Contents:

1. Appendix table

No.	Species	Definition	Molecular Weight
3	NO	Nitric oxide	30
3a	^{15}NO		31
4	NO_2	Nitrogen dioxide	46
4a	$^{15}NO_2$		47
5	NO_3	Nitrogen trioxide	62
5a	$^{15}NO_3$		63
6	N_2O_5	Dinitrogen pentoxide	108
6a	$^{15}NNO_5$		109
6b	$^{15}N_2O_5$		110
7	HONO	Nitrous acid	47
7a	$HO^{15}NO$		48
8	HNO_3	Nitric acid	63
8a	$H^{15}NO_3$		64
9	HNO_4	Pernitric acid	79
9a	$H^{15}NO_4$		80
14	N_2	Nitrogen	28
14a	^{15}NN		29
14b	$^{15}N_2$		30
46	ONIT	Organic nitrate	119
46a	^{15}ONIT		120
47	PAN	Peroxyacyl nitrate and higher saturated PANs	121
47a	^{15}PAN		122
48	TPAN	Unsaturated PANs	147
48a	^{15}TPAN		148
75	OLNN	NO_3-alkene adduct reacting to form carbonitrates + HO2	136
75a	^{15}OLNN		137
76	OLND	NO_3-alkene adduct reacting via decomposition	136
76a	^{15}OLND		137

Table S1a: ^{14}N and ^{15}N species

No.	Species	Definition	Molecular Weight
37	HCHO	Formaldehyde	30
38	ALD	Acetaldehyde and higher aldehydes	44
40	GLY	Glyoxal	58
43	MACR	Methacrolein and other unsaturated monoaldehydes	70
41	MGLY	Methylglyxal and other α-carbonyl aldehydes	72
42	DCB	unsaturated dicarbonyls	87
36	CSL	cresol and other hydroxy substituted aromatics	108

Table S1b: Hydrocarbon species

Reaction No.	Reaction	Photolysis Frequency, s-1	Cross Section	Quantum Yield	α
R1	NO_2 --> O^3P + NO	7.50 x 10^{-3}	DeMoretal. [1994]	DeMoretal. [1994]	1
R1a	$^{15}NO_2$ --> O^3P + ^{15}NO	7.50 x 10^{-3}	DeMoretal. [1994]	DeMoretal. [1994]	1.0042
R4	HONO --> HO + NO	1.63 x 10^{-3}	DeMoretal. [1994]	DeMoretal. [1995]	1
R4a	HO^{15}NO --> HO + ^{15}NO	1.63 x 10^{-3}	DeMoretal. [1994]	DeMoretal. [1996]	1
R5	HNO_3 --> HO + NO_2	4.50 x 10^{-7}	DeMoretal. [1994]	assumedto be unity	1
R5a	H$^{15}NO_3$ --> HO + $^{15}NO_2$	4.50 x 10^{-7}	DeMoretal. [1994]	assumedto be unity	1
R6	HNO_4 --> 0.65 HO_2 + 0.65 NO_2 + 0.35 HO + 0.35 NO_3	3.17 x 10^{-6}	DeMoretal. [1994]	assumedto be unity	1
R6a	H$^{15}NO_4$ --> 0.65 HO_2 + 0.65 $^{15}NO_2$ + 0.35 HO + 0.35 $^{15}NO_3$	3.17 x 10^{-6}	DeMoretal. [1994]	assumedto be unity	1
R7	NO_3--> NO + O_2	2.33 x 10^{-2}	Waynetal. [1991]	Waynetal. [1992]	1
R7a	$^{15}NO_3$--> ^{15}NO + O_2	2.33 x 10^{-2}	Waynetal. [1991]	Waynetal. [1992]	1
R8	NO_3 --> NO_2 + O^3P	1.87 x 10^{-1}	Waynetal. [1991]	Waynetal. [1992]	1
R8a	$^{15}NO_3$ --> $^{15}NO_2$ + O^3P	1.87 x 10^{-1}	Waynetal. [1991]	Waynetal. [1992]	1

Table S2a: Photolysis reactions involving N compounds

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R, K	k	α
R26	$O^1D + N_2 \rightarrow O^3P + N_2$	1.80×10^{-11}	-110	2.60×10^{-11}	1
R26a	$O^1D + {}^{15}NN \rightarrow O^3P + {}^{15}NN$	1.80×10^{-11}	-110	2.60×10^{-11}	1
R35	$O^3P + NO \rightarrow NO_2$	Table S2d		1.66×10^{-12}	1
R35a	$O^3P + {}^{15}NO \rightarrow {}^{15}NO_2$	Table S2d		1.66×10^{-12}	1
R36	$O^3P + NO_2 \rightarrow NO + O_2$	6.50×10^{-12}	-120	9.72×10^{-12}	1
R36a	$O^3P + {}^{15}NO_2 \rightarrow {}^{15}NO + O_2$	6.50×10^{-12}	-120	9.72×10^{-12}	1
R37	$O^3P + NO_2 \rightarrow NO_3$	Table S2d		1.58×10^{-12}	1
R37a	$O^3P + {}^{15}NO_2 \rightarrow {}^{15}NO_3$	Table S2d		1.58×10^{-12}	1
R38	$HO + NO \rightarrow HONO$	Table S2d		1.58×10^{-12}	1
R38a	$HO + {}^{15}NO \rightarrow HO{}^{15}NO$	Table S2d		1.58×10^{-12}	1
R39	$HO + NO_2 \rightarrow HNO_3$	Table S2d		1.58×10^{-12}	1
R39a	$HO + {}^{15}NO_2 \rightarrow H{}^{15}NO_3$	Table S2d		1.58×10^{-12}	1.04
R40	$HO + NO_3 \rightarrow NO_2 + HO_2$	2.20×10^{-11}		2.20×10^{-11}	1
R40a	$HO + {}^{15}NO_3 \rightarrow {}^{15}NO_2 + HO_2$	2.20×10^{-11}		2.20×10^{-11}	1
R41	$HO_2 + NO \rightarrow NO_2 + HO$	3.70×10^{-12}	-250	8.56×10^{-12}	1
R41a	$HO_2 + {}^{15}NO \rightarrow {}^{15}NO_2 + HO$	3.70×10^{-12}	-250	8.56×10^{-12}	1

R42	$HO_2 + NO_2$ --> HNO_4	Table S2d		1.39 x 10^{-12}	1
R42a	$HO_2 + {}^{15}NO_2$ --> $H{}^{15}NO_4$	Table S2d		1.39 x 10^{-12}	1
R43	HNO4 --> $HO_2 + NO_2$	Table S2e		8.62 x 10^{-2}	1
R43a	$H{}^{15}NO4$ --> $HO_2 + {}^{15}NO_2$	Table S2e		8.62 x 10^{-2}	1
R44	$HO_2 + NO_3$--> 0.3 HNO_3 + 0.7 NO_2 + 0.7 HO + O_2	3.50 x 10^{-12}		3.50 x 10^{-12}	1
R44a	$HO_2 + {}^{15}NO_3$--> 0.3 $H{}^{15}NO_3$ + 0.7 $^{15}NO_2$ + 0.7 HO + O_2	3.50 x 10^{-12}		3.50 x 10^{-12}	1
R45	HO + HONO --> $NO_2 + H_2O$	1.80 x 10^{-11}	390	4.86 x 10^{-12}	1
R45a	HO + $HO{}^{15}NO$ --> $^{15}NO_2$ + H_2O	1.80 x 10^{-11}	390	4.86 x 10^{-12}	1
R46	HO + HNO_3 --> $NO_3 + H_2O$	Table S2f		1.47 x 10^{-13}	1
R46a	HO + $H{}^{15}NO_3$ --> $^{15}NO_3$ + H_2O	Table S2f		1.47 x 10^{-13}	1
R47	HO + HNO_4 --> NO_2+ O_2 + H_2O	1.30 x 10^{-12}	-380	4.65 x 10^{-12}	1
R47a	HO + $H{}^{15}NO_4$ --> $^{15}NO_2$+ O_2 + H_2O	1.30 x 10^{-12}	-380	4.65 x 10^{-12}	1
R48	O_3 + NO --> $NO_2 + O_2$	2.00 x 10^{-12}	1400	1.82 x 10^{-14}	1
R48a	$O_3 + {}^{15}NO$ --> $^{15}NO_2 + O_2$	2.00 x 10^{-12}	1400	1.82 x 10^{-14}	0.9933
R49	$O_3 + NO_2$ --> $NO_3 + O_2$	1.20 x 10^{-13}	2450	3.23 x 10^{-17}	1
R49a	$O_3 + {}^{15}NO_2$ --> $^{15}NO_3 + O_2$	1.20 x 10^{-13}	2450	3.23 x 10^{-17}	1
R50	NO + NO + O_2 --> NO_2 + NO_2	3.30 x 10^{-39}	-530	1.95 x 10^{-38}	1

R50a	$NO + {}^{15}NO + O_2 \rightarrow NO_2 + {}^{15}NO_2$	3.30×10^{-39}	-530	1.95×10^{-38}	1
R50b	${}^{15}NO + {}^{15}NO + O_2 \rightarrow {}^{15}NO_2 + {}^{15}NO_2$	3.30×10^{-39}	-530	1.95×10^{-38}	1
R51	$NO_3 + NO \rightarrow NO_2 + NO_2$	1.50×10^{-11}	-170	2.65×10^{-11}	1
R51a	${}^{15}NO_3 + NO \rightarrow NO_2 + {}^{15}NO_2$	1.50×10^{-11}	-170	2.65×10^{-11}	1
R51b	$NO_3 + {}^{15}NO \rightarrow NO_2 + {}^{15}NO_2$	1.50×10^{-11}	-170	2.65×10^{-11}	1
R51c	${}^{15}NO_3 + {}^{15}NO \rightarrow {}^{15}NO_2 + {}^{15}NO_2$	1.50×10^{-11}	-170	2.65×10^{-11}	1
R52	$NO_3 + NO_2 \rightarrow NO + NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	1
R52a	$NO_3 + {}^{15}NO_2 \rightarrow {}^{15}NO + NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	0.5
R52b	$NO_3 + {}^{15}NO_2 \rightarrow NO + {}^{15}NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	0.5
R52c	${}^{15}NO_3 + NO_2 \rightarrow {}^{15}NO + NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	0.5
R52d	${}^{15}NO_3 + NO_2 \rightarrow NO + {}^{15}NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	0.5
R52e	${}^{15}NO_3 + {}^{15}NO_2 \rightarrow {}^{15}NO + {}^{15}NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}	1
R53	$NO_3 + NO_2 \rightarrow N_2O_5$	Table S2d		1.27×10^{-12}	1
R53a	$NO_3 + {}^{15}NO_2 \rightarrow {}^{15}NNO_5$	Table S2d		1.27×10^{-12}	1.0266
R53b	${}^{15}NO_3 + NO_2 \rightarrow {}^{15}NNO_5$	Table S2d		1.27×10^{-12}	1.0309
R53c	${}^{15}NO_3 + {}^{15}NO_2 \rightarrow {}^{15}N_2O_5$	Table S2d		1.27×10^{-12}	1.057
R54	$N_2O_5 \rightarrow NO_2 + NO_3$	Table S2e		4.36×10^{-2}	1
R54a	${}^{15}NNO_5 \rightarrow {}^{15}NO_2 + NO_3$	Table S2e		4.36×10^{-2}	0.5
R54b	${}^{15}NNO_5 \rightarrow NO_2 + {}^{15}NO_3$	Table S2e		4.36×10^{-2}	0.5

R54c	$^{15}N_2O_5$ --> $^{15}NO_2$ + $^{15}NO_3$	Table S2e		4.36 x 10^{-2}	1
R55	NO_3 + NO_3 --> NO_2 + NO_2 + O_2	8.50 x 10^{-13}	2450	2.29 x 10^{-16}	1
R55a	NO_3 + $15NO_3$ --> NO_2 + $^{15}NO_2$ + O_2	8.50 x 10^{-13}	2450	2.29 x 10^{-16}	1
R55b	$^{15}NO_3$ + $^{15}NO_3$ --> $^{15}NO_2$ + $^{15}NO_2$ + O_2	8.50 x 10^{-13}	2450	2.29 x 10^{-16}	1
R88	PAN + HO --> HCHO + XO_2 + H_2O + NO_3	4.00 x 10^{-14}		4.00 x 10^{-14}	1
R88a	^{15}PAN + HO --> HCHO + XO_2 + H_2O + $^{15}NO_3$	4.00 x 10^{-14}		4.00 x 10^{-14}	1
R89	TPAN + HO --> 0.60 HKET + 0.40 HCHO + 0.40 HO_2 + XO_2 + 0.40 PAN + 0.60 NO_3	3.25 x 10^{-13}	-500	1.74 x 10^{-12}	1
R89a	^{15}TPAN + HO --> 0.60 HKET + 0.40 HCHO + 0.40 HO_2 + XO_2 + 0.40 ^{15}PAN + 0.60 $^{15}NO_3$	3.25 x 10^{-13}	-500	1.74 x 10^{-12}	1
R90	ONIT + HO --> HC3P + NO_2 + H_2O	5.31 x 10^{-12}	260	2.22 x 10^{-12}	1
R90a	^{15}ONIT + HO --> HC3P + $^{15}NO_2$ + H_2O	5.31 x 10^{-12}	260	2.22 x 10^{-12}	1
R91	HCHO + NO_3 --> HO_2 + HNO_3 + CO	3.40 x 10^{-13}	1900	5.79 x 10^{-16}	1
R91a	HCHO + $^{15}NO_3$ --> HO_2 + H$^{15}NO_3$ + CO	3.40 x 10^{-13}	1900	5.79 x 10^{-16}	0.9974
R92	ALD + NO_3 --> ACO_3 + HNO_3	1.40 x 10^{-12}	1900	2.38 x 10^{-15}	1
R92a	ALD + $^{15}NO_3$ --> ACO_3 + H$^{15}NO_3$	1.40 x 10^{-12}	1900	2.38 x 10^{-15}	0.9967
R93	GLY + NO_3 --> HNO_3 + HO_2 + 2 CO	2.90 x 10^{-12}	1900	4.94 x 10^{-15}	1
R93a	GLY + $^{15}NO_3$ --> H$^{15}NO_3$ + HO_2 + 2 CO	2.90 x 10^{-12}	1900	4.94 x 10^{-15}	0.9962

R94	MGLY + NO_3 --> HNO_3 + ACO_3 + CO	1.40 x 10^{-12}	1900	2.38 x 10^{-15}	1
R94a	MGLY + $^{15}NO_3$ --> $H^{15}NO_3$ + ACO_3 + CO	1.40 x 10^{-12}	1900	2.38 x 10^{-15}	0.9957
R95	MACR + NO_3 --> 0.20 TCO_3 + 0.20 HNO_3 + 0.80 OLNN + 0.80 CO	8.27 x 10^{-15}	150	5.00 x 10^{-15}	1
R95a	MACR + $^{15}NO_3$ --> 0.20 TCO_3 + 0.20 $H^{15}NO_3$ + 0.80 ^{15}OLNN + 0.80 CO	8.27 x 10^{-15}	150	5.00 x 10^{-15}	0.9958
R96	DCB + NO_3 --> 0.50 TCO_3 + 0.50 HO_2 + 0.50 XO_2 + 0.25 GLY + 0.25 ALD + 0.03 KET + 0.25 MGLY + 0.5 HNO_3 + 0.5 NO_2	2.87 x 10^{-13}	1000	1.00 x 10^{-14}	1
R96a	DCB + $^{15}NO_3$ --> 0.50 TCO_3 + 0.50 HO_2 + 0.50 XO_2 + 0.25 GLY + 0.25 ALD + 0.03 KET + 0.25 MGLY + 0.5 $H^{15}NO_3$ + 0.5 $^{15}NO_2$	2.87 x 10^{-13}	1000	1.00 x 10^{-14}	0.9954
R97	CSL + NO_3 --> HNO_3 + PHO	2.20 x 10^{-11}		2.20 x 10^{-11}	1
R97a	CSL + $^{15}NO_3$ --> $H^{15}NO_3$ + PHO	2.20 x 10^{-11}		2.20 x 10^{-11}	0.9949
R98	ETE + NO_3 --> 0.80 OLNN + 0.20 OLND	Table S2c		2.05 x 10^{-16}	1
R98a	ETE + $^{15}NO_3$ --> 0.80 ^{15}OLNN + 0.20 ^{15}OLND	Table S2c		2.05 x 10^{-16}	1
R99	OLT + NO_3 --> 0.43 OLNN + 0.57 OLND	1.79 x 10^{-13}	450	3.95 x 10^{-14}	1
R99a	OLT + $^{15}NO_3$ --> ^{15}0.43 OLNN + 0.57 ^{15}OLND	1.79 x 10^{-13}	450	3.95 x 10^{-14}	1
R100	OLI + NO_3 --> 0.11 OLNN + 0.89 OLND	8.64 x 10^{-13}	-450	3.91 x 10^{-12}	1

R100a	OLI + $^{15}NO_3$ --> 0.11 ^{15}OLNN + 0.89 ^{15}OLND	8.64 x 10^{-13}	-450	3.91 x 10^{-12}	1
R101	DIEN + NO_3 --> 0.90 OLNN + 0.10 OLND + 0.90 MACR	1.0 x 10^{-13}		1.0 x 10^{-13}	1
R101a	DIEN + $^{15}NO_3$ --> 0.90 ^{15}OLNN + 0.10 ^{15}OLND + 0.90 MACR	1.0 x 10^{-13}		1.0 x 10^{-13}	1
R102	ISO + NO_3 --> 0.90 OLNN + 0.10 OLND + 0.90 MACR	4.00 x 10^{-12}	446	8.96 x 10^{-13}	1
R102a	ISO + $^{15}NO_3$ --> 0.90 ^{15}OLNN + 0.10 ^{15}OLND + 0.90 MACR	4.00 x 10^{-12}	446	8.96 x 10^{-13}	1
R103	API + NO_3 --> 0.10 OLNN + 0.90 OLND	1.19 x 10^{-12}	-490	6.16 x 10^{-12}	1
R103a	API + $^{15}NO_3$ --> 0.10 ^{15}OLNN + 0.90 ^{15}OLND	1.19 x 10^{-12}	-490	6.16 x 10^{-12}	1
R104	LIM + NO_3 --> 0.13 OLNN + 0.87 OLND	1.22 x 10^{-11}		1.22 x 10^{-11}	1
R104a	LIM + $^{15}NO_3$ --> 0.13 ^{15}OLNN + 0.87 ^{15}OLND	1.22 x 10^{-11}		1.22 x 10^{-11}	1
R105	TPAN + NO_3 --> 0.60 ONIT + 0.60 NO_3 + 0.40 PAN + 0.40 HCHO + 0.40 NO_2 + XO_2	2.20 x 10^{-14}	500	4.11 x 10^{-15}	1
R105a	TPAN + $^{15}NO_3$ --> 0.30 ONIT + 0.30 ^{15}ONIT + 0.30 NO_3 + 0.30 $^{15}NO_3$ + 0.20 PAN + 0.20 ^{15}PAN + 0.40 HCHO + 0.20 NO_2 + 0.20 $^{15}NO_2$ + XO_2	2.20 x 10^{-14}	500	4.11 x 10^{-15}	1
R105b	^{15}TPAN + $^{15}NO_3$ --> 0.60 ^{15}ONIT + 0.60 $^{15}NO_3$ + 0.40 ^{15}PAN + 0.40 HCHO + 0.40 $^{15}NO_2$ + XO_2	2.20 x 10^{-14}	500	4.11 x 10^{-15}	1

R115	TPAN + O_3 --> 0.70 HCHO + 0.30 PAN + 0.70 NO_2 + 0.13 CO + 0.04 H_2 + 0.11 ORA1 + 0.08 HO_2 + 0.036 HO + 0.70 ACO_3	2.46 x 10^{-15}	1700	8.19 x 10^{-18}	1
R115a	^{15}TPAN + O_3 --> 0.70 HCHO + 0.30 ^{15}PAN + 0.70 $^{15}NO_2$ + 0.13 CO + 0.04 H_2 + 0.11 ORA1 + 0.08 HO_2 + 0.036 HO + 0.70 ACO_3	2.46 x 10^{-15}	1700	8.19 x 10^{-18}	1
R116	PHO + NO_2 --> 0.10 CSL + ONIT	2.00 x 10^{-11}		2.00 x 10^{-11}	1
R116a	PHO + $^{15}NO_2$ --> 0.10 CSL + ^{15}ONIT	2.00 x 10^{-11}		2.00 x 10^{-11}	1
R117	ADDT + NO_2 --> CSL + HONO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R117a	ADDT + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R121	ADDX + NO_2 --> CSL + HONO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R121a	ADDX + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R124	ADDC + NO_2 --> CSL + HONO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R124a	ADDC + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60 x 10^{-11}		3.60 x 10^{-11}	1
R127	ACO_3 + NO_2 --> PAN	Table S2d		8.66 x 10^{-12}	1
R127a	ACO_3 + $^{15}NO_2$ --> ^{15}PAN	Table S2d		8.66 x 10^{-12}	1
R128	PAN --> ACO_3 + NO_2	Table S2e		4.63 x 10^{-4}	1
R128a	^{15}PAN --> ACO_3 + $^{15}NO_2$	Table S2e		4.63 x 10^{-4}	1

R129	$TCO_3 + NO_2$ --> TPAN	Table S2d		8.66 x 10^{-12}	1
R129a	$TCO_3 + {}^{15}NO_2$ --> ^{15}TPAN	Table S2d		8.66 x 10^{-12}	1
R130	TPAN --> $TCO_3 + NO_2$	Table S2e		4.63 x 10^{-4}	1
R130a	^{15}TPAN --> $TCO_3 + {}^{15}NO_2$	Table S2e		4.63 x 10^{-4}	1
R131	MO_2 + NO --> HCHO + HO_2 + NO_2	4.2 x 10^{-12}	-180	7.68 x 10^{-12}	1
R131a	$MO_2 + {}^{15}$NO --> HCHO + $HO_2 + {}^{15}NO_2$	4.2 x 10^{-12}	-180	7.68 x 10^{-12}	1
R132	ETHP + NO --> ALD + HO_2 + NO_2	8.7 x 10^{-12}		8.7 x 10^{-12}	1
R132a	ETHP + ^{15}NO --> ALD + $HO_2 + {}^{15}NO_2$	8.7 x 10^{-12}		8.7 x 10^{-12}	1
R133	HC3P + NO --> 0.047 HCHO + 0.233 ALD + 0.623 KET + 0.063 GLY + 0.742 HO_2 + 0.15 MO_2 + 0.048 ETHP + 0.048 XO_2 + 0.059 ONIT + 0.941 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R133a	HC3P + ^{15}NO --> 0.047 HCHO + 0.233 ALD + 0.623 KET + 0.063 GLY + 0.742 HO_2 + 0.15 MO_2 + 0.048 ETHP + 0.048 XO_2 + 0.059 ^{15}ONIT + 0.941 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R134	HC5P + NO --> 0.021 HCHO + 0.211 ALD + 0.722 KET + 0.599 HO_2 + 0.031 MO_2 + 0.245 ETHP + 0.334XO_2 + 0.124 ONIT + 0.876 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1

R134a	HC5P + ^{15}NO --> 0.021 HCHO + 0.211 ALD + 0.722 KET + 0.599 HO_2 + 0.031 MO_2 + 0.245 ETHP + 0.334XO_2 + 0.124 ^{15}ONIT + 0.876 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R135	HC8P + NO --> 0.15 ALD + 0.642 KET + 0.133 ETHP + 0.261 ONIT + 0.739 NO_2 + 0.606 HO_2 + 0.416 XO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R135a	HC8P + ^{15}NO --> 0.15 ALD + 0.642 KET + 0.133 ETHP + 0.261 ^{15}ONIT + 0.739 $^{15}NO_2$ + 0.606 HO_2 + 0.416 XO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R136	ETEP + NO --> 1.6 HCHO + HO_2 + NO_2 + 0.2 ALD	9.0 x 10^{-12}		9.0 x 10^{-12}	1
R136a	ETEP + ^{15}NO --> 1.6 HCHO + HO_2 + $^{15}NO_2$ + 0.2 ALD	9.0 x 10^{-12}		9.0 x 10^{-12}	1
R137	OLTP + NO --> 0.94 ALD + HCHO + HO_2 + NO_2 + 0.06 KET	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R137a	OLTP + ^{15}NO --> 0.94 ALD + HCHO + HO_2 + $^{15}NO_2$ + 0.06 KET	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R138	OLIP + NO --> HO2 + 1.71 ALD + 0.29 KET + NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R138a	OLIP + ^{15}NO --> HO2 + 1.71 ALD + 0.29 KET + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R139	ISOP + NO --> 0.446 MACR + 0.354 OLT + 0.847 HO_2 + 0.606 HCHO + 0.153 ONIT + 0.847 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1

R139a	ISOP + ^{15}NO --> 0.446 MACR + 0.354 OLT + 0.847 HO_2 + 0.606 HCHO + 0.153 ^{15}ONIT + 0.847 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R140	APIP + NO --> 0.80 HO_2 + 0.80 ALD + 0.80 KET + 0.20 ONIT + 0.80 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R140a	APIP + ^{15}NO --> 0.80 HO_2 + 0.80 ALD + 0.80 KET + 0.20 ^{15}ONIT + 0.80 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R141	LIMP + NO --> 0.65 HO_2 + 0.40 MACR + 0.25 OLI + 0.25 HCHO + 0.35 ONIT + 0.65 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R141a	LIMP + ^{15}NO --> 0.65 HO_2 + 0.40 MACR + 0.25 OLI + 0.25 HCHO + 0.35 ^{15}ONIT + 0.65 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R142	TOLP + NO --> 0.95 NO_2 + 0.95 HO_2 + 0.65 MGLY + 1.20 GLY + 0.50 DCB + 0.05 ONIT	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R142a	TOLP + ^{15}NO --> 0.95 $^{15}NO_2$ + 0.95 HO_2 + 0.65 MGLY + 1.20 GLY + 0.50 DCB + 0.05 ^{15}ONIT	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R143	XYLP + NO --> 0.95 NO_2 + 0.95 HO_2 + 0.60 MGLY + 0.35 GLY + 0.95 DCB + 0.05 ONIT	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R143a	XYLP + ^{15}NO --> 0.95 $^{15}NO_2$ + 0.95 HO_2 + 0.60 MGLY + 0.35 GLY + 0.95 DCB + 0.05 ^{15}ONIT	4.0 x 10^{-12}		4.0 x 10^{-12}	1

R144	CSLP + NO --> GLY + MGLY + HO_2 + NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R144a	CSLP + ^{15}NO --> GLY + MGLY + HO_2 + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R145	ACO_3 + NO --> MO_2 + NO_2	2.0 x 10^{-11}		2.0 x 10^{-11}	1
R145a	ACO_3 + ^{15}NO --> MO_2 + $^{15}NO_2$	2.0 x 10^{-11}		2.0 x 10^{-11}	1
R146	TCO_3 + NO --> ACO_3 + HCHO + NO_2	2.0 x 10^{-11}		2.0 x 10^{-11}	1
R146a	TCO_3 + ^{15}NO --> ACO_3 + HCHO + $^{15}NO_2$	2.0 x 10^{-11}		2.0 x 10^{-11}	1
R147	KETP + NO --> 0.54 MGLY + 0.46 ALD + 0.23 ACO_3 + 0.77 HO_2 + 0.16XO_2 + NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R147a	KETP + ^{15}NO --> 0.54 MGLY + 0.46 ALD + 0.23 ACO_3 + 0.77 HO_2 + 0.16XO_2 + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R148	OLNN + NO --> HO2 + ONIT + NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R148a	^{15}OLNN + NO --> HO_2 + 0.5 ^{15}ONIT + 0.5 NO_2 + 0.5 ONIT + 0.5 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R148b	OLNN + ^{15}NO --> HO_2 + 0.5 ONIT + 0.5 $^{15}NO_2$ + 0.5 ^{15}ONIT + 0.5 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R148c	^{15}OLNN + ^{15}NO --> HO_2 + ^{15}ONIT + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R149	OLND + NO --> 0.287 HCHO + 1.24 ALD + 0.464 KET + 2 NO_2	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R149a	OLND + ^{15}NO --> 0.287 HCHO + 1.24 ALD + 0.464 KET + NO_2 + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1

R149b	^{15}OLND + NO --> 0.287 HCHO + 1.24 ALD + 0.464 KET + NO_2 + $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R149c	^{15}OLND + ^{15}NO --> 0.287 HCHO + 1.24 ALD + 0.464 KET + 2 $^{15}NO_2$	4.0 x 10^{-12}		4.0 x 10^{-12}	1
R169	OLNN + HO_2 --> ONIT	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R169a	^{15}OLNN + HO_2 --> ^{15}ONIT	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R170	OLND + HO_2 --> ONIT	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R170a	^{15}OLND + HO_2 --> ^{15}ONIT	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R190	OLNN + MO_2 --> 0.75 HCHO + HO_2 + ONIT	1.60 x 10^{-13}	-708	1.72 x 10^{-12}	1
R190a	^{15}OLNN + MO_2 --> 0.75 HCHO + HO_2 + ^{15}ONIT	1.60 x 10^{-13}	-708	1.72 x 10^{-12}	1
R191	OLND + MO_2 --> 0.96 HCHO + 0.5 HO_2 + 0.64 ALD + 0.149 KET + 0.5 NO_2 + 0.5 ONIT	9.68 x 10^{-14}	-708	1.04 x 10^{-12}	1
R191a	^{15}OLND + MO_2 --> 0.96 HCHO + 0.5 HO_2 + 0.64 ALD + 0.149 KET + 0.5 $^{15}NO_2$ + 0.5 ^{15}ONIT	9.68 x 10^{-14}	-708	1.04 x 10^{-12}	1
R208	OLNN + ACO_3 --> ONIT + 0.5 ORA2 + 0.5 MO_2 + 0.50 HO_2	8.85 x 10^{-13}	-765	1.15 x 10^{-11}	1
R208a	^{15}OLNN + ACO_3 --> ^{15}ONIT + 0.5 ORA2 + 0.5 MO_2 + 0.50 HO_2	8.85 x 10^{-13}	-765	1.15 x 10^{-11}	1

R209	OLND + ACO_3 --> 0.207 HCHO + 0.65 ALD + 0.167 KET + 0.484 ORA2 + 0.484 ONIT + 0.516 NO_2 + 0.516 MO_2	5.37 x 10^{-13}	-765	7.00 x 10^{-12}	1
R209a	^{15}OLND + ACO_3 --> 0.207 HCHO + 0.65 ALD + 0.167 KET + 0.484 ORA2 + 0.484 ^{15}ONIT + 0.516 $^{15}NO_2$ + 0.516 MO_2	5.37 x 10^{-13}	-765	7.00 x 10^{-12}	1
R210	OLNN + OLNN --> 2 0NIT + HO_2	7.0 x 10^{-14}	-1000	2.00 x 10^{-12}	1
R210a	OLNN + ^{15}OLNN --> ONIT + ^{15}0NIT + HO_2	7.0 x 10^{-14}	-1000	2.00 x 10^{-12}	1
R210b	OLNN + ^{15}OLNN --> 2 ^{15}0NIT + HO_2	7.0 x 10^{-14}	-1000	2.00 x 10^{-12}	1
R211	OLNN + OLND --> 0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO_2 + 1.50 ONIT + 0.50 NO_2	4.25 x 10^{-14}	-1000	1.22 x 10^{-12}	1
R211a	^{15}OLNN + OLND --> 0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO_2 + 0.75 ONIT + 0.75 ^{15}ONIT + 0.25 NO_2 + 0.25 $^{15}NO_2$	4.25 x 10^{-14}	-1000	1.22 x 10^{-12}	1
R211b	OLNN + ^{15}OLND --> 0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO_2 + 0.75 ONIT + 0.75 ^{15}ONIT + 0.25 NO_2 + 0.25 $^{15}NO_2$	4.25 x 10^{-14}	-1000	1.22 x 10^{-12}	1
R211c	^{15}OLNN + ^{15}OLND --> 0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO_2 + 1.50 ^{15}ONIT + 0.50 $^{15}NO_2$	4.25 x 10^{-14}	-1000	1.22 x 10^{-12}	1

R212	OLND + OLND --> 0.504 HCHO + 1.21 ALD + 0.285 KET + ONIT + NO_2	2.96 x 10^{-14}	-1000	8.50 x 10^{-13}	1
R212a	OLND + ^{15}OLND --> 0.504 HCHO + 1.21 ALD + 0.285 KET + ^{15}ONIT + NO_2	2.96 x 10^{-14}	-1000	8.50 x 10^{-13}	1
R212b	OLND + ^{15}OLND --> 0.504 HCHO + 1.21 ALD + 0.285 KET + ONIT + $^{15}NO_2$	2.96 x 10^{-14}	-1000	8.50 x 10^{-13}	1
R212c	^{15}OLND + ^{15}OLND --> 0.504 HCHO + 1.21 ALD + 0.285 KET + ^{15}ONIT + $^{15}NO_2$	2.96 x 10^{-14}	-1000	8.50 x 10^{-13}	1
R213	MO_2 + NO_3 --> HCHO + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R213a	MO_2 + $^{15}NO_3$ --> HCHO + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R214	ETHP + NO_3 --> ALD + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R214a	ETHP + $^{15}NO_3$ --> ALD + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R215	HC3P + NO_3 --> 0.048 HCHO + 0.243 ALD + 0.67 KET + 0.063 GLY + 0.792 HO_2 + 0.155 MO_2 + 0.053 ETHP + 0.051 XO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R215a	HC3P + $^{15}NO_3$ --> 0.048 HCHO + 0.243 ALD + 0.67 KET + 0.063 GLY + 0.792 HO_2 + 0.155 MO_2 + 0.053 ETHP + 0.051 XO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R216	HC5P + NO_3 --> 0.021 HCHO + 0.239 ALD + 0.828 KET + 0.699 HO_2 + 0.04 MO_2 + 0.262 ETHP + 0.391 XO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1

R216a	HC5P + $^{15}NO_3$ --> 0.021 HCHO + 0.239 ALD + 0.828 KET + 0.699 HO_2 + 0.04 MO_2 + 0.262 ETHP + 0.391 XO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R217	HC8P + NO_3 --> 0.187 ALD + 0.88 KET + 0.845 HO_2 + 0.155 ETHP + 0.587 XO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R217a	HC8P + $^{15}NO_3$ --> 0.187 ALD + 0.88 KET + 0.845 HO_2 + 0.155 ETHP + 0.587 XO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R218	ETEP + NO_3 --> 1.6 HCHO + 0.2 ALD + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R218a	ETEP + $^{15}NO_3$ --> 1.6 HCHO + 0.2 ALD + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R219	OLTP + NO_3 --> HCHO + 0.94 ALD + 0.06 KET + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R219a	OLTP + $^{15}NO_3$ --> HCHO + 0.94 ALD + 0.06 KET + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R220	OLIP + NO_3 --> 1.71 ALD + 0.29 KET + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R220a	OLIP + $^{15}NO_3$ --> 1.71 ALD + 0.29 KET + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R221	ISOP + NO_3 --> 0.60 MACR + 0.40 OLT + 0.686 HCHO + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R221a	ISOP + $^{15}NO_3$ --> 0.60 MACR + 0.40 OLT + 0.686 HCHO + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R222	APIP + NO_3 --> ALD + KET + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1

R222a	APIP + $^{15}NO_3$ --> ALD + KET + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R223	LIMP + NO_3 --> 0.60 MACR + 0.40 OLI + 0.40 HCHO + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R223a	LIMP + $^{15}NO_3$ --> 0.60 MACR + 0.40 OLI + 0.40 HCHO + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R224	TOLP + NO_3 --> 0.70 MGLY + 1.30GLY + 0.50 DCB + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R224a	TOLP + $^{15}NO_3$ --> 0.70 MGLY + 1.30GLY + 0.50 DCB + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R225	XYLP + NO_3 --> 1.26 MGLY + 0.74 GLY + DCB + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R225a	XYLP + $^{15}NO_3$ --> 1.26 MGLY + 0.74 GLY + DCB + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R226	CSLP + NO_3 --> GLY + MGLY + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R226a	CSLP + $^{15}NO_3$ --> GLY + MGLY + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R227	ACO3 + NO_3 --> MO_2 + NO_2	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R227a	ACO3 + $^{15}NO_3$ --> MO_2 + $^{15}NO_2$	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R228	TCO3 + NO_3 --> HCHO + ACO_3 + NO_2	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R228a	TCO3 + $^{15}NO_3$ --> HCHO + ACO_3 + $^{15}NO_2$	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R229	KETP + NO_3 --> 0.54 MGLY + 0.46 ALD + 0.77 HO_2 + 0.23 ACO_3 + 0.16 XO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1

R229a	KETP + $^{15}NO_3$ --> 0.54 MGLY + 0.46 ALD + 0.77 HO_2 + 0.23 ACO_3 + 0.16 XO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R230	OLNN + NO_3 --> ONIT + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R230a	OLNN + $^{15}NO_3$ --> ONIT + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R230b	^{15}OLNN + NO_3 --> ^{15}ONIT + HO_2 + NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R230c	^{15}OLNN + $^{15}NO_3$ --> ^{15}ONIT + HO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R231	OLND + NO_3 --> 0.28 HCHO + 1.24 ALD + 0.469 KET + 2 NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R231a	^{15}OLND + NO_3 --> 0.28 HCHO + 1.24 ALD + 0.469 KET + NO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R231b	OLND + $^{15}NO_3$ --> 0.28 HCHO + 1.24 ALD + 0.469 KET + NO_2 + $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R231c	^{15}OLND + $^{15}NO_3$ --> 0.28 HCHO + 1.24 ALD + 0.469 KET + 2 $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R236	XO_2 + NO --> NO_2	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R236a	XO_2 + ^{15}NO --> $^{15}NO_2$	4.00 x 10^{-12}		4.00 x 10^{-12}	1
R237	XO_2 + NO3 --> NO_2	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R237a	XO_2 + ^{15}NO3 --> $^{15}NO_2$	1.20 x 10^{-12}		1.20 x 10^{-12}	1
R238	NO + $^{15}NO_2$ --> ^{15}NO + NO_2	3.60 x 10^{-14}		3.60 x 10^{-14}	1
R238a	^{15}NO + NO_2 --> NO + $^{15}NO_2$	3.60 x 10^{-14}	-18.467	3.83 x	0.9771

				10^{-14}	
R239	N_2O_5 --> HNO_3 + HNO_3	0.1		0.1	1
R239a	$^{15}NNO_5$ --> $^{15}HNO_3$ + HNO_3	0.1		0.1	0.9954
R239b	$^{15}N_2O_5$ --> $^{15}HNO_3$ + $^{15}HNO_3$	0.1		0.1	0.9909

Table S2b: Chemical reactions involving N compounds

Reaction No.	Reaction	C, K^{-2} cm^3 s^{-1}	D, K	α
R98	ETE + NO_3 --> 0.80 OLNN + 0.20 OLND	4.88 x 10^{-18}	2282	1
R98a	ETE + $^{15}NO_3$ --> 0.80 ^{15}OLNN + 0.20 ^{15}OLND	4.88 x 10^{-18}	2282	0.9975

Table S2c: Reaction rate constants of the form $k = T^2 C \exp(-D/T)$

Reaction No.	Reaction	K_0^{300}, $cm^6\ s^{-1}$	n	K_∞^{300}, $cm^6\ s^{-1}$	m
R35	$O^3P + NO \rightarrow NO_2$	9.00×10^{-32}	1.5	3.00×10^{-11}	0
R35a	$O^3P + {}^{15}NO \rightarrow {}^{15}NO_2$	9.00×10^{-32}	1.5	3.00×10^{-11}	0
R37	$O^3P + NO_2 \rightarrow NO_3$	9.00×10^{-32}	2	2.20×10^{-11}	0
R37a	$O^3P + {}^{15}NO_2 \rightarrow {}^{15}NO_3$	9.00×10^{-32}	2	2.20×10^{-11}	0
R38	$HO + NO \rightarrow HONO$	7.00×10^{-31}	2.6	1.50×10^{-11}	0.5
R38a	$HO + {}^{15}NO \rightarrow HO{}^{15}NO$	7.00×10^{-31}	2.6	1.50×10^{-11}	0.5
R39	$HO + NO_2 \rightarrow HNO_3$	2.60×10^{-30}	3.2	2.40×10^{-11}	1.3
R39a	$HO + {}^{15}NO_2 \rightarrow H{}^{15}NO_3$	2.60×10^{-30}	3.2	2.40×10^{-11}	1.3
R42	$HO_2 + NO_2 \rightarrow HNO_4$	2.80×10^{-31}	3.2	4.70×10^{-12}	1.4
R42a	$HO_2 + {}^{15}NO_2 \rightarrow H{}^{15}NO_4$	2.80×10^{-31}	3.2	4.70×10^{-12}	1.4
R53	$NO_3 + NO_2 \rightarrow N_2O_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7
R53a	$NO_3 + {}^{15}NO_2 \rightarrow {}^{15}NNO_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7
R53b	$^{15}NO_3 + NO_2 \rightarrow {}^{15}NNO_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7
R53c	$^{15}NO_3 + {}^{15}NO_2 \rightarrow {}^{15}N_2O_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7
R127	$ACO_3 + NO_2 \rightarrow PAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5
R127a	$ACO_3 + {}^{15}NO_2 \rightarrow {}^{15}PAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5
R129	$TCO_3 + NO_2 \rightarrow TPAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5
R129a	$TCO_3 + {}^{15}NO_2 \rightarrow {}^{15}TPAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5

Table S2d: Troe reactions

Reaction No.	Reaction	A	B	K_0^{300}, cm^6 s^{-1}	n	K_∞^{300}, cm^6 s^{-1}	m
R43	HNO4 --> HO_2 + NO_2	4.76 x 10^{+26}	10900	1.81 x 10^{-31}	3.2	4.70 x 10^{-12}	1.4
R43a	H^{15}NO4 --> HO_2 + $^{15}NO_2$	4.76 x 10^{+26}	10900	1.81 x 10^{-31}	3.2	4.70 x 10^{-12}	1.4
R54	N_2O_5 --> NO_2 + NO_3	3.70 x 10^{+26}	11000	2.20 x 10^{-30}	3.9	1.50 x 10^{-12}	0.7
R54a	$^{15}NNO_5$ --> $^{15}NO_2$ + NO_3	3.70 x 10^{+26}	11000	2.20 x 10^{-30}	3.9	1.50 x 10^{-12}	0.7
R54b	$^{15}NNO_5$ --> NO_2 + $^{15}NO_3$	3.70 x 10^{+26}	11000	2.20 x 10^{-30}	3.9	1.50 x 10^{-12}	0.7
R54c	$^{15}N_2O_5$ --> $^{15}NO_2$ + $^{15}NO_3$	3.70 x 10^{+26}	11000	2.20 x 10^{-30}	3.9	1.50 x 10^{-12}	0.7
R128	PAN --> ACO_3 + NO_2	1.16 x 10^{+28}	13954	9.70 x 10^{-29}	5.6	9.30 x 10^{-12}	1.5
R128a	^{15}PAN --> ACO_3 + $^{15}NO_2$	1.16 x 10^{+28}	13954	9.70 x 10^{-29}	5.6	9.30 x 10^{-12}	1.5
R130	TPAN --> TCO_3 + NO_2	1.16 x 10^{+28}	13954	9.70 x 10^{-29}	5.6	9.30 x 10^{-12}	1.5
R130a	^{15}TPAN --> TCO_3 + $^{15}NO_2$	1.16 x 10^{+28}	13954	9.70 x 10^{-29}	5.6	9.30 x 10^{-12}	1.5

Table S2e: Troe equilibrium reactions

Reaction No.	Reaction	Rate Constant Expression
R46	$HO + HNO_3 \rightarrow NO_3 + H_2O$	$k = k_o + k_3/(1 + k_3/k_2)$ $k_o = 7.2 \times 10^{-15} \times \exp(785/T)$ $k_2 = 4.1 \times 10^{-16} \times \exp(1440/T)$ $k_3 = 1.9 \times 10^{-33} \times \exp(725/T) \times [M]$ [M] is the concentration of air in molecules cm-3
R46a	$HO + H^{15}NO_3 \rightarrow {}^{15}NO_3 + H_2O$	

Table S2f: Reactions with special rate expressions

Compound	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1E+07	-
O_3	10	-
NO	0.2	2.59
^{15}NO	0.00072	9.32E-03
NO_2	0.25	-
$^{15}NO_2$	0.0009	-
HNO_3	-	-
$H^{15}NO_3$	-	-
CO	1000	5.6
CH_4	3000	-
H_2	500	-
H_2O_2	2	-
SO_2	-	0.52
ETH	-	0.24
HC3	-	2.94
HC5	-	0.77
HC8	-	0.45
ETE	-	0.46
OLI	-	0.19
OLT	-	0.22
TOL	-	0.57
XYL	-	0.52
HCHO	1	0.14
ALD	-	0.04
KET	-	0.50
O_2	2.09E+08	-
N_2	7.74394109E+08	-
^{15}NN	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-

Table S3a: Initial concentrations and emission rates for test cases

Meteorological conditions	Values
Start Date/Time	Mar 1, 0300 LT
End Date/Time	Mar 6, 0000 LT
Latitude	33 °N
Longitude	0
Elevation, km	0
Temperature, K	298
Pressure, atm	1

Table S3b: Meteorological conditions for test cases

Compound	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1.00E+07	-
O_3	10	-
NO	5	2.59
^{15}NO	0.018	9.32E-03
NO_2	10	-
$^{15}NO_2$	0.036	-
HNO_3	-	-
$H^{15}NO_3$	-	-
CO	1000	5.6
CH_4	3000	-
H_2	500	-
H_2O_2	2	-
SO_2	-	0.52
ETH	-	0.24
HC3	-	2.94
HC5	-	0.77
HC8	-	0.45
ETE	-	0.46
OLI	-	0.19
OLT	-	0.22
TOL	-	0.57
XYL	-	0.52
HCHO	1	0.14
ALD	-	0.04
KET	-	0.50
O_2	2.09E+08	-
N_2	7.74394109E+08	-
^{15}NN	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-

Table S3c: Initial concentrations and emission rates for the cases with low VOC emission rate

Compound	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1.00E+07	-
O_3	10	-
NO	50	2.59
^{15}NO	0.18	9.32E-03
NO_2	100	-
$^{15}NO_2$	0.36	-
HNO_3	-	-
$H^{15}NO_3$	-	-
CO	1000	5.6
CH_4	3000	-
H_2	500	-
H_2O_2	2	-
SO_2	-	0.52
ETH	-	1.20
HC3	-	14.7
HC5	-	3.85
HC8	-	2.26
ETE	-	2.28
OLI	-	0.94
OLT	-	1.09
TOL	-	2.86
XYL	-	2.59
HCHO	1	0.69
ALD	-	0.18
KET	-	2.51
O_2	2.09E+08	-
N_2	7.74394109E+08	-
^{15}NN	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-

Table S3d: Initial concentrations and emission rates for the cases with high NO_x concentration and high VOC emission rate

Compound	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1.00E+07	-
O_3	10	-
NO	5	2.59
^{15}NO	0.018	9.32E-03
NO_2	10	-
$^{15}NO_2$	0.036	-
HNO_3	-	-
$H^{15}NO_3$	-	-
CO	1000	5.6
CH_4	3000	-
H_2	500	-
H_2O_2	2	-
SO_2	-	0.52
ETH	-	1.20
HC3	-	14.7
HC5	-	3.85
HC8	-	2.26
ETE	-	2.28
OLI	-	0.94
OLT	-	1.09
TOL	-	2.86
XYL	-	2.59
HCHO	1	0.69
ALD	-	0.18
KET	-	2.51
O_2	2.09E+08	-
N_2	7.74394109E+08	-
^{15}NN	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-

Table S3e: Initial concentrations and emission rates for the cases with intermediate NO_x concentration and high VOC emission rate

Compound	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1.00E+07	-
O_3	10	-
NO	0.5	2.59
^{15}NO	0.0018	9.32E-03
NO_2	1	-
$^{15}NO_2$	0.0036	-
HNO_3	-	-
$H^{15}NO_3$	-	-
CO	1000	5.6
CH_4	3000	-
H_2	500	-
H_2O_2	2	-
SO_2	-	0.52
ETH	-	1.20
HC3	-	14.7
HC5	-	3.85
HC8	-	2.26
ETE	-	2.28
OLI	-	0.94
OLT	-	1.09
TOL	-	2.86
XYL	-	2.59
HCHO	1	0.69
ALD	-	0.18
KET	-	2.51
O_2	2.09E+08	-
N_2	7.74394109E+08	-
^{15}NN	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-

Table S3f: Initial concentrations and emission rates for the cases with low NO_x concentration and high VOC emission rate

	Rural								
Case	1	2	3	4	5	6	7	8	9
H_2O, %	1	1	1	1	1	1	1	1	1
NO, ppb	0.1	0.1	0.1	0.334	0.334	0.334	1	1	1
^{15}NO, ppb	3.600E-04	3.600E-04	3.600E-04	1.202E-03	1.202E-03	1.202E-03	3.600E-03	3.600E-03	3.600E-03
NO_2, ppb	0.4	0.4	0.4	1.336	1.336	1.336	4	4	4
$^{15}NO_2$, ppb	0.00144	0.00144	0.00144	0.00481	0.00481	0.00481	0.0144	0.0144	0.0144
HNO_3, ppb	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
$H^{15}NO_3$, ppb	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036
CH_4, ppb	1800	1800	1800	1800	1800	1800	1800	1800	1800
CO, ppb	200	200	200	200	200	200	200	200	200
SO_2, ppb	5	5	5	5	5	5	5	5	5
O_3, ppb	10	10	10	10	10	10	10	10	10
H_2, ppb	500	500	500	500	500	500	500	500	500
H_2O_2, ppb	2	2	2	2	2	2	2	2	2
ETH, ppb	0.79	2.607	7.9	0.79	2.607	7.9	0.79	2.607	7.9
HC3, ppb	0.6575	2.16975	6.575	0.6575	2.16975	6.575	0.6575	2.16975	6.575
HC5, ppb	0.295	0.9735	2.95	0.295	0.9735	2.95	0.295	0.9735	2.95
HC8, ppb	0.13	0.429	1.3	0.13	0.429	1.3	0.13	0.429	1.3
ETE, ppb	0.3	0.99	3	0.3	0.99	3	0.3	0.99	3
OLT, ppb	0.1	0.33	1	0.1	0.33	1	0.1	0.33	1
OLI, ppb	0	0	0	0	0	0	0	0	0
ISO, ppb	0.12	0.396	1.2	0.12	0.396	1.2	0.12	0.396	1.2
TOL,	0.2667	0.88011	2.667	0.2667	0.88011	2.667	0.2667	0.88011	2.667

ppb									
XYL, ppb	0.0375	0.12375	0.375	0.0375	0.12375	0.375	0.0375	0.12375	0.375
CSL, ppb	0	0	0	0	0	0	0	0	0
HCHO, ppb	0.1	0.33	1	0.1	0.33	1	0.1	0.33	1
ALD, ppb	0.05	0.165	0.5	0.05	0.165	0.5	0.05	0.165	0.5
O_2, %	20.9	20.9	20.9	20.9	20.9	20.9	20.9	20.9	20.9
N_2, %	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394
^{15}NN, %	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596
$^{15}N_2$, %	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010
	Urban								
Case	10	11	12	13	14	15	16	17	18
H_2O, %	1	1	1	1	1	1	1	1	1
NO, ppb	8	8	8	26.4	26.4	26.4	80	80	80
^{15}NO, ppb	2.880E-02	2.880E-02	2.880E-02	9.504E-02	9.504E-02	9.504E-02	2.880E-01	2.880E-01	2.880E-01
NO_2, ppb	2	2	2	6.6	6.6	6.6	20	20	20
$^{15}NO_2$, ppb	0.0072	0.0072	0.0072	0.02376	0.02376	0.02376	0.072	0.072	0.072
HNO_3, ppb	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
$H^{15}NO_3$, ppb	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036	0.00036
CH_4, ppb	3000	3000	3000	3000	3000	3000	3000	3000	3000
CO, ppb	1000	1000	1000	1000	1000	1000	1000	1000	1000
SO_2, ppb	30	30	30	30	30	30	30	30	30
O_3, ppb	10	10	10	10	10	10	10	10	10
H_2, ppb	500	500	500	500	500	500	500	500	500
H_2O_2, ppb	2	2	2	2	2	2	2	2	2
ETH, ppb	2.75	9.075	27.5	2.75	9.075	27.5	2.75	9.075	27.5
HC3,	4.842	15.9786	48.42	4.842	15.9786	48.42	4.842	15.9786	48.42

ppb									
HC5, ppb	3.043	10.0419	30.43	3.043	10.0419	30.43	3.043	10.0419	30.43
HC8, ppb	2.223	7.3359	22.23	2.223	7.3359	22.23	2.223	7.3359	22.23
ETE, ppb	3.5	11.55	35	3.5	11.55	35	3.5	11.55	35
OLT, ppb	2.667	8.8011	26.67	2.667	8.8011	26.67	2.667	8.8011	26.67
OLI, ppb	1.25	4.125	12.5	1.25	4.125	12.5	1.25	4.125	12.5
ISO, ppb	0	0	0	0	0	0	0	0	0
TOL, ppb	1.81	5.973	18.1	1.81	5.973	18.1	1.81	5.973	18.1
XYL, ppb	0.625	2.0625	6.25	0.625	2.0625	6.25	0.625	2.0625	6.25
CSL, ppb	0.333	1.0989	3.33	0.333	1.0989	3.33	0.333	1.0989	3.33
HCHO, ppb	2.5	8.25	25	2.5	8.25	25	2.5	8.25	25
ALD, ppb	1.25	4.125	12.5	1.25	4.125	12.5	1.25	4.125	12.5
O_2, %	20.9	20.9	20.9	20.9	20.9	20.9	20.9	20.9	20.9
N_2, %	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394	77.4394
^{15}NN, %	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596	0.5596
$^{15}N_2$, %	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010

Table S4a: Initial concentrations for inter-comparison cases 1-18

Meteorological conditions	Values
Start Date/Time	June 21, 0600 LT
End Date/Time	June 23, 0600 LT
Latitude	40 °N
Longitude	0
Elevation, km	0
Temperature, K	298
Pressure, atm	1

Table S4b: Meteorological conditions for inter-comparison cases 1-18

	Case 19		Case 20	
Compound	Initial Concentrations, ppb	Emissions, ppt/min	Initial Concentrations, ppb	Emissions, ppt/min
H_2O	1 x 10^7	-	1 x 10^7	-
O_3	50	-	30	-
NO	0.2	2.6	0.02	0.26
^{15}NO	7.20E-04	9.36E-03	7.20E-05	9.36E-04
NO_2	0.5	-	0.05	-
$^{15}NO_2$	0.0018	-	0.00018	-
HNO_3	0.1	-	0.01	-
$H^{15}NO_3$	0.00036	-	0.000036	-
CO	200	5.7	104	0.57
CH_4	1700	-	1700	-
H_2	500	-	500	-
H_2O_2	2	-	0.2	-
SO_2	-	0.52	-	0.052
ETH	-	0.24	-	0.024
HC3	-	2.6	-	0.26
HC5	-	0.76	-	0.076
HC8	-	0.45	-	0.045
ETE	-	0.46	-	0.046
OLI	-	0.19	-	0.019
OLT	-	0.22	-	0.022
TOL	-	0.57	-	0.057
XYL	-	0.52	-	0.052
HCHO	1	0.14	0.1	0.014
ALD	-	0.036	-	0.0036
KET	-	0.32	-	0.032
O_2	2.09E+08	-	2.09E+08	-
N_2	7.74394109E+08	-	7.74394109E+08	-
^{15}NN	5.59578240E+06	-	5.59578240E+06	-
$^{15}N_2$	1.01088000E+04	-	1.01088000E+04	-

Table S5a: Initial concentrations and emission rates for inter-comparison cases 19-20

Meteorological conditions	Values
Start Date/Time	June 21, 0600 LT
End Date/Time	June 26, 0600 LT
Latitude	40 °N
Longitude	0
Elevation, km	0
Temperature, K	298
Pressure, atm	1

Table S5b: Meteorological conditions for inter-comparison cases 19-20

Reaction No.	Reaction	α
R1	NO_2 --> O^3P + NO	1
R1a	$^{15}NO_2$ --> O^3P + ^{15}NO	1.0042
R39	HO + NO_2 --> HNO_3	1
R39a	HO + $^{15}NO_2$ --> $H^{15}NO_3$	1.04
R48	O_3 + NO --> NO_2 + O_2	1
R48a	O_3 + ^{15}NO --> $^{15}NO_2$ + O_2	0.9933
R91	HCHO + NO_3 --> HO_2 + HNO_3 + CO	1
R91a	HCHO + $^{15}NO_3$ --> HO_2 + $H^{15}NO_3$ + CO	0.9974
R92	ALD + NO_3 --> ACO_3 + HNO_3	1
R92a	ALD + $^{15}NO_3$ --> ACO_3 + $H^{15}NO_3$	0.9967
R93	GLY + NO_3 --> HNO_3 + HO_2 + 2 CO	1
R93a	GLY + $^{15}NO_3$ --> $H^{15}NO_3$ + HO_2 + 2 CO	0.9962
R94	MGLY + NO_3 --> HNO_3 + ACO_3 + CO	1
R94a	MGLY + $^{15}NO_3$ --> $H^{15}NO_3$ + ACO_3 + CO	0.9957
R95	MACR + NO_3 --> 0.20 TCO_3 + 0.20 HNO_3 + 0.80 OLNN + 0.80 CO	1
R95a	MACR + $^{15}NO_3$ --> 0.20 TCO_3 + 0.20 $H^{15}NO_3$ + 0.80 ^{15}OLNN + 0.80 CO	0.9958
R96	DCB + NO_3 --> 0.50 TCO_3 + 0.50 HO_2 + 0.50 XO_2 + 0.25 GLY + 0.25 ALD + 0.03 KET + 0.25 MGLY + 0.5 HNO_3 + 0.5 NO_2	1
R96a	DCB + $^{15}NO_3$ --> 0.50 TCO_3 + 0.50 HO_2 + 0.50 XO_2 + 0.25 GLY + 0.25 ALD + 0.03 KET + 0.25 MGLY + 0.5 $H^{15}NO_3$ + 0.5 $^{15}NO_2$	0.9954
R97	CSL + NO_3 --> HNO_3 + PHO	1
R97a	CSL + $^{15}NO_3$ --> $H^{15}NO_3$ + PHO	0.9949
R238	NO + $^{15}NO_2$ --> ^{15}NO + NO_2	1
R238a	^{15}NO + NO_2 --> NO + $^{15}NO_2$	0.9771

Table S6: Fractionation factors of Leighton cycle, NO_x isotope exchange, OH production of HNO_3, and KIE effects of NO3 reacting with hydrocarbons.

Reaction No.	Reaction	α
R1	NO_2 --> O^3P + NO	1
R1a	$^{15}NO_2$ --> O^3P + ^{15}NO	1.0042
R39	HO + NO_2 --> HNO_3	1
R39a	HO + $^{15}NO_2$ --> $H^{15}NO_3$	1.04
R48	O_3 + NO --> NO_2 + O_2	1
R48a	O_3 + ^{15}NO --> $^{15}NO_2$ + O_2	0.9933
R53	NO_3 + NO_2 --> N_2O_5	1
R53a	NO_3 + $^{15}NO_2$ --> $^{15}NNO_5$	1.0266
R53b	$^{15}NO_3$ + NO_2 --> $^{15}NNO_5$	1.0309
R53c	$^{15}NO_3$ + $^{15}NO_2$ --> $^{15}N_2O_5$	1.057
R54	N_2O_5 --> NO_2 + NO_3	1
R54a	$^{15}NNO_5$ --> $^{15}NO_2$ + NO_3	0.5
R54b	$^{15}NNO_5$ --> NO_2 + $^{15}NO_3$	0.5
R54c	$^{15}N_2O_5$ --> $^{15}NO_2$ + $^{15}NO_3$	1
R238	NO + $^{15}NO_2$ --> ^{15}NO + NO_2	1
R238a	^{15}NO + NO_2 --> NO + $^{15}NO_2$	0.9771
R239	N_2O_5 --> HNO_3 + HNO_3	1
R239a	$^{15}NNO_5$ --> $^{15}HNO_3$ + HNO_3	0.9954
R239b	$^{15}N_2O_5$ --> $^{15}HNO_3$ + $^{15}HNO_3$	0.9909

Table S7: Fractionation factors of Leighton cycle, NO_x isotope exchange, OH production of HNO_3, and N_2O_5 heterogeneous reactions.

	Urban		Rural		Forest		Marine	
Compound	Initial Concentrations ppb	Emissions ppt/min	Initial Concentrations ppb	Emissions ppt/min	Initial Concentrations ppb	Emissions ppt/min	Initial Concentrations ppb	Emissions ppt/min
H_2O	1 x 10^7	-	1 x 10^7	-	1 x 10^7	-	1 x 10^7	-
O_3	300	-	50	-	10	-	10	-
NO	90	156	4.9	3.9	0.054	0.156	0.027	0.208
^{15}NO	0.324	0.5616	0.01764	0.01404	1.944E-04	0.0005616	9.720E-05	0.0007488
NO_2	90	-	2.1	-	0.006	-	0.003	-
$^{15}NO_2$	0.324	-	0.00756	-	2.160E-05	-	1.080E-05	-
HNO_3	20	-	6	-	0.29	-	0.145	-
$H^{15}NO_3$	0.072	-	0.0216	-	1.044E-03	-	5.22E-04	-
PAN	20	-	3	-	0.05	-	0.025	-
^{15}PAN	0.072	-	0.0108	-	1.800E-04	-	9.00E-05	-
CO	1000	5.7	200	5.7	207	5.7	-	5.7
CH_4	3000	-	1800	-	1657	-	-	-
H_2	500	-	500	-	500	-	500	-
H_2O_2	2	-	2	-	2	-	2	-
SO_2	30	0.52	5	0.52	-	0.52	-	0.52
ETH	30.730	4.8	2.557	0.36	0.98	0.216	1.304	0.144
HC3	53.777	52	1.147	3.9	0.84	2.34	1.306	1.56
HC5	33.803	15.2	1.368	1.14	0.344	0.684	0.199	0.456
HC8	24.694	9	0.259	0.675	0.1	0.405	0.025	0.27
ETE	17.986	9.2	0.100	0.69	0.97	0.414	1.469	0.276
OLI	3.063	3.8	-	0.285	-	0.171	-	0.114
OLT	6.535	4.4	0.066	0.33	0.39	0.198	0.404	0.132
ISO	-	-	0.082	-	2.040	-	-	-
TOL	17.667	11.4	0.372	0.855	0.93	0.513	0.545	0.342
XYL	15.802	10.4	0.195	0.78	0.090	0.468	0.140	0.312
HCHO	22.610	2.8	1.748	0.21	-	0.126	-	0.084
ALD	25.694	0.72	0.368	0.054	-	0.0324	-	0.0216
KET	-	6.4	-	0.48	-	0.288	-	0.192
API	-	-	-	-	0.130	-	-	-
O_2	2.09E+08	-	2.09E+08	-	2.09E+08	-	2.09E+08	-

N_2	7.7439E+08	-	7.7439E+08	-	7.7439E+08	-	7.7439E+08	-
^{15}NN	5.5958E+06	-	5.5958E+06	-	5.5958E+06	-	5.5958E+06	-
$^{15}N_2$	1.0109E+04	-	1.0109E+04	-	1.0109E+04	-	1.0109E+04	-

Table S8: Initial concentrations and emission rates for test cases under different environments

2. Detail information for case studies inputs

The completed i_NRACM was tested with different cases with various initial concentrations and emission rates, which stands for urban, rural, forest, and marine conditions. Stockwell *(1997)* provided 18 test cases without emission (9 for urban condition, 9 for rural condition), and 2 test cases with emission (1 for polluted atmosphere, 1 for clean atmosphere), while the concentration of chemicals in these test cases does not agree with atmospheric observations *[Altshuller, 1989; Baugues, 1986; Greenberg & Zimmerman, 1984; Logan, 1989; National Research Council, 1992; Torres & Buchan, 1988; Zimmerman et al., 1988]*.

First, Stockwell used the exact same initial ozone concentration of 10 ppb all of the 18 test cases without emission, which is severely underestimated for both urban (100-400 ppb) and rural (50-120 ppb) conditions *[Cleveland et al., 1977; Gregory et al., 1988; Janach, 1989; Kirchhoff, 1988; LeFohn & Pinkerton, 1988; Logan, 1989]*. Even for the so-called polluted atmosphere case, the initial ozone concentration was set to 50 ppb, which is hard to recognize as "polluted". The constant ozone concentration among urban and rural in Stockwell's cases also causes the NO/NO_x ratio being not reasonable. According to Toores and Buchan *(1988)*, with higher ozone concentration during the day, NO/NO_x becomes lower. This agrees with R48 ($NO + O_3 \rightarrow NO_2 + O_2$), with higher ozone concentration, more NO is consumed, thus more NO_2 is produced. Thus, NO/NO_x ratio in rural condition will be higher than in urban condition, which is opposite to Stockwell's cases. Second, Stockwell's cases considered NO_x to be the only compounds of NO_y in all the test cases. In fact, as the distance between sampling site and major anthropogenic sources increases, the conversion of NO_x to HNO_3 and PAN increases. As a result, NO_x account for 30-60% of NO_y at rural sites, and 15% at forest sites and marine sites *[Carroll et al., 1992; Fahey et al., 1986; National Research Council, 1992; Parrish et al., 1986; Williams et al., 1987]*. Third, for Stockwell's 9 urban cases and 9 rural cases, the emission rates of all chemical compounds are set to zero. Without the emission of NO and VOC, the simulated NO_x and VOC deplete quickly, which decay the NO_x cycle and the conversion to NO_y, as well as ozone concentration (Fig. S1). Fourth, the NO_x concentration in Stockwell's urban cases is too low, with the maximum of 100 ppb at the initial state, but quickly deplete to be less than 10 ppb in 6 hours. Baugues *(1986)* measured NO_x concentration among 30 sites among major cities in the eastern and southern United States in 1984 and 1985. Baugues's measurement shows 17 out of 21 sites in 1984 and 15 out of 19 sites in 1985 with maximum concentration of NO_x higher than 100 ppb, 10 out of 21 sites in 1984 and 7 out of 19 sites in 1985 with maximum concentration of NO_x higher than 200 ppb, which indicate the obvious higher NO_x

concentration than Stockwell's cases. For the so-called polluted atmosphere, the initial concentration of NO_x is only 0.7 ppb, with emission rate of 2.6 ppt/min, the maximum concentration only reaches 2.4 ppb around 6 am at day 2 to day 6, which again cannot stand for "polluted".

Thus, instead of replicating Stockwell's cases, we set up four conditions that stands for urban, rural, forest, and marine, with the initial concentrations based on various measurements from previous studies. The emission rates of NO and total VOCs was tuned until the simulation results satisfied with these following features: a). The concentration of NO_x changes diurnally and stabilized through time; b). The concentration of O_3 changes diurnally and stabilized through time; c). HNO_3 is produced primarily during daytime; d). VOCs are produced primarily during nighttime (Fig. S2-5). The molar fraction of each VOC species with respect to total VOC emission rate was obtained from Stockwell's *(1997)* emission cases.

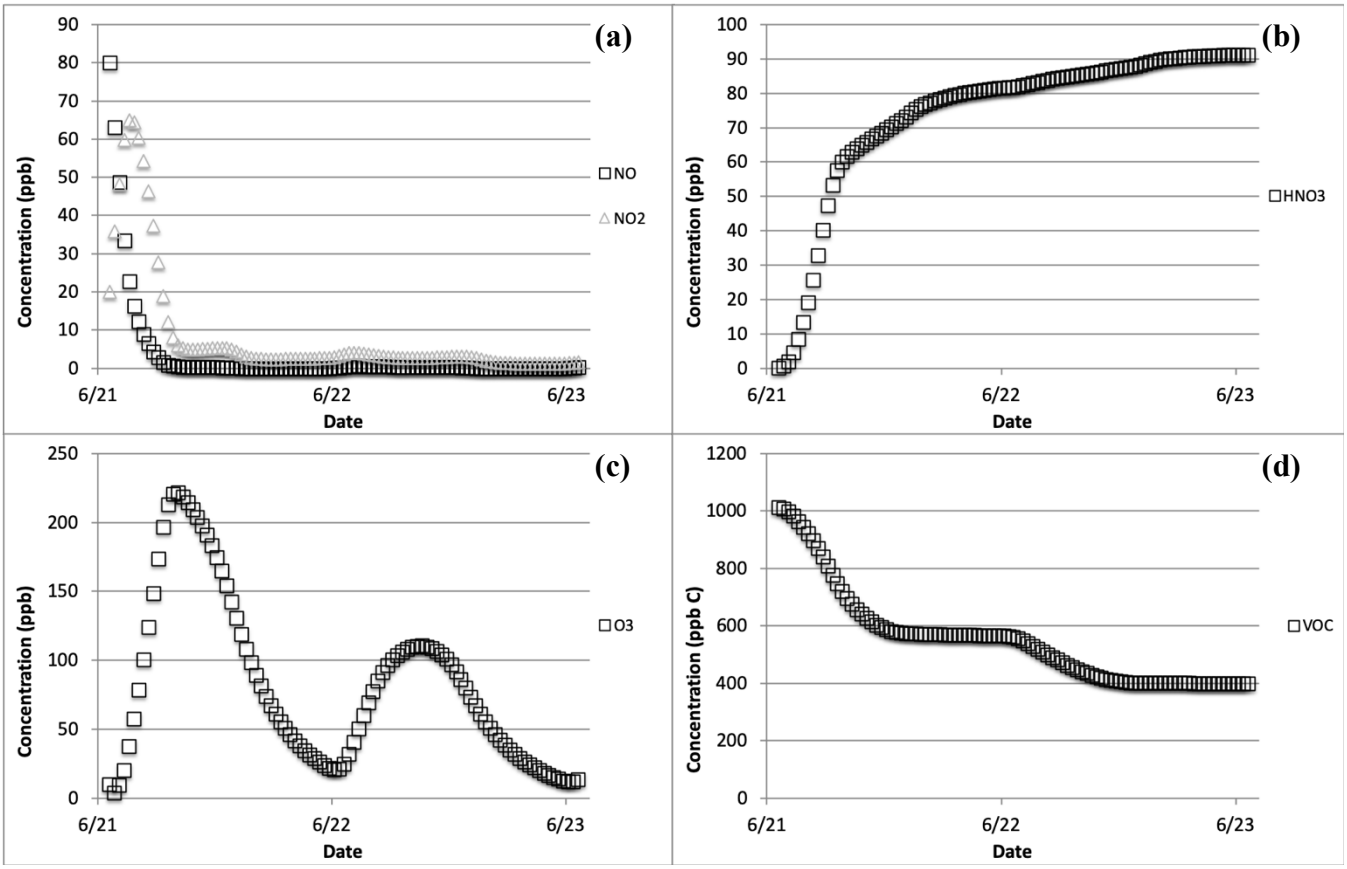

Figure S1. The concentrations of NO_x (top left, a), HNO_3 (top right, b), O_3 (bottom left, c), and total VOC (bottom right, d) for Stockwell's urban case with initial concentration of NO_x at 100 ppb, VOC at 1000 ppb C, simulation starts from Jun 21.

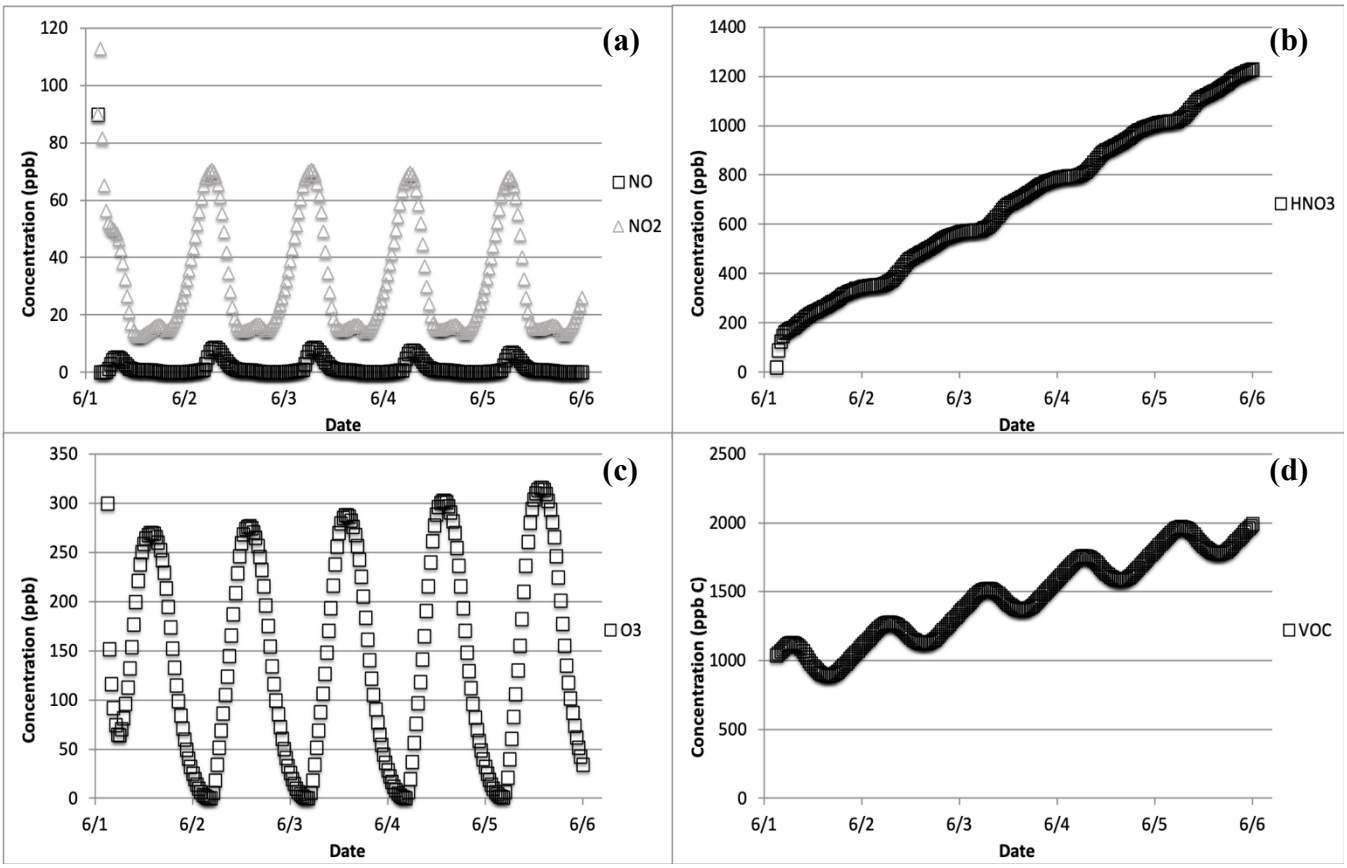

Figure S2. The concentrations of NO_x (top left, a), HNO_3 (top right, b), O_3 (bottom left, c), and total VOC (bottom right, d) for urban condition, with initial concentrations and emission rate listed in Table S8, simulation starts from Jun 1.

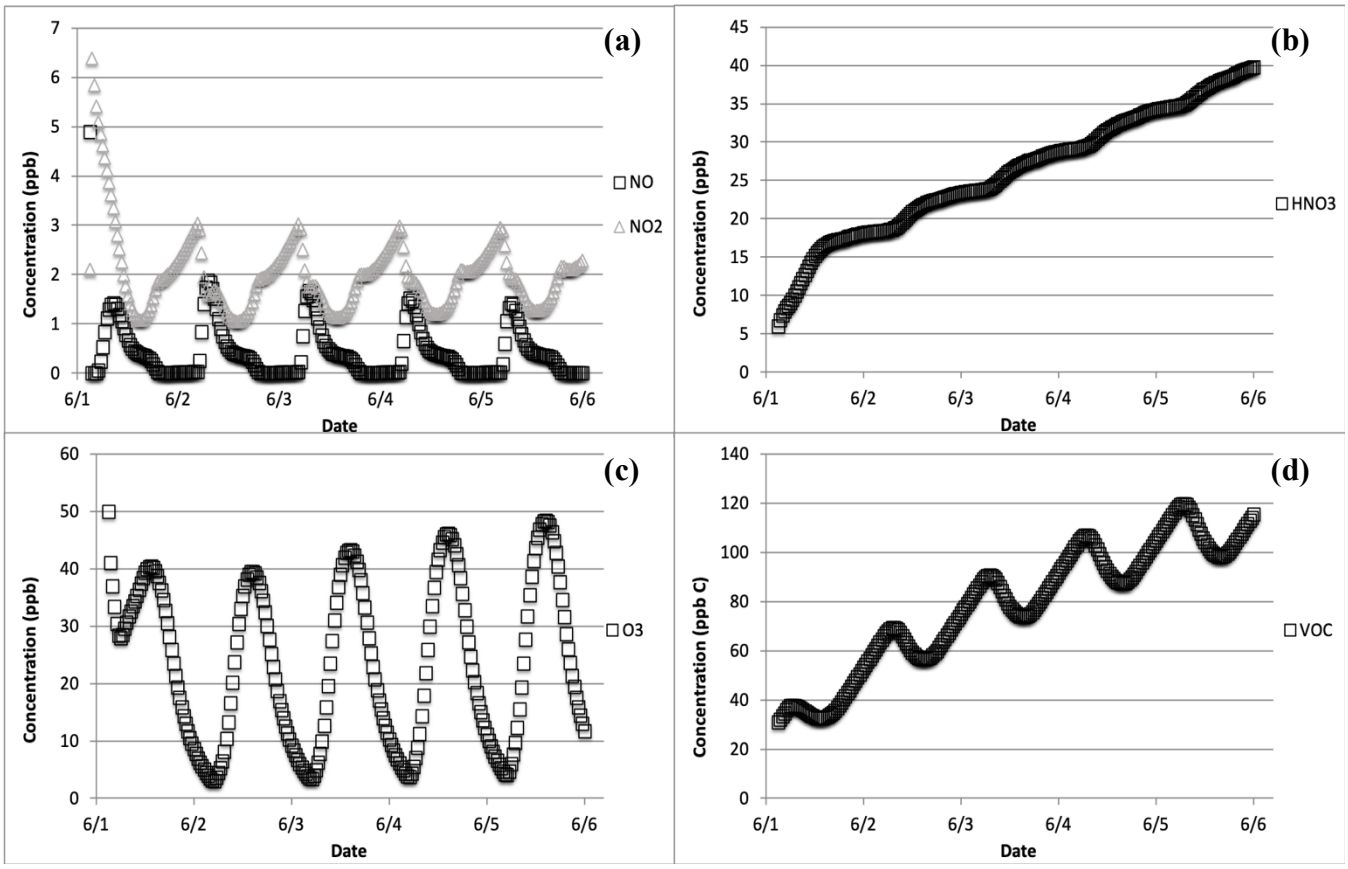

Figure S3. The concentrations of NO_x (top left, a), HNO_3 (top right, b), O_3 (bottom left, c), and total VOC (bottom right, d) for rural condition, with initial concentrations and emission rate listed in Table S8, simulation starts from Jun 1.

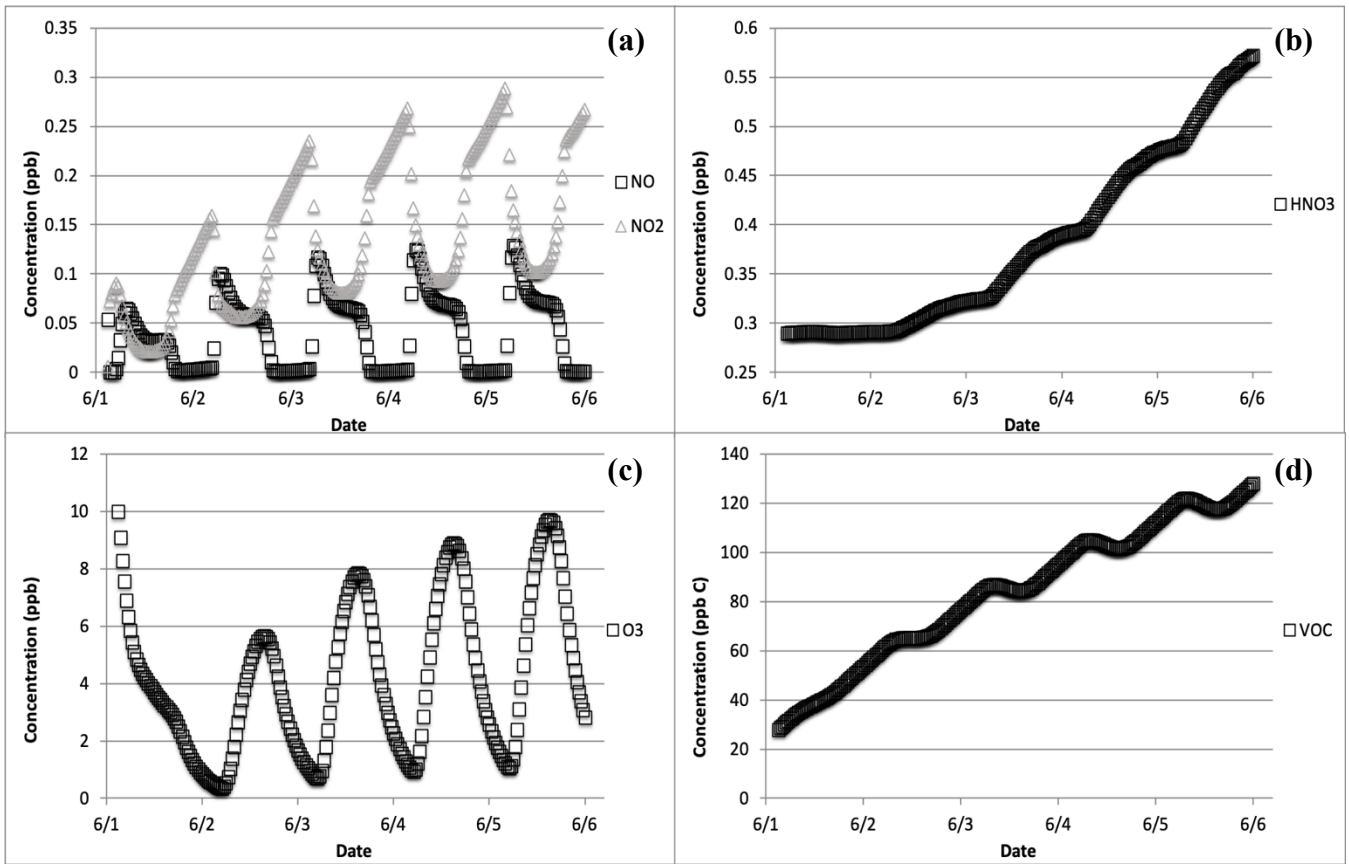

Figure S4. The concentrations of NO_x (top left, a), HNO_3 (top right, b), O_3 (bottom left, c), and total VOC (bottom right, d) for forest condition, with initial concentrations and emission rate listed in Table S8, simulation starts from Jun 1.

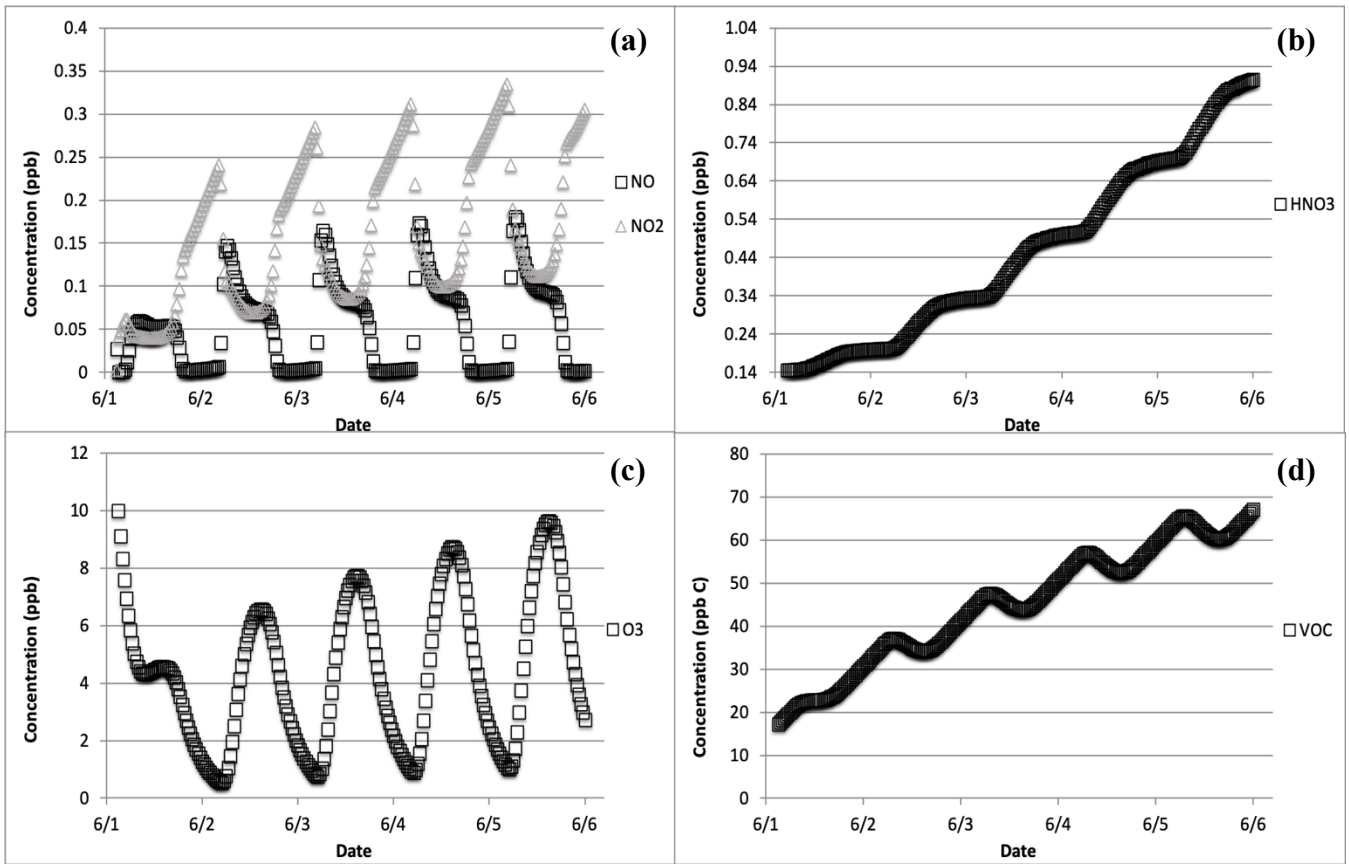

Figure S5. The concentrations of NO_x (top left), HNO_3 (top right), O_3 (bottom left), and total VOC (bottom right) for marine condition, with initial concentrations and emission rate listed in Table S8, simulation starts from Jun 1.

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