Bertram and Thornton (2009) have proposed kinetic equations to describe reactions between N_2O_5 and H_2O or HCl to form nitric acid or NO_2Cl, respectively. The process of NO_2Cl formation is complex and has the following major ingredients: (1) reaction occurs on the surface of an aerosol that may be sea salt or another type of aerosol; (2) reaction requires HCl that may be supplied by the aerosol or by the gas phase; (3) reaction requires N_2O_5 that is supplied by the gas phase.

2.2 MECHANISM IMPLEMENTATION

Rate constants may depend upon temperature and pressure requiring several types of rate expressions, as shown in Table 2-6. The reactions and rate expressions for CB6 are listed in Table 2-7. CB6 model species names are explained in Table 2-8.

Table 2-6. Rate constant expressions used in CB6.

Rate constant type	Expression
Temperature dependent rate constant	$k = A\left(\frac{T}{T_R}\right)^B \exp\left[\frac{-E_a}{T}\right]$
Temperature and pressure dependent rate constant defined using Troe's formula	$k = \left[\frac{k^o[M]}{1 + k^o[M]/k^\infty}\right] F^G$ $k^o = A\left(\frac{T}{T_R}\right)^B \exp\left[\frac{-E_a}{T}\right]$ $k^\infty = A'\left(\frac{T}{T_R'}\right)^{B'} \exp\left[\frac{-E_a'}{T}\right]$ $G = \left[1 + \left(\frac{\log(k^o[M]/k^\infty)}{n}\right)^2\right]^{-1}$
Previously defined rate constant (k_{ref}) multiplied by an equilibrium constant	$k = k_{ref} A\left(\frac{T}{T_R}\right)^B \exp\left[\frac{-E_a}{T}\right]$

Table notes:

T is the temperature (K)
T_R is a reference temperature of 300 K
E_A is an Arrhenius activation energy (K)
k_0 is the low pressure limit of the rate constant
k_∞ is the high pressure limit of the rate constant
[M] is the concentration of air

Table 2-7. Listing of reactions and rate parameters for CB6.

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
1	NO2 = NO + O	Photolysis				a
2	O + O2 + M = O3 + M	5.78E-34	5.68E-34	0.0	-2.60	a
3	O3 + NO = NO2	1.73E-14	1.40E-12	1310.0	0.00	a
4	O + NO + M = NO2 + M	1.01E-31	1.00E-31	0.0	-1.60	a
5	O + NO2 = NO	1.03E-11	5.50E-12	-188.0	0.00	a
6	O + NO2 = NO3	2.11E-12	Falloff, F=0.60 ,N=1.00			a
		k_0	1.30E-31	0.0	-1.50	
		k_∞	2.30E-11	0.0	0.24	
7	O + O3 =	7.96E-15	8.00E-12	2060.0	0.00	a
8	O3 = O	Photolysis				a
9	O3 = O1D	Photolysis				a
10	O1D + M = O + M	3.28E-11	2.23E-11	-115.0	0.00	a
11	O1D + H2O = 2 OH	2.14E-10	2.14E-10			a
12	O3 + OH = HO2	7.25E-14	1.70E-12	940.0	0.00	a
13	O3 + HO2 = OH	2.01E-15	2.03E-16	-693.0	4.57	a
14	OH + O = HO2	3.47E-11	2.40E-11	-110.0	0.00	a
15	HO2 + O = OH	5.73E-11	2.70E-11	-224.0	0.00	a
16	OH + OH = O	1.48E-12	6.20E-14	-945.0	2.60	a
17	OH + OH = H2O2	5.25E-12	Falloff, F=0.50 ,N=1.13			a
		k_0	6.90E-31	0.0	-0.80	
		k_∞	2.60E-11	0.0	0.00	
18	OH + HO2 =	1.11E-10	4.80E-11	-250.0	0.00	a
19	HO2 + HO2 = H2O2	2.90E-12	k = k1 + k2[M]			a
		k1	2.20E-13	-600.0	0.00	
		k2	1.90E-33	-980.0	0.00	
20	HO2 + HO2 + H2O = H2O2	6.53E-30	k = k1 + k2[M]			a
		k1	3.08E-34	-2800.0	0.00	
		k2	2.66E-54	-3180.0	0.00	
21	H2O2 = 2 OH	Photolysis				a
22	H2O2 + OH = HO2	1.70E-12	2.90E-12	160.0	0.00	a
23	H2O2 + O = OH + HO2	1.70E-15	1.40E-12	2000.0	0.00	a
24	NO + NO + O2 = 2 NO2	1.95E-38	3.30E-39	-530.0	0.00	a
25	HO2 + NO = OH + NO2	8.54E-12	3.45E-12	-270.0	0.00	a
26	NO2 + O3 = NO3	3.52E-17	1.40E-13	2470.0	0.00	a
27	NO3 = NO2 + O	Photolysis				b
28	NO3 = NO	Photolysis				b
29	NO3 + NO = 2 NO2	2.60E-11	1.80E-11	-110.0	0.00	a
30	NO3 + NO2 = NO + NO2	6.56E-16	4.50E-14	1260.0	0.00	b
31	NO3 + O = NO2	1.70E-11	1.70E-11			a
32	NO3 + OH = HO2 + NO2	2.00E-11	2.00E-11			a
33	NO3 + HO2 = OH + NO2	4.00E-12	4.00E-12			a
34	NO3 + O3 = NO2	1.00E-17	1.00E-17			c,k
35	NO3 + NO3 = 2 NO2	2.28E-16	8.50E-13	2450.0	0.00	b
36	NO3 + NO2 = N2O5	1.24E-12	Falloff, F=0.35 ,N=1.33			a
		k_0	3.60E-30	0.0	-4.10	
		k_∞	1.90E-12	0.0	0.20	
37	N2O5 = NO3 + NO2	4.46E-02	Falloff, F=0.35 ,N=1.33			a
		k_0	1.30E-03	11000.0	-3.50	
		k_∞	9.70E+14	11080.0	0.10	

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
38	N2O5 = NO2 + NO3	Photolysis				a
39	N2O5 + H2O = 2 HNO3	1.00E-22	1.00E-22			a
40	NO + OH = HONO	9.77E-12	Falloff, F=0.81 ,N=0.87			a
		k_0	7.40E-31	0.0	-2.40	
		k_∞	3.30E-11	0.0	-0.30	
41	NO + NO2 + H2O = 2 HONO	5.00E-40	5.00E-40			c,l
42	HONO + HONO = NO + NO2	1.00E-20	1.00E-20			c,m
43	HONO = NO + OH	Photolysis				a
44	HONO + OH = NO2	5.98E-12	2.50E-12	-260.0	0.00	a
45	NO2 + OH = HNO3	1.06E-11	Falloff, F=0.60 ,N=1.00			b
		k_0	1.80E-30	0.0	-3.00	
		k_∞	2.80E-11	0.0	0.00	
46	HNO3 + OH = NO3	1.54E-13	k = k1+k3M/(1+k3M/k2)			a
		k1	2.40E-14	-460.0	0.00	
		k2	2.70E-17	-2199.0	0.00	
		k3	6.50E-34	-1335.0	0.00	
47	HNO3 = OH + NO2	Photolysis				a
48	HO2 + NO2 = PNA	1.38E-12	Falloff, F=0.60 ,N=1.00			a
		k_0	1.80E-31	0.0	-3.20	
		k_∞	4.70E-12	0.0	0.00	
49	PNA = HO2 + NO2	8.31E-02	Falloff, F=0.60 ,N=1.00			a
		k_0	4.10E-05	10650.0	0.00	
		k_∞	4.80E+15	11170.0	0.00	
50	PNA = 0.59 HO2 + 0.59 NO2 + 0.41 OH + 0.41 NO3	Photolysis				a
51	PNA + OH = NO2	3.24E-12	3.20E-13	-690.0	0.00	a
52	SO2 + OH = SULF + HO2	8.12E-13	Falloff, F=0.53 ,N=1.10			a
		k_0	4.50E-31	0.0	-3.90	
		k_∞	1.30E-12	0.0	-0.70	
53	C2O3 + NO = NO2 + MEO2 + RO2	1.98E-11	7.50E-12	-290.0	0.00	a
54	C2O3 + NO2 = PAN	1.05E-11	Falloff, F=0.30 ,N=1.00			a
		k_0	2.70E-28	0.0	-7.10	
		k_∞	1.20E-11	0.0	-0.90	
55	PAN = NO2 + C2O3	3.31E-04	Falloff, F=0.30 ,N=1.00			a
		k_0	4.90E-03	12100.0	0.00	
		k_∞	5.40E+16	13830.0	0.00	
56	PAN = 0.6 NO2 + 0.6 C2O3 + 0.4 NO3 + 0.4 MEO2 + 0.4 RO2	Photolysis				a
57	C2O3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 MEO2 + 0.44 RO2 + 0.44 OH	1.39E-11	5.20E-13	-980.0	0.00	a
58	C2O3 + RO2 = C2O3	1.30E-11	8.90E-13	-800.0	0.00	a
59	C2O3 + C2O3 = 2 MEO2 + 2 RO2	1.55E-11	2.90E-12	-500.0	0.00	a
60	C2O3 + CXO3 = MEO2 + ALD2 + XO2H + 2 RO2	1.55E-11	2.90E-12	-500.0	0.00	a
61	CXO3 + NO = NO2 + ALD2 + XO2H + RO2	2.10E-11	6.70E-12	-340.0	0.00	a
62	CXO3 + NO2 = PANX	1.16E-11	Falloff, F=0.30 ,N=1.00			a
		k_0	3.00E-28	0.0	-7.10	
		k_∞	1.33E-11	0.0	-0.90	
63	PANX = NO2 + CXO3	3.68E-04	Falloff, F=0.30 ,N=1.00			a
		k_0	1.70E-03	11280.0	0.00	
		k_∞	8.30E+16	13940.0	0.00	

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
64	PANX = 0.6 NO2 +0.6 CXO3 + 0.4 NO3 + 0.4 ALD2 + 0.4 XO2H + 0.4 RO2	Photolysis				a
65	CXO3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALD2 + 0.44 XO2H + 0.44 RO2 + 0.44 OH	1.39E-11	5.20E-13	-980.0	0.00	a
66	CXO3 + RO2 = CXO3	1.30E-11	8.90E-13	-800.0	0.00	a
67	CXO3 + CXO3 = 2 ALD2 + 2 XO2H + 2 RO2	1.71E-11	3.20E-12	-500.0	0.00	a
68	RO2 + NO = NO	8.03E-12	2.40E-12	-360.0	0.00	a
69	RO2 + HO2 = HO2	7.03E-12	4.80E-13	-800.0	0.00	a
70	RO2 + RO2 =	3.48E-13	6.50E-14	-500.0	0.00	a
71	MEO2 + NO = FORM + HO2 + NO2	7.70E-12	2.30E-12	-360.0	0.00	a
72	MEO2 + HO2 = 0.9 MEPX + 0.1 FORM	5.21E-12	3.80E-13	-780.0	0.00	a
73	MEO2 + C2O3 = FORM + 0.9 HO2 + 0.9 MEO2 + 0.1 AACD + 0.9 RO2	1.07E-11	2.00E-12	-500.0	0.00	a
74	MEO2 + RO2 = 0.685 FORM + 0.315 MEOH + 0.37 HO2 + RO2	3.48E-13	k = kref*K			a
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
75	XO2H + NO = NO2 + HO2	9.04E-12	2.70E-12	-360.0	0.00	a
76	XO2H + HO2 = ROOH	9.96E-12	6.80E-13	-800.0	0.00	a
77	XO2H + C2O3 = 0.8 HO2 + 0.8 MEO2 + 0.2 AACD + 0.8 RO2	1.30E-11	k = kref*K			a
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
78	XO2H + RO2 = 0.6 HO2 + RO2	3.48E-13	k = kref*K			a
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
79	XO2 + NO = NO2	9.04E-12	k = kref*K			a
		k(ref)	ref = 75			
		K	1.00E+00	0.0	0.00	
80	XO2 + HO2 = ROOH	9.96E-12	k = kref*K			a
		k(ref)	ref = 76			
		K	1.00E+00	0.0	0.00	
81	XO2 + C2O3 = 0.8 MEO2 + 0.2 AACD + 0.8 RO2	1.30E-11	k = kref*K			a
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
82	XO2 + RO2 = 0.6 HO2 + RO2	3.48E-13	k = kref*K			a
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
83	XO2N + NO = NTR	9.04E-12	k = kref*K			a
		k(ref)	ref = 75			
		K	1.00E+00	0.0	0.00	
84	XO2N + HO2 = ROOH	9.96E-12	k = kref*K			a
		k(ref)	ref = 76			
		K	1.00E+00	0.0	0.00	
85	XO2N + C2O3 = 0.8 HO2 + 0.8 MEO2 + 0.2 AACD + 0.8 RO2	1.30E-11	k = kref*K			a
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
86	XO2N + RO2 = 0.6 HO2 + RO2	3.48E-13	k = kref*K			a
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
87	MEPX + OH = 0.6 MEO2 + 0.6 RO2 + 0.4 FORM + 0.4 OH	1.00E-11	5.30E-12	-190.0	0.00	a
88	MEPX = MEO2 + RO2 + OH	Photolysis				a
89	ROOH + OH = 0.54 XO2H + 0.06 XO2N + 0.6 RO2 + 0.4 OH	6.05E-12	3.20E-12	-190.0	0.00	a
90	ROOH = HO2 + OH	Photolysis				a
91	NTR + OH = HNO3 + XO2H + RO2	8.10E-13	8.10E-13			a,c
92	NTR = NO2 + XO2H + RO2	Photolysis				a,c
93	FACD + OH = HO2	4.50E-13	4.50E-13			a
94	AACD + OH = MEO2 + RO2	6.93E-13	4.00E-14	-850.0	0.00	a
95	PACD + OH = C2O3	6.93E-13	4.00E-14	-850.0	0.00	a
96	FORM + OH = HO2 + CO	8.49E-12	5.40E-12	-135.0	0.00	a
97	FORM = 2 HO2 + CO	Photolysis				a
98	FORM = CO + H2	Photolysis				a
99	FORM + O = OH + HO2 + CO	1.58E-13	3.40E-11	1600.0	0.00	b
100	FORM + NO3 = HNO3 + HO2 + CO	5.50E-16	5.50E-16			a
101	FORM + HO2 = HCO3	7.90E-14	9.70E-15	-625.0	0.00	a
102	HCO3 = FORM + HO2	1.51E+02	2.40E+12	7000.0	0.00	a
103	HCO3 + NO = FACD + NO2 + HO2	5.60E-12	5.60E-12			a
104	HCO3 + HO2 = 0.5 MEPX + 0.5 FACD + 0.2 OH + 0.2 HO2	1.26E-11	5.60E-15	-2300.0	0.00	a
105	ALD2 + O = C2O3 + OH	4.49E-13	1.80E-11	1100.0	0.00	b
106	ALD2 + OH = C2O3	1.50E-11	4.70E-12	-345.0	0.00	a
107	ALD2 + NO3 = C2O3 + HNO3	2.73E-15	1.40E-12	1860.0	0.00	a
108	ALD2 = MEO2 + RO2 + CO + HO2	Photolysis				a
109	ALDX + O = CXO3 + OH	7.02E-13	1.30E-11	870.0	0.00	c,n
110	ALDX + OH = CXO3	1.91E-11	4.90E-12	-405.0	0.00	a
111	ALDX + NO3 = CXO3 + HNO3	6.30E-15	6.30E-15			a
112	ALDX = MEO2 + RO2 + CO + HO2	Photolysis				f
113	GLYD + OH = 0.2 GLY + 0.2 HO2 + 0.8 C2O3	8.00E-12	8.00E-12			a
114	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				a,b,f
115	GLYD + NO3 = HNO3 + C2O3	2.73E-15	1.40E-12	1860.0	0.00	a
116	GLY + OH = 1.7 CO + 0.3 XO2 + 0.3 RO2 + HO2	9.70E-12	3.10E-12	-340.0	0.00	a
117	GLY = 2 HO2 + 2 CO	Photolysis				a,q
118	GLY + NO3 = HNO3 + CO + HO2 + XO2 + RO2	2.73E-15	1.40E-12	1860.0	0.00	a
119	MGLY = C2O3 + HO2 + CO	Photolysis				a
120	MGLY + NO3 = HNO3 + C2O3 + XO2 + RO2	2.73E-15	1.40E-12	1860.0	0.00	a
121	MGLY + OH = C2O3 + CO	1.31E-11	1.90E-12	-575.0	0.00	a
122	H2 + OH = HO2	6.70E-15	7.70E-12	2100.0	0.00	a
123	CO + OH = HO2	2.28E-13	k = k1 + k2[M]			a
		k1	1.44E-13	0.0	0.00	
		k2	3.43E-33	0.0	0.00	
124	CH4 + OH = MEO2 + RO2	6.37E-15	1.85E-12	1690.0	0.00	a
125	ETHA + OH = 0.991 ALD2 + 0.991 XO2H + 0.009 XO2N + RO2	2.41E-13	6.90E-12	1000.0	0.00	a
126	MEOH + OH = FORM + HO2	8.95E-13	2.85E-12	345.0	0.00	a
127	ETOH + OH = 0.95 ALD2 + 0.9 HO2 + 0.1 XO2H + 0.1 RO2 + 0.078 FORM + 0.011 GLYD	3.21E-12	3.00E-12	-20.0	0.00	a
128	KET = 0.5 ALD2 + 0.5 C2O3 + 0.5 XO2H +0.5 CXO3 + 0.5 MEO2 + RO2 - 2.5 PAR	Photolysis				a

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
129	ACET = 0.38 CO + 1.38 MEO2 + 1.38 RO2 + 0.62 C2O3	Photolysis				a
130	ACET + OH = FORM + C2O3 + XO2 + RO2	1.76E-13	1.41E-12	620.6	0.00	a
131	PRPA + OH = 0.71 ACET + 0.26 ALDX + 0.26 PAR + 0.97 XO2H + 0.03 XO2N + RO2	1.07E-12	7.60E-12	585.0	0.00	a
132	PAR + OH = 0.11 ALDX + 0.76 ROR + 0.13 XO2N + 0.11 XO2H + 0.76 XO2 + RO2 - 0.11 PAR	8.10E-13	8.10E-13			c
133	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	2.15E+04	5.70E+12	5780.0	0.00	a,c
134	ROR + O2 = KET + HO2	3.78E+04	1.50E-14	200.0	0.00	a,c
135	ROR + NO2 = NTR	3.29E-11	8.60E-12	-400.0	0.00	a,c
136	ETHY + OH = 0.7 GLY + 0.7 OH + 0.3 FACD + 0.3 CO + 0.3 HO2	7.52E-13	Falloff, F=0.37 ,N=1.30			a
		k_0	5.00E-30	0.0	-1.50	
		k_∞	1.00E-12	0.0	0.00	
137	ETH + O = FORM + HO2 + CO + 0.7 XO2H + 0.7 RO2 + 0.3 OH	7.29E-13	1.04E-11	792.0	0.00	c,o
138	ETH + OH = XO2H + RO2 + 1.56 FORM + 0.22 GLYD	7.84E-12	Falloff, F=0.48 ,N=1.15			a,g
		k_0	8.60E-29	0.0	-3.10	
		k_∞	9.00E-12	0.0	-0.85	
139	ETH + O3 = FORM + 0.51 CO + 0.16 HO2 + 0.16 OH + 0.37 FACD	1.58E-18	9.10E-15	2580.0	0.00	a,g
140	ETH + NO3 = 0.5 NO2 + 0.5 NTR + 0.5 XO2H + 0.5 XO2 + RO2 + 1.125 FORM	2.10E-16	3.30E-12	2880.0	0.00	a,g
141	OLE + O = 0.2 ALD2 + 0.3 ALDX + 0.1 HO2 + 0.2 XO2H + 0.2 CO + 0.2 FORM + 0.01 XO2N + 0.21 RO2 + 0.2 PAR + 0.1 OH	3.91E-12	1.00E-11	280.0	0.00	c,o
142	OLE + OH = 0.781 FORM + 0.488 ALD2 + 0.488 ALDX + 0.976 XO2H + 0.195 XO2 + 0.024 XO2N + 1.17 RO2 - 0.73 PAR	2.86E-11	Falloff, F=0.50 ,N=1.13			a,g
		k_0	8.00E-27	0.0	-3.50	
		k_∞	3.00E-11	0.0	-1.00	
143	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	1.00E-17	5.50E-15	1880.0	0.00	a,g
144	OLE + NO3 = 0.5 NO2 + 0.5 NTR + 0.48 XO2 + 0.48 XO2H + 0.04 XO2N + RO2 + 0.5 FORM + 0.25 ALD2 + 0.375 ALDX - PAR	9.54E-15	4.60E-13	1155.0	0.00	a,g
145	IOLE + O = 1.24 ALD2 + 0.66 ALDX + 0.1 XO2H + 0.1 RO2 + 0.1 CO + 0.1 PAR	2.30E-11	2.30E-11			c,o
146	IOLE + OH = 1.3 ALD2 + 0.7 ALDX + XO2H + RO2	5.99E-11	1.05E-11	-519.0	0.00	a,g
147	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	1.57E-16	4.70E-15	1013.0	0.00	a,g
148	IOLE + NO3 = 0.5 NO2 + 0.5 NTR + 0.48 XO2 + 0.48 XO2H + 0.04 XO2N + RO2 + 0.5 ALD2 + 0.625 ALDX + PAR	3.70E-13	3.70E-13			a,g
149	ISOP + OH = ISO2 + RO2	9.99E-11	2.70E-11	-390.0	0.00	a
150	ISO2 + NO = 0.117 INTR + 0.883 NO2 + 0.803 HO2 + 0.66 FORM + 0.66 ISPD + 0.08 XO2H + 0.08 RO2 + 0.05 IOLE + 0.042 GLYD + 0.115 PAR + 0.038 GLY + 0.042 MGLY + 0.093 OLE + 0.117 ALDX	8.13E-12	2.39E-12	-365.0	0.00	r,s
151	ISO2 + HO2 = 0.88 ISPX + 0.12 OH + 0.12 HO2 + 0.12 FORM + 0.12 ISPD	7.78E-12	7.43E-13	-700.0	0.00	r,s
152	ISO2 + C2O3 = 0.709 HO2 + 0.583 FORM + 0.583	1.30E-11	k = kref*K			r,s

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
	ISPD + 0.071 XO2H + 0.044 IOLE + 0.037 GLYD + 0.102 PAR + 0.034 GLY + 0.037 MGLY + 0.082 OLE + 0.103 ALDX + 0.8 MEO2 + 0.2 AACD + 0.871 RO2	k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
153	ISO2 + RO2 = 0.803 HO2 + 0.66 FORM + 0.66 ISPD + 0.08 XO2H + 0.05 IOLE + 0.042 GLYD + 0.115 PAR + 0.038 GLY + 0.042 MGLY + 0.093 OLE + 0.117 ALDX + 1.08 RO2	3.48E-13	k = kref*K			r,s
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
154	ISO2 = 0.8 HO2 + 0.04 OH + 0.04 FORM + 0.8 ISPD	1.00E+00	1.00E+00			j,t
155	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	1.27E-17	1.03E-14	1995.0	0.00	c
156	ISOP + NO3 = 0.35 NO2 + 0.65 INTR + 0.64 XO2H + 0.33 XO2 + 0.03 XO2N + RO2 + 0.35 FORM + 0.35 ISPD	6.74E-13	3.03E-12	448.0	0.00	u
157	ISPD + OH = 0.095 XO2N + 0.379 XO2 + 0.318 XO2H + 0.792 RO2 + 0.843 PAR + 0.379 C2O3 + 0.209 CXO3 + 0.379 GLYD + 0.24 MGLY + 0.24 FORM + 0.067 OLE + 0.079 CO + 0.028 ALDX	3.38E-11	6.31E-12	-500.0	0.00	r,s
158	ISPD + O3 = 0.02 ALD2 + 0.15 FORM + 0.225 CO + 0.85 MGLY + 0.36 PAR + 0.114 C2O3 + 0.064 XO2H + 0.064 RO2 + 0.268 OH + 0.09 HO2	7.10E-18	4.17E-15	1900.0	0.00	c
159	ISPD + NO3 = 0.643 CO + 0.282 FORM + 0.357 ALDX + 1.282 PAR + 0.85 HO2 + 0.075 CXO3 + 0.075 XO2H + 0.075 RO2 + 0.85 NTR + 0.15 HNO3	1.00E-15	1.00E-15			c
160	ISPD = 0.333 CO + 0.067 ALD2 + 0.9 FORM + 0.832 PAR + 0.333 HO2 + 0.7 XO2H + 0.7 RO2 + 0.967 C2O3	Photolysis				c,f
161	ISPX + OH = 0.904 EPOX + 0.933 OH + 0.067 ISO2 + 0.067 RO2 + 0.029 IOLE + 0.029 ALDX	7.77E-11	2.23E-11	-372.0	0.00	r,s
162	EPOX + OH = EPX2 + RO2	1.51E-11	5.78E-11	400.0	0.00	r,s
163	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	7.78E-12	7.43E-13	-700.0	0.00	r,s
164	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	8.13E-12	2.39E-12	-365.0	0.00	r,s
165	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	1.30E-11	k = kref*K			a,r,s
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
166	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	3.48E-13	k = kref*K			a,r,s
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
167	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 NTR	3.10E-11	3.10E-11			r,s
168	TERP + O = 0.15 ALDX + 5.12 PAR	3.60E-11	3.60E-11			c
169	TERP + OH = 0.75 XO2H + 0.5 XO2 + 0.25 XO2N + 1.5 RO2 + 0.28 FORM + 1.66 PAR + 0.47 ALDX	6.77E-11	1.50E-11	-449.0	0.00	c
170	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	7.63E-17	1.20E-15	821.0	0.00	c
171	TERP + NO3 = 0.47 NO2 + 0.28 XO2H + 0.75 XO2 + 0.25 XO2N + 1.28 RO2 + 0.47 ALDX + 0.53 NTR	6.66E-12	3.70E-12	-175.0	0.00	c
172	BENZ + OH = 0.53 CRES + 0.352 BZO2 + 0.352 RO2 + 0.118 OPEN + 0.118 OH + 0.53 HO2	1.22E-12	2.30E-12	190.0	0.00	a,d,e

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
173	BZO2 + NO = 0.918 NO2 + 0.082 NTR + 0.918 GLY + 0.918 OPEN + 0.918 HO2	9.04E-12	2.70E-12	-360.0	0.00	d,h
174	BZO2 + C2O3 = GLY + OPEN + HO2 + MEO2 + RO2	1.30E-11	k = kref*K			a,d,h
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
175	BZO2 + HO2 =	1.49E-11	1.90E-13	-1300.0	0.00	d
176	BZO2 + RO2 = GLY + OPEN + HO2 + RO2	3.48E-13	k = kref*K			a,d,h
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
177	TOL + OH = 0.18 CRES + 0.65 TO2 + 0.72 RO2 + 0.1 OPEN + 0.1 OH + 0.07 XO2H + 0.18 HO2	5.63E-12	1.80E-12	-340.0	0.00	a,d,e
178	TO2 + NO = 0.86 NO2 + 0.14 NTR + 0.417 GLY + 0.443 MGLY + 0.66 OPEN + 0.2 XOPN + 0.86 HO2	9.04E-12	2.70E-12	-360.0	0.00	d,h
179	TO2 + C2O3 = 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + MEO2 + RO2	1.30E-11	k = kref*K			a,d,h
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
180	TO2 + HO2 =	1.49E-11	1.90E-13	-1300.0	0.00	d
181	TO2 + RO2 = 0.48 GLY + 0.52 MGLY + 0.77 OPEN + 0.23 XOPN + HO2 + RO2	3.48E-13	k = kref*K			a,d,h
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
182	XYL + OH = 0.155 CRES + 0.544 XLO2 + 0.602 RO2 + 0.244 XOPN + 0.244 OH + 0.058 XO2H + 0.155 HO2	1.85E-11	1.85E-11			d,e,p
183	XLO2 + NO = 0.86 NO2 + 0.14 NTR + 0.221 GLY + 0.675 MGLY + 0.3 OPEN + 0.56 XOPN + 0.86 HO2	9.04E-12	2.70E-12	-360.0	0.00	d,h
184	XLO2 + HO2 =	1.49E-11	1.90E-13	-1300.0	0.00	d
185	XLO2 + C2O3 = 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + MEO2 + RO2	1.30E-11	k = kref*K			a,d,h
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
186	XLO2 + RO2 = 0.26 GLY + 0.77 MGLY + 0.35 OPEN + 0.65 XOPN + HO2 + RO2	3.48E-13	k = kref*K			a,d,h
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
187	CRES + OH = 0.06 CRO + 0.12 XO2H + HO2 + 0.13 OPEN + 0.732 CAT1 + 0.06 CO + 0.06 XO2N + 0.18 RO2 + 0.06 FORM	4.12E-11	1.70E-12	-950.0	0.00	d
188	CRES + NO3 = 0.3 CRO + HNO3 + 0.24 XO2 + 0.36 XO2H + 0.48 ALDX + 0.24 FORM + 0.24 MGLY + 0.12 OPEN + 0.1 XO2N + 0.7 RO2 + 0.24 CO	1.40E-11	1.40E-11			d
189	CRO + NO2 = CRON	2.10E-12	2.10E-12			d
190	CRO + HO2 = CRES	5.50E-12	5.50E-12			d
191	CRON + OH = CRNO	1.53E-12	1.53E-12			d
192	CRON + NO3 = CRNO + HNO3	3.80E-12	3.80E-12			d
193	CRNO + NO2 = 2 NTR	2.10E-12	2.10E-12			d
194	CRNO + O3 = CRN2	2.86E-13	2.86E-13			d
195	CRN2 + NO = CRNO + NO2	8.50E-12	2.54E-12	-360.0	0.00	d
196	CRN2 + HO2 = CRPX	1.88E-11	2.40E-13	-1300.0	0.00	d
197	CRPX = CRNO + OH	Photolysis				a,d
198	CRPX + OH = CRN2	3.59E-12	1.90E-12	-190.0	0.00	d
199	XOPN = CAO2 + 0.7 HO2 + 0.7 CO + 0.3 C2O3 + RO2	Photolysis				d,p
200	XOPN + OH = CAO2 + MGLY + XO2H + RO2	9.00E-11	9.00E-11			d,p
201	XOPN + O3 = 1.2 MGLY + 0.5 OH + 0.6 C2O3 + 0.1 ALD2 + 0.5 CO + 0.3 XO2H + 0.3 RO2	2.02E-17	1.08E-16	500.0	0.00	d,p

Number	Reactants and Products	k_{298}	Rate Parameters			Notes
			A	E_a	B	
202	XOPN + NO3 = 0.5 NO2 + 0.5 NTR + 0.45 XO2H + 0.45 XO2 + 0.1 XO2N + RO2 + 0.25 OPEN + 0.25 MGLY	3.00E-12	3.00E-12			d,p
203	OPEN = OPO3 + HO2 + CO	Photolysis				d,p
204	OPEN + OH = 0.6 OPO3 + 0.4 CAO2 + 0.4 RO2	4.40E-11	4.40E-11			d,p
205	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	1.01E-17	5.40E-17	500.0	0.00	d,p
206	OPEN + NO3 = OPO3 + HNO3	3.80E-12	3.80E-12			d,p
207	CAT1 + OH = CAO2 + RO2	7.00E-11	7.00E-11			d
208	CAT1 + NO3 = CRO + HNO3	1.70E-10	1.70E-10			d
209	CAO2 + NO = 0.86 NO2 + 0.14 NTR + 1.2 HO2 + 0.344 FORM + 0.344 CO	8.50E-12	2.54E-12	-360.0	0.00	d
210	CAO2 + HO2 =	1.88E-11	2.40E-13	-1300.0	0.00	d
211	CAO2 + C2O3 = HO2 + 0.4 GLY + MEO2 + RO2	1.30E-11	k = kref*K			d
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	
212	CAO2 + RO2 = HO2 + 0.4 GLY + RO2	3.48E-13	k = kref*K			d
		k(ref)	ref = 70			
		K	1.00E+00	0.0	0.00	
213	OPO3 + NO = NO2 + XO2H + RO2 + ALDX	1.00E-11	1.00E-11			d
214	OPO3 + NO2 = OPAN	1.16E-11	k = kref*K			d
		k(ref)	ref = 62			
		K	1.00E+00	0.0	0.00	
215	OPAN = OPO3 + NO2	9.92E-05	Falloff, F=0.30 ,N=1.00			d
		k_0	4.60E-04	11280.0	0.00	
		k_∞	2.24E+16	13940.0	0.00	
216	OPO3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALDX + 0.44 XO2H + 0.44 RO2 + 0.44 OH	1.39E-11	k = kref*K			d
		k(ref)	ref = 57			
		K	1.00E+00	0.0	0.00	
217	OPO3 + C2O3 = MEO2 + XO2 +ALDX + 2 RO2	1.55E-11	k = kref*K			d
		k(ref)	ref = 59			
		K	1.00E+00	0.0	0.00	
218	OPO3 + RO2 = 0.8 XO2H + 0.8 RO2 + 0.8 ALDX + 0.2 AACD	1.30E-11	k = kref*K			d
		k(ref)	ref = 58			
		K	1.00E+00	0.0	0.00	

Table notes:

k_{298} is the rate constant at 298 K and 1 atmosphere using units molecules cm^{-3} and s^{-1}

See Table 2-7 for species names

See Table 2-8 for information on photolysis reactions

a	IUPAC: Atkinson et al., (2010)	h	Arey et al. (2009)	o	Cvetanovic (1987)
b	JPL: Sander et al., (2006)	i	Hu et al. (2007)	p	Calvert et al. (2002)
c	CB05: Yarwood et al (2005)	j	Archibald et al. (2010)	q	Feierabend et al. (2009)
d	CB05-TU: Whitten et al., 2010)	k	Hjorth et al. (1992)	r	Paulot et al. (2009a)
e	Bloss et al. (2005)	l	Kaiser and Wu (1977)	s	Paulot et al. (2009b)
f	SAPRC-99: Carter (2000)	m	Jeffries et al. (2002)	t	Peeters et al. (2009)
g	Calvert et al. (2000)	n	Herron (1988)	u	Perring et al. (2009)

Table 2-8. Model species names for CB6.

Species	Description
AACD	Acetic acid
ACET	Acetone
ALD2	Acetaldehyde
ALDX	Propionaldehyde and higher aldehydes
BENZ	Benzene
BZO2	Peroxy radical from OH addition to benzene
C2O3	Acetylperoxy radical
CAO2	Peroxy radical from aromatic degradation products
CAT1	Methyl-catechols
CH4	Methane
CO	Carbon monoxide
CRES	Cresols
CRN2	Peroxy radical from nitro-cresol
CRNO	Alkoxy radical from nitro-cresols
CRO	Alkoxy radical from cresol
CRON	Nitro-cresols
CRPX	Nitro-cresol hydroperoxides
CXO3	C3 and higher acylperoxy radicals
EPOX	Epoxide formed from ISPX reaction with OH
EPX2	Peroxy radical from EPOX reaction with OH
ETH	Ethene
ETHA	Ethane
ETHY	Ethyne
ETOH	Ethanol
FACD	Formic acid
FORM	Formaldehyde
GLY	Glyoxal
GLYD	Glycolaldehyde
H2O2	Hydrogen peroxide
HCO3	Adduct from HO2 plus formaldehyde
HNO3	Nitric acid
HO2	Hydroperoxy radical
HONO	Nitrous acid
INTR	Organic nitrates from ISO2 reaction with NO
IOLE	Internal olefin carbon bond (R-C=C-R)
ISO2	Peroxy radical from OH addition to isoprene
ISOP	Isoprene
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)
ISPX	Hydroperoxides from ISO2 reaction with HO2
KET	Ketone carbon bond (C=O)
M	Air
MEO2	Methylperoxy radical
MEOH	Methanol
MEPX	Methylhydroperoxide
MGLY	Methylglyoxal
N2O5	Dinitrogen pentoxide
NO	Nitric oxide
NO2	Nitrogen dioxide
NO3	Nitrate radical
NTR	Organic nitrates
O	Oxygen atom in the O^3(P) electronic state
O1D	Oxygen atom in the O^1(D) electronic state

Species	Description
O2	Oxygen
O3	Ozone
OH	Hydroxyl radical
OLE	Terminal olefin carbon bond (R-C=C)
OPAN	Peroxyacyl nitrate (PAN compound) from OPO3
OPEN	Aromatic ring opening product (unsaturated dicarbonyl)
OPO3	Peroxyacyl radical from OPEN
PACD	Peroxyacetic and higher peroxycarboxylic acids
PAN	Peroxyacetyl Nitrate
PANX	C3 and higher peroxyacyl nitrate
PAR	Paraffin carbon bond (C-C)
PNA	Peroxynitric acid
PRPA	Propane
RO2	Operator to approximate total peroxy radical concentration
ROOH	Higher organic peroxide
ROR	Secondary alkoxy radical
SO2	Sulfur dioxide
SULF	Sulfuric acid (gaseous)
TERP	Monoterpenes
TO2	Peroxy radical from OH addition to TOL
TOL	Toluene and other monoalkyl aromatics
XLO2	Peroxy radical from OH addition to XYL
XO2	NO to NO2 conversion from alkylperoxy (RO2) radical
XO2H	NO to NO2 conversion (XO2) accompanied by HO2 production
XO2N	NO to organic nitrate conversion from alkylperoxy (RO2) radical
XOPN	Aromatic ring opening product (unsaturated dicarbonyl)
XYL	Xylene and other polyalkyl aromatics

2.3 REACTION RATE CHANGES FROM CB05

The rates for inorganic reactions included in CB6 (reactions 1-51) are compared to CB05 in Table 2-9 at 298 K and 1 atmosphere. Ten of the 51 reactions compared are photolysis reaction and they are discussed separately below. One reaction (O + O3) was not included in CB05. Of the remaining 40 reactions, there was no change in rate constant for 14 reactions and the change was smaller than 5% for another 8 reactions. Notable changes include:

- 5% increase in the rate constant for the OH + NO_2 reaction which will tend to shorten the atmospheric lifetime of NOx and thereby reduce ozone production in NOx-limited conditions.

- 60% decrease in the rate constant for the N_2O_5 + H_2O reaction (and elimination of the N_2O_5 + H_2O + H_2O reaction) which will prolong the atmospheric lifetime of NOx at night. As discussed above, heterogeneous reaction between N_2O_5 and $_{H2O}$ may offset this change and should be accounted for when CB6 is used in atmospheric models.

- 11% increase in the rate constant for $O(^1D)$ reaction with M (i.e., $O(^1D)$ quenching) and 3% decrease in the rate constant for $O(^1D)$ reaction with H_2O to produce OH. Both of these changes will reduce production of OH from O_3 photolysis.