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i_NRACM: incorporating ^{15}N into the Regional Atmospheric Chemistry Mechanism (RACM) for assessing the role photochemistry plays in controlling the isotopic composition of NO_x, NO_y, and atmospheric nitrate

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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}	DeMore et al. [1994]	DeMore et al. [1994]	1
R1a	$^{15}NO_2$ --> O^3P + ^{15}NO	7.50 x 10^{-3}	DeMore et al. [1994]	DeMore et al. [1994]	1.0042
R2	O_3 --> O^1D + O_2	1.62 x 10^{-5}	DeMore et al. [1994]	DeMore et al. [1994]	1
R3	O_3 --> O^3P + O_2	4.17 x 10^{-4}	DeMore et al. [1994]	assumed to be unity	
R4	HONO --> HO + NO	1.63 x 10^{-3}	DeMore et al. [1994]	DeMore et al. [1994]	1
R4a	HO^{15}NO --> HO + ^{15}NO	1.63 x 10^{-3}	DeMore et al. [1994]	DeMore et al. [1994]	1
R5	HNO_3 --> HO + NO_2	4.50 x 10^{-7}	DeMore et al. [1994]	assumed to be unity	1
R5a	H$^{15}NO_3$ --> HO + $^{15}NO_2$	4.50 x 10^{-7}	DeMore et al. [1994]	assumed to 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}	DeMore et al. [1994]	assumed to 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}	DeMore et al. [1994]	assumed to be unity	1
R7	NO_3--> NO + O_2	2.33 x 10^{-2}	Wayn et al. [1991]	Wayn et al. [1991]	1
R7a	$^{15}NO_3$--> ^{15}NO + O_2	2.33 x 10^{-2}	Wayn et al. [1991]	Wayn et al. [1991]	1
R8	NO_3 --> NO_2 + O^3P	1.87 x 10^{-1}	Wayn et al. [1991]	Wayn et al. [1991]	1
R8a	$^{15}NO_3$ --> $^{15}NO_2$ + O^3P	1.87 x 10^{-1}	Wayn et al. [1991]	Wayn et al. [1991]	1
R9	H_2O_2 --> HO + HO	6.00 x 10^{-6}	DeMore et al. [1994]	Wayn et al. [1991]	1
R10	HCHO --> H_2 + CO	3.50 x 10^{-5}	Moortgat et al. [1980] Cantrell et al. [1990]	Atkinson et al. [1994] DeMore et al. [1994]	1
R11	HCHO --> 2HO_2 + CO	2.17 x 10^{-5}	Moortgat et al. [1980] Cantrell et al. [1990]	Atkinson et al. [1994] DeMore et al. [1994]	1
R12	ALD --> MO_2 + HO_2 + CO	3.67 x 10^{-6}	Martinez et al. [1992]	Atkinson et al. [1994]	1
R13	OP1 --> HCHO + HO_2 + HO	4.17 x 10^{-6}	DeMore et al. [1994]	DeMore et al. [1994]	1

R14	OP2 --> ALD + HO_2 + HO	4.17 x 10^{-6}	DeMore et al. [1994]	DeMore et al. [1994]	1
R15	PAA --> MO_2 + HO	1.57 x 10^{-6}	Giguere and Olmos [1956]	assumed to be unity	1
R16	KET --> ETHP + ACO_3	6.67 x 10^{-7}	Martinez et al. [1992]	Atkinson et al. [1994]	1
R17	GLY --> 0.13 HCHO + 1.87 CO + 0.87 H_2	5.83 x 10^{-5}	Atkinson et al. [1992]	Atkinson et al. [1992]	1
R18	GLY --> 0.45 HCHO + 1.55 CO + 0.80 HO_2 + 0.15 H_2	2.00 x 10^{-5}	Atkinson et al. [1992]	Atkinson et al. [1992]	1
R19	MGLY --> CO + HO2 + ACO_3	9.33 x 10^{-5}	Atkinson et al. [1994] Staffelbach et al. [1995]	Koch and Moortgat et al. [1996]	1
R20	DCB --> TCO_3 + HO_2	4.33 x 10^{-5}	Stockwell et al. [1990]	Stockwell et al. [1990]	1
R21	ONIT--> 0.20 ALD + 0.80 KET + HO_2 + NO_2	2.17 x 10^{-6}	Atkinson et al. [1994]	Atkinson et al. [1994]	1
R22	MACR --> CO + HCHO + HO_2 + ACO_3	1.33 x 10^{-6}	Gardner et al. [1987]	Gardner et al. [1987]	1
R23	HKET --> HCHO + HO_2 + ACO_3	6.67 x 10^{-7}	Martinez et al. [1992]	Atkinson et al. [1994]	1

Table S2a: Photolysis reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R, K	k	α
R24	$O^3P + O_2$ --> O_3	Table S2f		1.50×10^{-14}	1
R25	$O^3P + O_3$ --> $2\ O_2$	8.00×10^{-12}	2060	7.96×10^{-15}	1
R26	$O^1D + N_2$ --> $O^3P + N_2$	1.80×10^{-11}	-110	2.60×10^{-11}	1
R26a	$O^1D + {}^{15}NN$ --> $O^3P + {}^{15}NN$	1.80×10^{-11}	-110	2.60×10^{-11}	1
R27	$O^1D + O_2$ --> $O^3P + O_2$	3.20×10^{-11}	-70	4.05×10^{-11}	1
R28	$O^1D + H_2O$ --> HO + HO	2.20×10^{-10}		2.20×10^{-10}	1
R29	O_3 + HO --> $HO_2 + O_2$	1.60×10^{-12}	940	6.83×10^{-14}	1
R30	$O_3 + HO_2$ --> HO + O_2	1.10×10^{-14}	500	2.05×10^{-15}	1
R31	HO + HO_2 --> $H_2O + O_2$	4.80×10^{-11}	-250	1.11×10^{-10}	1
R32	H_2O_2 + HO --> $HO_2 + H_2O$	2.90×10^{-12}	160	1.70×10^{-12}	1
R33	$HO_2 + HO_2$ --> $H_2O_2 + O_2$	Table S2f		2.92×10^{-12}	1
R34	$HO_2 + HO_2 + H_2O$ --> $H_2O_2 + O_2 + H_2O$	Table S2f		6.58×10^{-30}	1
R35	O^3P + NO --> NO_2	Table S2d		1.66×10^{-12}	1
R35a	$O^3P + {}^{15}NO$ --> $^{15}NO_2$	Table S2d		1.66×10^{-12}	1
R36	$O^3P + NO_2$ --> NO + O_2	6.50×10^{-12}	-120	9.72×10^{-12}	1
R36a	$O^3P + {}^{15}NO_2$ --> $^{15}NO + O_2$	6.50×10^{-12}	-120	9.72×10^{-12}	1
R37	$O^3P + NO_2$ --> NO_3	Table S2d		1.58×10^{-12}	1
R37a	$O^3P + {}^{15}NO_2$ --> $^{15}NO_3$	Table S2d		1.58×10^{-12}	1
R38	HO + NO --> HONO	Table S2d		4.87×10^{-12}	1
R38a	HO + ^{15}NO --> HO^{15}NO	Table S2d		4.87×10^{-12}	1
R39	HO + NO_2 --> HNO_3	Table S2d		1.15×10^{-11}	1
R39a	HO + $^{15}NO_2$ --> H$^{15}NO_3$	Table S2d		1.15×10^{-11}	1.04
R40	HO + NO_3 --> $NO_2 + HO_2$	2.20×10^{-11}		2.20×10^{-11}	1
R40a	HO + $^{15}NO_3$ --> $^{15}NO_2 + HO_2$	2.20×10^{-11}		2.20×10^{-11}	1
R41	HO_2 + NO --> NO_2 + HO	3.70×10^{-12}	-250	8.56×10^{-12}	1
R41a	$HO_2 + {}^{15}NO$ --> $^{15}NO_2$ + HO	3.70×10^{-12}	-250	8.56×10^{-12}	1
R42	$HO_2 + NO_2$ --> HNO_4	Table S2d		1.39×10^{-12}	1
R42a	$HO_2 + {}^{15}NO_2$ --> H$^{15}NO_4$	Table S2d		1.39×10^{-12}	1
R43	HNO4 --> $HO_2 + NO_2$	Table S2e		8.62×10^{-2}	1
R43a	H^{15}NO4 --> $HO_2 + {}^{15}NO_2$	Table S2e		8.62×10^{-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 --> NO_2 + $^{15}NO_2$	3.30 x 10^{-39}	-530	1.95 x 10^{-38}	1
R50b	^{15}NO + ^{15}NO + O_2 --> $^{15}NO_2$ + $^{15}NO_2$	3.30 x 10^{-39}	-530	1.95 x 10^{-38}	1
R51	NO_3 + NO --> $NO_2 + NO_2$	1.50 x 10^{-11}	-170	2.65 x 10^{-11}	1
R51a	$^{15}NO_3$ + NO --> NO_2 + $^{15}NO_2$	1.50 x 10^{-11}	-170	2.65 x 10^{-11}	1
R51b	NO_3 + ^{15}NO --> NO_2 + $^{15}NO_2$	1.50 x 10^{-11}	-170	2.65 x 10^{-11}	1
R51c	$^{15}NO_3$ + ^{15}NO --> $^{15}NO_2$ + $^{15}NO_2$	1.50 x 10^{-11}	-170	2.65 x 10^{-11}	1
R52	$NO_3 + NO_2$ --> NO + $NO_2 + O_2$	4.50 x 10^{-14}	1260	6.56 x 10^{-16}	1
R52a	NO_3 + $^{15}NO_2$ --> ^{15}NO + NO_2 + O_2	4.50 x 10^{-14}	1260	6.56 x 10^{-16}	0.5
R52b	NO_3 + $^{15}NO_2$ --> NO + $^{15}NO_2$ + O_2	4.50 x 10^{-14}	1260	6.56 x 10^{-16}	0.5
R52c	$^{15}NO_3$ + NO_2 --> ^{15}NO + NO_2 + O_2	4.50 x 10^{-14}	1260	6.56 x 10^{-16}	0.5
R52d	$^{15}NO_3$ + NO_2 --> NO + $^{15}NO_2$ + O_2	4.50 x 10^{-14}	1260	6.56 x 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	$^{15}N_2O_5 \rightarrow {}^{15}NO_2 + {}^{15}NO_3$	Table S2e		4.36×10^{-2}	1
R55	$NO_3 + NO_3 \rightarrow NO_2 + NO_2 + O_2$	8.50×10^{-13}	2450	2.29×10^{-16}	1
R55a	$NO_3 + 15NO_3 \rightarrow NO_2 + {}^{15}NO_2 + O_2$	8.50×10^{-13}	2450	2.29×10^{-16}	1
R55b	$^{15}NO_3 + {}^{15}NO_3 \rightarrow {}^{15}NO_2 + {}^{15}NO_2 + O_2$	8.50×10^{-13}	2450	2.29×10^{-16}	1
R56	$HO + H_2 \rightarrow H_2O + HO_2$	5.50×10^{-12}	2000	6.69×10^{-15}	1
R57	$HO + SO_2 \rightarrow$ SULF + HO_2	Table S2d		8.89×10^{-13}	1
R58	$CO + HO \rightarrow HO_2 + CO_2$	Table S2f		2.40×10^{-13}	1
R59	ISO + $O^3P \rightarrow$ 0.86 OLT + 0.05 HCHO + 0.02 HO + 0.01 CO + 0.13 DCB + 0.28 HO2 + 0.15 XO_2	6.00×10^{-11}		6.00×10^{-11}	1
R60	MACR + $O^3P \rightarrow$ALD	1.59×10^{-11}	-13	1.66×10^{-11}	1
R61	$CH4 + HO \rightarrow MO_2 + H_2O$	Table S2c		6.86×10^{-15}	1
R62	$ETH + HO \rightarrow$ ETHP + H_2O	Table S2c		2.57×10^{-13}	1
R63	HC3 + HO --> 0.583 HC3P + 0.381 HO_2 + 0.335 ALD + 0.036 ORA1 + 0.036 CO + 0.036 GLY + 0.036 HO + 0.010 HCHO + H_2O	5.26×10^{-12}	260	2.20×10^{-12}	1
R64	HC5 + HO --> 0.75 HC5P + 0.25 KET + 0.25 HO_2 + H_2O	8.02×10^{-12}	155	4.77×10^{-12}	1

R65	HC8 + HO --> 0.951 HC8P + 0.025 ALD + 0.024 HKET + 0.049 HO_2 + H_2O	1.64 x 10^{-11}	125	1.08 x 10^{-11}	1
R66	ETE + HO --> ETEP	1.96 x 10^{-12}	-438	8.52 x 10^{-12}	1
R67	OLT + HO --> OLTP	5.72 x 10^{-12}	-500	3.06 x 10^{-11}	1
R68	OLI + HO --> OLIP	1.33 x 10^{-11}	-500	7.12 x 10^{-11}	1
R69	DIEN + HO --> ISOP	1.48 x 10^{-11}	-448	6.65 x 10^{-11}	1
R70	ISO + HO --> ISOP	2.54 x 10^{-11}	-410	1.01 x 10^{-10}	1
R71	API + HO --> APIP	1.21 x 10^{-11}	-444	5.37 x 10^{-11}	1
R72	LIM + HO --> LIMP	1.70 x 10^{-10}		1.70 x 10^{-10}	1
R73	TOL + HO --> 0.90 ADDT + 0.10 XO_2 + 0.10 HO_2	1.81 x 10^{-12}	-355	5.96 x 10^{-12}	1
R74	XYL + HO --> 0.90 ADDX + 0.10 XO_2 + 0.10 HO_2	7.30 x 10^{-12}	-355	2.40 x 10^{-11}	1
R75	CSL + HO --> 0.85 ADDC + 0.10 PHO + 0.05 HO_2 + 0.05 XO_2	6.00 x 10^{-11}		6.00 x 10^{-11}	1
R76	HCHO + HO --> HO2 + CO + H_2O	1.00 x 10^{-11}		1.00 x 10^{-11}	1
R77	ALD + HO --> ACO_3+ H_2O	5.55 x 10^{-12}	-331	1.69 x 10^{-11}	1
R78	KET + HO --> KETP + H_2O	Table S2c		6.87 x 10^{-13}	1
R79	HKET + HO --> HO_2 + MGLY + H_2O	3.00 x 10^{-12}		3.00 x 10^{-12}	1
R80	GLY + HO --> HO_2+ 2 CO + H_2O	1.14 x 10^{-11}		1.14 x 10^{-11}	1
R81	MGLY + HO --> ACO_3 + CO + H_2O	1.72 x 10^{-11}		1.72 x 10^{-11}	1
R82	MACR + HO --> 0.51 TCO_3 + 0.41 HKET + 0.08 MGLY + 0.41 CO + 0.08 HCHO + 0.49 HO_2 + 0.49 XO_2	1.86 x 10^{-11}	-175	3.35 x 10^{-11}	1
R83	DCB + HO --> 0.50 TCO_3 + 0.50 HO_2 + 0.50 XO_2 + 0.35 UDD + 0.15 GLY + 0.15 MGLY	2.80 x 10^{-11}	-175	5.04 x 10^{-11}	1

R84	UDD + HO --> 0.88 ALD + 0.12 KET + HO_2	2.70 x 10^{-10}		2.70 x 10^{-10}	1
R85	OP1 + HO --> 0.65 MO_2 + 0.35 HCHO + 0.35 HO	2.93 x 10^{-12}	-190	5.54 x 10^{-12}	1
R86	OP2 + HO --> 0.44 HC3P + 0.08 ALD + 0.41 KET + 0.49 HO + 0.07 XO_2	3.40 x 10^{-12}	-190	6.43 x 10^{-12}	1
R87	PAA + HO --> 0.35 HCHO + 0.65 ACO_3 + 0.35 HO_2 + 0.35 XO_2	2.93 x 10^{-12}	-190	5.54 x 10^{-12}	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
R106	ETE + O_3 --> HCHO + 0.43 CO + 0.37 ORA1 + 0.26 HO_2+ 0.13 H_2 + 0.12 HO	9.14 x 10^{-15}	2580	1.59 x 10^{-18}	1
R107	OLT + O_3 --> 0.64 HCHO + 0.44 ALD + 0.37 CO + 0.14 ORA1 + 0.10 ORA2 + 0.25 HO_2 + 0.40 HO + 0.03 KET + 0.03 KETP + 0.06 CH_4 + 0.05 H_2 + 0.006 H_2O_2	4.33 x 10^{-15}	1800	1.03 x 10^{-17}	1

	+ 0.03 ETH + 0.19 MO_2 + 0.10 ETHP				
R108	OLI + O_3 --> 0.02 HCHO + 0.99 ALD + 0.16 KET + 0.30 CO + 0.011 H_2O_2 + ORA2 + 0.07 CH_4 + 0.22 HO_2 + 0.63 HO + 0.23 MO_2 + 0.12 KETP + 0.06 ETH + 0.18 ETHP	4.40×10^{-15}	845	2.58×10^{-16}	1
R109	DIEN + O_3 --> 0.90 HCHO + 0.39 MACR + 0.36 CO + 0.15 ORA1 + 0.09 O^3P + 0.30 HO_2 + 0.35 OLT + 0.28 HO + 0.05 H_2 + 0.15 ACO_3 + 0.03 MO_2 + 0.02 KETP + 0.13 XO_2 + 0.001 H_2O_2	1.34×10^{-14}	2283	6.33×10^{-18}	1
R110	ISO + O_3 --> 0.90 HCHO + 0.39 MACR + 0.36 CO + 0.15 ORA1 + 0.09 O^3P + 0.30 HO_2 + 0.35 OLT + 0.28 HO + 0.05 H_2 + 0.15 ACO_3 + 0.03 MO_2 + 0.02 KETP + 0.13 XO_2 + 0.001 H_2O_2	7.86×10^{-15}	1913	1.28×10^{-17}	1
R111	API + O_3 --> 0.65 ALD + 0.53 KET + 0.14 CO + 0.20 ETHP + 0.42 KETP + 0.85 HO + 0.10 HO_2 + 0.02 H_2O_2	1.01×10^{-15}	736	8.66×10^{-17}	1
R112	LIM + O_3 --> 0.04 HCHO + 0.46 OLT + 0.14 CO + 0.16 ETHP + 0.42 KETP + 0.85 HO + 0.10 HO_2 + 0.02 H_2O_2 + 0.79 MACR + 0.01 ORA1 + 0.07 ORA2	2.00×10^{-16}		2.00×10^{-16}	1
R113	MACR + O_3 --> 0.40 HCHO + 0.60 MGLY + 0.13 ORA2 + 0.54 CO + 0.08 H_2 + 0.22 ORA1 + 0.29 HO_2 + 0.07 HO + 0.13 OP2 + 0.13 ACO_3	1.36×10^{-15}	2112	1.14×10^{-18}	1

R114	DCB + O_3 --> 0.21 HO + 0.29 HO_2 + 0.66 CO + 0.50 GLY + 0.28 ACO_3 + 0.16 ALD + 0.62 MGLY + 0.11 PAA + 0.11 ORA1 + 0.21 ORA2	2.00×10^{-18}		2.00×10^{-18}	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	2.46×10^{-15}	1700	8.19×10^{-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	2.46×10^{-15}	1700	8.19×10^{-18}	1
R116	PHO + NO_2 --> 0.10 CSL + ONIT	2.00×10^{-11}		2.00×10^{-11}	1
R116a	PHO + $^{15}NO_2$ --> 0.10 CSL + ^{15}ONIT	2.00×10^{-11}		2.00×10^{-11}	1
R117	PHO + HO_2 --> CSL	1.00×10^{-11}		1.00×10^{-11}	1
R118	ADDT + NO_2 --> CSL + HONO	3.60×10^{-11}		3.60×10^{-11}	1
R118a	ADDT + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60×10^{-11}		3.60×10^{-11}	1
R119	ADDT + O_2 --> 0.98 TOLP + 0.02 CSL + 0.02 HO_2	1.66×10^{-17}	-1044	5.52×10^{-16}	1
R120	ADDT + O_3 --> CSL + HO	5.00×10^{-11}		5.00×10^{-11}	1
R121	ADDX + NO_2 --> CSL + HONO	3.60×10^{-11}		3.60×10^{-11}	1
R121a	ADDX + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60×10^{-11}		3.60×10^{-11}	1
R122	ADDX + O_2 --> 0.98 XYLP + 0.02 CSL + 0.02 HO_2	1.66×10^{-17}	-1044	5.52×10^{-16}	1
R123	ADDX + O_3 --> CSL + HO	1.00×10^{-11}		1.00×10^{-11}	1
R124	ADDC + NO_2 --> CSL + HONO	3.60×10^{-11}		3.60×10^{-11}	1
R124a	ADDC + $^{15}NO_2$ --> CSL + HO^{15}NO	3.60×10^{-11}		3.60×10^{-11}	1

R125	DDC + O_2 --> 0.98 CSLP + 0.02 CSL + 0.02 HO_2	1.66 x 10^{-17}	-1044	5.52 x 10^{-16}	1
R126	DDC + O3 --> CSL + HO_2	5.00 x 10^{-11}		5.00 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 + 0.334 XO_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 + 0.334 XO_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
R150	MO_2 + HO_2 --> OP1	3.80 x 10^{-13}	-800	5.57 x 10^{-12}	1
R151	ETHP + HO_2 --> OP2	7.50 x 10^{-13}	-700	7.86 x 10^{-12}	1
R152	HC3P + HO_2 --> OP2	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R153	HC5P + HO_2 --> OP2	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R154	HC8P + HO_2 --> OP2	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R155	ETEP + HO_2 --> OP2	1.90 x 10^{-13}	-1300	1.50 x 10^{-11}	1
R156	OLIP + HO_2 --> OP2	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1
R157	OLTP + HO_2 --> OP2	1.66 x 10^{-13}	-1300	1.30 x 10^{-11}	1

R158	ISOP + HO_2 --> OP2	1.28 x 10^{-13}	-1300	1.00 x 10^{-11}	1
R159	APIP + HO_2 --> OP2	1.50 x 10^{-13}		1.50 x 10^{-11}	1
R160	LIMP + HO_2 --> OP2	1.50 x 10^{-13}		1.50 x 10^{-11}	1
R161	TOLP + HO_2 --> OP2	3.75 x 10^{-13}	-980	1.01 x 10^{-11}	1
R162	XYLP + HO_2 --> OP2	3.75 x 10^{-13}	-980	1.01 x 10^{-11}	1
R163	CSLP + HO_2 --> OP2	3.75 x 10^{-13}	-980	1.01 x 10^{-11}	1
R164	ACO_3 + HO_2 --> PAA	1.15 x 10^{-13}	-550	7.28 x 10^{-12}	1
R165	ACO_3 + HO_2 --> ORA2 + O_3	3.86 x 10^{-13}	-2640	2.72 x 10^{-12}	1
R166	TCO_3 + HO_2 --> OP2	1.15 x 10^{-13}	-550	7.28 x 10^{-12}	1
R167	TCO_3 + HO_2 --> ORA2 + O_3	3.86 x 10^{-13}	-2640	2.72 x 10^{-12}	1
R168	KETP + HO_2 --> OP2	1.15 x 10^{-13}	-1300	9.02 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
R171	MO_2 + MO_2 --> 1.33 HCHO + 0.66 HO_2	9.10 x 10^{-14}	-416	3.68 x 10^{-13}	1
R172	ETHP + MO_2 --> 0.75 HCHO + HO_2 + 0.75 ALD	1.18 x 10^{-14}	-158	2.01 x 10^{-13}	1
R173	HC3P + MO_2 --> 0.81 HCHO + 0.992 HO_2 + 0.58 ALD + 0.018 KET + 0.007 MO_2 + 0.005 MGLY + 0.085 XO_2 + 0.119 GLY	9.46 x 10^{-14}	-431	4.02 x 10^{-13}	1
R174	HCSP + MO_2 --> 0.829 HCHO + 0.946 HO_2 + 0.523 ALD + 0.24 KET + 0.014 ETHP + 0.049 MO_2 + 0.245 XO_2	1.00 x 10^{-13}	-467	4.79 x 10^{-13}	1
R175	HC8P + MO_2 --> 0.753 HCHO + 0.993 HO_2 + 0.411 ALD + 0.419 KET + 0.322 XO_2 + 0.013 ETHP	4.34 x 10^{-14}	-633	3.63 x 10^{-13}	1
R176	ETEP + MO_2 --> 1.55 HCHO + HO_2 + 0.35 ALD	1.71 x 10^{-13}	-708	1.84 x 10^{-12}	1

R177	OLTP + MO_2 --> 1.25 HCHO + HO_2 + 0.669 ALD + 0.081 KET	1.46 x 10^{-13}	-708	1.57 x 10^{-12}	1
R178	OLIP + MO_2 --> 0.755 HCHO + HO_2 + 0.932 ALD + 0.313 KET	9.18 x 10^{-14}	-708	9.87 x 10^{-13}	1
R179	ISOP + MO_2 --> 0.550 MACR + 0.370 OLT + HO_2+ 0.08 OLI + 1.09 HCHO	1.36 x 10^{-13}	-708	1.46 x 10^{-12}	1
R180	APIP + MO_2 --> HCHO + ALD + KET + 2 HO_2	3.56 x 10^{-14}	-708	3.83 x 10^{-13}	1
R181	LIMP + MO_2 --> 1.4 HCHO + 0.60 MACR + 0.40 OLI + 2 HO_2	3.56 x 10^{-14}	-708	3.83 x 10^{-13}	1
R182	TOLP + MO_2 --> HCHO + HO_2 + 0.35 MGLY + 0.65 GLY + DCB	3.56 x 10^{-14}	-708	3.83 x 10^{-13}	1
R183	XYLP + MO_2 --> HCHO + HO_2 + 0.63 MGLY + 0.37 GLY + DCB	3.56 x 10^{-14}	-708	3.83 x 10^{-13}	1
R184	CSLP + MO_2 --> GLY + MGLY + HCHO + 2 HO_2	3.56 x 10^{-14}	-708	3.83 x 10^{-13}	1
R185	ACO_3 + MO_2 --> HCHO + HO_2 + MO_2	3.21 x 10^{-11}	440	7.33 x 10^{-12}	1
R186	ACO_3 + MO_2 --> HCHO + ORA2	2.68 x 10^{-16}	-2510	1.22 x 10^{-12}	1
R187	TCO_3 + MO_2 --> 2 HCHO + HO_2 + ACO_3	3.21 x 10^{-11}	440	7.33 x 10^{-12}	1
R188	TCO3 + MO_2 --> HCHO + ORA2	2.68 x 10^{-16}	-2510	1.22 x 10^{-12}	1
R189	KETP + MO_2 --> 0.75 HCHO + 0.88 HO_2 + 0.40 MGLY + 0.30 ALD + 0.30 HKET + 0.12 ACO_3 + 0.08 XO_2	6.91 x 10^{-13}	-508	3.80 x 10^{-12}	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
R192	ETHP + ACO_3 --> ALD + 0.5 HO_2 + 0.5 MO_2 + 0.5 ORA2	1.03 x 10^{-12}	-211	2.09 x 10^{-12}	1
R193	HC3P + ACO_3 --> 0.724 ALD + 0.127 KET + 0.488 HO_2 + 0.508 MO_2 + 0.006 ETHP + 0.071 XO_2 + 0.091 HCHO + 0.10 GLY + 0.499 ORA2 + 0.004 MGLY	6.90 x 10^{-14}	-460	3.23 x 10^{-12}	1
R194	HC5P + ACO_3 --> 0.677 ALD + 0.33 KET + 0.438 HO_2 + 0.554 MO_2 + 0.495 ORA2 + 0.018 ETHP + 0.237 XO_2 + 0.076 HCHO	5.59 x 10^{-13}	-522	3.22 x 10^{-12}	1
R195	HC8P + ACO_3 --> 0.497 ALD + 0.581 KET + 0.489 HO_2 + 0.507 MO_2 + 0.495 ORA2 + 0.015 ETHP + 0.318 XO_2	2.47 x 10^{-13}	-683	2.44 x 10^{-12}	1
R196	ETEP + ACO_3 --> 0.8 HCHO + 0.6 ALD + 0.5 HO_2 + 0.5 MO_2 + 0.5 ORA2	9.48 x 10^{-13}	-765	1.24 x 10^{-11}	1
R197	OLTP + ACO_3 --> 0.859 ALD + 0.501 HCHO + 0.501 HO_2 + 0.501 MO_2 + 0.499 ORA2 + 0.141 KET	8.11 x 10^{-13}	-765	1.06 x 10^{-11}	1
R198	OLIP + ACO_3 --> 0.941 ALD + 0.569 KET + 0.51 HO_2 + 0.51 MO_2 + 0.49 ORA2	5.09 x 10^{-13}	-765	6.63 x 10^{-12}	1
R199	ISOP + ACO_3 --> 0.771 MACR + 0.229 OLT + 0.506 HO_2 + 0.494	7.60 x 10^{-13}	-765	9.90 x 10^{-12}	1

	ORA2 + 0.340 HCHO + 0.506 MO_2				
R200	APIP + ACO_3 --> ALD + KET + HO_2 + MO_2	7.40 x 10^{-13}	-765	9.63 x 10^{-12}	1
R201	LIMP + ACO_3 --> 0.60 MACR + 0.40 OLI + 0.40 HCHO + HO_2 + MO_2	7.40 x 10^{-13}	-765	9.63 x 10^{-12}	1
R202	TOLP + ACO_3 --> MO_2 + HO_2 + 0.35 MGLY + 0.65 GLY + DCB	7.40 x 10^{-13}	-765	9.63 x 10^{-12}	1
R203	XYLP + ACO_3 --> MO_2 + HO_2 + 0.63 MGLY + 0.37 GLY + DCB	7.40 x 10^{-13}	-765	9.63 x 10^{-12}	1
R204	CSLP + ACO_3 --> GLY + MGLY + MO_2 + HO_2	7.40 x 10^{-13}	-765	9.63 x 10^{-12}	1
R205	ACO_3 + ACO_3 --> 2 MO_2	2.80 x 10^{-12}	-530	1.66 x 10^{-11}	1
R206	TCO_3 + ACO_3 --> MO_2 + ACO_3 + HCHO	2.80 x 10^{-12}	-530	1.66 x 10^{-11}	1
R207	KETP + ACO_3 --> 0.54 MGLY + 0.35 ALD + 0.11 KET + 0.12 ACO_3 + 0.38 HO_2+ 0.08 XO_2 + 0.5 MO_2 + 0.5 ORA2	7.51 x 10^{-13}	-765	5.00 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 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-12}	1
R214	ETHP + NO_3 --> ALD + HO_2 + NO_2	1.20×10^{-12}		1.20×10^{-12}	1
R214a	ETHP + $^{15}NO_3$ --> ALD + HO_2 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-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	1.20×10^{-12}		1.20×10^{-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 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-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	1.20×10^{-12}		1.20×10^{-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 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-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	1.20×10^{-12}		1.20×10^{-12}	1
R217a	HC8P + $^{15}NO_3$ --> 0.187 ALD + 0.88 KET + 0.845 HO_2 + 0.155 ETHP + 0.587 XO_2 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-12}	1
R218	ETEP + NO_3 --> 1.6 HCHO + 0.2 ALD + HO_2 + NO_2	1.20×10^{-12}		1.20×10^{-12}	1
R218a	ETEP + $^{15}NO_3$ --> 1.6 HCHO + 0.2 ALD + HO_2 + $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-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

R232	$XO_2 + HO_2$ --> OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	1
R233	$XO_2 + MO_2$ --> HCHO + HO_2	5.99×10^{-15}	-1510	9.50×10^{-13}	1
R234	$XO_2 + ACO_3$ --> MO_2	3.40×10^{-14}	-1516	6.38×10^{-12}	1
R235	$XO_2 + XO_2$ -->	7.13×10^{-17}	-2950	1.42×10^{-12}	1
R236	XO_2 + NO --> NO_2	4.00×10^{-12}		4.00×10^{-12}	1
R236a	$XO_2 + {}^{15}NO$ --> $^{15}NO_2$	4.00×10^{-12}		4.00×10^{-12}	1
R237	XO_2 + NO3 --> NO_2	1.20×10^{-12}		1.20×10^{-12}	1
R237a	$XO_2 + {}^{15}NO3$ --> $^{15}NO_2$	1.20×10^{-12}		1.20×10^{-12}	1
R238	NO + $^{15}NO_2$ --> ^{15}NO + NO_2	3.60×10^{-14}		3.60×10^{-14}	1
R238a	^{15}NO + NO_2 --> NO + $^{15}NO_2$	3.60×10^{-14}	-18.467	3.83×10^{-14}	0.9771
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: The RACM Mechanism

Reaction No.	Reaction	C, K^{-2} cm^3 s^{-1}	D, K	α
R61	CH_4 + HO --> MO_2 + H_2O	7.44 x 10^{-18}	1361	1
R62	ETH + HO --> ETHP + H_2O	1.51 x 10^{-17}	492	1
R78	KET + HO --> KETP + H_2O	5.68 x 10^{-18}	-92	1
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	α
R35	$O^3P + NO \rightarrow NO_2$	9.00×10^{-32}	1.5	3.00×10^{-11}	0	1
R35a	$O^3P + {}^{15}NO \rightarrow {}^{15}NO_2$	9.00×10^{-32}	1.5	3.00×10^{-11}	0	1
R37	$O^3P + NO_2 \rightarrow NO_3$	9.00×10^{-32}	2	2.20×10^{-11}	0	1
R37a	$O^3P + {}^{15}NO_2 \rightarrow {}^{15}NO_3$	9.00×10^{-32}	2	2.20×10^{-11}	0	1
R38	$HO + NO \rightarrow HONO$	7.00×10^{-31}	2.6	1.50×10^{-11}	0.5	1
R38a	$HO + {}^{15}NO \rightarrow HO{}^{15}NO$	7.00×10^{-31}	2.6	1.50×10^{-11}	0.5	1
R39	$HO + NO_2 \rightarrow HNO_3$	2.60×10^{-30}	3.2	2.40×10^{-11}	1.3	1
R39a	$HO + {}^{15}NO_2 \rightarrow H{}^{15}NO_3$	2.60×10^{-30}	3.2	2.40×10^{-11}	1.3	1.04
R42	$HO_2 + NO_2 \rightarrow HNO_4$	2.80×10^{-31}	3.2	4.70×10^{-12}	1.4	1
R42a	$HO_2 + {}^{15}NO_2 \rightarrow H{}^{15}NO_4$	2.80×10^{-31}	3.2	4.70×10^{-12}	1.4	1
R53	$NO_3 + NO_2 \rightarrow N_2O_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1
R53a	$NO_3 + {}^{15}NO_2 \rightarrow {}^{15}NNO_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1.0266
R53b	$^{15}NO_3 + NO_2 \rightarrow {}^{15}NNO_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1.0309
R53c	$^{15}NO_3 + {}^{15}NO_2 \rightarrow {}^{15}N_2O_5$	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1.057
R57	$HO + SO_2 \rightarrow SULF + HO_2$	3.0×10^{-31}	3.3	1.50×10^{-12}	0	1
R127	$ACO_3 + NO_2 \rightarrow PAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R127a	$ACO_3 + {}^{15}NO_2 \rightarrow {}^{15}PAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R129	$TCO_3 + NO_2 \rightarrow TPAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R129a	$TCO_3 + {}^{15}NO_2 \rightarrow {}^{15}TPAN$	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1

Table S2d: Troe reactions

Reaction No.	Reaction	A	B	K_0^{300}, $cm^6\ s^{-1}$	n	K_∞^{300}, $cm^6\ s^{-1}$	m	α
R43	$HNO4 \rightarrow HO_2 + NO_2$	$4.76 \times 10^{+26}$	10900	1.81×10^{-31}	3.2	4.70×10^{-12}	1.4	1
R43a	$H^{15}NO4 \rightarrow HO_2 + {}^{15}NO_2$	$4.76 \times 10^{+26}$	10900	1.81×10^{-31}	3.2	4.70×10^{-12}	1.4	1
R54	$N_2O_5 \rightarrow NO_2 + NO_3$	$3.70 \times 10^{+26}$	11000	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1
R54a	$^{15}NNO_5 \rightarrow {}^{15}NO_2 + NO_3$	$3.70 \times 10^{+26}$	11000	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	0.5
R54b	$^{15}NNO_5 \rightarrow NO_2 + {}^{15}NO_3$	$3.70 \times 10^{+26}$	11000	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	0.5
R54c	$^{15}N_2O_5 \rightarrow {}^{15}NO_2 + {}^{15}NO_3$	$3.70 \times 10^{+26}$	11000	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1
R128	$PAN \rightarrow ACO_3 + NO_2$	$1.16 \times 10^{+28}$	13954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R128a	$^{15}PAN \rightarrow ACO_3 + {}^{15}NO_2$	$1.16 \times 10^{+28}$	13954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R130	$TPAN \rightarrow TCO_3 + NO_2$	$1.16 \times 10^{+28}$	13954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R130a	$^{15}TPAN \rightarrow TCO_3 + {}^{15}NO_2$	$1.16 \times 10^{+28}$	13954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1

Table S2e: Troe equilibrium reactions

Reaction No.	Reaction	Rate Constant Expression	α
R24	$O^3P + O_2 \rightarrow O_3$	$[M] \times 6.0 \times 10^{-34} \times (T/300\ K)^{-23}$	1
R33	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$2.3 \times 10^{-13} \times \exp(600/T) + 1.7 \times 10^{-33} \times [M] \times \exp(1000/T)$	1
R34	$HO_2 + HO_2 + H_2O \rightarrow H_2O_2 + O_2 + H_2O$	$3.22 \times 10^{-34} \times \exp(2800/T) + 2.38 \times 10^{-54} \times [M] \times \exp(3200/T)$	1
R46	$HO + HNO_3 \rightarrow NO_3 + H_2O$	$k = k_o + k_3/(1 + k_3/k_2)$ ko = 7.2 x 10-15 x exp(785/T) k2 = 4.1 x 10-16 x exp(1440/T) k3 = 1.9 x 10-33 x exp(725/T) x [M]	1
R46a	$HO + H^{15}NO_3 \rightarrow {}^{15}NO_3 + H_2O$		1
R58	$CO + HO \rightarrow HO_2 + CO_2$	$1.5 \times 10^{-13} \times (1 + 2.439 \times 10^{-20} \times [M])$	1

Table S2f: Reactions with special rate expressions

*[M] is the concentration of air in molecules cm^{-3}

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

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 S4: 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 S5: Fractionation factors of Leighton cycle, NO_x isotope exchange, OH production of HNO_3, and N_2O_5 heterogeneous reactions.

Does NO_2OH equilibrate with NO_2 + OH?

$$NO_2 + OH \underset{k_r}{\overset{k_f}{\rightleftarrows}} NO2OH^* \xrightarrow{+M,\ k_q} HNO_3$$

3 body rate law

$dHNO3/dt = k_{obs} = k_f\, k_q[M]/ (k_r + k_q[M])$

Solve for the unimolecular decay, reverse constant k_r

$k_r + k_q[M] = k_f\, k_q[M]/ k_{obs}$

$k_r = k_f\, k_q[M]/ k_{obs} + k_q[M] = [M]\ (k_f\, k_q/ k_{obs} + k_q.)$ (4)

k_f = assume collisional frequency NO_2 + OH (Ea =0 no activation energy) = 2.9×10^{-10}
k_q = assume collisional frequency NO_2OH^* + N_2 (every collision deactivates, max rate) = 2.3×10^{-10}
K_{obs}= high pressure limit, surface pressure = 6.3×10^{-11} (from recent exp paper)
[M]=2.5×10^{19}

$k_r = (2.5 \times 10^{19})[(2.3 \times 10^{-10})(2.9 \times 10^{-10})/ 6.3 \times 10^{-11}) + 2.9 \times 10^{-10}]$
$= 3.23 \times 10^{10}$ (first order rate k unimolecular decay of [NO2OH*]

lifetime to decay = $1/k_r = 3.1 \times 10^{-11}$ s
lifetime to react = $[NO2OH^*]/ (k_q[NO2OH^*][M]) = 1/[M]k_q = 17.2 \times 10^{-11}$
complex will decay is 17.2/3.1 = 5.5 times faster than HNO_3 formation, even more at lower pressure.

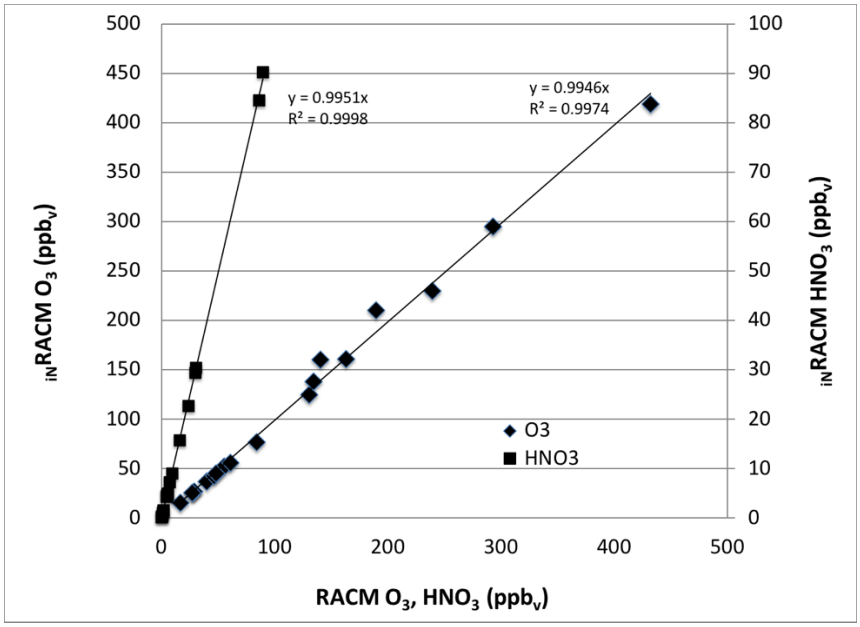

Fig. S1 Comparison of HNO_3 and O_3 mixing ratios (ppb_v) predicted by RACM and $_{iN}$RACM for 24 test cases described in Stockwell et al.(1997). $_{iN}$RACM was run with without the heterogeneous N_2O_5 reaction and without O_3 deposition in order to mimic the RACM simulations.

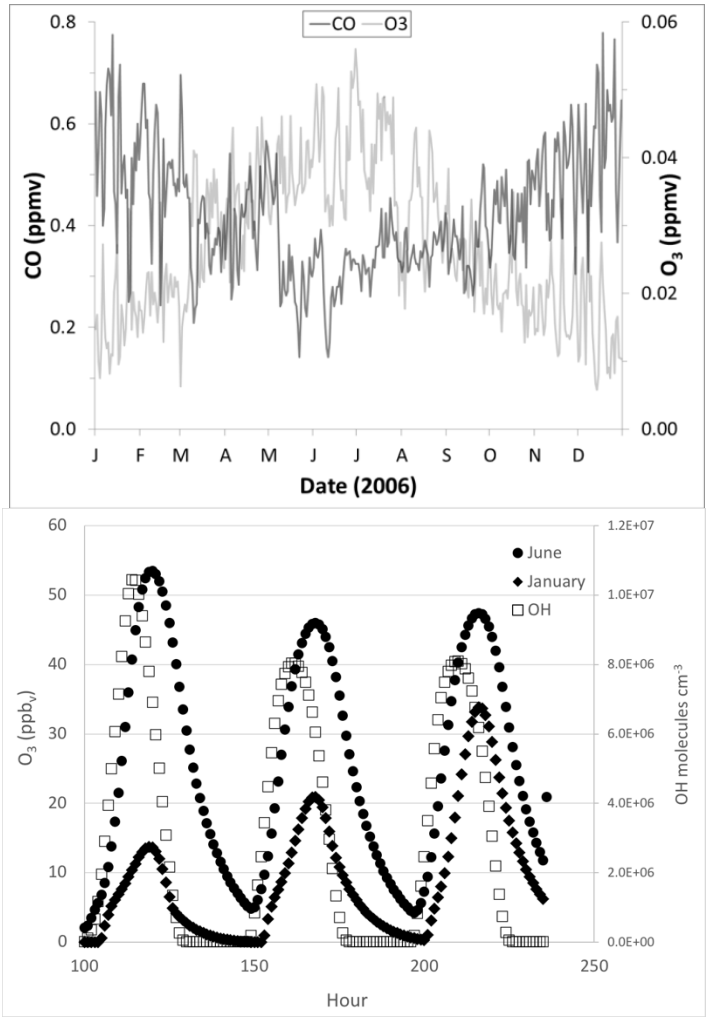

Fig. S2. Upper graph in the overserved O_3 mixing ratios in Tucson during 2006 (from Pima County Department of Environmental Quality's Air Quality Monitoring Division). Lower graph is O_3 mixing ratios for day 2-5 of 1 week simulations for June and January and OH concentrations (June only) using Tucson conditions. Observed seasonal and daily O_3 mixing ratio variations are captured reasonably well by $_{in}$RACM and OH concentrations match observations in urban environments like Tucson.

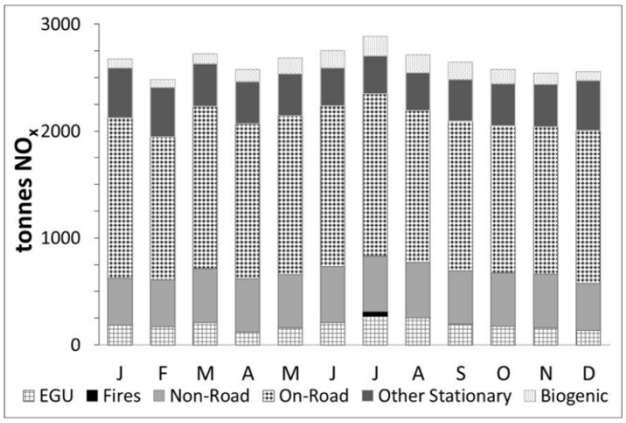

Figure S3. 2005 EPA NO_x Emission Inventory for Pima County, AZ (Riha, 2013).

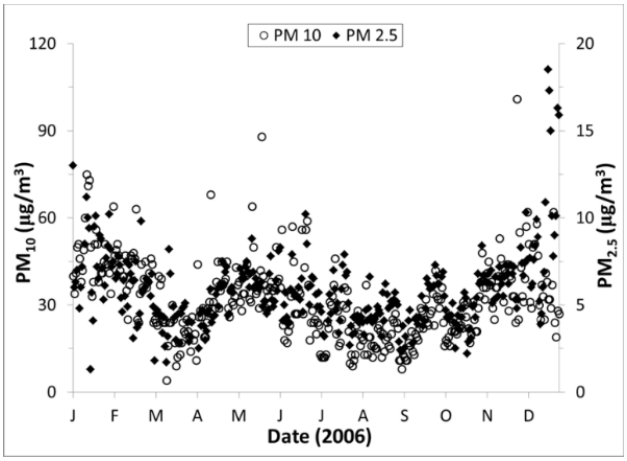

Figure S4. $PM_{2.5}$ and PM_{10} aerosol concentration ($\mu g/m^3$) in Tucson, AZ in 2006 (Riha, 2013).

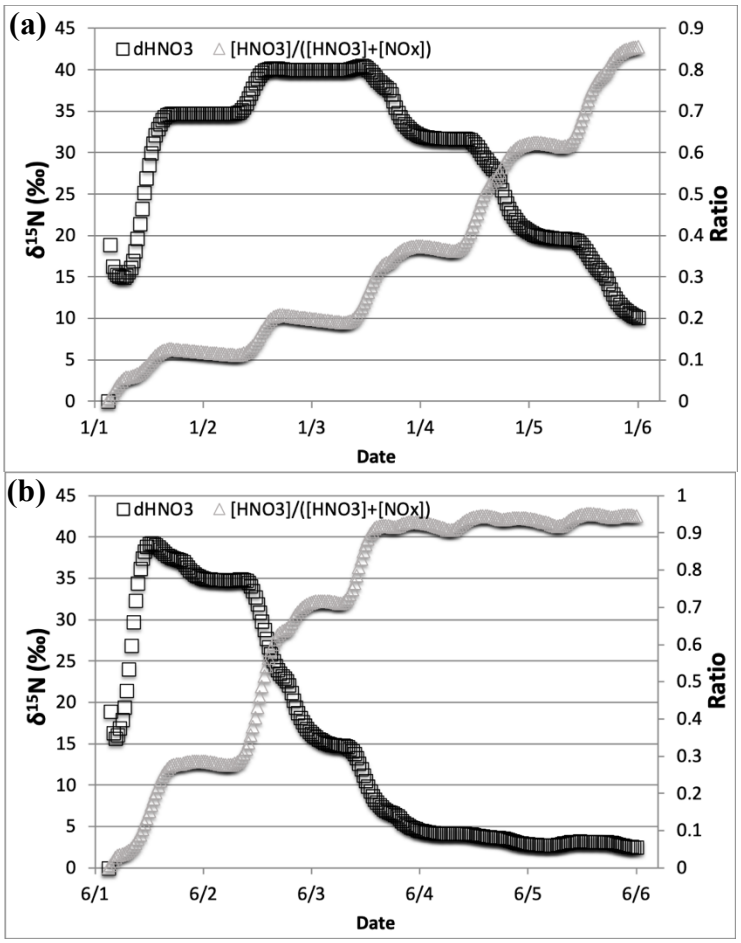

Figure S5. The $\delta^{15}N(HNO_3)$ (□) and $HNO_3/(HNO_3+NO_x)$ (Δ, right axis) based on i_NRACM mechanism, started on Jan 1 (a) and Jun 1 (b). The 5-day simulation was under the conditions list in Table S3c

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