ALD2 + 0.488 ALDX + 0.976 XO2H + 0.195 XO2 + 0.024 XO2N + 1.195 RO2 - 0.73 PAR	Falloff: F=0.5; n=1.13 k(0) = 8.00E-27 (T/300)^-3.5 k(inf) = 3.00E-11 (T/300)^-1	2.86E-11
138	OLE + O3 = 0.295 ALD2 + 0.555 FORM + 0.27 ALDX + 0.15 XO2H + 0.15 RO2 + 0.334 OH + 0.08 HO2 + 0.378 CO + 0.075 GLY + 0.075 MGLY + 0.09 FACD + 0.13 AACD + 0.04 H2O2 - 0.79 PAR	k = 5.50E-15 exp(-1880/T)	1.00E-17
139	OLE + NO3 = 0.5 NO2 + 0.5 NTR1 + 0.48 XO2 + 0.48 XO2H + 0.04 XO2N + RO2 + 0.5 FORM + 0.25 ALD2 + 0.375 ALDX - 1 PAR	k = 4.60E-13 exp(-1155/T)	9.54E-15
140	IOLE + OH = 1.3 ALD2 + 0.7 ALDX + XO2H + RO2	k = 1.05E-11 exp(519/T)	5.99E-11
141	IOLE + O3 = 0.732 ALD2 + 0.442 ALDX + 0.128 FORM + 0.245 CO + 0.5 OH + 0.3 XO2H + 0.3 RO2 + 0.24 GLY + 0.06 MGLY + 0.29 PAR + 0.08 AACD + 0.08 H2O2	k = 4.70E-15 exp(-1013/T)	1.57E-16
142	IOLE + NO3 = 0.5 NO2 + 0.5 NTR1 + 0.48 XO2 + 0.48 XO2H + 0.04 XO2N + RO2 + 0.5 ALD2 + 0.625 ALDX + PAR	k = 3.70E-13	3.70E-13
143	ISOP + OH = ISO2 + RO2	k = 2.70E-11 exp(390/T)	9.99E-11
144	ISO2 + NO = 0.1 INTR + 0.9 NO2 + 0.673 FORM + 0.9 ISPD + 0.818 HO2 + 0.082 XO2H + 0.082 RO2	k = 2.39E-12 exp(365/T)	8.13E-12
145	ISO2 + HO2 = 0.88 ISPX + 0.12 OH + 0.12 HO2 + 0.12 FORM + 0.12 ISPD	k = 7.43E-13 exp(700/T)	7.78E-12
146	ISO2 + C2O3 = 0.598 FORM + 1 ISPD + 0.728 HO2 + 0.072 XO2H + 0.8 MEO2 + 0.2 AACD + 0.872 RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
147	ISO2 + RO2 = 0.598 FORM + 1 ISPD + 0.728 HO2 + 0.072 XO2H + 1.072 RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
148	ISO2 = HO2 + HPLD	k = 3.30E+9 exp(-8300/T)	2.64E-3
149	ISOP + O3 = 0.6 FORM + 0.65 ISPD + 0.15 ALDX + 0.2 CXO3 + 0.35 PAR + 0.266 OH + 0.2 XO2 + 0.2 RO2 + 0.066 HO2 + 0.066 CO	k = 1.03E-14 exp(-1995/T)	1.27E-17
150	ISOP + NO3 = 0.35 NO2 + 0.65 NTR2 + 0.64 XO2H + 0.33 XO2 + 0.03 XO2N + RO2 + 0.35 FORM + 0.35 ISPD	k = 3.03E-12 exp(-448/T)	6.74E-13
151	ISPD + OH = 0.022 XO2N + 0.521 XO2 + 0.115 MGLY + 0.115 MEO2 + 0.269 GLYD + 0.269 C2O3 + 0.457 OPO3 + 0.117 PAR + 0.137 ACET + 0.137 CO + 0.137 HO2 + 0.658 RO2	k = 5.58E-12 exp(511/T)	3.10E-11
152	ISPD + O3 = 0.04 ALD2 + 0.231 FORM + 0.531 MGLY + 0.17 GLY + 0.17 ACET + 0.543 CO + 0.461 OH + 0.15 FACD + 0.398 HO2 + 0.143 C2O3	k = 3.88E-15 exp(-1770/T)	1.02E-17

Number	Reactants and Products	Rate Constant Expression	k_{298}
153	ISPD + NO3 = 0.717 HNO3 + 0.142 NTR2 + 0.142 NO2 + 0.142 XO2 + 0.142 XO2H + 0.113 GLYD + 0.113 MGLY + 0.717 PAR + 0.717 CXO3 + 0.284 RO2	k = 4.10E-12 exp(-1860/T)	7.98E-15
154	ISPD = 0.76 HO2 + 0.34 XO2H + 0.16 XO2 + 0.34 MEO2 + 0.208 C2O3 + 0.26 FORM + 0.24 OLE + 0.24 PAR + 0.17 ACET + 0.128 GLYD + 0.84 RO2	Photolysis	1.60E-5
155	ISPX + OH = 0.904 EPOX + 0.933 OH + 0.067 ISO2 + 0.067 RO2 + 0.029 IOLE + 0.029 ALDX	k = 2.23E-11 exp(372/T)	7.77E-11
156	HPLD = OH + ISPD	Photolysis	4.41E-4
157	HPLD + NO3 = HNO3 + ISPD	k = 6.00E-12 exp(-1860/T)	1.17E-14
158	EPOX + OH = EPX2 + RO2	k = 5.78E-11 exp(-400/T)	1.51E-11
159	EPX2 + HO2 = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 1.125 OH + 0.825 HO2 + 0.375 FORM + 0.074 FACD + 0.251 CO + 2.175 PAR	k = 7.43E-13 exp(700/T)	7.78E-12
160	EPX2 + NO = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + NO2 + 0.251 CO + 2.175 PAR	k = 2.39E-12 exp(365/T)	8.13E-12
161	EPX2 + C2O3 = 0.22 GLYD + 0.22 GLY + 0.22 MGLY + 0.1 OH + 0.66 HO2 + 0.3 FORM + 0.2 CO + 1.74 PAR + 0.8 MEO2 + 0.2 AACD + 0.8 RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
162	EPX2 + RO2 = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO2 + 0.375 FORM + 0.251 CO + 2.175 PAR + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
163	INTR + OH = 0.63 XO2 + 0.37 XO2H + RO2 + 0.444 NO2 + 0.185 NO3 + 0.104 INTR + 0.592 FORM + 0.331 GLYD + 0.185 FACD + 2.7 PAR + 0.098 OLE + 0.078 ALDX + 0.266 NTR2	k = 3.10E-11	3.10E-11
164	TERP + OH = 0.75 XO2H + 0.5 XO2 + 0.25 XO2N + 1.5 RO2 + 0.28 FORM + 1.66 PAR + 0.47 ALDX	k = 1.50E-11 exp(449/T)	6.77E-11
165	TERP + O3 = 0.57 OH + 0.07 XO2H + 0.69 XO2 + 0.18 XO2N + 0.94 RO2 + 0.24 FORM + 0.001 CO + 7 PAR + 0.21 ALDX + 0.39 CXO3	k = 1.20E-15 exp(-821/T)	7.63E-17
166	TERP + NO3 = 0.47 NO2 + 0.28 XO2H + 0.75 XO2 + 0.25 XO2N + 1.28 RO2 + 0.47 ALDX + 0.53 NTR2	k = 3.70E-12 exp(175/T)	6.66E-12
167	BENZ + OH = 0.53 CRES + 0.352 BZO2 + 0.352 RO2 + 0.118 OPEN + 0.118 OH + 0.53 HO2	k = 2.30E-12 exp(-190/T)	1.22E-12
168	BZO2 + NO = 0.918 NO2 + 0.082 NTR2 + 0.918 GLY + 0.918 OPEN + 0.918 HO2	k = 2.70E-12 exp(360/T)	9.04E-12
169	BZO2 + C2O3 = GLY + OPEN + HO2 + MEO2 + RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11

Number	Reactants and Products	Rate Constant Expression	k_{298}
170	BZO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
171	BZO2 + RO2 = GLY + OPEN + HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
172	TOL + OH = 0.18 CRES + 0.65 TO2 + 0.72 RO2 + 0.1 OPEN + 0.1 OH + 0.07 XO2H + 0.18 HO2	k = 1.80E-12 exp(340/T)	5.63E-12
173	TO2 + NO = 0.86 NO2 + 0.14 NTR2 + 0.417 GLY + 0.443 MGLY + 0.66 OPEN + 0.2 XOPN + 0.86 HO2	k = 2.70E-12 exp(360/T)	9.04E-12
174	TO2 + C2O3 = 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + MEO2 + RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
175	TO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
176	TO2 + RO2 = 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
177	XYL + OH = 0.155 CRES + 0.544 XLO2 + 0.602 RO2 + 0.244 XOPN + 0.244 OH + 0.058 XO2H + 0.155 HO2	k = 1.85E-11	1.85E-11
178	XLO2 + NO = 0.86 NO2 + 0.14 NTR2 + 0.221 GLY + 0.675 MGLY + 0.3 OPEN + 0.56 XOPN + 0.86 HO2	k = 2.70E-12 exp(360/T)	9.04E-12
179	XLO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
180	XLO2 + C2O3 = 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + MEO2 + RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
181	XLO2 + RO2 = 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
182	CRES + OH = 0.025 GLY + 0.025 OPEN + HO2 + 0.2 CRO + 0.732 CAT1 + 0.02 XO2N + 0.02 RO2	k = 1.70E-12 exp(950/T)	4.12E-11
183	CRES + NO3 = 0.3 CRO + HNO3 + 0.48 XO2 + 0.12 XO2H + 0.24 GLY + 0.24 MGLY + 0.48 OPO3 + 0.1 XO2N + 0.7 RO2	k = 1.40E-11	1.40E-11
184	CRO + NO2 = CRON	k = 2.10E-12	2.10E-12
185	CRO + HO2 = CRES	k = 5.50E-12	5.50E-12
186	CRON + OH = NTR2 + 0.5 CRO	k = 1.53E-12	1.53E-12
187	CRON + NO3 = NTR2 + 0.5 CRO + HNO3	k = 3.80E-12	3.80E-12
188	CRON = HONO + HO2 + FORM + OPEN	Photolysis	9.45E-5
189	XOPN = 0.4 GLY + XO2H + 0.7 HO2 + 0.7 CO + 0.3 C2O3	Photolysis	5.04E-4
190	XOPN + OH = MGLY + 0.4 GLY + 2 XO2H + 2 RO2	k = 9.00E-11	9.00E-11
191	XOPN + O3 = 1.2 MGLY + 0.5 OH + 0.6 C2O3 + 0.1 ALD2 + 0.5 CO + 0.3 XO2H + 0.3 RO2	k = 1.08E-16 exp(-500/T)	2.02E-17

Number	Reactants and Products	Rate Constant Expression	k_{298}
192	XOPN + NO3 = 0.5 NO2 + 0.5 NTR2 + 0.45 XO2H + 0.45 XO2 + 0.1 XO2N + RO2 + 0.25 OPEN + 0.25 MGLY	k = 3.00E-12	3.00E-12
193	OPEN = OPO3 + HO2 + CO	Photolysis	5.04E-4
194	OPEN + OH = 0.6 OPO3 + 0.4 XO2H + 0.4 RO2 + 0.4 GLY	k = 4.40E-11	4.40E-11
195	OPEN + O3 = 1.4 GLY + 0.24 MGLY + 0.5 OH + 0.12 C2O3 + 0.08 FORM + 0.02 ALD2 + 1.98 CO + 0.56 HO2	k = 5.40E-17 exp(-500/T)	1.01E-17
196	OPEN + NO3 = OPO3 + HNO3	k = 3.80E-12	3.80E-12
197	CAT1 + OH = 0.14 FORM + 0.2 HO2 + 0.5 CRO	k = 5.00E-11	5.00E-11
198	CAT1 + NO3 = CRO + HNO3	k = 1.70E-10	1.70E-10
199	OPO3 + NO = NO2 + 0.5 GLY + 0.5 CO + 0.8 HO2 + 0.2 CXO3	k = k(ref)/K k(ref) = k(61) K = 1.00E+0	2.10E-11
200	OPO3 + NO2 = OPAN	k = k(ref)/K k(ref) = k(62) K = 1.00E+0	8.28E-12
201	OPAN = OPO3 + NO2	k = k(ref)/K k(ref) = k(63) K = 1.00E+0	3.62E-4
202	OPO3 + HO2 = 0.37 PACD + 0.13 AACD + 0.13 O3 + 0.5 OH + 0.5 MEO2 + 0.5 RO2	k = k(ref)/K k(ref) = k(57) K = 1.00E+0	2.20E-11
203	OPO3 + C2O3 = MEO2 + XO2 + ALDX + 2 RO2	k = k(ref)/K k(ref) = k(59) K = 1.00E+0	1.55E-11
204	OPO3 + RO2 = 0.8 XO2H + 0.8 ALDX + 1.8 RO2 + 0.2 AACD	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.60E-11
205	OPAN + OH = 0.5 NO2 + 0.5 GLY + CO + 0.5 NTR2	k = 3.60E-11	3.60E-11
206	PANX + OH = ALD2 + NO2	k = 3.00E-12	3.00E-12
207	NTR2 = HNO3	k = 2.30E-5	2.30E-5
208	ECH4 + OH = MEO2 + RO2	k = 1.85E-12 exp(-1690/T)	6.37E-15
209	I2 = 2 I	Photolysis	1.30E-1
210	HOI = I + OH	Photolysis	6.38E-2
211	I + O3 = IO	k = 2.10E-11 exp(-830/T)	1.30E-12
212	IO = I + O	Photolysis	1.18E-1
213	IO + IO = 0.4 I + 0.4 OIO + 0.6 I2O2	k = 5.40E-11 exp(180/T)	9.88E-11
214	IO + HO2 = HOI	k = 1.40E-11 exp(540/T)	8.57E-11
215	IO + NO = I + NO2	k = 7.15E-12 exp(300/T)	1.96E-11
216	IO + NO2 = INO3	Falloff: F=0.4; n=1.26 k(0) = 7.70E-31 (T/300)^-5 k(inf) = 1.60E-11	3.54E-12
217	OIO = I	Photolysis	1.28E-1

Number	Reactants and Products	Rate Constant Expression	k_{298}
218	OIO + OH = HIO3	Falloff: F=0.3; n=1.41 k(0) = 1.50E-27 (T/300)^-3.93 k(inf) = 5.50E-10 exp(46/T)	3.96E-10
219	OIO + IO = IXOY	k = 1.00E-10	1.00E-10
220	OIO + NO = IO + NO2	k = 1.10E-12 exp(542/T)	6.78E-12
221	I2O2 = I + OIO	k = 1.00E+1	1.00E+1
222	I2O2 + O3 = IXOY	k = 1.00E-12	1.00E-12
223	INO3 = I + NO3	Photolysis	1.26E-2
224	INO3 + H2O = HOI + HNO3	k = 2.50E-22	2.50E-22
225	XPRP = XO2N + RO2	Falloff: F=0.41; n=1 k(0) = 2.37E-21 k(inf) = 4.30E-1 (T/298)^-8	3.09E-2
226	XPRP = 0.732 ACET + 0.268 ALDX + 0.268 PAR + XO2H + RO2	k = 1.00E+0	1.00E+0
227	XPAR = XO2N + RO2	Falloff: F=0.41; n=1 k(0) = 4.81E-20 k(inf) = 4.30E-1 (T/298)^-8	1.49E-1
228	XPAR = 0.126 ALDX + 0.874 ROR + 0.126 XO2H + 0.874 XO2 + RO2 - 0.126 PAR	k = 1.00E+0	1.00E+0
229	INTR = HNO3	k = 1.40E-4	1.40E-4
230	SO2 = SULF	k = 0.00E+0	0.00E+0
231	DMS + OH = SO2 + FORM + MEO2 + RO2	k = 1.12E-11 exp(-250/T)	4.84E-12
232	DMS + OH + O2 = SULF + MEO2 + RO2	k = 1.28E-37 exp(4480/T)	4.33E-31
233	DMS + NO3 = SO2 + FORM + HNO3 + MEO2 + RO2	k = 1.90E-13 exp(520/T)	1.09E-12
234	NO2 + OH + H2O = HNO3 + H2O	k = 1.10E-30	1.10E-30
235	CL2 = 2 CL	Photolysis	1.55E-3
236	ICL = I + CL	Photolysis	1.91E-2
237	HOCL = CL + OH	Photolysis	1.35E-4
238	CL + O3 = CLO	k = 2.30E-11 exp(-200/T)	1.18E-11
239	CL + HO2 = 0.78 HCL + 0.22 CLO + 0.22 OH	k = 3.00E-11 exp(120/T)	4.49E-11
240	CL + H2 = HCL + HO2	k = 3.05E-11 exp(-2270/T)	1.50E-14
241	CLO + CLO = 0.3 CL2 + 1.4 CL	k = 1.63E-14	1.63E-14
242	CLO + IO = CL + I	k = 5.00E-13 exp(300/T)	1.37E-12
243	CLO + HO2 = HOCL	k = 2.60E-12 exp(290/T)	6.88E-12
244	CLO + MEO2 = CL + FORM + HO2	k = 1.80E-11 exp(-600/T)	2.40E-12
245	CLO + NO = CL + NO2	k = 6.40E-12 exp(290/T)	1.69E-11
246	CLO + NO2 = CLN3	Falloff: F=0.6; n=1 k(0) = 1.80E-31 (T/300)^-3.4 k(inf) = 1.50E-11 (T/300)^-1.9	2.34E-12
247	CLN3 = CLO + NO2	k = k(ref)/K k(ref) = k(246) K = 2.98E-28 exp(13264/T)	3.67E-4
248	CLN3 = CLO + NO2	Photolysis	4.03E-6
249	CLN3 = CL + NO3	Photolysis	2.33E-5
250	CLN2 = CL + NO2	Photolysis	2.16E-4
251	HCL + N2O5 = CLN2 + HNO3	k = 6.00E-13	6.00E-13
252	CLN3 + H2O = HOCL + HNO3	k = 2.50E-22	2.50E-22
253	FORM + CL = HCL + CO + HO2	k = 8.10E-11 exp(-30/T)	7.32E-11

Number	Reactants and Products	Rate Constant Expression	k_{298}
254	ALD2 + CL = HCL + C2O3	k = 7.30E-11	7.30E-11
255	ALDX + CL = HCL + CXO3	k = 1.40E-10	1.40E-10
256	GLY + CL = HCL + 1.8 CO + HO2 + 0.2 XO2 + 0.2 RO2	k = 3.80E-11	3.80E-11
257	GLYD + CL = HCL + 0.2 GLY + 0.2 HO2 + 0.8 C2O3	k = 6.60E-11	6.60E-11
258	MGLY + CL = HCL + CO + C2O3	k = 4.80E-11	4.80E-11
259	ACET + CL = HCL + FORM + C2O3 + XO2 + RO2	k = 1.63E-11 exp(-610/T)	2.10E-12
260	KET + CL = HCL + 0.5 ALD2 + 0.5 C2O3 + 0.5 XO2H + 0.5 CXO3 + 0.5 MEO2 + RO2 - 2.5 PAR	k = 2.77E-11 exp(76/T)	3.57E-11
261	MEOH + CL = HCL + FORM + HO2	k = 5.50E-11	5.50E-11
262	ETOH + CL = 0.95 ALD2 + 0.9 HO2 + 0.1 XO2H + 0.1 RO2 + 0.078 FORM + 0.011 GLYD	k = 9.60E-11	9.60E-11
263	ISPD + CL = 0.17 HCL + 0.34 CLAO + 0.5 CLAD + 0.32 CO + 0.17 OPO3 + 0.48 C2O3 + 0.32 XO2H + 0.48 XO2 + 0.04 XO2N + 0.84 RO2	k = 2.20E-10	2.20E-10
264	FMCL = CO + HCL	k = 6.94E-5	6.94E-5
265	CLAD = MEO2 + XO2 + CO + CL + 2 RO2	Photolysis	4.04E-5
266	CLAD + OH = FMCL + XO2 + XO2H + 2 RO2	k = 3.10E-12	3.10E-12
267	CLAO + OH = FMCL + C2O3 + XO2 + 2 RO2	k = 4.20E-13	4.20E-13
268	CH4 + CL = HCL + MEO2 + RO2	k = 7.10E-12 exp(-1270/T)	1.00E-13
269	ECH4 + CL = HCL + MEO2 + RO2	k = 7.10E-12 exp(-1270/T)	1.00E-13
270	ETHA + CL = HCL + 0.991 ALD2 + 0.991 XO2H + 0.009 XO2N + RO2	k = 7.20E-11 exp(-70/T)	5.69E-11
271	PRPA + CL = HCL + XPRP	k = 1.40E-10	1.40E-10
272	PAR + CL = HCL + XPAR	k = 4.50E-11	4.50E-11
273	ETHY + CL = 0.53 HCL + 0.26 FMCL + 1.32 CO + 0.79 HO2 + 0.21 GLY + 0.21 CL	Falloff: F=0.6; n=1 k(0) = 5.30E-30 (T/300)^-2.4 k(inf) = 2.20E-10 (T/300)^-0.7	5.09E-11
274	ETH + CL = CLAD + XO2H + RO2	Falloff: F=0.6; n=1 k(0) = 1.60E-29 (T/300)^-3.3 k(inf) = 3.10E-10 (T/300)^-1	1.06E-10
275	OLE + CL = 0.2 HCL + 0.3 CLAD + 0.5 CLAO + 0.18 ALDX + 0.08 XO2N + 0.92 XO2H + RO2 - 1. PAR	k = 2.15E-10	2.15E-10
276	IOLE + CL = 0.44 HCL + 0.56 CLAO + 0.23 ALDX + 0.17 ALD2 + 0.17 C2O3 + 0.1 XO2N + 0.73 XO2H + 0.83 RO2	k = 3.50E-10	3.50E-10
277	ISOP + CL = 0.15 HCL + 0.58 CLAD + 0.22 CLAO + 0.05 FMCL + 0.15 ISPD + 0.1 FORM + 0.12 XO2N + 0.88 XO2H + 0.88 XO2 + 1.88 RO2	k = 7.60E-11 exp(500/T)	4.07E-10
278	TERP + CL = 0.55 HCL + 0.15 CLAO + 0.15 CLAD + 0.15 FMCL + 0.3 XO2N + 0.7 XO2H + RO2	k = 5.30E-10	5.30E-10

Number	Reactants and Products	Rate Constant Expression	k_{298}
279	TOL + CL = HCL + 0.9 CRES + 0.1 XO2N + 0.9 XO2H + RO2	k = 5.60E-11	5.60E-11
280	XYL + CL = HCL + 0.9 CRES + 0.1 XO2N + 0.9 XO2H + RO2	k = 1.40E-10	1.40E-10
281	CRES + CL = HCL + 0.025 GLY + 0.025 OPEN + 0.2 CRO + 0.732 CAT1 + HO2 + 0.02 XO2N + 0.02 RO2	k = 1.90E-10	1.90E-10
282	DMS + CL = HCL + SO2 + FORM + MEO2 + RO2	k = 1.80E-10	1.80E-10
283	BR2 = 2 BR	Photolysis	2.79E-2
284	IBR = I + BR	Photolysis	5.90E-2
285	BRCL = CL + BR	Photolysis	7.36E-3
286	HOBR = BR + OH	Photolysis	1.51E-3
287	BR + O3 = BRO	k = 1.60E-11 exp(-780/T)	1.17E-12
288	BR + HO2 = HBR	k = 4.80E-12 exp(-310/T)	1.70E-12
289	BR + NO2 = BRN2	Falloff: F=0.6; n=1 k(0) = 6.45E-32 (T/300)^-2.4 k(inf) = 4.05E-12	7.43E-13
290	BR + NO3 = BRO + NO2	k = 1.60E-11	1.60E-11
291	BR2 + OH = HOBR + BR	k = 2.10E-11 exp(240/T)	4.70E-11
292	HBR + OH = BR	k = 5.50E-12 exp(200/T)	1.08E-11
293	BRO = BR + O	Photolysis	2.13E-2
294	BRO + BRO = 1.7 BR + 0.15 BR2	k = 1.50E-12 exp(230/T)	3.25E-12
295	BRO + CLO = BR + CL	k = 3.10E-12 exp(420/T)	1.27E-11
296	BRO + IO = BR + I	k = 5.50E-12 exp(760/T)	7.05E-11
297	BRO + HO2 = HOBR	k = 4.50E-12 exp(460/T)	2.11E-11
298	BRO + NO = BR + NO2	k = 8.80E-12 exp(260/T)	2.11E-11
299	BRO + NO2 = BRN3	Falloff: F=0.6; n=1 k(0) = 5.50E-31 (T/300)^-3.1 k(inf) = 6.60E-12 (T/300)^-2.9	2.84E-12
300	BRN2 = BR + NO2	Photolysis	3.21E-3
301	BRN3 = 0.85 BR + 0.85 NO3 + 0.15 BRO + 0.15 NO2	Photolysis	9.73E-4
302	BRN3 + H2O = HOBR + HNO3	k = 2.50E-22	2.50E-22
303	BR + FORM = HBR + CO + HO2	k = 1.70E-11 exp(-800/T)	1.16E-12
304	BR + ALD2 = HBR + C2O3	k = 1.80E-11 exp(-460/T)	3.84E-12
305	BR + ALDX = HBR + CXO3	k = 5.75E-11 exp(-575/T)	8.35E-12
306	BR + ETH = FMBR + FORM + XO2H + RO2	k = 6.35E-15 exp(-440/T)	1.45E-15
307	BR + OLE = FMBR + ALD2 + 0.08 XO2N + 0.92 XO2H + RO2 - 1. PAR	k = 3.60E-12	3.60E-12
308	BR + IOLE = FMBR + 0.5 ALDX + 0.5 ACET + 0.1 XO2N + 0.9 XO2H + RO2	k = 9.30E-12	9.30E-12
309	BR + ISOP = FMBR + ISPD + 0.12 XO2N + 0.88 XO2H + RO2	k = 7.40E-11	7.40E-11
310	BR + TERP = FMBR + 0.3 XO2N + 0.7 XO2H + RO2	k = 2.50E-11	2.50E-11
311	FMBR = HBR + CO	k = 2.78E-4	2.78E-4
312	CH3I = I + MEO2	Photolysis	3.17E-6
313	MI2 = 2 I + FORM	Photolysis	4.74E-3

Number	Reactants and Products	Rate Constant Expression	k_{298}
314	MIB = I + BR + FORM	Photolysis	2.51E-4
315	MIC = I + CL + FORM	Photolysis	7.44E-5
316	MB3 = 3 BR + HO2 + CO	Photolysis	5.10E-7
317	MB3 + OH = 3 BR + CO	k = 9.00E-13 exp(-360/T)	2.69E-13
318	MB2 + OH = 2 BR + HO2 + CO	k = 2.00E-12 exp(-840/T)	1.19E-13
319	MBC + OH = BR + MEO2	k = 2.10E-12 exp(-880/T)	1.10E-13
320	MBC2 + OH = BR + MEO2	k = 9.40E-13 exp(-510/T)	1.70E-13
321	MB2C + OH = BR + MEO2	k = 9.00E-13 exp(-420/T)	2.20E-13
322	I + HO2 = HI	k = 1.50E-11 exp(-1090/T)	3.87E-13
323	HI + OH = I	k = 3.00E-11	3.00E-11
324	I + NO2 = INO2	Falloff: F=0.63; n=1 k(0) = 3.00E-31 (T/300)^-1 k(inf) = 6.60E-11	5.24E-12
325	INO2 = I + NO2	Photolysis	2.01E-3
326	INO2 + INO2 = I2 + 2 NO2	k = 4.70E-12 exp(-1670/T)	1.73E-14
327	BR + BRN2 = BR2 + NO2	k = 5.00E-11	5.00E-11
328	GLY = CGLY	k = 1.00E-6	1.00E-6
329	MGLY = CGLY	k = 1.00E-6	1.00E-6

Table C-2. CB6r5h species names and descriptions.

Name	Description	C	H	O	N	S	Cl	Br	I	MW
BZO2	Peroxy radical from OH addition to benzene	6	7	5						159.1
C2O3	Acetylperoxy radical	2	3	3						75.0
CRO	Alkoxy radical from cresol	7	7	1						107.1
CXO3	C3 and higher acylperoxy radicals	2	3	3						75.0
EPX2	Peroxy radical from EPOX reaction with OH	5	9	5						149.1
HCO3	Adduct from HO2 plus formaldehyde	1	3	3						63.0
HO2	Hydroperoxy radical		1	2						33.0
ISO2	Peroxy radical from OH addition to isoprene	5	9	3						117.1
MEO2	Methylperoxy radical	1	3	2						47.0
O	Oxygen atom in the $O^3(P)$ electronic state			1						16.0
O1D	Oxygen atom in the $O^1(D)$ electronic state			1						16.0
OH	Hydroxyl radical		1	1						17.0
OPO3	Peroxyacyl radical from OPEN and other model species	4	3	4						115.1
RO2	Operator to approximate total peroxy radical concentration	4	7	2						87.1
ROR	Secondary alkoxy radical from PAR	4	7	1						71.1
TO2	Peroxy radical from OH addition to TOL	7	9	5						173.1
XLO2	Peroxy radical from OH addition to XYL	8	11	5						187.2
XO2	NO to NO2 conversion from a peroxy radical	4	7	2						87.1
XO2H	NO to NO2 conversion (XO2) accompanied by HO2 production from a peroxy radical	4	7	2						87.1
XO2N	NO to organic nitrate conversion from a peroxy radical	4	7	2						87.1
XPRP	Operator to enable T-dependent organic nitrate yield from PRPA	3	7	2						75.1
XPAR	Operator to enable T-dependent organic nitrate yield from PAR	1	2.5	2						46.5
AACD	Acetic acid	2	4	2						60.1
ACET	Acetone	3	6	1						58.1
ALD2	Acetaldehyde	2	4	1						44.1
ALDX	Higher aldehydes (R-C-CHO)	2	3	1						43.0
BENZ	Benzene	6	6							78.1
CAT1	Methyl-catechols	7	8	2						124.1
CO	Carbon monoxide	1		1						28.0
CH4	Methane	1	4							16.0
CRES	Cresols	7	8	1						108.1
CRON	Nitro-cresols	7	7	3	1					153.1
DMS	Dimethyl sulfide	2	6			1				62.1
ECH4	Emitted methane (to enable tracking seperate from CH4)	1	4							16.0
EPOX	Epoxide formed from ISPX reaction with OH	5	10	3						118.1
ETH	Ethene	2	4							28.1

Name	Description	C	H	O	N	S	Cl	Br	I	MW
ETHA	Ethane	2	6							30.1
ETHY	Ethyne	2	2							26.0
ETOH	Ethanol	2	6	1						46.1
FACD	Formic acid	1	2	2						46.0
FORM	Formaldehyde	1	2	1						30.0
GLY	Glyoxal	2	2	2						58.0
GLYD	Glycolaldehyde	2	4	2						60.1
H2O2	Hydrogen peroxide		2	2						34.0
HNO3	Nitric acid		1	3	1					63.0
HONO	Nitrous acid		1	2	1					47.0
HPLD	Hydroperoxyaldehyde from ISO2 isomerization	5	8	3						116.1
INTR	Organic nitrates from ISO2 reaction with NO	5	9	4	1					147.1
IOLE	Internal olefin carbon bond (R-C=C-R)	4	8							56.1
ISOP	Isoprene	5	8							68.1
ISPD	Isoprene product (methacrolein, methyl vinyl ketone, etc.)	4	6	1						70.1
ISPX	Hydroperoxides from ISO2 reaction with HO2	5	10	3						118.1
KET	Ketone carbon bond (C=O)	1		1						28.0
MEOH	Methanol	1	4	1						32.0
MEPX	Methylhydroperoxide	1	4	2						48.0
MGLY	Methylglyoxal	3	4	2						72.1
N2O5	Dinitrogen pentoxide			5	2					108.0
NO	Nitric oxide			1	1					30.0
NO2	Nitrogen dioxide			2	1					46.0
NO3	Nitrate radical			3	1					62.0
NTR1	Simple organic nitrates	4	9	3	1					119.1
NTR2	Multi-functional organic nitrates	4	9	4	1					135.1
O3	Ozone			3						48.0
OLE	Terminal olefin carbon bond (R-C=C)	2	5							29.1
OPAN	Other peroxyacyl nitrates (PAN compounds) from OPO3	4	3	6	1					161.1
OPEN	Aromatic ring opening product (unsaturated dicarbonyl)	4	4	2						84.1
PACD	Peroxyacetic and higher peroxycarboxylic acids	2	4	3						76.1
PAN	Peroxyacetyl Nitrate	2	3	5	1					121.0
PANX	Larger alkyl peroxyacyl nitrates (from CXO3)	3	5	5	1					135.1
PAR	Paraffin carbon bond (C-C)	1	2.5							14.5
PNA	Peroxynitric acid		1	4	1					79.0
PRPA	Propane	3	8							44.1
ROOH	Higher organic peroxide	4	10	2						90.1
SO2	Sulfur dioxide			2		1				64.1
SULF	Sulfuric acid (gaseous)		2	4		1				98.1

Name	Description	C	H	O	N	S	Cl	Br	I	MW
TERP	Monoterpenes	10	16							136.2
TOL	Toluene and other monoalkyl aromatics	7	8							92.1
XOPN	Aromatic ring opening product (unsaturated dicarbonyl)	5	6	2						98.1
XYL	Xylene and other polyalkyl aromatics	8	10							106.2
CL2	Molecular chlorine						2			70.9
CL	Chlorine atom						1			35.5
CLO	Chlorine monoxide			1			1			51.5
HCL	Hydrogen chloride		1				1			36.5
HOCL	Hypochlorous acid		1	1			1			52.5
CLN2	Nitryl chloride			2	1		1			81.5
CLN3	Chlorine nitrate			3	1		1			97.5
FMCL	Formyl chloride	1	1	1			1			64.5
CLAD	Chloroacetaldehyde	2	3	1			1			78.5
CLAO	Chloroacetone	3	5	1			1			92.5
BR2	Molecular bromine							2		159.8
BRCL	Bromine monochloride						1	1		115.4
BR	Bromine atom							1		79.9
BRO	Bromine monoxide			1				1		95.9
HBR	Hydrogen bromide		1					1		80.9
HOBR	Hypobromous acid		1	1				1		96.9
BRN2	Nitryl bromide			2	1			1		125.9
BRN3	Bromine nitrate			3	1			1		141.9
FMBR	Formyl bromide	1	1	1				1		108.9
I2	Molecular iodine								2	253.8
IBR	Iodine monobromide							1	1	206.8
ICL	Iodine monochloride						1		1	162.4
I	Iodine atom								1	126.9
IO	Iodine monoxide			1					1	142.9
OIO	Iodine dioxide			2					1	158.9
I2O2	Diiodine dioxide			2					2	285.8
IXOY	Condensable iodine oxides			3					2	301.8
HI	Hydrogen iodide		1						1	127.9
HOI	Hypoiodous acid		1	1					1	143.9
HIO3	Iodic acid		1	3					1	175.9
INO2	Nitryl iodide			2	1				1	172.9
INO3	Iodine nitrate			3	1				1	188.9
CH3I	Iodomethane (CH3I)	1	3						1	141.9
MI2	Diiodomethane (CH2I2)	1	2						2	267.8
MIB	Bromoiodomethane (CH2IBr)	1	2					1	1	220.8
MIC	Chloroiodomethane (CH2IClO	1	2				1		1	176.4
MBC	Chlorobromomethane (CH2BrCl)	1	2				1	1		129.4

Name	Description	C	H	O	N	S	Cl	Br	I	MW
MB2	Dibromomethane (CH2Br2)	1	2					2		173.8
MBC2	Dichlorobromomethane (CHBrCl2)	1	3				2	1		165.8
MB2C	Chlorodibromomethane (CHBr2Cl)	1	3				1	2		210.3
MB3	Bromoform (CHBr3)	1	1					3		252.7

Table C-3. Zenith angle (degrees) dependence of photolysis frequencies (s^{-1}) for CB6r5h reactions.

Reaction ID	Solar zenith angle (degree)					
	0	20	40	60	78	86
1	1.01E-02	9.77E-03	8.75E-03	6.30E-03	2.09E-03	5.12E-04
8	4.26E-04	4.19E-04	3.94E-04	3.33E-04	1.79E-04	4.27E-05
9	4.55E-05	3.99E-05	2.54E-05	8.78E-06	9.20E-07	1.52E-07
21	8.79E-06	8.26E-06	6.64E-06	3.78E-06	8.81E-07	2.03E-07
27	1.88E-01	1.86E-01	1.79E-01	1.56E-01	8.22E-02	1.79E-02
28	2.32E-02	2.31E-02	2.23E-02	1.98E-02	1.12E-02	2.63E-03
38	5.54E-05	5.23E-05	4.26E-05	2.52E-05	6.30E-06	1.48E-06
43	1.74E-03	1.68E-03	1.49E-03	1.04E-03	3.29E-04	8.35E-05
47	8.47E-07	7.70E-07	5.57E-07	2.54E-07	4.20E-08	7.98E-09
50	7.02E-06	6.46E-06	4.84E-06	2.36E-06	4.16E-07	7.73E-08
56	9.53E-07	8.81E-07	6.72E-07	3.47E-07	7.05E-08	1.52E-08
64	9.53E-07	8.81E-07	6.72E-07	3.47E-07	7.05E-08	1.52E-08
88	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07	1.53E-07
90	6.02E-06	5.68E-06	4.61E-06	2.68E-06	6.52E-07	1.53E-07
92	3.29E-06	3.01E-06	2.22E-06	1.06E-06	1.85E-07	3.60E-08
97	4.16E-05	3.90E-05	3.10E-05	1.69E-05	3.55E-06	7.35E-07
98	5.43E-05	5.18E-05	4.35E-05	2.69E-05	7.06E-06	1.73E-06
106	7.29E-06	6.59E-06	4.65E-06	1.96E-06	2.54E-07	3.93E-08
109	6.88E-05	6.41E-05	4.99E-05	2.62E-05	5.17E-06	1.04E-06
111	9.03E-06	8.24E-06	6.01E-06	2.76E-06	4.40E-07	7.94E-08
114	1.35E-04	1.30E-04	1.14E-04	7.95E-05	2.57E-05	6.08E-06
116	2.36E-04	2.29E-04	2.04E-04	1.46E-04	4.92E-05	1.16E-05
125	1.16E-06	1.02E-06	6.50E-07	2.27E-07	2.34E-08	3.59E-09
126	1.02E-06	9.02E-07	5.83E-07	2.08E-07	2.25E-08	3.51E-09
154	2.96E-05	2.84E-05	2.45E-05	1.60E-05	4.60E-06	1.16E-06
156	7.04E-04	6.84E-04	6.12E-04	4.41E-04	1.46E-04	3.58E-05
188	1.51E-04	1.47E-04	1.31E-04	9.45E-05	3.13E-05	7.68E-06
189	8.04E-04	7.82E-04	7.00E-04	5.04E-04	1.67E-04	4.09E-05
193	8.04E-04	7.82E-04	7.00E-04	5.04E-04	1.67E-04	4.09E-05
209	1.57E-01	1.56E-01	1.49E-01	1.30E-01	6.88E-02	1.50E-02
210	1.02E-01	9.90E-02	8.87E-02	6.38E-02	2.12E-02	5.18E-03
212	1.88E-01	1.82E-01	1.63E-01	1.18E-01	3.90E-02	9.56E-03
217	1.55E-01	1.53E-01	1.47E-01	1.28E-01	6.77E-02	1.48E-02
223	2.53E-02	2.42E-02	2.03E-02	1.26E-02	3.29E-03	8.06E-04
235	2.48E-03	2.41E-03	2.16E-03	1.55E-03	5.15E-04	1.26E-04
236	2.31E-02	2.29E-02	2.19E-02	1.91E-02	1.01E-02	2.20E-03
237	2.72E-04	2.60E-04	2.18E-04	1.35E-04	3.54E-05	8.66E-06
248	9.89E-06	9.28E-06	7.36E-06	4.03E-06	8.45E-07	1.75E-07
249	4.71E-05	4.49E-05	3.77E-05	2.33E-05	6.12E-06	1.50E-06

Reaction ID	Solar zenith angle (degree)					
	0	20	40	60	78	86
250	4.36E-04	4.15E-04	3.49E-04	2.16E-04	5.66E-05	1.39E-05
265	9.92E-05	9.30E-05	7.38E-05	4.04E-05	8.47E-06	1.75E-06
283	3.37E-02	3.34E-02	3.21E-02	2.79E-02	1.47E-02	3.22E-03
284	7.12E-02	7.06E-02	6.77E-02	5.90E-02	3.12E-02	6.80E-03
285	1.18E-02	1.14E-02	1.02E-02	7.36E-03	2.44E-03	5.98E-04
286	2.41E-03	2.34E-03	2.10E-03	1.51E-03	5.01E-04	1.23E-04
293	4.29E-02	4.09E-02	3.43E-02	2.13E-02	5.57E-03	1.37E-03
300	5.13E-03	4.99E-03	4.46E-03	3.21E-03	1.07E-03	2.61E-04
301	1.55E-03	1.51E-03	1.35E-03	9.73E-04	3.23E-04	7.91E-05
312	7.80E-06	7.31E-06	5.80E-06	3.17E-06	6.66E-07	1.38E-07
313	9.57E-03	9.13E-03	7.66E-03	4.74E-03	1.24E-03	3.04E-04
314	6.18E-04	5.79E-04	4.60E-04	2.51E-04	5.28E-05	1.09E-05
315	1.83E-04	1.71E-04	1.36E-04	7.44E-05	1.56E-05	3.23E-06
316	1.70E-06	1.54E-06	1.12E-06	5.10E-07	8.42E-08	1.60E-08
325	3.21E-03	3.12E-03	2.79E-03	2.01E-03	6.66E-04	1.63E-04