APPENDIX B: Listing of Carbon Bond-IV Mechanisms

Table B1. Regulatory Version of the Carbon Bond Mechanism, CB-IV.1

Rxn No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
	NO2 Photolysis	
1]	NO2 = NO + O	j1
2]	O = O3	k_{hi} = 2.8E-12(TK/300)^0 k_{lo} = 6.0E-34(TK/300)^-2.3 F_c = 0.6
3]	O3 + NO = NO2	1.8E-12 exp (-1370/TK)
4]	O + NO2 = NO	9.3E-12
5]	O + NO2 = NO3	k_{hi} = 2.2E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-2.0 F_c = 0.6
6]	O + NO = NO2	k_{hi} = 3.0E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-1.5 F_c = 0.6
	OZONE Photolysis	
7]	O3 + NO2 = NO3	1.2E-13 exp (-2450/TK)
8]	O3 {hv} = O	j8
9]	O3 {hv} = O1D	j9
10]	O1D = O	1.9E08 exp (390/TK)
11]	O1D + H2O = 2.0*OH	2.2E-10
12]	O3 + OH = HO2	1.6E-12 exp (-940/TK)
13]	O3 + HO2 = OH	1.4E-14 exp (-580/TK)
	NO3 Chemistry	
14]	NO3 {hv} = 0.89*NO2 + 0.89*O + 0.11*NO	j14
15]	NO3 + NO = 2.0*NO2	1.3E-11 exp (250/TK)
16]	NO3 + NO2 = NO + NO2	2.5E-14 exp (-1230/TK)
17]	NO3 + NO2 = N2O5	k_{hi} =1.5E-12^-0.5 k_{lo} = 2.2E-30^-4.3 F_c = 0.6
18]	N2O5 {hv} = NO3 + NO2	K17*3.7E26 exp (11000/TK)
19]	N2O5 + H2O = 2.0*HNO3	1.3E-21
	HONO Chemistry	
20]	NO + NO = 2.0*NO2	1.80E-20 exp (530/TK)
21]	NO + NO2 + H2O = 2.0*HONO	4.4E-40
22]	OH + NO = HONO	k_{hi} = 3.0E-11(TK/300)^-1.0 k_{lo} = 6.7E-31(TK/300)^-3.3 F_c = 0.6
23]	HONO = OH + NO	0.171*j1
24]	OH + HONO = NO2	6.6E-12

Table B1. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
25]	HONO + HONO = NO + NO2	1.0E-20
	OH/HO2 Termination Reactions	
26]	OH + NO2 = HNO3	k_{hi} = 2.4E-11(TK/300)^-1.3 k_{lo} = 2.6E-30(TK/300)^-3.2 F_c = 0.6
27]	OH + HNO3 = NO3	k_0 = 7.2E-15 exp (785/TK) k_2 = 4.1E-16 exp (1440/TK) k_3 = 1.9E-33 exp (725/TK)
28]	HO2 + NO = OH + NO2	3.7E-12 exp (240/TK)
29]	HO2 + NO2 = PNA	k_{hi} = 4.2E-12(TK/300)^0.2 k_{lo} = 2.3E-31(TK/300)^-4.6 F_c = 0.6
30]	PNA = HO2 + NO2	k29*4.76E26 exp (10900/TK)
31]	OH + PNA = NO2	1.3E-12 exp (380/TK)
32]	HO2 + HO2 = H2O2	5.9E-14 exp (1150/TK)
33]	HO2 + HO2 + H2O = H2O2	2.2E-38 exp (5800/TK)
34]	H2O2 = 2*OH	k34
35]	OH + H2O2 = HO2	3.1E-12 exp (-187/TK)
	Propagation Reactions	
36]	OH + CO = HO2	2.2E-13
	Formaldehyde Chemistry	
37]	HCHO + OH = HO2 + CO	1.0E-11
38]	HCHO {hv} = 2*HO2 + CO	j38
39]	HCHO {hv} = CO + H2	j39
40]	HCHO + O = OH + HO2 + CO	3.0E-11 exp (-1550/TK)
41]	HCHO + NO3 = HNO3 + HO2 + CO	6.3E-16
	Higher Aldehyde Chemistry	
42]	RCHO + O = C2O3 + OH	1.2E-11 exp (-986/TK)
43]	RCHO + OH = C2O3	7.0E-12 exp (250/TK)
44]	RCHO + NO3 = C2O3 + HNO3	2.5E-15
45]	RCHO = XO2 + 2*HO2 + CO + HCHO	j45
	PAN Chemistry	
46]	C2O3 + NO = NO2 + XO2 + HCHO + HO2	5.4E-12 exp (250/TK)
47]	C2O3 + NO2 = PAN	8.0E-20 exp (5500/TK)
48]	PAN = C2O3 + NO2	9.4E16 exp (-14000/TK)
49]	C2O3+ C2O3 = 2*XO2 + 2*HCHO + 2*HO2	2.0E-12

Table B1. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
50]	C2O3+ HO2 = 0.75*C2O3H +0.79*HCHO + 0.79*XO2 +0.25*C2O2H + 0.79*HO2 +0.79*OH	6.5E-12
	Paraffin Chemistry	
51]	OH = HCHO + XO2 + HO2	1.1E02 exp (-1710/TK)
52]	OH + PAR = 0.87*XO2 + 0.13*XO2N + 0.11*HO2 +0.11*RCHO + 0.76*ROR +-0.11*PAR	8.14E-13
53]	ROR = 1.1*RCHO + 0.96*XO2 + 0.94*HO2 +-2.1*PAR + 0.04*XO2N +0.02*ROR	1.0E15 exp (-8000/TK)
54]	ROR = HO2 + KETENE	1.6E03
55]	ROR + NO2 = NTR	1.50E-11
	Olefin Chemistry	
56]	O + OLE = 0.63*RCHO + 0.38*HO2 + 0.28*XO2 +0.30*CO + 0.20*HCHO +0.02*XO2N + 0.22*PAR +0.20*OH	1.2E-11exp (-324/TK)
57]	OH + OLE = HCHO + RCHO + XO2 + HO2 + -1*PAR	5.2E-12 exp (504/TK)
58]	O3 + OLE = 0.5*RCHO + 0.74*HCHO + 0.33*CO + 0.44*HO2 + 0.22*XO2+ 0.10*OH + -1.0*PAR	1.4E-14 exp (-2105/TK)
59]	NO3 + OLE = 0.91*XO2 + 0.09*XO2N + HCHO + RCHO +-1*PAR + NO2	7.7E-15
	Ethene Chemistry	
60]	O + C:C = HCHO + 0.70*XO2 + CO + 1.70*HO2+ 0.30*OH	1.0E-11 exp (-792/TK)
61]	OH + C:C = XO2 + 1.56*HCHO + HO2 + 0.22*RCHO	2.0E-12 exp (411/TK)
62]	O3 + C:C = HCHO + 0.42*CO + 0.12*HO2	1.3E-14 exp (-2633/TK)
	Aromatic Chemistry	
63]	OH + TOL = 0.08*[XO2+HO2] + 0.36*[CRES+HO2] + 0.56*TO2	2.1E-12 exp (322/TK)
64]	TO2 + NO = 0.90*[NO2+HO2+OPEN] + 0.1*NTR	8.12E-12
65]	TO2 = CRES + HO2	4.2
66]	OH + CRES = 0.40*CRO + 0.60*[XO2 + HO2] + 0.30*OPEN	4.1E-11
67]	NO3 + CRES = CRO + HNO3	2.2E-11
68]	CRO + NO2 = ARONTR	1.4E-11

Table B1. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
69]	OH + XYL = 0.10*[HO2+XO2+PAR] + 0.20*[CRES+HO2+PAR] + 0.30*TO2 + 0.40*[2*MGLY + 2*PAR+HO2]	1.7E-11 exp (116/TK)
70]	OPEN + OH = XO2 + 2.0*CO +2.0*HO2 + C2O3 + HCHO	3.0E-11
71]	OPEN = C2O3 + HO2 + CO	9.04*j38
72]	OPEN + O3 = 0.03*RCHO + 0.62*C2O3 + 0.70*HCHO +0.03*XO2 + 0.69*CO + 0.08*OH + 0.76*HO2 + 0.2*MGLY	5.4E-17 exp (-500/TK)
73]	OH + MGLY = XO2 + C2O3	1.7E-11
74]	MGLY = C2O3 + HO2 + CO	9.62*j38
	Isoprene Chemistry - Condensed	
75]	O + ISOP = 0.6*HO2 + 0.80*RCHO + 0.55*OLE + 0.50*XO2 + 0.50*CO + 0.45*C:C + 0.9*PAR	1.8E-11
76]	OH + ISOP = XO2 + HCHO + 0.67*HO2 +0.13*XO2N + 1.0*C:C + 0.4*MGLY + 0.2*C2O3 + 0.2*RCHO	9.6E-11
77]	O3 + ISOP = HCHO + 0.4*RCHO + 0.55*C:C + 0.2*MGLY + 0.10*PAR + 0.06*CO + 0.44*HO2 +0.1*OH	1.2E-17
78]	NO3 + ISOP = XO2N	3.2E-13
	Operator Chemistry	
79]	XO2 + NO = NO2	8.1E-12
80]	XO2 + XO2 =	1.7E-14 exp (1300/TK)
81]	XO2N + NO = {NTR}	6.8E-13

Table B1b. Sources of Data Used to Calculate Photolysis Rates in CB-IV.1 (Gery, et al., 1989)

Species	Quantum Yield	Absorption Cross Section
NO_2	*DeMore et al.* [1985]	*DeMore et al.* [1985]
O_3 to $O(^3P)$	*Atkinson and Lloyd* [1984]	*Molina and Molina* [1987]
O_3 to $O(^1D)$	*DeMore et al.* [1985]	*Bass* [1985]
NO_3	*Atkinson and Lloyd* [1984]	*Atkinson and Lloyd* [1984]
HONO	*Baulch et al.* [1984]	*DeMore et al.* [1985]
H_2O_2	assumed to be 1.0	*Baulch et al.* [1984]
HCHO to $2HO_2$	*Calvert* [1980]	*Bass et al.* [1980]
HCHO to H_2 + CO	*Calvert* [1980]	*Bass et al.* [1980]
ALD2	*Baulch et al.* [1984]	*Baulch et al.* [1984]

Table B2. Current Operational Version of CB-IV, Mechanism Used in MAQSIP Testing (1998, Docket #)

Rxn No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
	NO2 Photolysis	
1]	NO2 = NO + O	j1
2]	O = O3	k_{hi} = 2.8E-12(TK/300)^0 k_{lo} = 6.0E-34(TK/300)^-2.3 F_c = 0.6
3]	O3 + NO = NO2	1.8E-12 exp (-1370/TK)
4]	O + NO2 = NO	9.3E-12
5]	O + NO2 = NO3	k_{hi} = 2.2E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-2.0 F_c = 0.6
6]	O + NO = NO2	k_{hi} = 3.0E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-1.5 F_c = 0.6
	OZONE Photolysis	
7]	O3 + NO2 = NO3	1.2E-13 exp (-2450/TK)
8]	O3 {hv} = O	0.053*j1
9]	O3 {hv} = O1D	j9
10a]	O1D + N2 = O	1.8E-11 exp (107/TK)
10b]	O1D + O2 = O	3.2E-11exp (67/TK)
11]	O1D + H2O = 2.0*OH	2.2E-10
12]	O3 + OH = HO2	1.6E-12 exp (-940/TK)
13]	O3 + HO2 = OH	1.4E-14 exp (-580/TK)
	NO3 Chemistry	
14]	NO3 {hv} = 0.89*NO2 +0.89*O +0.11*NO	33.9*j1

Table B2. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
15]	NO3 + NO = 2.0*NO2	1.3E-11 exp (250/TK)
16]	NO3 + NO2 = NO + NO2	2.5E-14 exp (-1230/TK)
17]	NO3 + NO2 = N2O5	k_{hi} = 1.5E-12(TK/300)^-0.5 k_{lo} = 2.2E-30(TK/300)^-4.3 F_c = 0.6
18]	N2O5 = NO3 + NO2	k17*3.7E26 exp (11000/TK)
19]	N2O5 + H2O = 2.0*HNO3	1.3E-21
	HONO Chemistry	
20]	NO + NO + O2 = 2.0*NO2	3.30E-39 exp (530/TK)
21]	NO + NO2 + H2O = 2.0*HONO	4.4E-40
22]	OH + NO = HONO	k_{hi} = 3.0E-11^-1.0 k_{lo} = 6.7E-31^-3.3 F_c = 0.6^1
23]	HONO = OH + NO	0.1975*j1
24]	OH + HONO = NO2	6.6E-12
25]	HONO + HONO = NO + NO2	1.0E-20
	OH/HO2 Termination Reactions	
26]	OH + NO2 = HNO3	k_{hi} = 2.4E-11(TK/300)^-1.3 k_{lo} = 2.6E-30(TK/300)^-3.2 F_c = 0.6
27]	OH + HNO3 = NO3	k_0 = 7.2E-15 exp (785/TK) & k_2 = 4.1E-16 exp (1440/TK) & k_3 = 1.9E-33 exp (725/TK)
28]	HO2 + NO = OH + NO2	3.7E-12 exp (240/TK)
29]	HO2 + NO2 = PNA	k_{hi} = 4.2E-12(TK/300)^0.2 k_{lo} = 2.3E-31(TK/300)^-4.6 F_c = 0.6
30]	PNA = HO2 + NO2	k29*4.76E26 exp (10900/TK)
31]	OH + PNA = NO2	1.3E-12 exp (380/TK)
32]	HO2 + HO2 = H2O2	5.9E-14 exp (1150/TK)
33]	HO2 + HO2 + H2O = H2O2	2.2E-38 exp (5800/TK)
34]	H2O2 = 2*OH	0.255*k39
35]	OH + H2O2 = HO2	3.1E-12 exp (-187/TK)
	Propagation Reactions	
36a]	OH + CO = HO2	1.5E-13
36b]	OH + CO = HO2	k36a*0.6*Pressure
	Formaldehyde Chemistry	
37]	HCHO + OH = HO2 + CO	1.0E-11
38]	HCHO {hv} = 2*HO2 + CO	j38

Table B2. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
39]	HCHO {hv} = CO + H2	j39
40]	HCHO + O = OH + HO2 + CO	3.0E-11 exp (-1550/TK)
41]	HCHO + NO3 = HNO3 + HO2 + CO	6.3E-16
	Higher Aldehyde Chemistry	
42]	RCHO + O = C2O3 + OH	1.2E-11 exp (-986/TK)
43]	RCHO + OH = C2O3	7.0E-12 exp (250/TK)
44]	RCHO + NO3 = C2O3 + HNO3	2.5E-15
45]	RCHO = XO2 + 2*HO2 + CO + HCHO	j45
	PAN Chemistry	
46]	C2O3 + NO = NO2 + XO2 + HCHO + HO2	3.49E-11 exp (-180/TK)
47]	C2O3 + NO2 = PAN	2.63E-12exp (380/TK)
48]	PAN = C2O3 + NO2	2.0E16exp (-13500/TK)
49]	C2O3+ C2O3 = 2*XO2 + 2*HCHO + 2*HO2	2.5E-12
50]	C2O3 + HO2 = 0.75*C2O3H + 0.79*HCHO + 0.79*XO2 + 0.25*C2O2H + 0.79*HO2 +0.79*OH	6.5E-12
	Paraffin Chemistry	
51]	OH = HCHO + XO2 + HO2	1.1E02 exp (-1710/TK)
52]	OH + PAR = 0.87*XO2 + 0.13*XO2N + 0.11*HO2 + 0.11*RCHO + 0.76*ROR + -0.11*PAR	8.1E-13
53]	ROR = 1.1*RCHO + 0.96*XO2 + 0.94*HO2 + -2.1*PAR + 0.04*XO2N + 0.02*ROR	1.0E15 exp (-8000/TK)
54]	ROR = HO2 + KETENE	1.6E03
55]	ROR + NO2 = NTR	1.50E-11
	Olefin Chemistry	
56]	O + OLE = 0.63*RCHO + 0.38*HO2 + 0.28*XO2 + 0.30*CO + 0.20*HCHO + 0.02*XO2N + 0.22*PAR + 0.20*OH	1.2E-11exp (-324/TK)
57]	OH + OLE = HCHO + RCHO + XO2 + HO2 + -1*PAR	5.2E-12 exp (504/TK)
58]	O3 + OLE = 0.5*RCHO + 0.74*HCHO + 0.33*CO + 0.44*HO2 + 0.22*XO2 + 0.10*OH + -1.0*PAR	1.4E-14 exp (-2105/TK)
59]	NO3 + OLE = 0.91*XO2 + 0.09*XO2N + HCHO + RCHO + -1*PAR + NO2	7.7E-15

Table B2. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
	Ethene Chemistry	
60]	O + C:C = HCHO + 0.70*XO2 + CO + 1.70*HO2+ 0.30*OH	1.0E-11 exp (-792/TK)
61]	OH + C:C = XO2 + 1.56*HCHO + HO2 + 0.22*RCHO	2.0E-12 exp (411/TK)
62]	O3 + C:C = HCHO + 0.42*CO +0.12*HO2	1.3E-14 exp (-2633/TK)
	Aromatic Chemistry	
63]	OH + TOL = 0.08*[XO2+HO2] + 0.36*[CRES+HO2] + 0.56*TO2	2.1E-12 exp (322/TK)
64]	TO2 + NO = 0.90*[NO2 + HO2 + OPEN] + 0.1*NTR	8.1E-12
65]	TO2 = CRES + HO2	4.2
66]	OH + CRES = 0.40*CRO + 0.60*[XO2 + HO2] + 0.30*OPEN	4.1E-11
67]	NO3 + CRES = CRO + HNO3	2.2E-11
68]	CRO + NO2 = ARONTR	1.4E-11
69]	OH + XYL = 0.10*[HO2+XO2+PAR] + 0.20*[CRES+HO2+PAR] + 0.30*TO2 +0.40*[2*MGLY + 2*PAR + HO2]	1.7E-11 exp (116/TK)
70]	OPEN + OH = XO2 + 2.0*CO + 2.0*HO2 + C2O3 + HCHO	3.0E-11
71]	OPEN = C2O3 + HO2 + CO	9.04 *j38
72]	OPEN + O3 = 0.03*RCHO + 0.62*C2O3 + 0.70*HCHO + 0.03*XO2 + 0.69*CO + 0.08*OH + 0.76*HO2 + 0.2*MGLY	5.4E-17 exp (-500/TK)
73]	OH + MGLY = XO2 + C2O3	1.7E-11
74]	MGLY = C2O3 + HO2 + CO	9.64*j38
	Isoprene Chemistry - Condensed	
75]	O + ISOP = 0.6*HO2 + 0.80*RCHO + 0.55*OLE + 0.50*XO2 + 0.50*CO + 0.45*C:C + 0.9*PAR	3.6E-11
76]	OH + ISOP = XO2 + HCHO + 0.67*HO2 + 0.13*XO2N + 1.0*C:C + 0.4*MGLY + 0.2*C2O3 + 0.2*RCHO	2.54E-11 exp (407.6/TK)
77]	O3 + ISOP = HCHO + 0.4*RCHO + 0.55*C:C + 0.2*MGLY + 0.10*PAR + 0.06*CO + 0.44*HO2 +0.1*OH	7.86E-15 exp (-1912/TK)
78]	NO3 + ISOP = XO2N	3.03E-12 exp (-448/TK)
	Operator Chemistry	
79]	XO2 + NO = NO2	8.1E-12

Table B2. Continued

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}
80]	XO2 + XO2 =	1.7E-14 exp (1300/TK)
81]	XO2N + NO = {NTR}	8.12E-12
82]	SO2 + OH = SULF + HO2	4.39E-13 exp (160/TK)
83]	SO2 = SULF	1.36E-06
84]	MEOH + OH =	1.08E-12
85]	ETOH + OH =	1.61E-12 exp (176/TK)
86]	XO2 + HO2 =	7.67E-14 exp (1300/TK)
87]	XO2N + HO2 =	7.67E-14 exp (1300/TK)
88]	XO2N + XO2N =	1.73E-14 exp (1300/TK)
89]	XO2N + XO2 =	3.45E-14 exp (1300/TK)
	Additional Isoprene Chemistry	
90]	ISPD + OH = 1.565*PAR + 0.167*HCHO + 0.713*XO2 + 0.503*HO2 + 0.334*CO + 0.168*MGLY + 0.273*RCHO +0.498*C2O3	3.36E-11
91]	ISPD + O3 = 0.114*C2O3 + 0.150*HCHO + 0.850*MGLY + 0.154*HO2 + 0.268*OH + 0.064*XO2 + 0.020*RCHO + 0.360*PAR + 0.225*CO	7.11E-18
92]	ISPD + NO3 = 0.357*RCHO + 0.282*HCHO + 1.282*PAR + 0.925*HO2 + 0.643*CO + 0.850*NTR + 0.075*C2O3 + 0.075*XO2 + 0.075*HNO3	1.00E-15
93]	ISPD = 0.333*CO + 0.067*RCHO + 0.900*HCHO + 0.832*PAR + 1.033*HO2 + 0.700*XO2 + 0.967*C2O3	0.0036*j93
94]	ISOP + NO2 = 0.20*ISPD + 0.80*NTR + 1.00*XO2 + 0.80*HO2 + 0.20*NO + 0.80*RCHO + 2.4*PAR	1.49E-19

Table B2b. Sources of Data Used to Calculate Photolysis Rates in a Current Operational Version of CB-IV; Mechanism Used in MAQSIP (Hanna, personal communication, 1998)

Species	Quantum Yield	Absorption Cross Section
NO_2	*DeMore et al.* [1994] *	*DeMore et al.* [1994] *
O_3 to $O(^3P)$	*DeMore et al.* [1994]	*DeMore et al.* [1994]
O_3 to $O(^1D)$	*DeMore et al.* [1994]	*DeMore et al.* [1994]
NO_3	*DeMore et al.* [1994]	*DeMore et al.* [1994]
HONO	*DeMore et al.* [1994]	*DeMore et al.* [1994] *
H_2O_2	assumed to be 1.0	*DeMore et al.* [1984] *
HCHO to $2HO_2$	*DeMore et al.* [1994]	*DeMore et al.* [1994] *
HCHO to H_2 + CO	*DeMore et al.* [1994]	*DeMore et al.* [1994] *
RCHO	*DeMore et al.* [1994]	*DeMore et al.* [1994]

*Updated sets of photolyis data from those published with CB-IV.1

Table B3. CB-IV_99: Updated CB-IV Mechanism, Most Current Kinetic and Mechanistic Updates from UNC

Rxn No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}	Ref.
	NO2 Photolysis		
1]	NO2 = NO + O	j1	
2]	O = O3	6.0E-34^-2.3	2
3]	O3 + NO = NO2	2.0E-12 exp (-1400/TK)	2
4]	O + NO2 = NO	6.5E-12 exp (120/TK)	2
5]	O + NO2 = NO3	k_{hi} = 2.2E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-2.0 F_c = 0.6	2
6]	O + NO = NO2	k_{hi} = 3.0E-11(TK/300)^0 k_{lo} = 9.0E-32(TK/300)^-1.5 F_c = 0.6	2
	OZONE Photolysis		
7]	O3 + NO2 = NO3	1.2E-13 exp (-2450/TK)	2
8]	O3 {hv} = O	j8	
9]	O3 {hv} = O1D	j9	
10]	O1D + M = O	1.92E-11 exp (126/TK)	2
11]	O1D + H2O = 2.0*OH	2.2E-10	2
12]	O3 + OH = HO2	1.6E-12 exp (-940/TK)	2
13]	O3 + HO2 = OH	1.1E-14 exp (-580/TK)	2

Table B3. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}	Ref.
	NO3 Chemistry		
14a]	NO3 {hv} = NO + O2	j14a	
14b]	NO3 {hv} = NO2 + O	j14b	
15]	NO3 + NO = 2.0*NO2	1.8E-11 exp (110/TK)	3
16]	NO3 + NO2 = NO + NO2	2.5E-14 exp (-1260/TK)	2
17]	NO3 + NO2 = N2O5	k_{hi} = 1.5E-12(TK/300)^-0.7 k_{lo} = 2.2E-30(TK/300)^-3.9 F_c = 0.6	2
18]	N2O5 = NO3 + NO2	K_e=2.7E-27 exp (11000/TK)	2
19]	N2O5 + H2O = 2.0*HNO3	1.5E-21	2
	HONO Chemistry		
20]	NO + NO + O2 = 2.0*NO2	3.3E-39 exp (530/TK)	3
21]	NO + NO2 + H2O = 2.0*HONO	4.4E-40	2
22]	OH + NO = HONO	k_{hi} = 3.6E-11(TK/300)^-0.1 k_{lo} = 7.0E-31(TK/300)^-2.6 F_c = 0.6	2
23]	HONO = OH + NO	j23	
24]	OH + HONO = NO2	2.7E-12 exp (260/TK)	3
25]	HONO + HONO = NO + NO2	1.0E-20	2
	OH/HO2 Termination Reactions		
26]	OH + NO2 = HNO3	k_{hi} = 7.5E-11(TK/300)^-0.6 k_{lo} = 2.6E-30(TK/300)^-2.9 F_c = 0.41	3
27]	OH + HNO3 = NO3	k_0 = 7.2E-15 exp (785/TK) k_2 = 4.1E-16 exp (1440/TK) k_3 = 1.9E-33 exp (725/TK)	2
28]	HO2 + NO = OH + NO2	3.7E-12 exp (240/TK)	3
29]	HO2 + NO2 = PNA	k_{hi} = 4.7E-12^0 k_{lo} = 1.8E-31^-3.2 F_c = 0.6	2
30]	PNA = HO2 + NO2	K_e=2.1E-27exp (10900)	2
31]	OH + PNA = NO2	1.5E-12 exp (360/TK)	2
32]	HO2 + HO2 = H2O2 {+ O2}	2.3E-13 exp (600/TK)	2
33]	HO2 + HO2 + M = H2O2 + O2 {+ H2O}	1.9E-33 exp (980/TK)	3
34]	H2O2 = 2*OH	j34	
35]	OH + H2O2 = HO2	2.9E-12 exp (-160/TK)	2
	Propagation Reactions		
36a]	OH + CO = HO2	1.3E-13(TK/300)^1	2
36b]	OH + CO = HO2	k36a*0.6*Pressure	2
37]	OH + CH4 = XO2 + HCHO + HO2	2.45E-12 exp (-1775/TK)	2

Table B3. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}	Ref.
	Formaldehyde Chemistry		
38]	HCHO + OH = HO2 + CO	8.6E-12 exp (20/TK)	3
39]	HCHO {hv} = 2*HO2 + CO	j39	
40]	HCHO {hv} = CO + H2	j40	
41]	HCHO + O = OH + HO2 + CO	3.4E-11 exp (-1600/TK)	2
42]	HCHO + NO3 = HNO3 + HO2 + CO	5.8E-16	2
	Higher Aldehyde Chemistry		
43]	RCHO + O = C2O3 + OH	1.8E-11 exp (-1100/TK)	2
44]	RCHO + OH = C2O3	5.6E-12 exp (270/TK)	2
45]	RCHO + NO3 = C2O3 + HNO3	1.4E-12 exp (-1900/TK)	2
46]	RCHO = XO2 + 2*HO2 + CO + HCHO	j46	
	PAN Chemistry		
47]	C2O3 + NO = NO2 + XO2 + HCHO + HO2	5.3E-12 exp (360/TK)	2
48]	C2O3 + NO2 = PAN	k_{hi} = 9.3E-12^-1.5 k_{lo} = 9.7E-29^-5.6 F_c = 0.6	2
49]	PAN = C2O3 + NO2	K_e = 9.0E-29 exp (14000/TK)	2
50]	C2O3 + C2O3 = 2*XO2 + 2*HCHO + 2*HO2	2.9E-12 exp (500/TK)	2
51]	C2O3+ HO2 = 0.75*C2O3H + 0.75*O2 + 0.25*O3 + 0.25*C2O2H	4.5E-13 exp (1000/TK)	2
	Paraffin Chemistry		
52]	OH = HCHO + XO2 + HO2 {Omit in Chamber modeling, included in wall reactions}	1.1E02 exp (-1710/TK)	1
53]	OH + PAR = 0.87*XO2 + 0.13*XO2N + 0.11*HO2 + 0.11*RCHO + 0.76*ROR + -0.11*PAR	8.1E-13	1
54]	ROR = 1.1*RCHO + 0.96*XO2 + 0.94*HO2 + -2.1*PAR + 0.04*XO2N + 0.02*ROR	1.0E15 exp (-8000/TK)	1
55]	ROR = HO2 + KETENE	1.6E03	1
56]	ROR + NO2 = NTR	1.50E-11	1
	Olefin Chemistry		
57]	O + OLE = 0.49*RCHO + 0.29*HO2 + 0.19*XO2 + 0.20*CO + 0.20*HCHO + 0.007*XO2N + 0.61*PAR + 0.10*OH	4.0E-12	4
58]	OH + OLE = 0.71*HCHO + 0.95*RCHO + 0.71*XO2 + 0.95*HO2 + -0.71*PAR	k_{hi} = 2.8E-11(TK/300)^-1.3 k_{lo} = 3.0E-27(TK/300)^-3.0 F_c = 0.5	4

Table B3. (Continued)

Rxn. No	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}	Ref.
59]	O3 + OLE = 0.52*RCHO + 0.86*HCHO + 0.395*CO + 0.42*HO2 + 0.45*XO2 + 0.31*OH + -1.0*PAR + 0.08*H2O2	5.5E-15 exp (-1880/TK)	4
60]	NO3 + OLE = 0.91*XO2 + 0.09*XO2N + HCHO + RCHO + -1*PAR + NO2	4.6E-13 exp (-1155/TK)	4
	Ethene Chemistry		
61]	O + C:C = 0.95*HCHO + 0.60*XO2 + 0.95*CO + 1.55*HO2 + 0.35*OH	1.04E-11 exp (-792/TK)	1
62]	OH + C:C = XO2 + 1.56*HCHO + HO2 + 0.22*RCHO	k_{hi} = 9.0E-12(TK/300)^0.0 k_{lo} = 7.0E-29(TK/300)^-3.1 F_c = 0.7	3
63]	O3 + C:C = 1.02*HCHO + 0.325*CO + 0.08*HO2 + 0.02*H2O2	9.14E-15 exp (-2580/TK)	3
	Aromatic Chemistry		
64]	OH + TOL = 0.08*[XO2+HO2]+0.36*[CRES + HO2] + 0.56*TO2	1.81E-12 exp (355/TK)	5
65]	TO2 + NO = 0.90*[NO2 + HO2 + OPEN] + 0.1*NTR	8.1E-12	1
66]	TO2 = CRES + HO2	4.2	1
67]	OH + CRES = 0.40*CRO + 0.60*[XO2 + HO2] + 0.30*OPEN	4.1E-11	1
68]	NO3 + CRES = CRO + HNO3	2.2E-11	1
70]	OH + XYL = 0.10*[HO2+XO2+PAR] + 0.20*[CRES+HO2+PAR] + 0.30*TO2 + 0.40*[2MGLY + 2PAR + HO2]	1.7E-11 exp (116/TK)	1
71]	OPEN + OH = XO2 + 2.0*CO + 2.0*HO2 + C2O3+ HCHO	3.0E-11	1
72]	OPEN = C2O3 + HO2 + CO	6.0*j39	
73]	OPEN + O3 = 0.03*RCHO + 0.62*C2O3 + 0.70*HCHO + 0.03*XO2 + 0.69*CO + 0.08*OH + 0.76*HO2 + 0.2*MGLY	5.4E-17 exp (-500/TK)	1
74]	OH + MGLY = XO2 + C2O3	1.7E-11	1
75]	MGLY = C2O3 + HO2 + CO	6.0*j39	
	Isoprene Chemistry – Condensed		
76]	O + ISOP = 0.1*HO2 + 0.5*HCHO + 0.25*XO2 + 0.25*C2O3 + 0.75*ISPD +0.25*PAR	3.6E-11	6
77]	OH + ISOP = 0.991*XO2 + 0.629*HCHO + 0.912*HO2 + 0.088*XO2N + 0.912*ISPD	2.54E-11exp (407.6/TK)	6

Table B3a. (Continued)

Rxn. No.	Reaction	Rate Constant cm^3 $molecule^{-1}$ sec^{-1}	Ref.
78]	O3 + ISOP = 0.6*HCHO + 0.15*RCHO + 0.066*HO2 + 0.2*C2O3 + 0.35*PAR + 0.066*CO + 0.2*XO2 +0.266*OH + 0.65*ISPD	7.86E-15 exp (-1912/TK)	6
79]	NO3 + ISOP = XO2 + 0.2*ISPD + 0.8*NTR + 0.8*HO2 + 0.2*NO2 + 0.8*RCHO + 2.4*PAR	3.03E-12 exp (-448/TK)	6
80]	NO2 + ISOP = XO2 + 0.2*ISPD + 0.8*NTR + 0.8*HO2 + 0.2*NO2 + 0.8*RCHO + 2.4*PAR	1.5E-19	6
	Operator Chemistry		
81]	XO2 + NO = NO2	3.0E-12 exp (280/TK)	2
82]	XO2 + XO2 =	2.5E-13 exp (190/TK)	2
83]	XO2N + NO = {NTR}	k81	2
84]	SO2 + OH = SULF + HO2	k_{hi} = 1.5E-12(TK/300)^0.0 k_{lo} = 3.0E-31(TK/300)^-3.3 F_c = 0.6	2
85]	SO2 = SULF	1.4E-06	2
86]	MEOH + OH =	6.7E-12 exp (600/TK)	2
87]	ETOH + OH =	7.0E-12 exp (235/TK)	2
88]	XO2 + HO2 =	3.8E-13 exp (800/TK)	2
89]	XO2N + HO2 =	k88	2
90]	XO2N + XO2N =	k82	2
91]	XO2N + XO2 =	2*k82	2
	Additional Isoprene Chemistry		
92]	ISPD + O3 = 0.114*C2O3 + 0.150*HCHO + 0.850*MGLY + 0.154*HO2 + 0.268*OH + 0.064*XO2 + 0.020*RCHO + 0.360*PAR + 0.225*CO	7.11E-18	6
93]	ISPD + NO3 = 0.357*RCHO + 0.282*HCHO + 1.282*PAR + 0.925*HO2 + 0.643*CO + 0.850*NTR + 0.075*C2O3 + 0.075*XO2 + 0.075*HNO3	1.00E-15	6
94]	ISPD = 0.333*CO + 0.067*RCHO + 0.900*HCHO + 0.832*PAR + 1.033*HO2 + 0.700*XO2 + 0.967*C2O3	j94	
95]	ISPD + OH = 0.167*HCHO + 0.713*XO2 + 0.503*HO2 + 0.334*CO + 0.168*MGLY + 0.273*RCHO + 1.565*PAR+0.498*C2O3	3.36E-11	6

References: 1) Gery, et al. (1989) 2) DeMore, et al. (1997) 3) Atkinson, et al. (1997) 4) Atkinson (1997a) 5) Le Bras (1997) 6) Carter (1996)

Table B3b. CB-IV_99 Photolysis Rate Data References

Rxn. No.	Species	Quantum Yield	Absorption Cross Section
1	NO_2	Gardner, et al (1987)	Bass et al. (1976)
8	O_3 to $O(^3P)$	= 1 - Φ_{j9}	Bass and Paur (1985); Carter et al. (1986) for $\lambda > 320$ nm
9	O_3 to $O(^1D)$	Atkinson et al. (1997c); Ravishankara et al. (1998)*	Bass and Paur (1985); Carter et al. (1986) for $\lambda > 320$ nm
14a	NO_3 to NO	Orlando et al. (1993)	Atkinson et al. (1997c) based on Sander (1986)
14b	NO_3 to NO_2	Orlando et al. (1993)	Atkinson et al. (1997c) based on Sander (1986)
23	HONO	Atkinson, et al (1997c)	DeMore, et al. (1997)
34	H_2O_2	Assumed to be 1	Stockwell (1988)
39	HCHO to $2HO_2$	Gery	Moortgat
40	HCHO to H_2 + CO	Gery	Moortgat
46	RCHO	Atkinson et al. (1997c)*	Martinez et al. (1992)*
94	ACROLEIN	Gardner et al. (1987)	Gardner et al. (1987)

*Updated sets of photolysis data from the current operational versions of the mechanism