Supplement

On the role of monoterpene chemistry in the remote continental boundary layer

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Abbreviation	Name	Abbreviation	Name
ACD	acetaldehyde	HC3P	peroxy radicals from alkanes, alcohols, esters, and alkynes with OH rate constants less than 3.4 $\times 10^{-12}$ cm^3 s^{-1} at 298 K, 1 atm
ACO3	acetyl peroxy radical	HC5P	peroxy radicals from alkanes, alcohols, esters, and alkynes with OH rate constants between 3.4 $\times 10^{-12}$ cm^3 s^{-1} and 6.8×10^{-12} cm^3 s^{-1} at 298 K, 1 atm
ACT	acetone	HC8P	peroxy radicals from alkanes, alcohols, esters, and alkynes with OH rate constants greater than 6.8 $\times 10^{-12}$ cm^3 s^{-1} at 298 K, 1 atm
ACTP	peroxy radical from acetone	HKET	hydroxy ketone
ADCN	aromatic-NO3 adduct	HONIT	2nd generation monoterpene nitrate
ALD	C-3 and higher aldehydes	HPALD	C-5 hydroperoxyaldehyde
AONIT	aromatic-derived organic nitrates	IAP	hydroxy ketone/aldehyde peroxide from isoprene chemistry
API	α -pinene and other cyclic terpenes with one double bond	IEPOX	isoprene-derived dihydroxy epoxide
APIP	peroxy radical from API	IEPOXOO	peroxy radical from IEPOX
BAL2	peroxy radicals from BALD	IMONIT	multifunctional organic nitrate from isoprene chemistry
BALD	benzaldehyde and other aromatic aldehydes	ISHP	hydroxy hydro peroxides
BENP	peroxy radicals from benzene	ISNP	peroxide from isoprene nitrate peroxy radicals
CHO	phenoxy radical from cresol and other hydroxy substituted aromatics	ISO	isoprene
DCB1	unsaturated dicarbonyls	ISOP	peroxy radical from ISOP
DCB2	unsaturated dicarbonyls	ISOPNB	β-hydroxy isoprene nitrate
DCB3	unsaturated dicarbonyls	ISOPNBO2	peroxy radical from ISOPNB
DHMOB	multi-hydroxy ketone/aldehyde from isoprene chemistry	ISOPND	δ-hydroxy isoprene nitrate
DIBOO	dibble peroxy radical (see Paulot et al. (2009a))	ISOPNDO2	peroxy radical from ISOPND
DONIT	unsaturated, multifunctional organic nitrates	KET	ketone
ETHLN	ethanal nitrate	KETP	peroxy radical from KET
ETHP	peroxy radicals from ethane	LIM	limonene and other cyclic diene-terpenes
GLY	glyoxal	LIMP	peroxy radical from LIM
GLYC	glycoaldehyde	MACP	acyl peroxy radicals from MACR
HAC	hydroxy acetone	MACR	methacrolein

Table S1 Chemical species in expanded organic nitrate chemistry.

Abbreviation	Name	Abbreviation	Name
MACRN	methacrolein nitrate	OP2	> C-1 organic peroxides
MACRO2	peroxy radicals from MACR	ORA1	formic acid
MAHP	methyl acrylic acid	ORA2	acetic and higher acids
MCTO	alkoxy radicals from methyl catechol oxidation	PER1	peroxy intermediate from toluene oxidation
MEK	methyl ethyl ketone	PER2	peroxy intermediate from toluene oxidation
MGLY	methyl glyoxal	PROPNN	propanone nitrate
MO2	methyl peroxy radical	PYAC	pyruvic acid
MOBA	organic acids	ROH	C-3 and higher alcohols
MOBAOO	peroxy radical from MOBA	TOLND	NO_3-alkene adduct from monoterpenes that primarily decomposes
MOH	methanol	TOLNN	NO_3-alkene adduct from monoterpenes that primarily retains the NO_3 functional group
MONIT	multifunctional organic nitrate	TOLP	peroxy radicals from toluene
MPAN	methacryloyl peroxy nitrate	TONIT	saturated first generation monoterpene organic nitrate
MVK	methyl vinyl ketone	UALD	unsaturated aldehydes
MVKN	methyl vinyl ketone nitrate	UHC	multifunctional alkene from isoprene chemistry
MVKP	peroxy radical from MVK	UHCAP	acyl peroxy radical from UHC
OLI	internal alkene	UHCP	peroxy radical from UHC
OLIP	peroxy radical from OLI	UTONIT	unsaturated first generation monoterpene organic nitrate
OLND	NO_3-alkene adduct that primarily decomposes	VRP	peroxide from MVK peroxy radical
OLNN	NO_3-alkene adduct that primarily retains the NO_3 functional group	XO2	accounts for additional NO to NO_2 conversions in peroxy radical reactions
OLT	terminal alkene	XYLP	peroxy radicals from m and p-xylene
OLTP	peroxy radical from OLT	XYOP	peroxy radicals from o-xylene
ONIT	monofunctional organic nitrate		

Table S1 (continued) Chemical species in expanded organic nitrate chemistry.

Species	H* (M atm-1)	-ΔH/R (K)	f0	Reference
ISON, ETHLN, ISOPND, ISOPNB, TONIT, IMONIT, UTONIT, MACRN, MVKN	17000	9200	0	Ito et al. (2007) for biogenic hydroxy nitrates
MAHP, VRP, IAP, ISNP	340	6000	0.1	Ito et al. (2007) for organic peroxides
MONIT, PROPNN, DONIT, AONIT, ONIT	1.13	5487	0	WRF-Chem ONIT
ISHP, HONIT	2.69×10^{13}	8684	0	WRF-Chem HNO_3
IEPOX	75400	6615	1	WRF-Chem H_2O_2

Table S2 Dry deposition parameters for additional isoprene chemistry and organic nitrate species. H* is the Henry's law coefficient and f0 is the reactivity factor as defined in Wesely, (1989).

Reactants		Products	Rate	Notes
APIP + NO	→	0.82 HO2 + 0.43 ALD + 0.82 NO2 + 0.44 KET + 0.12 TONIT + 0.06 UTONIT + 0.23 HCHO + 0.11 ACT + 0.07 ORA1	4.00×10^{-12}	RACM2 renamed
LIMP + NO	→	0.22 UTONIT + 0.686 HO2 + 0.491 UALD + 0.231 HCHO + 0.058 HAC + 0.78 NO2 + 0.289 OLI + 0.289 KET	4.00×10^{-12}	MCM products
API + NO3	→	0.10 TOLNN + 0.90 TOLND	$1.19\times10^{-12}\times\exp(490.0/T)$	RACM2 renamed
LIM + NO3	→	0.71 TOLNN + 0.29 TOLND	1.22×10^{-11}	RACM2 renamed
TOLNN + NO	→	TONIT + NO2 + HO2	4.00×10^{-12}	RACM2 renamed
TOLNN + HO2	→	0.7 TONIT + 0.3 UTONIT	$1.66\times10^{-13}\times\exp(1300.0/T)$	RACM2 renamed
TOLNN + MO2	→	HCHO + 2.0 HO2 + 0.7 TONIT + 0.3 UTONIT	$1.60\times10^{-13}\times\exp(708.0/T)$	RACM2 renamed
TOLNN + ACO3	→	0.7 TONIT + 0.3 UTONIT + MO2 + HO2	$8.85\times10^{-13}\times\exp(765.0/T)$	RACM2 renamed
TOLNN + NO3	→	0.7 TONIT + 0.3 UTONIT + NO2 + HO2	1.20×10^{-12}	RACM2 renamed
TOLNN + TOLNN	→	1.4 TONIT + 0.6 UTONIT + HO2	$7.00\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TOLNN + OLND	→	0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO2 + 0.50 NO2 + 0.7 TONIT + 0.3 UTONIT + 0.5 MONIT	$4.25\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TOLNN + OLNN	→	MONIT + 0.7 TONIT + 0.3 UTONIT + HO2	$7.00\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TOLND + NO	→	0.287 HCHO + 1.24 ALD + 0.464 KET + 2.0 NO2	4.00×10^{-12}	RACM2 renamed
TOLND + HO2	→	0.7 TONIT + 0.3 UTONIT	$1.66\times10^{-13}\times\exp(1300.0/T)$	RACM2 renamed
TOLND + MO2	→	0.965 HCHO + 0.500 HO2 + 0.930 ALD + 0.348 KET + 0.500 NO2 + 0.250 MOH + 0.25 ROH + 0.350 TONIT + 0.15 UTONIT	$9.68\times10^{-14}\times\exp(708.0/T)$	RACM2 renamed
TOLND + ACO3	→	0.287 HCHO + 1.24 ALD + 0.464 KET + 0.500 MO2 + 0.500 ORA2 + NO2	$5.37\times10^{-13}\times\exp(765.0/T)$	RACM2 renamed
TOLND + NO3	→	0.287 HCHO + 1.24 ALD + 0.464 KET + 2.00 NO2	1.20×10^{-12}	RACM2 renamed
TOLND + TOLND	→	0.504 HCHO + 1.21 ALD + 0.285 KET + 0.7 TONIT + 0.3 UTONIT + NO2	$2.96\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TOLND + OLND	→	0.504 HCHO + 1.21 ALD + 0.285 KET + NO2 + 0.35 TONIT + 0.15 UTONIT + 0.5 MONIT	$2.96\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TOLND + OLNN	→	0.202 HCHO + 0.64 ALD + 0.149 KET + 0.50 HO2 + 0.50 NO2 + MONIT + 0.35 TONIT + 0.15 UTONIT	$4.25\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed

Table S3 Monoterpene reactions added to/revised from RACM2.

Reactants		Products	Rate	Notes
TOLNN + TOLND	→	0.202 HCHO + 0.640 ALD + 0.149 KET + 0.500 HO2 + 0.500 NO2 + 1.05 TONIT + 0.45 UTONIT	$4.25\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
TONIT + hv	→	KET + NO2	J(onitOH3)	MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
TONIT + HO	→	HONIT	4.8×10^{-12}	Assuming a 50-50 α,β-pinene mixture and using the MCM nitrates formed from the OH addition to the double bond
UTONIT + hv	→	UALD + NO2	J(onitOH3)	MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
UTONIT + HO	→	HONIT	7.29×10^{-11}	Average of MCM limonene nitrate rates
UTONIT + O3	→	HONIT	1.67×10^{-16}	EPA EPI v4.1 rates weighted by MCM isomers
HONIT + hv	→	HKET + NO2	J(onitOH3)	MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
HO + HONIT	→	NO3 + HKET	$k_0=2.4\times10^{-14}\times\exp(460/T)$ $k_1=2.7\times10^{-17}\times\exp(2199/T)$ $k_2=6.5\times10^{-34}\times\exp(1335/T)\times M$ $rate=k_0+k_2/(1+k_2./k_1)$	same as RACM2 HNO_3

[#] Cross sections are calculated using the Fast-JX cross-section generator (Wild et al., 2000).
Table S3 (continued) Monoterpene reactions added to/revised from RACM2.

Reactants		Products	Rate	Notes
HC3P + NO	→	0.063 ONIT + 0.002 MONIT + 0.132 ALD + 0.165 ACT + 0.504 ACD + 0.207 HO2 + 0.131 MO2 + 0.500 ETHP + 0.089 XO2 + 0.935 NO2 + 0.042 MEK	4.00×10^{-12}	RACM2 renamed
HC5P + NO	→	0.018 HCHO + 0.203 ALD + 0.039 KET + 0.438 HO2 + 0.051 MO2 + 0.231 ETHP + 0.435 XO2 + 0.114 ONIT + 0.022 MONIT + 0.864 NO2 + 0.033 MEK + 0.217 ACT + 0.045 ACD + 0.272 HKET	4.00×10^{-12}	RACM2 renamed
HC8P + NO	→	0.163 ALD + 0.698 KET + 0.145 ETHP + 0.197 ONIT + 0.803 NO2 + 0.658 HO2 + 0.452 XO2	4.00×10^{-12}	RACM2 renamed and nitrate yield re-scaled based on Arey et al. (2001)
OLTP + NO	→	0.44 ALD + 0.78 HCHO + 0.78 HO2 + 0.97 NO2 + 0.13 MEK + 0.012 ACD + 0.06 ACT + 0.03 MONIT	4.00×10^{-12}	RACM2 renamed
OLIP + NO	→	0.83 HO2 + 0.68 ALD + 0.09 KET + 0.95 NO2 + 0.035 MONIT + 0.015 DONIT + 0.81 ACD + 0.02 HKET + 0.20 ACT	4.00×10^{-12}	RACM2 renamed
BENP + NO	→	0.082 AONIT + 0.918 HO2 + 0.459 DCB2 + 0.918 NO2 + 0.459 DCB3 + 0.918 GLY	$2.54\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
TOLP + NO	→	0.95 DCB2 + 0.95 NO2 + 0.95 HO2 + 0.05 AONIT	$2.70\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
PER1 + NO	→	0.95 DCB1 + 0.95 NO2 + 0.95 MGLY + 0.95 HO2 + 0.050 AONIT + 0.95 BALD	$2.70\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
XYLP + NO	→	0.95 DCB3 + 0.95 NO2 + 0.95 HO2 + 0.05 AONIT	$2.70\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
PER2 + NO	→	0.95 DCB1 + 0.95 NO2 + 0.95 MGLY + 0.95 HO2 + 0.050 AONIT + 1.05 DCB3	$2.70\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
XYOP + NO	→	0.95 HO2 + 0.350 GLY + 0.600 MGLY + 0.700 DCB1 + 0.073 DCB2 + 0.177 DCB3 + 0.05 AONIT + 0.95 NO2	$2.70\times10^{-12}\times\exp(360.0/T)$	RACM2 renamed
KETP + NO	→	0.531 MGLY + 0.452 ALD + 0.226 ACO3 + 0.757 HO2 + 0.157 XO2 + 0.983 NO2 + 0.017 MONIT	4.00×10^{-12}	Added nitrate
OLNN + NO	→	MONIT + NO2 + HO2	4.00×10^{-12}	RACM2 renamed
BAL2 + NO2	→	AONIT	2.00×10^{-11}	RACM2 renamed
CHO + NO2	→	AONIT	2.00×10^{-11}	RACM2 renamed

Table S4 Non-biogenic organic nitrates added to RACM2.

Reactants		Products	Rate	Notes
MCTO + NO2	→	AONIT	2.08×10^{-12}	RACM2 renamed
ADCN + HO2	→	AONIT	$3.75\times10^{-13}\times\exp(980.0/T)$	RACM2 renamed
OLNN + HO2	→	MONIT	$1.66\times10^{-13}\times\exp(1300.0/T)$	RACM2 renamed
OLND + HO2	→	MONIT	$1.66\times10^{-13}\times\exp(1300.0/T)$	RACM2 renamed
OLNN + MO2	→	HCHO + 2.0 HO2 + MONIT	$1.60\times10^{-13}\times\exp(708.0/T)$	RACM2 renamed
OLND + MO2	→	0.965 HCHO + 0.500 HO2 + 0.930 ALD + 0.348 KET + 0.500 NO2 + 0.250 MOH + 0.25 ROH + 0.500 MONIT	$9.68\times10^{-14}\times\exp(708.0/T)$	RACM2 renamed
ADCN + MO2	→	HCHO + HO2 + 0.7 OP2 + 0.7 GLY + 0.7 NO2 + 0.3 AONIT	3.56×10^{-14}	RACM2 renamed
OLNN + ACO3	→	MONIT + MO2 + HO2	$8.85\times10^{-13}\times\exp(765.0/T)$	RACM2 renamed
ADCN + ACO3	→	MO2 + HO2 + 0.7 OP2 + 0.7 GLY + 0.7 NO2 + 0.3 AONIT	$7.40\times10^{-13}\times\exp(708.0/T)$	RACM2 renamed
OLNN + NO3	→	MONIT + NO2 + HO2	1.20×10^{-12}	RACM2 renamed
OLNN + OLNN	→	2.00 MONIT + HO2	$7.00\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
OLNN + OLND	→	0.202 HCHO + 0.640 ALD + 0.149 KET + 0.500 HO2 + 0.500 NO2 + 1.50 MONIT	$4.25\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
OLND + OLND	→	0.504 HCHO + 1.21 ALD + 0.285 KET + MONIT + NO2	$2.96\times10^{-14}\times\exp(1000.0/T)$	RACM2 renamed
AONIT + hv	→	KET + NO2	J(onitOH3)	MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
DONIT + hv	→	UALD + NO2	J(onitOH1)	MCM n-propyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
MONIT + hv	→	KET + NO2	J(onitOH1)	Same as above
AONIT + HO	→	DCB2 + NO2	7.3×10^{-11}	MCM rate for major peroxy radical formed from benzene
DONIT + HO	→	UALD + NO2	4.1×10^{-11}	MCM weighted average based on butadiene nitrates
MONIT + HO	→	HKET + NO2	1.79×10^{-12}	Rate is from MCM hydroxy nitrate from 2-butene

[#] Cross sections are calculated using the Fast-JX cross-section generator (Wild et al., 2000).
MCM - (Jenkin et al., 1997; Saunders et al., 2003)
Table S4 (continued) Non-biogenic organic nitrates added to RACM2.

Reactants		Products	Rate	Notes
ISO + HO	→	ISOP	$3.1\times10^{-11}\times\exp(350.0/T)$	Rate from Sander et al. (2011)
ISOP + NO	→	0.4 MVK + 0.26 MACR + 0.883 NO2 + 0.07 ISOPND + 0.047 ISOPNB + 0.66 HCHO + 0.143 UHC + 0.08 DIBOO + 0.803 HO2	$2.7\times10^{-12}\times\exp(360.0/T)$	Products from Paulot et al. (2009a), rate from MCM
ISOP + HO2	→	0.88 ISHP + 0.12 HO + 0.047 MACR + 0.073 MVK + 0.12 HO2 + 0.12 HCHO	$7.4\times10^{-13}\times\exp(700.0/T)$	Paulot et al. (2009b)
ISOP	→	HPALD + HO2	$4.12\times10^{8}\times\exp(-7700.0/T)$	Products from Peeters and Müller (2010), rate from Crounse et al. (2011)
ISOPND + hv	→	ISOP + NO2	J(onit1)	MCM n-propyl nitrate photolysis cross-section#
ISOPND + HO	→	ISOPNDO2	$1.77\times10^{-11}\times\exp(500.0/T)$	Paulot et al. (2009a) products and rate with temperature dependence of RACM2 internal alkene
ISOPND + O3	→	0.266 PROPNN + 0.017 ORA2 + 0.249 GLYC + 0.075 H2O2 + 0.89 HO + 0.445 HO2 + 0.214 CO + 0.214 HCHO + 0.445 NO2 + 0.271 ETHLN + 0.018 IMONIT + 0.445 MGLY + 0.289 HAC + 0.231 GLY	$9.03\times10^{-16}\times\exp(-845.0/T)$	Products based on MCM, rate from Lockwood et al. (2010) with temperature dependence of RACM2 internal alkene
ISOPNDO2 + NO	→	0.15 PROPNN + 0.44 HAC + 0.07 MVKN + 0.13 ETHLN + 0.31 ORA1 + 0.31 NO3 + 0.72 HCHO + 0.15 GLYC + 1.34 NO2 + 0.35 HO2 + 0.34 HKET	$2.7\times10^{-12}\times\exp(360.0/T)$	Paulot et al. (2009a) products and MCM rate
ISOPNDO2 + HO2	→	ISNP	$2.06\times10^{-13}\times\exp(1300.0/T)$	MCM rate
ISOPNDO2 + MO2	→	1.506 HCHO + 0.949 HO2 + 0.3 IMONIT + 0.055 MVKN + 0.309 HAC + 0.093 ETHLN + 0.216 ORA1 + 0.235 HKET + 0.101 PROPNN + 0.101 GLYC + 0.216 NO3 + 0.235 NO2	7.5×10^{-14}	Madronich and Calvert (1990) RO_2 products and rate*
ISOPNDO2 + ACO3	→	0.078 MVKN + 0.442 HAC + 0.133 ETHLN + 0.309 ORA1 + 0.336 HKET + 0.144 PROPNN + 0.144 GLYC + 0.723 HCHO + 0.355 HO2 + 0.309 NO3 + MO2 + CO2 + 0.336 NO2	$9.53\times10^{-14}\times\exp(500.0/T)$	Madronich and Calvert (1990) RO_2 products and rate*

Table S5 Reactions of isoprene and related species added to RACM2.

Reactants		Products	Rate	Notes
ISOPNDO2 + NO3	→	0.078 MVKN + 0.442 HAC + 0.133 ETHLN + 0.309 ORA1 + 0.336 HKET + 0.144 PROPNN + 0.144 GLYC + 0.723 HCHO + 0.355 HO2 + 0.309 NO3 + 1.336 NO2	2.3×10^{-12}	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
ISOPNB + hv	→	ISOP + NO2	J(onitOH3)	MCM tert-butyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
ISOPNB + HO	→	ISOPNBO2	2.43×10^{-12} ×exp(500.00/T)	Paulot et al. (2009a) products and rate with temperature dependence of RACM2 terminal alkene
ISOPNB + O3	→	0.541 HCHO + 0.506 CO + 0.526 HO + 0.327 NO2 + 0.179 HAC + 0.102 H2O2 + 0.349 MACRN + 0.112 IMONIT + 0.128 CO2 + 0.327 HO2 + 0.068 ORA1 + 0.212 MVKN + 0.148 MGLY	5.04×10^{-14}×exp(-1800/T)	Products based on MCM, rate from Lockwood et al. (2010) with temperature dependence of RACM2 terminal alkene
ISOPNBO2 + NO	→	0.6 GLYC + 0.6 HAC + 0.4 HCHO + 0.4 HO2 + 0.26 MACRN + 0.14 MVKN + 1.6 NO2	2.7×10^{-12} ×exp(360.0/T)	Paulot et al. (2009a) products, MCM rate
ISOPNBO2 + HO2	→	ISNP	2.06×10^{-13} ×exp(1300.0/T)	MCM
ISOPNBO2 + MO2	→	0.128 MACRN + 0.16 MOH + 0.101 MVKN + 0.801 HO2 + 1.069 HCHO + 0.343 HAC + 0.343 GLYC + 0.343 NO2 + 0.428 IMONIT	6.7×10^{-13}	Madronich and Calvert (1990) RO_2 products and rate*, RO follows same fate as in the NO reaction
ISOPNBO2 + ACO3	→	0.064 IMONIT + 0.23 MACRN + 0.144 MVKN + 0.374 HCHO + 0.562 HAC + 0.562 GLYC + 0.562 NO2 + 0.936 CO2 + 0.936 MO2 + 0.374 HO2 + 0.064 ORA2	8.16×10^{-13} ×exp(500.0/T)	Madronich and Calvert (1990)/Tyndall et al. (2001) products and rate*
ISOPNBO2 + NO3	→	0.256 MACRN + 0.144 MVKN + 0.6 HAC + 0.6 GLYC + 0.4 HCHO + 0.4 HO2 + 1.6 NO2	2.3×10^{-12}	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
HPALD + hv	→	1.0 HO + HO2 + 0.5 HAC + 0.5 MGLY + 0.25 GLYC + 0.25 GLY + HCHO	J(hpald)	Peeters and Müller (2010)
HPALD + HO	→	HO	4.6×10^{-11}	Peeters and Müller (2010)
IEPOX + HO	→	IEPOXOO	5.78×10^{-11}×exp(-400.0/T)	Paulot et al. (2009b)

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants		Products	Rate	Notes
IEPOXOO + NO	→	0.725 HAC + 0.275 GLYC + 0.275 GLY + 0.275 MGLY + 0.125 HO + 0.825 HO2 + 0.2 CO2 + 0.375 HCHO + 0.074 ORA1 + 0.251 CO + NO2	2.7×10^{-12} ×exp(360.0/T)	MCM
IEPOXOO + HO2	→	0.725 HAC + 0.275 GLYC + 0.275 GLY + 0.275 MGLY + 1.125 HO + 0.825 HO2 + 0.2 CO2 + 0.375 HCHO + 0.074 ORA1 + 0.251 CO	7.4×10^{-13} ×exp(700.0/T)	Paulot et al. (2009b)
IEPOXOO + NO3	→	0.725 HAC + 0.275 GLYC + 0.275 GLY + 0.275 MGLY + 0.125 HO + 0.825 HO2 + 0.2 CO2 + 0.375 HCHO + 0.074 ORA1 + 0.251 CO + NO2	2.3×10^{-12}	MCM
ISHP + hv	→	HO + 0.202 UHC + 0.108 DIBOO + 0.44 MVK + 0.25 MACR + 0.69 HCHO + 0.892 HO2	J(ch3o2h)	MCM CH_3OOH cross section [#]
ISHP + HO	→	IEPOX + HO	1.9×10^{-11} ×exp(390.0/T)	Paulot et al. (2009b)
ISHP + HO	→	0.7 ISOP + 0.3 UHC + 0.3 HO	3.8×10^{-12} ×exp(200.0/T)	Paulot et al. (2009b)
PROPNN + hv	→	NO2 + ACO3 + HCHO	J(noa)	MCM nitroxy acetone cross section[#]
PROPNN + HO	→	NO2 + MGLY	1.0×10^{-12}	Paulot et al. (2009a)
ETHLN + hv	→	HO2 + CO + HCHO + NO2	J(noa)	MCM nitroxy acetone cross section[#]
ETHLN + HO	→	HCHO + CO2 + NO2	1.0×10^{-11}	Paulot et al. (2009a)
IMONIT + hv	→	HKET + NO2	J(onitOH1)	MCM n-propyl nitrate photolysis cross-section, divided by 3 due to the hydroxy group (Roberts and Fajer, 1989)[#]
IMONIT + HO	→	HKET + NO2	7.2×10^{-12}	MCM weighted average
ISNP + hv	→	HO + 0.686 HO2 + 0.298 PROPNN + 0.612 GLYC + 0.632 HAC + 0.318 ETHLN + 0.314 NO2 + 0.07 MVKN + 0.07 HCHO	J(ch3o2h)	MCM CH_3OOH cross section [#]
ISNP + HO	→	0.460 ISOPNDO2 + 0.097 ISOPNBO2 + 0.443 IMONIT + 0.443 HO	1.67×10^{-11} ×exp(200.0/T)	Calculated using Kwok and Atkinson (1995) with temperature dependence and products of CH_3OOH from Sander et al. (2011)
UHC + hv	→	0.5 UHCAP + 1.24 HO2 + 0.26 ACO3 + 0.74 CO + 0.26 GLYC + 0.24 HAC	J(macr)	IUPAC cross section

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants		Products	Rate	Notes
UHC + HO	→	0.74 UHCP + 0.26 UHCAP	1.1×10^{-10}	Paulot et al. (2009a)
UHC + O3	→	0.503 MGLY + 0.89 HO + 0.89 CO + 0.659 HO2 + 0.231 HCHO + 0.018 MOH + 0.018 CO2 + 0.271 GLYC + 0.076 H2O2 + 0.266 HAC + 0.266 GLY + 0.231 ACO3	4.0×10^{-17}	Rate from Jenkin et al. (1997) lowered by a factor of 10 due to the aldehyde
UHC + NO3	→	HNO3 + UHCAP	$5.95\times10^{-12}\times\exp(-1860/T)$	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
UHCP + NO	→	0.39 DHMOB + 0.32 GLYC + 0.32 MGLY + 0.29 HAC + 0.29 GLY + HO2 + NO2	$2.7\times10^{-12}\times\exp(360.0/T)$	Paulot et al. (2009a) products, MCM rate
UHCP + HO2	→	0.652 IAP + 0.136 DHMOB + 0.212 MGLY + 0.212 GLYC + 0.348 HO + 0.348 HO2	$2.06\times10^{-13}\times\exp(1300.0/T)$	Hasson et al. (2004) products, MCM rate
UHCP + MO2	→	0.573 DHMOB + HCHO + 1.4 HO2 + 0.222 GLYC + 0.222 MGLY + 0.205 HAC + 0.205 GLY	8.24×10^{-14}	Madronich and Calvert (1990) RO_2 products and rate*
UHCP + ACO3	→	MO2 + CO2 + 0.39 DHMOB + 0.32 GLYC + 0.32 MGLY + 0.29 HAC + 0.29 GLY + HO2	$1.04\times10^{-13}\times\exp(500.0/T)$	Madronich and Calvert (1990) RO_2 products and rate*
UHCP + NO3	→	NO2 + 0.39 DHMOB + 0.317 GLYC + 0.317 MGLY + 0.293 GLY + 0.293 HAC + HO2	2.3×10^{-12}	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
UHCAP + NO	→	NO2 + 0.65 MOBA + 0.35 ALD + 0.35 CO + HO2	$7.5\times10^{-12}\times\exp(290.0/T)$	Paulot et al. (2009a) products, MCM rate
UHCAP + HO2	→	0.4 IAP + 0.2 ORA2 + 0.2 O3 + 0.4 HO + 0.26 MOBA + 0.14 ALD + 0.14 CO	$5.2\times10^{-13}\times\exp(980.0/T)$	Hasson et al. (2004) branching MCM rate
UHCAP + MO2	→	0.1 ORA2 + HCHO + 1.8 HO2 + 0.585 MOBA + 0.315 ALD + 0.315 CO	$8.83\times10^{-13}\times\exp(500.0/T)$	Tyndall et al. (2001)
UHCAP + ACO3	→	MO2 + CO2 + HO2 + 0.65 MOBA + 0.35 ALD + 0.35 CO	$2.9\times10^{-12}\times\exp(500.0/T)$	Tyndall et al. (2001)
UHCAP + NO3	→	NO2 + HO2 + 0.65 MOBA + 0.35 ALD + 0.35 CO	4.0×10^{-12}	MCM
UHCAP + NO2	→	MPAN	TROE(9.0×10^{-28} , 8.9, 7.7×10^{-12} , 0.2, T, M)	Sander et al. (2011) rate for PPN
IAP + HO	→	0.165 UHCAP + 0.495 UHCP + 0.34 DIBOO	$2.7\times10^{-11}\times\exp(200.0/T)$	Calculated using Kwok and Atkinson (1995) with temperature dependence and products of CH_3OOH from Sander et al. (2011)

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants		Products	Rate	Notes
IAP + hv	→	HO + 0.107 MOBA + 0.058 ALD + 0.058 CO + 0.193 DHMOB + 0.335 GLYC + 0.335 MGLY + 0.307 HAC + 0.307 GLY + HO2	J(ch3o2h)	MCM CH_3OOH cross section [#]
DIBOO + NO	→	NO2 + HO2 + 0.52 GLYC + 0.52 MGLY + 0.48 GLY + 0.48 HAC	2.7×10^{-12} ×exp(360.0/T)	Paulot et al. (2009a) products, MCM rate
DIBOO + HO2	→	0.33 IAP + 0.67 HO + 0.67 HO2 + 0.348 GLYC + 0.348 MGLY + 0.322 GLY + 0.322 HAC	2.06×10^{-13} ×exp(1300.0/T)	Hasson et al. (2004) branching MCM rate
DIBOO + MO2	→	0.396 DHMOB + 0.88 HCHO + 0.364 GLYC + 0.364 MGLY + 1.208 HO2 + 0.12 MOH + 0.24 GLY + 0.24 HAC	4.6×10^{-13}	Madronich and Calvert (1990) RO_2 products and rate*
DIBOO + ACO3	→	0.52 GLYC + 0.52 MGLY + 0.952 HO2 + 0.952 MO2 + 0.952 CO2 + 0.432 GLY + 0.432 HAC + 0.048 ORA2 + 0.048 DHMOB	5.8×10^{-13} ×exp(500.0/T)	Tyndall et al. (2001)
DIBOO + NO3	→	NO2 + HO2 + 0.52 GLYC + 0.52 MGLY + 0.48 GLY + 0.48 HAC	2.3×10^{-12}	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
MOBA + hv	→	0.53 PYAC + 0.48 GLY + 1.52 HO2 + 2.0 CO + 0.48 MO2	J(macr)	IUPAC cross section
MOBA + HO	→	MOBAOO	3.0×10^{-12}	Paulot et al. (2009a)
MOBA + O3	→	0.555 MGLY + 0.89 HO + 0.89 CO + 0.445 HO2 + 0.076 H2O2 + 0.555 GLY + 0.231 KETP + 0.214 ACO3 + 0.214 CO2	2.0×10^{-17}	Paulot et al. (2009a), MCM
MOBAOO + NO	→	ALD + CO2 + HO2 + NO2	8.0×10^{-12}	Paulot et al. (2009a)
MOBAOO + HO2	→	OP2	2.06×10^{-13} ×exp(1300.0/T)	MCM
MOBAOO + MO2	→	0.7 CO2 + 0.7 ALD + 1.4 HO2 + HCHO + 0.3 ROH	3.55×10^{-12}	Madronich and Calvert (1990) RO_2 products and rate assuming 3^o beta hydroxy
MOBAOO + ACO3	→	ALD + 2.0 CO2 + HO2 + MO2	4.23×10^{-12} ×exp(500.0/T)	Tyndall et al. (2001)
MOBAOO + NO3	→	NO2 + HO2 + ALD + CO2	2.3×10^{-12}	Jenkin et al. (1997) RO_2+NO_3 products with MCM rate
HAC + hv	→	ACO3 + HCHO + HO2	J(ch3coch3)	MCM products assume same cross-section as acetone
HAC + HO	→	MGLY + HO2	1.6×10^{-12}×exp(305.0/T)	MCM products, IUPAC rate
GLYC + hv	→	2.0 HO2 + HCHO + CO	J(glyc)	MCM cross section[#]
GLYC + HO	→	0.2 GLY + 0.2 HO2 + 0.8 RCO3	1.0×10^{-11}	MCM

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants		Products	Rate	Notes
GLYC + NO3	→	RCO3 + HNO3	$1.4\times10^{-12}\times\exp(-1860.0/T)$	MCM
DHMOB + hv	→	HO2 + CO + KETP	J(ald)	Assume aldehyde
DHMOB + HO	→	1.5 CO + 0.5 HO2 + 0.5 HAC + 0.5 ALD	1.0×10^{-11}	Paulot et al. (2009a)
PYAC + HO	→	ACO3 + CO2	8.0×10^{-13}	MCM
PYAC + hv	→	ACO3 + CO2 + HO2	j(Pj_ch3cocho)	Fast-JX 6.5 cross section#
MACR + hv		0.5 MACP + 0.175 ACO3 + 0.5 HCHO + 0.325 MO2 + 0.825 CO + HO2	J(macr)	IUPAC cross section
MACR + HO		0.53 MACP + 0.47 MACRO2	$8.0\times10^{-12}\times\exp(380.0/T)$	Paulot et al. (2009a) products, IUPAC rate
MACR + O3		0.902 MGLY + 0.242 HCHO + 0.238 HO + 0.652 CO + 0.098 ACO3 + 0.204 ORA1 + 0.14 HO2 + 0.144 H2O2	$1.4\times10^{-15}\times\exp(-2100.0/T)$	MCM
MACR + NO3		MACP + HNO3	3.4×10^{-15}	MCM
MACP + NO		NO2 + CO + CO2 + HCHO + MO2	$7.5\times10^{-12}\times\exp(290.0/T)$	rate MCM AP + NO prdts Paulot ACP
MACP + HO2		0.4 MAHP + 0.2 O3 + 0.2 ORA2 + 0.4 HO + 0.4 CO2 + 0.26 MO2 + 0.4 HCHO + 0.14 ACO3 + 0.26 CO	$5.2\times10^{-13}\times\exp(980.0/T)$	Hasson et al. (2004) products, MCM rate
MACP + MO2		0.9 HO2 + 0.9 CO2 + 0.585 MO2 + 0.585 CO + 0.315 ACO3 + 0.1 ORA2 + 1.9 HCHO	$2.0\times10^{-12}\times\exp(500.0/T)$	Tyndall et al. (2001)
MACP + ACO3		1.65 MO2 + 2.0 CO2 + 0.35 ACO3 + HCHO + 0.65 CO	$2.9\times10^{-12}\times\exp(500.0/T)$	Tyndall et al. (2001) and IUPAC rate
MACP + NO3		NO2 + CO2 + HCHO + 0.65 MO2 + 0.65 CO + 0.35 ACO3	4.0×10^{-12}	MCM
MACP + NO2		MPAN	TROE(9.0×10^{-28} , 8.9, 7.7×10^{-12} , 0.2, T, M)	Sander et al. (2011) rate for PPN
MPAN		MACP + NO2	TROEE(1.11×10^{28} , 14000.0, 9.0×10^{-28} , 8.9 , 7.7×10^{-12} , 0.2, T , M)	Sander et al. (2011) rate for PPN
MAHP + HO		MACP	1.66×10^{-11}	MCM
UALD + NO3		MACP + HNO3	$5.02\times10^{-13}\times\exp(-1076/T)$	MCM
MAHP + hv		ACO3 + HO + CO2	J(ch3o2h)	MCM CH_3OOH cross section #
MACRO2		HAC + CO + HO	$2.9\times\exp10^{7}\times\exp(-5297/T)$	Crounse et al. (2012)

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants	Products	Rate	Notes
MACRO2 + NO	0.85 NO2 + 0.85 HO2 + 0.425 HAC + 0.425 CO + 0.425 HCHO + 0.425 MGLY + 0.15 MACRN	2.7×10^{-12} ×exp(360.0/T)	Paulot et al. (2009a) products, MCM rate
MACRO2 + HO2	OP2	1.8×10^{-13} ×exp(1300.0/T)	MCM
MACRO2 + MO2	0.328 HKET + 1.037 HCHO + 1.344 HO2 + 0.599 HAC + 0.599 CO + 0.036 MOH + 0.073 MGLY	2.04×10^{-13}	Madronich and Calvert (1990) RO_2 products and rate*, from initial $2^o/3^o$ split from MCM
MACRO2 + ACO3	0.855 HAC + 0.855 CO + 0.131 MGLY + 0.131 HCHO + 0.014 HKET + 0.014 ORA2 + 0.986 MO2 + 0.986 HO2 + 0.986 CO2	2.58×10^{-13} ×exp(500.0/T)	MCM peroxy branching ratio, Madronich and Calvert (1990) RO_2 products and rate*
MACRO2 + NO3	0.855 HAC + 0.855 CO + 0.855 HO2 + 0.145 HO2 + 0.145 MGLY + 0.145 HCHO + NO2	2.3×10^{-12}	MCM
MVK + hv	0.6 OLT + 0.6 CO + 0.4 ACO3 + 0.4 MO2	J(mvk)	Fast-JX 6.5 products and cross-section#
MVK + O3	0.28 ACO3 + 0.56 CO + 0.075 ORA1 + 0.09 H2O2 + 0.28 HO2 + 0.2 CO2 + 0.1 ACD + 0.545 HCHO + 0.36 HO + 0.545 MGLY + 0.075 PYAC	8.5×10^{-16}×exp(-1520.0/T)	MCM products assuming that the Criegee radical reacts only with H_2O, IUPAC rate
MVKP + NO	0.625 GLYC + 0.625 ACO3 + 0.265 MGLY + 0.265 HCHO + 0.265 HO2 + 0.11 MVKN + 0.89 NO2	2.7×10^{-12} ×exp(360.0/T)	Paulot et al (2009a) products, MCM rate
MVKP + HO2	0.531 VRP + 0.469 GLYC + 0.469 ACO3 + 0.469 HO	1.82×10^{-13} ×exp(1300.0/T)	MCM rate and $1^o/2^o$ RO^2 branching, Hasson et al. (2004) products
MVKP + MO2	0.25 ROH + 0.9 HCHO + 0.25 HKET + 0.25 MOH + 0.15 MGLY + 0.35 GLYC + 0.35 ACO3 + 0.65 HO2	1.38×10^{-12}	MCM initial branching ratio, Madronich and Calvert (1990) RO_2 products and rate*
MVKP + ACO3	0.1 HKET + 0.1 ORA2 + 0.27 MGLY + 0.27 HO2 + 0.27 HCHO + 0.63 GLYC + 0.63 ACO3 + 0.9 CO2 + 0.9 MO2	1.7×10^{-12} ×exp(500.0/T)	Tyndall et al. (2001)
MVKP + NO3	NO2 + 0.3 MGLY + 0.3 HO2 + 0.3 HCHO + 0.7 GLYC + 0.7 ACO3	2.3×10^{-12}	MCM
VRP + hv	HO + 0.7 ACO3 + 0.7 GLYC + 0.3 MGLY + 0.3 HCHO + 0.3 HO2	J(ch3o2h)	MCM CH_3OOH cross section, products split by initial MCM branching ratio for MVKP#
VRP + HO	0.7 MVKP + 0.3 KET + 0.3 HO	3.8×10^{-12} ×exp(200.0/T)	CH3OOH + OH rate and radical branching ratio from Sander et al. (2011)

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

Reactants	Products	Rate	Notes
MACRN + hv	NO2 + CO + HAC + HO2	J(ibutald)	MCM iso-butyraldehyde cross-section#
MVKN + hv	GLYC + NO2 + ACO3	J(noa)	MCM nitroxy acetone cross section#
MACRN + HO	0.08 ORA2 + 0.08 HCHO + 0.15 NO3 + 0.07 ORA1 + 0.07 MGLY + 0.85 HAC + 0.85 NO2 + 0.93 CO2	5.0×10^{-11}	Paulot et al. (2009a)
MVKN + HO	0.65 ORA1 + 0.65 MGLY + 0.35 HCHO + 0.35 PYAC + NO3	5.6×10^{-12}	Paulot et al. (2009a)

*Using updated rates (Atkinson et al., 2004, 2006; Sander et al., 2011), IUPAC rate or cross section (Atkinson et al., 2006), # Cross sections are calculated using the Fast-JX cross-section generator (Wild et al., 2000)., MCM - (Jenkin et al., 1997; Saunders et al., 2003), TROE(k_0(300K),n,k_∞(300K),m,T,M): $k_0(T) = k_0\_300K \times (300/T)^n \times M$, $k_\infty(T) = k_\infty(300K) \times (300/T)^m$, $k_{ratio} = k_0(T)/k_\infty(T)$, rate $= k_0(T)./(1+k_{ratio}) \times 0.6$^(1/(1+log10($k_{ratio}$)^2)), TROEE(A, B, k_0(300K),n,k_∞(300K),m,T,M): $k_0(T) = k_0\_300K \times (300/T)^n \times M$, $k_\infty(T) = k_\infty(300K) \times (300/T)^m$, $k_{ratio} = k_0(T)/k_\infty(T)$, k $= k_{0(}T)/(1+k_{ratio}) \times 0.6$^(1/(1+log10($k_{ratio}$)^2)), rate = A×exp(-BT/) × k

Table S5 (continued) Reactions of isoprene and related species added to RACM2.

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