Comprehensive Air Quality Model With Extensions, v7.20: Formulation and Evaluation for Ozone and Particulate Matter Over the US

Supplemental Information

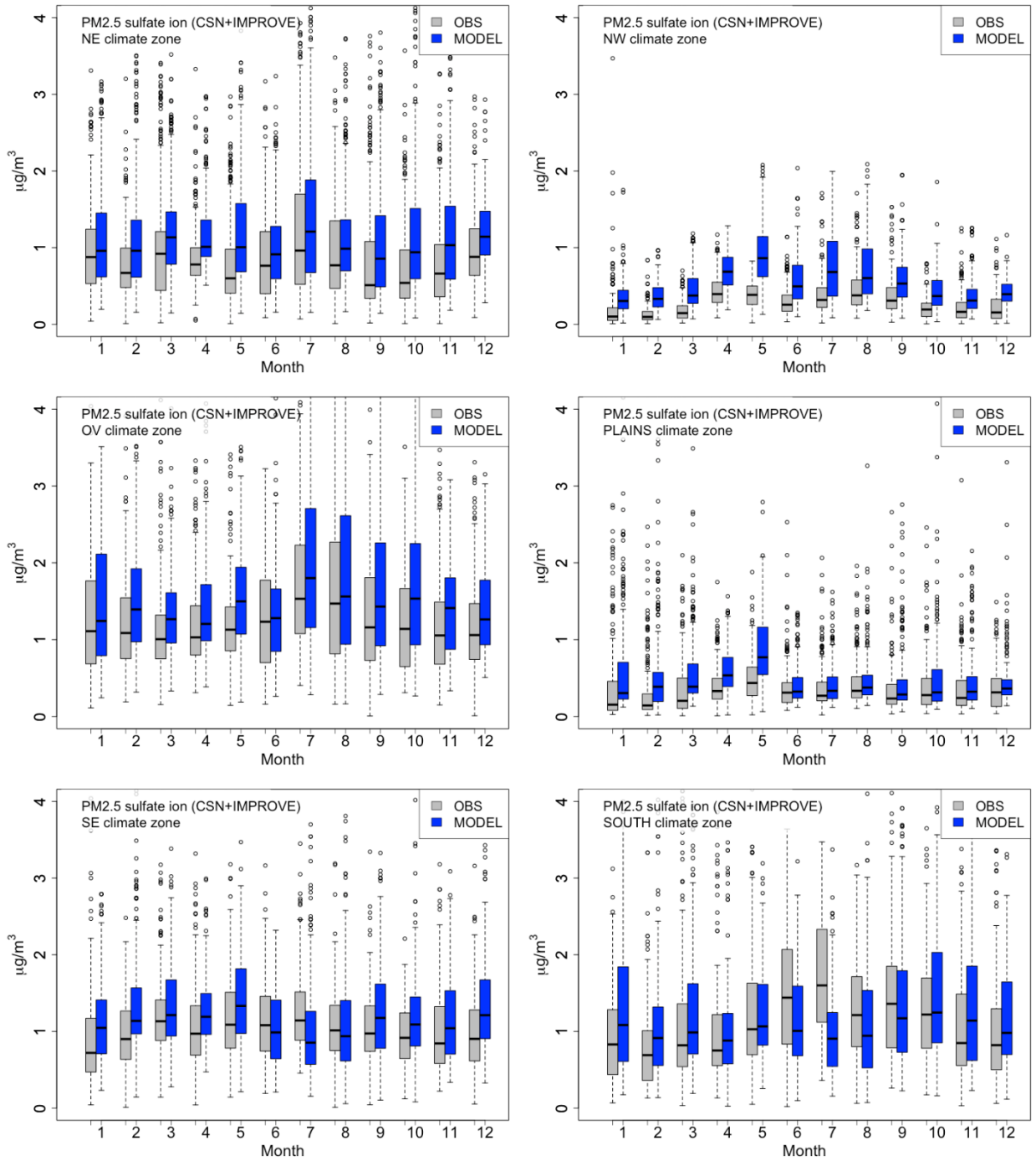


Figure S1. Monthly comparison between 2016 observed (grey) and simulated (blue) 24-h particulate sulfate concentration for each of the nine NOAA climate regions shown in Figure 12. Boxes represent the interquartile range (25th to 75th percentile with median shown by the center line), dashed whiskers represent 1.5 times the interquartile range, and circles represent individual outlier values.

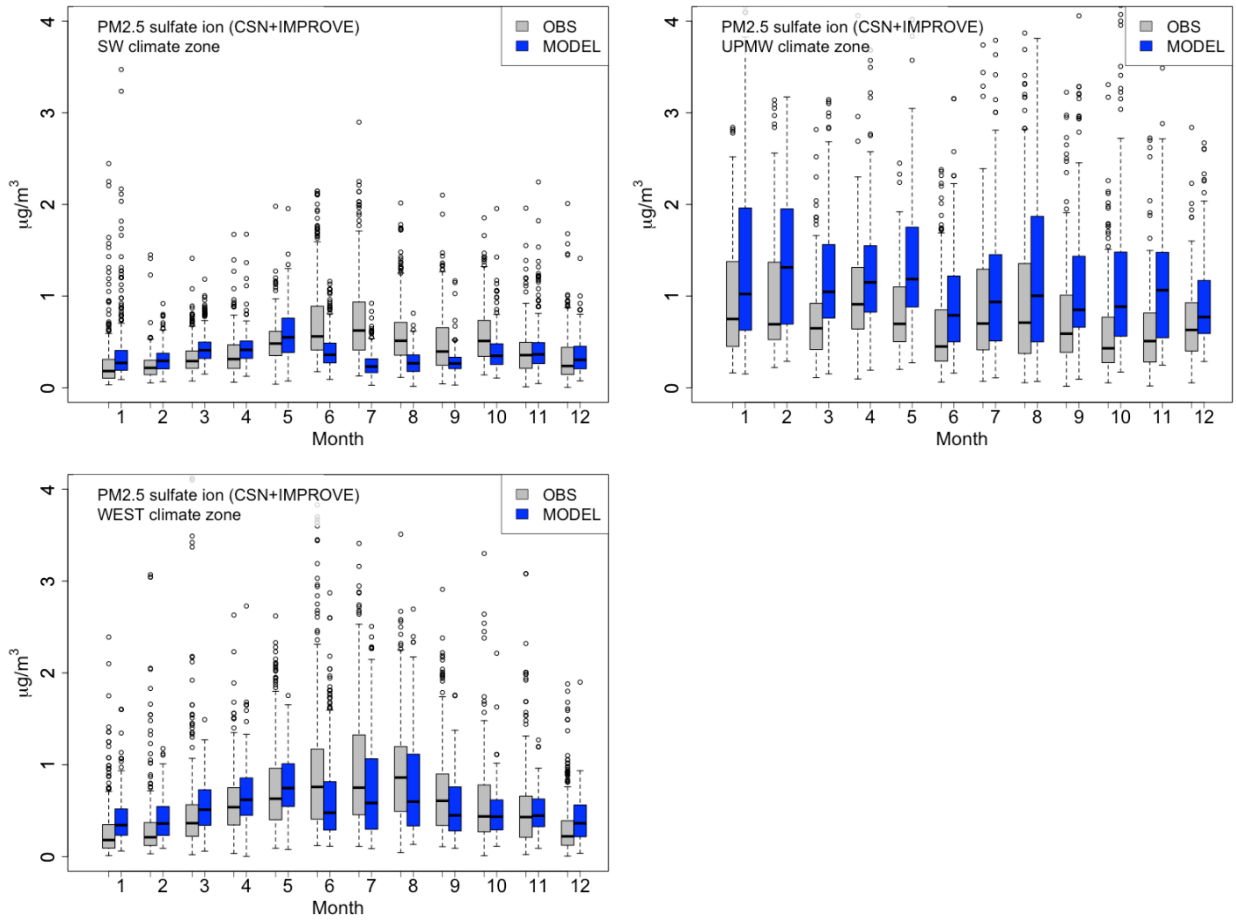


Figure S1 (Concluded).

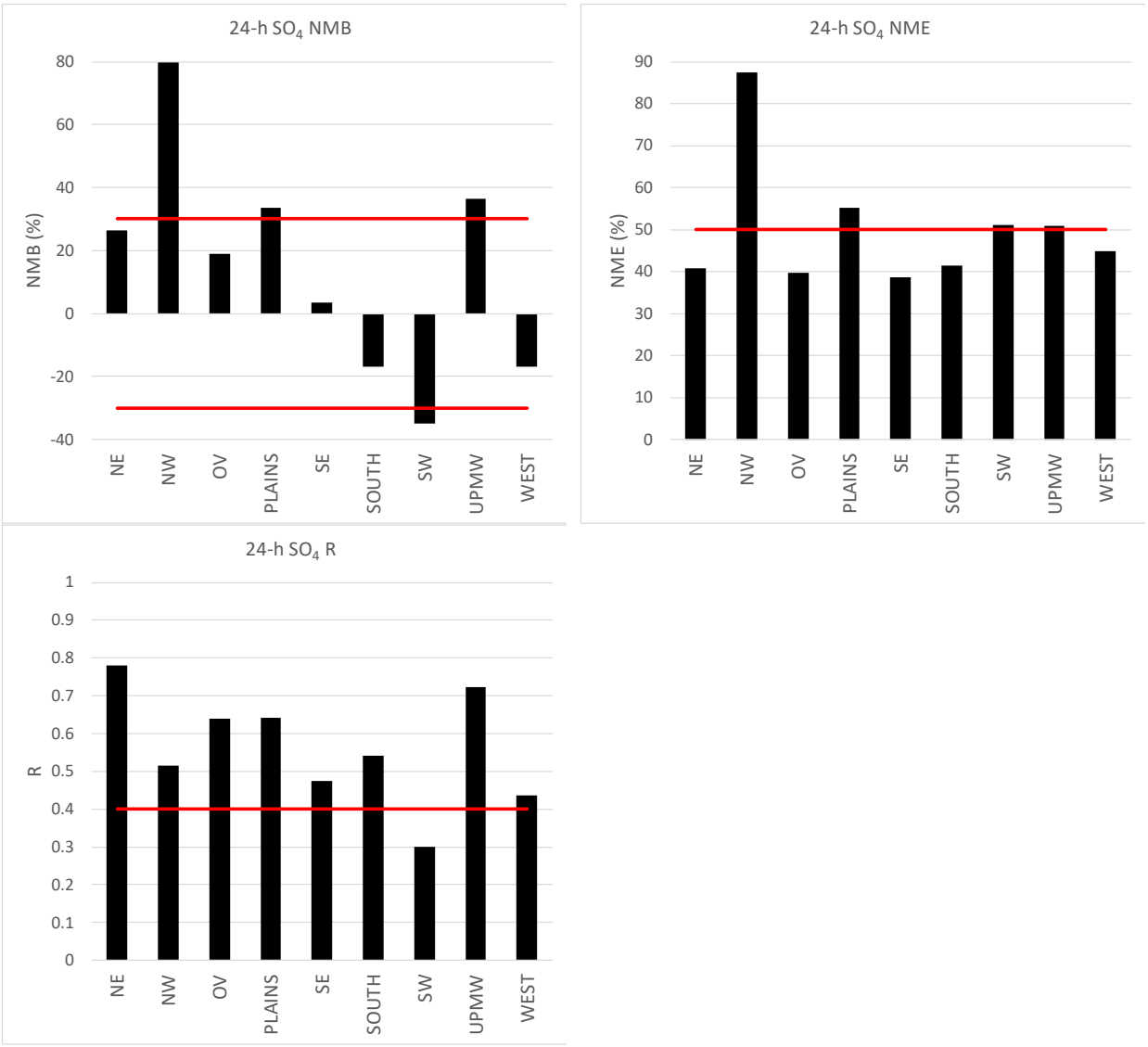


Figure S2. Statistical model performance (NMB, NME, r) in replicating 24-h particulate sulfate over the April-September, 2016 warm season by US climate zone. Criteria benchmarks are shown as red lines.

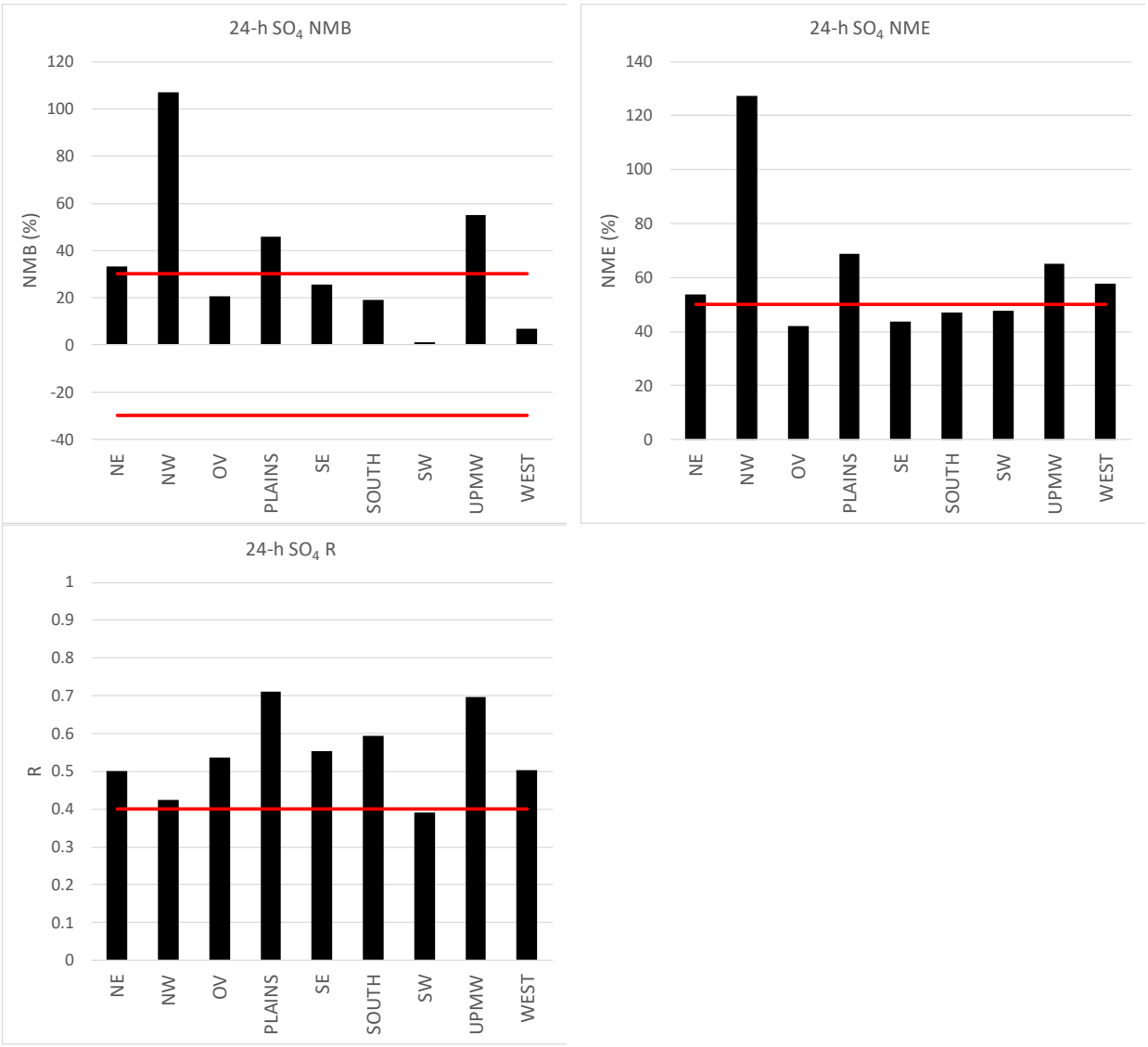


Figure S3. Statistical model performance (NMB, NME, r) in replicating 24-h particulate sulfate over the combined January-March and October-December, 2016 cool seasons by US climate zone. Criteria benchmarks are shown as red lines.

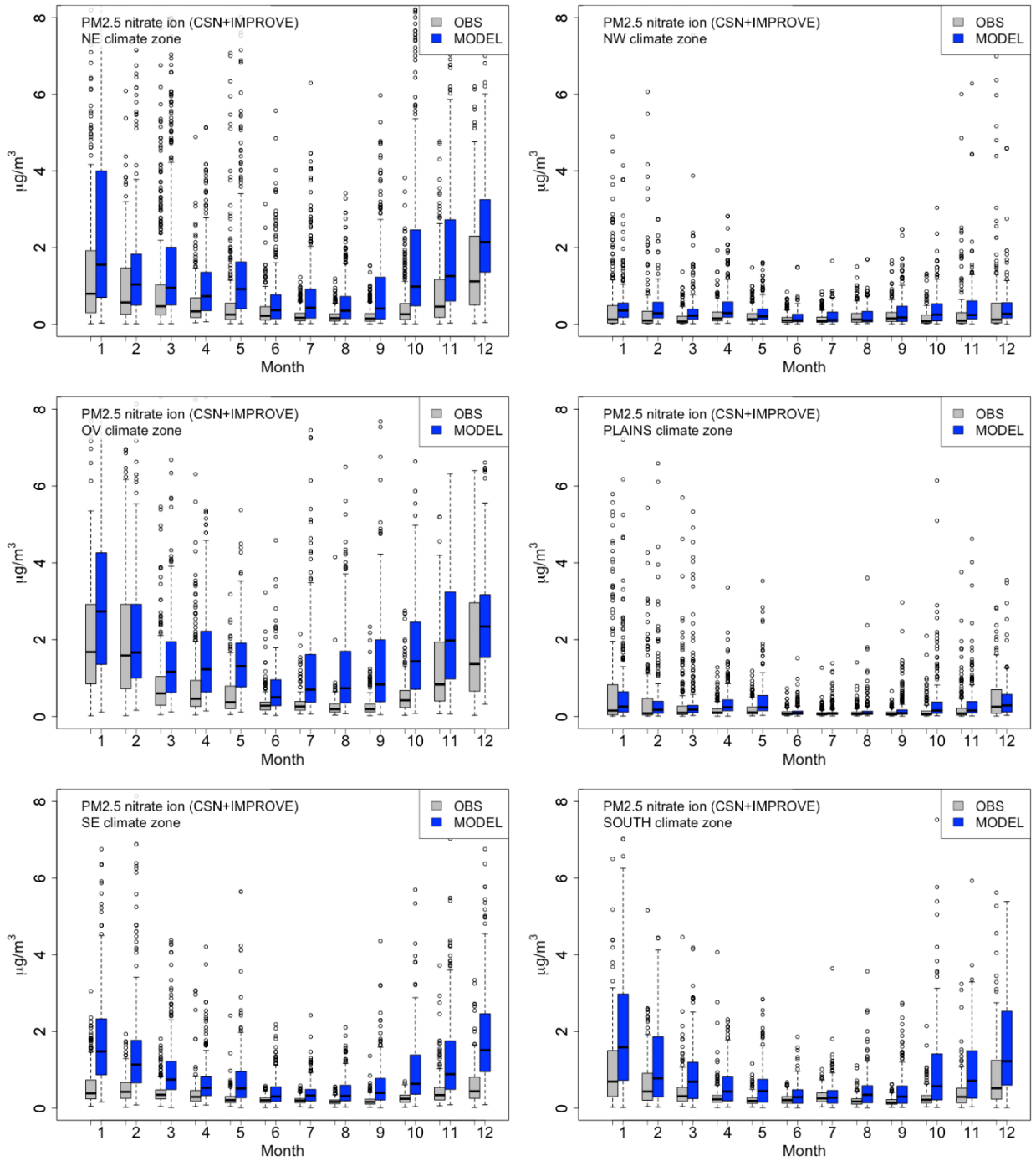


Figure S4. Monthly comparison between 2016 observed (grey) and simulated (blue) 24-h particulate nitrate concentration for each of the nine NOAA climate regions shown in Figure 12. Boxes represent the interquartile range (25th to 75th percentile with median shown by the center line), dashed whiskers represent 1.5 times the interquartile range, and circles represent individual outlier values.

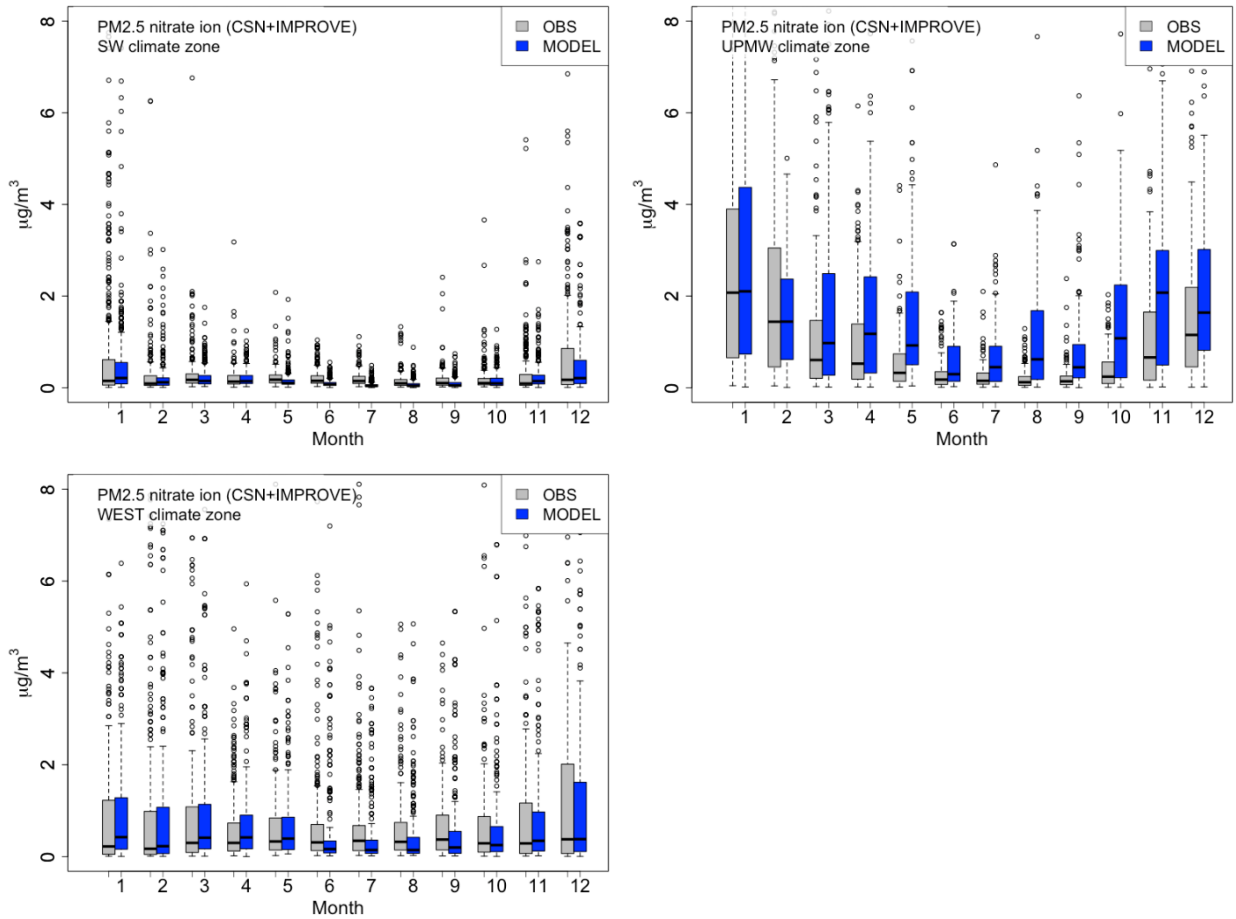


Figure S4 (Concluded).

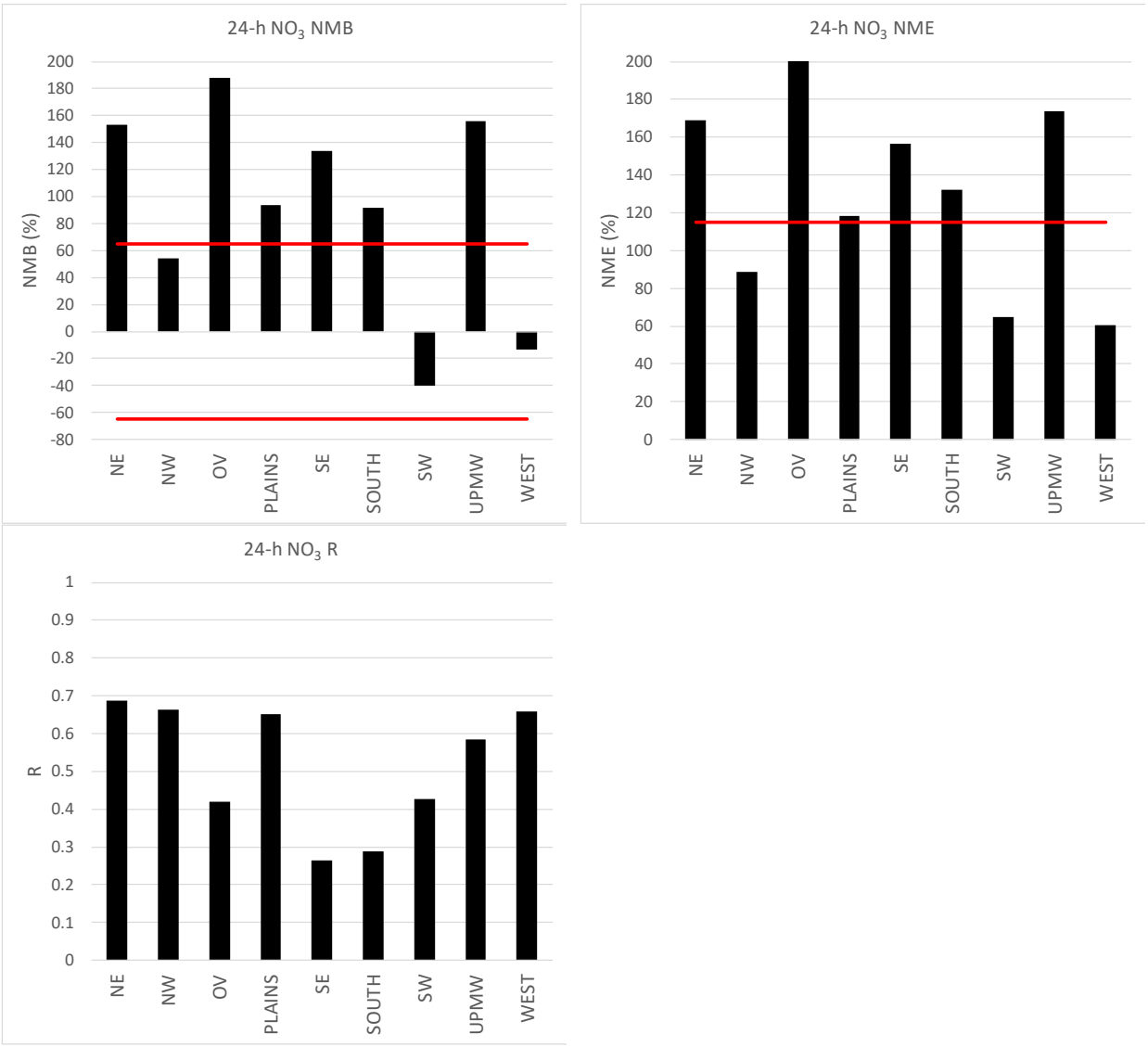


Figure S5. Statistical model performance (NMB, NME, r) in replicating 24-h particulate nitrate over the April-September, 2016 warm season by US climate zone. Criteria benchmarks are shown as red lines.

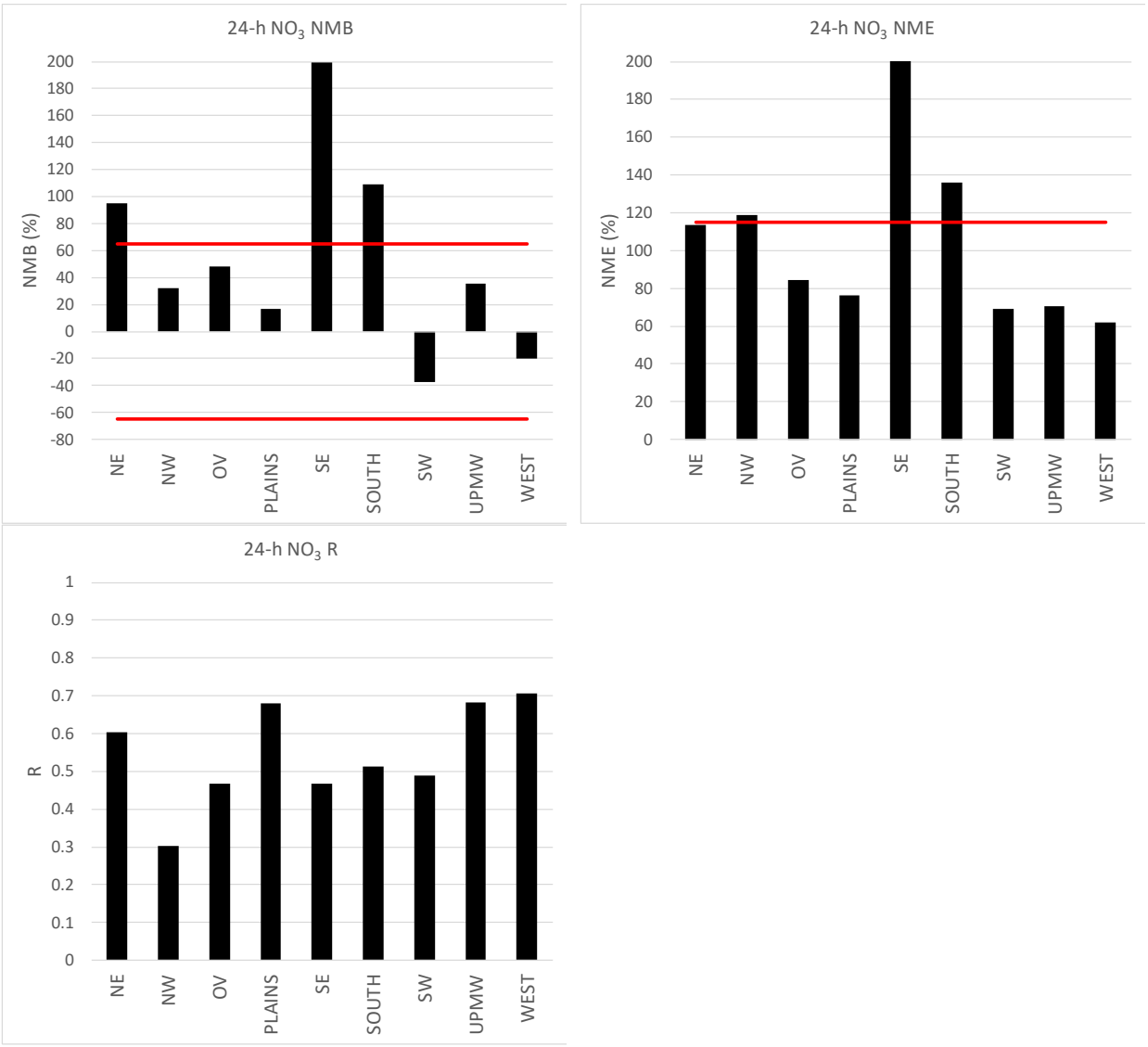


Figure S6. Statistical model performance (NMB, NME, r) in replicating 24-h particulate nitrate over the combined January-March and October-December, 2016 cool seasons by US climate zone. Criteria benchmarks are shown as red lines.

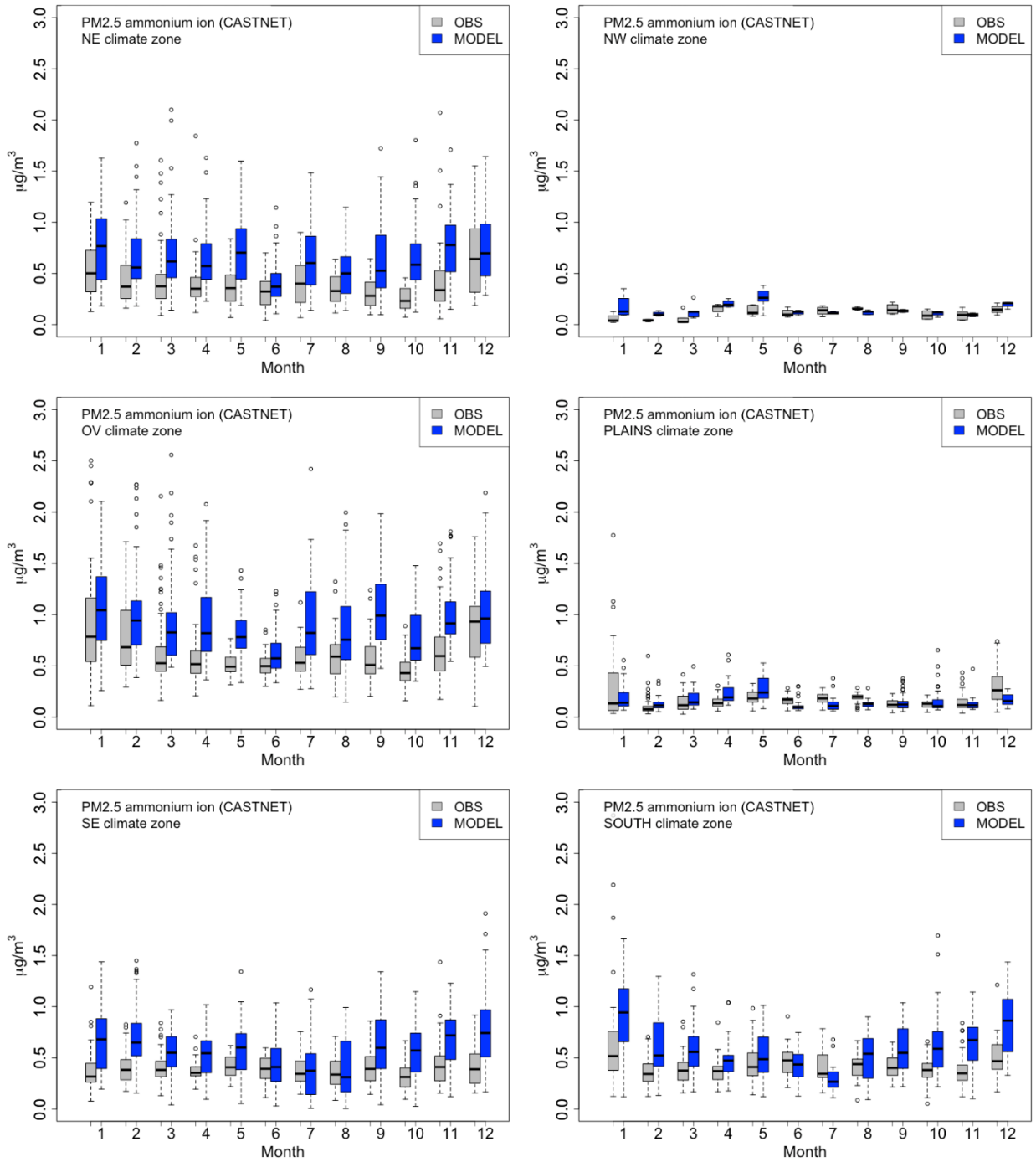
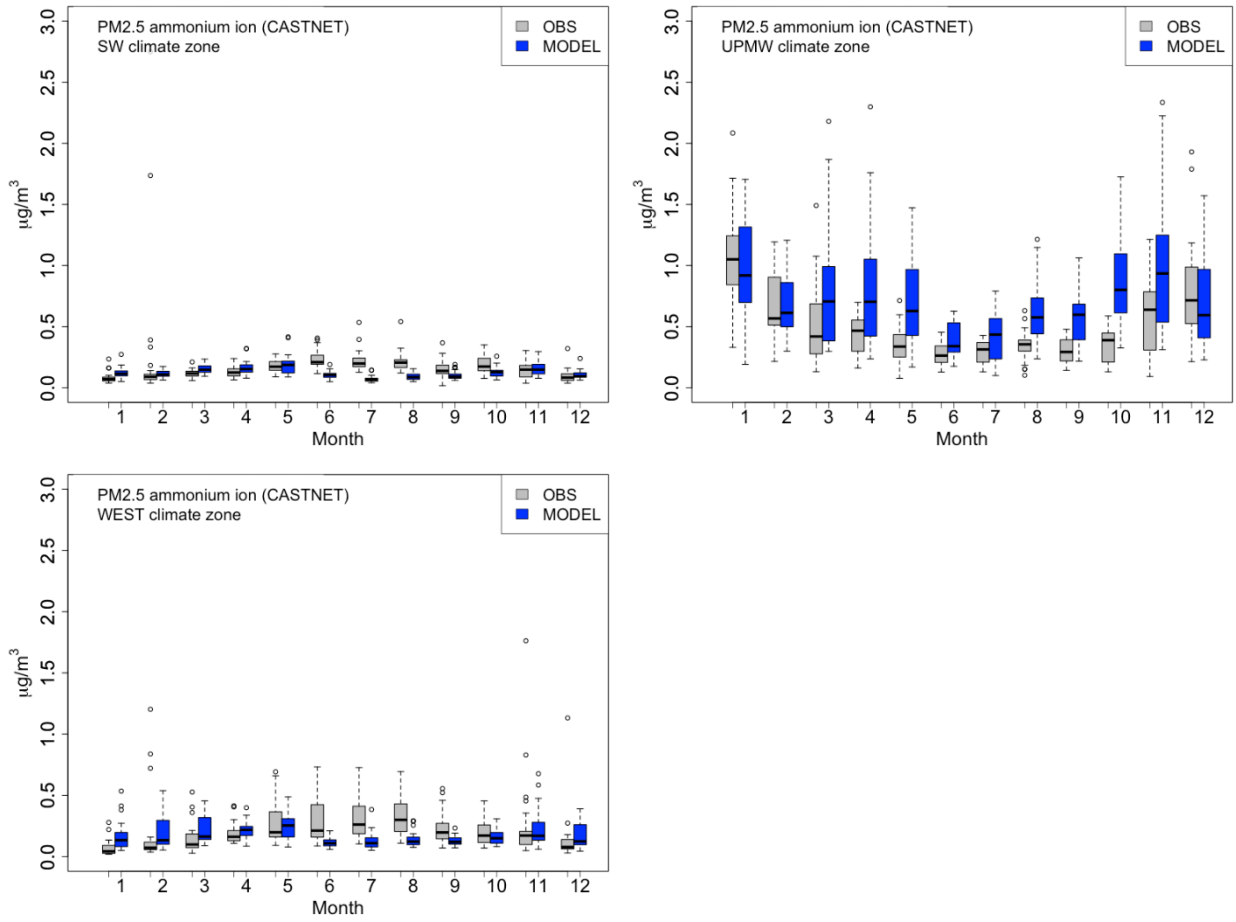


Figure S7. Monthly comparison between 2016 observed (grey) and simulated (blue) 24-h particulate ammonium concentration for each of the nine NOAA climate regions shown in Figure 12. Boxes represent the interquartile range (25th to 75th percentile with median shown by the center line), dashed whiskers represent 1.5 times the interquartile range, and circles represent individual outlier values.



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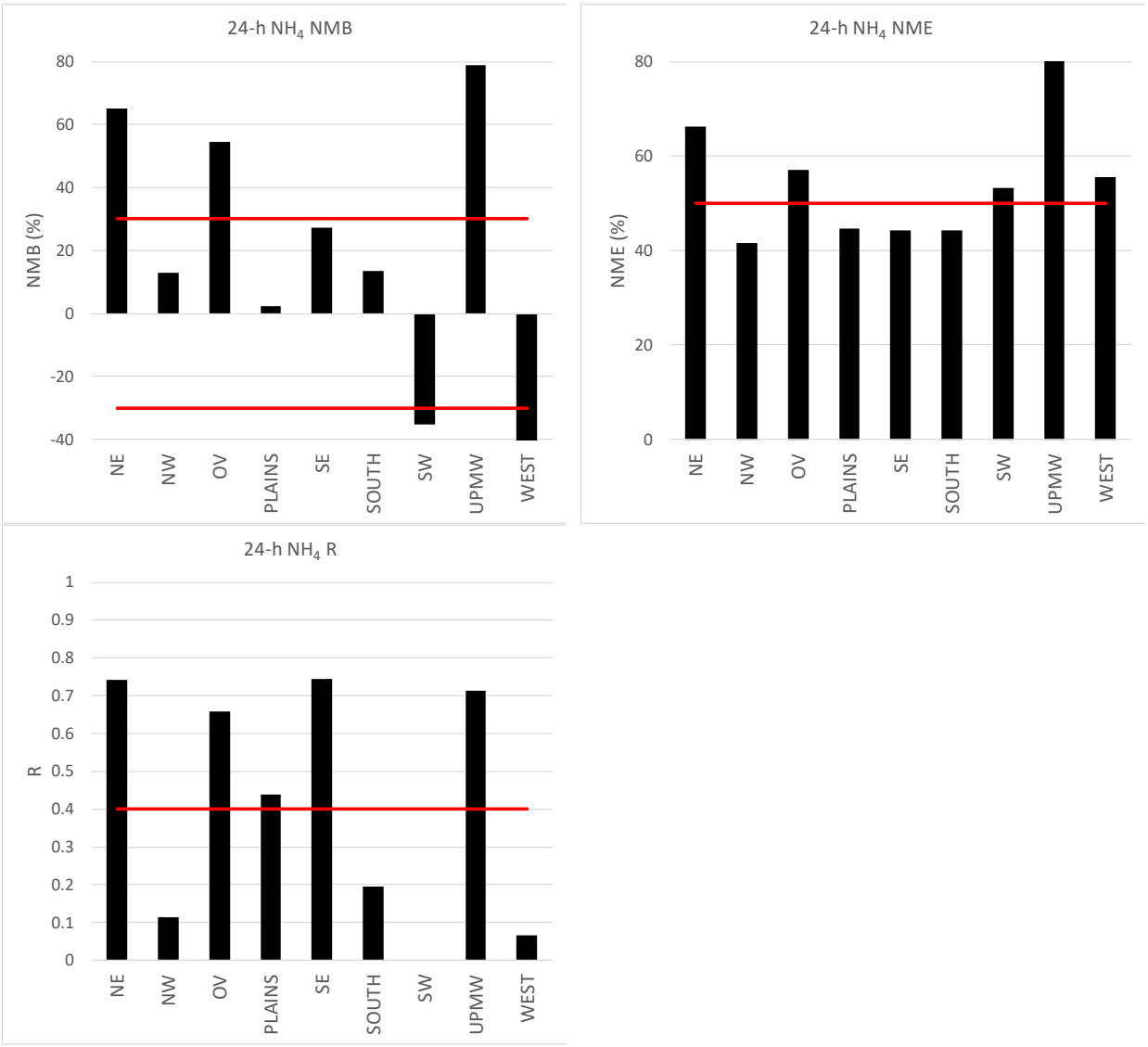

Figure S8. Statistical model performance (NMB, NME, r) in replicating 24-h particulate ammonium over the April-September, 2016 warm season by US climate zone. Criteria benchmarks are shown as red lines.

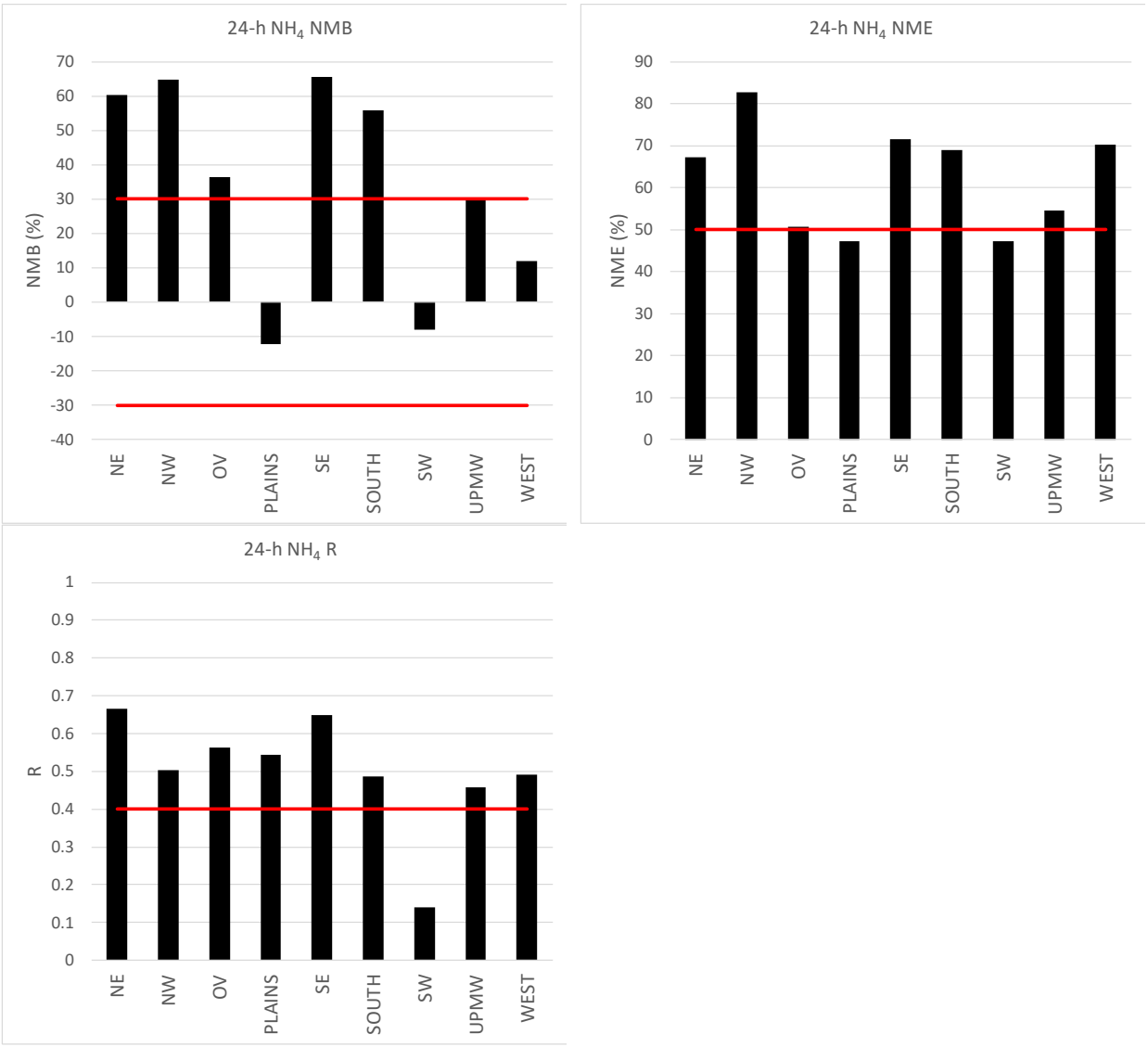

Figure S9. Statistical model performance (NMB, NME, r) in replicating 24-h particulate ammonium over the combined January-March and October-December, 2016 cool seasons by US climate zone. Criteria benchmarks are shown as red lines.

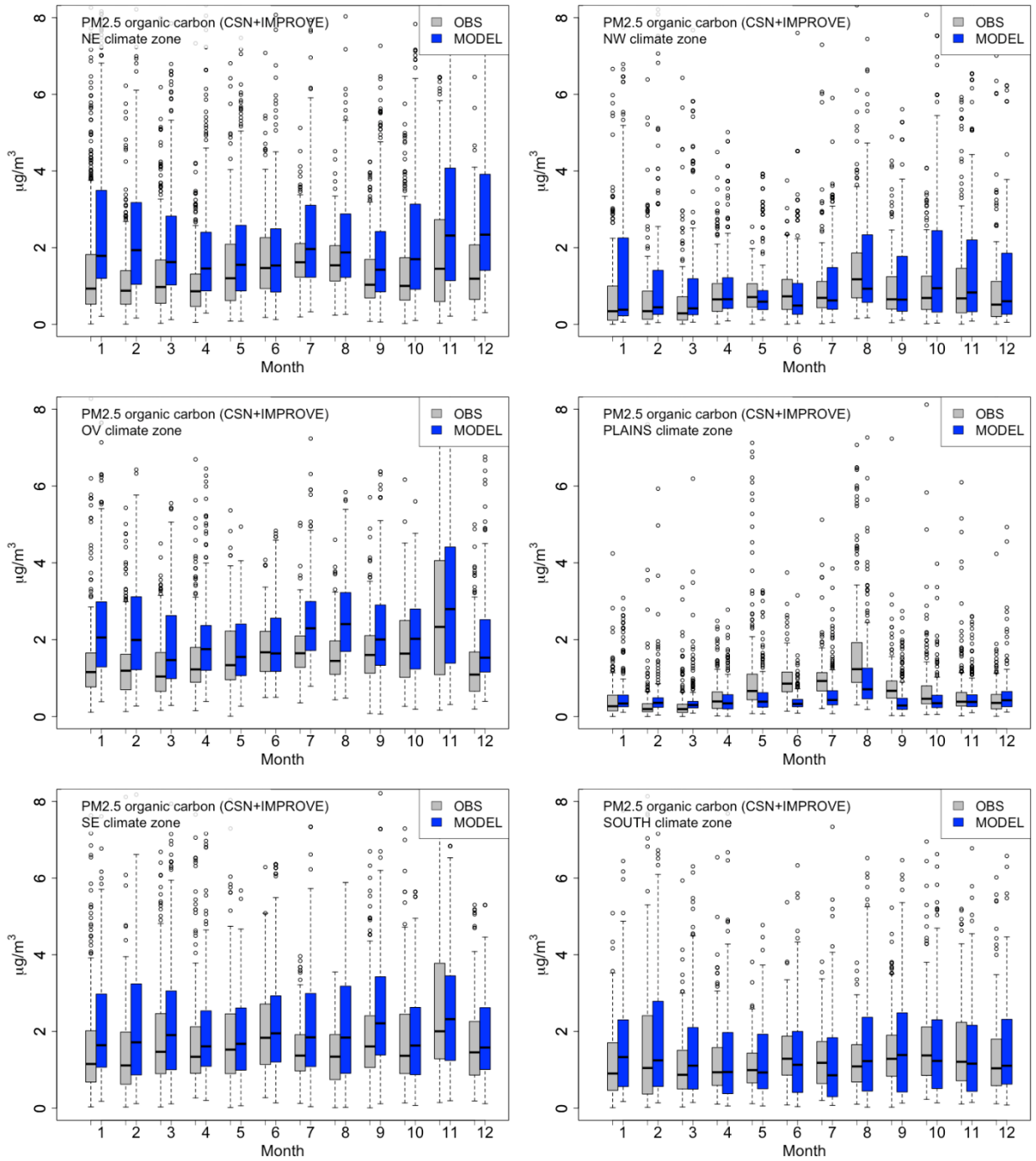

Figure S10. Monthly comparison between 2016 observed (grey) and simulated (blue) 24-h particulate organic carbon concentration for each of the nine NOAA climate regions shown in Figure 12. Boxes represent the interquartile range (25th to 75th percentile with median shown by the center line), dashed whiskers represent 1.5 times the interquartile range, and circles represent individual outlier values.

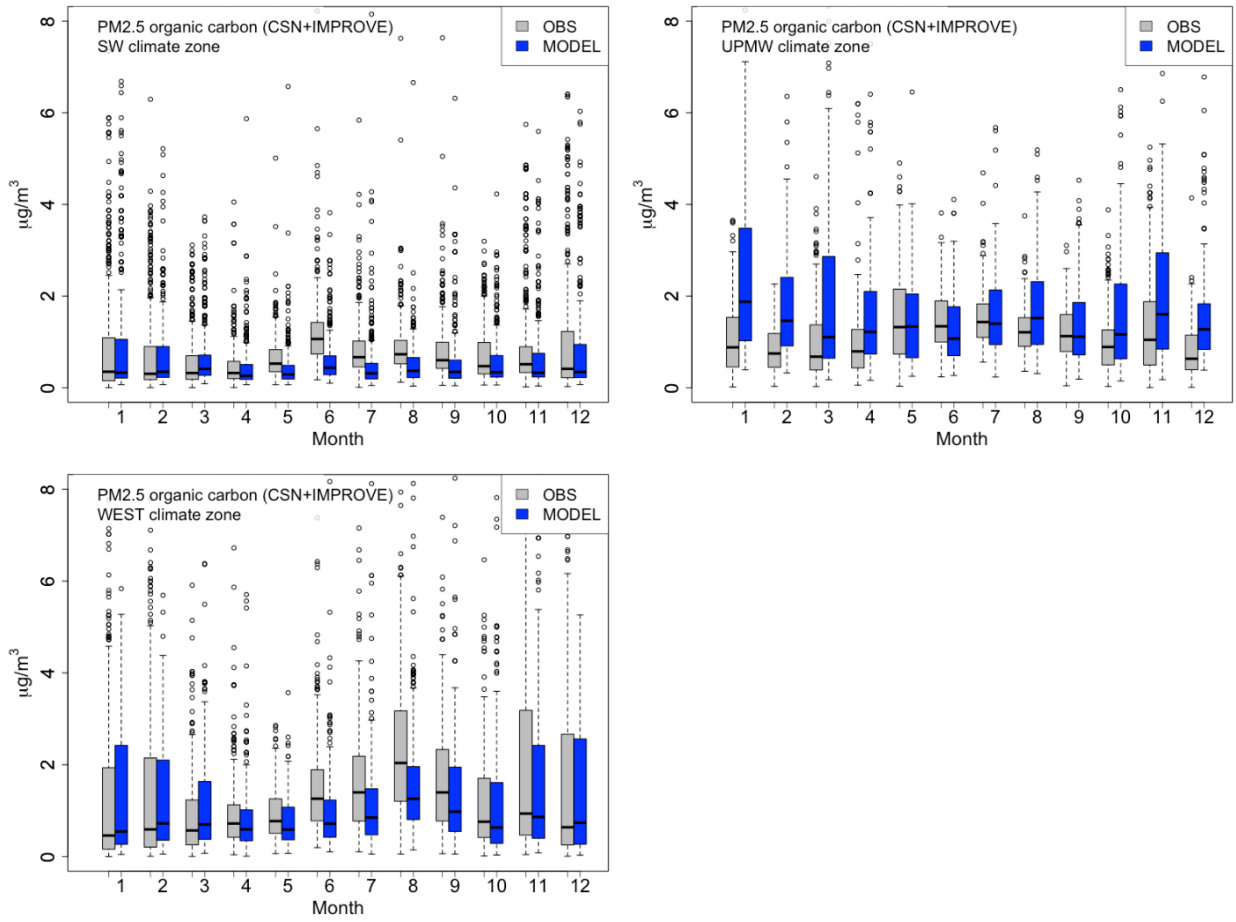

Figure S10 (Concluded).

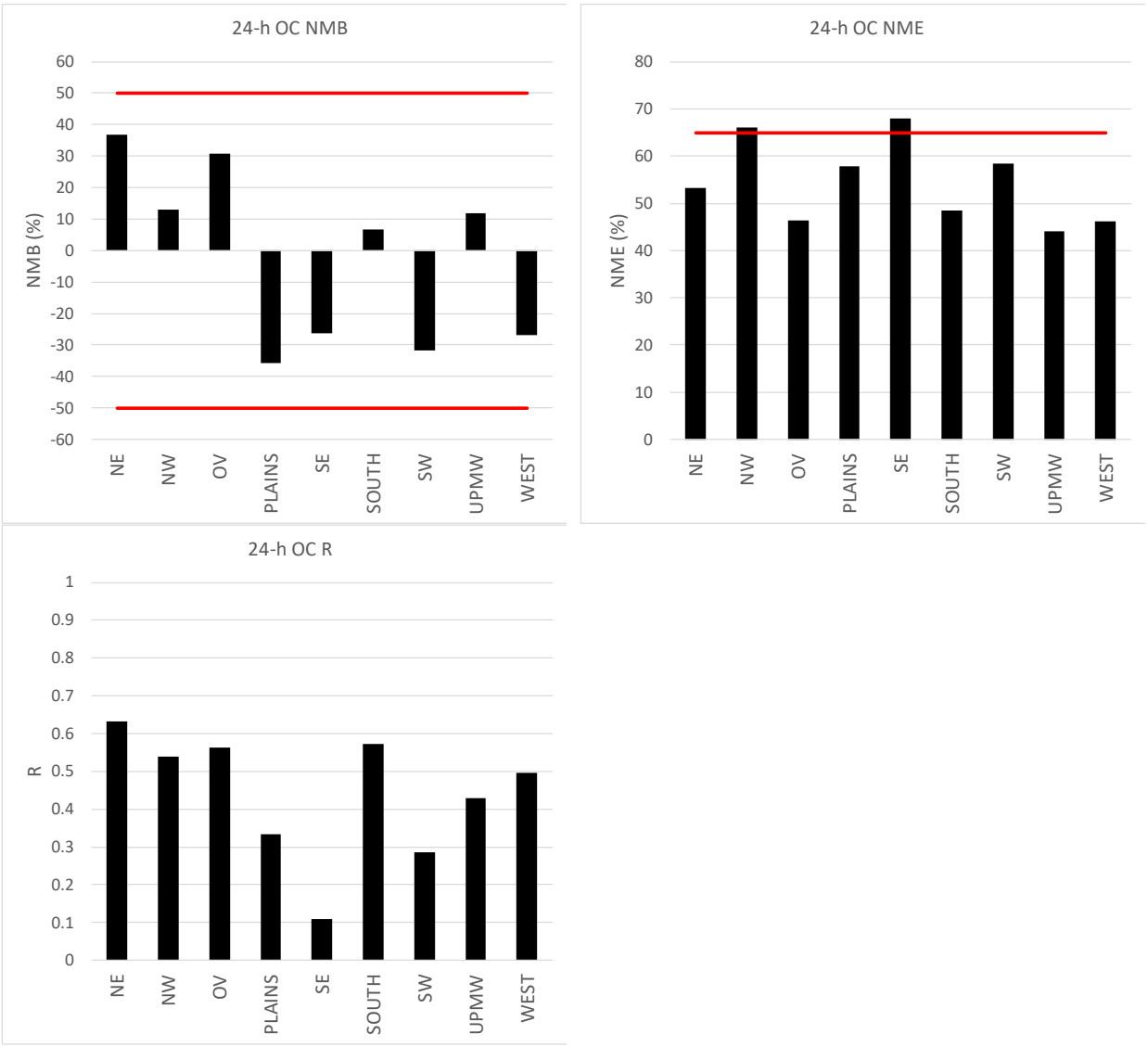

Figure S11. Statistical model performance (NMB, NME, r) in replicating 24-h particulate organic carbon over the April-September, 2016 warm season by US climate zone. Criteria benchmarks are shown as red lines.

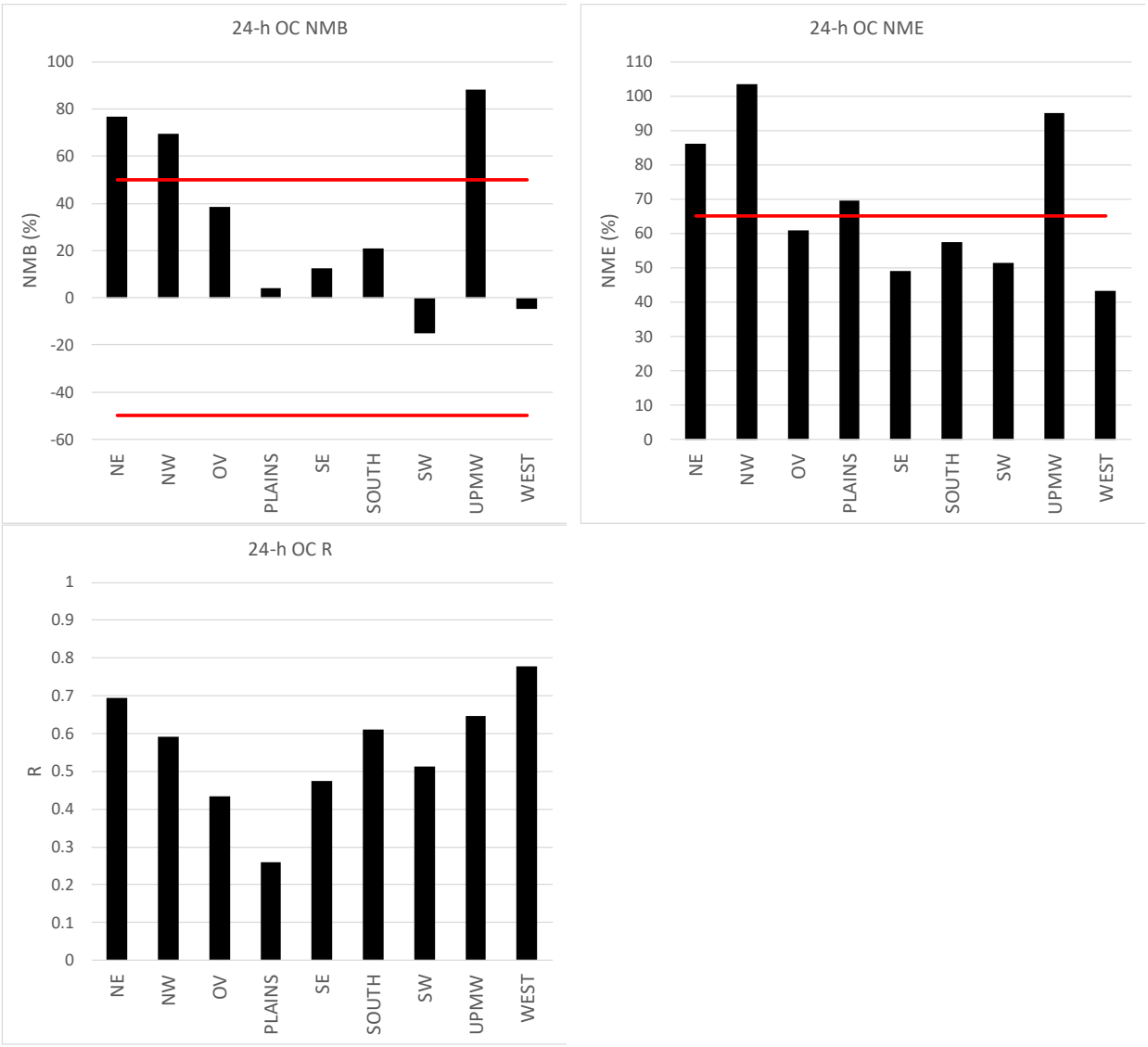

Figure S12. Statistical model performance (NMB, NME, r) in replicating 24-h particulate organic carbon over the combined January-March and October-December, 2016 cool seasons by US climate zone. Criteria benchmarks are shown as red lines.

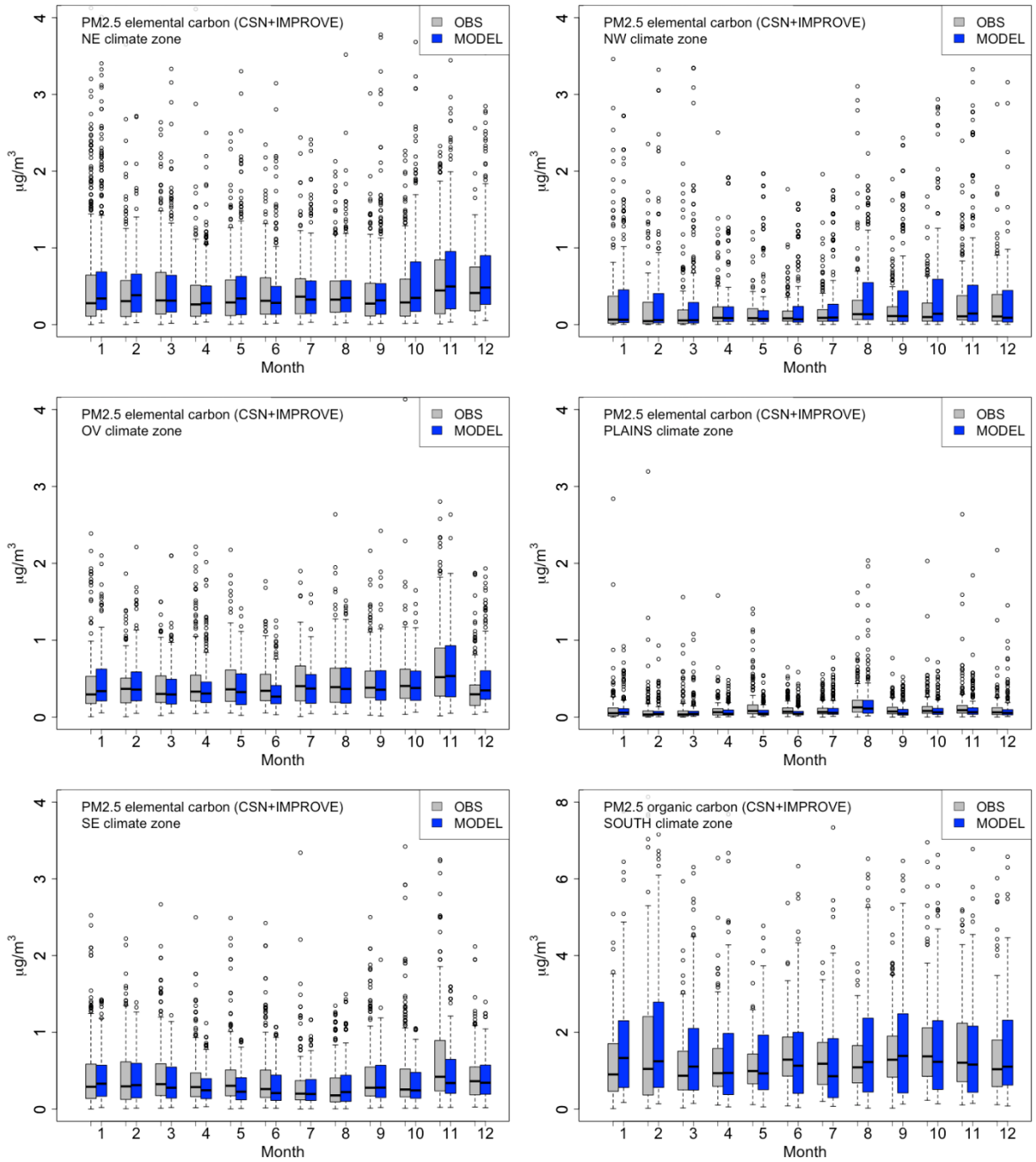

Figure S13. Monthly comparison between 2016 observed (grey) and simulated (blue) 24-h particulate elemental carbon concentration for each of the nine NOAA climate regions shown in Figure 12. Boxes represent the interquartile range (25th to 75th percentile with median shown by the center line), dashed whiskers represent 1.5 times the interquartile range, and circles represent individual outlier values.

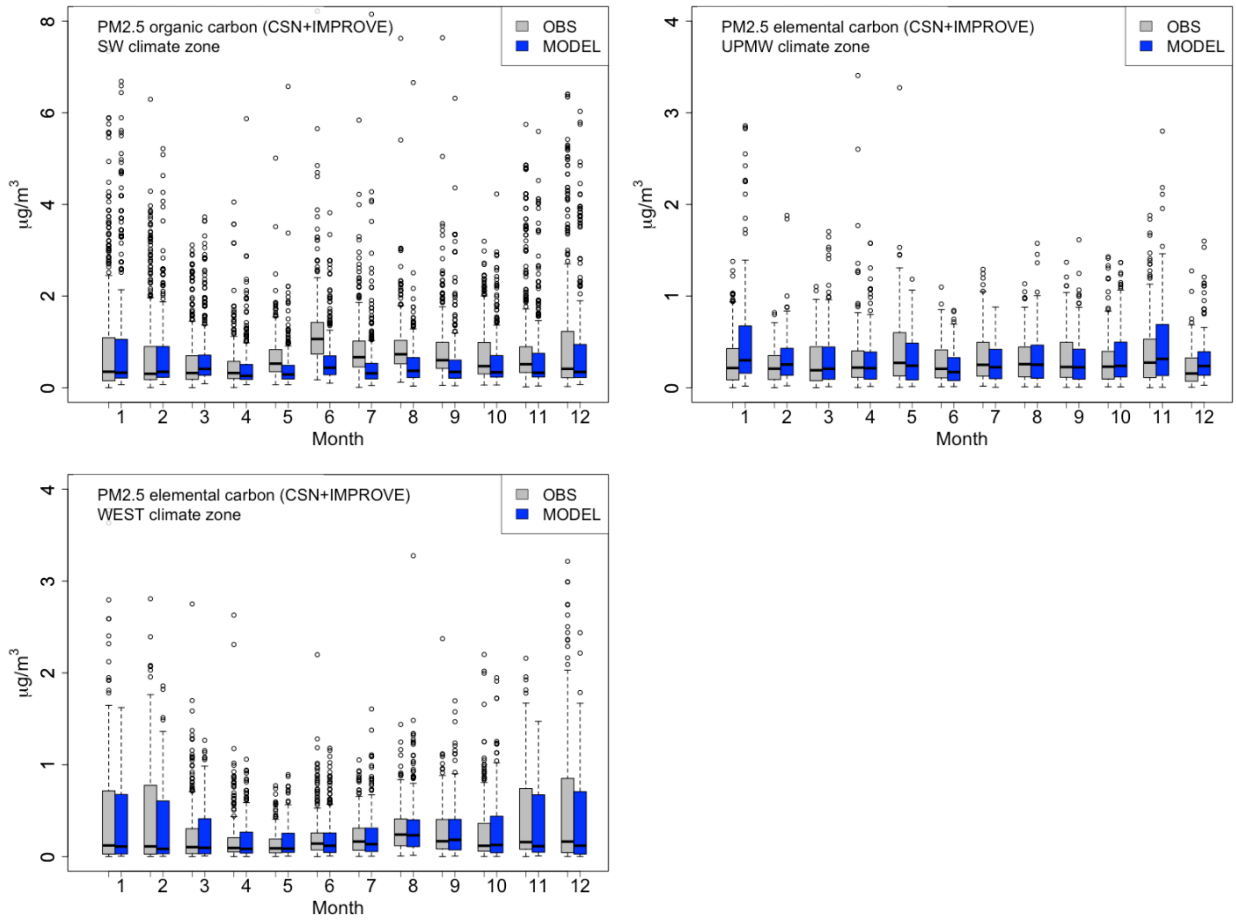

Figure S13 (Concluded).

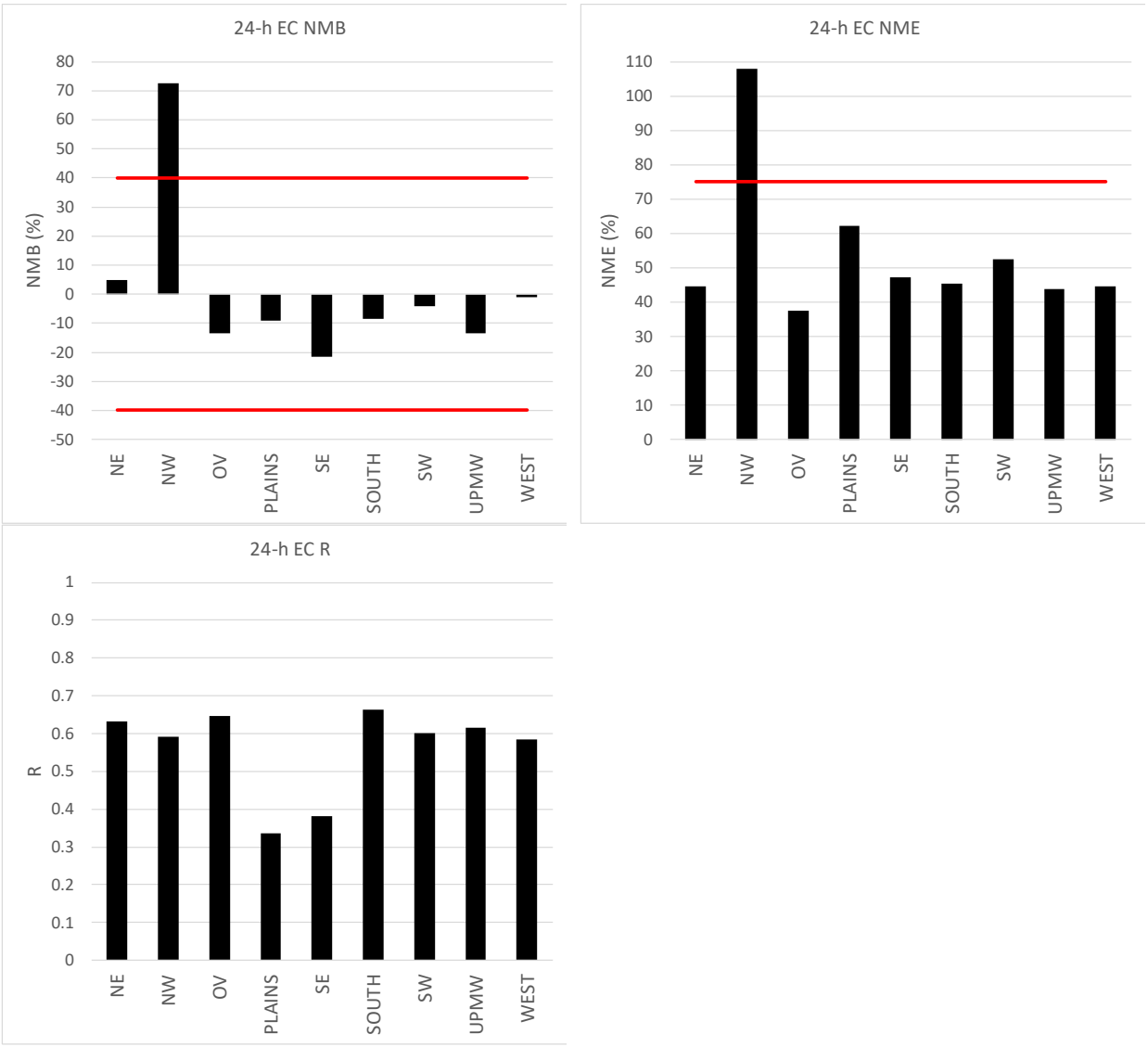

Figure S14. Statistical model performance (NMB, NME, r) in replicating 24-h particulate elemental carbon over the April-September, 2016 warm season by US climate zone. Criteria benchmarks are shown as red lines.

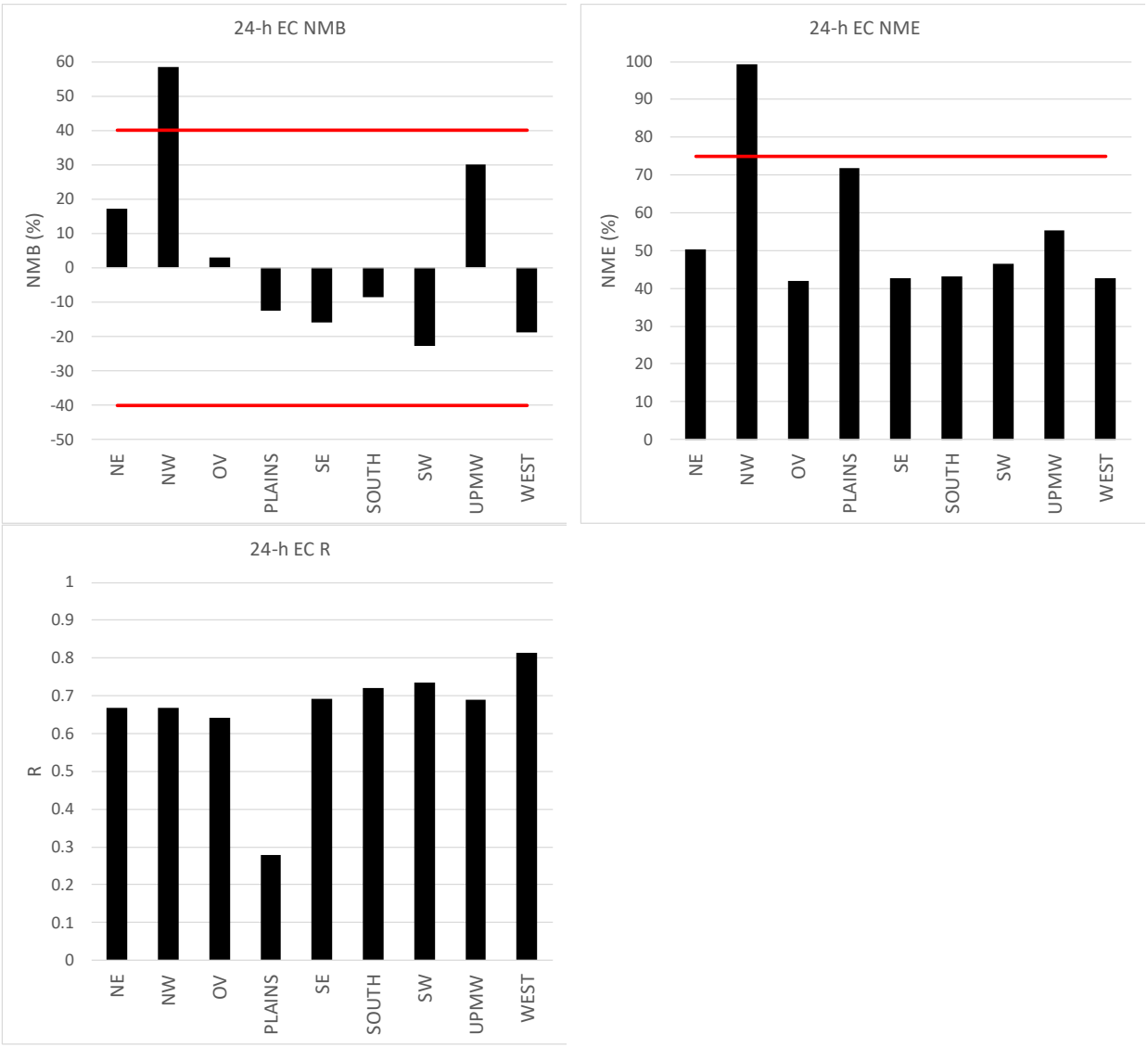

Figure S15. Statistical model performance (NMB, NME, r) in replicating 24-h particulate elemental carbon over the combined January-March and October-December, 2016 cool seasons by US climate zone. Criteria benchmarks are shown as red lines.

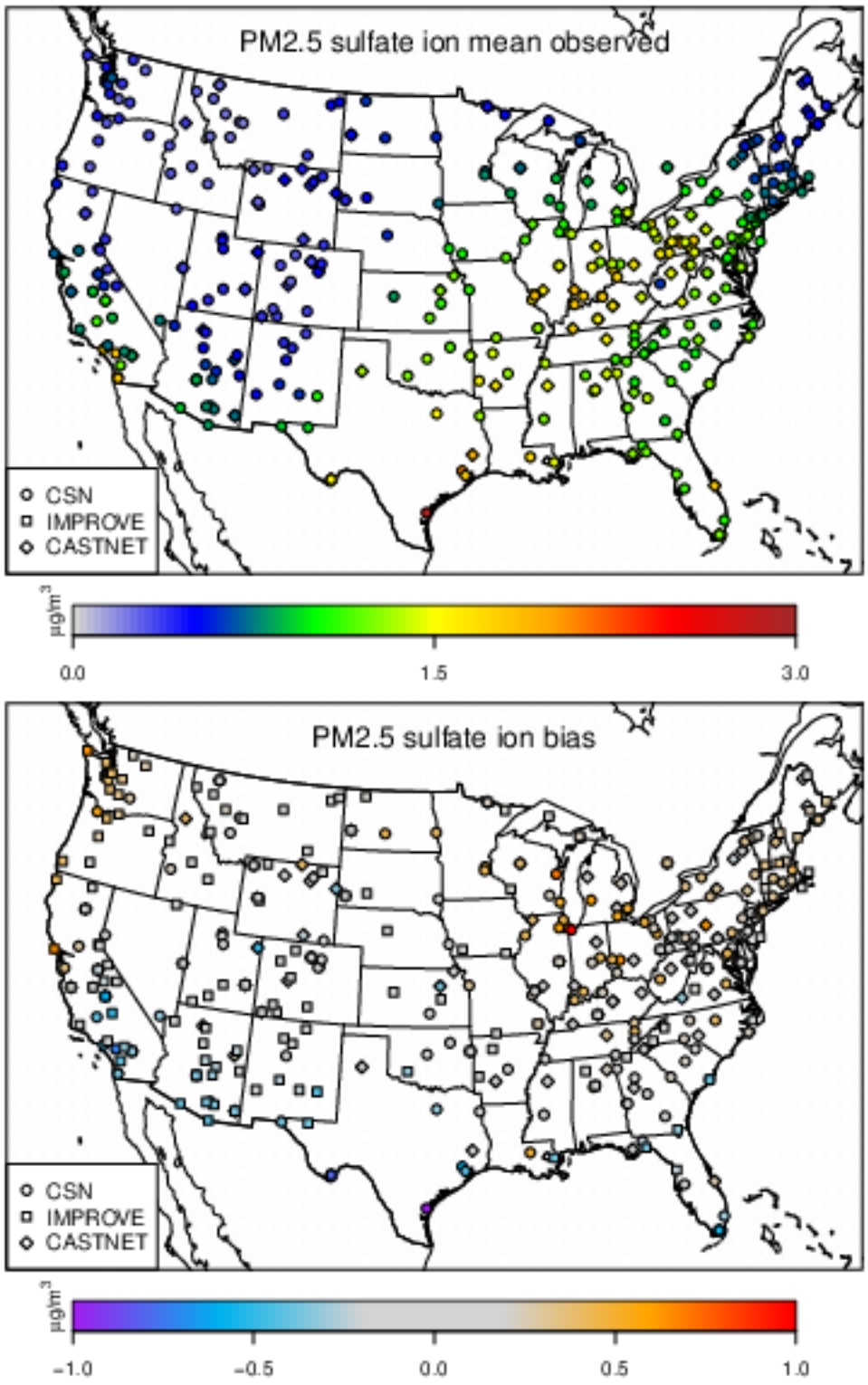

Figure S16. Observed April-September average sulfate concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

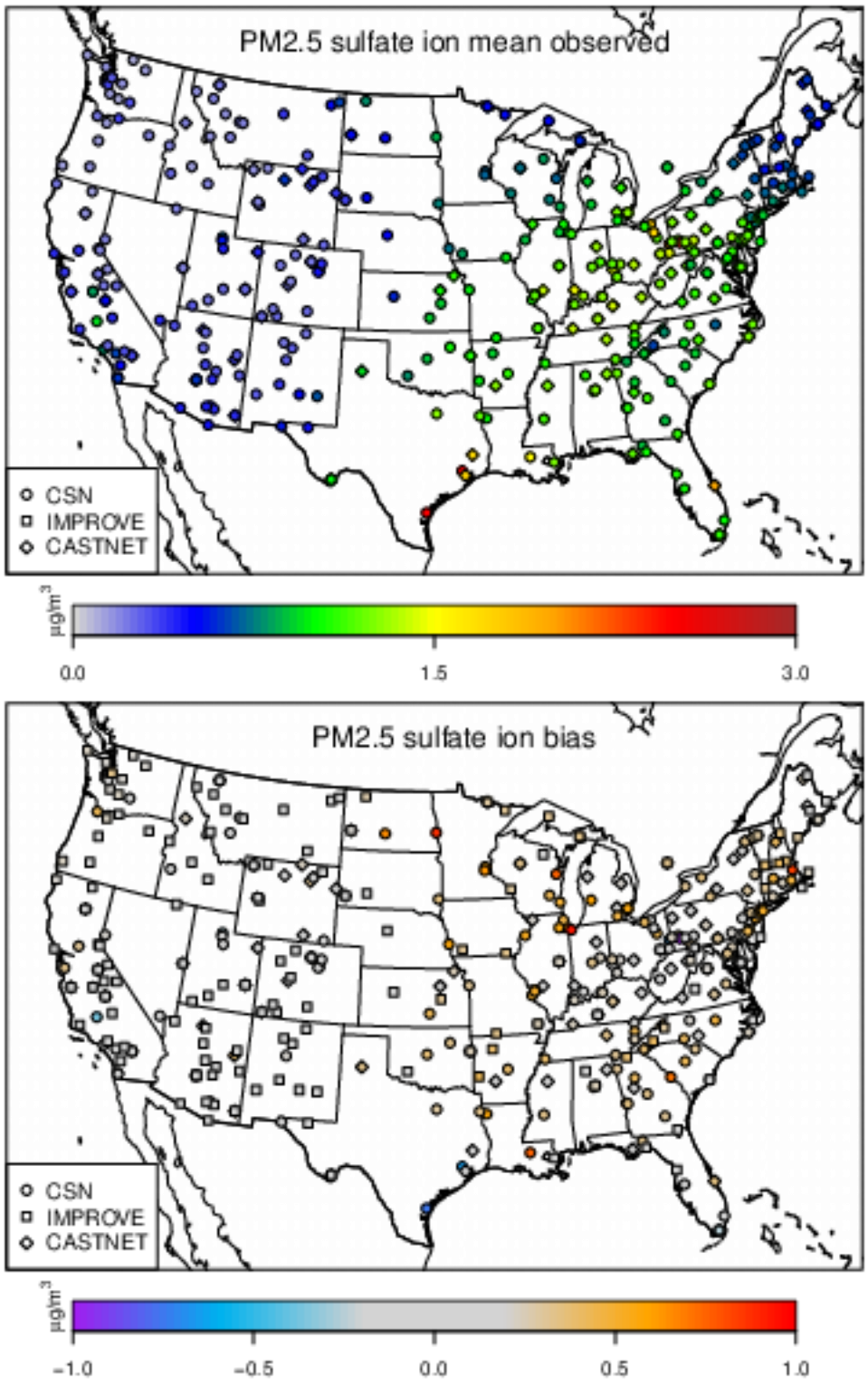

Figure S17. Observed October-March average sulfate concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

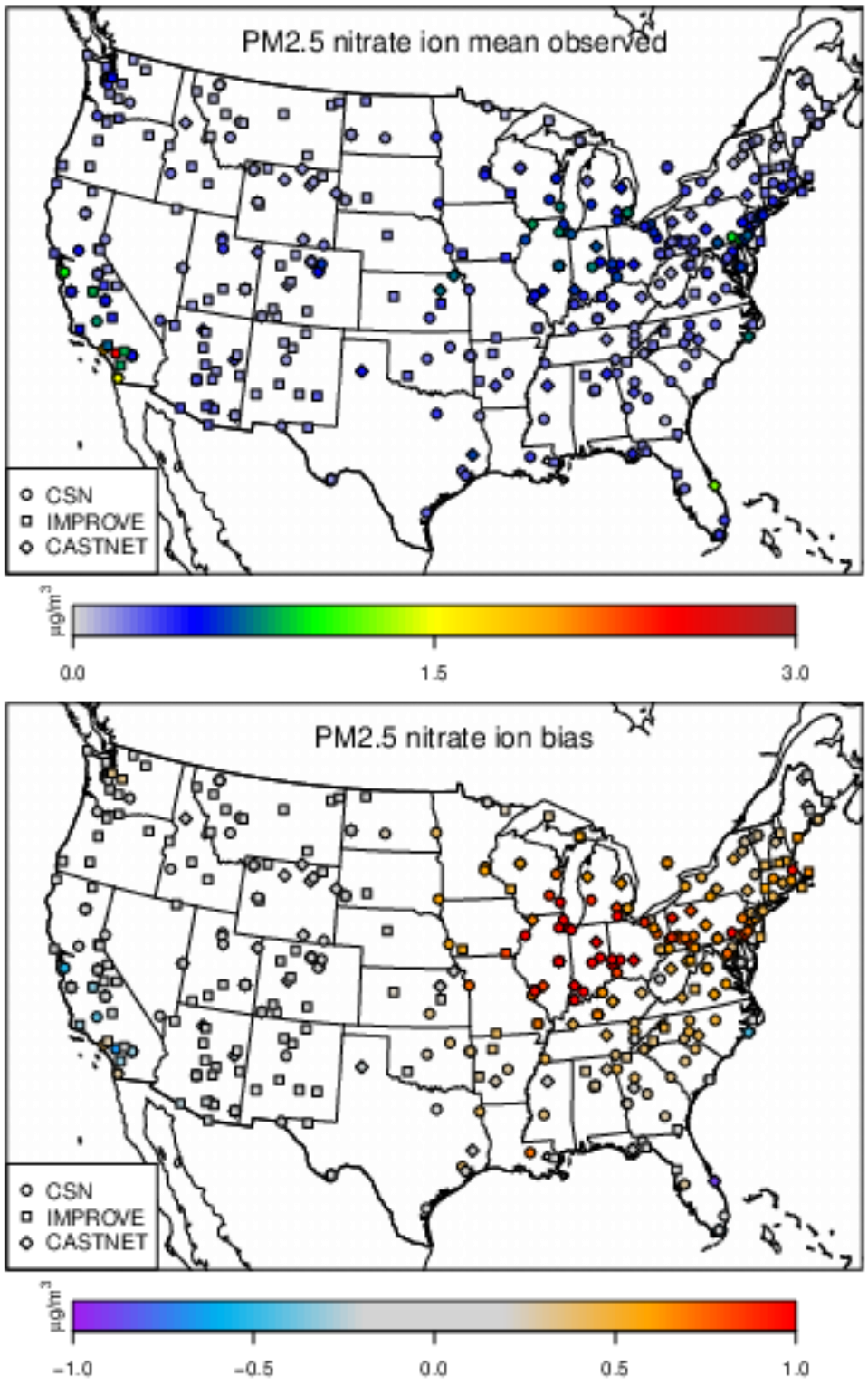

Figure S18. Observed April-September average nitrate concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

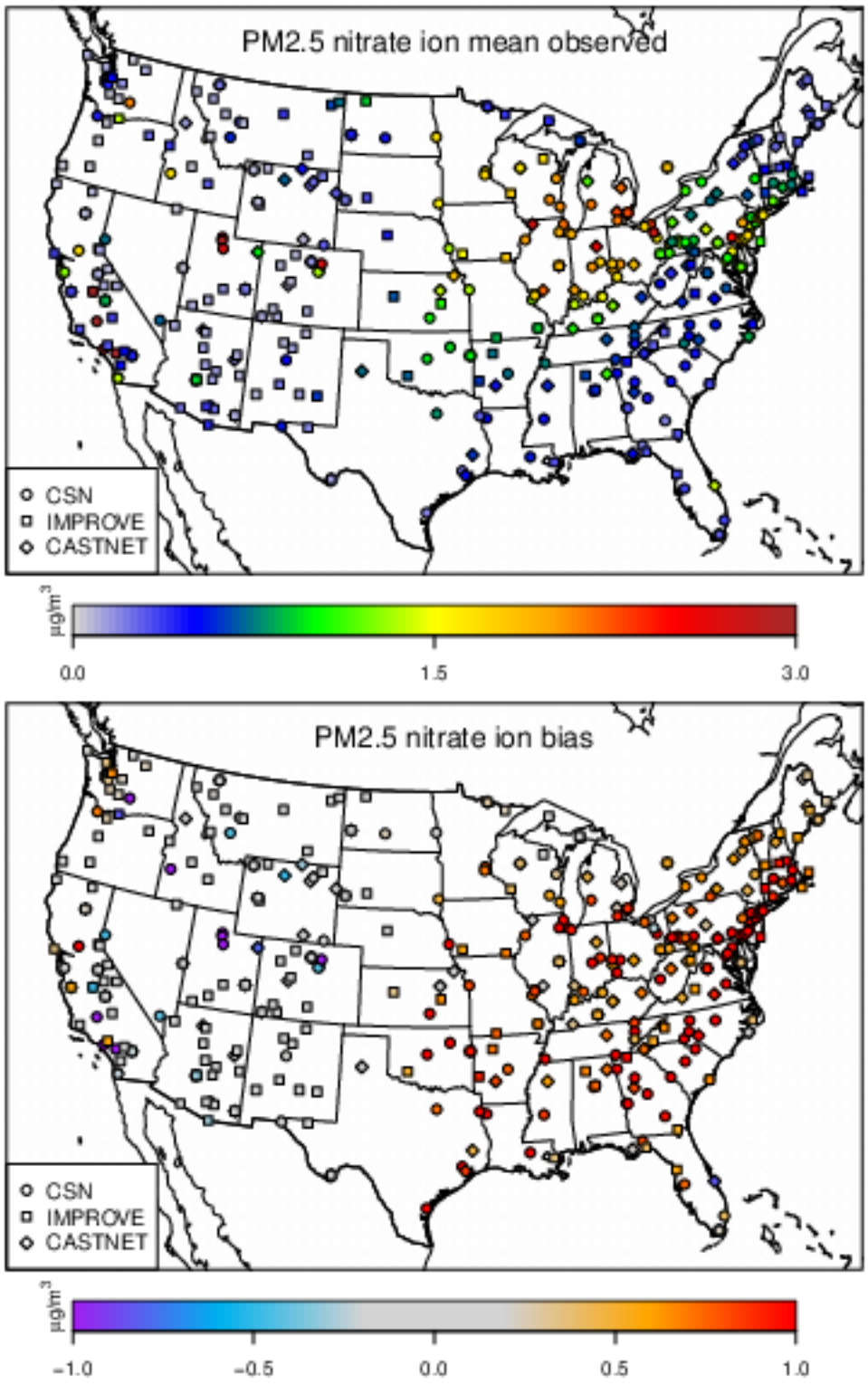

Figure S19. Observed October-March average nitrate concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

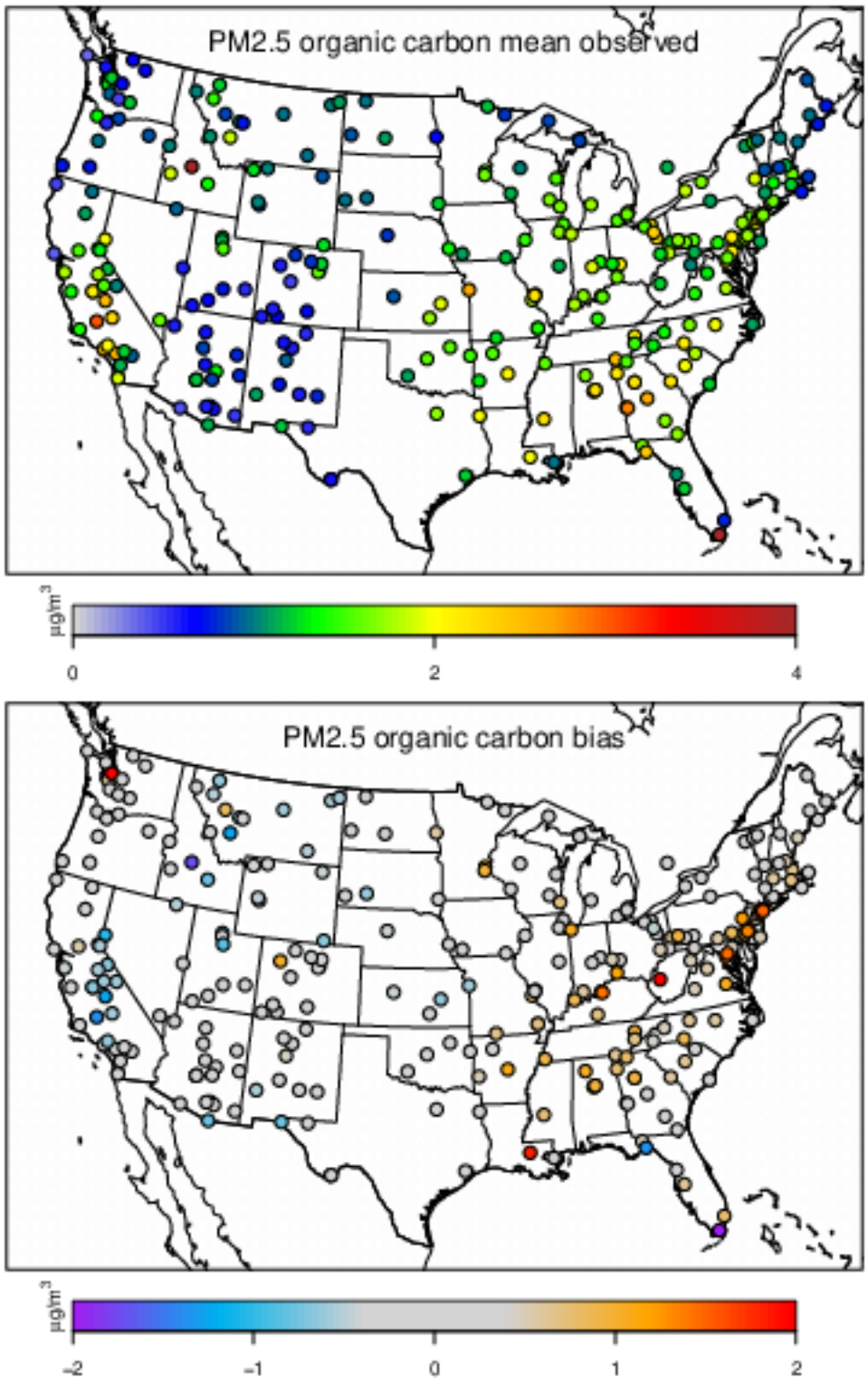

Figure S20. Observed April-September average organic carbon concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

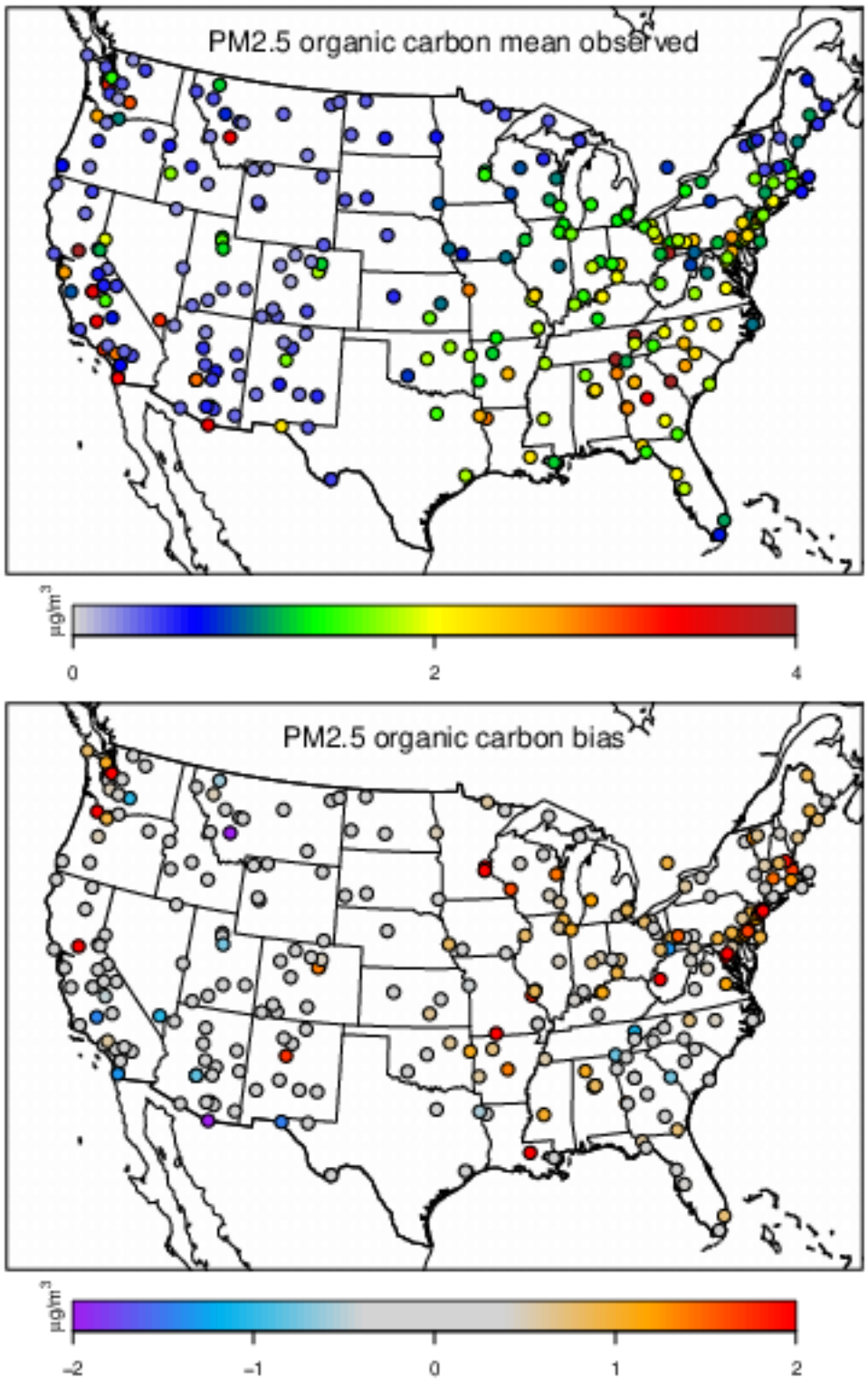

Figure S21. Observed October-March average organic carbon concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

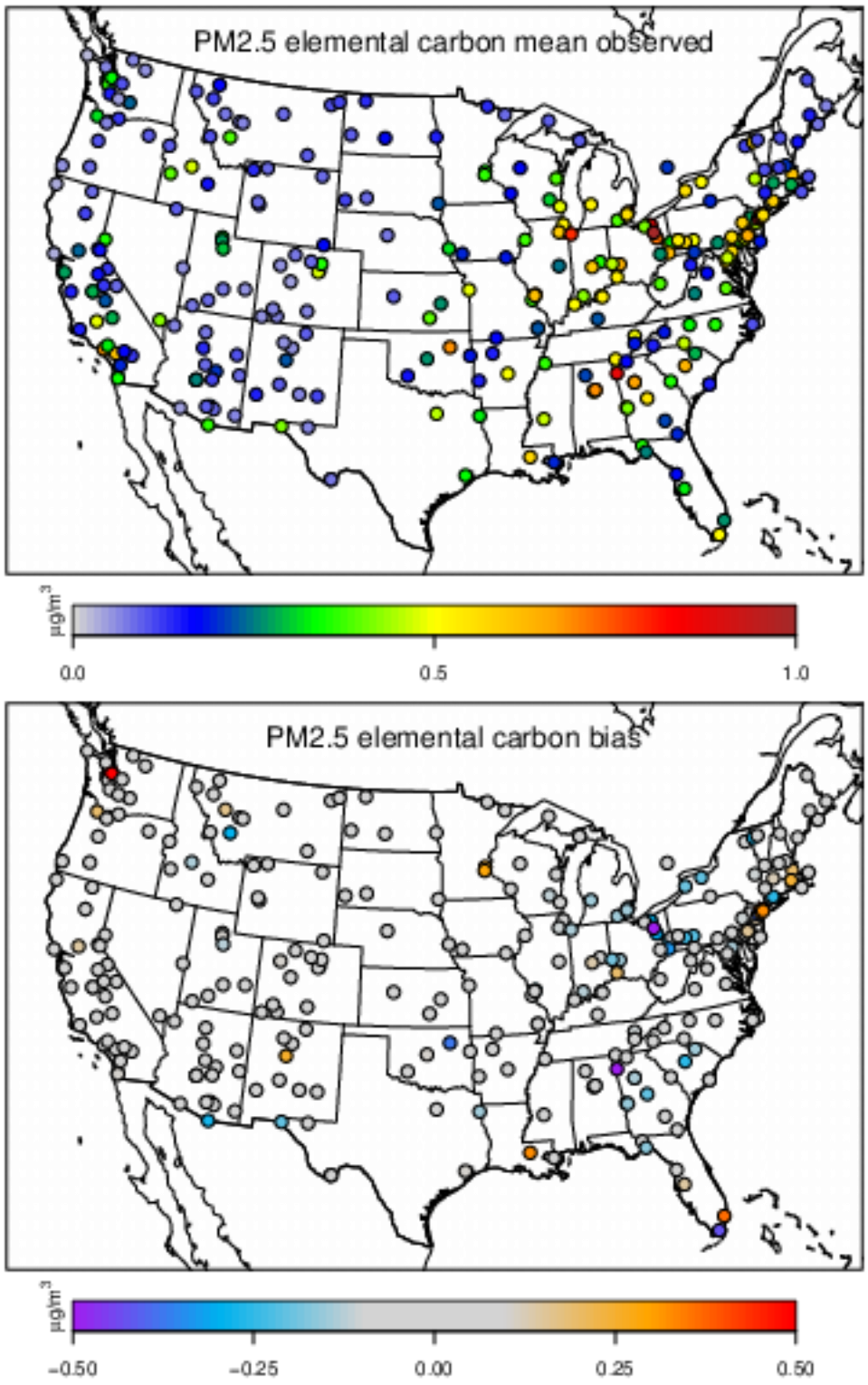

Figure S22. Observed April-September average elemental carbon concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

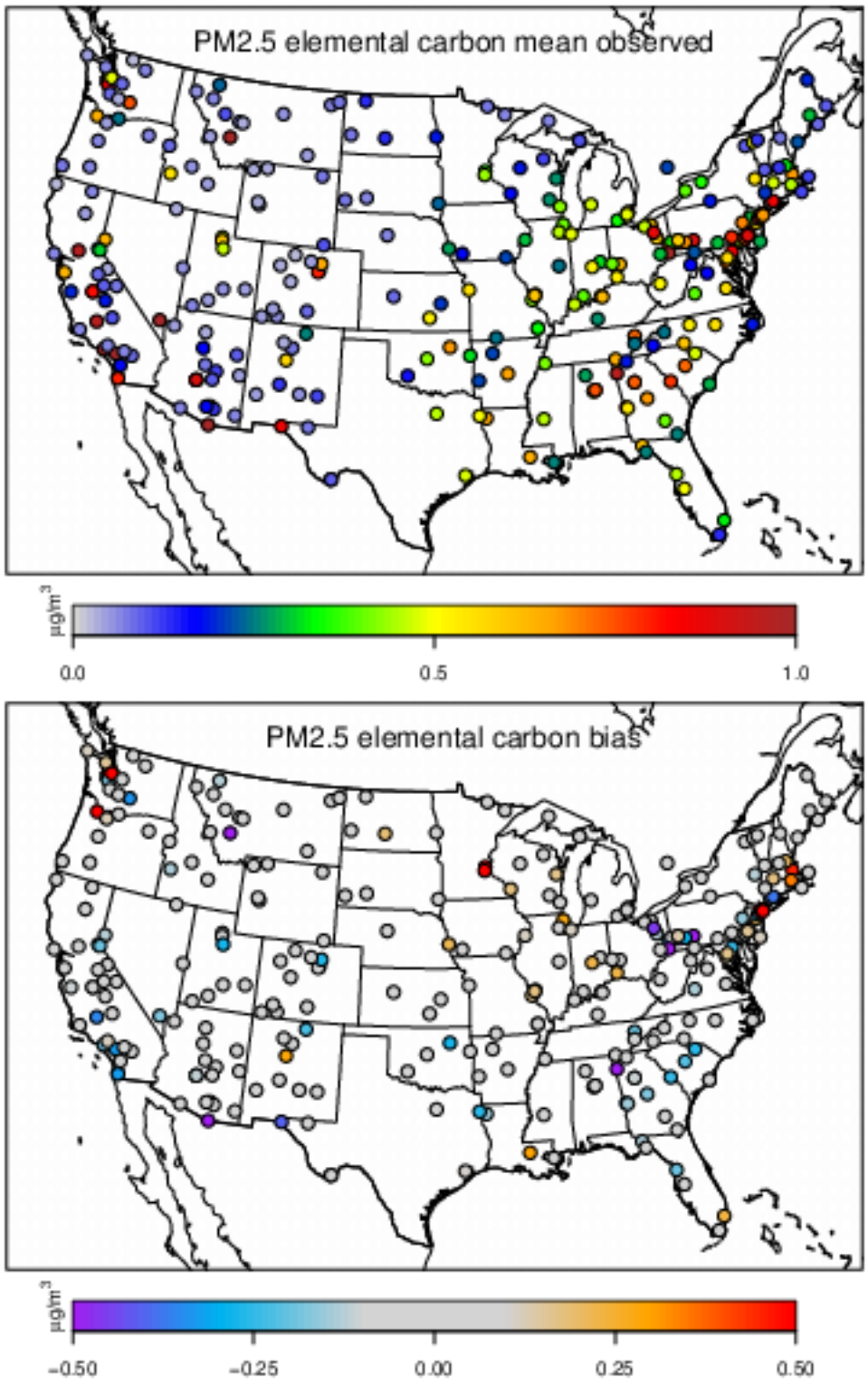

Figure S23. Observed October-March average elemental carbon concentrations (ug/m3) at AMON sites (top) and simulated mean bias (MB, ug/m3) with the bidirectional scheme (bottom).

CB6r2 Gas-Phase Chemistry

Table S1. Reactions and rate constant expressions for the CB6r2 mechanism. See Table S2 for species names. k_{298} is the rate constant at 298 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

Number	Reactants and Products	Rate Constant Expression	k_{298}
1	NO2 = NO + O	Photolysis	6.30E-3
2	O + O2 + M = O3 + M	k = 5.68E-34 (T/300)^-2.6	5.78E-34
3	O3 + NO = NO2	k = 1.40E-12 exp(-1310/T)	1.73E-14
4	O + NO + M = NO2 + M	k = 1.00E-31 (T/300)^-1.6	1.01E-31
5	O + NO2 = NO	k = 5.50E-12 exp(188/T)	1.03E-11
6	O + NO2 = NO3	Falloff: F=0.6; n=1 k(0) = 1.30E-31 (T/300)^-1.5 k(inf) = 2.30E-11 (T/300)^0.24	2.11E-12
7	O + O3 =	k = 8.00E-12 exp(-2060/T)	7.96E-15
8	O3 = O	Photolysis	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 = 2.70E-11 exp(224/T)	5.73E-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=0.5; n=1.13 k(0) = 6.90E-31 (T/300)^-0.8 k(inf) = 2.60E-11	5.25E-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 = 2.90E-12 exp(-160/T)	1.70E-12
23	H2O2 + O = OH + HO2	k = 1.40E-12 exp(-2000/T)	1.70E-15
24	NO + NO + O2 = 2 NO2	k = 3.30E-39 exp(530/T)	1.95E-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	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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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=0.6; n=1 k(0) = 1.80E-31 (T/300)^-3.2 k(inf) = 4.70E-12	1.38E-12
49	PNA = HO2 + NO2	Falloff: F=0.6; n=1 k(0) = 4.10E-5 exp(-10650/T) k(inf) = 4.80E+15 exp(-11170/T)	8.31E-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) = 4.50E-31 (T/300)^-3.9 k(inf) = 1.30E-12 (T/300)^-0.7	8.12E-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) = 2.70E-28 (T/300)^-7.1 k(inf) = 1.20E-11 (T/300)^-0.9	9.40E-12
55	PAN = NO2 + C2O3	Falloff: F=0.3; n=1.41 k(0) = 4.90E-3 exp(-12100/T) k(inf) = 5.40E+16 exp(-13830/T)	2.98E-4
56	PAN = 0.6 NO2 + 0.6 C2O3 + 0.4 NO3 + 0.4 MEO2 + 0.4 RO2	Photolysis	3.47E-7
57	C2O3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 MEO2 + 0.44 RO2 + 0.44 OH	k = 5.20E-13 exp(980/T)	1.39E-11
58	C2O3 + RO2 = C2O3	k = 8.90E-13 exp(800/T)	1.30E-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 = 2.90E-12 exp(500/T)	1.55E-11
61	CXO3 + NO = NO2 + ALD2 + XO2H + RO2	k = 6.70E-12 exp(340/T)	2.10E-11

Number	Reactants and Products	Rate Constant Expression	k_{298}
62	CXO3 + NO2 = PANX	k = k(ref)/K k(ref) = k(54) K = 1.00E+0	9.40E-12
63	PANX = NO2 + CXO3	k = k(ref)/K k(ref) = k(55) K = 1.00E+0	2.98E-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 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALD2 + 0.44 XO2H + 0.44 RO2 + 0.44 OH	k = 5.20E-13 exp(980/T)	1.39E-11
66	CXO3 + RO2 = 0.8 ALD2 + 0.8 XO2H + 0.8 RO2	k = 8.90E-13 exp(800/T)	1.30E-11
67	CXO3 + CXO3 = 2 ALD2 + 2 XO2H + 2 RO2	k = 3.20E-12 exp(500/T)	1.71E-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	1.30E-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
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	1.30E-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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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	1.30E-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 = 5.30E-12 exp(190/T)	1.00E-11
96	FORM + OH = HO2 + CO	k = 5.40E-12 exp(135/T)	8.49E-12
97	FORM = 2 HO2 + CO	Photolysis	1.78E-5
98	FORM = CO + H2	Photolysis	2.38E-5
99	FORM + O = OH + HO2 + CO	k = 3.40E-11 exp(-1600/T)	1.58E-13
100	FORM + NO3 = HNO3 + HO2 + CO	k = 5.50E-16	5.50E-16
101	FORM + HO2 = HCO3	k = 9.70E-15 exp(625/T)	7.90E-14
102	HCO3 = FORM + HO2	k = 2.40E+12 exp(-7000/T)	1.51E+2
103	HCO3 + NO = FACD + NO2 + HO2	k = 5.60E-12	5.60E-12
104	HCO3 + HO2 = 0.5 MEPX + 0.5 FACD + 0.2 OH + 0.2 HO2	k = 5.60E-15 exp(2300/T)	1.26E-11
105	ALD2 + O = C2O3 + OH	k = 1.80E-11 exp(-1100/T)	4.49E-13
106	ALD2 + OH = C2O3	k = 4.70E-12 exp(345/T)	1.50E-11
107	ALD2 + NO3 = C2O3 + HNO3	k = 1.40E-12 exp(-1860/T)	2.73E-15
108	ALD2 = MEO2 + RO2 + CO + HO2	Photolysis	1.76E-6
109	ALDX + O = CXO3 + OH	k = 1.30E-11 exp(-870/T)	7.02E-13
110	ALDX + OH = CXO3	k = 4.90E-12 exp(405/T)	1.91E-11
111	ALDX + NO3 = CXO3 + HNO3	k = 6.30E-15	6.30E-15
112	ALDX = ALD2 + XO2H + RO2 + CO + HO2	Photolysis	6.96E-6
113	GLYD + OH = 0.2 GLY + 0.2 HO2 + 0.8 C2O3	k = 8.00E-12	8.00E-12
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	1.56E-6
115	GLYD + NO3 = HNO3 + C2O3	k = 1.40E-12 exp(-1860/T)	2.73E-15
116	GLY + OH = 1.8 CO + 0.2 XO2 + 0.2 RO2 + HO2	k = 3.10E-12 exp(340/T)	9.70E-12
117	GLY = 2 HO2 + 2 CO	Photolysis	5.50E-5
118	GLY + NO3 = HNO3 + 1.5 CO + 0.5 XO2 + 0.5 RO2 + HO2	k = 1.40E-12 exp(-1860/T)	2.73E-15
119	MGLY = C2O3 + HO2 + CO	Photolysis	1.46E-4
120	MGLY + NO3 = HNO3 + C2O3 + XO2 + RO2	k = 1.40E-12 exp(-1860/T)	2.73E-15
121	MGLY + OH = C2O3 + CO	k = 1.90E-12 exp(575/T)	1.31E-11
122	H2 + OH = HO2	k = 7.70E-12 exp(-2100/T)	6.70E-15

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123	CO + OH = HO2	k = k1 + k2 [M] k1 = 1.44E-13 k2 = 3.43E-33	2.28E-13
124	CH4 + OH = MEO2 + RO2	k = 1.85E-12 exp(-1690/T)	6.37E-15
125	ETHA + OH = 0.991 ALD2 + 0.991 XO2H + 0.009 XO2N + RO2	k = 6.90E-12 exp(-1000/T)	2.41E-13
126	MEOH + OH = FORM + HO2	k = 2.85E-12 exp(-345/T)	8.95E-13
127	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
128	KET = 0.5 ALD2 + 0.5 C2O3 + 0.5 XO2H + 0.5 CXO3 + 0.5 MEO2 + RO2 - 2.5 PAR	Photolysis	2.27E-7
129	ACET = 0.38 CO + 1.38 MEO2 + 1.38 RO2 + 0.62 C2O3	Photolysis	2.08E-7
130	ACET + OH = FORM + C2O3 + XO2 + RO2	k = 1.41E-12 exp(-620.6/T)	1.76E-13
131	PRPA + OH = 0.71 ACET + 0.26 ALDX + 0.26 PAR + 0.97 XO2H + 0.03 XO2N + RO2	k = 7.60E-12 exp(-585/T)	1.07E-12
132	PAR + OH = 0.11 ALDX + 0.76 ROR + 0.13 XO2N + 0.11 XO2H + 0.76 XO2 + RO2 - 0.11 PAR	k = 8.10E-13	8.10E-13
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	k = 5.70E+12 exp(-5780/T)	2.15E+4
134	ROR + O2 = KET + HO2	k = 1.50E-14 exp(-200/T)	7.67E-15
135	ROR + NO2 = NTR1	k = 8.60E-12 exp(400/T)	3.29E-11
136	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
137	ETH + O = FORM + HO2 + CO + 0.7 XO2H + 0.7 RO2 + 0.3 OH	k = 1.04E-11 exp(-792/T)	7.29E-13
138	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
139	ETH + O3 = FORM + 0.51 CO + 0.16 HO2 + 0.16 OH + 0.37 FACD	k = 9.10E-15 exp(-2580/T)	1.58E-18
140	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
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	k = 1.00E-11 exp(-280/T)	3.91E-12
142	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
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	k = 5.50E-15 exp(-1880/T)	1.00E-17
144	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

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145	IOLE + O = 1.24 ALD2 + 0.66 ALDX + 0.1 XO2H + 0.1 RO2 + 0.1 CO + 0.1 PAR	k = 2.30E-11	2.30E-11
146	IOLE + OH = 1.3 ALD2 + 0.7 ALDX + XO2H + RO2	k = 1.05E-11 exp(519/T)	5.99E-11
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	k = 4.70E-15 exp(-1013/T)	1.57E-16
148	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
149	ISOP + OH = ISO2 + RO2	k = 2.70E-11 exp(390/T)	9.99E-11
150	ISOP + O = 0.75 ISPD + 0.5 FORM + 0.25 XO2 + 0.25 RO2 + 0.25 HO2 + 0.25 CXO3 + 0.25 PAR	k = 3.00E-11	3.00E-11
151	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
152	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
153	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	1.30E-11
154	ISO2 + RO2 = 0.598 FORM + 1 ISPD + 0.728 HO2 + 0.072 XO2H + 0.072 RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
155	ISO2 = HO2 + HPLD	k = 3.30E+9 exp(-8300/T)	2.64E-3
156	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
157	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
158	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
159	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
160	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
161	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

Number	Reactants and Products	Rate Constant Expression	k_{298}
162	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
163	HPLD = OH + ISPD	Photolysis	4.41E-4
164	HPLD + NO3 = HNO3 + ISPD	k = 6.00E-12 exp(-1860/T)	1.17E-14
165	EPOX + OH = EPX2 + RO2	k = 5.78E-11 exp(-400/T)	1.51E-11
166	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
167	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
168	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	1.30E-11
169	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
170	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
171	TERP + O = 0.15 ALDX + 5.12 PAR	k = 3.60E-11	3.60E-11
172	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
173	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
174	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
175	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
176	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
177	BZO2 + C2O3 = GLY + OPEN + HO2 + MEO2 + RO2	k = k(ref)/K k(ref) = k(58) K = 1.00E+0	1.30E-11
178	BZO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
179	BZO2 + RO2 = GLY + OPEN + HO2 + RO2	k = k(ref)/K k(ref) = k(70) K = 1.00E+0	3.48E-13
180	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

Number	Reactants and Products	Rate Constant Expression	k_{298}
181	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
182	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	1.30E-11
183	TO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
184	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
185	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
186	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
187	XLO2 + HO2 =	k = 1.90E-13 exp(1300/T)	1.49E-11
188	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	1.30E-11
189	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
190	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
191	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
192	CRO + NO2 = CRON	k = 2.10E-12	2.10E-12
193	CRO + HO2 = CRES	k = 5.50E-12	5.50E-12
194	CRON + OH = NTR2 + 0.5 CRO	k = 1.53E-12	1.53E-12
195	CRON + NO3 = NTR2 + 0.5 CRO + HNO3	k = 3.80E-12	3.80E-12
196	CRON = HONO + HO2 + FORM + OPEN	Photolysis	9.45E-5
197	XOPN = 0.4 GLY + XO2H + 0.7 HO2 + 0.7 CO + 0.3 C2O3	Photolysis	5.04E-4
198	XOPN + OH = MGLY + 0.4 GLY + 2 XO2H + 2 RO2	k = 9.00E-11	9.00E-11
199	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
200	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
201	OPEN = OPO3 + HO2 + CO	Photolysis	5.04E-4
202	OPEN + OH = 0.6 OPO3 + 0.4 XO2H + 0.4 RO2 + 0.4 GLY	k = 4.40E-11	4.40E-11
203	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
204	OPEN + NO3 = OPO3 + HNO3	k = 3.80E-12	3.80E-12
205	CAT1 + OH = 0.14 FORM + 0.2 HO2 + 0.5 CRO	k = 5.00E-11	5.00E-11

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206	CAT1 + NO3 = CRO + HNO3	k = 1.70E-10	1.70E-10
207	OPO3 + NO = NO2 + 0.5 GLY + 0.5 CO + 0.8 HO2 + 0.2 CXO3	k = 1.00E-11	1.00E-11
208	OPO3 + NO2 = OPAN	k = k(ref)/K k(ref) = k(54) K = 1.00E+0	9.40E-12
209	OPAN = OPO3 + NO2	k = k(ref)/K k(ref) = k(55) K = 1.00E+0	2.98E-4
210	OPO3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALDX + 0.44 XO2H + 0.44 RO2 + 0.44 OH	k = k(ref)/K k(ref) = k(57) K = 1.00E+0	1.39E-11
211	OPO3 + C2O3 = MEO2 + XO2 + ALDX + 2 RO2	k = k(ref)/K k(ref) = k(59) K = 1.00E+0	1.55E-11
212	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	1.30E-11
213	OPAN + OH = 0.5 NO2 + 0.5 GLY + CO + 0.5 NTR2	k = 3.60E-11	3.60E-11
214	PANX + OH = ALD2 + NO2	k = 3.00E-12	3.00E-12
215	NTR2 = HNO3	k = 2.30E-5	2.30E-5
216	ECH4 + OH = MEO2 + RO2	k = 1.85E-12 exp(-1690/T)	6.37E-15

Table S2. CAMx species names and descriptions for CB6 mechanisms.

Model Species	Description	Carbon #[1]	Mol. Wt.[2]
APO2	Peroxy radical from OH addition to α-pinene	10	185.2
BZO2	Peroxy radical from OH addition to benzene	6	159.1
C2O3	Acetylperoxy radical	2	75.0
CRO	Alkoxy radical from cresol	7	107.1
CXO3	C3 and higher acylperoxy radicals	3	89.0
EPX2	Peroxy radical from EPOX reaction with OH	5	149.1
HCO3	Adduct from HO2 plus formaldehyde	1	63.0
HO2	Hydroperoxy radical	1	28.0
ISO2	Peroxy radical from OH addition to isoprene	5	117.1
MEO2	Methylperoxy radical	1	47.0
NO3	Nitrate radical		62.0
O	Oxygen atom in the $O^3(P)$ electronic state		16.0
O1D	Oxygen atom in the $O^1(D)$ electronic state		16.0
OH	Hydroxyl radical		17.0
OPO3	Peroxyacyl radical from OPEN	4	115.0
RO2	Operator to approximate total peroxy radical concentration		87.1
ROR	Secondary alkoxy radical	1	71.1
SQO2	Peroxy radical from OH addition to SQT	15	253.3
TO2	Peroxy radical from OH addition to TOL	7	173.1
TPO2	Peroxy radical from OH addition to TERP	10	185.2
XLO2	Peroxy radical from OH addition to XYL	8	187.1
XO2	NO to NO2 conversion from alkylperoxy (RO2) radical		87.1
XO2H	NO to NO2 conversion (XO2) accompanied by HO2 production		87.1
XO2N	NO to organic nitrate conversion from alkylperoxy (RO2) radical		87.1
I	Iodine atom		126.90
IO	Iodine monoxide		142.89
OIO	Iodine dioxide		158.88
AACD	Acetic acid	2	60.0
ACET	Acetone	3	58.1
ALD2	Acetaldehyde	2	44.0
ALDX	Propionaldehyde and higher aldehydes	2	58.1
APIN	α-Pinene	10	136.2
BENZ	Benzene	6	78.1
CAT1	Methyl-catechols	7	124.1
CO	Carbon monoxide	1	28.0
CH4	Methane	1	16.0
CRES	Cresols	7	108.1
CRON	Nitro-cresols	7	153.1
EPOX	Epoxide formed from ISPX reaction with OH	5	118.1
ETH	Ethene	2	28.0

Model Species	Description	Carbon #[1]	Mol. Wt.[2]
ETHA	Ethane	2	30.1
ETHY	Ethyne	2	26.0
ETOH	Ethanol	2	46.1
FACD	Formic acid	1	46.0
FORM	Formaldehyde	1	30.0
GLY	Glyoxal	2	58.0
GLYD	Glycolaldehyde	2	60.0
H2O2	Hydrogen peroxide		34.0
HACT	Hydroxyacetone	3	74.1
HNO3	Nitric acid		63.0
HONO	Nitrous acid		47.0
HPLD	Hydroperoxyaldehyde	5	116.1
INTR	Organic nitrates from ISO2 reaction with NO	5	147.1
IOLE	Internal olefin carbon bond (R-C=C-R)	4	56.1
ISOP	Isoprene	5	68.1
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)	4	70.1
ISPX	Hydroperoxides from ISO2 reaction with HO2	5	118.1
KET	Ketone carbon bond (C=O)	1	72.1
MEOH	Methanol	1	32.0
MEPX	Methylhydroperoxide	1	48.0
MGLY	Methylglyoxal	3	72.0
N2O5	Dinitrogen pentoxide		108.0
NO	Nitric oxide		30.0
NO2	Nitrogen dioxide		46.0
NTR	Organic nitrates	4	119.1
O3	Ozone		48.0
OLE	Terminal olefin carbon bond (R-C=C)	3	42.1
OPAN	Peroxyacyl nitrate (PAN compound) from OPO3	4	161.0
OPEN	Aromatic ring opening product (unsaturated dicarbonyl)	4	84.0
PACD	Peroxyacetic and higher peroxycarboxylic acids	2	76.0
PAN	Peroxyacetyl Nitrate	2	121.0
PANX	C3 and higher peroxyacyl nitrate	3	135.0
PAR	Paraffin carbon bond (C-C)	1	72.1
PNA	Peroxynitric acid		79.0
PRPA	Propane	3	44.1
ROOH	Higher organic peroxide		90.1
SQT	Sesquiterpenes	15	204.3
SO2	Sulfur dioxide		64.0
SULF	Sulfuric acid (gaseous)		98.0
TERP	Monoterpenes	10	136.2
TOL	Toluene and other monoalkyl aromatics	7	92.1
XOPN	Aromatic ring opening product (unsaturated dicarbonyl)	5	98.1

Model Species	Description	Carbon #[1]	Mol. Wt.[2]
XYL	Xylene and other polyalkyl aromatics	8	106.2
NTR1	Simple organic nitrates		119.1
NTR2	Multi-functional organic nitrates		135.1
ECH4	Emitted methane (to enable tracking separate from CH4)	1	16.0
XPRP	Operator for organic nitrates from PRPA	3	89.1
XPAR	Operator for organic nitrates from PAR	1	117.1
CRNO	Nitro-cresol oxy radical	7	152.1
CRN2	Nitro-cresol peroxy radical	7	168.1
CRPX	Nitro-cresol hydroperoxide	7	169.1
CAO2	Ring-opening product from methyl catechol	7	173.1
I2	Molecular iodine		253.80
I2O2	Diiodine dioxide		285.78
IXOY	Condensable iodine oxides		301.77
HOI	Hypoiodous acid		143.90
HIO3	Iodic acid		175.88
INO3	Iodine nitrate		188.87
DMS	Dimethyl sulfate	2	62.10

[1] Carbon # is the precise number of carbon atoms for each model species.

[2] Mol. Wt. is a representative molecular weight, intended only for estimating molecular diffusivity, e.g. in dry deposition calculations. Diffusivity requires a different interpretation (complete molecules) than Carbon Bond chemistry (chemical groups).

Table S3. Listing of the CB6r2h halogen mechanism (see Table S1 for a complete listing of CB6r2). See Tables S2 and S4 for species names. k_{298} is the rate constant at 298 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

Number	Reactants and Products	Rate Constant Expression	k_{298}
1	CL2 = 2 CL	Photolysis	1.56E-3
2	HOCL = CL + OH	Photolysis	1.34E-4
3	CL + O3 = CLO	k = 2.30E-11 exp(-200/T)	1.18E-11
4	CLO + CLO = 0.3 CL2 + 1.4 CL	k = 1.63E-14	1.63E-14
5	CLO + NO = CL + NO2	k = 6.40E-12 exp(290/T)	1.69E-11
6	CLO + HO2 = HOCL	k = 2.70E-12 exp(220/T)	5.65E-12
7	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
8	CLN3 = CLO + NO2	Falloff: F=0.6; n=1 k(0) = 4.48E-5 (T/300)^-1 exp(-12530/T) k(inf) = 3.71E+15 (T/300)^3.5 exp(-12530/T)	3.11E-4
9	CLN3 = CLO + NO2	Photolysis	4.97E-6
10	CLN3 = CL + NO3	Photolysis	4.67E-4
11	CLN3 + H2O = HOCL + HNO3	k = 2.50E-22	2.50E-22
12	OH + HCL = CL	k = 6.58E-13 (T/300)^1.2 exp(58/T)	7.93E-13
13	OH + FMCL = CL + CO	k = 3.67E-11 exp(-1419/T)	3.14E-13
14	FMCL = CL + CO + HO2	Photolysis	6.10E-8
15	CLO + MEO2 = CL + FORM + HO2	k = 4.10E-13 exp(-800/T)	2.80E-14
16	CL + CH4 = HCL + MEO2	k = 6.60E-12 exp(-1240/T)	1.03E-13
17	CL + PAR = HCL	k = 5.00E-11	5.00E-11
18	CL + ETHA = HCL + 0.991 ALD2 + 0.991 XO2H + 0.009 XO2N + RO2	k = 8.30E-11 exp(-100/T)	5.93E-11
19	CL + PRPA = HCL + ACET + 0.97 XO2H + 0.03 XO2N + RO2	k = 1.40E-10	1.40E-10
20	CL + ISOP = FMCL + ISPD + 0.96 XO2H + 0.04 XO2N + RO2	k = 4.30E-10	4.30E-10
21	HCL + N2O5 = CLN2 + HNO3	k = 6.00E-13	6.00E-13
22	CLN2 = CL + NO2	Photolysis	2.86E-4
23	BR2 = 2 BR	Photolysis	2.79E-2
24	HOBR = BR + OH	Photolysis	1.51E-3
25	BR2 + OH = HOBR + BR	k = 5.40E-11 exp(180/T)	9.88E-11
26	HBR + OH = BR	k = 5.50E-12 exp(-200/T)	2.81E-12
27	BR + O3 = BRO	k = 1.60E-11 exp(780/T)	2.19E-10
28	BR + HO2 = HBR	k = 4.80E-12 exp(310/T)	1.36E-11
29	BR + NO2 = BRN2	Falloff: F=0.6; n=1 k(0) = 4.20E-31 (T/300)^-2.4 k(inf) = 2.70E-11	4.89E-12
30	BR + NO3 = BRO + NO2	k = 1.60E-11	1.60E-11
31	BRO = BR + O	Photolysis	2.05E-2
32	BRO + HO2 = HOBR	k = 4.50E-12 exp(460/T)	2.11E-11
33	BRO + OH = BR + HO2	k = 1.70E-11 exp(250/T)	3.93E-11
34	BRO + BRO = 2 BR	k = 2.40E-12 exp(40/T)	2.74E-12
35	BRO + BRO = BR2	k = 2.80E-14 exp(860/T)	5.02E-13
36	BRO + NO = BR + NO2	k = 8.80E-12 exp(260/T)	2.11E-11
37	BRO + NO2 = BRN3	Falloff: F=0.6; n=1 k(0) = 5.20E-31 (T/300)^-3.2 k(inf) = 6.90E-12	2.81E-12
38	BRN2 = BR + NO2	Photolysis	3.21E-3

Number	Reactants and Products	Rate Constant Expression	k_{298}
39	BRN3 = BR + NO3	Photolysis	9.76E-4
40	BRN3 + H2O = HOBR + HNO3	k = 2.50E-22	2.50E-22
41	FMBR + OH = BR + CO	k = 5.00E-12	5.00E-12
42	FMBR = BR + CO + HO2	Photolysis	4.15E-6
43	BRO + MEO2 = 0.75 HOBR + 0.25 BR + FORM	k = 4.10E-13 exp(-800/T)	2.80E-14
44	BR + FORM = HBR + CO + HO2	k = 7.70E-11 exp(-580/T)	1.10E-11
45	BR + ALD2 = HBR + C2O3	k = 1.80E-11 exp(-460/T)	3.84E-12
46	BR + OLE = FMBR + ALD2 + XO2H - 1 PAR + RO2	k = 3.60E-12	3.60E-12
47	BR + ISOP = FMBR + ISPD + 0.96 XO2H + 0.04 XO2N + RO2	k = 5.00E-12	5.00E-12
48	I2 = 2 I	Photolysis	1.30E-1
49	HOI = I + OH	Photolysis	6.36E-2
50	I2 + OH = I + HOI	k = 2.10E-10	2.10E-10
51	I2 + NO3 = I + INO3	k = 1.50E-12	1.50E-12
52	HI + OH = I	k = 1.60E-11 exp(440/T)	7.00E-11
53	I + O3 = IO	k = 2.10E-11 exp(-830/T)	1.30E-12
54	I + HO2 = HI	k = 1.50E-11 exp(-1090/T)	3.87E-13
55	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
56	IO = I + O	Photolysis	1.18E-1
57	IO + IO = 0.4 I + 0.4 OIO + 0.6 I2O2	k = 5.40E-11 exp(180/T)	9.88E-11
58	IO + HO2 = HOI	k = 1.40E-11 exp(540/T)	8.57E-11
59	IO + NO = I + NO2	k = 7.15E-12 exp(300/T)	1.96E-11
60	IO + NO2 = INO3	Falloff: F=0.4; n=1 k(0) = 7.70E-31 (T/300)^-5 k(inf) = 1.60E-11	3.55E-12
61	HOI + OH = IO	k = 5.00E-12	5.00E-12
62	OIO = I	Photolysis	1.28E-1
63	OIO + OH = HIO3	Falloff: F=0.3; n=1 k(0) = 1.50E-27 (T/300)^-3.93 k(inf) = 5.50E-10 exp(46/T)	4.72E-10
64	OIO + IO = IXOY	k = 1.00E-10	1.00E-10
65	OIO + OIO = IXOY	k = 1.50E-10	1.50E-10
66	OIO + NO = IO + NO2	k = 1.10E-12 exp(542/T)	6.78E-12
67	I2O2 = I + OIO	k = 1.00E+1	1.00E+1
68	I2O2 + O3 = IXOY	k = 1.00E-12	1.00E-12
69	INO2 = I + NO2	Photolysis	3.21E-3
70	INO2 + INO2 = I2 + 2 NO2	k = 4.70E-13 exp(-1670/T)	1.73E-15
71	INO3 = I + NO3	Photolysis	1.25E-2
72	INO3 + H2O = HOI + HNO3	k = 2.50E-22	2.50E-22
73	CLO + BRO = CL + BR	k = 4.70E-12 exp(320/T)	1.38E-11
74	CLO + IO = CL + I	k = 4.70E-12 exp(280/T)	1.20E-11
75	BRO + IO = BR + I	k = 1.50E-11 exp(510/T)	8.31E-11
76	CH3I = I + MEO2	Photolysis	3.19E-6
77	MI2 = 2 I + FORM	Photolysis	4.69E-3
78	MIB = I + BR + FORM	Photolysis	2.53E-4
79	MIC = I + CL + FORM	Photolysis	7.48E-5
80	MB3 = 3 BR + HO2 + CO	Photolysis	4.64E-7
81	MB3 + OH = 3 BR + CO	k = 1.35E-12 exp(-600/T)	1.80E-13
82	MB2 + OH = 2 BR + HO2 + CO	k = 2.00E-12 exp(-840/T)	1.19E-13

Number	Reactants and Products	Rate Constant Expression	k_{298}
83	MBC + OH = BR + MEO2	k = 2.35E-12 exp(-1300/T)	3.00E-14
84	MBC2 + OH = BR + MEO2	k = 9.00E-13 exp(-600/T)	1.20E-13
85	MB2C + OH = BR + MEO2	k = 9.00E-13 exp(-600/T)	1.20E-13
86	IALK = I + ALDX + XO2H + RO2	Photolysis	5.88E-7
87	SSCL + HNO3 = HCL + SSN3	k = 1.00E-12	1.00E-12
88	SSBR + HOBR = BR2	k = 1.00E-12	1.00E-12

Table S4. CAMx halogen species names and descriptions for CB6r2h.

Species	Description	Constituents							Mol. Wt.
		C	H	O	N	Cl	Br	I	
CL2	Molecular chlorine					2			70.9
CL	Chlorine atom					1			35.5
CLO	Chlorine monoxide			1		1			51.4
HCL	Hydrogen chloride		1			1			36.5
HOCL	Hypochlorous acid		1	1		1			52.4
CLN2	Nitryl chloride: $ClNO_2$			2		1			81.4
CLN3	Chlorine nitrate: $ClONO_2$			3		1			97.4
FMCL	Formyl chloride: HC(O)Cl	1	1	1		1			64.5
BR2	Molecular bromine						2		159.8
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 broride: $BrNO_2$			2			1		125.9
BRN3	Bromine nitrate: $BrONO_2$			3			1		141.9
FMBR	Formyl bromide: HC(O)Br	1	1	1			1		108.9
I2	Molecular iodine							2	253.8
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 (> I_2O_2)			3				2	301.8
HI	Hydrogen iodide		1					1	127.9
HOI	Hypoiodous acid		1	1				1	143.9
HIO3	Iodic acid: $HONO_2$		1	3				1	175.9
INO2	Nitryl iodide: INO_2			2				1	172.9
INO3	Iodine nitrate: $IONO_2$			3				1	188.9
CH3I	Iodomethane	1	3					1	141.9
MI2	Diiodomethane: CH_2I_2	1	2					2	267.8
MIB	Bromoiodomethane: CH_2BrI	1	2				1	1	220.8
MIC	Chloroiodomethane: CH_2ClI	1	2			1		1	176.4
MBC	Chlorobromomethane: CH_2ClBr	1	2			1	1		129.4
MB2	Dibromomethane: CH_2Br_2	1	2				2		173.8
MBC2	Dichlorobromomethane: $CHCl_2Br$	1	3			2	1		165.8
MB2C	Chlorodibromomethane: $CHClBr_2$	1	3			1	2		210.3
MB3	Bromoform $CHBr_3$	1	1				3		252.7
IALK	Alkyl iodides	3	7					1	170.0
SSCL	Pseudo gas-phase species for sea salt chloride	0				1			58.4
SSBR	Pseudo gas-phase species for sea salt bromide	0					1		102.9
SSN3	Pseudo gas-phase species for sea salt nitrate	0		3	1				85.0

CB6r4 Gas-Phase Chemistry

Table S5. Reactions and rate constant expressions for the CB6r4 mechanism. See Table S2 for species names. k_{298} is the rate constant at 298 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

Number	Reactants and Products	Rate Constant Expression	k_{298}
1	NO2 = NO + O	Photolysis	6.30E-3
2	O + O2 + M = O3 + M	k = 5.68E-34 (T/300)^-2.6	5.78E-34
3	O3 + NO = NO2	k = 1.40E-12 exp(-1310/T)	1.73E-14
4	O + NO + M = NO2 + M	k = 1.00E-31 (T/300)^-1.6	1.01E-31
5	O + NO2 = NO	k = 5.50E-12 exp(188/T)	1.03E-11
6	O + NO2 = NO3	Falloff: F=0.6; n=1 k(0) = 1.30E-31 (T/300)^-1.5 k(inf) = 2.30E-11 (T/300)^0.24	2.11E-12
7	O + O3 =	k = 8.00E-12 exp(-2060/T)	7.96E-15
8	O3 = O	Photolysis	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 = 2.70E-11 exp(224/T)	5.73E-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=0.5; n=1.13 k(0) = 6.90E-31 (T/300)^-0.8 k(inf) = 2.60E-11	5.25E-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 = 2.90E-12 exp(-160/T)	1.70E-12
23	H2O2 + O = OH + HO2	k = 1.40E-12 exp(-2000/T)	1.70E-15
24	NO + NO + O2 = 2 NO2	k = 3.30E-39 exp(530/T)	1.95E-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	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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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=0.6; n=1 k(0) = 1.80E-31 (T/300)^-3.2 k(inf) = 4.70E-12	1.38E-12
49	PNA = HO2 + NO2	Falloff: F=0.6; n=1 k(0) = 4.10E-5 exp(-10650/T) k(inf) = 4.80E+15 exp(-11170/T)	8.31E-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) = 4.50E-31 (T/300)^-3.9 k(inf) = 1.30E-12 (T/300)^-0.7	8.12E-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) = 2.70E-28 (T/300)^-7.1 k(inf) = 1.20E-11 (T/300)^-0.9	9.40E-12
55	PAN = NO2 + C2O3	Falloff: F=0.3; n=1.41 k(0) = 4.90E-3 exp(-12100/T) k(inf) = 5.40E+16 exp(-13830/T)	2.98E-4
56	PAN = 0.6 NO2 + 0.6 C2O3 + 0.4 NO3 + 0.4 MEO2 + 0.4 RO2	Photolysis	3.47E-7
57	C2O3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 MEO2 + 0.44 RO2 + 0.44 OH	k = 5.20E-13 exp(980/T)	1.39E-11
58	C2O3 + RO2 = C2O3	k = 8.90E-13 exp(800/T)	1.30E-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 = 2.90E-12 exp(500/T)	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 = 1.00E+0	9.40E-12
63	PANX = NO2 + CXO3	k = k(ref)/K k(ref) = k(55) K = 1.00E+0	2.98E-4

Number	Reactants and Products	Rate Constant Expression	k_{298}
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 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALD2 + 0.44 XO2H + 0.44 RO2 + 0.44 OH	k = 5.20E-13 exp(980/T)	1.39E-11
66	CXO3 + RO2 = 0.8 ALD2 + 0.8 XO2H + 0.8 RO2	k = 8.90E-13 exp(800/T)	1.30E-11
67	CXO3 + CXO3 = 2 ALD2 + 2 XO2H + 2 RO2	k = 3.20E-12 exp(500/T)	1.71E-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	1.30E-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
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	1.30E-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	1.30E-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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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 = 5.30E-12 exp(190/T)	1.00E-11
96	FORM + OH = HO2 + CO	k = 5.40E-12 exp(135/T)	8.49E-12
97	FORM = 2 HO2 + CO	Photolysis	1.78E-5
98	FORM = CO + H2	Photolysis	2.38E-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	1.76E-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	6.96E-6
110	GLYD + OH = 0.2 GLY + 0.2 HO2 + 0.8 C2O3	k = 8.00E-12	8.00E-12
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	1.56E-6
112	GLYD + NO3 = HNO3 + C2O3	k = 1.40E-12 exp(-1860/T)	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	5.50E-5
115	GLY + NO3 = HNO3 + 1.5 CO + 0.5 XO2 + 0.5 RO2 + HO2	k = 1.40E-12 exp(-1860/T)	2.73E-15
116	MGLY = C2O3 + HO2 + CO	Photolysis	1.46E-4
117	MGLY + NO3 = HNO3 + C2O3 + XO2 + RO2	k = 1.40E-12 exp(-1860/T)	2.73E-15
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

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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 + 0.51 CO + 0.16 HO2 + 0.16 OH + 0.37 FACD	k = 9.10E-15 exp(-2580/T)	1.58E-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
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	1.30E-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

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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
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	1.30E-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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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	1.30E-11
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	1.30E-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	1.30E-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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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 = 1.00E-11	1.00E-11
200	OPO3 + NO2 = OPAN	k = k(ref)/K k(ref) = k(54) K = 1.00E+0	9.40E-12
201	OPAN = OPO3 + NO2	k = k(ref)/K k(ref) = k(55) K = 1.00E+0	2.98E-4
202	OPO3 + HO2 = 0.41 PACD + 0.15 AACD + 0.15 O3 + 0.44 ALDX + 0.44 XO2H + 0.44 RO2 + 0.44 OH	k = k(ref)/K k(ref) = k(57) K = 1.00E+0	1.39E-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	1.30E-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	1.44E-1
210	HOI = I + OH	Photolysis	6.36E-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 k(0) = 7.70E-31 (T/300)^-5 k(inf) = 1.60E-11	3.55E-12
217	OIO = I	Photolysis	1.41E-1
218	OIO + OH = HIO3	Falloff: F=0.3; n=1 k(0) = 1.50E-27 (T/300)^-3.93 k(inf) = 5.50E-10 exp(46/T)	4.72E-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	1.25E-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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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	0	0
231	DMS + OH = SO2 + FORM + MEO2	k = 1.12E-11 exp(-250/T)	4.84E-12
232	DMS + OH + O2 = SULF + MEO2	k = 1.28E-37 exp(4480/T)	4.33E-31
233	DMS + NO3 = SO2 + FORM + MEO2 + HNO3	k = 1.9E-13 exp(520/T)	1.09E-12

CB6r5 Gas-Phase Chemistry

Table S6. Reactions and rate constant expressions for the CB6r5 mechanism. See Table S2 for species names. k_{298} is the rate constant at 298 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

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	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	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
31	NO3 + O = NO2	k = 1.70E-11	1.70E-11

Number	Reactants and Products	Rate Constant Expression	k_{298}
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=0.41; n=1.24 k(0) = 3.20E-30 (T/300)^-4.5 k(inf) = 3.00E-11	9.89E-12
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) = 3.28E-28 (T/300)^-6.87 k(inf) = 1.12E-11 (T/300)^-1.11	8.92E-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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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 = 1.21E+0	7.37E-12
63	PANX = NO2 + CXO3	k = k(ref)/K k(ref) = k(55) K = 1.21E+0	3.56E-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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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 = 5.30E-12 exp(190/T)	1.00E-11
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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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	5.01E-4
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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
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
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

Number	Reactants and Products	Rate Constant Expression	k_{298}
200	OPO3 + NO2 = OPAN	k = k(ref)/K k(ref) = k(62) K = 1.00E+0	7.37E-12
201	OPAN = OPO3 + NO2	k = k(ref)/K k(ref) = k(63) K = 1.00E+0	3.56E-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(65) 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	1.44E-1
210	HOI = I + OH	Photolysis	6.36E-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	1.41E-1
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	1.25E-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

Number	Reactants and Products	Rate Constant Expression	k_{298}
230	SO2 = SULF	k = 0.00E+0	0.00E+0
231	DMS + OH = SO2 + FORM + MEO2	k = 1.12E-11 exp(-250/T)	4.84E-12
232	DMS + OH + O2 = SULF + MEO2	k = 1.28E-37 exp(4480/T)	4.33E-31
233	DMS + NO3 = SO2 + FORM + MEO2 + HNO3	k = 1.90E-13 exp(520/T)	1.09E-12
234	NO2 + OH + H2O = HNO3 + H2O	k = 1.10E-30	1.10E-30

SAPRC07TC Gas-Phase Chemistry

Table S7. Reactions and rate constants for the SAPRC07TC mechanism. See Table S8 for species names. k_{300} is the rate constant at 300 K and 1 atmosphere using units in cm^3 $molecule^{-1}$ s^{-1}. For photolysis reactions k_{298} shows the photolysis rate at a solar zenith angle of 60° and height of 600 m MSL/AGL.

Number	Reactants and Products	Rate Constant Expression	k_{300}
1	NO2 = NO + O3P	Photolysis	6.37E-3
2	O3P + O2 + M = O3	k = 5.68E-34 (T/300)^-2.6	5.68E-34
3	O3P + O3 =	k = 8.00E-12 exp(-2060/T)	8.34E-15
4	O3P + NO = NO2	Falloff: F=0.6; n=1 k(0) = 9.00E-32 (T/300)^-1.5 k(inf) = 3.00E-11	1.64E-12
5	O3P + NO2 = NO	k = 5.50E-12 exp(188/T)	1.03E-11
6	O3P + NO2 = NO3	Falloff: F=0.6; n=1 k(0) = 2.50E-31 (T/300)^-1.8 k(inf) = 2.20E-11 (T/300)^-0.7	3.24E-12
7	O3 + NO = NO2	k = 3.00E-12 exp(-1500/T)	2.02E-14
8	O3 + NO2 = NO3	k = 1.40E-13 exp(-2470/T)	3.72E-17
9	NO + NO3 = 2. NO2	k = 1.80E-11 exp(110/T)	2.60E-11
10	NO + NO + O2 = 2. NO2	k = 3.30E-39 exp(530/T)	1.93E-38
11	NO2 + NO3 = 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
12	N2O5 = NO2 + NO3	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)	5.69E-2
13	N2O5 + H2O = 2. HNO3	k = 1.00E-22	1.00E-22
14	N2O5 + H2O + H2O = 2. HNO3	k = 0.00E+0	0.00E+0
15	NO2 + NO3 = NO + NO2	k = 4.50E-14 exp(-1260/T)	6.75E-16
16	NO3 = NO	Photolysis	1.98E-2
17	NO3 = NO2 + O3P	Photolysis	1.56E-1
18	O3 = O1D	Photolysis	9.47E-6
19	O3 = O3P	Photolysis	3.40E-4
20	O1D + H2O = 2. OH	k = 1.63E-10 exp(60/T)	1.99E-10
21	O1D + M = O3P	k = 2.38E-11 exp(96/T)	3.28E-11
22	OH + NO = HONO	Falloff: F=0.6; n=1 k(0) = 7.00E-31 (T/300)^-2.6 k(inf) = 3.60E-11 (T/300)^-0.1	7.31E-12
23	HONO = OH + NO	Photolysis	9.88E-4
24	OH + HONO = NO2	k = 2.50E-12 exp(260/T)	5.95E-12
25	OH + NO2 = HNO3	Falloff: F=0.6; n=1 k(0) = 1.80E-30 (T/300)^-3 k(inf) = 2.80E-11	1.05E-11
26	OH + NO3 = HO2 + NO2	k = 2.00E-11	2.00E-11
27	OH + HNO3 = 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)	1.51E-13
28	HNO3 = OH + NO2	Photolysis	2.55E-7
29	OH + CO = HO2 + CO2	k = k1 + k2 [M] k1 = 1.44E-13 k2 = 3.43E-33	2.28E-13
30	OH + O3 = HO2	k = 1.70E-12 exp(-940/T)	7.41E-14
31	HO2 + NO = OH + NO2	k = 3.60E-12 exp(270/T)	8.85E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
32	HO2 + NO2 = PNA	Falloff: F=0.6; n=1 k(0) = 2.00E-31 (T/300)^-3.4 k(inf) = 2.90E-12 (T/300)^-1.1	1.12E-12
33	PNA = HO2 + NO2	Falloff: F=0.6; n=1 k(0) = 3.72E-5 (T/300)^-2.4 exp(-10650/T) k(inf) = 5.42E+15 (T/300)^-2.3 exp(-11170/T)	1.07E-1
34	PNA = 0.61 HO2 + 0.61 NO2 + 0.39 OH + 0.39 NO3	Photolysis	3.17E-6
35	PNA + OH = NO2	k = 1.30E-12 exp(380/T)	4.61E-12
36	HO2 + O3 = OH	k = 2.03E-16 (T/300)^4.57 exp(693/T)	2.05E-15
37	HO2 + HO2 = H2O2	k = k1 + k2 [M] k1 = 2.20E-13 exp(600/T) k2 = 1.90E-33 exp(980/T)	2.84E-12
38	HO2 + HO2 + H2O = H2O2	k = k1 + k2 [M] k1 = 3.08E-34 exp(2800/T) k2 = 2.66E-54 exp(3180/T)	6.09E-30
39	NO3 + HO2 = 0.8 OH + 0.8 NO2 + 0.2 HNO3	k = 4.00E-12	4.00E-12
40	NO3 + NO3 = 2. NO2	k = 8.50E-13 exp(-2450/T)	2.41E-16
41	H2O2 = 2. OH	Photolysis	3.78E-6
42	H2O2 + OH = HO2	k = 1.80E-12	1.80E-12
43	OH + HO2 =	k = 4.80E-11 exp(250/T)	1.10E-10
44	OH + SO2 = HO2 + SULF	Falloff: F=0.6; n=1 k(0) = 3.30E-31 (T/300)^-4.3 k(inf) = 1.60E-12	9.49E-13
45	OH + H2 = HO2	k = 7.70E-12 exp(-2100/T)	7.02E-15
46	MEO2 + NO = NO2 + HCHO + HO2	k = 2.30E-12 exp(360/T)	7.64E-12
47	MEO2 + HO2 = COOH	k = 3.46E-13 (T/300)^0.36 exp(780/T)	4.66E-12
48	MEO2 + HO2 = HCHO	k = 3.34E-14 (T/300)^-3.53 exp(780/T)	4.50E-13
49	MEO2 + NO3 = HCHO + HO2 + NO2	k = 1.30E-12	1.30E-12
50	MEO2 + MEO2 = MEOH + HCHO	k = 6.39E-14 (T/300)^-1.8 exp(365/T)	2.16E-13
51	MEO2 + MEO2 = 2. HCHO + 2. HO2	k = 7.40E-13 exp(-520/T)	1.31E-13
52	RO2C + NO = NO2	k = 2.60E-12 exp(380/T)	9.23E-12
53	RO2C + HO2 =	k = 3.80E-13 exp(900/T)	7.63E-12
54	RO2C + NO3 = NO2	k = 2.30E-12	2.30E-12
55	RO2C + MEO2 = 0.5 HO2 + 0.75 HCHO + 0.25 MEOH	k = 2.00E-13	2.00E-13
56	RO2C + RO2C =	k = 3.50E-14	3.50E-14
57	RO2X + NO = XN	k = k(52)	9.23E-12
58	RO2X + HO2 =	k = k(53)	7.63E-12
59	RO2X + NO3 = NO2	k = k(54)	2.30E-12
60	RO2X + MEO2 = 0.5 HO2 + 0.75 HCHO + 0.25 MEOH	k = k(55)	2.00E-13
61	RO2X + RO2C =	k = k(56)	3.50E-14
62	RO2X + RO2X =	k = k(56)	3.50E-14
63	MCO3 + NO2 = PAN	Falloff: F=0.3; n=1.41 k(0) = 2.70E-28 (T/300)^-7.1 k(inf) = 1.21E-11 (T/300)^-0.9	9.38E-12
64	PAN = MCO3 + NO2	Falloff: F=0.3; n=1.41 k(0) = 4.90E-3 exp(-12100/T) k(inf) = 4.00E+16 exp(-13600/T)	6.27E-4
65	PAN = 0.6 MCO3 + 0.6 NO2 + 0.4 MEO2 + 0.4 CO2 + 0.4 NO3	Photolysis	3.50E-7
66	MCO3 + NO = MEO2 + CO2 + NO2	k = 7.50E-12 exp(290/T)	1.97E-11
67	MCO3 + HO2 = 0.7 CO3H + 0.3 AACD + 0.3 O3	k = 5.20E-13 exp(980/T)	1.36E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
68	MCO3 + NO3 = MEO2 + CO2 + NO2	k = k(54)	2.30E-12
69	MCO3 + MEO2 = 0.1 AACD + HCHO + 0.9 HO2 + 0.9 MEO2 + 0.9 CO2	k = 2.00E-12 exp(500/T)	1.06E-11
70	MCO3 + RO2C = MEO2 + CO2	k = 4.40E-13 exp(1070/T)	1.56E-11
71	MCO3 + RO2X = MEO2 + CO2	k = k(70)	1.56E-11
72	MCO3 + MCO3 = 2. MEO2 + 2. CO2	k = 2.90E-12 exp(500/T)	1.54E-11
73	RCO3 + NO2 = PAN2	k = 1.21E-11 (T/300)^-1.07	1.21E-11
74	PAN2 = RCO3 + NO2	k = 8.30E+16 exp(-13940/T)	5.48E-4
75	PAN2 = 0.6 RCO3 + 0.6 NO2 + 0.4 RO2C + 0.4 XHO2 + 0.4 YRPX + 0.4 XCCH + 0.4 CO2 + 0.4 NO3	Photolysis	3.50E-7
76	RCO3 + NO = NO2 + RO2C + XHO2 + YRPX + XCCH + CO2	k = 6.70E-12 exp(340/T)	2.08E-11
77	RCO3 + HO2 = 0.75 RO3H + 0.25 PACD + 0.25 O3	k = k(67)	1.36E-11
78	RCO3 + NO3 = NO2 + RO2C + XHO2 + YRPX + XCCH + CO2	k = k(54)	2.30E-12
79	RCO3 + MEO2 = HCHO + HO2 + RO2C + XHO2 + XCCH + YRPX + CO2	k = k(69)	1.06E-11
80	RCO3 + RO2C = RO2C + XHO2 + XCCH + YRPX + CO2	k = k(70)	1.56E-11
81	RCO3 + RO2X = RO2C + XHO2 + XCCH + YRPX + CO2	k = k(70)	1.56E-11
82	RCO3 + MCO3 = 2. CO2 + MEO2 + RO2C + XHO2 + YRPX + XCCH	k = k(72)	1.54E-11
83	RCO3 + RCO3 = 2. RO2C + 2. XHO2 + 2. XCCH + 2. YRPX + 2. CO2	k = k(72)	1.54E-11
84	BZC3 + NO2 = PBZN	k = 1.37E-11	1.37E-11
85	PBZN = BZC3 + NO2	k = 7.90E+16 exp(-14000/T)	4.27E-4
86	PBZN = 0.6 BZC3 + 0.6 NO2 + 0.4 CO2 + 0.4 BZO + 0.4 RO2C + 0.4 NO3	Photolysis	3.50E-7
87	BZC3 + NO = NO2 + CO2 + BZO + RO2C	k = k(76)	2.08E-11
88	BZC3 + HO2 = 0.75 RO3H + 0.25 PACD + 0.25 O3 + 4. XC	k = k(67)	1.36E-11
89	BZC3 + NO3 = NO2 + CO2 + BZO + RO2C	k = k(54)	2.30E-12
90	BZC3 + MEO2 = HCHO + HO2 + RO2C + BZO + CO2	k = k(69)	1.06E-11
91	BZC3 + RO2C = RO2C + BZO + CO2	k = k(70)	1.56E-11
92	BZC3 + RO2X = RO2C + BZO + CO2	k = k(70)	1.56E-11
93	BZC3 + MCO3 = 2. CO2 + MEO2 + BZO + RO2C	k = k(72)	1.54E-11
94	BZC3 + RCO3 = 2. CO2 + 2. RO2C + XHO2 + YRPX + XCCH + BZO	k = k(72)	1.54E-11
95	BZC3 + BZC3 = 2. BZO + 2. RO2C + 2. CO2	k = k(72)	1.54E-11
96	MAC3 + NO2 = MPAN	k = k(73)	1.21E-11
97	MPAN = MAC3 + NO2	k = 1.60E+16 exp(-13486/T)	4.80E-4
98	MPAN = 0.6 MAC3 + 0.6 NO2 + 0.4 CO2 + 0.4 HCHO + 0.4 MCO3 + 0.4 NO3	Photolysis	3.50E-7
99	MAC3 + NO = NO2 + CO2 + HCHO + MCO3	k = k(76)	2.08E-11
100	MAC3 + HO2 = 0.75 RO3H + 0.25 PACD + 0.25 O3 + XC	k = k(67)	1.36E-11
101	MAC3 + NO3 = NO2 + CO2 + HCHO + MCO3	k = k(54)	2.30E-12
102	MAC3 + MEO2 = 2. HCHO + HO2 + CO2 + MCO3	k = k(69)	1.06E-11
103	MAC3 + RO2C = CO2 + HCHO + MCO3	k = k(70)	1.56E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
104	MAC3 + RO2X = CO2 + HCHO + MCO3	k = k(70)	1.56E-11
105	MAC3 + MCO3 = 2. CO2 + MEO2 + HCHO + MCO3	k = k(72)	1.54E-11
106	MAC3 + RCO3 = HCHO + MCO3 + RO2C + XHO2 + YRPX + XCCH + 2. CO2	k = k(72)	1.54E-11
107	MAC3 + BZC3 = HCHO + MCO3 + BZO + RO2C + 2. CO2	k = k(72)	1.54E-11
108	MAC3 + MAC3 = 2. HCHO + 2. MCO3 + 2. CO2	k = k(72)	1.54E-11
109	TBUO + NO2 = RNO3 - 2. XC	k = 2.40E-11	2.40E-11
110	TBUO = ACET + MEO2	k = 7.50E+14 exp(-8152/T)	1.19E+3
111	BZO + NO2 = NPHE	k = 2.30E-11 exp(150/T)	3.79E-11
112	BZO + HO2 = CRES - 1. XC	k = k(53)	7.63E-12
113	BZO = CRES + RO2C + XHO2 - 1. XC	k = 1.00E-3	1.00E-3
114	XHO2 + NO = NO + HO2	k = k(52)	9.23E-12
115	XHO2 + HO2 = HO2	k = k(53)	7.63E-12
116	XHO2 + NO3 = NO3 + HO2	k = k(54)	2.30E-12
117	XHO2 + MEO2 = MEO2 + 0.5 HO2	k = k(55)	2.00E-13
118	XHO2 + RO2C = RO2C + 0.5 HO2	k = k(56)	3.50E-14
119	XHO2 + RO2X = RO2X + 0.5 HO2	k = k(56)	3.50E-14
120	XHO2 + MCO3 = MCO3 + HO2	k = k(70)	1.56E-11
121	XHO2 + RCO3 = RCO3 + HO2	k = k(70)	1.56E-11
122	XHO2 + BZC3 = BZC3 + HO2	k = k(70)	1.56E-11
123	XHO2 + MAC3 = MAC3 + HO2	k = k(70)	1.56E-11
124	XOH + NO = NO + OH	k = k(52)	9.23E-12
125	XOH + HO2 = HO2	k = k(53)	7.63E-12
126	XOH + NO3 = NO3 + OH	k = k(54)	2.30E-12
127	XOH + MEO2 = MEO2 + 0.5 OH	k = k(55)	2.00E-13
128	XOH + RO2C = RO2C + 0.5 OH	k = k(56)	3.50E-14
129	XOH + RO2X = RO2X + 0.5 OH	k = k(56)	3.50E-14
130	XOH + MCO3 = MCO3 + OH	k = k(70)	1.56E-11
131	XOH + RCO3 = RCO3 + OH	k = k(70)	1.56E-11
132	XOH + BZC3 = BZC3 + OH	k = k(70)	1.56E-11
133	XOH + MAC3 = MAC3 + OH	k = k(70)	1.56E-11
134	XNO2 + NO = NO + NO2	k = k(52)	9.23E-12
135	XNO2 + HO2 = HO2 + XN	k = k(53)	7.63E-12
136	XNO2 + NO3 = NO3 + NO2	k = k(54)	2.30E-12
137	XNO2 + MEO2 = MEO2 + 0.5 NO2 + 0.5 XN	k = k(55)	2.00E-13
138	XNO2 + RO2C = RO2C + 0.5 NO2 + 0.5 XN	k = k(56)	3.50E-14
139	XNO2 + RO2X = RO2X + 0.5 NO2 + 0.5 XN	k = k(56)	3.50E-14
140	XNO2 + MCO3 = MCO3 + NO2	k = k(70)	1.56E-11
141	XNO2 + RCO3 = RCO3 + NO2	k = k(70)	1.56E-11
142	XNO2 + BZC3 = BZC3 + NO2	k = k(70)	1.56E-11
143	XNO2 + MAC3 = MAC3 + NO2	k = k(70)	1.56E-11
144	XMEO + NO = NO + MEO2	k = k(52)	9.23E-12
145	XMEO + HO2 = HO2 + XC	k = k(53)	7.63E-12
146	XMEO + NO3 = NO3 + MEO2	k = k(54)	2.30E-12
147	XMEO + MEO2 = 1.5 MEO2 + 0.5 XC	k = k(55)	2.00E-13
148	XMEO + RO2C = RO2C + 0.5 MEO2 + 0.5 XC	k = k(56)	3.50E-14
149	XMEO + RO2X = RO2X + 0.5 MEO2 + 0.5 XC	k = k(56)	3.50E-14
150	XMEO + MCO3 = MCO3 + MEO2	k = k(70)	1.56E-11
151	XMEO + RCO3 = RCO3 + MEO2	k = k(70)	1.56E-11
152	XMEO + BZC3 = BZC3 + MEO2	k = k(70)	1.56E-11
153	XMEO + MAC3 = MAC3 + MEO2	k = k(70)	1.56E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
154	XMC3 + NO = NO + MCO3	k = k(52)	9.23E-12
155	XMC3 + HO2 = HO2 + 2. XC	k = k(53)	7.63E-12
156	XMC3 + NO3 = NO3 + MCO3	k = k(54)	2.30E-12
157	XMC3 + MEO2 = MEO2 + 0.5 MCO3 + XC	k = k(55)	2.00E-13
158	XMC3 + RO2C = RO2C + 0.5 MCO3 + XC	k = k(56)	3.50E-14
159	XMC3 + RO2X = RO2X + 0.5 MCO3 + XC	k = k(56)	3.50E-14
160	XMC3 + MCO3 = 2. MCO3	k = k(70)	1.56E-11
161	XMC3 + RCO3 = RCO3 + MCO3	k = k(70)	1.56E-11
162	XMC3 + BZC3 = BZC3 + MCO3	k = k(70)	1.56E-11
163	XMC3 + MAC3 = MAC3 + MCO3	k = k(70)	1.56E-11
164	XRC3 + NO = NO + RCO3	k = k(52)	9.23E-12
165	XRC3 + HO2 = HO2 + 3. XC	k = k(53)	7.63E-12
166	XRC3 + NO3 = NO3 + RCO3	k = k(54)	2.30E-12
167	XRC3 + MEO2 = MEO2 + 0.5 RCO3 + 1.5 XC	k = k(55)	2.00E-13
168	XRC3 + RO2C = RO2C + 0.5 RCO3 + 1.5 XC	k = k(56)	3.50E-14
169	XRC3 + RO2X = RO2X + 0.5 RCO3 + 1.5 XC	k = k(56)	3.50E-14
170	XRC3 + MCO3 = MCO3 + RCO3	k = k(70)	1.56E-11
171	XRC3 + RCO3 = 2. RCO3	k = k(70)	1.56E-11
172	XRC3 + BZC3 = BZC3 + RCO3	k = k(70)	1.56E-11
173	XRC3 + MAC3 = MAC3 + RCO3	k = k(70)	1.56E-11
174	XMA3 + NO = NO + MAC3	k = k(52)	9.23E-12
175	XMA3 + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
176	XMA3 + NO3 = NO3 + MAC3	k = k(54)	2.30E-12
177	XMA3 + MEO2 = MEO2 + 0.5 MAC3 + 2. XC	k = k(55)	2.00E-13
178	XMA3 + RO2C = RO2C + 0.5 MAC3 + 2. XC	k = k(56)	3.50E-14
179	XMA3 + RO2X = RO2X + 0.5 MAC3 + 2. XC	k = k(56)	3.50E-14
180	XMA3 + MCO3 = MCO3 + MAC3	k = k(70)	1.56E-11
181	XMA3 + RCO3 = RCO3 + MAC3	k = k(70)	1.56E-11
182	XMA3 + BZC3 = BZC3 + MAC3	k = k(70)	1.56E-11
183	XMA3 + MAC3 = 2. MAC3	k = k(70)	1.56E-11
184	XTBU + NO = NO + TBUO	k = k(52)	9.23E-12
185	XTBU + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
186	XTBU + NO3 = NO3 + TBUO	k = k(54)	2.30E-12
187	XTBU + MEO2 = MEO2 + 0.5 TBUO + 2. XC	k = k(55)	2.00E-13
188	XTBU + RO2C = RO2C + 0.5 TBUO + 2. XC	k = k(56)	3.50E-14
189	XTBU + RO2X = RO2X + 0.5 TBUO + 2. XC	k = k(56)	3.50E-14
190	XTBU + MCO3 = MCO3 + TBUO	k = k(70)	1.56E-11
191	XTBU + RCO3 = RCO3 + TBUO	k = k(70)	1.56E-11
192	XTBU + BZC3 = BZC3 + TBUO	k = k(70)	1.56E-11
193	XTBU + MAC3 = MAC3 + TBUO	k = k(70)	1.56E-11
194	XCO + NO = NO + CO	k = k(52)	9.23E-12
195	XCO + HO2 = HO2 + XC	k = k(53)	7.63E-12
196	XCO + NO3 = NO3 + CO	k = k(54)	2.30E-12
197	XCO + MEO2 = MEO2 + 0.5 CO + 0.5 XC	k = k(55)	2.00E-13
198	XCO + RO2C = RO2C + 0.5 CO + 0.5 XC	k = k(56)	3.50E-14
199	XCO + RO2X = RO2X + 0.5 CO + 0.5 XC	k = k(56)	3.50E-14
200	XCO + MCO3 = MCO3 + CO	k = k(70)	1.56E-11
201	XCO + RCO3 = RCO3 + CO	k = k(70)	1.56E-11
202	XCO + BZC3 = BZC3 + CO	k = k(70)	1.56E-11
203	XCO + MAC3 = MAC3 + CO	k = k(70)	1.56E-11
204	HCHO = 2. HO2 + CO	Photolysis	1.78E-5
205	HCHO = CO	Photolysis	2.38E-5
206	HCHO + OH = HO2 + CO	k = 5.40E-12 exp(135/T)	8.47E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
207	HCHO + NO3 = HNO3 + HO2 + CO	k = 2.00E-12 exp(-2431/T)	6.05E-16
208	CCHO + OH = MCO3	k = 4.40E-12 exp(365/T)	1.49E-11
209	CCHO = CO + HO2 + MEO2	Photolysis	1.77E-6
210	CCHO + NO3 = HNO3 + MCO3	k = 1.40E-12 exp(-1860/T)	2.84E-15
211	RCHO + OH = 0.965 RCO3 + 0.035 RO2C + 0.035 XHO2 + 0.035 XCO + 0.035 XCCH + 0.035 YRPX	k = 5.10E-12 exp(405/T)	1.97E-11
212	RCHO = RO2C + XHO2 + YRPX + XCCH + CO + HO2	Photolysis	6.95E-6
213	RCHO + NO3 = HNO3 + RCO3	k = 1.40E-12 exp(-1601/T)	6.74E-15
214	ACET + OH = RO2C + XMC3 + XHCH + YRPX	k = 4.56E-14 (T/300)^3.65 exp(429/T)	1.91E-13
215	ACET = 0.62 MCO3 + 1.38 MEO2 + 0.38 CO	Photolysis	1.04E-7
216	MEK + OH = 0.967 RO2C + 0.039 RO2X + 0.039 ZRN3 + 0.376 XHO2 + 0.51 XMC3 + 0.074 XRC3 + 0.088 XHCH + 0.504 XCCH + 0.376 XRCH + YRPX + 0.3 XC	k = 1.30E-12 (T/300)^2 exp(-25/T)	1.20E-12
217	MEK = MCO3 + RO2C + XHO2 + XCCH + YRPX	Photolysis	8.13E-7
218	MEOH + OH = HCHO + HO2	k = 2.85E-12 exp(-345/T)	9.02E-13
219	FACD + OH = HO2 + CO2	k = 4.50E-13	4.50E-13
220	AACD + OH = 0.509 MEO2 + 0.491 RO2C + 0.509 CO2 + 0.491 XHO2 + 0.491 XMGL + 0.491 YRPX - 0.491 XC	k = 4.20E-14 exp(855/T)	7.26E-13
221	PACD + OH = RO2C + XHO2 + 0.143 CO2 + 0.142 XCCH + 0.4 XRCH + 0.457 XBAC + YRPX - 0.455 XC	k = 1.20E-12	1.20E-12
222	COOH + OH = 0.3 HCHO + 0.3 OH + 0.7 MEO2	k = 3.80E-12 exp(200/T)	7.40E-12
223	COOH = HCHO + HO2 + OH	Photolysis	2.72E-6
224	ROOH + OH = 0.744 OH + 0.251 RO2C + 0.004 RO2X + 0.004 ZRN3 + 0.744 RCHO + 0.239 XHO2 + 0.012 XOH + 0.012 XHCH + 0.012 XCCH + 0.205 XRCH + 0.034 XPD2 + 0.256 YRPX - 0.115 XC	k = 2.50E-11	2.50E-11
225	ROOH = RCHO + HO2 + OH	Photolysis	2.72E-6
226	R6PX + OH = 0.84 OH + 0.222 RO2C + 0.029 RO2X + 0.029 ZRN3 + 0.84 PRD2 + 0.09 XHO2 + 0.041 XOH + 0.02 XCCH + 0.075 XRCH + 0.084 XPD2 + 0.16 YRPX + 0.02 XC	k = 5.60E-11	5.60E-11
227	R6PX = OH + 0.142 HO2 + 0.782 RO2C + 0.077 RO2X + 0.077 ZRN3 + 0.085 RCHO + 0.142 PRD2 + 0.782 XHO2 + 0.026 XCCH + 0.058 XRCH + 0.698 XPD2 + 0.858 Y6PX + 0.017 XC	Photolysis	2.72E-6
228	RAPX + OH = 0.139 OH + 0.148 HO2 + 0.589 RO2C + 0.124 RO2X + 0.124 ZRN3 + 0.074 PRD2 + 0.147 MGLY + 0.139 IPRD + 0.565 XHO2 + 0.024 XOH + 0.448 XRCH + 0.026 XGLY + 0.03 XMEK + 0.252 XMGL + 0.073 XAF1 + 0.073 XAF2 + 0.713 Y6PX + 2.674 XC	k = 1.41E-10	1.41E-10
229	RAPX = OH + HO2 + 0.5 GLY + 0.5 MGLY + 0.5 AFG1 + 0.5 AFG2 + 0.5 XC	Photolysis	2.72E-6
230	GLY = 2. CO + 2. HO2	Photolysis	7.88E-5
231	GLY = HCHO + CO	Photolysis	2.23E-5
232	GLY + OH = 0.63 HO2 + 1.26 CO + 0.37 RCO3 - 0.37 XC	k = 1.10E-11	1.10E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
233	GLY + NO3 = HNO3 + 0.63 HO2 + 1.26 CO + 0.37 RCO3 - 0.37 XC	k = 2.80E-12 exp(-2376/T)	1.02E-15
234	MGLY = HO2 + CO + MCO3	Photolysis	1.39E-4
235	MGLY + OH = CO + MCO3	k = 1.50E-11	1.50E-11
236	MGLY + NO3 = HNO3 + CO + MCO3	k = 1.40E-12 exp(-1895/T)	2.53E-15
237	BACL = 2. MCO3	Photolysis	2.45E-4
238	CRES + OH = 0.2 BZO + 0.8 RO2C + 0.8 XHO2 + 0.8 Y6PX + 0.25 XMGL + 5.05 XC	k = 1.70E-12 exp(950/T)	4.03E-11
239	CRES + NO3 = HNO3 + BZO + XC	k = 1.40E-11	1.40E-11
240	NPHE + OH = BZO + XN	k = 3.50E-12	3.50E-12
241	NPHE = HONO + 6. XC	Photolysis	9.55E-6
242	NPHE = 6. XC + XN	Photolysis	9.55E-5
243	BALD + OH = BZC3	k = 1.20E-11	1.20E-11
244	BALD = 7. XC	Photolysis	2.48E-5
245	BALD + NO3 = HNO3 + BZC3	k = 1.34E-12 exp(-1860/T)	2.72E-15
246	AFG1 + OH = 0.217 MAC3 + 0.723 RO2C + 0.06 RO2X + 0.06 ZRN3 + 0.521 XHO2 + 0.201 XMC3 + 0.334 XCO + 0.407 XRCH + 0.129 XMEK + 0.107 XGLY + 0.267 XMGL + 0.783 Y6PX + 0.284 XC	k = 7.40E-11	7.40E-11
247	AFG1 + O3 = 0.826 OH + 0.522 HO2 + 0.652 RO2C + 0.522 CO + 0.174 CO2 + 0.432 GLY + 0.568 MGLY + 0.652 XRC3 + 0.652 XHCH + 0.652 Y6PX - 0.872 XC	k = 9.66E-18	9.66E-18
248	AFG1 = 1.023 HO2 + 0.173 MEO2 + 0.305 MCO3 + 0.5 MAC3 + 0.695 CO + 0.195 GLY + 0.305 MGLY + 0.217 XC	Photolysis	3.07E-3
249	AFG2 + OH = 0.217 MAC3 + 0.723 RO2C + 0.06 RO2X + 0.06 ZRN3 + 0.521 XHO2 + 0.201 XMC3 + 0.334 XCO + 0.407 XRCH + 0.129 XMEK + 0.107 XGLY + 0.267 XMGL + 0.783 Y6PX + 0.284 XC	k = 7.40E-11	7.40E-11
250	AFG2 + O3 = 0.826 OH + 0.522 HO2 + 0.652 RO2C + 0.522 CO + 0.174 CO2 + 0.432 GLY + 0.568 MGLY + 0.652 XRC3 + 0.652 XHCH + 0.652 Y6PX - 0.872 XC	k = 9.66E-18	9.66E-18
251	AFG2 = PRD2 - 1. XC	Photolysis	3.07E-3
252	AFG3 + OH = 0.206 MAC3 + 0.733 RO2C + 0.117 RO2X + 0.117 ZRN3 + 0.561 XHO2 + 0.117 XMC3 + 0.114 XCO + 0.274 XGLY + 0.153 XMGL + 0.019 XBAC + 0.195 XAF1 + 0.195 XAF2 + 0.231 XIPR + 0.794 Y6PX + 0.938 XC	k = 9.35E-11	9.35E-11
253	AFG3 + O3 = 0.471 OH + 0.554 HO2 + 0.013 MCO3 + 0.258 RO2C + 0.007 RO2X + 0.007 ZRN3 + 0.58 CO + 0.19 CO2 + 0.366 GLY + 0.184 MGLY + 0.35 AFG1 + 0.35 AFG2 + 0.139 AFG3 + 0.003 MACR + 0.004 MVK + 0.003 IPRD + 0.095 XHO2 + 0.163 XRC3 + 0.163 XHCH + 0.095 XMGL + 0.264 Y6PX - 0.575 XC	k = 1.43E-17	1.43E-17
254	MACR + OH = 0.5 MAC3 + 0.5 RO2C + 0.5 XHO2 + 0.416 XCO + 0.084 XHCH + 0.416 XMEK + 0.084 XMGL + 0.5 YRPX - 0.416 XC	k = 8.00E-12 exp(380/T)	2.84E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
255	MACR + O3 = 0.208 OH + 0.108 HO2 + 0.1 RO2C + 0.45 CO + 0.117 CO2 + 0.1 HCHO + 0.9 MGLY + 0.333 FACD + 0.1 XRC3 + 0.1 XHCH + 0.1 YRPX - 0.1 XC	k = 1.40E-15 exp(-2100/T)	1.28E-18
256	MACR + NO3 = 0.5 MAC3 + 0.5 RO2C + 0.5 HNO3 + 0.5 XHO2 + 0.5 XCO + 0.5 YRPX + 1.5 XC + 0.5 XN	k = 1.50E-12 exp(-1815/T)	3.54E-15
257	MACR + O3P = RCHO + XC	k = 6.34E-12	6.34E-12
258	MACR = 0.33 OH + 0.67 HO2 + 0.34 MCO3 + 0.33 MAC3 + 0.33 RO2C + 0.67 CO + 0.34 HCHO + 0.33 XMC3 + 0.33 XHCH + 0.33 YRPX	Photolysis	1.39E-6
259	MVK + OH = 0.975 RO2C + 0.025 RO2X + 0.025 ZRN3 + 0.3 XHO2 + 0.675 XMC3 + 0.3 XHCH + 0.675 XGLD + 0.3 XMGL + YRPX - 0.05 XC	k = 2.60E-12 exp(610/T)	1.99E-11
260	MVK + O3 = 0.164 OH + 0.064 HO2 + 0.05 RO2C + 0.05 XHO2 + 0.475 CO + 0.124 CO2 + 0.05 HCHO + 0.95 MGLY + 0.351 FACD + 0.05 XRC3 + 0.05 XHCH + 0.05 YRPX - 0.05 XC	k = 8.50E-16 exp(-1520/T)	5.36E-18
261	MVK + O3P = 0.45 RCHO + 0.55 MEK + 0.45 XC	k = 4.32E-12	4.32E-12
262	MVK = 0.4 MEO2 + 0.6 CO + 0.6 PRD2 + 0.4 MAC3 - 2.2 XC	Photolysis	5.25E-7
263	IPRD + OH = 0.289 MAC3 + 0.67 RO2C + 0.67 XHO2 + 0.041 RO2X + 0.041 ZRN3 + 0.336 XCO + 0.055 XHCH + 0.129 XGLD + 0.013 XRCH + 0.15 XMEK + 0.332 XPD2 + 0.15 XGLY + 0.174 XMGL - 0.504 XC + 0.711 Y6PX	k = 6.19E-11	6.19E-11
264	IPRD + O3 = 0.285 OH + 0.4 HO2 + 0.048 RO2C + 0.048 XRC3 + 0.498 CO + 0.14 CO2 + 0.124 HCHO + 0.21 MEK + 0.023 GLY + 0.742 MGLY + 0.1 FACD + 0.372 PACD + 0.047 XGLD + 0.001 XHCH + 0.048 Y6PX - 0.329 XC	k = 4.18E-18	4.18E-18
265	IPRD + NO3 = 0.15 MAC3 + 0.15 HNO3 + 0.799 RO2C + 0.799 XHO2 + 0.051 RO2X + 0.051 ZRN3 + 0.572 XCO + 0.227 XHCH + 0.218 XRCH + 0.008 XMGL + 0.572 XRN3 + 0.85 Y6PX + 0.278 XN - 0.815 XC	k = 1.00E-13	1.00E-13
266	IPRD = 1.233 HO2 + 0.467 MCO3 + 0.3 RCO3 + 1.233 CO + 0.3 HCHO + 0.467 GLYD + 0.233 MEK - 0.233 XC	Photolysis	1.39E-6
267	PRD2 + OH = 0.472 HO2 + 0.379 XHO2 + 0.029 XMC3 + 0.049 XRC3 + 0.473 RO2C + 0.071 RO2X + 0.071 ZRN3 + 0.002 HCHO + 0.211 XHCH + 0.001 CCHO + 0.083 XCCH + 0.143 RCHO + 0.402 XRCH + 0.115 XMEK + 0.329 PRD2 + 0.007 XPD2 + 0.528 Y6PX + 0.877 XC	k = 1.55E-11	1.55E-11
268	PRD2 = 0.913 XHO2 + 0.4 MCO3 + 0.6 RCO3 + 1.59 RO2C + 0.087 RO2X + 0.087 ZRN3 + 0.303 XHCH + 0.163 XCCH + 0.78 XRCH + Y6PX - 0.091 XC	Photolysis	2.26E-8

Number	Reactants and Products	Rate Constant Expression	k_{300}
269	RNO3 + OH = 0.189 HO2 + 0.305 XHO2 + 0.019 NO2 + 0.313 XNO2 + 0.976 RO2C + 0.175 RO2X + 0.175 ZRN3 + 0.011 XHCH + 0.429 XCCH + 0.001 RCHO + 0.036 XRCH + 0.004 XACE + 0.01 MEK + 0.17 XMEK + 0.008 PRD2 + 0.031 XPD2 + 0.189 RNO3 + 0.305 XRN3 + 0.157 YRPX + 0.636 Y6PX + 0.174 XN + 0.04 XC	k = 7.20E-12	7.20E-12
270	RNO3 = 0.344 HO2 + 0.554 XHO2 + NO2 + 0.721 RO2C + 0.102 RO2X + 0.102 ZRN3 + 0.074 HCHO + 0.061 XHCH + 0.214 CCHO + 0.23 XCCH + 0.074 RCHO + 0.063 XRCH + 0.008 XACE + 0.124 MEK + 0.083 XMEK + 0.19 PRD2 + 0.261 XPD2 + 0.066 YRPX + 0.591 Y6PX + 0.396 XC	Photolysis	1.20E-6
271	GLYD + OH = MCO3	k = k(208)	1.49E-11
272	GLYD = CO + 2. HO2 + HCHO	Photolysis	2.75E-6
273	GLYD + NO3 = HNO3 + MCO3	k = k(210)	2.84E-15
274	ACRO + OH = 0.25 XHO2 + 0.75 MAC3 + 0.25 RO2C + 0.167 XCO + 0.083 XHCH + 0.167 XCCH + 0.083 XGLY + 0.25 YRPX - 0.75 XC	k = 1.99E-11	1.99E-11
275	ACRO + O3 = 0.83 HO2 + 0.33 OH + 1.005 CO + 0.31 CO2 + 0.5 HCHO + 0.185 FACD + 0.5 GLY	k = 1.40E-15 exp(-2528/T)	3.07E-19
276	ACRO + NO3 = 0.031 XHO2 + 0.967 MAC3 + 0.031 RO2C + 0.002 RO2X + 0.002 ZRN3 + 0.967 HNO3 + 0.031 XCO + 0.031 XRN3 + 0.033 YRPX + 0.002 XN - 1.097 XC	k = 1.18E-15	1.18E-15
277	ACRO + O3P = RCHO	k = 2.37E-12	2.37E-12
278	ACRO = 1.066 HO2 + 0.178 OH + 0.234 MEO2 + 0.33 MAC3 + 1.188 CO + 0.102 CO2 + 0.34 HCHO + 0.05 AACD - 0.284 XC	Photolysis	1.28E-6
279	CO3H + OH = 0.98 MCO3 + 0.02 RO2C + 0.02 CO2 + 0.02 XOH + 0.02 XHCH + 0.02 YRPX	k = 5.28E-12	5.28E-12
280	CO3H = MEO2 + CO2 + OH	Photolysis	3.60E-7
281	RO3H + OH = 0.806 RCO3 + 0.194 RO2C + 0.194 YRPX + 0.11 CO2 + 0.11 XOH + 0.11 XCCH + 0.084 XHO2 + 0.084 XRCH	k = 6.42E-12	6.42E-12
282	RO3H = XHO2 + XCCH + YRPX + CO2 + OH	Photolysis	3.60E-7
283	XHCH + NO = NO + HCHO	k = k(52)	9.23E-12
284	XHCH + HO2 = HO2 + XC	k = k(53)	7.63E-12
285	XHCH + NO3 = NO3 + HCHO	k = k(54)	2.30E-12
286	XHCH + MEO2 = MEO2 + 0.5 HCHO + 0.5 XC	k = k(55)	2.00E-13
287	XHCH + RO2C = RO2C + 0.5 HCHO + 0.5 XC	k = k(56)	3.50E-14
288	XHCH + RO2X = RO2X + 0.5 HCHO + 0.5 XC	k = k(56)	3.50E-14
289	XHCH + MCO3 = MCO3 + HCHO	k = k(70)	1.56E-11
290	XHCH + RCO3 = RCO3 + HCHO	k = k(70)	1.56E-11
291	XHCH + BZC3 = BZC3 + HCHO	k = k(70)	1.56E-11
292	XHCH + MAC3 = MAC3 + HCHO	k = k(70)	1.56E-11
293	XCCH + NO = NO + CCHO	k = k(52)	9.23E-12
294	XCCH + HO2 = HO2 + 2. XC	k = k(53)	7.63E-12
295	XCCH + NO3 = NO3 + CCHO	k = k(54)	2.30E-12
296	XCCH + MEO2 = MEO2 + 0.5 CCHO + XC	k = k(55)	2.00E-13
297	XCCH + RO2C = RO2C + 0.5 CCHO + XC	k = k(56)	3.50E-14
298	XCCH + RO2X = RO2X + 0.5 CCHO + XC	k = k(56)	3.50E-14
299	XCCH + MCO3 = MCO3 + CCHO	k = k(70)	1.56E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
300	XCCH + RCO3 = RCO3 + CCHO	k = k(70)	1.56E-11
301	XCCH + BZC3 = BZC3 + CCHO	k = k(70)	1.56E-11
302	XCCH + MAC3 = MAC3 + CCHO	k = k(70)	1.56E-11
303	XRCH + NO = NO + RCHO	k = k(52)	9.23E-12
304	XRCH + HO2 = HO2 + 3. XC	k = k(53)	7.63E-12
305	XRCH + NO3 = NO3 + RCHO	k = k(54)	2.30E-12
306	XRCH + MEO2 = MEO2 + 0.5 RCHO + 1.5 XC	k = k(55)	2.00E-13
307	XRCH + RO2C = RO2C + 0.5 RCHO + 1.5 XC	k = k(56)	3.50E-14
308	XRCH + RO2X = RO2X + 0.5 RCHO + 1.5 XC	k = k(56)	3.50E-14
309	XRCH + MCO3 = MCO3 + RCHO	k = k(70)	1.56E-11
310	XRCH + RCO3 = RCO3 + RCHO	k = k(70)	1.56E-11
311	XRCH + BZC3 = BZC3 + RCHO	k = k(70)	1.56E-11
312	XRCH + MAC3 = MAC3 + RCHO	k = k(70)	1.56E-11
313	XACE + NO = NO + ACET	k = k(52)	9.23E-12
314	XACE + HO2 = HO2 + 3. XC	k = k(53)	7.63E-12
315	XACE + NO3 = NO3 + ACET	k = k(54)	2.30E-12
316	XACE + MEO2 = MEO2 + 0.5 ACET + 1.5 XC	k = k(55)	2.00E-13
317	XACE + RO2C = RO2C + 0.5 ACET + 1.5 XC	k = k(56)	3.50E-14
318	XACE + RO2X = RO2X + 0.5 ACET + 1.5 XC	k = k(56)	3.50E-14
319	XACE + MCO3 = MCO3 + ACET	k = k(70)	1.56E-11
320	XACE + RCO3 = RCO3 + ACET	k = k(70)	1.56E-11
321	XACE + BZC3 = BZC3 + ACET	k = k(70)	1.56E-11
322	XACE + MAC3 = MAC3 + ACET	k = k(70)	1.56E-11
323	XMEK + NO = NO + MEK	k = k(52)	9.23E-12
324	XMEK + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
325	XMEK + NO3 = NO3 + MEK	k = k(54)	2.30E-12
326	XMEK + MEO2 = MEO2 + 0.5 MEK + 2. XC	k = k(55)	2.00E-13
327	XMEK + RO2C = RO2C + 0.5 MEK + 2. XC	k = k(56)	3.50E-14
328	XMEK + RO2X = RO2X + 0.5 MEK + 2. XC	k = k(56)	3.50E-14
329	XMEK + MCO3 = MCO3 + MEK	k = k(70)	1.56E-11
330	XMEK + RCO3 = RCO3 + MEK	k = k(70)	1.56E-11
331	XMEK + BZC3 = BZC3 + MEK	k = k(70)	1.56E-11
332	XMEK + MAC3 = MAC3 + MEK	k = k(70)	1.56E-11
333	XPD2 + NO = NO + PRD2	k = k(52)	9.23E-12
334	XPD2 + HO2 = HO2 + 6. XC	k = k(53)	7.63E-12
335	XPD2 + NO3 = NO3 + PRD2	k = k(54)	2.30E-12
336	XPD2 + MEO2 = MEO2 + 0.5 PRD2 + 3. XC	k = k(55)	2.00E-13
337	XPD2 + RO2C = RO2C + 0.5 PRD2 + 3. XC	k = k(56)	3.50E-14
338	XPD2 + RO2X = RO2X + 0.5 PRD2 + 3. XC	k = k(56)	3.50E-14
339	XPD2 + MCO3 = MCO3 + PRD2	k = k(70)	1.56E-11
340	XPD2 + RCO3 = RCO3 + PRD2	k = k(70)	1.56E-11
341	XPD2 + BZC3 = BZC3 + PRD2	k = k(70)	1.56E-11
342	XPD2 + MAC3 = MAC3 + PRD2	k = k(70)	1.56E-11
343	XGLY + NO = NO + GLY	k = k(52)	9.23E-12
344	XGLY + HO2 = HO2 + 2. XC	k = k(53)	7.63E-12
345	XGLY + NO3 = NO3 + GLY	k = k(54)	2.30E-12
346	XGLY + MEO2 = MEO2 + 0.5 GLY + XC	k = k(55)	2.00E-13
347	XGLY + RO2C = RO2C + 0.5 GLY + XC	k = k(56)	3.50E-14
348	XGLY + RO2X = RO2X + 0.5 GLY + XC	k = k(56)	3.50E-14
349	XGLY + MCO3 = MCO3 + GLY	k = k(70)	1.56E-11
350	XGLY + RCO3 = RCO3 + GLY	k = k(70)	1.56E-11
351	XGLY + BZC3 = BZC3 + GLY	k = k(70)	1.56E-11
352	XGLY + MAC3 = MAC3 + GLY	k = k(70)	1.56E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
353	XMGL + NO = NO + MGLY	k = k(52)	9.23E-12
354	XMGL + HO2 = HO2 + 3. XC	k = k(53)	7.63E-12
355	XMGL + NO3 = NO3 + MGLY	k = k(54)	2.30E-12
356	XMGL + MEO2 = MEO2 + 0.5 MGLY + 1.5 XC	k = k(55)	2.00E-13
357	XMGL + RO2C = RO2C + 0.5 MGLY + 1.5 XC	k = k(56)	3.50E-14
358	XMGL + RO2X = RO2X + 0.5 MGLY + 1.5 XC	k = k(56)	3.50E-14
359	XMGL + MCO3 = MCO3 + MGLY	k = k(70)	1.56E-11
360	XMGL + RCO3 = RCO3 + MGLY	k = k(70)	1.56E-11
361	XMGL + BZC3 = BZC3 + MGLY	k = k(70)	1.56E-11
362	XMGL + MAC3 = MAC3 + MGLY	k = k(70)	1.56E-11
363	XBAC + NO = NO + BACL	k = k(52)	9.23E-12
364	XBAC + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
365	XBAC + NO3 = NO3 + BACL	k = k(54)	2.30E-12
366	XBAC + MEO2 = MEO2 + 0.5 BACL + 2. XC	k = k(55)	2.00E-13
367	XBAC + RO2C = RO2C + 0.5 BACL + 2. XC	k = k(56)	3.50E-14
368	XBAC + RO2X = RO2X + 0.5 BACL + 2. XC	k = k(56)	3.50E-14
369	XBAC + MCO3 = MCO3 + BACL	k = k(70)	1.56E-11
370	XBAC + RCO3 = RCO3 + BACL	k = k(70)	1.56E-11
371	XBAC + BZC3 = BZC3 + BACL	k = k(70)	1.56E-11
372	XBAC + MAC3 = MAC3 + BACL	k = k(70)	1.56E-11
373	XBAL + NO = NO + BALD	k = k(52)	9.23E-12
374	XBAL + HO2 = HO2 + 7. XC	k = k(53)	7.63E-12
375	XBAL + NO3 = NO3 + BALD	k = k(54)	2.30E-12
376	XBAL + MEO2 = MEO2 + 0.5 BALD + 3.5 XC	k = k(55)	2.00E-13
377	XBAL + RO2C = RO2C + 0.5 BALD + 3.5 XC	k = k(56)	3.50E-14
378	XBAL + RO2X = RO2X + 0.5 BALD + 3.5 XC	k = k(56)	3.50E-14
379	XBAL + MCO3 = MCO3 + BALD	k = k(70)	1.56E-11
380	XBAL + RCO3 = RCO3 + BALD	k = k(70)	1.56E-11
381	XBAL + BZC3 = BZC3 + BALD	k = k(70)	1.56E-11
382	XBAL + MAC3 = MAC3 + BALD	k = k(70)	1.56E-11
383	XAF1 + NO = NO + AFG1	k = k(52)	9.23E-12
384	XAF1 + HO2 = HO2 + 5. XC	k = k(53)	7.63E-12
385	XAF1 + NO3 = NO3 + AFG1	k = k(54)	2.30E-12
386	XAF1 + MEO2 = MEO2 + 0.5 AFG1 + 2.5 XC	k = k(55)	2.00E-13
387	XAF1 + RO2C = RO2C + 0.5 AFG1 + 2.5 XC	k = k(56)	3.50E-14
388	XAF1 + RO2X = RO2X + 0.5 AFG1 + 2.5 XC	k = k(56)	3.50E-14
389	XAF1 + MCO3 = MCO3 + AFG1	k = k(70)	1.56E-11
390	XAF1 + RCO3 = RCO3 + AFG1	k = k(70)	1.56E-11
391	XAF1 + BZC3 = BZC3 + AFG1	k = k(70)	1.56E-11
392	XAF1 + MAC3 = MAC3 + AFG1	k = k(70)	1.56E-11
393	XAF2 + NO = NO + AFG2	k = k(52)	9.23E-12
394	XAF2 + HO2 = HO2 + 5. XC	k = k(53)	7.63E-12
395	XAF2 + NO3 = NO3 + AFG2	k = k(54)	2.30E-12
396	XAF2 + MEO2 = MEO2 + 0.5 AFG2 + 2.5 XC	k = k(55)	2.00E-13
397	XAF2 + RO2C = RO2C + 0.5 AFG2 + 2.5 XC	k = k(56)	3.50E-14
398	XAF2 + RO2X = RO2X + 0.5 AFG2 + 2.5 XC	k = k(56)	3.50E-14
399	XAF2 + MCO3 = MCO3 + AFG2	k = k(70)	1.56E-11
400	XAF2 + RCO3 = RCO3 + AFG2	k = k(70)	1.56E-11
401	XAF2 + BZC3 = BZC3 + AFG2	k = k(70)	1.56E-11
402	XAF2 + MAC3 = MAC3 + AFG2	k = k(70)	1.56E-11
403	XAF3 + NO = NO + AFG3	k = k(52)	9.23E-12
404	XAF3 + HO2 = HO2 + 7. XC	k = k(53)	7.63E-12
405	XAF3 + NO3 = NO3 + AFG3	k = k(54)	2.30E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
406	XAF3 + MEO2 = MEO2 + 0.5 AFG3 + 3.5 XC	k = k(55)	2.00E-13
407	XAF3 + RO2C = RO2C + 0.5 AFG3 + 3.5 XC	k = k(56)	3.50E-14
408	XAF3 + RO2X = RO2X + 0.5 AFG3 + 3.5 XC	k = k(56)	3.50E-14
409	XAF3 + MCO3 = MCO3 + AFG3	k = k(70)	1.56E-11
410	XAF3 + RCO3 = RCO3 + AFG3	k = k(70)	1.56E-11
411	XAF3 + BZC3 = BZC3 + AFG3	k = k(70)	1.56E-11
412	XAF3 + MAC3 = MAC3 + AFG3	k = k(70)	1.56E-11
413	XMAC + NO = NO + MACR	k = k(52)	9.23E-12
414	XMAC + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
415	XMAC + NO3 = NO3 + MACR	k = k(54)	2.30E-12
416	XMAC + MEO2 = MEO2 + 0.5 MACR + 2. XC	k = k(55)	2.00E-13
417	XMAC + RO2C = RO2C + 0.5 MACR + 2. XC	k = k(56)	3.50E-14
418	XMAC + RO2X = RO2X + 0.5 MACR + 2. XC	k = k(56)	3.50E-14
419	XMAC + MCO3 = MCO3 + MACR	k = k(70)	1.56E-11
420	XMAC + RCO3 = RCO3 + MACR	k = k(70)	1.56E-11
421	XMAC + BZC3 = BZC3 + MACR	k = k(70)	1.56E-11
422	XMAC + MAC3 = MAC3 + MACR	k = k(70)	1.56E-11
423	XMVK + NO = NO + MVK	k = k(52)	9.23E-12
424	XMVK + HO2 = HO2 + 4. XC	k = k(53)	7.63E-12
425	XMVK + NO3 = NO3 + MVK	k = k(54)	2.30E-12
426	XMVK + MEO2 = MEO2 + 0.5 MVK + 2. XC	k = k(55)	2.00E-13
427	XMVK + RO2C = RO2C + 0.5 MVK + 2. XC	k = k(56)	3.50E-14
428	XMVK + RO2X = RO2X + 0.5 MVK + 2. XC	k = k(56)	3.50E-14
429	XMVK + MCO3 = MCO3 + MVK	k = k(70)	1.56E-11
430	XMVK + RCO3 = RCO3 + MVK	k = k(70)	1.56E-11
431	XMVK + BZC3 = BZC3 + MVK	k = k(70)	1.56E-11
432	XMVK + MAC3 = MAC3 + MVK	k = k(70)	1.56E-11
433	XIPR + NO = NO + IPRD	k = k(52)	9.23E-12
434	XIPR + HO2 = HO2 + 5. XC	k = k(53)	7.63E-12
435	XIPR + NO3 = NO3 + IPRD	k = k(54)	2.30E-12
436	XIPR + MEO2 = MEO2 + 0.5 IPRD + 2.5 XC	k = k(55)	2.00E-13
437	XIPR + RO2C = RO2C + 0.5 IPRD + 2.5 XC	k = k(56)	3.50E-14
438	XIPR + RO2X = RO2X + 0.5 IPRD + 2.5 XC	k = k(56)	3.50E-14
439	XIPR + MCO3 = MCO3 + IPRD	k = k(70)	1.56E-11
440	XIPR + RCO3 = RCO3 + IPRD	k = k(70)	1.56E-11
441	XIPR + BZC3 = BZC3 + IPRD	k = k(70)	1.56E-11
442	XIPR + MAC3 = MAC3 + IPRD	k = k(70)	1.56E-11
443	XRN3 + NO = NO + RNO3	k = k(52)	9.23E-12
444	XRN3 + HO2 = HO2 + 6. XC + XN	k = k(53)	7.63E-12
445	XRN3 + NO3 = NO3 + RNO3	k = k(54)	2.30E-12
446	XRN3 + MEO2 = MEO2 + 0.5 RNO3 + 0.5 XN + 3. XC	k = k(55)	2.00E-13
447	XRN3 + RO2C = RO2C + 0.5 RNO3 + 0.5 XN + 3. XC	k = k(56)	3.50E-14
448	XRN3 + RO2X = RO2X + 0.5 RNO3 + 0.5 XN + 3. XC	k = k(56)	3.50E-14
449	XRN3 + MCO3 = MCO3 + RNO3	k = k(70)	1.56E-11
450	XRN3 + RCO3 = RCO3 + RNO3	k = k(70)	1.56E-11
451	XRN3 + BZC3 = BZC3 + RNO3	k = k(70)	1.56E-11
452	XRN3 + MAC3 = MAC3 + RNO3	k = k(70)	1.56E-11
453	YRPX + NO = NO	k = k(52)	9.23E-12
454	YRPX + HO2 = HO2 + ROOH - 3. XC	k = k(53)	7.63E-12
455	YRPX + NO3 = NO3	k = k(54)	2.30E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
456	YRPX + MEO2 = MEO2 + 0.5 MEK - 2. XC	k = k(55)	2.00E-13
457	YRPX + RO2C = RO2C + 0.5 MEK - 2. XC	k = k(56)	3.50E-14
458	YRPX + RO2X = RO2X + 0.5 MEK - 2. XC	k = k(56)	3.50E-14
459	YRPX + MCO3 = MCO3	k = k(70)	1.56E-11
460	YRPX + RCO3 = RCO3	k = k(70)	1.56E-11
461	YRPX + BZC3 = BZC3	k = k(70)	1.56E-11
462	YRPX + MAC3 = MAC3	k = k(70)	1.56E-11
463	Y6PX + NO = NO	k = k(52)	9.23E-12
464	Y6PX + HO2 = HO2 + R6PX - 6. XC	k = k(53)	7.63E-12
465	Y6PX + NO3 = NO3	k = k(54)	2.30E-12
466	Y6PX + MEO2 = MEO2 + 0.5 PRD2 - 3. XC	k = k(55)	2.00E-13
467	Y6PX + RO2C = RO2C + 0.5 PRD2 - 3. XC	k = k(56)	3.50E-14
468	Y6PX + RO2X = RO2X + 0.5 PRD2 - 3. XC	k = k(56)	3.50E-14
469	Y6PX + MCO3 = MCO3	k = k(70)	1.56E-11
470	Y6PX + RCO3 = RCO3	k = k(70)	1.56E-11
471	Y6PX + BZC3 = BZC3	k = k(70)	1.56E-11
472	Y6PX + MAC3 = MAC3	k = k(70)	1.56E-11
473	YAPX + NO = NO	k = k(52)	9.23E-12
474	YAPX + HO2 = HO2 + RAPX - 8. XC	k = k(53)	7.63E-12
475	YAPX + NO3 = NO3	k = k(54)	2.30E-12
476	YAPX + MEO2 = MEO2 + 0.5 PRD2 - 3. XC	k = k(55)	2.00E-13
477	YAPX + RO2C = RO2C + 0.5 PRD2 - 3. XC	k = k(56)	3.50E-14
478	YAPX + RO2X = RO2X + 0.5 PRD2 - 3. XC	k = k(56)	3.50E-14
479	YAPX + MCO3 = MCO3	k = k(70)	1.56E-11
480	YAPX + RCO3 = RCO3	k = k(70)	1.56E-11
481	YAPX + BZC3 = BZC3	k = k(70)	1.56E-11
482	YAPX + MAC3 = MAC3	k = k(70)	1.56E-11
483	ZRN3 + NO = NO + RNO3 - 1. XN	k = k(52)	9.23E-12
484	ZRN3 + HO2 = HO2 + 6. XC	k = k(53)	7.63E-12
485	ZRN3 + NO3 = NO3 + PRD2 + HO2	k = k(54)	2.30E-12
486	ZRN3 + MEO2 = MEO2 + 0.5 PRD2 + 0.5 HO2 + 3. XC	k = k(55)	2.00E-13
487	ZRN3 + RO2C = RO2C + 0.5 PRD2 + 0.5 HO2 + 3. XC	k = k(56)	3.50E-14
488	ZRN3 + RO2X = RO2X + 0.5 PRD2 + 0.5 HO2 + 3. XC	k = k(56)	3.50E-14
489	ZRN3 + MCO3 = MCO3 + PRD2 + HO2	k = k(70)	1.56E-11
490	ZRN3 + RCO3 = RCO3 + PRD2 + HO2	k = k(70)	1.56E-11
491	ZRN3 + BZC3 = BZC3 + PRD2 + HO2	k = k(70)	1.56E-11
492	ZRN3 + MAC3 = MAC3 + PRD2 + HO2	k = k(70)	1.56E-11
493	XGLD + NO = NO + GLYD	k = k(52)	9.23E-12
494	XGLD + HO2 = HO2 + 2. XC	k = k(53)	7.63E-12
495	XGLD + NO3 = NO3 + GLYD	k = k(54)	2.30E-12
496	XGLD + MEO2 = MEO2 + 0.5 GLYD + XC	k = k(55)	2.00E-13
497	XGLD + RO2C = RO2C + 0.5 GLYD + XC	k = k(56)	3.50E-14
498	XGLD + RO2X = RO2X + 0.5 GLYD + XC	k = k(56)	3.50E-14
499	XGLD + MCO3 = MCO3 + GLYD	k = k(70)	1.56E-11
500	XGLD + RCO3 = RCO3 + GLYD	k = k(70)	1.56E-11
501	XGLD + BZC3 = BZC3 + GLYD	k = k(70)	1.56E-11
502	XGLD + MAC3 = MAC3 + GLYD	k = k(70)	1.56E-11
503	XACR + NO = NO + ACRO	k = k(52)	9.23E-12
504	XACR + HO2 = HO2 + 3. XC	k = k(53)	7.63E-12
505	XACR + NO3 = NO3 + ACRO	k = k(54)	2.30E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
506	XACR + MEO2 = MEO2 + 0.5 ACRO + 1.5 XC	k = k(55)	2.00E-13
507	XACR + RO2C = RO2C + 0.5 ACRO + 1.5 XC	k = k(56)	3.50E-14
508	XACR + RO2X = RO2X + 0.5 ACRO + 1.5 XC	k = k(56)	3.50E-14
509	XACR + MCO3 = MCO3 + ACRO	k = k(70)	1.56E-11
510	XACR + RCO3 = RCO3 + ACRO	k = k(70)	1.56E-11
511	XACR + BZC3 = BZC3 + ACRO	k = k(70)	1.56E-11
512	XACR + MAC3 = MAC3 + ACRO	k = k(70)	1.56E-11
513	CH4 + OH = MEO2	k = 1.85E-12 exp(-1690/T)	6.62E-15
514	ETHE + OH = XHO2 + RO2C + 1.61 XHCH + 0.195 XGLD + YRPX	Falloff: F=0.6; n=1 k(0) = 1.00E-28 (T/300)^-4.5 k(inf) = 8.80E-12 (T/300)^-0.85	8.15E-12
515	ETHE + O3 = 0.16 HO2 + 0.16 OH + 0.51 CO + 0.12 CO2 + HCHO + 0.37 FACD	k = 9.14E-15 exp(-2580/T)	1.68E-18
516	ETHE + NO3 = XHO2 + RO2C + XRCH + YRPX + XN - 1. XC	k = 3.30E-12 (T/300)^2 exp(-2880/T)	2.24E-16
517	ETHE + O3P = 0.8 HO2 + 0.29 XHO2 + 0.51 MEO2 + 0.29 RO2C + 0.51 CO + 0.278 XCO + 0.278 XHCH + 0.1 CCHO + 0.012 XGLY + 0.29 YRPX + 0.2 XC	k = 1.07E-11 exp(-800/T)	7.43E-13
518	PRPE + OH = 0.984 XHO2 + 0.984 RO2C + 0.016 RO2X + 0.016 ZRN3 + 0.984 XHCH + 0.984 XCCH + YRPX - 0.048 XC	k = 4.85E-12 exp(504/T)	2.60E-11
519	PRPE + O3 = 0.165 HO2 + 0.35 OH + 0.355 MEO2 + 0.525 CO + 0.215 CO2 + 0.5 HCHO + 0.5 CCHO + 0.185 FACD + 0.075 AACD + 0.07 XC	k = 5.51E-15 exp(-1878/T)	1.05E-17
520	PRPE + NO3 = 0.949 XHO2 + 0.949 RO2C + 0.051 RO2X + 0.051 ZRN3 + YRPX + XN + 2.694 XC	k = 4.59E-13 exp(-1156/T)	9.73E-15
521	PRPE + O3P = 0.45 RCHO + 0.55 MEK - 0.55 XC	k = 1.02E-11 exp(-280/T)	4.01E-12
522	BD13 + OH = 0.951 XHO2 + 1.189 RO2C + 0.049 RO2X + 0.049 ZRN3 + 0.708 XHCH + 0.48 XACR + 0.471 XIPR + YRPX - 0.797 XC	k = 1.48E-11 exp(448/T)	6.59E-11
523	BD13 + O3 = 0.08 HO2 + 0.08 OH + 0.255 CO + 0.185 CO2 + 0.5 HCHO + 0.185 FACD + 0.5 ACRO + 0.375 MVK + 0.125 PRD2 - 0.875 XC	k = 1.34E-14 exp(-2283/T)	6.64E-18
524	BD13 + NO3 = 0.815 XHO2 + 0.12 XNO2 + 1.055 RO2C + 0.065 RO2X + 0.065 ZRN3 + 0.115 XHCH + 0.46 XMVK + 0.12 XIPR + 0.355 XRN3 + YRPX + 0.525 XN - 1.075 XC	k = 1.00E-13	1.00E-13
525	BD13 + O3P = 0.25 HO2 + 0.117 XHO2 + 0.118 XMA3 + 0.235 RO2C + 0.015 RO2X + 0.015 ZRN3 + 0.115 XCO + 0.115 XACR + 0.001 XAF1 + 0.001 XAF2 + 0.75 PRD2 + 0.25 YRPX - 1.532 XC	k = 2.26E-11 exp(-40/T)	1.98E-11
526	ISOP + OH = 0.907 XHO2 + 0.986 RO2C + 0.093 RO2X + 0.093 ZRN3 + 0.624 XHCH + 0.23 XMAC + 0.32 XMVK + 0.357 XIPR + Y6PX - 0.167 XC	k = 2.54E-11 exp(410/T)	9.96E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
527	ISOP + O3 = 0.066 HO2 + 0.266 OH + 0.192 XMA3 + 0.192 RO2C + 0.008 RO2X + 0.008 ZRN3 + 0.275 CO + 0.122 CO2 + 0.4 HCHO + 0.192 XHCH + 0.204 FACD + 0.39 MACR + 0.16 MVK + 0.15 IPRD + 0.1 PRD2 + 0.2 Y6PX - 0.559 XC	k = 7.86E-15 exp(-1912/T)	1.34E-17
528	ISOP + NO3 = 0.749 XHO2 + 0.187 XNO2 + 0.936 RO2C + 0.064 RO2X + 0.064 ZRN3 + 0.936 XIPR + Y6PX + 0.813 XN - 0.064 XC	k = 3.03E-12 exp(-448/T)	6.81E-13
529	ISOP + O3P = 0.25 MEO2 + 0.24 XMA3 + 0.24 RO2C + 0.01 RO2X + 0.01 ZRN3 + 0.24 XHCH + 0.75 PRD2 + 0.25 Y6PX - 1.01 XC	k = 3.50E-11	3.50E-11
530	APIN + OH = 0.799 XHO2 + 0.004 XRC3 + 1.042 RO2C + 0.197 RO2X + 0.197 ZRN3 + 0.002 XCO + 0.022 XHCH + 0.776 XRCH + 0.034 XACE + 0.02 XMGL + 0.023 XBAC + Y6PX + 6.2 XC	k = 1.21E-11 exp(436/T)	5.18E-11
531	APIN + O3 = 0.009 HO2 + 0.102 XHO2 + 0.728 OH + 0.001 XMC3 + 0.297 XRC3 + 1.511 RO2C + 0.337 RO2X + 0.337 ZRN3 + 0.029 CO + 0.051 XCO + 0.017 CO2 + 0.344 XHCH + 0.24 XRCH + 0.345 XACE + 0.008 MEK + 0.002 XGLY + 0.081 XBAC + 0.255 PRD2 + 0.737 Y6PX + 2.999 XC	k = 5.00E-16 exp(-530/T)	8.55E-17
532	APIN + NO3 = 0.056 XHO2 + 0.643 XNO2 + 0.007 XRC3 + 1.05 RO2C + 0.293 RO2X + 0.293 ZRN3 + 0.005 XCO + 0.007 XHCH + 0.684 XRCH + 0.069 XACE + 0.002 XMGL + 0.056 XRN3 + Y6PX + 0.301 XN + 5.608 XC	k = 1.19E-12 exp(490/T)	6.09E-12
533	APIN + O3P = PRD2 + 4. XC	k = 3.20E-11	3.20E-11
534	ACYE + OH = 0.3 HO2 + 0.7 OH + 0.3 CO + 0.3 FACD + 0.7 GLY	Falloff: F=0.6; n=1 k(0) = 5.50E-30 (T/300)^-2 k(inf) = 8.30E-13	7.56E-13
535	ACYE + O3 = 1.5 HO2 + 0.5 OH + 1.5 CO + 0.5 CO2	k = 1.00E-14 exp(-4100/T)	1.16E-20
536	BENZ + OH = 0.57 HO2 + 0.29 XHO2 + 0.116 OH + 0.29 RO2C + 0.024 RO2X + 0.024 ZRN3 + 0.29 XGLY + 0.57 CRES + 0.029 XAF1 + 0.261 XAF2 + 0.116 AFG3 + 0.314 YAPX - 0.976 XC	k = 2.33E-12 exp(-193/T)	1.22E-12
537	TOLU + OH = 0.181 HO2 + 0.454 XHO2 + 0.312 OH + 0.454 RO2C + 0.054 RO2X + 0.054 ZRN3 + 0.238 XGLY + 0.151 XMGL + 0.181 CRES + 0.065 XBAL + 0.195 XAF1 + 0.195 XAF2 + 0.312 AFG3 + 0.073 Y6PX + 0.435 YAPX - 0.109 XC	k = 1.81E-12 exp(338/T)	5.58E-12
538	MXYL + OH = 0.159 HO2 + 0.52 XHO2 + 0.239 OH + 0.52 RO2C + 0.082 RO2X + 0.082 ZRN3 + 0.1 XGLY + 0.38 XMGL + 0.159 CRES + 0.041 XBAL + 0.336 XAF1 + 0.144 XAF2 + 0.239 AFG3 + 0.047 Y6PX + 0.555 YAPX + 0.695 XC	k = 2.31E-11	2.31E-11
539	OXYL + OH = 0.161 HO2 + 0.554 XHO2 + 0.198 OH + 0.554 RO2C + 0.087 RO2X + 0.087 ZRN3 + 0.084 XGLY + 0.238 XMGL + 0.185 XBAC + 0.161 CRES + 0.047 XBAL + 0.253 XAF1 + 0.253 XAF2 + 0.198 AFG3 + 0.055 Y6PX + 0.586 YAPX + 0.484 XC	k = 1.36E-11	1.36E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
540	PXYL + OH = 0.159 HO2 + 0.487 XHO2 + 0.278 OH + 0.487 RO2C + 0.076 RO2X + 0.076 ZRN3 + 0.286 XGLY + 0.112 XMGL + 0.159 CRES + 0.088 XBAL + 0.045 XAF1 + 0.067 XAF2 + 0.278 AFG3 + 0.286 XAF3 + 0.102 Y6PX + 0.461 YAPX + 0.399 XC	k = 1.43E-11	1.43E-11
541	B124 + OH = 0.022 HO2 + 0.627 XHO2 + 0.23 OH + 0.627 RO2C + 0.121 RO2X + 0.121 ZRN3 + 0.074 XGLY + 0.405 XMGL + 0.112 XBAC + 0.022 CRES + 0.036 XBAL + 0.088 XAF1 + 0.352 XAF2 + 0.23 AFG3 + 0.151 XAF3 + 0.043 Y6PX + 0.705 YAPX + 1.19 XC	k = 3.25E-11	3.25E-11
542	ETOH + OH = 0.95 HO2 + 0.05 XHO2 + 0.05 RO2C + 0.081 XHCH + 0.95 CCHO + 0.01 XGLD + 0.05 YRPX - 0.001 XC	k = 5.49E-13 (T/300)^2 exp(530/T)	3.21E-12
543	ALK1 + OH = XHO2 + RO2C + XCCH + YRPX	k = 1.34E-12 (T/300)^2 exp(-499/T)	2.54E-13
544	ALK2 + OH = 0.965 XHO2 + 0.965 RO2C + 0.035 RO2X + 0.035 ZRN3 + 0.261 XRCH + 0.704 XACE + YRPX - 0.105 XC	k = 1.49E-12 (T/300)^2 exp(-87/T)	1.11E-12
545	ALK3 + OH = 0.695 XHO2 + 0.236 XTBU + 1.253 RO2C + 0.07 RO2X + 0.07 ZRN3 + 0.026 XHCH + 0.445 XCCH + 0.122 XRCH + 0.024 XACE + 0.332 XMEK + 0.983 YRPX + 0.017 Y6PX - 0.046 XC	k = 1.51E-12 exp(126/T)	2.30E-12
546	ALK4 + OH = 0.83 XHO2 + 0.01 XMEO + 0.011 XMC3 + 1.763 RO2C + 0.149 RO2X + 0.149 ZRN3 + 0.002 XCO + 0.029 XHCH + 0.438 XCCH + 0.236 XRCH + 0.426 XACE + 0.106 XMEK + 0.146 XPD2 + Y6PX - 0.119 XC	k = 3.75E-12 exp(44/T)	4.34E-12
547	ALK5 + OH = 0.647 XHO2 + 1.605 RO2C + 0.353 RO2X + 0.353 ZRN3 + 0.04 XHCH + 0.106 XCCH + 0.209 XRCH + 0.071 XACE + 0.086 XMEK + 0.407 XPD2 + Y6PX + 2.004 XC	k = 2.70E-12 exp(374/T)	9.39E-12
548	OLE1 + OH = 0.871 XHO2 + 0.001 XMEO + 1.202 RO2C + 0.128 RO2X + 0.128 ZRN3 + 0.582 XHCH + 0.01 XCCH + 0.007 XGLD + 0.666 XRCH + 0.007 XACE + 0.036 XACR + 0.001 XMAC + 0.012 XMVK + 0.009 XIPR + 0.168 XPD2 + 0.169 YRPX + 0.831 Y6PX + 0.383 XC	k = 6.72E-12 exp(501/T)	3.57E-11
549	OLE1 + O3 = 0.095 HO2 + 0.057 XHO2 + 0.128 OH + 0.09 RO2C + 0.005 RO2X + 0.005 ZRN3 + 0.303 CO + 0.088 CO2 + 0.5 HCHO + 0.011 XCCH + 0.5 RCHO + 0.044 XRCH + 0.003 XACE + 0.009 MEK + 0.185 FACD + 0.159 PACD + 0.268 PRD2 + 0.011 YRPX + 0.052 Y6PX + 0.11 XC	k = 3.19E-15 exp(-1701/T)	1.10E-17
550	OLE1 + NO3 = 0.772 XHO2 + 1.463 RO2C + 0.228 RO2X + 0.228 ZRN3 + 0.013 XCCH + 0.003 XRCH + 0.034 XACE + 0.774 XRN3 + 0.169 YRPX + 0.831 Y6PX + 0.226 XN - 1.149 XC	k = 5.37E-13 exp(-1047/T)	1.64E-14
551	OLE1 + O3P = 0.45 RCHO + 0.39 MEK + 0.16 PRD2 + 1.13 XC	k = 1.61E-11 exp(-326/T)	5.43E-12

Number	Reactants and Products	Rate Constant Expression	k_{300}
552	OLE2 + OH = 0.912 XHO2 + 0.953 RO2C + 0.088 RO2X + 0.088 ZRN3 + 0.179 XHCH + 0.835 XCCH + 0.51 XRCH + 0.144 XACE + 0.08 XMEK + 0.002 XMVK + 0.012 XIPR + 0.023 XPD2 + 0.319 YRPX + 0.681 Y6PX + 0.135 XC	k = 1.26E-11 exp(488/T)	6.41E-11
553	OLE2 + O3 = 0.094 HO2 + 0.041 XHO2 + 0.443 OH + 0.307 MEO2 + 0.156 XMC3 + 0.008 XRC3 + 0.212 RO2C + 0.003 RO2X + 0.003 ZRN3 + 0.299 CO + 0.161 CO2 + 0.131 HCHO + 0.114 XHCH + 0.453 CCHO + 0.071 XCCH + 0.333 RCHO + 0.019 XRCH + 0.051 ACET + 0.033 MEK + 0.001 XMEK + 0.024 FACD + 0.065 AACD + 0.235 PACD + 0.037 PRD2 + 0.073 YRPX + 0.136 Y6PX + 0.16 XC	k = 8.59E-15 exp(-1255/T)	1.31E-16
554	OLE2 + NO3 = 0.4 XHO2 + 0.426 XNO2 + 0.035 XMEO + 1.193 RO2C + 0.14 RO2X + 0.14 ZRN3 + 0.072 XHCH + 0.579 XCCH + 0.163 XRCH + 0.116 XACE + 0.002 XMEK + 0.32 XRN3 + 0.319 YRPX + 0.681 Y6PX + 0.254 XN + 0.13 XC	k = 2.31E-13 exp(382/T)	8.25E-13
555	OLE2 + O3P = 0.079 RCHO + 0.751 MEK + 0.17 PRD2 + 0.739 XC	k = 1.43E-11 exp(111/T)	2.07E-11
556	ARO1 + OH = 0.123 HO2 + 0.566 XHO2 + 0.202 OH + 0.566 RO2C + 0.11 RO2X + 0.11 ZRN3 + 0.158 XGLY + 0.1 XMGL + 0.123 CRES + 0.072 XAF1 + 0.185 XAF2 + 0.202 AFG3 + 0.309 XPD2 + 0.369 Y6PX + 0.31 XC	k = 7.84E-12	7.84E-12
557	ARO2 + OH = 0.077 HO2 + 0.617 XHO2 + 0.178 OH + 0.617 RO2C + 0.128 RO2X + 0.128 ZRN3 + 0.088 XGLY + 0.312 XMGL + 0.134 XBAC + 0.077 CRES + 0.026 XBAL + 0.221 XAF1 + 0.247 XAF2 + 0.178 AFG3 + 0.068 XAF3 + 0.057 XPD2 + 0.101 Y6PX + 1.459 XC	k = 3.09E-11	3.09E-11
558	TERP + OH = 0.734 XHO2 + 0.064 XRC3 + 1.211 RO2C + 0.201 RO2X + 0.201 ZRN3 + 0.001 XCO + 0.411 XHCH + 0.385 XRCH + 0.037 XACE + 0.007 XMEK + 0.003 XMGL + 0.009 XBAC + 0.003 XMVK + 0.002 XIPR + 0.409 XPD2 + Y6PX + 4.375 XC	k = 2.27E-11 exp(435/T)	9.68E-11
559	TERP + O3 = 0.078 HO2 + 0.046 XHO2 + 0.499 OH + 0.202 XMC3 + 0.059 XRC3 + 0.49 RO2C + 0.121 RO2X + 0.121 ZRN3 + 0.249 CO + 0.063 CO2 + 0.127 HCHO + 0.033 XHCH + 0.208 XRCH + 0.057 XACE + 0.002 MEK + 0.172 FACD + 0.068 PACD + 0.003 XMGL + 0.039 XBAC + 0.002 XMAC + 0.001 XIPR + 0.502 PRD2 + 0.428 Y6PX + 3.852 XC	k = 8.28E-16 exp(-785/T)	6.05E-17
560	TERP + NO3 = 0.227 XHO2 + 0.287 XNO2 + 0.026 XRC3 + 1.786 RO2C + 0.46 RO2X + 0.46 ZRN3 + 0.012 XCO + 0.023 XHCH + 0.002 XGLD + 0.403 XRCH + 0.239 XACE + 0.005 XMAC + 0.001 XMVK + 0.004 XIPR + 0.228 XRN3 + Y6PX + 0.485 XN + 3.785 XC	k = 1.33E-12 exp(490/T)	6.81E-12
561	TERP + O3P = 0.237 RCHO + 0.763 PRD2 + 4.711 XC	k = 4.02E-11	4.02E-11

Number	Reactants and Products	Rate Constant Expression	k_{300}
562	SESQ + OH = 0.734 XHO2 + 0.064 XRC3 + 1.211 RO2C + 0.201 RO2X + 0.201 ZRN3 + 0.001 XCO + 0.411 XHCH + 0.385 XRCH + 0.037 XACE + 0.007 XMEK + 0.003 XMGL + 0.009 XBAC + 0.003 XMVK + 0.002 XIPR + 0.409 XPD2 + Y6PX + 9.375 XC	k = k(558)	9.68E-11
563	SESQ + O3 = 0.078 HO2 + 0.046 XHO2 + 0.499 OH + 0.202 XMC3 + 0.059 XRC3 + 0.49 RO2C + 0.121 RO2X + 0.121 ZRN3 + 0.249 CO + 0.063 CO2 + 0.127 HCHO + 0.033 XHCH + 0.208 XRCH + 0.057 XACE + 0.002 MEK + 0.172 FACD + 0.068 PACD + 0.003 XMGL + 0.039 XBAC + 0.002 XMAC + 0.001 XIPR + 0.502 PRD2 + 0.428 Y6PX + 8.852 XC	k = k(559)	6.05E-17
564	SESQ + NO3 = 0.227 XHO2 + 0.287 XNO2 + 0.026 XRC3 + 1.786 RO2C + 0.46 RO2X + 0.46 ZRN3 + 0.012 XCO + 0.023 XHCH + 0.002 XCCH + 0.403 XRCH + 0.239 XACE + 0.005 XMAC + 0.001 XMVK + 0.004 XIPR + 0.228 XRN3 + Y6PX + 0.485 XN + 8.785 XC	k = k(560)	6.81E-12
565	SESQ + O3P = 0.237 RCHO + 0.763 PRD2 + 9.711 XC	k = k(561)	4.02E-11

Table S8. Explicit species in the SAPRC07TC mechanism.

Species Name	Description
BD13	1,3-butadiene
AACD	Acetic acid
ACET	Acetone
ACRO	Acrolein
ACYE	Acetylene
AFG1	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form radicals
AFG2	Lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form non-radical products
AFG3	Lumped diunsaturatred dicarbonyl aromatic fragmentation product.
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 2 and 5E2 ppm^{-1} min^{-1}. (Primarily ethane)
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 5E2 and 2.5E3 ppm^{-1} min^{-1}. (Primarily propane and acetylene)
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 2.5E3 and 5E3 ppm^{-1} min^{-1}.
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} between 5E3 and 1E4 ppm^{-1} min^{-1}.
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have k_{OH} greater than 1E4 ppm^{-1} min^{-1}.
APIN	α-pinene
ARO1	Aromatics with k_{OH} < 2E4 ppm^{-1} min^{-1}.
ARO2	Aromatics with k_{OH} > 2E4 ppm^{-1} min^{-1}.
B124	1,2,4-trimethyl benzene
BACL	Biacetyl
BALD	Aromatic aldehydes (e.g., benzaldehyde)
BENZ	Benzene
BZC3	Peroxyacyl radical formed from Aromatic Aldehydes
BZO	Phenoxy Radicals
CCHO	Acetaldehyde
CO3H	Peroxyacetic acid
CH4	Methane
CO	Carbon Monoxide
CO2	Carbon Dioxide
COOH	Methyl Hydroperoxide
CRES	Phenols and Cresols
ETHE	Ethene
ETOH	Ethanol
FACD	Formic Acid
GLY	Glyoxal
H2	Hydrogen
H2O	Water
HCHO	Formaldehyde
HNO3	Nitric Acid
PNA	Peroxynitric Acid
HO2	Hydroperoxide Radicals
H2O2	Hydrogen Peroxide
GLYD	Glycolaldehyde

Species Name	Description
HONO	Nitrous Acid
IPRD	Lumped isoprene product species
ISOP	Isoprene
M	Atmospheric pressure
MAC3	Peroxyacyl radicals formed from methacrolein and other acroleins.
MACR	Methacrolein
MPAN	PAN analogue formed from Methacrolein
MCO3	Acetyl Peroxy Radicals
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5E-13 but slower than 5E-12 cm^3 $molec^{-2}$ sec^{-1}. (Based on mechanism for methyl ethyl ketone).
MEO2	Methyl Peroxy Radicals
MEOH	Methanol
MGLY	Methyl Glyoxal
MVK	Methyl Vinyl Ketone
MXYL	m-xylene
N2O5	Nitrogen Pentoxide
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
NPHE	Nitrophenols
O1D	Excited Oxygen Atoms
O2	Oxygen
O3	Ozone
O3P	Ground State Oxygen Atoms
OH	Hydroxyl Radicals
OLE1	Alkenes (other than ethene) with k_{OH} < 7E4 ppm^{-1} min^{-1}.
OLE2	Alkenes with k_{OH} > 7E4 ppm^{-1} min^{-1}.
OXYL	o-xylene
PACD	Propanoic acid
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
PBZN	PAN analogues formed from Aromatic Aldehydes
PRD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5E-12 cm^3 $molec^{-2}$ sec^{-1}
PRPE	Propene
PXYL	p-xylene
R6PX	Lumped organic hydroperoxides with 5 or more carbons (other than those formed following OH addition to aromatic rings, which is reprsented separately). Mechanism based on that estimated for 3-hexyl hydroperoxide.
RAPX	Organic hydroperoxides formed following OH addition to aromatic rings, which is reprsented separately because of their probable role in SOA formation. Mechanism based on two isomers expected to be formed in the m-xylene system.
RCHO	Lumped C3+ Aldehydes (mechanism based on propionaldehyde)
RCO3	Peroxy Propionyl and higher peroxy acyl Radicals
RO3H	Higher organic peroxy acids (mechanism based on peroxypropionic acid).
RNO3	Lumped Organic Nitrates

Species Name	Description
RO2C	Peroxy Radical Operator representing NO to NO2 and NO3 to NO2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals.
RO2X	Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO3, acyl peroxy radicals, and other peroxy radicals.
ROOH	Lumped organic hydroperoxides with 2-4 carbons. Mechanism based on that estimated for n-propyl hydroperoxide.
SESQ	Sesquiterpenes
SO2	Sulfur Dioxide
SULF	Sulfates (SO3 or H2SO4)
TBUO	t-Butoxy Radicals
TERP	Terpenes
TOLU	Toluene
XACE	As for xHO2
XACR	As for xHO2
XAF1	As for xHO2
XAF2	As for xHO2
XAF3	As for xHO2
XBAC	As for xHO2
XBAL	As for xHO2
XC	Lost Carbon or carbon in unreactive products
XCCH	As for xHO2
XCO	As for xHO2
XGLY	As for xHO2
XHCH	As for xHO2
XHO2	Formation of HO2 from alkoxy radicals formed in peroxy radical reactions with NO and NO3 (100% yields) and RO2 (50% yields)
XGLD	As for xHO2
XIPR	As for xHO2
XMA3	As for xHO2
XMAC	As for xHO2
XMC3	As for xHO2
XMEK	As for xHO2
XMEO	As for xHO2
XMGL	As for xHO2
XMVK	As for xHO2
XN	Lost Nitrogen or nitrogen in unreactive products
XNO2	As for xHO2
XOH	As for xHO2
XPD2	As for xHO2
XRCH	As for xHO2
XRC3	As for xHO2
XRN3	As for xHO2
XTBU	As for xHO2
Y6PX	As for ROOH, but for R6PX
YAPX	As for ROOH, but for RAPX
YRPX	Formation of ROOH following RO2 + HO2 reactions
ZRN3	Formation of RNO3 in the RO2 + NO, reaction.