Supplemental Information for

The Regional Atmospheric Chemistry Mechanism, Version 2

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Table S1. RACM2 species list.

Species	Definition	Carbon #	MW	Species	Definition	Carbon #	MW
CO	Carbon monoxide	1	28	ACD	Acetaldehyde	2	44
CO2	Carbon dioxide	1	44	ACE	Acetylene	2	26
H2	Hydrogen		2	ACO3	Acetyl peroxy radicals	2	75
H2O	Water		18	ACT	acetone	3	58
H2O2	Hydrogen peroxide		34	ACTP	Peroxy radicals formed from ACT	3	89
HNO3	Nitric acid		63	ADCN	Aromatic-NO3 adduct from PHEN	6	156
HNO4	Pernitric acid		79	ADDC	Aromatic-HO adduct from CSL	7	125
HO	Hydroxy radical		17	ALD	C3 and higher aldehydes	3	58
HO2	Hydroperoxy radical		33	API	Alpha-pinenes and other cyclic terpenes with one double bond	10	136
HONO	Nitrous acid		47	APIP	Peroxy radicals formed from API	10	185
N2	Nitrogen		28	BALD	Benzaldehyde and other aromatic aldehydes	7	106
N2O5	Dinitrogen pentoxide		108	BALP	Peroxy radicals formed from BALD	7	137
NO	Nitric oxide		30	BAL1	Peroxy radicals formed from BALD	7	121
NO2	Nitrogen dioxide		46	BAL2	Peroxy radicals formed from BALD	7	105
NO3	Nitrogen trioxide		62	BEN	Benzene	6	78

O1D	Excited state oxygen atom, $O(^1D)$	16	BENP	Peroxy radicals formed from BEN	6	127
O2	Oxygen	32	CH4	methane	1	16
O3	Ozone	48	CHO	Phenoxy radical formed from CSL	7	139
O3P	Ground state oxygen atom, $O(^3P)$	16	CSL	Cresol and other hydroxy substituted aromatics	7	108
SO2	Sulfur dioxide	64	DCB1	Unsaturated dicarbonyls	4.5	91
SULF	Sulfuric acid	98	DCB2	Unsaturated dicarbonyls	7	110
			DCB3	Unsaturated dicarbonyls	4	84
			DIEN	Butadiene and other anthropogenic dienes	4	54
			EOH	Ethanol	2	46
			EPX	Epoxide formed in TOL, XYL and XYO reactions	7.75	122.5
			ETE	ethene	2	28
			ETEG	Ethylene glycol	2	62
			ETEP	Peroxy radicals formed from ETE	2	77
			ETH	ethane	2	30
			ETHP	Peroxy radicals formed from ETH	2	61
			GLY	Glyoxal	2	58
			HC3	Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) less than 3.4x10-12 cm3 s-1	3.6	44
			HC3P	Peroxy radicals formed from HC3	3.6	75

HC5	Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) between 3.4x10-12 and 6.8x10-12 cm3 s-1	5.6	72
HC5P	Peroxy radicals formed from HC5	5.6	103
HC8	Alkanes, esters and alkynes with HO rate constant (298 K, 1 atm) greater than 6.8x10-12 cm3 s-1	7.9	114
HC8P	Peroxy radicals formed from HC8	7.9	145
HCHO	Formaldehyde	1	30
HKET	Hydroxy ketone	3	74
ISHP	Beta-hydroxy hydroperoxides from ISOP+HO2	5	118
ISO	Isoprene	5	68
ISON	Beta-hydroxyalkylnitrates from ISOP+NO alkylnitrates from ISO+NO3	5	147
ISOP	Peroxy radicals formed from ISO+HO	5	117
KET	ketones	5	86
KETP	Peroxy radicals formed from KET	5	117
LIM	d-limonene and other cyclic diene-terpenes	10	136
LIMP	Peroxy radicals formed from LIM	10	185
MACP	Peroxy radicals formed from MACR+HO	4	101

MACR	methacrolein	4	70
MAHP	Hydroperoxides from MACP+HO2	4	102
MCP	Peroxy radical formed from MACR + HO which does not form MPAN	4	119
MCT	Methyl catechol	7	124
MCTO	Alkoxy radical formed from MCT+HO and MCT+NO3	7	123
MCTP	Radical formed fro MCT+O3 reaction	7	172
MEK	Methyl ethyl ketone	4	72
MEKP	Peroxy radicals formed from MEK	4	103
MGLY	Methylglyoxal and other alpha-carbonyl aldehydes	3	72
MO2	Methyl peroxy radical	1	47
MOH	methanol	1	32
MPAN	Peroxymethacryloylnitrate and other higher peroxyacylnitrates from isoprene oxidation	4	148
MVK	Methyl vinyl ketone	4	70
MVKP	Peroxy radicals formed from MVK	4	119
NALD	nitrooxyacetaldehyde	2	105
OLI	Internal alkenes	5	68
OLIP	Peroxy radicals formed from OLI	5	117
OLND	NO3-alkene adduct reacting via decomposition	3	136

OLNN	NO3-alkene adduct reacting to form carbonitrates + HO2	3	136
OLT	Terminal alkenes	3.8	42
OLTP	Peroxy radicals formed from OLT	3.8	91
ONIT	Organic nitrate	3.5	119
OP1	Methyl hydrogen peroxide	1	48
OP2	Higher organic peroxides	2	62
ORA1	Formic acid	1	46
ORA2	Acetic acid and higher acids	2	60
ORAP	Peroxy radical formed from ORA2 + HO reaction	2	109
PAA	Peroxyacetic acids and higher analogs	2	76
PAN	Peroxyacetyl nitrate and higher saturated PANs	2	121
PER1	Peroxy intermediate formed from TOL	7.1	141
PER2	Peroxy intermediate formed from TOL	7.1	157
PHEN	phenol	6	94
PHO	Phenoxy radical formed from phenol	6	93
PPN	Peroxypropionyl nitrate	3	135
RCO3	Higher saturated acyl peroxy radicals	3	90
ROH	C3 and higher alcohols	3	60
TLP1	Peroxy radicals formed from TOL	7.1	91

TOL	Toluene and less reactive aromatics	7.1	92
TOLP	Peroxy radicals formed from TOL	7.1	141
TR2	Peroxy radicals formed from TOL	7.1	109
UALD	Unsaturated aldehydes	5	84
UALP	Peroxy radicals formed from UALD	5	133
XO2	Accounts for addition NO to NO2 conversions	N/a	N/a
XY2	Peroxy radicals formed from XYL	8.9	124
XYL1	Peroxy radicals formed from XYL	8.9	156
XYM	M-xylene	8.9	106
XYP	P-xylene	8.9	106
XYLP	Peroxy radicals formed from XYL	8.9	155
XYO	o-xylene	8.9	106
XYO2	Peroxy radicals formed from XYO	8.9	155
XYOP	Peroxy radicals formed from XYO	8.9	155

Table S2a. The RACM2 Chemical Mechanism: Photolysis Reactions

Reaction No.	Reaction	Photolysis Frequency s^{-1}	Cross Section Notes	Quantum Yield Notes
R001	$O_3 + h\nu \rightarrow O^3P + O_2$	4.31×10^{-4}	JPL 2011	1
R002	$O_3 + h\nu \rightarrow O^1D + O_2$	1.67×10^{-5}	JPL 2011	JPL 2011
R003	$H_2O_2 + h\nu \rightarrow 2\ HO$	5.98×10^{-6}	JPL 2011	2
R004	$NO_2 + h\nu \rightarrow O^3P + NO$	8.41×10^{-3}	JPL 2011	JPL 2011
R005	$NO_3 + h\nu \rightarrow NO + O_2$	2.28×10^{-2}	JPL 2011	JPL 2011
R006	$NO_3 + h\nu \rightarrow O^3P + NO_2$	1.80×10^{-1}	JPL 2011	JPL 2011
R007	$HONO + h\nu \rightarrow HO + NO$	1.22×10^{-3}	JPL 2011	JPL 2011
R008	$HNO_3 + h\nu \rightarrow HO + NO_2$	4.59×10^{-7}	JPL 2011	2
R009	$HNO_4 + h\nu \rightarrow 0.20\ HO + 0.80\ HO_2 + 0.80\ NO_2 + 0.20\ NO_3$	5.21×10^{-6}	JPL 2011	2,3
R010	$HCHO + h\nu \rightarrow H_2 + CO$	4.02×10^{-5}	JPL 2011	JPL 2011
R011	$HCHO + h\nu \rightarrow 2\ HO_2 + CO$	4.02×10^{-5}	JPL 2011	JPL 2011
R012	$ACD + h\nu \rightarrow HO_2 + MO_2 + CO$	3.45×10^{-6}	JPL 2011	JPL 2011
R013	$ALD + h\nu \rightarrow HO_2 + ETHP + CO$	4.41×10^{-6}	JPL 2011	4
R014	$ACT + h\nu \rightarrow MO_2 + ACO_3$	9.91×10^{-7}	JPL 2011	JPL 2011
R015	$UALD + h\nu \rightarrow 1.22\ HO_2 + 0.784\ ACO_3 + 1.22\ CO + 0.35\ HCHO + 0.434\ ALD + 0.216\ KET$	1.15×10^{-5}	5	6
R016	$MEK + h\nu \rightarrow 0.50\ MO_2 + 0.50\ ETHP + ACO_3$	1.10×10^{-6}	7	8
R017	$KET + h\nu \rightarrow ETHP + ACO_3$	8.60×10^{-6}	9	8
R018	$HKET + h\nu \rightarrow HO_2 + ACO_3 + HCHO$	1.48×10^{-6}	10, R17 (KET)	R17 (KET)
R019	$MACR + h\nu \rightarrow 0.34\ HO + 0.66\ HO_2 + 0.67\ ACO_3 + 0.33\ MACP + 0.34\ XO_2 + 0.67\ CO + 0.67\ HCHO$	3.55×10^{-6}	JPL 2011	JPL 2011
R020	$MVK + h\nu \rightarrow 0.3\ MO_2 + 0.3\ MACP + 0.7\ CO + 0.7\ UALD$	7.59×10^{-7}	JPL 2011	JPL 2011
R021	$GLY + h\nu \rightarrow H_2 + 2\ CO$	4.95×10^{-6}	JPL 2011	JPL 2011
R022	$GLY + h\nu \rightarrow 2\ CO + HCHO$	2.37×10^{-5}	JPL 2011	JPL 2011
R023	$GLY + h\nu \rightarrow 2\ HO_2 + 2\ CO$	6.03×10^{-5}	JPL 2011	JPL 2011
R024	$MGLY + h\nu \rightarrow HO_2 + ACO_3 + CO$	6.03×10^{-4}	JPL 2011	JPL 2011
R025	$DCB1 + h\nu \rightarrow 1.5\ HO_2 + 0.5\ ACO_3 + 2\ XO_2 + CO + 0.5\ GLY + 0.5\ MGLY$	6.03×10^{-4}	R24 (MGLY)	R24 (MGLY)

Table S2a – Continued. The RACM2 Chemical Mechanism: Photolysis Reactions

Reaction No.	Reaction	Photolysis Frequency s^{-1}	Cross Section	Quantum Yield
R026	$DCB2 + h\nu \rightarrow 1.5\ HO_2 + 0.5\ ACO_3 + 2\ XO_2 + CO + 0.5\ GLY + 0.5\ MGLY$	6.03×10^{-4}	R24 (MGLY)	R24 (MGLY)
R027	$BALD + h\nu \rightarrow CHO + HO_2 + CO$	3.32×10^{-5}	12, SAPRC07	SAPRC07
R028	$OP1 + h\nu \rightarrow HO + HO_2 + HCHO$	4.11×10^{-6}	JPL 2011	13, JPL 2011
R029	$OP2 + h\nu \rightarrow HO + HO_2 + ALD$	4.11×10^{-6}	R29 (OP1)	R29 (OP1)
R030	$PAA + h\nu \rightarrow HO + MO_2$	5.93×10^{-7}	JPL 2011	14
R031	$ONIT + h\nu \rightarrow HO_2 + NO_2 + 0.20\ ALD + 0.80\ KET$	1.96×10^{-6}	15	15
R032	$PAN + h\nu \rightarrow ACO_3 + NO_2$	3.81×10^{-7}	JPL (2011)	JPL (2011)
R033	$PAN + h\nu \rightarrow MO_2 + NO_3 + CO_2$	2.26×10^{-7}	JPL (2011)	JPL (2011)

1. Assumed to be equal to 1.00 minus the quantum yield of R002 (O^1D).
2. Assumed to be unity
3. Stoichiometry: JPL 2011 above 200 nm
4. Heicklen et al. (1986)
5. Based upon crotonaldehyde
6. Magneron et al. 2002
7. Yujing and Mellouki 2000
8. Set to 0.34, Raben and Moortgat (1996)
9. $C_2H_5COC_2H_5$ used as surrogate Yujing and Mellouki 2000
10. Products from hydroxyacetone
11. OLIP added for mass balance
12. Products Zhu and Cronin (2000)
13. Set to 1.00
14. Orlando, J. J. and G. S. Tyndall, 2003 – assumed to be unity
15. Talukdar et al. (1997)

Table S2b. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3 s^{-1}$	E/R K	k^*	Note
	Inorganic Reactions				
R034	$O_3 + HO \rightarrow HO_2 + O_2$	1.70×10^{-12}	940	7.26×10^{-14}	1
R035	$O_3 + HO_2 \rightarrow HO + 2\ O_2$	1.00×10^{-14}	490	1.93×10^{-15}	2
R036	$O_3 + NO \rightarrow NO_2 + O_2$	1.40×10^{-12}	1310	1.73×10^{-14}	1
R037	$O_3 + NO_2 \rightarrow NO_3 + O_2$	1.40×10^{-13}	2470	3.53×10^{-17}	1
R038	$O^3P + O_2 \rightarrow O_3$	Table 2f		1.40×10^{-14}	1
R039	$O^3P + O_3 \rightarrow 2\ O_2$	8.00×10^{-12}	2060	7.99×10^{-15}	1
R040	$O^1D + O_2 \rightarrow O^3P + O_2$	3.20×10^{-11}		3.20×10^{-11}	1
R041	$O^1D + N_2 \rightarrow O^3P + N_2$	1.80×10^{-11}	-107	2.58×10^{-11}	1
R042	$O^1D + H_2O \rightarrow 2\ HO$	2.20×10^{-10}		2.20×10^{-10}	1
R043	$H_2 + HO \rightarrow H_2O + HO_2$	7.70×10^{-12}	2100	6.72×10^{-15}	1
R044	$HO + HO_2 \rightarrow H_2O + O_2$	4.80×10^{-11}	-250	1.11×10^{-10}	1
R045	$2\ HO_2 \rightarrow H_2O_2 + O_2$	Table 2f		2.90×10^{-12}	1
R046	$2\ HO_2 + H_2O \rightarrow H_2O_2 + H_2O + O_2$	Table 2f		6.42×10^{-30}	1
R047	$H_2O_2 + HO \rightarrow HO_2 + H_2O$	2.90×10^{-12}	160	1.70×10^{-12}	1
R048	$NO + O^3P \rightarrow NO_2$	Table 2d		1.66×10^{-12}	2
R049	$NO + HO \rightarrow HONO$	Table 2d		7.40×10^{-12}	2
R050	$NO + HO_2 \rightarrow NO_2 + HO$	3.45×10^{-12}	-270	8.90×10^{-12}	1
R51	$NO + HO_2 \rightarrow HNO_3$	Table 2f			1

Table SS2b2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	K^*	Note
R052	$2\ NO + O_2 \rightarrow 2\ NO_2$	3.30×10^{-39}	-530	1.95×10^{-38}	1
R053	$HONO + HO \rightarrow NO_2 + H_2O$	2.50×10^{-12}	-260	5.98×10^{-12}	1
R054	$NO_2 + O^3P \rightarrow NO + O_2$	5.50×10^{-12}	-188	1.03×10^{-11}	1
R055	$NO_2 + O^3P \rightarrow NO_3$	Table 2d		3.28×10^{-12}	2
R056	$NO_2 + HO \rightarrow HNO_3$	Table 2d		1.06×10^{-11}	2
R057	$HNO_3 + HO \rightarrow NO_3 + H_2O$	Table 2f		1.50×10^{-13}	1
R058	$NO_3 + HO \rightarrow NO_2 + HO_2$	2.00×10^{-11}		2.00×10^{-11}	1
R059	$NO_3 + HO_2 \rightarrow 0.7\ HO + 0.7\ NO_2 + 0.3\ HNO_3$ Products Le Bras 1997	4.00×10^{-12}		4.00×10^{-12}	1
R060	$NO_3 + NO \rightarrow 2\ NO_2$	1.80×10^{-11}	-110	2.60×10^{-11}	1
R061	$NO_3 + NO_2 \rightarrow NO + NO_2 + O_2$	4.50×10^{-14}	1260	6.57×10^{-16}	2
R062	$2\ NO_3 \rightarrow 2\ NO_2 + O_2$	8.50×10^{-13}	2450	2.29×10^{-16}	2
R063	$NO_3 + NO_2 \rightarrow N_2O_5$	Table 2d		1.18×10^{-12}	2
R064	$N_2O_5 \rightarrow NO_2 + NO_3$	Table 2e		4.44×10^{-2}	2
R065	$N_2O_5 + H_2O \rightarrow HNO_3 + HNO_3$	2.50×10^{-22}		2.50×10^{-22}	1
R066	$NO_2 + HO_2 \rightarrow HNO_4$	Table 2d		1.14×10^{-12}	2
R067	$HNO_4 \rightarrow HO_2 + NO_2$	Table 2e		7.19×10^{-2}	2
R068	$HNO_4 + HO \rightarrow NO_2 + H_2O + O_2$	1.30×10^{-12}	-380	4.65×10^{-12}	1, 3
R069	$SO_2 + HO \rightarrow SULF + HO_2$	Table 2d		9.58×10^{-13}	2
R070	$CO + HO \rightarrow HO_2 + CO_2$	Table 2f		2.15×10^{-13}	1

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
	Alkanes + HO				
R071	$CH_4 + HO \rightarrow MO_2 + H_2O$	1.85×10^{-12}	1690	6.39×10^{-15}	1
R072	$ETH + HO \rightarrow ETHP + H_2O$	6.90×10^{-12}	1000	2.41×10^{-13}	1
R073	$HC3 + HO \rightarrow HC3P + H_2O$	7.68×10^{-12}	370	2.22×10^{-12}	4
R074	$HC5 + HO \rightarrow HC5P + H_2O$	1.01×10^{-11}	245	4.44×10^{-12}	5
R075	$HC8 + HO \rightarrow 0.049\ HO_2 + 0.951\ HC8P + H_2O + 0.025\ ALD + 0.024\ HKET$	2.82×10^{-11}	273	1.13×10^{-11}	6
	Alkenes + HO				
R076	$ETE + HO \rightarrow ETEP$	Table 2d		8.20×10^{-12}	2
R077	$OLT + HO \rightarrow OLTP$	5.72×10^{-12}	-500	3.06×10^{-11}	7
R078	$OLI + HO \rightarrow OLIP$	1.33×10^{-11}	-500	7.11×10^{-11}	7
R079	$DIEN + HO \rightarrow OLIP$	1.48×10^{-11}	-448	6.65×10^{-11}	8
	Alkynes + HO				
R080	$ACE + HO \rightarrow 0.65\ HO + 0.35\ HO_2 + 0.35\ CO + 0.650\ GLY + 0.35\ ORA1$	Table 2d		7.47×10^{-13}	2
	Aromatics + HO				
R081	$BEN + HO \rightarrow 0.648\ HO_2 + 0.352\ BENP + 0.118\ EPX + 0.53\ PHEN$	2.33×10^{-12}	193	1.22×10^{-12}	9
R082	$TOL + HO \rightarrow 0.177\ HO_2 + 0.763\ TR2 + 0.06\ TLP1 + 0.177\ CSL$	1.81×10^{-12}	-354	5.93×10^{-12}	10
R083	$XYM + HO \rightarrow 0.177\ HO_2 + 0.763\ XY2 + 0.06\ XYL1 + 0.117\ CSL$	2.31×10^{-11}		2.31×10^{-11}	10
R084	$XYP + HO \rightarrow 0.177\ HO_2 + 0.763\ XY2 + 0.06\ XYL1 + 0.117\ CSL$	1.43×10^{-11}		2.13×10^{-11}	10

Table 2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3 s^{-1}$	E/R K	K^*	Note
R085	XYO + HO $\rightarrow$ 0.177 HO_2 + 0.763 XYO2 + 0.06 XYL1 + 0.117 CSL	1.36×10^{-11}		1.36×10^{-11}	10
	Biogenic Hydrocarbons + HO				
R086	ISO + HO $\rightarrow$ ISOP	2.54×10^{-11}	-410	1.00×10^{-10}	11
R087	API + HO $\rightarrow$ APIP	1.21×10^{-11}	-440	5.29×10^{-11}	1
R088	LIM + HO $\rightarrow$ LIMP	4.20×10^{-11}	-401	1.61×10^{-10}	12
	Aldehydes + HO				
R089	HCHO + HO $\rightarrow$ HO_2 + H_2O + CO	5.50×10^{-12}	-125	8.36×10^{-12}	2
R090	ACD + HO $\rightarrow$ ACO_3 + H_2O	4.38×10^{-12}	-366	1.49×10^{-11}	13
R091	ALD + HO $\rightarrow$ RCO_3 + H_2O	5.10×10^{-12}	-405	1.98×10^{-11}	1
	Ketones + HO				
R092	ACT + HO $\rightarrow$ ACTP + H_2O	Table 2f		1.78×10^{-13}	14
R093	MEK + HO $\rightarrow$ MEKP + H_2O	1.30×10^{-12}	25	1.20×10^{-12}	1
R094	KET + HO $\rightarrow$ KETP + H_2O	2.80×10^{-12}	- 10	2.90×10^{-12}	15
R095	HKET + HO $\rightarrow$ HO_2 + H_2O + MGLY	3.00×10^{-12}		3.00×10^{-12}	16
	Unsaturated Carbonyls + HO				
R096	MACR + HO $\rightarrow$ 0.57 MACP + 0.43 MCP	8.0×10^{-12}	-380	2.9×10^{-11}	1
R097	MVK + HO $\rightarrow$ MVKP	2.60×10^{-12}	-610	2.01×10^{-11}	8
R098	UALD + HO $\rightarrow$ 0.313 ACO_3 + 0.687 UALP	5.77×10^{-12}	-533	3.45×10^{-11}	17
	Dicarbonyls + HO				

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R099	GLY + HO $\rightarrow$ HO_2 + H_2O + 2 CO	1.10×10^{-11}		1.10×10^{-11}	8
R100	MGLY + HO $\rightarrow$ ACO_3 + H_2O + CO	9.26×10^{-13}	-830	1.50×10^{-11}	18, 19
R101	DCB1 + HO $\rightarrow$ 0.52 HO_2 + 0.33 CO + 0.40 ALD + 0.78 KET + 0.10 GLY + 0.01 MGLY	2.8×10^{-11}	-175	5.04×10^{-11}	20
R102	DCB2 + HO $\rightarrow$ 0.52 HO_2 + 0.33 CO + 0.13 MEK + 0.10 GLY + 0.01 MGLY + 0.78 OP2	2.8×10^{-11}	-175	5.04×10^{-11}	20
R103	DCB3 + HO $\rightarrow$ 0.56 HO_2 + 0.21 MACP + 0.11 CO + 0.27 GLY + 0.01 MGLY + 0.79 OP2	1.00×10^{-13}		1.00×10^{-13}	20
	Oxygenated Aromatics + HO				
R104	BALD + HO $\rightarrow$ BALP + H_2O	5.32×10^{-12}	-243	1.20×10^{-11}	21
R105	PHEN + HO $\rightarrow$ 0.73 HO_2 + 0.20 ADDC + 0.07 CHO + 0.73 MCT	6.75×10^{-12}	-405	2.63×10^{-11}	9
R106	CSL + HO $\rightarrow$ 0.73 HO_2 + 0.20 ADDC + 0.07 CHO + 0.73 MCT	4.65×10^{-11}		4.65×10^{-11}	9
R107	EPX + HO $\rightarrow$ HO_2 + XO_2 + CO + ALD	2.8×10^{-11}	-175	5.04×10^{-11}	20
R108	MCT + HO $\rightarrow$ MCTO	2.05×10^{-10}		2.05×10^{-10}	9
	Alcohols and Glycols + HO				
R109	MOH + HO $\rightarrow$ HO_2 + HCHO	2.85×10^{-12}	345	8.96×10^{-13}	1
R110	EOH + HO $\rightarrow$ HO_2 + ACD	3.00×10^{-12}	-20	2.81×10^{-12}	1
R111	ROH + HO $\rightarrow$ HO_2 + 0.719 ALD + 0.184 ACD	2.60×10^{-12}	-200	1.33×10^{-12}	1

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R112	ETEG + HO → HO_2 + ALD	1.47×10^{-11}		1.47×10^{-11}	22
	Organic Peroxides + HO				
R113	OP1 + HO → 0.35 HO + 0.65 MO_2 + 0.35 HCHO	2.90×10^{-12}	-190	5.48×10^{-12}	8
R114	OP2 + HO → 0.49 HO + 0.44 HC3P + 0.07 XO_2 + 0.08 ALD + 0.41 KET	3.40×10^{-12}	-190	6.43×10^{-12}	23
R115	ISHP + HO → HO + MACR	1.00×10^{-10}		1.00×10^{-10}	11
R116	MAHP + HO → MACP	3.00×10^{-11}		3.00×10^{-11}	11
	Organic Acids + HO				
R117	ORA1 + HO → HO_2 + H_2O+ CO_2	4.50×10^{-13}		4.50×10^{-13}	24
R118	ORA2 + HO → 0.64 MO_2 + 0.36 ORAP + 0.64 CO_2	2.20×10^{-14}	-1012	6.55×10^{-13}	25
R119	PAA + HO → 0.35 HO + 0.65 ACO_3 + 0.35 XO_2 + 0.35 HCHO	2.93×10^{-12}	-190	5.54×10^{-12}	26
	Organic Nitrogen Containing Compounds + HO				
R120	PAN + HO → XO_2 + H_2O + NO_3 + HCHO	4.00×10^{-14}		4.00×10^{-14}	2
R121	PPN + HO → XO_2 + H_2O + NO_3 + HCHO	4.00×10^{-14}		4.00×10^{-14}	2
R122	MPAN + HO → NO_2 + HKET	3.20×10^{-11}		3.20×10^{-11}	27
R123	ONIT + HO → HC3P + H_2O + NO_2	5.31×10^{-12}	260	2.22×10^{-12}	
R124	NALD + HO → NO_2 + XO_2 + HKET	5.60×10^{-12}	-270	1.39×10^{-11}	9, 11
R125	ISON + HO → NALD + 0.07 HKET + 0.07 HCHO	1.30×10^{-11}		1.30×10^{-11}	9, 11

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
	Alkenes + O_3				
R126	ETE + O_3 $\rightarrow$ 0.08 HO + 0.15 HO_2 + 0.13 H_2 + 0.43 CO + HCHO + 0.37 ORA1	9.14×10^{-15}	2580	1.60×10^{-18}	1
R127	OLT + O_3 $\rightarrow$ 0.22 HO + 0.32 HO_2 + 0.08 MO_2 + 0.06 ETHP + 0.068 H_2O_2 + 0.43 CO + 0.01 CH_4 + 0.02 ETH + 0.56 HCHO + 0.44 ALD + 0.06 MEK + 0.03 ORA1 + 0.06 ORA2 + 0.01 ACD + 0.01 HKET + 0.015 HC3 + 0.04 HC3P + 0.03 ACT + 0.006 HC5 + 0.02 HC5P + 0.02 BALD + 0.032 BEN	4.33×10^{-15}	1800	1.03×10^{-17}	1
R128	OLI + O_3 $\rightarrow$ 0.46 HO + 0.07 HO_2 + 0.32 MO_2 + 0.07 ETHP + 0.026 H_2O_2 + 0.37 CO + 0.04 CH_4 + 0.01 ETH + 0.09 HCHO + 0.73 ALD + 0.017 KET + 0.017 ORA2 + 0.04 HC3P + 0.09 ACO3 + 0.01 HC3 + 0.457 ACD + 0.11 ACT + 0.44 HKET	4.40×10^{-15}	845	2.59×10^{-16}	1
R129	DIEN + O_3 $\rightarrow$ 0.09 O^3P + 0.28 HO + 0.30 HO_2 + 0.03 MO_2 + 0.15 ACO_3 + 0.02 KETP + 0.13 XO_2 + 0.05 H_2 + 0.001 H_2O_2 + 0.36 CO + 0.35 OLT + 0.90 HCHO + 0.39 MACR + 0.15 ORA1	1.34×10^{-14}	2283	6.33×10^{-18}	8
R130	ISO + O_3 $\rightarrow$ 0.25 HO + 0.25 HO_2 + 0.08 MO_2 + 0.1 ACO_3 + 0.1 MACP + 0.09 H_2O_2 + 0.14 CO + 0.58 HCHO + 0.461 MACR + 0.189 MVK + 0.28 ORA1 + 0.153 OLT	7.86×10^{-15}	1913	1.28×10^{-17}	11, 28
R131	API + O_3 $\rightarrow$ 0.85 HO + 0.10 HO_2 + 0.20 ETHP + 0.42 KETP + 0.02 H_2O_2 + 0.14 CO + 0.65 ALD + 0.53 KET	5.00×10^{-16}	530	8.45×10^{-17}	8

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R132	LIM + O_3 → 0.85 HO + 0.10 HO_2 + 0.16 ETHP + 0.42 KETP 0.02 H_2O_2 + 0.14 CO + 0.46 OLT + 0.04 HCHO + 0.79 MACR + 0.01 ORA1 + 0.07 ORA2	2.95×10^{-15}	783	2.13×10^{-16}	8
R133	MACR + O_3 → 0.19 HO + 0.14 HO_2 + 0.10 ACO_3 + 0.22 CO + 0.50 MGLY + 0.45 ORA1	1.36×10^{-15}	2112	1.14×10^{-18}	1, 11
R134	MVK + O_3 → 0.16 HO + 0.11 HO_2 + 0.28 ACO_3 + 0.01 XO_2 + 0.56 CO 0.1 HCHO + 0.54 MGLY + 0.07 ORA1 +0.07 ORA2 + 0.1 ALD	7.51×10^{-16}	1520	4.59×10^{-18}	9, 20
R135	UALD + O_3 → 0.1 HO + 0.072 HO_2 + 0.008 MO_2 + 0.002 ACO_3 + 0.1 XO_2 + 0.243 CO + 0.080 HCHO + 0.420 ACD + 0.028 KET + 0.491 GLY + 0.003 MGLY + 0.044 ORA1	1.66×10^{-18}		1.66×10^{-18}	29
R136	DCB1 + O_3 → 0.05 HO + HO_2 + 0.60 RCO3 + 0.6 XO2 +1.5 CO + 0.5 CO_2 + 0.05 GLY + 0.08 MGLY + 0.65 OP2 + 0.05 HCHO	2.0×10^{-16}		2.00×10^{-16}	30
R137	DCB2 + O_3 → 0.05 HO + HO_2 + 0.60 RCO3 + 0.60 XO2 +1.5 CO + 0.5 CO_2 + 0.05 GLY + 0.08 MGLY + 0.70 DCB1 + 0.65 OP2 + 0.05 HCHO	2.0×10^{-16}		2.00×10^{-16}	30
R138	DCB3 + O_3 → 0.05 HO + HO_2 + 1.5 CO + 0.5 CO_2 + 0.48 GLY + 0.70 DCB1 + 0.25 ORA1 + 0.25 ORA2 + 0.11 PAA	9.0×10^{-17}		9.00×10^{-17}	30
R139	EPX + O_3 → 0.05 HO + 1.5 HO_2 + 1.5 CO + 0.5 CO_2 + GLY + 0.85 BALD	1.0×10^{-16}		1.00×10^{-16}	20
R140	MCTO + O_3 → MCTP	2.86×10^{-13}		2.86×10^{-13}	9

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
	Stable Organics + NO_3				
R141	ETE + NO_3 $\rightarrow$ 0.80 OLNN + 0.20 OLND	Table S2c		9.15×10^{-10}	8
R142	OLT + NO_3 $\rightarrow$ 0.43 OLNN + 0.57 OLND	1.79×10^{-13}	450	3.96×10^{-14}	7
R143	OLI + NO_3 $\rightarrow$ 0.11 OLNN + 0.89 OLND	8.64×10^{-13}	-450	3.91×10^{-12}	7
R144	DIEN + NO_3 $\rightarrow$ 0.90 OLNN + 0.10 OLND + 0.90 MACR	1.00×10^{-13}		1.00×10^{-13}	8
R145	ISO + NO_3 $\rightarrow$ ISON	3.03×10^{-12}	446	6.79×10^{-13}	11
R146	API + NO_3 $\rightarrow$ 0.10 OLNN + 0.90 OLND	1.19×10^{-12}	-490	6.16×10^{-12}	8
R147	LIM + NO_3 $\rightarrow$ 0.71 OLNN + 0.29 OLND	1.22×10^{-11}		1.22×10^{-11}	8, 31
R148	HCHO + NO_3 $\rightarrow$ HO_2 + CO + HNO_3	2.00×10^{-12}	2440	5.58×10^{-16}	18
R149	ACD + NO_3 $\rightarrow$ ACO_3 + HNO_3	1.40×10^{-12}	1900	2.39×10^{-15}	2
R150	ALD + NO_3 $\rightarrow$ RCO_3 + HNO_3	3.76×10^{-12}	1900	6.42×10^{-15}	32
R151	MACR + NO_3 $\rightarrow$ 0.32 MACP + 0.68 XO_2 + 0.32 HNO_3 + 0.68 HCHO + 0.68 MGLY + 0.68 NO2	3.40×10^{-15}		3.40×10^{-12}	1, 18
R152	UALD + NO_3 $\rightarrow$ HO_2 + XO_2 + 0.668 CO + 0.332 HCHO + 0.332 ALD + ONIT	5.02×10^{-13}	1076	1.36×10^{-14}	33
R153	GLY + NO_3 $\rightarrow$ HO_2 + 2 CO + HNO_3	2.90×10^{-12}	1900	4.95×10^{-15}	34
R154	MGLY + NO_3 $\rightarrow$ ACO_3 + CO + HNO_3	3.76×10^{-12}	1900	6.42×10^{-15}	35

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	K^*	Note
R155	$PHEN + NO_3 \rightarrow 0.4\ CHO + 0.1\ ADDC + 0.5\ ADCN + 0.5\ HNO_3$	3.78×10^{-12}		3.78×10^{-12}	20
R156	$CSL + NO_3 \rightarrow 0.4\ CHO + 0.1\ ADDC + 0.5\ ADCN + 0.5\ HNO_3$	1.06×10^{-12}		1.06×10^{-12}	9
R157	$EPX + NO_3 \rightarrow 0.50\ HO + 1.50\ HO_2 + 1.50\ CO + 0.50\ CO_2 + GLY + 0.50\ NO_2 + 0.50\ HNO_3$	2.87×10^{-13}	1000	1.00×10^{-14}	8, 36
R158	$MCT + NO_3 \rightarrow MCTO + HNO_3$	2.01×10^{-10}		2.01×10^{-10}	9
R159	$MPAN + NO_3 \rightarrow MACP + NO_2$	2.20×10^{-14}	500	4.11×10^{-15}	11
	Decomposition of Intermediates From Aromatics				
R160	$TR2 \rightarrow 0.28\ HO + 0.29\ HO_2 + 0.28\ TOLP + 0.15\ PER1 + 0.28\ DCB2 + 0.01\ CSL + 0.28\ EPX$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10
R161	$TOLP \rightarrow 0.49\ HO + 0.01\ HO_2 + 0.50\ PER1 + 0.49\ DCB2 + 0.01\ CSL$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10
R162	$XY2 \rightarrow 0.158\ HO + 0.308\ HO_2 + 0.25\ RCO3 + 0.308\ XYLP + 0.150\ PER2 + 0.224\ DCB2 + 0.01\ CSL + 0.84\ EPX$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10
R163	$XYLP \rightarrow 0.39\ HO + 0.01\ HO_2 + 0.50\ PER2 + 0.49\ DCB2 + 0.01\ CSL$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10
R164	$XYO2 \rightarrow 0.158\ HO + 0.308\ HO_2 + 0.25\ RCO3 + 0.308\ XYLP + 0.150\ PER2 + 0.224\ DCB2 + 0.01\ CSL + 0.84\ EPX$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10
R165	$XYOP \rightarrow 0.390\ HO + 0.010\ HO_2 + 0.500\ PER2 + 0.490\ DCB2 + 0.010\ CSL$	$1.00 \times 10^{+3}$		$1.00 \times 10^{+3}$	10

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
	Peroxyacetynitrate Formation and Decomposition				
R166	$ACO_3 + NO_2 \rightarrow PAN$	Table 2d		8.68×10^{-12}	2
R167	$PAN \rightarrow ACO_3 + NO_2$	Table 2e		4.76×10^{-4}	2
R168	$RCO_3 + NO_2 \rightarrow PPN$	Table 2d		8.68×10^{-12}	2
R169	$PPN \rightarrow RCO_3 + NO_2$	Table 2e		4.76×10^{-4}	2
R170	$MACP + NO_2 \rightarrow MPAN$	Table 2d		5.14×10^{-12}	
R171	$MPAN \rightarrow MACP + NO_2$	$1.60 \times 10^{+16}$	13486	3.63×10^{-4}	11, 37, 38
	Organic Peroxy Radicals + NO				
R172	$MO_2 + NO \rightarrow HO_2 + NO_2 + HCHO$	2.80×10^{-12}	-300	7.66×10^{-12}	2
R173	$ETHP + NO \rightarrow HO_2 + NO_2 + ACD$	2.60×10^{-12}	-365	8.84×10^{-12}	2
R174	$HC3P + NO \rightarrow 0.66\ HO_2 + 0.131\ MO_2 + 0.048\ ETHP + 0.089\ XO_2 + 0.935\ NO_2 + 0.504\ ACD + 0.132\ ALD + 0.165\ ACT + 0.042\ MEK + 0.065\ ONIT$	4.00×10^{-12}		4.00×10^{-12}	39
R175	$HC5P + NO \rightarrow 0.200\ HO_2 + 0.051\ MO_2 + 0.231\ ETHP + 0.235\ XO_2 + 0.864\ NO_2 + 0.018\ HCHO + 0.045\ ACD + 0.203\ ALD + 0.217\ ACT + 0.033\ MEK + 0.039\ KET + 0.272\ HKET + 0.136\ ONIT$	4.00×10^{-12}		4.00×10^{-12}	39
R176	$HC8P + NO \rightarrow 0.606\ HO_2 + 0.133\ ETHP + 0.416\ XO_2 + 0.739\ NO_2 + 0\ .150\ ALD + 0.642\ KET + 0.261\ ONIT$	4.00×10^{-12}		4.00×10^{-12}	39
R177	$ETEP + NO \rightarrow HO_2 + NO_2 + 1.6\ HCHO + 0.2\ ALD$	9.00×10^{-12}		9.00×10^{-12}	8

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R178	OLTP + NO $\rightarrow$ 0.78 HO_2+ 0.97 NO_2 + 0.78 HCHO + 0.012 ACD + 0.44 ALD + 0.06 ACT + 0.13 MEK + 0.03 ONIT	4.00×10^{-12}		4.00×10^{-12}	39
R179	OLIP + NO $\rightarrow$ 0.83 HO_2 + 0.95 NO_2 + 0.81 ACD + 0.20 ACT + 0.68 ALD + 0.09 KET + 0.02 HKET + 0.05 ONIT	4.00×10^{-12}		4.00×10^{-12}	39
R180	BENP + NO $\rightarrow$ 0.918 HO_2 + 0.918 NO_2 + 0.459 DCB2 + 0.459 DCB3 + 0.918 GLY + 0.082 ONIT	2.54×10^{-12}	-360	8.50×10^{-12}	9
R181	TLP1 + NO $\rightarrow$ NO_2 + BALD	4.00×10^{-12}		4.00×10^{-12}	10
R182	TOLP + NO $\rightarrow$ 0.95 HO_2 + 0.95 NO_2 + 0.95 DCB2 + 0.050 ONIT	2.70×10^{-12}	-360	9.03×10^{-12}	10
R183	PER1 + NO $\rightarrow$ 0.5 HO_2 + 0.95 NO_2 + 0.5 BALD + 0.5 MGLY + 0.5 DCB1 + 0.05 ONIT	2.70×10^{-12}	-360	9.03×10^{-12}	10
R184	XYL1 + NO $\rightarrow$ NO_2 + BALD	4.00×10^{-12}		4.00×10^{-12}	10
R185	XYLP + NO $\rightarrow$ 0.95 HO_2 + 0.95 NO_2 + 0.95 DCB3 + 0.050 ONIT	2.70×10^{-12}	-360	9.03×10^{-12}	10
R186	PER2 + NO $\rightarrow$ 0.95 HO_2 + 0.95 NO_2 + 0.95 MGLY + 0.95 DCB1 + 1.05 DCB3 + 0.05 ONIT	2.70×10^{-12}	-360	9.03×10^{-12}	10
R187	XYOP + NO $\rightarrow$ 0.95 HO2 + 0.95 NO_2 + 0.350 GLY + 0.600 MGLY + 0.700 DCB1 + 0.073 DCB2 + 0.177 DCB3 + 0.05 ONIT	2.70×10^{-12}	-360	9.03×10^{-12}	40
R188	ISOP + NO$\rightarrow$ 0.88 HO_2 + 0.88 NO_2 + 0.2 HCHO + 0.28 MACR + 0.44 MVK + 0.12 ISON + 0.021 GLY + 0.029 HKET + 0.27 ALD	2.43×10^{-12}	-360	8.13×10^{-12}	11, 28
R189	APIP + NO $\rightarrow$ 0.82 HO_2 + 0.82 NO_2 + 0.23 HCHO + 0.43 ALD + 0.11 ACT + 0.44 KET + 0.07 ORA1 + 0.18 ONIT	4.00×10^{-12}		4.00×10^{-12}	8, 39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R190	LIMP + NO → HO_2 + NO_2 + 0.05 OLI + 0.43 HCHO + 0.68 UALD + 0.07 ORA1	4.00×10^{-12}		4.00×10^{-12}	8, 39
R191	ACO_3 + NO → MO_2 + NO_2	8.10×10^{-12}	-270	2.00×10^{-11}	40
R192	RCO_3 + NO → ETHP + NO_2	8.10×10^{-12}	-270	2.00×10^{-11}	40
R193	ACTP + NO → ACO_3 + NO_2 + HCHO	2.90×10^{-12}	-300	7.93×10^{-12}	2
R194	MEKP + NO → 0.67 HO_2 + NO_2 + 0.33 HCHO + 0.67 DCB1	4.00×10^{-12}		4.00×10^{-12}	39
R195	KETP + NO → 0.77 HO_2 + 0.23 ACO_3 + 0.16 XO_2 + NO_2 + 0.46 ALD + 0.54 MGLY	4.00×10^{-12}		4.00×10^{-12}	41
R196	MACP + NO → 0.75 HO_2 + 0.25 ACO_3 + NO_2 + 0.25 CO + 0.75 HCHO + 0.50 MGLY + 0.25 HKET	2.54×10^{-12}	-360	8.50×10^{-12}	11
R197	MCP + NO → NO2 + 0.50 HO2 + 0.50 HCHO + HKET	2.54×10^{-12}	-360	8.50×10^{-12}	
R198	MVKP + NO → 0.3 HO_2 + 0.7 ACO_3 + 0.7 XO_2 + NO_2 + 0.3 HCHO + 0.7 ALD + 0.3 MGLY	2.54×10^{-12}	-360	8.50×10^{-12}	9
R199	UALP + NO → HO_2 + NO_2 + 0.61 CO + 0.03 HCHO + 0.27 ALD + 0.18 GLY + 0.7 KET + 0.21 MGLY	2.54×10^{-12}	-360	8.50×10^{-12}	9
R200	BALP + NO → BAL1 + NO_2	4.00×10^{-12}		4.00×10^{-12}	21
R201	BAL1 + NO → BAL2 + NO_2	4.00×10^{-12}		4.00×10^{-12}	21
R202	ADDC + NO → HO2 + NO_2 + 0.32 HKET + 0.68 GLY + 0.68 OP2	2.70×10^{-12}	-360	9.03×10^{-12}	9
R203	MCTP + NO → MCTO + NO2	2.70×10^{-12}	-360	9.03×10^{-12}	9

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R204	ORAP + NO → HO_2 + NO_2 + GLY	4.00×10^{-12}		4.00×10^{-12}	42
R205	OLNN + NO → HO_2 + NO_2 + ONIT	4.00×10^{-12}		4.00×10^{-12}	41
R206	OLND + NO → 2 NO_2 + 0.287 HCHO + 1.24 ALD + 0.464 KET	4.00×10^{-12}		4.00×10^{-12}	41
R207	ADCN + NO → 2 NO_2 + GLY + OP2	2.70×10^{-12}	-360	9.03×10^{-12}	9
R208	XO_2 + NO → NO_2	4.00×10^{-12}		4.00×10^{-12}	39
	Organic Radical Termination with Nitrogen Dioxide				
R209	BAL2 + NO_2 → ONIT	2.00×10^{-11}		2.00×10^{-11}	20, 21
R210	CHO + NO_2 → ONIT	2.00×10^{-11}		2.00×10^{-11}	20
R211	MCTO + NO_2 → ONIT	2.08×10^{-12}		2.08×10^{-12}	9
	Organic Peroxy Radicals + HO_2				
R212	MO_2 + HO_2 → OP1	4.10×10^{-13}	-750	5.07×10^{-12}	2
R213	ETHP + HO_2 → OP2	7.50×10^{-13}	-700	7.85×10^{-12}	2
R214	HC3P + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R215	HC5P + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R216	HC8P + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R217	ETEP + HO_2 → OP2	1.90×10^{-13}	-1300	1.49×10^{-11}	39, 43
R218	OLTP + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R219	OLIP + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R220	BENP + HO_2 → OP2	2.91×10^{-13}	-1300	2.28×10^{-11}	9

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3 s^{-1}$	E/R K	k^*	Note
R221	$TLP1 + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R222	$TOLP + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R223	$PER1 + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R224	$XYL1 + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R225	$XYLP + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R226	$PER2 + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R227	$XYOP + HO_2 \rightarrow OP2$	3.75×10^{-13}	-980	1.00×10^{-11}	20
R228	$ISOP + HO_2 \rightarrow ISHP$	2.05×10^{-13}	-1300	1.60×10^{-11}	11
R229	$APIP + HO_2 \rightarrow OP2$	1.50×10^{-11}		1.50×10^{-11}	39
R230	$LIMP + HO_2 \rightarrow OP2$	1.50×10^{-11}		1.50×10^{-11}	39
R231	$ACO_3 + HO_2 \rightarrow 0.44\ HO + 0.44\ MO_2 + 0.44\ CO_2 + 0.15\ ORA2 + 0.41\ PAA$	4.3×10^{-13}	-1040	1.41×10^{-11}	1
R232	$RCO_3 + HO_2 \rightarrow 0.44\ HO + 0.44\ ETHP + 0.44\ CO2 + 0.15\ ORA2 + 0.41\ PAA$	4.3×10^{-13}	-1040	1.41×10^{-11}	1
R233	$ACTP + HO_2 \rightarrow 0.15\ HO + 0.15\ ACO_3 + 0.15\ HCHO + 0.850\ OP2$	1.15×10^{-13}	-1300	9.00×10^{-12}	1
R234	$MEKP + HO_2 \rightarrow OP2$	1.15×10^{-13}	-1300	9.00×10^{-12}	9
R235	$KETP + HO_2 \rightarrow OP2$	1.15×10^{-13}	-1300	9.00×10^{-12}	39
R236	$MACP + HO_2 \rightarrow MAHP$	1.82×10^{-13}	-1300	1.42×10^{-11}	11
R237	$MCP + HO_2 \rightarrow MAHP$	1.82×10^{-13}	-1300	1.42×10^{-11}	11
R238	$MVKP + HO_2 \rightarrow OP2$	7.70×10^{-14}	-1298	5.99×10^{-12}	9

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k*	Note
R239	UALP + HO_2 → OP2	7.70×10^{-14}	-1298	5.99×10^{-12}	9
R240	ADDC + HO_2 → OP2	3.75×10^{-13}	-980	1.00×10^{-11}	20
R241	CHO + HO_2 → CSL	1.00×10^{-11}		1.00×10^{-11}	20
R242	MCTP + HO_2 → OP2	3.75×10^{-13}	-980	1.00×10^{-11}	9
R243	ORAP + HO_2 → ONIT	1.15×10^{-13}	-1300	9.00×10^{-12}	44
R244	OLNN + HO_2 → ONIT	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R245	OLND + HO_2 → ONIT	1.66×10^{-13}	-1300	1.30×10^{-11}	39
R246	ADCN + HO_2 → OP2	3.75×10^{-13}	-980	1.00×10^{-11}	9
R247	XO_2 + HO_2 → OP2	1.66×10^{-13}	-1300	1.30×10^{-11}	39
	Organic Peroxy Radicals + Methyl Peroxy Radical				
R248	MO_2 + MO_2 → 0.74 HO_2 + 1.37 HCHO + 0.63 MOH	9.50×10^{-14}	-390	3.51×10^{-13}	19, 45
R249	ETHP + MO_2 → HO_2 + 0.75 HCHO + 0.75 ACD + 0.25 MOH + 0.25 EOH	1.18×10^{-13}	-158	2.00×10^{-13}	39, 43
R250	HC3P + MO_2 → 0.894 HO_2 + 0.080 MO_2 + 0.026 ETHP + 0.026 XO_2 + 0.827 HCHO + 0.198 ALD + 0.497 KET + 0.050 GLY + 0.25 MOH + 0.25 ROH	9.46×10^{-14}	-431	4.02×10^{-13}	39
R251	HC5P + MO_2 → 0.842 HO_2 + 0.018 MO_2 + 0.14 ETHP + 0.191 XO_2 + 0.777 HCHO + 0.251 ALD + 0.618 KET + 0.25 MOH + 0.25 ROH	1.00×10^{-13}	-467	4.79×10^{-13}	39
R252	HC8P + MO_2 → 0.910 HO_2 + 0.090 ETHP + 0.281 XO_2 + 0.750 HCHO + 0.197 ALD + 0.652 KET + 0.250 MOH + 0.250 ROH	4.34×10^{-14}	-633	3.63×10^{-13}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3 s^{-1}$	E/R K	k^*	Note
R253	ETEP + MO_2 → HO_2 + 1.95 HCHO + 0.15 ALD + 0.25 MOH + 0.25 ETEG	1.71×10^{-13}	-708	1.84×10^{-12}	39
R254	OLTP + MO_2 → HO_2 + 1.5 HCHO + 0.705 ALD + 0.045 KET + 0.25 MOH + 0.25 ROH	1.46×10^{-13}	-708	1.57×10^{-12}	39
R255	OLIP + MO_2 → HO_2 + 0.750 HCHO + 1.28 ALD + 0.218 KET + 0.250 MOH + 0.250 ROH	9.18×10^{-14}	-708	9.87×10^{-13}	39
R256	BENP + MO_2 → 1.6 HO_2 + HCHO + 0.459 DCB2 + 0.459 DCB3 + 0.6 GLY	3.56×10^{-14}	-708	3.83×10^{-13}	9
R257	TLP1 + MO_2 → HO_2 + HCHO + BALD	3.56×10^{-14}	-708	3.83×10^{-13}	20
R258	TOLP + MO_2 → 2 HO_2 + HCHO + 0.271 GLY + DCB2	3.56×10^{-14}	-708	3.83×10^{-13}	20
R259	PER1 + MO_2 → 2 HO_2 + HCHO + MGLY + DCB1	3.56×10^{-14}	-708	3.83×10^{-13}	20
R260	XYL1 + MO_2 → HO_2 + HCHO + BALD	3.56×10^{-14}	-708	3.83×10^{-13}	20
R261	XYLP + MO_2 → 2 HO_2 + HCHO + DCB2	3.56×10^{-14}	-708	3.83×10^{-13}	20
R262	PER2 + MO_2 → 2 HO_2 + HCHO + MGLY + DCB1 + 1.05 DCB3	3.56×10^{-14}	-708	3.83×10^{-13}	20
R263	XYOP + MO_2 → 2 HO_2 + HCHO + 0.368 GLY + 0.632 MGLY + 0.737 DCB1 + 0.077 DCB2 + 0.186 DCB3	3.56×10^{-14}	-708	3.83×10^{-13}	20
R264	ISOP + MO_2 → HO_2 + 1.31 HCHO + 0.159 MACR + 0.250 MVK + 0.250 MOH + 0.250 ROH .+ 023 ALD + .018 GLY + .016 HKET	3.40×10^{-14}	-221	7.14×10^{-14}	11, 28
R265	APIP + MO_2 → HO_2 + 0.75 HCHO + 0.75 ALD + 0.75 KET + 0.25 MOH + 0.25 ROH	3.56×10^{-14}	-708	3.83×10^{-13}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R266	LIMP + MO_2 → HO_2 + 1.04 HCHO + 0.192 OLI + 0.308 MACR + 0.25 MOH + 0.25 ROH	3.56×10^{-14}	-708	3.83×10^{-13}	39
R267	ACO_3 + MO_2 → 0.9 HO_2 + 0.90 MO_2 + 0.4 CO_2 + HCHO + 0.1 ORA2	2.0×10^{-11}	-500	1.07×10^{-10}	40
R268	RCO_3 + MO_2 → 0.9 HO_2 + 0.90 MO_2 + 0.4 CO_2 + HCHO + 0.1 ORA2	2.0×10^{-11}	-500	1.07×10^{-10}	40
R269	ACTP + MO_2 → 0.5 HO_2 + 0.5 ACO_3 + 1.5 HCHO + 0.25 MOH + 0.25 ROH + 0.125 ORA2	7.50×10^{-13}	-500	4.01×10^{-12}	41
R270	MEKP + MO_2 → 0.834 HO_2 + HCHO + 0.334 DCB1 + 0.25 MOH + 0.25 ROH	6.91×10^{-13}	-508	3.80×10^{-12}	39
R271	KETP + MO_2 → HO_2 + 0.75 HCHO + 0.50 DCB1 + 0.25 MOH + 0.25 ROH	6.91×10^{-13}	-508	3.80×10^{-12}	39
R272	MACP + MO_2 → 0.5 HO_2 + 0.269 ACO_3 + 0.5 CO + 1.66 HCHO + 0.250 MOH + 0.250 ROH + 0.067 ORA2 + 0.25 MO_2	3.40×10^{-14}	-221	7.14×10^{-14}	11
R273	MCP + MO_2 → NO_2 + HO_2 + 1.5 HCHO + .5 HKET + .25 MOH + .25 ROH	3.40×10^{-14}	-221	7.14×10^{-14}	11
R274	MVKP + MO_2 → HO_2 + 1.16 ACO_3 + 1.16 XO_2 + 1.5 HCHO + 1.75 ALD + 0.50 MGLY + 0.25 MOH + 0.25 ROH + 0.292 ORA2	3.40×10^{-14}	-221	7.14×10^{-14}	11
R275	UALP + MO_2 → HO_2 + 0.305 CO + 0.773 HCHO + 0.203 ALD + 0.525 KET + 0.135 GLY + 0.105 MGLY + 0.25 MOH + 0.25 ROH	3.40×10^{-14}	-221	7.14×10^{-14}	11
R276	BALP + MO_2 → HO_2 + BAL1 + HCHO	3.56×10^{-14}	-708	3.83×10^{-13}	39
R277	BAL1 + MO_2 → HO_2 + BAL2 + HCHO	3.56×10^{-14}	-708	3.83×10^{-13}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R278	ADDC + MO_2 → 2 HO_2 + HCHO + 0.32 HKET + 0.68 GLY + 0.68 OP2	3.56×10^{-14}	-708	3.83×10^{-13}	9, 39
R279	MCTP + MO_2 → HO_2 + MCTO + HCHO	3.56×10^{-14}	-708	3.83×10^{-13}	9, 39
R280	ORAP + MO_2 → HO_2 + HCHO + GLY	7.50×10^{-13}	-500	4.01×10^{-12}	46
R281	OLNN + MO_2 → 2 HO_2 + HCHO + ONIT	1.60×10^{-13}	-708	1.72×10^{-12}	39
R282	OLND + MO_2 → 0.50 HO_2 + 0.50 NO_2 + 0.965 HCHO + 0.93 ALD + 0.348 KET + 0.25 MOH + 0.25 ROH + 0.50 ONIT	9.68×10^{-14}	-708	1.04×10^{-12}	39
R283	ADCN + MO_2 → HO_2 + 0.7 NO_2 + HCHO + 0.7 GLY + 0.7 OP2 + 0.3 ONIT	3.56×10^{-14}		3.56×10^{-14}	9
R284	XO_2 + MO_2 → HO_2 + HCHO	5.99×10^{-15}	-1510	9.48×10^{-13}	39
	Organic Peroxy Radicals + Acetyl Peroxy Radical				39
R285	ETHP + ACO_3 → 0.500 HO_2 + 0.5 MO_2 + ACD + 0.5 ORA2	1.03×10^{-12}	-211	2.09×10^{-12}	39
R286	HC3P + ACO_3 → 0.394 HO_2 + 0.580 MO_2 + 0.026 ETHP + 0.026 XO_2 + 0.130 HCHO + 0.273 ALD + 0.662 KET + 0.067 GLY + 0.500 ORA2	6.90×10^{-13}	-460	3.23×10^{-12}	39
R287	HC5P + ACO_3 → 0.342 HO_2 + 0.518 MO_2 + 0.140 ETHP + 0.191 XO_2 + 0.042 HCHO + 0.381 ALD + 0.824 KET + 0.500 ORA2	5.59×10^{-13}	-522	3.22×10^{-12}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R288	$HC8P + ACO_3 \rightarrow 0.303\ HO_2 + 0.5\ MO_2 + 0.067\ ETHP + 0.208\ XO_2 + 0.217\ ALD + 0.642\ KET + 0.495\ ORA2$	2.47×10^{-13}	-683	2.44×10^{-12}	39
R289	$ETEP + ACO_3 \rightarrow 0.5\ HO_2 + 0.5\ MO_2 + 1.6\ HCHO + 0.2\ ALD + 0.5\ ORA2$	9.48×10^{-13}	-765	1.23×10^{-11}	39
R290	$OLTP + ACO_3 \rightarrow 0.50\ HO_2 + 0.50\ MO_2 + HCHO + 0.94\ ALD + 0.06\ KET + 0.50\ ORA2$	8.11×10^{-13}	-765	1.06×10^{-11}	39
R291	$OLIP + ACO_3 \rightarrow 0.50\ HO_2 + 0.50\ MO_2 + 1.71\ ALD + 0.29\ KET + 0.50\ ORA2$	5.09×10^{-13}	-765	6.62×10^{-12}	39
R292	$BENP + ACO_3 \rightarrow 0.60\ HO_2 + MO_2 + 0.459\ DCB2 + 0.458\ DCB3 + 0.60\ GLY$	7.40×10^{-13}	-765	9.63×10^{-12}	9
R293	$TLP1 + ACO_3 \rightarrow MO_2 + BALD$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R294	$TOLP + ACO_3 \rightarrow HO_2 + MO_2 + DCB2$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R295	$PER1 + ACO_3 \rightarrow HO_2 + MO_2 + MGLY + DCB1$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R296	$XYL1 + ACO_3 \rightarrow MO_2 + BALD$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R297	$XYLP + ACO_3 \rightarrow HO_2 + MO_2 + DCB2$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R298	$PER2 + ACO_3 \rightarrow HO_2 + MO_2 + MGLY + DCB1 + 1.05\ DCB3$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R299	$XYOP + ACO_3 \rightarrow HO_2 + MO_2 + 0.368\ GLY + 0.632\ MGLY + 0.737\ DCB1 + 0.077\ DCB2 + 0.186\ DCB3$	7.40×10^{-13}	-765	9.63×10^{-12}	10
R300	$ISOP + ACO_3 \rightarrow 0.5\ HO_2 + 0.5\ MO_2 + 0.75\ HCHO + 0.159\ MACR + 0.25\ MVK + 0.5\ ORA2 + .031\ ALD + .024\ GLY + .033\ HKET$	8.40×10^{-14}	-221	1.76×10^{-13}	11, 28
R301	$APIP + ACO_3 \rightarrow 0.5\ HO_2 + 0.5\ MO_2 + ALD + KET + ORA2$	7.40×10^{-13}	-765	9.63×10^{-12}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R302	LIMP + ACO_3 → 0.5 HO_2 + 0.5 MO_2 + 0.192 OLI + 0.385 HCHO + 0.308 MACR + 0.5 ORA2	7.40×10^{-13}	-765	9.63×10^{-12}	39
R303	ACO3 + ACO_3 → 2 MO_2 + 2 CO_2	2.50×10^{-12}	-500	1.34×10^{-11}	47, 48
R304	RCO3 + ACO_3 → MO_2 + ETHP + 2 CO_2	2.50×10^{-12}	-500	1.34×10^{-11}	47, 48
R305	ACTP + ACO_3 → 0.50 MO_2 + 0.50 ACO_3 + HCHO + 0.75 ORA2	7.51×10^{-13}	-565	5.00×10^{-12}	39, 49
R306	MEKP + ACO_3 → 0.33 HO_2 + 0.50 MO_2 + 0.33 HCHO + 0.334 DCB1 + 0.50 ORA2	7.51×10^{-13}	-565	5.00×10^{-12}	39
R307	KETP + ACO_3 → 0.50 HO_2 + 0.50 MO_2 + 0.50 DCB1 + 0.50 ORA2	7.51×10^{-13}	-565	5.00×10^{-12}	39
R308	MACP + ACO_3 → 0.50 HO_2 + 0.50 MO_2 + 0.167 ACO_3 + 0.167 CO + HCHO + 0.167 HKET + 0.33 MGLY + 0.583 ORA2	8.40×10^{-14}	-221	1.76×10^{-13}	11
R309	MCP + ACO_3 → NO_2 + .5 HO_2 + HCHO .5 HKET + .5 MO_2 + .5 ORA2	8.40×10^{-14}	-221	1.76×10^{-13}	11
R310	MVKP + ACO_3 → 0.5 HO_2 + 0.5 MO_2 + 1.16 ACO_3 + 1.16 XO_2 + HCHO + 2.3 ALD + 0.50 MGLY + 1.083 ORA2	8.40×10^{-14}	-221	1.76×10^{-13}	11, 50
R311	UALP + ACO_3 → 0.50 HO_2 + 0.50 MO_2 + 0.50 CO + 0.030 HCHO + 0.27 ALD + 0.70 KET + 0.18 GLY + 0.105 MGLY + 0.5 ORA2	8.40×10^{-14}	-221	1.76×10^{-13}	50
R312	BALP + ACO_3 → MO_2 + BAL1	7.40×10^{-13}	-765	9.63×10^{-12}	51
R313	BAL1 + ACO_3 → MO_2 + BAL2	7.40×10^{-13}	-765	9.63×10^{-12}	51
R314	ADDC + ACO_3 → 2 HO_2 + MO_2 + 0.32 HKET + 0.68 GLY + 0.68 OP2	7.40×10^{-13}	-708	7.95×10^{-12}	20

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R315	$MCTP + ACO_3 \rightarrow HO_2 + MO_2 + MCTO$	7.40×10^{-13}	-708	7.95×10^{-12}	9
R316	$ORAP + ACO_3 \rightarrow MO_2 + GLY$	7.51×10^{-13}	-565	5.00×10^{-12}	52
R317	$OLNN + ACO_3 \rightarrow HO_2 + MO2 + ONIT$	8.85×10^{-13}	-765	1.15×10^{-11}	39
R318	$OLND + ACO_3 \rightarrow 0.50\ MO_2 + NO_2 + 0.287\ HCHO + 1.24\ ALD + 0.464\ KET + 0.50\ ORA2$	5.37×10^{-13}	-765	6.99×10^{-12}	39
R319	$ADCN + ACO_3 \rightarrow HO_2 + MO_2 + 0.7\ NO_2 + 0.7\ GLY + 0.7\ OP2 + 0.3\ ONIT$	7.40×10^{-13}	-708	7.95×10^{-12}	9
R320	$XO_2 + ACO_3 \rightarrow MO_2$	3.40×10^{-14}	-1560	6.37×10^{-12}	39
	Organic Peroxy Radicals + NO_3				
R321	$MO_2 + NO_3 \rightarrow HO_2 + NO_2 + HCHO$	1.20×10^{-12}		1.20×10^{-12}	39
R322	$ETHP + NO_3 \rightarrow HO_2 + NO_2 + ACD$	1.20×10^{-12}		1.20×10^{-12}	39
R323	$HC3P + NO_3 \rightarrow 0.254\ HO_2 + NO_2 + 0.140\ MO_2 + 0.503\ ETHP + 0.092\ XO_2 + 0.095\ ACT + 0.519\ ACD + 0.147\ ALD + 0.075\ MEK$	1.20×10^{-12}		1.20×10^{-12}	39
R324	$HC5P + NO_3 \rightarrow 0.488\ HO_2 + 0.055\ MO_2 + 0.28\ ETHP + 0.485\ XO_2 + NO_2 + 0.024\ HCHO + 0.241\ ALD + 0.06\ KET + 0.063\ MEK + 0.247\ ACT + 0.048\ ACD + 0.275\ HKET$	1.20×10^{-12}		1.20×10^{-12}	39
R325	$HC8P + NO_3 \rightarrow 0.82\ HO_2 + 0.18\ ETHP + 0.563\ XO_2 + NO_2 + 0.203\ ALD + 0.869\ KET$	1.20×10^{-12}		1.20×10^{-12}	39
R326	$ETEP + NO_3 \rightarrow HO_2 + NO_2 + 1.6\ HCHO + 0.2\ ALD$	1.20×10^{-12}		1.20×10^{-12}	39
R327	$OLTP + NO_3 \rightarrow 0.79\ HO_2 + NO_2 + 0.79\ HCHO + 0.47\ ALD + 0.09\ ACT + 0.02\ ACD + 0.18\ MEK$	1.20×10^{-12}		1.20×10^{-12}	39

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R328	$OLIP + NO_3 \rightarrow 0.86\ HO_2 + NO_2 + 0.72\ ALD + 0.20\ ACT + 0.85\ ACD + 0.04\ HKET + 0.11\ KET$	1.20×10^{-12}		1.20×10^{-12}	39
R329	$BENP + NO_3 \rightarrow HO_2 + NO_2 + 0.50\ DCB2 + 0.50\ DCB3 + GLY$	1.20×10^{-12}		1.20×10^{-12}	9
R330	$TLP1 + NO_3 \rightarrow NO_2 + BALD$	1.20×10^{-12}		1.20×10^{-12}	10
R331	$TOLP + NO_3 \rightarrow HO_2 + NO_2 + DCB2$	1.20×10^{-12}		1.20×10^{-12}	10
R332	$PER1 + NO_3 \rightarrow 0.5\ HO_2 + NO_2 + 0.5\ MGLY + 0.5\ DCB1 + 0.5\ BALD$	1.20×10^{-12}		1.20×10^{-12}	10
R333	$XYL1 + NO_3 \rightarrow NO_2 + BALD$	1.20×10^{-12}		1.20×10^{-12}	10
R334	$XYLP + NO_3 \rightarrow HO_2 + NO_2 + DCB3$	1.20×10^{-12}		1.20×10^{-12}	10
R335	$PER2 + NO_3 \rightarrow HO_2 + NO_2 + MGLY + DCB1 + 1.05\ DCB3$	1.20×10^{-12}		1.20×10^{-12}	10
R336	$XYOP + NO_3 \rightarrow HO_2 + NO_2 + 0.368\ GLY + 0.632\ MGLY + 0.737\ DCB1 + 0.077\ DCB2 + 0.186\ DCB3$	1.20×10^{-12}		1.20×10^{-12}	20
R337	$ISOP + NO_3 \rightarrow HO_2 + NO_2 + 0.75\ HCHO + 0.318\ MACR + 0.5\ MVK + 0.024\ GLY + .033\ HKET + .031\ ALD$	1.20×10^{-12}		1.20×10^{-12}	11, 28
R338	$APIP + NO_3 \rightarrow HO_2 + NO_2 + ALD + KET$	1.20×10^{-12}		1.20×10^{-12}	39
R339	$LIMP + NO_3 \rightarrow HO_2 + NO_2 + 0.385\ OLI + 0.385\ HCHO + 0.615\ MACR$	1.20×10^{-12}		1.20×10^{-12}	39
R340	$ACO_3 + NO_3 \rightarrow MO_2 + NO_2$	4.00×10^{-12}		4.00×10^{-12}	39, 53
R341	$RCO_3 + NO_3 \rightarrow ETHP + NO_2$	4.00×10^{-12}		4.00×10^{-12}	39, 53

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R K	k^*	Note
R342	ACTP + NO_3 → ACO_3 + NO_2 + HCHO	1.20×10^{-12}		1.20×10^{-12}	39
R343	MEKP + NO_3 → 0.67 HO_2 + NO_2 + 0.33 HCHO + 0.67 DCB1	1.20×10^{-12}		1.20×10^{-12}	39
R344	KETP + NO_3 → HO_2 + NO_2 + DCB1	1.20×10^{-12}		1.20×10^{-12}	39
R345	MACP + NO_3 → HO_2 + 0.33 ACO_3 + NO_2 + 0.33 CO + HCHO + 0.33 HKET + 0.667 MGLY	1.20×10^{-12}		1.20×10^{-12}	11
R346	MCP + NO_3 → NO_2 + HO_2 + HCHO HKET	1.20×10^{-12}		1.20×10^{-12}	49
R347	MVKP + NO_3 → 0.3 HO_2 + 0.7 ACO_3 + 0.7 XO_2 + NO_2 + 0.3 HCHO + 0.7 ALD + MGLY	1.20×10^{-12}		1.20×10^{-12}	9
R348	UALP + NO_3 → HO_2 + NO_2 + 0.61 CO + 0.03 HCHO + 0.27 ALD + 0.7 KET + 0.18 GLY + 0.21 MGLY	1.20×10^{-12}		1.20×10^{-12}	9
R349	BALP + NO_3 → BAL1 + NO_2	1.20×10^{-12}		1.20×10^{-12}	9
R350	BAL1 + NO_3 → BAL2 + NO_2	1.20×10^{-12}		1.20×10^{-12}	9
R351	ADDC + NO_3 → HO_2 + NO_2 + 0.32 HKET + 0.68 GLY + 0.68 OP2	1.20×10^{-12}		1.20×10^{-12}	9
R352	MCTP + NO_3 → NO_2 + MCTO	1.20×10^{-12}		1.20×10^{-12}	39
R353	ORAP + NO_3 → HO_2 + NO_2 + GLY	1.20×10^{-12}		1.20×10^{-12}	39
R354	OLNN + NO_3 → HO_2 + NO_2 + ONIT	1.20×10^{-12}		1.20×10^{-12}	39
R355	OLND + NO_3 → 2 NO_2 + 0.287 HCHO + 1.24 ALD + 0.464 KET	1.20×10^{-12}		1.20×10^{-12}	39
R356	ADCN + NO_3 → 2 NO_2 + GLY + OP2	1.20×10^{-12}		1.20×10^{-12}	9

Table S2b – Continued. The RACM2 Chemical Mechanism, Thermal Reactions

Reaction No.	Reaction	A, $cm^3 s^{-1}$	E/R K	K^*	Note
R357	$XO_2 + NO_3 \rightarrow NO_2$	1.20×10^{-12}		1.20×10^{-12}	39
	Self Reaction of RCO3 Radical				
R358	$RCO_3 + RCO_3 \rightarrow$ 2 ETHP + 2 CO_2				40, 47
	Organic Nitrate Radical Cross Reactions				
R359	OLNN + OLNN $\rightarrow HO_2$ + 2 ONIT	7.00×10^{-14}	-1000	2.00×10^{-12}	39
R360	OLNN + OLND $\rightarrow$ 0.50 HO_2 + 0.50 NO_2 + 0.202 HCHO + 0.640 ALD + 0.149 KET + 1.50 ONIT	4.25×10^{-14}	-1000	1.22×10^{-12}	39
R361	OLND + OLND $\rightarrow NO_2$ + 0.504 HCHO + 1.21 ALD + 0.285 KET + ONIT	2.96×10^{-14}	-1000	8.47×10^{-13}	39
	Operator Radical + Operator Radical				
R362	$XO_2 + XO_2 \rightarrow$	7.13×10^{-17}	-2950	1.41×10^{-12}	39
	Operator Radical + RCO3 Radical				
R363	$XO_2 + RCO_3 \rightarrow$ ETHP + CO_2	$2.50 \text{ x } 10^{-12}$	-500	1.34×10^{-11}	40, 47

The rate constants are calculated for 298 K and 1 atm. The units for first order reactions are s^{-1}, second order rate constants are $cm^3 s^{-1}$ and for third order the units are $cm^6 s^{-1}$.

Note 1: IUPAC Web version [January 2010]; Note 2: Sander et al. [2011]; Note 3: Uselman et al. In Nitrogeneous Air Pollutants, Chemical and Biological Implications, 1979; Note 4: Rate constants used for aggregated species taken from Atkinson, 2003; El Boudali et al., 2001; IUPAC 2010; Talukdar et al., 1994.; Note 5: Rate constants used for aggregated species taken from Veillerot et al., 1996; El Boudali et al., 1996; Picquet et al., 1998; Wilson et al., 2006; Note 6: Rate constants used for aggregated species taken from Wilson et al., 2006, Atkinson, 2003 and Aschmann and Atkinson, 1998; Note 7: no change from RACM1; Note 8: Atkinson and Arey, 2003; Note 9: MCM V3.2; Note 10: Calvert et al., 2002; Note 11: Geiger et al., 2003; Note 12: Gill and Hites, 2002; Note 13: Sivakumaran and Crowley, 2003; Note 14: Gierczak et al., 2003; Note 15: Wallington and Kurylo, 1987; Note 16: Orlando et al., 1999; Note 17: Magneron et al., 2002; Note 18: Atkinson et al., 2006; Note 19: Tyndall et al., 1995; Note 20: Carter, 2010; Note 21: Ferri et al., 2001 and Semadeni et al., 1995; Note 22: Aschmann and Atkinson, 1998; Note 23: Estimated for propyl hydroperoxide ; Note 24: Singleton et al., 1988; Note 25: Butkovskaya et al., 2004 and De Smedt et al., 2005; Note 26: Assumed the same as OP1 + HO; Note 27: Orlando et al., 2002; Note 28: Rate constant is average of Grosjean and Grosjean, 1998 and Sato et al., 2004; MVK, MACR and ISON from Sprengnether et al. 2002, small compounds from Galloway et al. 2011; Note 29: MACR-MVK split according to Carter, 1996; Note 30: Determined by fitting model simulations to chamber data. Experiment EC331 (toluene + n-butane) was used; Note 31: Rate constant from Atkinson and Arey 2003 and products from Spittler et al., 2006; Note 32: Based on propanal. The E/R of ACD together with the recommended k(298) for propanal was used to determine the A factor for ALD; Note 33: Rate constant take to be $2*k_{ALD}$ - k_{ETH}; E/R same as ALD + NO_3; Note 34: Salgado et al., 2008; Note 35: assumed the same as ALD + NO3; Note 36: Rate from Bierbach et al.,1994, Products from DCB1 + O3; Note 37: Kirchner and Stockwell, 1996; Note 38: using RACM1 product yields and dividing DCB value among DCB1,2,3; Note 33: Tyndall et al., 2001; Note 39: Roberts and Bertman, 1992; Note 40: Carter and Atkinson, 1996; Note 41: Rate from HCP3 + NO; Note 42: Rate from ACTP + NO; Note 43: Lebras, 1997; Note 44: Rate from ACTP + HO2; Note 45: Same as ACTP + MO2; Note 46: Lightfoot, 1992; Note 47: Tyndall et al., 2001; Note 48: Bridier et al., 1993; Note 49: Rate constant from GEOS-CHEM version 5-07-8; Note 50: Rate assumed same as MVKP+ACO3; Note 51: Rate constant assumed same as TOLP+ACO3; Note 52: Rate assumed same as ACTP+ACO3; Note 53: Wayne, 2000.

Table S2c. The RACM2 Chemical Mechanism: Reaction Rate Constants of the Form k = T2 C exp (-D/T)

Reaction No.	Reaction	C K^{-2} cm^3 s^{-1}	D K	Note
R137	ETE + NO_3 $\rightarrow$ 0.80 OLNN + 0.20 OLND	4.88×10^{-18}	2282	1

Note 1: Atkinson and Arey, 2003

Table S2d. The RACM2 Chemical Mechanism: Troe Reaction Parameters

Reaction No.	Reaction	k_o^{300} cm^6 s^{-1}	n	k_∞^{300} cm^3 s^{-1}	m	Note
R48	NO + O^3P $\rightarrow$ NO_2	9.00×10^{-32}	1.5	3.00×10^{-11}	0	1
R49	NO + HO $\rightarrow$ HONO	7.00×10^{-31}	2.6	3.60×10^{-11}	0.1	1
R54	NO_2 + O^3P $\rightarrow$ NO_3	2.50×10^{-31}	1.8	2.20×10^{-11}	0.7	1
R55	NO_2 + HO $\rightarrow$ HNO_3	1.80×10^{-30}	3.0	2.80×10^{-11}	0	1
R62	NO_3 + NO_2 $\rightarrow$ N_2O_5	2.00×10^{-30}	4.4	1.40×10^{-12}	0.7	1
R65	NO_2 + HO_2 $\rightarrow$ HNO_4	2.0×10^{-31}	3.4	2.90×10^{-12}	1.1	1
R68	SO_2 + HO $\rightarrow$ SULF + HO_2	3.30×10^{-31}	4.3	1.60×10^{-12}	0	1
R75	ETE + HO $\rightarrow$ ETEP	1.00×10^{-28}	4.5	8.80×10^{-12}	0.85	1
R79	ACE + HO $\rightarrow$ 0.65 HO + 0.35 HO_2 + 0.35 CO + 0.650 GLY + 0.35 ORA1	5.50×10^{-30}	0.0	8.30×10^{-13}	-2.0	1
R164	ACO_3 + NO_2 $\rightarrow$ PAN	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R166	RCO_3 + NO_2 $\rightarrow$ PPN	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1

Note 1, Sander et al. [2011]

Table S2e. The RACM2 Chemical Mechanism: Troe Equilibrium Reactions

Reaction No.	Reaction	A	B	k_o^{300} $cm^6\ s^{-1}$	n	k_∞^{300} $cm^3\ s^{-1}$	m	Note
R63	$N_2O_5 \rightarrow NO_2 + NO_3$	$3.70 \times 10^{+26}$	11,000	2.20×10^{-30}	3.9	1.50×10^{-12}	0.7	1
R66	$HNO_4 \rightarrow HO_2 + NO_2$	$4.76 \times 10^{+26}$	10,900	2.00×10^{-31}	3.4	2.90×10^{-12}	1.1	1
R165	$PAN \rightarrow ACO_3 + NO_2$	$1.16 \times 10^{+28}$	13,954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1
R167	$PPN \rightarrow RCO_3 + NO_2$	$1.16 \times 10^{+28}$	13,954	9.70×10^{-29}	5.6	9.30×10^{-12}	1.5	1

Note 1, Sander et al. [2011]

Table S2f. The RACM2 Chemical Mechanism: Reactions With Special Rate Expressions

Reaction No.	Reaction	Rate Constant Expression[a] $cm^3\ s^{-1}$	Note
R38	$O^3P + O_2 \rightarrow O_3$	$[M] \times 5.60 \times 10^{-34} \times (T/300)^{**}(-2.6)$	1
R45	$2\ HO_2 \rightarrow H_2O_2 + O_2$	$2.2 \times 10^{-13} \times \exp(600/T) + 1.90 \times 10^{-33} \times$ $[M] \times \exp(980/T)$	1
R46	$2\ HO_2 + H_2O \rightarrow H_2O_2 + H_2O + O_2$	$3.08 \times 10^{-34} \times \exp(2800/T) + 2.59 \times 10^{-54} \times$ $[M] \times \exp(3180/T)$	1
R51	$NO + HO_2 \rightarrow HNO_3$	$k_1 = 3.45e\text{-}12^*\exp(270/T)$ $k_2 = (530/Y)+(4.8 \text{ x } 10^{-6})^*\text{pressure} - 1.73$ $k = k_1^*k_2/100$	1
R56	$HNO_3 + HO \rightarrow NO_3 + H_2O$	$k = k_0 + k_3/(1 + k_3 / k_2)$ $k_0 = 2.4 \times 10^{-14} \times \exp(460/T)$ $k_2 = 2.4 \times 10^{-17} \times \exp(2199/T)$ $k_3 = 6.5 \times 10^{-34} \times \exp(1335/T) \times [M]$	1

R69	$CO + HO \rightarrow HO_2 + CO_2$	$1.44 \times 10^{-13} \times (1. + 0.8 \times [M] / 4 \times 10^{+19})$	1
R90	$ACT + HO \rightarrow ACTP + H_2O$	$1.39 \times 10^{-13} + 3.72 \times 10^{-11} \times \exp(-2044/T)$	2

Note 1, IUPAC Web version [January 2010]
Note 2: Gierczak et al., 2003

[a]The unit of T is K. The units for second order rate constants are $cm^3\ s^{-1}$ and for third order the units are $cm^6\ s^{-1}$. Pressure is in units of Pascal. For all of the above, [M] is the concentration of air in molecules cm^3.

Comparison of RACM1 and RACM2 Mechanisms for “Real Atmosphere” Cases

Box-model simulations made with the RACM1 and RACM2 were compared to provide an assessment of their differences in calculated ozone, HNO_3, H_2SO_4, PAN, H_2O_2 and HCHO. The simulations were made based on the urban case discussed in [Stockwell et al., 2012]. The two-day simulations were made for surface conditions with a pressure of 1 atmosphere, a temperature of 298 K and a relative humidity of 50%, Table S3. Physical losses, such as deposition, of ozone, HNO_3, H_2O_2, H_2SO_4 etc. were not included because the purpose was to compare their chemical production by the two mechanisms.

The initial ozone concentration was taken to be a near background value of 30 ppb for all simulations. The photolysis rate coefficients were calculated for a latitude of 40° at summer solstice. The photolysis rate coefficients for the photochemical reactions of both mechanisms were calculated using the delta-Eddington radiative transfer model. To make the simulations as equivalent as possible the revised photolysis rate coefficients for the RACM2 mechanism were used for both mechanisms or they were mapped from the RACM2 mechanism to those of RACM1 as appropriate.

The initial conditions consisted of four inorganic variations, Table S4, and four organic variations, Table S5. The four inorganic variations were run with the four organic variations for a total of sixteen simulations. The sixteen simulations represent a wide range of initial conditions. Although not all combinations are representative of typical conditions, the simulations provide an extensive comparison of the two mechanisms.

For the inorganic variations A, B and C represent somewhat aged air masses that range from rural to moderately polluted while case D represents a polluted case with fresh emissions. For the inorganic variations A, B and C the initial carbon monoxide concentration was 100 ppb and D was 1000 ppb. The initial SO_2 was taken similarly to be 5 ppb for A, B and C and increased to 30 ppb for case D. The NO and NO_2 concentrations were varied from case A in multiples of 5 and 10 to give cases B and C and in Case D the initial NO_x was 10 ppb with a NO/NO_2 ratio of 4.

The initial organic mixture is a relatively realistic mixture based on measurements made at Howard University’s atmospheric field site near Beltsville, Maryland [Stockwell et al., 2012]. Table S5 shows the initial organic mixing ratios used for the simulations. The NMOC2 column represents an approximation to the Beltsville measurements and in general the NMOC1, NMOC3 and NMOC4 represent multiples of 0.1, 5 and 10 of NMOC2. The total organic mixing ratios were 19.09, 190.9, 954.5 and 1909 ppbC for NMOC1, NMOC2, NMOC3 and NMOC4, respectively. These when combined with the inorganic variations lead to a wide range of VOC to NO_x ratios, Table S6. These ratios are not always typical of atmospheric conditions but provide a wide range of conditions for comparing RACM1 and RACM2.

Tables S7 and S8 show the peak ozone simulated by the two mechanisms. The maximum ozone is 30.00 ppb for RACM1 and RACM2 in cases NMOC1-C and NMOC1-D and for RACM2 in case NMOC-D because the mechanisms yielded a net ozone loss from the 30.00 ppb initial conditions. Otherwise the tables show that RACM2 predicts lower ozone concentrations than RACM1 for most of the simulations. Figure S1 shows that the RACM2 mechanism forecasts less ozone than RACM1 for most of the initial conditions simulated and that this trend to lower predictions increases at the higher ozone mixing ratios.

RACM2 forecasts less HNO_3 than RACM1, Figure S2. This indicated that there is less reactive nitrogen available for ozone and HNO_3 formation in the RACM2 simulations than in the RACM1 simulations. The tendency of RACM2 to produce less ozone and HNO_3 than RACM1 is consistent with the forecasted mixing ratios of PAN, Figure S3. The formation of PAN removes NO_2 and acetyl-peroxy radicals from the system. The higher mixing ratios of PAN suggest that RACM2 has lower levels of NO_x available for ozone formation under the more polluted conditions. The lower levels of NO_x in RACM2 forecasts lead also to higher mixing ratios of hydrogen peroxide forecasted by RACM2 than RACM1, Figure S4.

RACM2 forecasts more HCHO than RACM1; this may be due to the greater level of detail of the organic chemistry in RACM2, Figure S5. Although the photolysis of HCHO produces HO_2; the two mechanisms predict almost the same mixing ratios of H_2SO_4. The mixing ratio of H_2SO_4 is indicative of integrated hydroxyl concentrations. This agreement indicates that there is considerable agreement for the integrated hydroxyl concentrations between the two mechanisms, Figure S6.

Table S3. Conditions used for all simulations.

Initial Condition	**Value**
Start-Time	6:00
Duration	48 hr
Temperature	298.15 K
Pressure	1013.25 mbar
Date for photolysis calculation	June 21
Latitude	40°
<u>Mixing Ratio</u>	
H_2O	15500 ppm
Methane	1800. ppb
H_2	550 ppb
O_3	30 ppb

Table S4. Inorganic initial concentrations as varied in simulations.

Case	A (ppb)	B (ppb)	C (ppb)	D (ppb)
Carbon Monoxide	100.	100.	100.	1000.
Nitric Oxide	0.1	0.5	1.0	8.0
Nitrogen Dioxide	0.4	2.0	4.0	2.0
Sulfur Dioxide	5.0	5.0	5.0	30.0

Table S5. Non-methane organic compound initial concentrations as varied in simulations.

	NMOC1 (ppb)	NMOC2 (ppb)	NMOC3 (ppb)	NMOC4 (ppb)
Ethane	0.30	3.0	15.0	30.
Slow Reacting Alkanes	1.00	10.	50.0	100.
Medium Reacting Alkanes	0.25	2.5	12.5	25.
Fast Reacting Alkanes	0.15	1.5	7.50	15.
Ethene	0.20	2.0	10.0	20.
Internal Alkenes	0.10	1.0	5.0	10.
Terminal Alkenes	0.20	2.0	10.0	20.
Dienes	0.05	0.5	2.5	5.
Benzene	0.09	0.9	4.5	9.
Toluene	0.20	2.0	10.0	20.
Xylene	0.20	2.0	10.0	20.
o-Xylene	0.10	1.0	5.0	10.
Methanol	0.01	0.1	0.5	1.
Ethanol	0.01	0.1	0.5	1.
Higher Alcohols	0.01	0.1	0.5	1.
Formaldehyde	0.25	2.5	12.5	25.
Acetylene	0.20	2.0	10.0	20.
Acetaldehyde	0.10	1.0	5.0	10.
Higher Aldehyde	0.05	0.5	2.5	5.
Acetone	0.03	0.3	1.5	3.
Methyl Ethyl Ketone	0.20	2.0	10.0	20.
Higher Ketone	0.20	2.0	10.0	20.
Glyoxal	0.02	0.2	1.0	2.
Methylglyoxal	0.01	0.05	0.25	0.5
Methacrolein	0.01	0.1	0.5	1.0
Methyl Vinyl Ketone	0.01	0.1	0.5	1.0
Isoprene	0.34	3.4	17.0	34.
α-Pinenes	0.10	1.0	5.0	10.
d-Limonene	0.10	1.0	5.0	10.

Table S6. NOx/VOC ratios for cases simulated.

		Total NMOC (ppbC)			
		NMOC1	**NMOC2**	**NMOC3**	**NMOC4**
NOx	**(ppbN)**	19.09	190.9	954.5	1909.
A	0.5	38.18	381.80	1909.00	3818.0
B	2.5	7.64	76.36	381.80	763.6
C	5.0	3.82	38.18	190.90	381.8
D	10.	1.91	19.09	95.45	190.9

Table S7. RACM1 maximum ozone mixing ratios.

	RACM1 O_3 (ppb)			
	A	B	**C**	**D**
NMOC1	38.74	34.96	30.00	30.00
NMOC2	55.81	80.45	56.61	41.48
NMOC3	62.85	110.99	94.43	71.24
NMOC4	105.59	157.19	153.30	122.59

Table S8 RACM2 maximum ozone mixing ratios.

	RACM2 O_3 (ppb)			
	A	B	**C**	**D**
NMOC1	36.33	31.54	30.00	30.00
NMOC2	57.51	54.11	38.57	30.00
NMOC3	66.58	90.85	58.82	43.30
NMOC4	105.20	145.87	94.70	73.97

Figure Captions

Figure S1. Plot of maximum ozone mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 6 – 10. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

Figure S2. Plot of maximum HNO_3 mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 6 – 10. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

Figure S3. Plot of maximum PAN mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 1 – 4. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

Figure S4. Plot of maximum H_2O_2 mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 1 – 4. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

Figure S5. Plot of maximum HCHO mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 1 – 4. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

Figure S6. Plot of maximum H_2SO_4 mixing ratios estimated from RACM2 versus those estimated by RACM1 for the conditions given in Tables 1 – 4. The solid line is the 1-1 line of perfect agreement while the dashed line is the regression line between the two mechanisms.

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