Supplement 1 of
Schultz et al., 2017,
"The Chemistry Climate Model ECHAM-HAMMOZ"
in Geosci. Model Dev. (2017), available at:
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The supplement provides:
The Chemical Mechanism of HAMMOZ
List of Henry coefficients

The Chemical Mechanism of ECHAM6.3-HAM2.3-MOZ1.0

JAM version: 002b

Number of reactions:

Tropospheric photolysis (S1):	97
Stratospheric photolysis (S2):	45
(Tropospheric) O_x (S3):	7
(Tropospheric) HO_x (S4):	17
NOx (S5):	25
C1 oxidation (S6):	20
C2 oxidation (S7):	48
C3 oxidation (S8):	31
C4 oxidation (S9):	63
C5 oxidation (S10):	137
C6 oxidation (S11):	31
C7 oxidation (S12):	20
C8 oxidation (S13):	13
C10/C15 oxidation (terpenes, sesqui-terpenes; S14):	36
Tropospheric halogen + organics (S15):	21
Sulfur (S16):	11
Stratospheric O(1D) (S17):	28
Stratospheric inorganic halogen (S18):	48
Stratospheric organic halogen (S19):	12
(Tropospheric) heterogeneous (S20):	7
Stratospheric Sulfate aerosol (S21):	6
Stratospheric Nitric acid dihydrate (S22):	5
Stratospheric Ice aerosol (S23):	6
All equations:	734

Table S1: Tropospheric photolysis reactions

reaction	reference
$O_3 + hv \longrightarrow O_1D + O_2$	
$O_3 + hv \longrightarrow O + O_2$	
$H_2O_2 + hv \longrightarrow 2 \cdot OH$	
$N_2O + hv \longrightarrow N_2 + O_1D$	
$NO + hv \longrightarrow N + O$	
$NO_2 + hv \longrightarrow NO + O$	
$NO_3 + hv \longrightarrow NO_2 + O$	
$NO_3 + hv \longrightarrow NO + O_2$	
$HNO_3 + hv \longrightarrow NO_2 + OH$	
$HONO + hv \longrightarrow NO + OH$	
$HO_2NO_2 + hv \longrightarrow NO_3 + OH$	
$HO_2NO_2 + hv \longrightarrow HO_2 + NO_2$	
$N_2O_5 + hv \longrightarrow NO_2 + NO_3$	
$N_2O_5 + hv \longrightarrow NO + O + NO_3$	
$CO_2 + hv \longrightarrow CO + O$	
$CH_4 + hv \longrightarrow CH_3O_2 + H$	
$CH_4 + hv \longrightarrow 1.44 \cdot H_2 + 0.18 \cdot CH_2O + 0.18 \cdot O + 0.66 \cdot OH + 0.44 \cdot CO_2 + 0.38 \cdot CO + 0.05 \cdot H_2O$	
$CH_2O + hv \longrightarrow CO + 2 \cdot H$	
$CH_2O + hv \longrightarrow CO + H_2$	
$CH_3OOH + hv \longrightarrow CH_2O + H + OH$	
$CH_3O_2NO_2 + hv \longrightarrow HO_2 + NO_3 + HCHO$	
$CH_3O_2NO_2 + hv \longrightarrow CH_3O_2 + NO_2$	
$CH_3CHO + hv \longrightarrow CH_3O_2 + CO + HO_2$	
$CH_3COOOH + hv \longrightarrow CH_3O_2 + OH + CO_2$	
$C_2H_5OOH + hv \longrightarrow CH_3CHO + HO_2 + OH$	
$PAN + hv \longrightarrow 0.6 \cdot CH_3CO_3 + 0.6 \cdot NO_2 + 0.4 \cdot CH_3O_2 + 0.4 \cdot NO_3 + 0.4 \cdot CO_2$	
$EOOH + hv \longrightarrow EO + OH$	
$GLYOXAL + hv \longrightarrow 2 \cdot CO + 2 \cdot HO_2$	
$GLYALD + hv \longrightarrow 2 \cdot HO_2 + CO + CH_2O$	
$HOCH_2CO_3H + hv \longrightarrow CH_2O + HO_2 + OH + CO_2$	
$HCOCO_2H + hv \longrightarrow 2 \cdot HO_2 + CO + CO_2$	
$HCOCO_3H + hv \longrightarrow CO + HO_2 + OH + CO_2$	
$CH_3COCH_3 + hv \longrightarrow CH_3CO_3 + CH_3O_2$	

Table S1: Tropospheric photolysis reactions (... continued)

reaction	reference
$C_3H_7OOH + hv \longrightarrow 0.82 \cdot CH_3COCH_3 + OH + HO_2 + 0.27 \cdot CH_3CHO$	
$POOH + hv \longrightarrow CH_2O + CH_3CHO + HO_2 + OH$	
$HYAC + hv \longrightarrow CH_3CO_3 + HO_2 + CH_2O$	
$CH_3COCHO + hv \longrightarrow CH_3CO_3 + CO + HO_2$	
$ROOH + hv \longrightarrow CH_2O + CH_3CO_3 + OH$	
$PR_2O_2HNO_3 + hv \longrightarrow 0.83 \cdot HO_2 + 0.83 \cdot NOA + 0.17 \cdot CH_2O + 0.17 \cdot CH_3CHO + OH$	
$NOA + hv \longrightarrow CH_2O + CH_3CO_3 + NO_2$	Müller et al. (2014)
$MEK + hv \longrightarrow C_2H_5O_2 + CH_3CO_3$	
$MEKOOH + hv \longrightarrow CH_3CO_3 + OH + CH_3CHO$	
$MEKNO_3 + hv \longrightarrow CH_3CHO + CH_3CO_3 + NO_2$	Müller et al. (2014)
$MACR + hv \longrightarrow HO_2 + 0.5 \cdot MCO_3 + 0.5 \cdot CH_2O + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO$	
$MACR + hv \longrightarrow HO_2 + 0.5 \cdot MCO_3 + 0.5 \cdot CH_2O + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO$	
$MACROOH + hv \longrightarrow HO_2 + HYAC + OH + CO$	
$MACROH + hv \longrightarrow CO + HYAC + 2 \cdot HO_2 + H_2O$	
$MPAN + hv \longrightarrow MCO_3 + NO_2$	
$MACO_3H + hv \longrightarrow CH_2O + CH_3CO_3 + OH + CO_2$	
$MVK + hv \longrightarrow 0.5 \cdot C_3H_6 + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CH_2O + CO + 0.5 \cdot HO_2$	
$LHMVKABOOH + hv \longrightarrow 0.3 \cdot CH_3COCHO + OH + 0.3 \cdot CH_2O + 0.3 \cdot HO_2 + 0.7 \cdot CH_3CO_3 + 0.7 \cdot GLYALD$	
$MVKN + hv \longrightarrow CH_3CO_3 + GLYALD + NO_2$	Müller et al. (2014)
$MACRN + hv \longrightarrow CO + HYAC + HO_2 + NO_2$	Müller et al. (2014)
$CO_2H_3CHO + hv \longrightarrow CH_3COCHO + CO + 2 \cdot HO_2$	
$CO_2H_3CO_3H + hv \longrightarrow CH_3COCHO + HO_2 + OH + CO_2$	
$BIACETOH + hv \longrightarrow CH_3CO_3 + HOCH_2CO_3$	
$ALKOOH + hv \longrightarrow 0.4 \cdot CH_3CHO + 0.25 \cdot CH_2O + 0.25 \cdot CH_3COCH_3 + HO_2 + 0.8 \cdot MEK + OH$	
$ALKNO_3 + hv \longrightarrow 0.4 \cdot CH_3CHO + 0.25 \cdot CH_2O + 0.25 \cdot CH_3COCH_3 + HO_2 + 0.8 \cdot MEK + NO_2$	
$LISOPACOOH + hv \longrightarrow HO_2 + LHC_4ACCHO + OH$	
$LISOPACNO_3 + hv \longrightarrow HO_2 + LHC_4ACCHO + NO_2$	
$HPALD + hv \longrightarrow LHC_4ACCO_3 + OH$	D. Taraborrelli: $J(MACR)/phi(MACR) = 2. * jmacr\_a/0.004 = 500. * jmacr\_a$
$PACALD + hv \longrightarrow OH + 0.5 \cdot HO_2 + 0.5 \cdot CO + 0.5 \cdot CH_3COCHO + 0.5 \cdot GLYOX + 0.5 \cdot CH_3CO_3$	D. Taraborrelli: average of product yields of C5PACALD 1 and 2 in MCMv3.3.1, 2*J(MACR)/phi(MACR)=2.*jhpald = 1000.*jmacr_a

Table S1: Tropospheric photolysis reactions (... continued)

reaction	reference
$LIECHO + hv \longrightarrow CO + HO_2 + 0.6 \cdot LHMVKABO_2 + 0.4 \cdot MACRO_2$	
$LIECO_3H + hv \longrightarrow 0.6 \cdot LHMVKABO_2 + 0.4 \cdot MACRO_2 + CO_2 + OH$	
$ISOPBOOH + hv \longrightarrow CH_2O + MVK + HO_2 + OH$	
$ISOPBNO_3 + hv \longrightarrow CH_2O + MVK + HO_2 + NO_2$	
$ISOPDOOH + hv \longrightarrow CH_2O + MACR + HO_2 + OH$	
$ISOPDNO_3 + hv \longrightarrow CH_2O + MACR + HO_2 + NO_2$	
$NISOPOOH + hv \longrightarrow HO_2 + NC_4CHO + OH$	
$NC_4CHO + hv \longrightarrow LHC_4ACCO_3 + NO_2$	Müller et al. (2014)
$LNISOOH + hv \longrightarrow NOA + OH + 0.5 \cdot GLYOXAL + 0.5 \cdot CO + HO_2 + 0.5 \cdot CO_2$	
$LHC_4ACCHO + hv \longrightarrow 0.5 \cdot LHC_4ACCO_3 + 0.25 \cdot HYAC + 0.25 \cdot GLYALD + 0.25 \cdot CH_3CO_3 + 0.75 \cdot CO + 1.25 \cdot HO_2$	
$LC_{578}OOH + hv \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot CH_3COCHO + 0.5 \cdot GLYOXAL + 0.5 \cdot GLYALD + HO_2 + OH$	
$LHC_4ACCO_3H + hv \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot GLYALD + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO + 0.5 \cdot HO_2 + OH + CO_2$	
$HCOC_5 + hv \longrightarrow CH_2O + CH_3CO_3 + HOCH_2CO_3$	
$C_{59}OOH + hv \longrightarrow HOCH_2CO_3 + HYAC + NO_2 + OH$	
$LISOPOOHOOH + hv \longrightarrow 0.25 \cdot CH_3COCHO + 0.25 \cdot GLYALD + 0.25 \cdot GLYOXAL + 0.25 \cdot HYAC + 0.25 \cdot CO + 0.25 \cdot MACROH + 0.25 \cdot CH_2O + 0.25 \cdot CO_2H_3CHO + HO_2$	
$LISOPNO_3OOH + hv \longrightarrow HOCH_2CO_3 + HYAC + NO_2 + OH$	
$LISOPNO_3NO_3 + hv \longrightarrow HOCH_2CO_3 + HYAC + NO_2 + NO_2$	
$MBOOOH + hv \longrightarrow HO_2 + OH + 0.67 \cdot GLYALD + 0.67 \cdot CH_3COCH_3 + 0.33 \cdot IBUTALOH + 0.33 \cdot CH_2O$	
$IBUTALOH + hv \longrightarrow 2 \cdot HO_2 + CO + CH_3COCH_3$	
$IBUTALOHOOH + hv \longrightarrow CH_3COCH_3 + OH + CO_2 + HO_2$	
$BEPOMUC + hv \longrightarrow BIGALD_1 + 1.5 \cdot HO_2 + 1.5 \cdot CO$	
$BIGALD_1 + hv \longrightarrow 0.6 \cdot MALO_2 + HO_2$	
$TOLOOH + hv \longrightarrow OH + 0.6 \cdot GLYOXAL + 0.4 \cdot CH_3COCHO + HO_2 + 0.2 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.2 \cdot BIGALD_3$	
$TEPOMUC + hv \longrightarrow 0.5 \cdot CH_3CO_3 + HO_2 + 1.5 \cdot CO$	
$CATEC_1OOH + hv \longrightarrow CATEC_1O + OH$	
$BIGALD_2 + hv \longrightarrow 0.6 \cdot DICARBO_2 + 0.6 \cdot HO_2$	
$BIGALD_3 + hv \longrightarrow 0.6 \cdot CO + 0.6 \cdot HO_2 + 0.6 \cdot MDIALO_2$	
$BIGALD_4 + hv \longrightarrow CO + HO_2 + CH_3COCHO + CH_3CO_3$	
$TERPOOH + hv \longrightarrow 0.4 \cdot CH_2O + 0.05 \cdot CH_3COCH_3 + 0.945 \cdot TERPROD_1 + HO_2 + OH$	

Table S1: Tropospheric photolysis reactions (... continued)

reaction	reference
$TERPROD_1 + hv \longrightarrow CO + HO_2 + TERPROD_2$	
$TERP_2OOH + hv \longrightarrow OH + 0.372 \cdot CH_2O + 0.3 \cdot CH_3COCH_3 + 0.25 \cdot CO + CO_2 + TERPROD_2 + HO_2 + 0.25 \cdot GLYALD$	
$TERPROD_2 + hv \longrightarrow 0.15 \cdot CH_3COCH_2O_2 + 0.68 \cdot CH_2O + 0.8 \cdot CO_2 + 0.5 \cdot CH_3COCH_3 + 1.2 \cdot HO_2 + 1.7 \cdot CO$	
$ISOPBNO_3 + hv \longrightarrow HO_2 + NO_2 + TERPROD_1$	
$NTERPNO_3 + hv \longrightarrow NO_2 + OH + TERPROD_1$	
$ELVOC + hv \longrightarrow HO_2 + OH + TERPROD_2$	

Table S2: Stratospheric photolysis reactions

reaction	reference
$O_2 + hv \longrightarrow O + O_1D$	
$O_2 + hv \longrightarrow 2 \cdot O$	
$H_2O + hv \longrightarrow H + OH$	
$H_2O + hv \longrightarrow H_2 + O_1D$	
$H_2O + hv \longrightarrow 2 \cdot H + O$	
$CL_2 + hv \longrightarrow 2 \cdot CL$	
$CL_2O_2 + hv \longrightarrow 2 \cdot CL$	
$CLO + hv \longrightarrow CL + O$	
$HCL + hv \longrightarrow CL + H$	
$HOCL + hv \longrightarrow CL + OH$	
$CLONO_2 + hv \longrightarrow CL + NO_3$	
$CLONO_2 + hv \longrightarrow CLO + NO_2$	
$OCLO + hv \longrightarrow CLO + O$	
$BRO + hv \longrightarrow BR + O$	
$HBR + hv \longrightarrow BR + H$	
$HOBR + hv \longrightarrow BR + OH$	
$BRONO + hv \longrightarrow BR + NO_2$	50% branching ratio assigned to both possible channels. Cross-sections consistent with Burkholder and Orlando (2000)
$BRONO + hv \longrightarrow BRO + NO$	50% branching ratio assigned to both possible channels. Cross-sections consistent with Burkholder and Orlando (2000)
$BRNO_2 + hv \longrightarrow BR + NO_2$	
$BRONO_2 + hv \longrightarrow BR + NO_3$	

Table S2: Stratospheric photolysis reactions (... continued)

reaction	reference
$BRONO_2 + hv \longrightarrow BRO + NO_2$	
$BR_2 + hv \longrightarrow 2 \cdot BR$	
$BRCL + hv \longrightarrow BR + CL$	
$HF + hv \longrightarrow F + H$	
$SF_6 + hv \longrightarrow$	
$CH_3BR + hv \longrightarrow BR + CH_3O_2$	
$CH_2BR_2 + hv \longrightarrow 2 \cdot BR$	
$CHBR_3 + hv \longrightarrow 3 \cdot BR$	
$CH_3CL + hv \longrightarrow CH_3O_2 + CL$	
$CH_3CCL_3 + hv \longrightarrow 3 \cdot CL$	
$CF_3BR + hv \longrightarrow BR + F + COF_2$	
$CF_2CLBR + hv \longrightarrow BR + CL + COF_2$	
$CCL_4 + hv \longrightarrow 4 \cdot CL + CO_2$	
$CFC_{11} + hv \longrightarrow 2 \cdot CL + COFCL$	
$CFC_{12} + hv \longrightarrow 2 \cdot CL + COF_2$	
$CFC_{113} + hv \longrightarrow 2 \cdot CL + COFCL + COF_2$	
$CFC_{114} + hv \longrightarrow 2 \cdot CL + 2 \cdot COF_2$	
$CFC_{115} + hv \longrightarrow CL + F + 2 \cdot COF_2$	
$HCFC_{22} + hv \longrightarrow CL + COF_2$	
$HCFC_{141}B + hv \longrightarrow CL + COFCL$	
$HCFC_{142}B + hv \longrightarrow CL + COF_2$	
$H_{1202} + hv \longrightarrow 2 \cdot BR + COF_2$	
$H_{2402} + hv \longrightarrow 2 \cdot BR + 2 \cdot COF_2$	
$COF_2 + hv \longrightarrow 2 \cdot F$	
$COFCL + hv \longrightarrow CL + F$	

Table S3: (Tropospheric) O_x reactions

reaction	rate coefficient	reference
$O + O_2 + M \longrightarrow M + O_3$	O_{O_2}	
$O + O_3 \longrightarrow 2 \cdot O_2$	$8.000 \cdot 10^{-12} \exp(-2060./T)$	JPL (2011)
$O + O + M \longrightarrow M + O_2$	O_O	not in JPL (2011)
$O_1D + N_2 \longrightarrow N_2 + O$	$2.150 \cdot 10^{-11} \exp(110./T)$	
$O_1D + O_2 \longrightarrow O + O_2$	$3.135 \cdot 10^{-11} \exp(55./T)$	

Table S3: (Tropospheric) O_x reactions (... continued)

reaction	rate coefficient	reference
$O_1D + O_2 \longrightarrow O + O_2$	$1.650 \cdot 10^{-12}\exp(55./T)$	
$O_1D + H_2O \longrightarrow 2 \cdot OH$	$1.630 \cdot 10^{-10}\exp(60./T)$	JPL (2011)

Table S4: (Tropospheric) HO_x reactions

reaction	rate coefficient	reference
$H + O_2 + M \longrightarrow HO_2 + M$	$ktroe(4.400 \cdot 10^{-32}, 1.3, 7.500 \cdot 10^{-11}, -0.2, 0.6)$	JPL (2011)
$H + O_3 \longrightarrow O_2 + OH$	$1.400 \cdot 10^{-10}\exp(-470./T)$	JPL (2011)
$H + HO_2 \longrightarrow 2 \cdot OH$	$7.200 \cdot 10^{-11}$	JPL (2011)
$H + HO_2 \longrightarrow H_2O + O$	$1.600 \cdot 10^{-12}$	JPL (2011)
$H + HO_2 \longrightarrow H_2 + O_2$	$6.900 \cdot 10^{-12}$	JPL (2011)
$H_2 + O \longrightarrow H + OH$	$1.600 \cdot 10^{-11}\exp(-4570./T)$	
$H_2 + OH \longrightarrow H + H_2O$	$2.800 \cdot 10^{-12}\exp(-1800./T)$	JPL (2011)
$OH + O \longrightarrow H + O_2$	$1.800 \cdot 10^{-11}\exp(180./T)$	JPL (2011)
$OH + OH \longrightarrow H_2O + O$	$1.800 \cdot 10^{-12}$	JPL (2011)
$OH + OH + M \longrightarrow H_2O_2 + M$	$ktroe(6.900 \cdot 10^{-31}, 1., 2.600 \cdot 10^{-11}, 0., 0.6)$	JPL (2011)
$OH + O_3 \longrightarrow HO_2 + O_2$	$1.700 \cdot 10^{-12}\exp(-940./T)$	JPL (2011)
$HO_2 + O \longrightarrow O_2 + OH$	$3.000 \cdot 10^{-11}\exp(200./T)$	JPL (2011)
$HO_2 + OH \longrightarrow H_2O + O_2$	$4.800 \cdot 10^{-11}\exp(250./T)$	JPL (2011)
$HO_2 + O_3 \longrightarrow OH + 2 \cdot O_2$		IUPAC (2004)
$HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$	$HO_2{-}HO_2$	
$H_2O_2 + O \longrightarrow HO_2 + OH$	$1.400 \cdot 10^{-12}\exp(-2000./T)$	JPL (2011)
$H_2O_2 + OH \longrightarrow H_2O + HO_2$	$1.800 \cdot 10^{-12}$	JPL (2011)

Table S5: NO_x reactions

reaction	rate coefficient	reference
$N + OH \longrightarrow H + NO$	$5.000 \cdot 10^{-11}$	
$N + O_2 \longrightarrow NO + O$	$1.500 \cdot 10^{-11}\exp(-3600./T)$	JPL (2011)
$N + NO \longrightarrow N_2 + O$	$2.100 \cdot 10^{-11}\exp(100./T)$	JPL (2011)
$N + NO_2 \longrightarrow 0.5 \cdot N_2O + 0.5 \cdot O + 0.5 \cdot NO + 0.25 \cdot N_2 + 0.25 \cdot O_2$	$5.800 \cdot 10^{-12}\exp(220./T)$	JPL (2011), products: D. Kinnison
$NO + O + M \longrightarrow M + NO_2$	$ktroe(9.000 \cdot 10^{-32}, 1.5, 3.000 \cdot 10^{-11}, 0., 0.6)$	JPL (2011)
$NO + O_3 \longrightarrow NO_2 + O_2$	$3.000 \cdot 10^{-12}\exp(-1500./T)$	JPL (2011)

Table S5: NOx reactions (... continued)

reaction	rate coefficient	reference
$NO + HO_2 \longrightarrow NO_2 + OH$	$3.300 \cdot 10^{-12} \exp(270./T)$	JPL (2011)
$NO_2 + O \longrightarrow NO + O_2$	$5.100 \cdot 10^{-12} \exp(210./T)$	JPL (2011)
$NO_2 + O + M \longrightarrow M + NO_3$	$ktroe(2.500 \cdot 10^{-31}, 1.8, 2.200 \cdot 10^{-11}, 0.7, 0.6)$	JPL (2011)
$NO_2 + O_3 \longrightarrow NO_3 + O_2$	$1.200 \cdot 10^{-13} \exp(-2450./T)$	JPL (2011)
$NO_2 + H \longrightarrow NO + OH$	$4.000 \cdot 10^{-10} \exp(-340./T)$	JPL (2011)
$NO_2 + OH + M \longrightarrow HNO_3 + M$	$ktroe(1.800 \cdot 10^{-30}, 3., 2.800 \cdot 10^{-11}, 0., 0.6)$	JPL (2011)
$NO_3 + O \longrightarrow NO_2 + O_2$	$1.000 \cdot 10^{-11}$	JPL (2011)
$NO_3 + OH \longrightarrow HO_2 + NO_2$	$2.200 \cdot 10^{-11}$	JPL (2011)
$NO_3 + HO_2 \longrightarrow NO_2 + OH + O_2$	$3.500 \cdot 10^{-12}$	JPL (2011)
$NO_3 + NO \longrightarrow 2 \cdot NO_2$	$1.500 \cdot 10^{-11} \exp(170./T)$	JPL (2011)
$HNO_3 + OH \longrightarrow H_2O + NO_3$		$X/(1 + X/(2.7 \cdot 10^{-17} \exp(2199/T))) + 2.4 \cdot 10^{-14} \exp(460/T)$; $X = M6.5 \cdot 10^{-34} \exp(1335/T)$ - JPL (2011)
$NO + OH \longrightarrow HONO$	$ktroe(7.000 \cdot 10^{-31}, 2.6, 3.600 \cdot 10^{-11}, 0.1, 0.6)$	JPL (2011)
$HONO + OH \longrightarrow H_2O + NO_2$	$1.800 \cdot 10^{-11} \exp(-390./T)$	JPL (2011)
$NO_2 + HO_2 + M \longrightarrow HO_2NO_2 + M$	$ktroe(2.000 \cdot 10^{-31}, 3.4, 2.900 \cdot 10^{-12}, 1.1, 0.6)$	JPL (2011)
$HO_2NO_2 + OH \longrightarrow H_2O + NO_2 + O_2$	$1.300 \cdot 10^{-12} \exp(380./T)$	JPL (2011)
$HO_2NO_2 + M \longrightarrow HO_2 + NO_2 + M$		$[NO_2{-}NO_3] * \exp(-10900./T)/2.1 \cdot 10^{-27}$ JPL (2011)
$NO_2 + NO_3 + M \longrightarrow M + N_2O_5$	$ktroe(2.000 \cdot 10^{-30}, 4.4, 1.400 \cdot 10^{-12}, 0.7, 0.6)$	JPL (2011)
$N_2O_5 + M \longrightarrow NO_2 + NO_3 + M$	$kN2O5$	$[NO_2{-}NO_3] * \exp(-11000/T)/2.7 \cdot 10^{-27}$ JPL (2011)
$NH_3 + OH \longrightarrow$	$1.700 \cdot 10^{-12} \exp(-710./T)$	JPL (2011)

Table S6: C1 oxidation

reaction	rate coefficient	reference
$CO + OH \longrightarrow CO_2 + H$	$kactiv(1.5 \cdot 10^{-13}, -0.6, 2.1 \cdot 10^{9}, -6.1)$	JPL (2011)
$CO + OH + M \longrightarrow CO_2 + HO_2 + M$	$ktroe(5.900 \cdot 10^{-33}, 1.4, 1.100 \cdot 10^{-12}, -1.3, 0.6)$	
$CH_4 + OH \longrightarrow CH_3O_2 + H_2O$	$2.450 \cdot 10^{-12} \exp(-1775./T)$	JPL (2011)
$CH_3OH + OH \longrightarrow CH_2O + HO_2 + H_2O$	$2.900 \cdot 10^{-12} \exp(-345./T)$	JPL (2011)
$CH_3O_2 + NO \longrightarrow CH_2O + NO_2 + HO_2$	$1.960 \cdot 10^{-12} \exp(403./T)$	Orlando and Tyndall (2012)
$CH_3O_2 + HO_2 \longrightarrow CH_3OOH + O_2$	$3.800 \cdot 10^{-13} \exp(730./T)$	Orlando and Tyndall (2012)
$CH_3O_2 + CH_3O_2 \longrightarrow 2 \cdot CH_2O + 2 \cdot HO_2$	$7.400 \cdot 10^{-13} \exp(-520./T)$	IUPAC (2006)

Table S6: C1 oxidation (... continued)

reaction	rate coefficient	reference
$CH_3O_2 + CH_3O_2 \longrightarrow CH_2O + CH_3OH$	$2.330 \cdot 10^{-14} \exp(678./T)$	own fit for $T = 240 - 300$K
$CH_2O + O \longrightarrow HO_2 + OH + CO$	$3.400 \cdot 10^{-11} \exp(-1600./T)$	JPL (2011)
$CH_2O + OH \longrightarrow CO + H_2O + H$	$5.500 \cdot 10^{-12} \exp(125./T)$	JPL (2011)
$CH_2O + HO_2 \longrightarrow HOCH_2OO$	$9.700 \cdot 10^{-15} \exp(625./T)$	IUPAC (2006)
$CH_2O + NO_3 \longrightarrow CO + HO_2 + HNO_3$	$6.000 \cdot 10^{-13} \exp(-2058./T)$	
$CH_3OOH + OH \longrightarrow 0.7 \cdot CH_3O_2 + 0.3 \cdot OH + 0.3 \cdot CH_2O + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	JPL (2011)
$HCOOH + OH \longrightarrow CO_2 + HO_2 + H_2O$	$4.000 \cdot 10^{-13}$	JPL (2011)
$HOCH_2OO \longrightarrow CH_2O + HO_2$	$2.400 \cdot 10^{12} \exp(-7000./T)$	Lamarque et al. (2012)
$HOCH_2OO + NO \longrightarrow HCOOH + NO_2 + HO_2$	$2.600 \cdot 10^{-12} \exp(265./T)$	Lamarque et al. (2012)
$HOCH_2OO + HO_2 \longrightarrow H_2O + HCOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	Lamarque et al. (2012)
$HCN + OH \longrightarrow CO + NO + H_2O$	$1.200 \cdot 10^{-13} \exp(-400./T)$	JPL (2011), products: Tyndall
$CH_3O_2 + NO_2 + M \longrightarrow CH_3O_2NO_2 + M$	$ktroe(1.000 \cdot 10^{-30}, 4.8, 7.200 \cdot 10^{-12}, 2.1, 0.6)$	JPL (2011)
$CH_3O_2NO_2 + M \longrightarrow CH_3O_2 + NO_2 + M$		

Table S7: C2 oxidation

reaction	rate coefficient	reference
$C_2H_2 + OH + M \longrightarrow 0.65 \cdot GLYOXAL + 0.65 \cdot OH + 0.35 \cdot HCOOH + 0.35 \cdot HO_2 + 0.35 \cdot CO + M$	$ktroe(5.500 \cdot 10^{-30}, 0., 8.300 \cdot 10^{-13}, -2., 0.6)$	JPL (2011)
$C_2H_4 + OH + M \longrightarrow EO_2 + M$	$ktroe(1.000 \cdot 10^{-28}, 4.5, 7.500 \cdot 10^{-12}, 0.85, 0.6)$	JPL (2011)
$C_2H_4 + O_3 \longrightarrow CH_2O + 0.65 \cdot CO + 0.15 \cdot OH + 0.15 \cdot HO_2 + 0.5 \cdot H_2O + 0.35 \cdot HCOOH$	$9.100 \cdot 10^{-15} \exp(-2580./T)$	IUPAC (2006)
$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	$7.660 \cdot 10^{-12} \exp(-1020./T)$	JPL (2011)
$C_2H_5OH + OH \longrightarrow CH_3CHO + HO_2 + H_2O$	$3.350 \cdot 10^{-12} \exp(0./T)$	JPL (2011)
$CH_3CHO + OH \longrightarrow CH_3CO_3 + H_2O$	$4.630 \cdot 10^{-12} \exp(350./T)$	JPL (2011)
$CH_3CHO + NO_3 \longrightarrow CH_3CO_3 + HNO_3$	$1.400 \cdot 10^{-12} \exp(-1900./T)$	JPL (2011)
$CH_3COOOH + OH \longrightarrow 0.5 \cdot CH_3CO_3 + H_2O + 0.5 \cdot CH_2O + 0.5 \cdot CO_2 + 0.5 \cdot OH$	$1.000 \cdot 10^{-12}$	Orlando (p.c.) added OH
$C_2H_5O_2 + NO \longrightarrow CH_3CHO + HO_2 + NO_2$	$2.620 \cdot 10^{-12} \exp(373./T)$	Orlando and Tyndall (2012)
$C_2H_5O_2 + HO_2 \longrightarrow C_2H_5OOH + O_2$	$7.400 \cdot 10^{-13} \exp(700./T)$	Orlando and Tyndall (2012)
$C_2H_5O_2 + CH_3O_2 \longrightarrow 0.7 \cdot CH_2O + 0.8 \cdot CH_3CHO + HO_2 + 0.3 \cdot CH_3OH + 0.2 \cdot C_2H_5OH$	$2.000 \cdot 10^{-13}$	Orlando (p.c.), products: Tyndall (p.c.)
$C_2H_5O_2 + CH_3CO_3 \longrightarrow CH_3CHO + HO_2 + CH_3O_2 + CO_2$	$1.800 \cdot 10^{-12} \exp(500./T)$	10% lower than $CH_3O_2 + CH_3CO_3$; Orlando and Tyndall (2012) only give k@298K

Table S7: C2 oxidation (... continued)

reaction	rate coefficient	reference
$C_2H_5O_2 + C_2H_5O_2 \longrightarrow 1.6 \cdot CH_3CHO + 1.2 \cdot HO_2 + 0.4 \cdot C_2H_5OH$	$7.600 \cdot 10^{-14}$	Orlando and Tyndall (2012)
$C_2H_5OOH + OH \longrightarrow 0.5 \cdot C_2H_5O_2 + 0.5 \cdot CH_3CHO + 0.5 \cdot OH + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	no data, analog to CH_3OOH^+OH
$CH_3CO_3 + NO \longrightarrow CH_3O_2 + CO_2 + NO_2$	$7.500 \cdot 10^{-12} \exp(290./T)$	Orlando and Tyndall (2012)
$CH_3CO_3 + NO_2 + M \longrightarrow M + PAN$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	
$CH_3CO_3 + HO_2 \longrightarrow 0.4 \cdot CH_3COOOH + 0.2 \cdot CH_3COOH + 0.2 \cdot O_3 + 0.4 \cdot CH_3O_2 + 0.4 \cdot OH + 0.4 \cdot CO_2$	$5.200 \cdot 10^{-13} \exp(980./T)$	Orlando and Tyndall (2012)
$CH_3CO_3 + CH_3O_2 \longrightarrow CH_2O + 0.9 \cdot CH_3O_2 + 0.9 \cdot HO_2 + 0.9 \cdot CO_2 + 0.1 \cdot CH_3COOH$	$2.000 \cdot 10^{-12} \exp(500./T)$	Orlando and Tyndall (2012)
$CH_3CO_3 + CH_3CO_3 \longrightarrow 2 \cdot CH_3O_2 + 2 \cdot CO_2$	$2.900 \cdot 10^{-12} \exp(500./T)$	Orlando and Tyndall (2012)
$CH_3COOH + OH \longrightarrow CH_3O_2 + CO_2 + H_2O$	$3.150 \cdot 10^{-14} \exp(920./T)$	JPL (2011)
$PAN + M \longrightarrow CH_3CO_3 + NO_2 + M$		
$PAN + OH \longrightarrow CH_2O + CO_2 + NO_3$	$4.000 \cdot 10^{-14}$	JPL (2011), includes implicit $NO \longrightarrow NO_2$ conversion
$EO_2 + NO \longrightarrow 0.75 \cdot EO + NO_2 + 0.5 \cdot CH_2O + 0.25 \cdot HO_2$	$4.200 \cdot 10^{-12} \exp(180./T)$	Lamarque et al. (2012)
$EO_2 + HO_2 \longrightarrow EOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$EO_2 + CH_3O_2 \longrightarrow 0.5 \cdot EO + 0.5 \cdot O_2 + 0.5 \cdot CH_2O + 0.5 \cdot HO_2 + 0.5 \cdot CH_3OH + 0.5 \cdot GLYALD$	$4.000 \cdot 10^{-12} \exp(1000./T)$	Tyndall (p.c.)
$EO_2 + CH_3CO_3 \longrightarrow CH_3O_2 + EO + CO_2$	$1.000 \cdot 10^{-11}$	
$EO + O_2 \longrightarrow GLYALD + HO_2$	$1.000 \cdot 10^{-14}$	Lamarque et al. (2012)
$EO \longrightarrow 2 \cdot CH_2O + HO_2$	$1.600 \cdot 10^{11} \exp(-4150./T)$	Lamarque et al. (2012)
$GLYOXAL + OH \longrightarrow 0.6 \cdot HO_2 + 1.2 \cdot CO + H_2O + 0.4 \cdot HCOCO_3$	$3.100 \cdot 10^{-12} \exp(340./T)$	MCM3.2
$GLYOXAL + NO_3 \longrightarrow 0.6 \cdot HO_2 + 1.2 \cdot CO + 0.4 \cdot HCOCO_3 + HNO_3$	$2.500 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$GLYALD + OH \longrightarrow 0.2 \cdot GLYOXAL + 0.2 \cdot HO_2 + 0.8 \cdot HOCH_2CO_3 + H_2O$	$1.000 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$GLYALD + NO_3 \longrightarrow HNO_3 + HOCH_2CO_3$	$1.440 \cdot 10^{-12} \exp(-1862./T)$	Taraborrelli et al. (2009)
$HOCH_2CO_3 + NO_2 + M \longrightarrow CH_2O + CO_2 + HNO_3 + M$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	Orlando and Tyndall (2012)
$HOCH_2CO_3 + HO_2 \longrightarrow 0.4 \cdot HOCH_2CO_3H + 0.2 \cdot HOCH_2CO_2H + 0.2 \cdot O_3 + 0.4 \cdot CO_2 + 0.4 \cdot OH + 0.4 \cdot HO_2 + 0.4 \cdot CH_2O$	$4.300 \cdot 10^{-13} \exp(1040./T)$	Orlando (p.c.)
$HOCH_2CO_3 + CH_3O_2 \longrightarrow 2 \cdot CH_2O + CO_2 + 2 \cdot HO_2$	$1.000 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$HOCH_2CO_3 + CH_3CO_3 \longrightarrow CH_3O_2 + 2 \cdot CO_2 + HO_2 + CH_2O$	$1.000 \cdot 10^{-11}$	Taraborrelli et al. (2009)

Table S7: C2 oxidation (... continued)

reaction	rate coefficient	reference
$HOCH_2CO_3 + NO \longrightarrow HO_2 + NO_2 + CH_2O + CO_2$	$8.100 \cdot 10^{-12} \exp(270./T)$	Taraborrelli et al. (2009)
$HOCH_2CO_3 + NO_3 \longrightarrow HO_2 + NO_2 + CH_2O + CO_2$	$4.000 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$HOCH_2CO_2H + OH \longrightarrow CH_2O + HO_2 + CO_2 + H_2O$	$2.730 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$HOCH_2CO_3H + OH \longrightarrow H_2O + HOCH_2CO_3$	$6.190 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$HCOCO_3 + CH_3O_2 \longrightarrow CO + 2 \cdot HO_2 + CO_2 + CH_2O$	$1.000 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$HCOCO_3 + CH_3CO_3 \longrightarrow CO + HO_2 + CH_3O_2 + 2 \cdot CO_2$	$1.000 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$HCOCO_3 + HO_2 \longrightarrow 0.7 \cdot HCOCO_3H + 0.7 \cdot O_2 + 0.3 \cdot HCOCO_2H + 0.3 \cdot O_3$	$4.300 \cdot 10^{-13} \exp(1040./T)$	Taraborrelli et al. (2009)
$HCOCO_3 + NO \longrightarrow CO + HO_2 + NO_2 + CO_2$	$8.100 \cdot 10^{-12} \exp(270./T)$	Taraborrelli et al. (2009)
$HCOCO_3 + NO_3 \longrightarrow CO + HO_2 + NO_2 + CO_2$	$4.000 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$HCOCO_2H + OH \longrightarrow CO + HO_2 + CO_2 + H_2O$	$1.230 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$HCOCO_3H + OH \longrightarrow H_2O + HCOCO_3$	$1.580 \cdot 10^{-11}$	Taraborrelli et al. (2009)
$CH_3CN + OH \longrightarrow CH_2O + H_2O + CO + NO_2$	$7.800 \cdot 10^{-13} \exp(-1050./T)$	products: Tyndall

Table S8: C3 oxidation

reaction	rate coefficient	reference
$C_3H_6 + OH + M \longrightarrow M + PO_2$	$ktroe(8.000 \cdot 10^{-27}, 3.5, 3.000 \cdot 10^{-11}, 0., 0.5)$	IUPAC (2006)
$C_3H_6 + O_3 \longrightarrow 0.28 \cdot CH_3O_2 + 0.1 \cdot CH_4 + 0.075 \cdot CH_3COOH + 0.56 \cdot CO + 0.075 \cdot HCOOH + 0.09 \cdot H_2O_2 + 0.28 \cdot HO_2 + 0.2 \cdot CO_2 + 0.545 \cdot CH_3CHO + 0.545 \cdot CH_2O + 0.36 \cdot OH$	$5.500 \cdot 10^{-15} \exp(-1880./T)$	IUPAC (2006)
$C_3H_6 + NO_3 \longrightarrow PRONO_3BO_2$	$4.600 \cdot 10^{-13} \exp(-1156./T)$	IUPAC (2006)
$C_3H_8 + OH \longrightarrow C_3H_7O_2 + H_2O$	$7.600 \cdot 10^{-12} \exp(-585./T)$	IUPAC (2006)
$CH_3COCH_3 + OH \longrightarrow CH_3COCH_2O_2 + H_2O$	$CH_3COCH_3 - OH$	
$C_3H_7O_2 + NO \longrightarrow 0.82 \cdot CH_3COCH_3 + NO_2 + HO_2 + 0.27 \cdot CH_3CHO$	$2.900 \cdot 10^{-12} \exp(350./T)$	Orlando and Tyndall (2012)
$C_3H_7O_2 + HO_2 \longrightarrow C_3H_7OOH + O_2$	$7.500 \cdot 10^{-13} \exp(700./T)$	Lamarque et al. (2012)
$C_3H_7O_2 + CH_3O_2 \longrightarrow CH_2O + 2 \cdot HO_2 + 0.82 \cdot CH_3COCH_3 + 0.27 \cdot CH_3CHO$	$3.750 \cdot 10^{-13} \exp(-40./T)$	Lamarque et al. (2012)
$C_3H_7O_2 + CH_3CO_3 \longrightarrow 0.82 \cdot CH_3COCH_3 + HO_2 + 0.27 \cdot CH_3CHO + CO_2 + CH_3O_2$	$1.000 \cdot 10^{-11}$	Lamarque et al. (2012)
$C_3H_7OOH + OH \longrightarrow 0.41 \cdot CH_3COCH_3 + 0.5 \cdot OH + 0.5 \cdot C_3H_7O_2 + 0.5 \cdot H_2O + 0.135 \cdot CH_3CHO$	$3.800 \cdot 10^{-12} \exp(200./T)$	Lamarque et al. (2012); $1.5 \cdot CH_3CHO$ as surrogate for propanal
$PO_2 + NO \longrightarrow CH_2O + CH_3CHO + HO_2 + NO_2$	$4.200 \cdot 10^{-12} \exp(180./T)$	Lamarque et al. (2012)

Table S8: C3 oxidation (... continued)

reaction	rate coefficient	reference
$PO_2 + NO_3 \longrightarrow CH_2O + CH_3CHO + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$PO_2 + HO_2 \longrightarrow O_2 + POOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	Lamarque et al. (2012)
$PO_2 + CH_3O_2 \longrightarrow 0.5 \cdot CH_3CHO + 1.25 \cdot CH_2O + HO_2 + 0.5 \cdot HYAC + 0.25 \cdot CH_3OH$	$8.300 \cdot 10^{-13}$	products: Tyndall (p.c.)
$PO_2 + CH_3CO_3 \longrightarrow CH_2O + CH_3CHO + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$POOH + OH \longrightarrow 0.5 \cdot PO_2 + 0.5 \cdot HYAC + 0.5 \cdot OH + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	Lamarque et al. (2012)
$HYAC + OH \longrightarrow CH_3COCHO + HO_2 + H_2O$	$3.000 \cdot 10^{-12}$	IUPAC (2006)
$CH_3COCHO + OH \longrightarrow CH_3CO_3 + CO + H_2O$	$8.400 \cdot 10^{-13} \exp(830./T)$	Lamarque et al. (2012)
$CH_3COCHO + NO_3 \longrightarrow CO + HNO_3 + CH_3CO_3$	$1.400 \cdot 10^{-12} \exp(-1860./T)$	Lamarque et al. (2012)
$CH_3COCH_2O_2 + NO \longrightarrow CH_2O + CH_3CO_3 + NO_2$	$2.900 \cdot 10^{-12} \exp(300./T)$	Lamarque et al. (2012)
$CH_3COCH_2O_2 + HO_2 \longrightarrow 0.85 \cdot O_2 + 0.85 \cdot ROOH + 0.15 \cdot CH_2O + 0.15 \cdot CH_3CO_3 + 0.15 \cdot OH + 0.15 \cdot H_2O$	$8.600 \cdot 10^{-13} \exp(700./T)$	Lamarque et al. (2012) + MCM3.2
$CH_3COCH_2O_2 + CH_3O_2 \longrightarrow 0.3 \cdot CH_3CO_3 + 0.8 \cdot CH_2O + 0.3 \cdot HO_2 + 0.2 \cdot HYAC + 0.5 \cdot CH_3COCHO + 0.5 \cdot CH_3OH$	$7.100 \cdot 10^{-13} \exp(500./T)$	Lamarque et al. (2012)
$CH_3COCH_2O_2 + CH_3CO_3 \longrightarrow CH_2O + CH_3CO_3 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$ROOH + OH \longrightarrow CH_3COCH_2O_2 + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	Lamarque et al. (2012)
$PRONO_3BO_2 + NO \longrightarrow 0.83 \cdot HO_2 + 0.83 \cdot NOA + 0.17 \cdot CH_2O + 0.17 \cdot CH_3CHO + 1.17 \cdot NO_2$	$2.540 \cdot 10^{-12} \exp(360./T)$	Taraborrelli et al. (2009)
$PRONO_3BO_2 + NO_3 \longrightarrow 0.83 \cdot HO_2 + 0.83 \cdot NOA + 0.17 \cdot CH_2O + 0.17 \cdot CH_3CHO + 1.17 \cdot NO_2$	$2.500 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$PRONO_3BO_2 + HO_2 \longrightarrow PR_2O_2HNO_3$	$1.320 \cdot 10^{-12} \exp(360./T)$	Taraborrelli et al. (2009)
$PRONO_3BO_2 + CH_3O_2 \longrightarrow 0.915 \cdot HO_2 + 0.915 \cdot NOA + 0.835 \cdot CH_2O + 0.085 \cdot CH_3CHO + 0.25 \cdot CH_3OH$	$1.000 \cdot 10^{-12}$	
$PRONO_3BO_2 + CH_3CO_3 \longrightarrow 0.83 \cdot HO_2 + 0.83 \cdot NOA + 0.17 \cdot CH_2O + 0.17 \cdot CH_3CHO + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$PR_2O_2HNO_3 + OH \longrightarrow 0.5 \cdot PRONO_3BO_2 + 0.5 \cdot NOA + 0.5 \cdot OH + H_2O$	$7.000 \cdot 10^{-12}$	Taraborrelli et al. (2009)
$NOA + OH \longrightarrow CH_3COCHO + NO_2 + H_2O$	$1.300 \cdot 10^{-13}$	Taraborrelli et al. (2009)

Table S9: C4 oxidation

reaction	rate coefficient	reference
$BIGENE + OH \longrightarrow ENEO_2$	$5.400 \cdot 10^{-11}$	Lamarque et al. (2012)

Table S9: C4 oxidation (... continued)

reaction	rate coefficient	reference
$MEK + OH \longrightarrow H_2O + MEKO_2$	$2.300 \cdot 10^{-12} \exp(-170./T)$	Lamarque et al. (2012)
$MEKO_2 + NO \longrightarrow CH_3CHO + CH_3CO_3 + NO_2$	$4.032 \cdot 10^{-12} \exp(180./T)$	treated like $MEKBO_2$ from MCM3.2; $A = 4.200 \cdot 10^{-12} \cdot 0.96$; 4% nitrate yield as for MVKN
$MEKO_2 + NO \longrightarrow MEKNO_3$	$1.680 \cdot 10^{-13} \exp(180./T)$	$A = 4.200 \cdot 10^{-12} \cdot 0.04$; 4% nitrate yield as for MVKN
$MEKO_2 + HO_2 \longrightarrow MEKOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	Lamarque et al. (2012)
$MEKO_2 + CH_3O_2 \longrightarrow 0.3 \cdot CH_3CHO + 0.3 \cdot CH_3CO_3 + CH_2O + 0.3 \cdot HO_2 + 0.3 \cdot O_2 + 0.5 \cdot BIACETOH + 0.5 \cdot CH_3OH + 0.266 \cdot HYAC$	$1.000 \cdot 10^{-12}$	Tyndall (p.c.) added CH_2O to first and third channel
$MEKO_2 + CH_3CO_3 \longrightarrow CH_3CHO + CH_3CO_3 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$MEKOOH + OH \longrightarrow H_2O + MEKO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	Lamarque et al. (2012)
$ENEO_2 + NO \longrightarrow CH_3CHO + 0.5 \cdot CH_2O + 0.5 \cdot CH_3COCH_3 + HO_2 + NO_2$	$4.200 \cdot 10^{-12} \exp(180./T)$	Lamarque et al. (2012)
$ENEO_2 + HO_2 \longrightarrow 1.333 \cdot POOH + O_2$	$7.500 \cdot 10^{-13} \exp(700./T)$	factor 4/3 to preserve carbon
$ENEO_2 + CH_3O_2 \longrightarrow 0.665 \cdot HYAC + 0.5 \cdot CH_3OH + 0.5 \cdot CH_3CHO + 0.25 \cdot CH_3COCH_3 + 0.75 \cdot CH_2O + HO_2$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$ENEO_2 + CH_3CO_3 \longrightarrow CH_3CHO + 0.5 \cdot CH_2O + 0.5 \cdot CH_3COCH_3 + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$MACR + OH \longrightarrow 0.45 \cdot MCO_3 + 0.55 \cdot MACRO_2$	$1.860 \cdot 10^{-11} \exp(175./T)$	Tnydall (p.c.)
$MACR + O_3 \longrightarrow 0.59 \cdot CH_3COCHO + 0.41 \cdot CH_3CO_3 + 0.82 \cdot CO + 0.41 \cdot HO_2 + 0.82 \cdot OH + 0.033750 \cdot HCOOH + 0.556250 \cdot CH_2O + 0.123750 \cdot H_2O_2$	$1.360 \cdot 10^{-15} \exp(-2112./T)$	
$MACR + NO_3 \longrightarrow HNO_3 + MCO_3$	$2.880 \cdot 10^{-12} \exp(-1862./T)$	
$MCO_3 + CH_3O_2 \longrightarrow 0.315 \cdot CH_3CO_3 + 0.585 \cdot CH_3O_2 + 0.585 \cdot CO + 1.9 \cdot CH_2O + 0.9 \cdot CO_2 + 0.9 \cdot HO_2 + 0.1 \cdot MACO_2H$	$1.000 \cdot 10^{-11}$	MCO_3 is an acyl radical, therefore $kRO_2CH_3CO_3$
$MCO_3 + CH_3CO_3 \longrightarrow CH_2O + 0.35 \cdot CH_3CO_3 + 1.65 \cdot CH_3O_2 + 0.65 \cdot CO + 2 \cdot CO_2$	$1.000 \cdot 10^{-11}$	
$MCO_3 + HO_2 \longrightarrow 0.44 \cdot OH + 0.154 \cdot CH_3CO_3 + 0.286 \cdot CH_3O_2 + 0.286 \cdot CO + 0.44 \cdot CH_2O + 0.44 \cdot CO_2 + 0.15 \cdot MACO_2H + 0.15 \cdot O_3 + 0.41 \cdot MACO_3H + 0.41 \cdot O_2$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$MCO_3 + NO \longrightarrow CH_2O + 0.35 \cdot CH_3CO_3 + 0.65 \cdot CH_3O_2 + 0.65 \cdot CO + NO_2 + CO_2$	$8.700 \cdot 10^{-12} \exp(290./T)$	
$MCO_3 + NO_3 \longrightarrow CH_2O + 0.35 \cdot CH_3CO_3 + 0.65 \cdot CH_3O_2 + 0.65 \cdot CO + NO_2 + CO_2$	$4.000 \cdot 10^{-12}$	

Table S9: C4 oxidation (... continued)

reaction	rate coefficient	reference
$MCO_3 + NO_2 + M \longrightarrow M + MPAN$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.3)$	
$MACRO_2 + CH_3O_2 \longrightarrow 0.75 \cdot CO + 0.75 \cdot HYAC + CH_2O + 1.5 \cdot HO_2 + 0.25 \cdot MACROH + 0.25 \cdot O_2$	$9.200 \cdot 10^{-14}$	products: Tyndall (p.c.)
$MACRO_2 + CH_3CO_3 \longrightarrow 0.85 \cdot CO + 0.85 \cdot HYAC + 0.15 \cdot CH_2O + 0.15 \cdot CH_3COCHO + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$MACRO_2 + NO \longrightarrow NO_2 + 0.85 \cdot CO + 0.85 \cdot HYAC + HO_2 + 0.15 \cdot CH_2O + 0.15 \cdot CH_3COCHO$	$2.464 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.97$; 3% MACRN-yield inferred from HYAC 42% yield at high-NO from Crounse et al. (2011) (Tyndall, p.c.)
$MACRO_2 + NO \longrightarrow MACRN$	$7.620 \cdot 10^{-14} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.03$; 3% MACRN-yield inferred from HYAC 42% yield at high-NO from Crounse et al. (2011) (Tyndall, p.c.)
$MACRO_2 + NO_3 \longrightarrow 0.85 \cdot CO + 0.85 \cdot HYAC + 0.15 \cdot CH_2O + 0.15 \cdot CH_3COCHO + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	
$MACRO_2 + HO_2 \longrightarrow 0.6 \cdot MACROOH + 0.4 \cdot CO + 0.4 \cdot HYAC + 0.4 \cdot HO_2 + 0.4 \cdot OH$	$1.820 \cdot 10^{-13} \exp(1300./T)$	
$MACRO_2 \longrightarrow CO + HYAC + OH$	$2.900 \cdot 10^{7} \exp(-5297./T)$	Isomerisation according to Crounse et al. (2012)
$MACROOH + OH \longrightarrow CO + HYAC + OH + H_2O$	$1.800 \cdot 10^{-11}$	
$MACROH + OH \longrightarrow CO_2 + HYAC + HO_2 + H_2O$	$1.800 \cdot 10^{-11}$	
$MPAN + M \longrightarrow MCO_3 + NO_2 + M$		
$MPAN + OH \longrightarrow CO + HYAC + NO_2$	$3.200 \cdot 10^{-11}$	rate: Orlando et al. (2002)
$MACO_2H + OH \longrightarrow CH_2O + CH_3CO_3 + CO_2 + H_2O$	$1.510 \cdot 10^{-11}$	products should be pyruvic acid + CH_2O + HO_2
$MACO_3H + OH \longrightarrow H_2O + MCO_3$	$1.870 \cdot 10^{-11}$	
$MVK + OH \longrightarrow LHMVKABO_2$	$4.130 \cdot 10^{-12} \exp(452./T)$	
$MVK + O_3 \longrightarrow 0.85 \cdot CH_3COCHO + 0.85 \cdot HCOOH + 0.15 \cdot CH_3CO_3 + 0.15 \cdot OH + 0.15 \cdot CO + 0.15 \cdot CH_2O$	$7.510 \cdot 10^{-16} \exp(-1521./T)$	products according to IUPAC (2006)
$LHMVKABO_2 + CH_3O_2 \longrightarrow 0.9 \cdot CH_2O + 0.35 \cdot GLYALD + 0.65 \cdot HO_2 + 0.35 \cdot CH_3CO_3 + 0.175 \cdot BIACETOH + 0.25 \cdot CH_3OH + 0.25 \cdot MACROH + 0.15 \cdot CH_3COCHO + 0.075 \cdot CO_2H_3CHO$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$LHMVKABO_2 + CH_3CO_3 \longrightarrow 0.3 \cdot CH_3COCHO + 0.7 \cdot GLYALD + 0.7 \cdot CH_3CO_3 + 0.3 \cdot CH_2O + 0.3 \cdot HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	

Table S9: C4 oxidation (... continued)

reaction	rate coefficient	reference
$LHMVKABO_2 + HO_2 \longrightarrow 0.34 \cdot LHMVKABOOH + 0.66 \cdot CH_3CO_3 + 0.66 \cdot OH + 0.66 \cdot GLYALD$	$1.820 \cdot 10^{-13} \exp(1300./T)$	Praske et al. (2015)
$LHMVKABO_2 + NO \longrightarrow NO_2 + 0.3 \cdot CH_2O + 0.3 \cdot CH_3COCHO + 0.3 \cdot HO_2 + 0.7 \cdot CH_3CO_3 + 0.7 \cdot GLYALD$	$2.438 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.96$; 4% nitrate yield Praske et al. (2015)
$LHMVKABO_2 + NO \longrightarrow MVKN$	$1.020 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.04$; 4% nitrate yield Praske et al. (2015)
$LHMVKABO_2 + NO_3 \longrightarrow 0.3 \cdot CH_3COCHO + 0.7 \cdot GLYALD + 0.7 \cdot CH_3CO_3 + 0.3 \cdot CH_2O + 0.3 \cdot HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	
$MVKN + OH \longrightarrow CH_3COCHO + HO_2 + CO_2 + NO_2 + H_2O$	$5.600 \cdot 10^{-12}$	k from Paulot et al. (2009); simplified products
$MACRN + OH \longrightarrow CO_2 + HYAC + NO_2 + H_2O$	$5.000 \cdot 10^{-11}$	k from Paulot et al. (2009); simplified products
$LHMVKABOOH + OH \longrightarrow 0.3 \cdot CO_2H_3CHO + OH + H_2O + 0.7 \cdot BIACETOH$	$4.500 \cdot 10^{-12}$	
$CO_2H_3CHO + OH \longrightarrow CO_2H_3CO_3 + H_2O$	$2.450 \cdot 10^{-11}$	
$CO_2H_3CHO + NO_3 \longrightarrow CO_2H_3CO_3 + HNO_3$	$5.760 \cdot 10^{-12} \exp(-1862./T)$	
$CO_2H_3CO_3 + CH_3O_2 \longrightarrow CH_3COCHO + 2 \cdot HO_2 + CO_2 + CH_2O$	$1.000 \cdot 10^{-11}$	products: Tyndall (p.c.)
$CO_2H_3CO_3 + CH_3CO_3 \longrightarrow CH_3COCHO + HO_2 + CH_3O_2 + 2 \cdot CO_2$	$1.000 \cdot 10^{-11}$	
$CO_2H_3CO_3 + HO_2 \longrightarrow 0.6 \cdot CO_2H_3CO_3H + 0.4 \cdot CO_2 + 0.4 \cdot OH + 0.4 \cdot HO_2 + 0.4 \cdot CH_3COCHO$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$CO_2H_3CO_3 + NO \longrightarrow CH_3COCHO + HO_2 + NO_2 + CO_2$	$8.100 \cdot 10^{-12} \exp(270./T)$	
$CO_2H_3CO_3 + NO_3 \longrightarrow CH_3COCHO + HO_2 + NO_2 + CO_2$	$4.000 \cdot 10^{-12}$	
$CO_2H_3CO_3H + OH \longrightarrow CO_2H_3CO_3 + H_2O$	$1.000 \cdot 10^{-12}$	Orlando (p.c.)
$MALO_2 + NO_2 + M \longrightarrow 0.8 \cdot LC_5PAN_{1719} + M$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	Orlando and Tyndall (2012) - Same as $k(CH_3CO_3 + NO_2)$; LC_5PAN as a surrogate
$MALO_2 + NO \longrightarrow 0.4 \cdot GLYOXAL + HO_2 + 0.4 \cdot CO + 0.4 \cdot CO_2 + NO_2 + 0.6 \cdot CO_2H_3CHO$	$7.500 \cdot 10^{-12} \exp(290./T)$	products: Tyndall (p.c.)
$MALO_2 + HO_2 \longrightarrow 0.16 \cdot GLYOXAL + HO_2 + 0.16 \cdot CO + 0.16 \cdot CO_2 + 0.16 \cdot OH + 0.84 \cdot CO_2H_3CHO$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$MALO_2 + CH_3O_2 \longrightarrow 0.4 \cdot GLYOXAL + 2 \cdot HO_2 + 0.4 \cdot CO + 0.4 \cdot CO_2 + 0.6 \cdot CO_2H_3CHO + CH_2O$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$MALO_2 + CH_3CO_3 \longrightarrow 0.4 \cdot GLYOXAL + HO_2 + 0.4 \cdot CO + 1.4 \cdot CO_2 + 0.6 \cdot CO_2H_3CHO + CH_3O_2$	$1.000 \cdot 10^{-11}$	

Table S9: C4 oxidation (... continued)

reaction	rate coefficient	reference
$MDIALO_2 + HO_2 \longrightarrow 0.4 \cdot OH + 0.332 \cdot HO_2 + 0.068 \cdot CH_3COCHO + 0.136 \cdot CO + 0.068 \cdot CH_3O_2 + 0.068 \cdot GLYOXAL$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$MDIALO_2 + NO \longrightarrow NO_2 + 0.83 \cdot HO_2 + 0.17 \cdot CH_3COCHO + 0.34 \cdot CO + 0.17 \cdot CH_3O_2 + 0.17 \cdot GLYOXAL$	$7.500 \cdot 10^{-12} \exp(290./T)$	
$MDIALO_2 + NO_2 + M \longrightarrow M$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	Orlando and Tyndall (2012); Same as $k(CH_3CO_3 + NO_2)$
$MDIALO_2 + CH_3O_2 \longrightarrow 1.83 \cdot HO_2 + 0.17 \cdot CH_3COCHO + 0.34 \cdot CO + 0.17 \cdot CH_3O_2 + 0.17 \cdot GLYOXAL + CH_2O$	$1.000 \cdot 10^{-12}$	
$MDIALO_2 + CH_3CO_3 \longrightarrow 0.83 \cdot HO_2 + 0.17 \cdot CH_3COCHO + 0.34 \cdot CO + 1.17 \cdot CH_3O_2 + 0.17 \cdot GLYOXAL + CO_2$	$1.000 \cdot 10^{-11}$	

Table S10: C5 oxidation

reaction	rate coefficient	reference
$BIGALKANE + OH \longrightarrow ALKO_2 + H_2O$	$3.500 \cdot 10^{-12}$	
$C_5H_8 + OH \longrightarrow 0.4 \cdot LISOPACO_2 + 0.35 \cdot ISOPBO_2 + 0.25 \cdot ISOPDO_2$	$2.700 \cdot 10^{-11} \exp(390./T)$	Tyndall (p.c.); MCM3.2 has yields .25, .5, .25
$C_5H_8 + O_3 \longrightarrow 0.051 \cdot CH_3O_2 + 0.1575 \cdot CH_3CO_3 + 0.054 \cdot LHMVKABO_2 + 0.522 \cdot CO + 0.068750 \cdot HCOOH + 0.11 \cdot H_2O_2 + 0.324750 \cdot MACR + 0.1275 \cdot C_3H_6 + 0.2625 \cdot HO_2 + 0.255 \cdot CO_2 + 0.749750 \cdot CH_2O + 0.041250 \cdot MACO_2H + 0.27 \cdot OH + 0.244 \cdot MVK$	$7.860 \cdot 10^{-15} \exp(-1913./T)$	
$C_5H_8 + NO_3 \longrightarrow NISOPO_2$	$3.030 \cdot 10^{-12} \exp(-446./T)$	
$MBO + OH \longrightarrow MBOO_2$	$8.100 \cdot 10^{-12} \exp(610./T)$	
$MBO + O_3 \longrightarrow 0.35 \cdot CO + 0.5 \cdot CH_2O + 0.1 \cdot CH_3COCH_3 + 0.9 \cdot IBUTALOH + 0.25 \cdot HCOOH + 0.06 \cdot HO_2 + 0.06 \cdot OH$	$1.000 \cdot 10^{-17}$	
$MBO + NO_3 \longrightarrow MBONO_3O_2$	$4.600 \cdot 10^{-14} \exp(-400./T)$	
$ALKO_2 + NO \longrightarrow 0.4 \cdot CH_3CHO + 0.25 \cdot CH_2O + 0.25 \cdot CH_3COCH_3 + HO_2 + 0.8 \cdot MEK + NO_2$	$3.780 \cdot 10^{-12} \exp(180./T)$	$A = 4.200 \cdot 10^{-12} \cdot 0.9$; 10% $ALKNO_3$-yield
$ALKO_2 + NO \longrightarrow ALKNO_3$	$4.200 \cdot 10^{-13} \exp(180./T)$	10% $ALKNO_3$-yield
$ALKO_2 + HO_2 \longrightarrow ALKOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$ALKO_2 + CH_3O_2 \longrightarrow 0.3 \cdot CH_3CHO + 1.1875 \cdot CH_2O + 0.1875 \cdot CH_3COCH_3 + 0.75 \cdot HO_2 + 0.6 \cdot MEK + 0.25 \cdot ALKOH$	$1.000 \cdot 10^{-12}$	

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$ALKO_2 + CH_3CO_3 \longrightarrow 0.4 \cdot CH_3CHO + 0.25 \cdot CH_2O + 0.25 \cdot CH_3COCH_3 + HO_2 + 0.8 \cdot MEK + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$ALKOOH + OH \longrightarrow ALKO_2 + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$ALKOH + OH \longrightarrow 1.25 \cdot MEK + HO_2 + H_2O$	$5.000 \cdot 10^{-12}$	Tyndall (p.c.), MEK yield to account for C
$ALKNO_3 + OH \longrightarrow 0.4 \cdot CH_3CHO + 0.25 \cdot CH_2O + 0.25 \cdot CH_3COCH_3 + HO_2 + 0.8 \cdot MEK + NO_2$	$2.000 \cdot 10^{-12}$	
$LISOPACO_2 + HO_2 \longrightarrow LISOPACOOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	add OH channel
$LISOPACO_2 + NO \longrightarrow HO_2 + 0.977 \cdot LHC_4ACCHO + NO_2 + 0.0277 \cdot CH_3COCHO + 0.0277 \cdot GLYOXAL + 0.0277 \cdot HYAC + 0.0277 \cdot GLYALD$	$2.235 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.88$; average 12% nitrate yield from Paulot et al. (2009); Tyndall (p.c.); direct GLYOXAL channel from lab meas.
$LISOPACO_2 + NO \longrightarrow LISOPACNO_3$	$3.050 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009)
$LISOPACO_2 + NO_3 \longrightarrow HO_2 + LHC_4ACCHO + NO_2$	$2.500 \cdot 10^{-12}$	
$LISOPACO_2 + CH_3O_2 \longrightarrow 0.75 \cdot CH_2O + 0.75 \cdot LHC_4ACCHO + 0.25 \cdot CH_3OH + 0.25 \cdot ISOPAOH + HO_2$	$2.400 \cdot 10^{-12}$	products: Tyndall (p.c.)
$LISOPACO_2 + CH_3CO_3 \longrightarrow HO_2 + LHC_4ACCHO + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$LISOPACO_2 \longrightarrow HO_2 + HPALD$	$4.1 \cdot 10^{8} \exp(-7700./T)$	Bulk isomerization rate constant for all ISOPO2 by Crounse et al. (2011)
$ISOPBO_2 \longrightarrow HO_2 + HPALD$	$4.1 \cdot 10^{8} \exp(-7700./T)$	see note of [LISOPACO2]
$ISOPDO_2 \longrightarrow HO_2 + HPALD$	$4.1 \cdot 10^{8} \exp(-7700./T)$	see note of [LISOPACO2]
$LISOPACOOH + OH \longrightarrow 0.415 \cdot LIEPOX + 0.415 \cdot OH + 0.415 \cdot LISOPOOHO_2 + 0.14 \cdot LHC_4ACCHO + 0.03 \cdot H_2O + 0.03 \cdot LISOPACO_2$	$1.540 \cdot 10^{-10}$	k from MCMv3.3.1 and OH-addition branching ratios estimated with site-specific SAR by Peeters et al. (2007) and H-abstraction channel assumed to be like the one for $CH_3OOH + OH$ reaction and abstraction from the alpha-hydroperoxyl allyl hydrogen estimated by SAR of MOM (Taraborrelli in prep.) being $2.12 \cdot 10^{-11}$
$ISOPAOH + OH \longrightarrow LISOPOOHO_2$	$9.300 \cdot 10^{-11}$	OH-addition to double bond and products approximated with the one from $ISOPOOH + OH$ reaction leading to similar SOA precursors.
$LISOPACNO_3 + OH \longrightarrow LISOPNO_3O_2$	$6.000 \cdot 10^{-11}$	
$LIEPOX + OH \longrightarrow 0.29 \cdot IEC_1O_2 + 0.71 \cdot LIECHO + 0.71 \cdot HO_2 + H_2O$	$1.500 \cdot 10^{-11}$	MCM3.2
$LIECHO + OH \longrightarrow H_2O + LIECO_3$	$1.760 \cdot 10^{-11}$	MCM3.2
$LIECHO + NO_3 \longrightarrow HNO_3 + LIECO_3$	$1.050 \cdot 10^{-11} \exp(-1860./T)$	MCM3.2

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$LIECO_3 + HO_2 \longrightarrow 0.6 \cdot LIECO_3H + 0.4 \cdot CO_2 + 0.4 \cdot OH + 0.25 \cdot LHMVKABO_2 + 0.15 \cdot MACRO_2$	$5.200 \cdot 10^{-13} \exp(980./T)$	MCM3.2
$LIECO_3 + NO \longrightarrow 0.6 \cdot LHMVKABO_2 + 0.4 \cdot MACRO_2 + NO_2 + CO_2$	$7.500 \cdot 10^{-12} \exp(290./T)$	MCM3.2
$LIECO_3 + NO_3 \longrightarrow 0.6 \cdot LHMVKABO_2 + 0.4 \cdot MACRO_2 + NO_2 + CO_2$	$4.000 \cdot 10^{-12}$	MCM3.2
$LIECO_3H + OH \longrightarrow H_2O + LIECO_3$	$1.040 \cdot 10^{-11}$	MCM3.2
$IEC_1O_2 + HO_2 \longrightarrow LIECO_3H$	$2.050 \cdot 10^{-13} \exp(1300./T)$	MCM3.2 plus shortcut
$IEC_1O_2 + NO \longrightarrow BIACETOH + NO_2 + CH_2O + HO_2$	$2.700 \cdot 10^{-12} \exp(360./T)$	MCM3.2
$IEC_1O_2 + NO_3 \longrightarrow BIACETOH + NO_2 + CH_2O + HO_2$	$2.300 \cdot 10^{-12}$	MCM3.2
$ISOPBO_2 + HO_2 \longrightarrow ISOPBOOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$ISOPBO_2 + NO \longrightarrow CH_2O + MVK + HO_2 + NO_2$	$2.235 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.88$; average 12% nitrate yield from Paulot et al. (2009);
$ISOPBO_2 + NO \longrightarrow ISOPBNO_3$	$3.050 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009);
$ISOPBO_2 + NO_3 \longrightarrow CH_2O + MVK + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	
$ISOPBO_2 + CH_3O_2 \longrightarrow 0.75 \cdot MVK + 1.75 \cdot CH_2O + 1.5 \cdot HO_2 + 0.25 \cdot ISOPBOH$	$8.000 \cdot 10^{-13}$	products: Tyndall (p.c.)
$ISOPBO_2 + CH_3CO_3 \longrightarrow CH_2O + MVK + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$ISOPBOOH + OH \longrightarrow 0.63 \cdot LIEPOX + 0.63 \cdot OH + 0.12 \cdot LISOPOOHO_2 + 0.15 \cdot H_2O + 0.15 \cdot ISOPBO_2$	$7.500 \cdot 10^{-11}$	St. Clair et al. (2015)
$ISOPBOH + OH \longrightarrow LISOPOOHO_2$	$3.850 \cdot 10^{-11}$	OH-addition to double bond and products approximated with the one from $ISOPOOH + OH$ reaction leading to similar SOA precursors.
$ISOPBNO_3 + OH \longrightarrow LISOPNO_3O_2$	$1.360 \cdot 10^{-11}$	
$ISOPDO_2 + HO_2 \longrightarrow ISOPDOOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$ISOPDO_2 + NO \longrightarrow CH_2O + MACR + HO_2 + NO_2$	$2.235 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.88$; average 12% nitrate yield from Paulot et al. (2009);
$ISOPDO_2 + NO \longrightarrow ISOPDNO_3$	$3.050 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009);
$ISOPDO_2 + NO_3 \longrightarrow CH_2O + MACR + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	
$ISOPDO_2 + CH_3O_2 \longrightarrow 0.5 \cdot MACR + 1.25 \cdot CH_2O + HO_2 + 0.25 \cdot CH_3OH + 0.25 \cdot HCOC_5 + 0.25 \cdot ISOPDOH$	$2.900 \cdot 10^{-12}$	products: Tyndall (p.c.)
$ISOPDO_2 + CH_3CO_3 \longrightarrow CH_2O + MACR + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$ISOPDOOH + OH \longrightarrow 0.79 \cdot LIEPOX + 0.79 \cdot OH + 0.14 \cdot LISOPOOHO_2 + 0.07 \cdot H_2O + 0.07 \cdot ISOPDO_2$	$1.180 \cdot 10^{-10}$	St. Clair et al. (2015)
$ISOPDOH + OH \longrightarrow LISOPOOHO_2$	$7.380 \cdot 10^{-11}$	OH-addition to double bond and products approximated with the one from ISOPOOH + OH reaction leading to similar SOA precursors.
$ISOPDNO_3 + OH \longrightarrow LISOPNO_3O_2$	$6.100 \cdot 10^{-11}$	OH-addition to double bond
$NISOPO_2 + HO_2 \longrightarrow NISOPOOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$NISOPO_2 + NO \longrightarrow HO_2 + NC_4CHO + NO_2$	$2.540 \cdot 10^{-12} \exp(360./T)$	
$NISOPO_2 + NO_3 \longrightarrow HO_2 + NC_4CHO + NO_2$	$2.500 \cdot 10^{-12}$	
$NISOPO_2 + CH_3O_2 \longrightarrow 0.75 \cdot CH_2O + 0.75 \cdot NC_4CHO + HO_2 + 0.25 \cdot CH_3OH + 0.25 \cdot LISOPACNO_3$	$1.300 \cdot 10^{-12}$	products: Tyndall (p.c.)
$NISOPO_2 + CH_3CO_3 \longrightarrow HO_2 + NC_4CHO + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$NISOPOOH + OH \longrightarrow NC_4CHO + OH + H_2O$	$1.030 \cdot 10^{-10}$	
$NC_4CHO + OH \longrightarrow H_2O + LNISO_3$	$4.160 \cdot 10^{-11}$	
$NC_4CHO + O_3 \longrightarrow 0.445 \cdot NO_2 + 0.89 \cdot CO + 0.075625 \cdot H_2O_2 + 0.034375 \cdot HCOCO_2H + 0.555 \cdot NOA + 0.445 \cdot HO_2 + 0.520625 \cdot GLYOXAL + 0.89 \cdot OH + 0.445 \cdot CH_3COCHO$	$2.400 \cdot 10^{-17}$	
$NC_4CHO + NO_3 \longrightarrow HNO_3 + LNISO_3$	$6.120 \cdot 10^{-12} \exp(-1862./T)$	
$LNISO_3 + HO_2 \longrightarrow 0.8 \cdot LNISOOH + 0.2 \cdot NOA + 0.2 \cdot OH + 0.2 \cdot CO_2 + 0.2 \cdot CO + 0.2 \cdot HO_2$	$1.930 \cdot 10^{-13} \exp(1300./T)$	products: Tyndall (p.c.)
$LNISO_3 + NO \longrightarrow NOA + 0.5 \cdot GLYOXAL + 0.5 \cdot CO + HO_2 + NO_2 + 0.5 \cdot CO_2$	$4.270 \cdot 10^{-12} \exp(360./T)$	
$LNISO_3 + NO_3 \longrightarrow NOA + 0.5 \cdot GLYOXAL + 0.5 \cdot CO + HO_2 + NO_2 + 0.5 \cdot CO_2$	$3.302 \cdot 10^{-12} \exp(360./T)$	
$LNISO_3 + CH_3O_2 \longrightarrow 0.375 \cdot GLYOXAL + 0.875 \cdot NOA + CH_2O + 1.75 \cdot HO_2 + 0.625 \cdot CO_2 + 0.0625 \cdot MACRN + 0.0625 \cdot MVKN + 0.5 \cdot CO$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$LNISO_3 + CH_3CO_3 \longrightarrow NOA + 0.5 \cdot GLYOXAL + 0.5 \cdot CO + HO_2 + CH_3O_2 + 1.5 \cdot CO_2$	$1.000 \cdot 10^{-11}$	
$LNISOOH + OH \longrightarrow H_2O + LNISO_3$	$2.650 \cdot 10^{-11}$	
$LHC_4ACCHO + OH \longrightarrow 0.52 \cdot LC_{578}O_2 + 0.48 \cdot LHC_4ACCO_3 + H_2O$	$4.520 \cdot 10^{-11}$	

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$LHC_4ACCHO + O_3 \longrightarrow 0.2225 \cdot CH_3CO_3 + 0.89 \cdot CO + 0.017188 \cdot HOCH_2CO_2H + 0.075625 \cdot H_2O_2 + 0.017188 \cdot HCOCO_2H + 0.2775 \cdot HYAC + 0.6675 \cdot HO_2 + 0.260313 \cdot GLYOXAL + 0.2225 \cdot CH_2O + 0.89 \cdot OH + 0.260313 \cdot GLYALD + 0.5 \cdot CH_3COCHO$	$2.400 \cdot 10^{-17}$	
$LHC_4ACCHO + NO_3 \longrightarrow HNO_3 + LHC_4ACCO_3$	$6.120 \cdot 10^{-12} \exp(-1862./T)$	
$LC_{578}O_2 + NO \longrightarrow 0.25 \cdot CH_3COCHO + 0.25 \cdot GLYALD + 0.25 \cdot GLYOXAL + 0.25 \cdot HYAC + 0.25 \cdot CO + 0.25 \cdot MACROH + 0.25 \cdot CH_2O + 0.25 \cdot CO_2H_3CHO + HO_2 + NO_2$	$2.540 \cdot 10^{-12} \exp(360./T)$	products: Tyndall (p.c.)
$LC_{578}O_2 + NO_3 \longrightarrow 0.25 \cdot CH_3COCHO + 0.25 \cdot GLYALD + 0.25 \cdot GLYOXAL + 0.25 \cdot HYAC + 0.25 \cdot CO + 0.25 \cdot MACROH + 0.25 \cdot CH_2O + 0.25 \cdot CO_2H_3CHO + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	products: Tyndall (p.c.)
$LC_{578}O_2 + HO_2 \longrightarrow LC_{578}OOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	add OH channel
$LC_{578}O_2 + CH_3O_2 \longrightarrow 0.156250 \cdot CH_3COCHO + 0.156250 \cdot GLYALD + 0.156250 \cdot GLYOXAL + 0.156250 \cdot HYAC + 0.156250 \cdot CO + 0.468750 \cdot MACROH + 1.031250 \cdot CH_2O + 0.3125 \cdot CO_2H_3CHO + 1.25 \cdot HO_2 + 0.125 \cdot CH_3OH$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$LC_{578}O_2 + CH_3CO_3 \longrightarrow 0.25 \cdot CH_3COCHO + 0.25 \cdot GLYALD + 0.25 \cdot GLYOXAL + 0.25 \cdot HYAC + 0.25 \cdot CO + 0.25 \cdot MACROH + 0.25 \cdot CH_2O + 0.25 \cdot CO_2H_3CHO + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$LC_{578}OOH + OH \longrightarrow H_2O + LC_{578}O_2$	$3.160 \cdot 10^{-11}$	
$LHC_4ACCO_3 \longrightarrow HO_2 + PACALD$	$4.1 \cdot 10^{8} \exp(-7700./T)$	see note of [LISOPACO2]
$LHC_4ACCO_3 + CH_3O_2 \longrightarrow CH_2O + 0.1 \cdot LHC_4ACCO_2H + 0.45 \cdot GLYALD + 0.45 \cdot HYAC + 0.45 \cdot CH_3CO_3 + 0.45 \cdot CO + 0.45 \cdot HO_2 + 0.9 \cdot CO_2$	$1.000 \cdot 10^{-11}$	products: Tyndall (p.c.)
$LHC_4ACCO_3 + CH_3CO_3 \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot GLYALD + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO + 0.5 \cdot HO_2 + CH_3O_2 + 2 \cdot CO_2$	$1.000 \cdot 10^{-11}$	
$LHC_4ACCO_3 + HO_2 \longrightarrow 0.4 \cdot LHC_4ACCO_3H + 0.2 \cdot LHC_4ACCO_2H + 0.2 \cdot O_3 + 0.4 \cdot CO_2 + 0.4 \cdot OH + 0.2 \cdot HYAC + 0.2 \cdot GLYALD + 0.2 \cdot CH_3CO_3 + 0.2 \cdot CO + 0.2 \cdot HO_2$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$LHC_4ACCO_3 + NO \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot GLYALD + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO + 0.5 \cdot HO_2 + NO_2 + CO_2$	$8.100 \cdot 10^{-12} \exp(270./T)$	
$LHC_4ACCO_3 + NO_3 \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot GLYALD + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO + 0.5 \cdot HO_2 + NO_2 + CO_2$	$4.000 \cdot 10^{-12}$	

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$LHC_4ACCO_3 + NO_2 + M \longrightarrow LC_5PAN_{1719} + M$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.3)$	
$LHC_4ACCO_2H + OH \longrightarrow 0.5 \cdot HYAC + 0.5 \cdot GLYALD + 0.5 \cdot CH_3CO_3 + 0.5 \cdot CO + 0.5 \cdot HO_2 + CO_2 + H_2O$	$2.520 \cdot 10^{-11}$	
$LHC_4ACCO_3H + OH \longrightarrow H_2O + LHC_4ACCO_3$	$2.880 \cdot 10^{-11}$	
$LC_5PAN_{1719} + M \longrightarrow LHC_4ACCO_3 + NO_2 + M$		$k0 = 4.9 \cdot 10^{-3} \exp(-12100./T) * M,\ kinf = 5.4 \cdot 10^{16} \exp(-13830./T),\ fc = 0.3$
$LC_5PAN_{1719} + OH \longrightarrow CO + MACROH + NO_2$	$2.520 \cdot 10^{-11}$	
$HCOC_5 + OH \longrightarrow C_{59}O_2$	$3.810 \cdot 10^{-11}$	
$C_{59}O_2 + CH_3O_2 \longrightarrow 0.75 \cdot HOCH_2CO_3 + 0.75 \cdot HYAC + CH_2O + 0.75 \cdot HO_2 + 0.3125 \cdot MACROH$	$1.000 \cdot 10^{-12}$	Tyndall (p.c.)
$C_{59}O_2 + CH_3CO_3 \longrightarrow HOCH_2CO_3 + HYAC + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$C_{59}O_2 + NO \longrightarrow HOCH_2CO_3 + HYAC + NO_2$	$2.540 \cdot 10^{-12} \exp(360./T)$	
$C_{59}O_2 + NO_3 \longrightarrow HOCH_2CO_3 + HYAC + NO_2$	$2.500 \cdot 10^{-12}$	
$C_{59}O_2 + HO_2 \longrightarrow C_{59}OOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$C_{59}OOH + OH \longrightarrow C_{59}O_2 + H_2O$	$9.700 \cdot 10^{-12}$	
$MBOO_2 + NO \longrightarrow HO_2 + 0.67 \cdot CH_3COCH_3 + 0.67 \cdot GLYALD + 0.33 \cdot CH_2O + 0.33 \cdot IBUTALOH + NO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$MBOO_2 + CH_3O_2 \longrightarrow 0.9165 \cdot CH_2O + 0.625 \cdot MACROH + 0.25 \cdot CH_3OH + HO_2 + 0.3335 \cdot CH_3COCH_3 + 0.3335 \cdot GLYALD + 0.1665 \cdot IBUTALOH$	$3.750 \cdot 10^{-13} \exp(-40./T)$	
$MBOO_2 + CH_3CO_3 \longrightarrow 0.67 \cdot CH_3COCH_3 + 0.67 \cdot GLYALD + 0.33 \cdot CH_2O + 0.33 \cdot IBUTALOH + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$MBOO_2 + HO_2 \longrightarrow MBOOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$MBOOOH + OH \longrightarrow 0.5 \cdot MBOO_2 + 0.625 \cdot MACROH + 0.5 \cdot OH + H_2O$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$IBUTALOH + OH \longrightarrow H_2O + IBUTALOHO_2$	$1.400 \cdot 10^{-11}$	
$IBUTALOHO_2 + NO \longrightarrow CO_2 + NO_2 + HO_2 + CH_3COCH_3$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$IBUTALOHO_2 + HO_2 \longrightarrow 0.6 \cdot IBUTALOHOOH + 0.4 \cdot HO_2 + 0.4 \cdot OH + 0.4 \cdot CH_3COCH_3 + 0.4 \cdot CO_2$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$IBUTALOHO_2 + CH_3O_2 \longrightarrow CH_3COCH_3 + 2 \cdot HO_2 + CO_2 + CH_2O$	$1.000 \cdot 10^{-12}$	products: Tyndall (p.c.)
$IBUTALOHO_2 + CH_3CO_3 \longrightarrow CH_3COCH_3 + HO_2 + CH_3O_2 + 2 \cdot CO_2$	$1.000 \cdot 10^{-11}$	
$IBUTALOHOOH + OH \longrightarrow H_2O + IBUTALOHO_2$	$1.000 \cdot 10^{-12}$	Tyndall (p.c.)

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$MBONO_3O_2 + HO_2 \longrightarrow$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$MBONO_3O_2 + NO \longrightarrow 0.25 \cdot CH_2O + 0.25 \cdot IBUTALOH + 1.25 \cdot NO_2 + 0.500250 \cdot NOA + 0.75 \cdot CH_3COCH_3 + 0.75 \cdot HO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$MBONO_3O_2 + NO_3 \longrightarrow 0.25 \cdot CH_2O + 0.25 \cdot IBUTALOH + 1.25 \cdot NO_2 + 0.500250 \cdot NOA + 0.75 \cdot CH_3COCH_3 + 0.75 \cdot HO_2$	$2.400 \cdot 10^{-12}$	
$MBONO_3O_2 + CH_3O_2 \longrightarrow 0.875 \cdot CH_2O + 0.125 \cdot IBUTALOH + 0.125 \cdot NO_2 + 0.250125 \cdot NOA + 0.375 \cdot CH_3COCH_3 + 0.875 \cdot HO_2 + 0.25 \cdot CH_3OH + 0.625 \cdot MACROH$	$1.000 \cdot 10^{-12}$	Tyndall (p.c.)
$MBONO_3O_2 + CH_3CO_3 \longrightarrow 0.25 \cdot CH_2O + 0.25 \cdot IBUTALOH + 0.25 \cdot NO_2 + 0.500250 \cdot NOA + 0.75 \cdot CH_3COCH_3 + 0.75 \cdot HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$DICARBO_2 + HO_2 \longrightarrow 0.4 \cdot OH + 0.068 \cdot CH_3COCHO + 0.068 \cdot HO_2 + 0.068 \cdot CO + 0.4 \cdot CO_2 + 0.332 \cdot CH_3CO_3 + 0.332 \cdot GLYOXAL$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$DICARBO_2 + NO \longrightarrow 0.17 \cdot CH_3COCHO + 0.17 \cdot HO_2 + 0.17 \cdot CO + CO_2 + 0.83 \cdot CH_3CO_3 + 0.83 \cdot GLYOXAL + NO_2$	$7.500 \cdot 10^{-12} \exp(290./T)$	
$DICARBO_2 + NO_2 + M \longrightarrow M$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	Orlando and Tyndall (2012), Same as $k(CH_3CO_3 + NO_2)$
$DICARBO_2 + CH_3O_2 \longrightarrow 0.17 \cdot CH_3COCHO + 1.17 \cdot HO_2 + 0.17 \cdot CO + CO_2 + 0.83 \cdot CH_3CO_3 + 0.83 \cdot GLYOXAL + CH_2O$	$1.000 \cdot 10^{-12}$	
$DICARBO_2 + CH_3CO_3 \longrightarrow 0.17 \cdot CH_3COCHO + 0.17 \cdot HO_2 + 0.17 \cdot CO + 2 \cdot CO_2 + 0.83 \cdot CH_3CO_3 + 0.83 \cdot GLYOXAL + CH_3O_2$	$1.000 \cdot 10^{-11}$	
$HPALD + OH \longrightarrow 0.641 \cdot OH + 0.385 \cdot PACALD + 0.256 \cdot BIGALD_3 + 0.359 \cdot CH_3COCHO + 0.359 \cdot GLYOX + 0.359 \cdot HO_2$	$5.200 \cdot 10^{-11}$	simplification of chemistry in MCMv3.3.1
$PACALD + OH \longrightarrow CH_3COCHO + HCOCO_3H + HO_2$	$4.720 \cdot 10^{-11}$	k and products for $C_5PACALD_2$ from MCMv3.3.1 assuming an implict $RO_2 \longrightarrow RO$ conversion
$LISOPOOHO_2 + HO_2 \longrightarrow LISOPOOHOOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$LISOPOOHO_2 + NO \longrightarrow CH_2O + HO_2 + 0.5 \cdot MACROOH + 0.5 \cdot LHMVKABOOH + NO_2$	$2.540 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009); nitrate yield left for the moment equal to the one of the simple ISOPO2 (it should be higher)
$LISOPOOHO_2 + NO \longrightarrow LISOPNO_3OOH$	$3.050 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009); nitrate yield left for the moment equal to the one of the simple ISOPO2 (it should be higher)

Table S10: C5 oxidation (... continued)

reaction	rate coefficient	reference
$LISOPOOHO_2 + NO_3 \longrightarrow CH_2O + HO_2 + 0.5 \cdot MACROOH + 0.5 \cdot LHMVKABOOH + NO_2$	$2.500 \cdot 10^{-12}$	
$LISOPOOHO_2 + CH_3O_2 \longrightarrow 1.5 \cdot CH_2O + 0.75 \cdot HO_2 + 0.375 \cdot MACROOH + 0.375 \cdot LHMVKABOOH + 0.25 \cdot LISOPOOHOOH$	$8.000 \cdot 10^{-13}$	
$LISOPOOHO_2 + CH_3CO_3 \longrightarrow CH_2O + HO_2 + 0.5 \cdot MACROOH + 0.5 \cdot LHMVKABOOH + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$LISOPNO_3O_2 + HO_2 \longrightarrow LISOPNO_3OOH$	$2.050 \cdot 10^{-13} \exp(1300./T)$	
$LISOPNO_3O_2 + NO \longrightarrow CH_2O + 0.5 \cdot MACRN + 0.5 \cdot MVKN + HO_2 + NO_2$	$2.235 \cdot 10^{-12} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.88$; average 12% nitrate yield from Paulot et al. (2009); nitrate yield left for the moment equal to the one of the simple ISOPO2 (it should be higher); previous $RONO_2$ split into 50% MACRN + 50% MVKN
$LISOPNO_3O_2 + NO \longrightarrow LISOPNO_3NO_3$	$3.050 \cdot 10^{-13} \exp(360./T)$	$A = 2.54 \cdot 10^{-12} \cdot 0.12$; average 12% nitrate yield from Paulot et al. (2009); nitrate yield left for the moment equal to the one of the simple ISOPO2 (it should be higher)
$LISOPNO_3O_2 + NO_3 \longrightarrow CH_2O + 0.5 \cdot MACRN + 0.5 \cdot MVKN + HO_2 + NO_2$	$2.500 \cdot 10^{-12}$	
$LISOPNO_3O_2 + CH_3O_2 \longrightarrow 0.3525 \cdot MACRN + 0.3525 \cdot MVKN + 1.75 \cdot CH_2O + 1.5 \cdot HO_2 + 0.25 \cdot LISOPNO_3OOH$	$8.000 \cdot 10^{-13}$	
$LISOPNO_3O_2 + CH_3CO_3 \longrightarrow CH_2O + 0.5 \cdot MACRN + 0.5 \cdot MVKN + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$LISOPOOHOOH + OH \longrightarrow H_2O + LISOPOOHO_2$	$7.600 \cdot 10^{-12} \exp(200./T)$	twice the $k(CH_3OOH + OH \longrightarrow CH_3O_2)$
$LISOPOOHOOH + OH \longrightarrow LC_{578}OOH + OH$	$2.104 \cdot 10^{-11}$	k for H-abstractions from SAR in MOM by a secondary carbon bearing a -OH group and a secondary and a tertiary carbon atoms bearing an -OOH group: $8.42 \cdot 10^{-13} \cdot 3.44 + (8.42 \cdot 10^{-13} + 1.75 \cdot 10^{-12}) \cdot 7$
$LISOPNO_3OOH + OH \longrightarrow H_2O + LISOPNO_3O_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$LISOPNO_3OOH + OH \longrightarrow C_{59}OOH + OH$	$1.515 \cdot 10^{-11}$	k for H-abstractions from SAR in MOM by a secondary carbon bearing a -OH group and a tertiary carbon atom bearing an -OOH group: $8.42 \cdot 10^{-13} \cdot 3.44 + 1.75 \cdot 10^{-12} \cdot 7$
$LISOPNO_3NO_3 + OH \longrightarrow 0.5 \cdot MACRN + 0.5 \cdot MVKN + NO_2 + CH_2O + HO_2$	$8.916 \cdot 10^{-12}$	k for H-abstractions from SAR in MOM by a secondary and a tertiary carbon bearing a -OH group: $(8.42 \cdot 10^{-13} + 1.75 \cdot 10^{-12}) \cdot 3.44$; previous $RONO_2$ split into 50% MACRN + 50% MVKN

Table S11: C6 oxidation

reaction	rate coefficient	reference
$BENZ + OH \longrightarrow 0.53 \cdot PHENOL + 0.12 \cdot BEPOMUC + 0.65 \cdot HO_2 + 0.35 \cdot BENZO_2$	$2.300 \cdot 10^{-12} \exp(-193./T)$	
$PHENOL + OH \longrightarrow 0.14 \cdot PHENO_2 + 0.8 \cdot HO_2 + 0.8 \cdot CATECHOL + 0.06 \cdot C_6H_5O$	$4.700 \cdot 10^{-13} \exp(1220./T)$	
$PHENOL + NO_3 \longrightarrow 0.26 \cdot PHENO_2 + 0.74 \cdot C_6H_5O + 0.74 \cdot HNO_3$	$3.800 \cdot 10^{-12}$	NPHENO2 approximated with $PHENO_2$
$PHENO_2 + NO \longrightarrow HO_2 + 0.7 \cdot GLYOXAL + NO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$PHENO_2 + HO_2 \longrightarrow PHENOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$PHENO_2 + CH_3O_2 \longrightarrow 2 \cdot HO_2 + 0.7 \cdot GLYOXAL + CH_2O$	$1.000 \cdot 10^{-12}$	
$PHENO_2 + CH_3CO_3 \longrightarrow HO_2 + 0.7 \cdot GLYOXAL + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$PHENOOH + OH \longrightarrow H_2O + PHENO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$C_6H_5O + NO_2 \longrightarrow$	$2.100 \cdot 10^{-12}$	
$C_6H_5O + O_3 \longrightarrow C_6H_5O_2$	$2.800 \cdot 10^{-13}$	
$C_6H_5O_2 + NO \longrightarrow C_6H_5O + NO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$C_6H_5O_2 + NO_3 \longrightarrow C_6H_5O + NO_2$	$2.300 \cdot 10^{-12}$	MCM3.2
$C_6H_5O_2 + HO_2 \longrightarrow C_6H_5OOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$C_6H_5O_2 + CH_3O_2 \longrightarrow C_6H_5O + CH_2O + HO_2$	$1.000 \cdot 10^{-12}$	
$C_6H_5O_2 + CH_3CO_3 \longrightarrow C_6H_5O + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$C_6H_5OOH + OH \longrightarrow C_6H_5O_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$BENZO_2 + NO \longrightarrow GLYOXAL + NO_2 + 0.5 \cdot BIGALD_1 + HO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	MCM3.2
$BENZO_2 + HO_2 \longrightarrow BENZOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$BENZO_2 + CH_3O_2 \longrightarrow GLYOXAL + 0.5 \cdot BIGALD_1 + 2 \cdot HO_2 + CH_2O$	$1.000 \cdot 10^{-12}$	
$BENZO_2 + CH_3CO_3 \longrightarrow GLYOXAL + 0.5 \cdot BIGALD_1 + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$BENZOOH + OH \longrightarrow BENZO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$CATECHOL + OH \longrightarrow CATEC_1O$	$1.000 \cdot 10^{-10}$	
$CATECHOL + NO_3 \longrightarrow CATEC_1O + HNO_3$	$9.900 \cdot 10^{-11}$	
$CATEC_1O + NO_2 \longrightarrow$	$2.100 \cdot 10^{-12}$	
$CATEC_1O + O_3 \longrightarrow CATEC_1O_2$	$2.800 \cdot 10^{-13}$	
$CATEC_1O_2 + HO_2 \longrightarrow CATEC_1OOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$CATEC_1O_2 + NO \longrightarrow CATEC_1O + NO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$CATEC_1O_2 + NO_3 \longrightarrow CATEC_1O + NO_2$	$2.300 \cdot 10^{-12}$	MCM3.2
$CATEC_1O_2 + CH_3O_2 \longrightarrow CATEC_1O + CH_2O + HO_2$	$1.000 \cdot 10^{-12}$	
$CATEC_1O_2 + CH_3CO_3 \longrightarrow CATEC_1OCH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$CATEC_1OOH + OH \longrightarrow CATEC_1O_2$	$1.900 \cdot 10^{-12} \exp(190./T)$	

Table S12: C7 oxidation

reaction	rate coefficient	reference
$TOL + OH \longrightarrow 0.18 \cdot CRESOL + 0.1 \cdot TEPOMUC + 0.07 \cdot BZOO + 0.65 \cdot TOLO_2 + 0.28 \cdot HO_2$	$1.700 \cdot 10^{-12} \exp(352./T)$	
$CRESOL + OH \longrightarrow 0.2 \cdot PHENO_2 + 0.73 \cdot HO_2 + 0.73 \cdot CATECHOL + 0.07 \cdot C_6H_5O$	$4.700 \cdot 10^{-11}$	CATECHOL and $PHENO_2$ omits one CH_3 group of MCATECHOL and $CRESO_2$
$CRESOL + NO_3 \longrightarrow 0.61 \cdot PHENO_2 + 0.39 \cdot C_6H_5O + 0.49 \cdot HNO_3$	$1.400 \cdot 10^{-11}$	$CRESO_2$ and $NCRESO_2$ approximated with $PHENO_2$; TOL_1O with C_6H_5O (see MCM3.2 for details)
$TOLO_2 + HO_2 \longrightarrow TOLOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$TOLO_2 + NO \longrightarrow NO_2 + 0.6 \cdot GLYOXAL + 0.4 \cdot CH_3COCHO + HO_2 + 0.2 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.2 \cdot BIGALD_3$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$TOLO_2 + CH_3O_2 \longrightarrow 0.6 \cdot GLYOXAL + 0.4 \cdot CH_3COCHO + 2 \cdot HO_2 + CH_2O$	$1.000 \cdot 10^{-12}$	
$TOLO_2 + CH_3CO_3 \longrightarrow 0.6 \cdot GLYOXAL + 0.4 \cdot CH_3COCHO + HO_2 + CH_3O_2 + CO_2 + 0.2 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.2 \cdot BIGALD_3$	$1.000 \cdot 10^{-11}$	
$TOLOOH + OH \longrightarrow TOLO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$BZOO + HO_2 \longrightarrow BZOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$BZOO + NO \longrightarrow BZALD + NO_2 + HO_2$	$2.600 \cdot 10^{-12} \exp(365./T)$	MCM3.2 forms 10% nitrate
$BZOO + CH_3O_2 \longrightarrow BZALD + 2 \cdot HO_2 + CH_2O$	$1.000 \cdot 10^{-12}$	
$BZOO + CH_3CO_3 \longrightarrow BZALD + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$BZOOH + OH \longrightarrow BZOO$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$BZALD + OH \longrightarrow ACBZO_2$	$5.900 \cdot 10^{-12} \exp(225./T)$	
$ACBZO_2 + NO_2 + M \longrightarrow M + PBZNIT$	$ktroe(2.700 \cdot 10^{-28}, 7.1, 1.200 \cdot 10^{-11}, 0.9, 0.6)$	Orlando and Tyndall (2012) - Same as $k(CH_3CO_3 + NO_2)$
$PBZNIT + M \longrightarrow ACBZO_2 + NO_2 + M$		
$ACBZO_2 + NO \longrightarrow C_6H_5O_2 + NO_2$	$7.500 \cdot 10^{-12} \exp(290./T)$	
$ACBZO_2 + HO_2 \longrightarrow 0.4 \cdot C_6H_5O_2 + 0.4 \cdot OH$	$4.300 \cdot 10^{-13} \exp(1040./T)$	
$ACBZO_2 + CH_3O_2 \longrightarrow C_6H_5O_2 + CH_2O + HO_2$	$1.000 \cdot 10^{-12}$	
$ACBZO_2 + CH_3CO_3 \longrightarrow C_6H_5O_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	

Table S13: C8 oxidation

reaction	rate coefficient	reference
$XYL + OH \longrightarrow 0.15 \cdot XYLOL + 0.23 \cdot TEPOMUC + 0.06 \cdot BZOO + 0.56 \cdot XYLENO_2 + 0.38 \cdot HO_2$	$1.700 \cdot 10^{-11}$	

Table S13: C8 oxidation (... continued)

reaction	rate coefficient	reference
$XYLOL + OH \longrightarrow 0.3 \cdot XYLOLO_2 + 0.63 \cdot HO_2 + 0.63 \cdot CATECHOL + 0.07 \cdot C_6H_5O$	$8.400 \cdot 10^{-11}$	CATECHOL omits two CH_3 groups of O-, M- and P-XYCATECH
$XYLOL + NO_3 \longrightarrow 0.61 \cdot PHENO_2 + 0.39 \cdot C_6H_5O + 0.49 \cdot HNO_3$	$3.200 \cdot 10^{-11}$	$XYLOLO_2$ and $NXYLOLO_2$ approximated with $PHENO_2$; XY1O with C_6H_5O (see MCM3.2 for details)
$XYLOLO_2 + NO \longrightarrow HO_2 + NO_2 + 0.17 \cdot GLYOXAL + 0.51 \cdot CH_3COCHO$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$XYLOLO_2 + HO_2 \longrightarrow XYLOLOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$XYLOLO_2 + CH_3O_2 \longrightarrow 0.17 \cdot GLYOXAL + 0.51 \cdot CH_3COCHO + 2 \cdot HO_2 + CH_2O$	$1.000 \cdot 10^{-12}$	
$XYLOLO_2 + CH_3CO_3 \longrightarrow HO_2 + 0.17 \cdot GLYOXAL + 0.51 \cdot CH_3COCHO + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$XYLOLOOH + OH \longrightarrow XYLOLO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	
$XYLENO_2 + HO_2 \longrightarrow XYLENOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$XYLENO_2 + NO \longrightarrow HO_2 + NO_2 + 0.34 \cdot GLYOXAL + 0.54 \cdot CH_3COCHO + 0.06 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.15 \cdot BIGALD_3 + 0.21 \cdot BIGALD_4$	$2.600 \cdot 10^{-12} \exp(365./T)$	
$XYLENO_2 + CH_3O_2 \longrightarrow 0.34 \cdot GLYOXAL + 0.54 \cdot CH_3COCHO + 2 \cdot HO_2 + CH_2O + 0.06 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.15 \cdot BIGALD_3 + 0.21 \cdot BIGALD_4$	$1.000 \cdot 10^{-12}$	
$XYLENO_2 + CH_3CO_3 \longrightarrow HO_2 + 0.34 \cdot GLYOXAL + 0.54 \cdot CH_3COCHO + 0.06 \cdot BIGALD_1 + 0.2 \cdot BIGALD_2 + 0.15 \cdot BIGALD_3 + 0.21 \cdot BIGALD_4 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$XYLENOOH + OH \longrightarrow XYLENO_2$	$3.800 \cdot 10^{-12} \exp(200./T)$	

Table S14: C10/C15 oxidation (terpenes, sesqui-terpenes)

reaction	rate coefficient	reference
$APIN + OH \longrightarrow TERPO_2$	$1.200 \cdot 10^{-11} \exp(440./T)$	
$BPIN + OH \longrightarrow TERPO_2$	$1.600 \cdot 10^{-11} \exp(470./T)$	
$LIMON + OH \longrightarrow TERPO_2$	$4.200 \cdot 10^{-11} \exp(400./T)$	
$MYRC + OH \longrightarrow TERPO_2$	$2.100 \cdot 10^{-10}$	
$BCARY + OH \longrightarrow TERPO_2$	$2.000 \cdot 10^{-10}$	
$APIN + O_3 \longrightarrow 0.07 \cdot ELVOC + 0.39 \cdot TERPROD_1 + 0.27 \cdot TERPROD_2 + 0.63 \cdot OH + 0.57 \cdot HO_2 + 0.23 \cdot CO + 0.27 \cdot CO_2 + 0.52 \cdot CH_3COCH_3 + 0.34 \cdot CH_2O + 0.05 \cdot HCOOH + 0.05 \cdot BIGALKANE + 0.06 \cdot CH_3CO_3 + 0.06 \cdot CH_3COCH_2O_2$	$6.300 \cdot 10^{-16} \exp(-580./T)$	7% ELVOC-yield according to Ehn et al. (2014) for endocyclic alkenes
$BPIN + O_3 \longrightarrow 0.43 \cdot TERPROD_1 + 0.3 \cdot TERPROD_2 + 0.63 \cdot OH + 0.57 \cdot HO_2 + 0.23 \cdot CO + 0.27 \cdot CO_2 + 0.52 \cdot CH_3COCH_3 + 0.34 \cdot CH_2O + 0.05 \cdot HCOOH + 0.05 \cdot BIGALKANE + 0.06 \cdot CH_3CO_3 + 0.06 \cdot CH_3COCH_2O_2$	$1.700 \cdot 10^{-15} \exp(-1300./T)$	

Table S14: C10/C15 oxidation (terpenes, sesqui-terpenes; ... continued)

reaction	rate coefficient	reference
$LIMON + O_3 \longrightarrow 0.07 \cdot ELVOC + 0.39 \cdot TERPROD_1 + 0.27 \cdot TERPROD_2 + 0.63 \cdot OH + 0.57 \cdot HO_2 + 0.23 \cdot CO + 0.27 \cdot CO_2 + 0.52 \cdot CH_3COCH_3 + 0.34 \cdot CH_2O + 0.05 \cdot HCOOH + 0.05 \cdot BIGALKANE + 0.06 \cdot CH_3CO_3 + 0.06 \cdot CH_3COCH_2O_2$	$3.000 \cdot 10^{-15} \exp(-780./T)$	7% ELVOC-yield according to Ehn et al. (2014) for endocyclic alkenes
$MYRC + O_3 \longrightarrow 0.43 \cdot TERPROD_1 + 0.3 \cdot TERPROD_2 + 0.63 \cdot OH + 0.57 \cdot HO_2 + 0.23 \cdot CO + 0.27 \cdot CO_2 + 0.52 \cdot CH_3COCH_3 + 0.34 \cdot CH_2O + 0.05 \cdot HCOOH + 0.05 \cdot BIGALKANE + 0.06 \cdot CH_3CO_3 + 0.06 \cdot CH_3COCH_2O_2$	$4.700 \cdot 10^{-16}$	
$BCARY + O_3 \longrightarrow 0.645 \cdot TERPROD_1 + 0.45 \cdot TERPROD_2 + 0.63 \cdot OH + 0.57 \cdot HO_2 + 0.23 \cdot CO + 0.27 \cdot CO_2 + 0.52 \cdot CH_3COCH_3 + 0.34 \cdot CH_2O + 0.05 \cdot HCOOH + 0.05 \cdot BIGALKANE + 0.06 \cdot CH_3CO_3 + 0.06 \cdot CH_3COCH_2O_2$	$1.200 \cdot 10^{-14}$	
$APIN + NO_3 \longrightarrow NTERPO_2$	$1.200 \cdot 10^{-12} \exp(490./T)$	
$BPIN + NO_3 \longrightarrow NTERPO_2$	$2.500 \cdot 10^{-12}$	
$LIMON + NO_3 \longrightarrow NTERPO_2$	$1.100 \cdot 10^{-11}$	
$MYRC + NO_3 \longrightarrow NTERPO_2$	$1.200 \cdot 10^{-11}$	
$BCARY + NO_3 \longrightarrow NTERPO_2 + 0.5 \cdot TERPROD_1$	$1.900 \cdot 10^{-11}$	
$TERPO_2 + NO \longrightarrow 0.26 \cdot TERPNO_3 + 0.74 \cdot NO_2 + 0.36 \cdot CH_2O + 0.045 \cdot CH_3COCH_3 + 0.695 \cdot TERPROD_1 + 0.74 \cdot HO_2$	$4.200 \cdot 10^{-12} \exp(180./T)$	alkyl nitrate yield according to Rindelaub et al. (2015) for alpha-pinene
$TERPO_2 + HO_2 \longrightarrow TERPOOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$TERPO_2 + CH_3O_2 \longrightarrow 1.15 \cdot CH_2O + 0.05 \cdot CH_3COCH_3 + 0.945 \cdot TERPROD_1 + HO_2 + 0.25 \cdot CH_3OH$	$2.000 \cdot 10^{-12} \exp(500./T)$	
$TERPO_2 + CH_3CO_3 \longrightarrow 0.4 \cdot CH_2O + 0.05 \cdot CH_3COCH_3 + 0.945 \cdot TERPROD_1 + HO_2 + CH_3O_2 + CO_2$	$1.000 \cdot 10^{-11}$	
$TERPOOH + OH \longrightarrow H_2O + TERPO_2$	$3.300 \cdot 10^{-11}$	
$TERPROD_1 + OH \longrightarrow TERP_2O_2$	$5.700 \cdot 10^{-11}$	
$TERPROD_1 + NO_3 \longrightarrow 0.5 \cdot TERP_2O_2 + 0.5 \cdot NTERPO_2 + 0.5 \cdot NO_2$	$1.000 \cdot 10^{-12}$	
$TERPNO_3 + OH \longrightarrow NO_2 + TERPROD_1 + H_2O$	$3.500 \cdot 10^{-12}$	
$TERP_2O_2 + NO \longrightarrow 0.1 \cdot TERPNO_3 + 0.9 \cdot NO_2 + 0.34 \cdot CH_2O + 0.27 \cdot CH_3COCH_3 + 0.225 \cdot CO + 0.9 \cdot CO_2 + 0.9 \cdot TERPROD_2 + 0.9 \cdot HO_2 + 0.225 \cdot GLYALD$	$4.200 \cdot 10^{-12} \exp(180./T)$	
$TERP_2O_2 + HO_2 \longrightarrow TERP_2OOH$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$TERP_2O_2 + CH_3O_2 \longrightarrow TERPROD_2 + 0.93 \cdot CH_2O + 0.25 \cdot CH_3OH + HO_2 + 0.5 \cdot CO_2 + 0.125 \cdot CO + 0.125 \cdot GLYALD + 0.15 \cdot CH_3COCH_3$	$2.000 \cdot 10^{-12} \exp(500./T)$	
$TERP_2O_2 + CH_3CO_3 \longrightarrow 0.34 \cdot CH_2O + 0.27 \cdot CH_3COCH_3 + 0.225 \cdot CO + 2 \cdot CO_2 + TERPROD_2 + HO_2 + 0.225 \cdot GLYALD + CH_3O_2$	$1.000 \cdot 10^{-11}$	
$TERP_2OOH + OH \longrightarrow H_2O + TERP_2O_2$	$2.300 \cdot 10^{-11}$	

Table S14: C10/C15 oxidation (terpenes, sesqui-terpenes; ... continued)

reaction	rate coefficient	reference
$TERPROD_2 + OH \longrightarrow 0.15 \cdot CH_3COCH_2O_2 + 0.68 \cdot CH_2O + 1.8 \cdot CO_2 + 0.5 \cdot CH_3COCH_3 + 0.65 \cdot CH_3CO_3 + 0.2 \cdot HO_2 + 0.7 \cdot CO$	$3.400 \cdot 10^{-11}$	
$NTERPO_2 + NO \longrightarrow 0.26 \cdot NTERPNO_3 + 1.48 \cdot NO_2 + 0.74 \cdot TERPROD_1$	$4.200 \cdot 10^{-12} \exp(180./T)$	alkyl nitrate yield according to Rindelaub et al. (2015) for alpha-pinene
$NTERPO_2 + HO_2 \longrightarrow NTERPNO_3$	$7.500 \cdot 10^{-13} \exp(700./T)$	
$NTERPO_2 + CH_3O_2 \longrightarrow 0.5 \cdot NTERPNO_3 + 0.75 \cdot CH_2O + 0.25 \cdot CH_3OH + 0.5 \cdot HO_2 + 0.5 \cdot TERPROD_1 + 0.5 \cdot NO_2$	$2.000 \cdot 10^{-12} \exp(500./T)$	
$NTERPO_2 + CH_3CO_3 \longrightarrow CH_3O_2 + TERPROD_1 + CO_2 + NO_2$	$1.000 \cdot 10^{-11}$	
$NTERPO_2 + NO_3 \longrightarrow 2 \cdot NO_2 + TERPROD_1$	$2.400 \cdot 10^{-12}$	
$NTERPNO_3 + OH \longrightarrow NO_2 + TERPROD_1 + H_2O$	$3.500 \cdot 10^{-12}$	
$ELVOC + OH \longrightarrow HO_2 + TERPROD_1$	$1.000 \cdot 10^{-11}$	a general rate coefficient for oxygenated VOC

Table S15: Tropospheric halogen + organics reactions

reaction	rate coefficient	reference
$CL + CH_2O \longrightarrow HCL + HO_2 + CO$	$8.100 \cdot 10^{-11} \exp(-30./T)$	
$CL + CH_4 \longrightarrow CH_3O_2 + HCL$	$7.300 \cdot 10^{-12} \exp(-1280./T)$	
$CL + CH_3CN \longrightarrow CH_2O + HCL + CO + NO$	$1.600 \cdot 10^{-11} \exp(-2140./T)$	JPL (2011), products: Tyndall
$CL + C_2H_2 + M \longrightarrow 0.1 \cdot CL + 0.1 \cdot GLYOXAL + 0.9 \cdot HCL + 0.9 \cdot HO_2 + 1.8 \cdot CO + M$	$ktroe(5.200 \cdot 10^{-30}, 2.4, 2.200 \cdot 10^{-10}, 0.7, 0.6)$	
$CL + C_2H_4 + M \longrightarrow HO_2 + 2 \cdot CO + HCL + M$	$ktroe(1.600e-29, 3.3, 3.100 \cdot 10^{-10}, 1., 0.6)$	
$CL + C_2H_6 \longrightarrow C_2H_5O_2 + HCL$	$7.200 \cdot 10^{-11} \exp(-70./T)$	
$CL + CH_3O_2 \longrightarrow 0.5 \cdot CLO + 0.5 \cdot CH_2O + 0.5 \cdot HCL + 0.5 \cdot OH + 0.5 \cdot CO + HO_2$	$1.600 \cdot 10^{-10}$	50% CH2OO is produced and assumed to be produced mostly in dry environments and thus decomposing
$CL + CH_3OH \longrightarrow CH_2O + HO_2 + HCL$	$7.100 \cdot 10^{-11} \exp(-75./T)$	IUPAC (2008)
$CL + CH_3OOH \longrightarrow CH_2O + OH + HCL$	$5.900 \cdot 10^{-11}$	IUPAC (2008)
$CL + CH_3CHO \longrightarrow CH_3CO_3 + HCL$	$8.000 \cdot 10^{-11}$	IUPAC (2008)
$CL + GLYALD \longrightarrow 0.35 \cdot GLYOXAL + 0.35 \cdot HO_2 + 0.65 \cdot HOCH_2CO_3 + HCL$	$7.600 \cdot 10^{-11}$	k by Bacher et al. (2001); products by Niki et al. (1987)
$CL + GLYOXAL \longrightarrow HCL + HCOCO_3$	$3.441 \cdot 10^{-11}$	k(298K) from Niki et al. (1985); k(CH_2O + Cl) has been adjusted for the k(CH_2O + Cl) by JPL (2011) used here
$CL + C_3H_8 \longrightarrow C_3H_7O_2 + HCL$	$1.400 \cdot 10^{-10}$	IUPAC (2008)

Table S15: Tropospheric halogen + organics reactions (... continued)

reaction	rate coefficient	reference
$CL + CH_3COCH_3 \longrightarrow CH_3COCH_2O_2 + HCL$	$1.500 \cdot 10^{-11} \exp(-590./T)$	IUPAC (2008)
$CL + HYAC \longrightarrow CH_3COCHO + HO_2 + HCL$	$5.400 \cdot 10^{-11}$	Calvert et al. (2008a)
$CL + BIGALKANE \longrightarrow ALKO_2 + HCL$	$1.935e - 10$	from the reaction with OH, BIGALKANE seems to be methyl-butane whose k is an average of k given by Qian et al. (2002) and Anderson et al. (2007)
$CL + MEK \longrightarrow HCL + MEKO_2$	$3.800 \cdot 10^{-11} \exp(16./T)$	Calvert et al. (2008b)
$CLO + CH_3O_2 \longrightarrow CL + HO_2 + CH_2O$	$3.300 \cdot 10^{-12} \exp(-115./T)$	
$BR + CH_2O \longrightarrow HBR + HO_2 + CO$	$1.700 \cdot 10^{-11} \exp(-800./T)$	
$BR + CH_3CHO \longrightarrow CH_3CO_3 + HBR$	$1.800 \cdot 10^{-11} \exp(-460./T)$	IUPAC (2008)
$BRO + CH_3O_2 \longrightarrow HOBR + OH + HO_2 + CO$	$2.420 \cdot 10^{-14} \exp(1617./T)$	Shallcross et al. (2015); CH_2OO assumed to be produced mostly in dry environments and thus decomposing

Table S16: Sulfur reactions

reaction	rate coefficient	reference
$SO_2 + OH + M \longrightarrow H_2SO_4 + HO_2$	$ktroe(3.300 \cdot 10^{-31}, 4.3, 1.600 \cdot 10^{-12}, 0., 0.6)$	JPL (2011)
$DMS + OH \longrightarrow CH_3SO_2 + HCHO$	$1.130 \cdot 10^{-11} \exp(-253./T)$	
$DMS + OH \longrightarrow DMSO + HO_2$	$1. \cdot 10^{-9} \exp(5820./T) \cdot [O_2]/(1. \cdot 10^{30} + 5. \cdot \exp(6280./T) \cdot [O_2])$	
$DMS + NO_3 \longrightarrow CH_3SO_2 + HNO_3 + HCHO$	$1.900 \cdot 10^{-13} \exp(520./T)$	
$DMS + CL \longrightarrow CH_3SO_2 + HCL + HCHO$	$3.300 \cdot 10^{-10}$	
$DMS + BR \longrightarrow CH_3SO_2 + HBR + HCHO$	$9.000 \cdot 10^{-11} \exp(-2386./T)$	
$DMS + BRO \longrightarrow BR + DMSO$	$4.400 \cdot 10^{-13}$	
$DMSO + OH \longrightarrow 0.6 \cdot SO_2 + HCHO + 0.6 \cdot CH_3O_2 + 0.4 \cdot HO_2 + 0.4 \cdot CH_3SO_3H$	$1.000 \cdot 10^{-10}$	
$CH_3SO_2 \longrightarrow CH_3O_2 + SO_2$	$1.800 \cdot 10^{13} \exp(-8661./T)$	
$CH_3SO_2 + O_3 \longrightarrow CH_3SO_3$	$3.000 \cdot 10^{-13}$	
$CH_3SO_3 + HO_2 \longrightarrow CH_3SO_3H$	$5.000 \cdot 10^{-11}$	

Table S17: Stratospheric O(1D) reactions (... continued)

reaction	rate coefficient	reference

Table S17: Stratospheric O(1D) reactions

reaction	rate coefficient	reference
$O_1D + N_2O \longrightarrow 2 \cdot NO$	$7.250 \cdot 10^{-11} \exp(20./T)$	
$O_1D + N_2O \longrightarrow N_2 + O_2$	$4.630 \cdot 10^{-11} \exp(20./T)$	
$O_1D + O_3 \longrightarrow 2 \cdot O_2$	$1.200 \cdot 10^{-10}$	
$O_1D + CFC_{11} \longrightarrow 2 \cdot CL + COFCL$	$2.020 \cdot 10^{-10}$	
$O_1D + CFC_{12} \longrightarrow 2 \cdot CL + COF_2$	$1.204 \cdot 10^{-10}$	
$O_1D + CFC_{113} \longrightarrow 2 \cdot CL + COFCL + COF_2$	$1.500 \cdot 10^{-10}$	
$O_1D + CFC_{114} \longrightarrow 2 \cdot CL + 2 \cdot COF_2$	$9.750 \cdot 10^{-11}$	
$O_1D + CFC_{115} \longrightarrow CL + F + 2 \cdot COF_2$	$1.500 \cdot 10^{-11}$	
$O_1D + HCFC_{22} \longrightarrow CL + COF_2$	$7.200 \cdot 10^{-11}$	
$O_1D + HCFC_{141}B \longrightarrow CL + COFCL$	$1.794 \cdot 10^{-10}$	
$O_1D + HCFC_{142}B \longrightarrow CL + COF_2$	$1.628 \cdot 10^{-10}$	
$O_1D + CCL_4 \longrightarrow 4 \cdot CL$	$2.840 \cdot 10^{-10}$	
$O_1D + CH_3BR \longrightarrow BR$	$1.674 \cdot 10^{-10}$	
$O_1D + CF_2CLBR \longrightarrow BR + CL + COF_2$	$9.600 \cdot 10^{-11}$	
$O_1D + CF_3BR \longrightarrow BR + F + COF_2$	$4.100 \cdot 10^{-11}$	
$O_1D + H_{1202} \longrightarrow 2 \cdot BR + COF_2$	$1.012 \cdot 10^{-10}$	
$O_1D + H_{2402} \longrightarrow 2 \cdot BR + 2 \cdot COF_2$	$1.200 \cdot 10^{-10}$	
$O_1D + CHBR_3 \longrightarrow 3 \cdot BR$	$4.490 \cdot 10^{-10}$	
$O_1D + CH_2BR_2 \longrightarrow 2 \cdot BR$	$2.570 \cdot 10^{-10}$	
$O_1D + COF_2 \longrightarrow 2 \cdot F$	$2.140 \cdot 10^{-11}$	
$O_1D + COFCL \longrightarrow CL + F$	$1.900 \cdot 10^{-10}$	
$O_1D + CH_4 \longrightarrow CH_3O_2 + OH$	$1.310 \cdot 10^{-10}$	
$O_1D + CH_4 \longrightarrow CH_2O + H + HO_2$	$3.500 \cdot 10^{-11}$	
$O_1D + CH_4 \longrightarrow CH_2O + H_2$	$9.000 \cdot 10^{-12}$	
$O_1D + H_2 \longrightarrow H + OH$	$1.200 \cdot 10^{-10}$	
$O_1D + HCL \longrightarrow CL + OH$	$1.500 \cdot 10^{-10}$	
$O_1D + HBR \longrightarrow BR + OH$	$1.200 \cdot 10^{-10}$	
$O_1D + HCN \longrightarrow CO + OH + NO$	$7.700 \cdot 10^{-11} \exp(100./T)$	Strekowski et al. (2001), products: Tyndall

Table S18: Stratospheric inorganic halogen reactions

reaction	rate coefficient	reference
$CL + O_3 \longrightarrow CLO + O_2$	$2.300 \cdot 10^{-11} \exp(-200./T)$	
$CL + H_2 \longrightarrow H + HCL$	$3.050 \cdot 10^{-11} \exp(-2270./T)$	
$CL + H_2O_2 \longrightarrow HCL + HO_2$	$1.100 \cdot 10^{-11} \exp(-980./T)$	
$CL + HO_2 \longrightarrow HCL + O_2$	$1.400 \cdot 10^{-11} \exp(270./T)$	
$CL + HO_2 \longrightarrow CLO + OH$	$3.600 \cdot 10^{-11} \exp(-375./T)$	
$CL_2O_2 + M \longrightarrow 2 \cdot CLO + M$	$kCL2O2$	
$CLO + O \longrightarrow CL + O_2$	$2.800 \cdot 10^{-11} \exp(85./T)$	
$CLO + OH \longrightarrow CL + HO_2$	$7.400 \cdot 10^{-12} \exp(270./T)$	
$CLO + OH \longrightarrow HCL + O_2$	$6.000 \cdot 10^{-13} \exp(230./T)$	
$CLO + HO_2 \longrightarrow HOCL + O_2$	$2.600 \cdot 10^{-12} \exp(290./T)$	
$CLO + NO \longrightarrow CL + NO_2$	$6.400 \cdot 10^{-12} \exp(290./T)$	
$CLO + NO_2 + M \longrightarrow CLONO_2 + M$	$ktroe(1.800 \cdot 10^{-31}, 3.4, 1.500 \cdot 10^{-11}, 1.9, 0.6)$	
$CLO + CLO \longrightarrow 2 \cdot CL + O_2$	$3.000 \cdot 10^{-11} \exp(-2450./T)$	
$CLO + CLO \longrightarrow CL_2 + O_2$	$1.000 \cdot 10^{-12} \exp(-1590./T)$	
$CLO + CLO \longrightarrow CL + OCLO$	$3.500 \cdot 10^{-13} \exp(-1370./T)$	
$CLO + CLO + M \longrightarrow CL_2O_2 + M$	$ktroe(1.600 \cdot 10^{-32}, 4.5, 3.000 \cdot 10^{-12}, 2., 0.6)$	
$HCL + OH \longrightarrow CL + H_2O$	$1.800 \cdot 10^{-12} \exp(-250./T)$	
$HCL + O \longrightarrow CL + OH$	$1.000 \cdot 10^{-11} \exp(-3300./T)$	
$HOCL + O \longrightarrow CLO + OH$	$1.700 \cdot 10^{-13}$	
$HOCL + CL \longrightarrow CLO + HCL$	$3.400 \cdot 10^{-12} \exp(-130./T)$	
$HOCL + OH \longrightarrow CLO + H_2O$	$3.000 \cdot 10^{-12} \exp(-500./T)$	
$CLONO_2 + O \longrightarrow CLO + NO_3$	$3.600 \cdot 10^{-12} \exp(-840./T)$	
$CLONO_2 + OH \longrightarrow HOCL + NO_3$	$1.200 \cdot 10^{-12} \exp(-330./T)$	
$CLONO_2 + CL \longrightarrow CL_2 + NO_3$	$6.500 \cdot 10^{-12} \exp(135./T)$	
$BR + O_3 \longrightarrow BRO + O_2$	$1.600 \cdot 10^{-11} \exp(-780./T)$	
$BR + HO_2 \longrightarrow HBR + O_2$	$4.800 \cdot 10^{-12} \exp(-310./T)$	
$BR + NO_2 + M \longrightarrow 0.85 \cdot BRONO + 0.15 \cdot BRNO_2 + M$	$ktroe(4.200 \cdot 10^{-31}, 2.4, 2.700 \cdot 10^{-11}, 0., 0.6)$	
$BRONO + M \longrightarrow BR + NO_2 + M$	$1.648 \cdot 10^{11} \exp(-7399./T)$	fit to upper limit by Wine et al. (1993) and scaled 1.5 factor to match data by Orlando and Burkholder (2000)
$BRO + O \longrightarrow BR + O_2$	$1.900 \cdot 10^{-11} \exp(230./T)$	
$BRO + OH \longrightarrow BR + HO_2$	$1.700 \cdot 10^{-11} \exp(250./T)$	
$BRO + HO_2 \longrightarrow HOBR + O_2$	$4.500 \cdot 10^{-12} \exp(460./T)$	

Table S18: Stratospheric inorganic halogen reactions (... continued)

reaction	rate coefficient	reference
$BRO + NO \longrightarrow BR + NO_2$	$8.800 \cdot 10^{-12} \exp(260./T)$	
$BRO + NO_2 + M \longrightarrow BRONO_2 + M$	$ktroe(5.200 \cdot 10^{-31}, 3.2, 6.900 \cdot 10^{-12}, 2.9, 0.6)$	
$BRO + CLO \longrightarrow BR + OCLO$	$9.500 \cdot 10^{-13} \exp(550./T)$	
$BRO + CLO \longrightarrow BR + CL + O_2$	$2.300 \cdot 10^{-12} \exp(260./T)$	
$BRO + CLO \longrightarrow BRCL + O_2$	$4.100 \cdot 10^{-13} \exp(290./T)$	
$BRO + BRO \longrightarrow 2 \cdot BR + O_2$	$2.400 \cdot 10^{-12} \exp(40./T)$	
$BRO + BRO \longrightarrow BR_2 + O_2$	$2.800 \cdot 10^{-14} \exp(860./T)$	
$HBR + OH \longrightarrow BR + H_2O$	$5.500 \cdot 10^{-12} \exp(200./T)$	
$HBR + O \longrightarrow BR + OH$	$5.800 \cdot 10^{-12} \exp(-1500./T)$	
$HOBR + O \longrightarrow BRO + OH$	$1.200 \cdot 10^{-10} \exp(-430./T)$	
$BRONO_2 + O \longrightarrow BRO + NO_3$	$1.900 \cdot 10^{-11} \exp(215./T)$	
$BRONO_2 + BR \longrightarrow BR_2 + NO_3$	$5.805 \cdot 10^{-11}$	Average of k at 298K by Orlando and Tyndall (1996) and Harwood et al. (1998)
$BR_2 + OH \longrightarrow BR + HOBR$	$2.100 \cdot 10^{-11} \exp(240./T)$	
$F + H_2O \longrightarrow HF + OH$	$1.400 \cdot 10^{-11}$	
$F + H_2 \longrightarrow H + HF$	$1.400 \cdot 10^{-10} \exp(-500./T)$	
$F + CH_4 \longrightarrow CH_3O_2 + HF$	$1.600 \cdot 10^{-10} \exp(-260./T)$	
$F + HNO_3 \longrightarrow HF + NO_3$	$6.000 \cdot 10^{-12} \exp(400./T)$	

Table S19: Stratospheric organic halogen reactions

reaction	rate coefficient	reference
$CH_3BR + OH \longrightarrow BR + H_2O + HO_2$	$2.350 \cdot 10^{-12} \exp(-1300./T)$	
$CH_3BR + CL \longrightarrow HCL + HO_2 + BR$	$1.400 \cdot 10^{-11} \exp(-1030./T)$	
$CH_2BR_2 + OH \longrightarrow 2 \cdot BR + H_2O$	$2.000 \cdot 10^{-12} \exp(-840./T)$	
$CHBR_3 + OH \longrightarrow 3 \cdot BR$	$1.350 \cdot 10^{-12} \exp(-600./T)$	
$CH_2BR_2 + CL \longrightarrow 2 \cdot BR + HCL$	$6.300 \cdot 10^{-12} \exp(-800./T)$	
$CHBR_3 + CL \longrightarrow 3 \cdot BR + HCL$	$4.850 \cdot 10^{-12} \exp(-850./T)$	
$CH_3CL + CL \longrightarrow CO + HO_2 + 2 \cdot HCL$	$2.170 \cdot 10^{-11} \exp(-1130./T)$	
$CH_3CL + OH \longrightarrow CO + HO_2 + HCL + H_2O$	$2.400 \cdot 10^{-12} \exp(-1250./T)$	products: Tyndall(p.c.), implicitly includes $NO \longrightarrow NO_2$ conversion with CH_2ClO_2
$CH_3CCL_3 + OH \longrightarrow H_2O + 3 \cdot CL$	$1.640 \cdot 10^{-12} \exp(-1520./T)$	
$HCFC_{22} + OH \longrightarrow CL + H_2O + COF_2$	$1.050 \cdot 10^{-12} \exp(-1600./T)$	
$HCFC_{141}B + OH \longrightarrow CL + COFCL$	$1.250 \cdot 10^{-12} \exp(-1600./T)$	

Table S19: Stratospheric organic halogen reactions (... continued)

reaction	rate coefficient	reference
$HCFC_{142}B + OH \longrightarrow CL + COF_2$	$1.300 \cdot 10^{-12} \exp(-1770./T)$	

Table S20: (Tropospheric) heterogeneous reactions

reaction	reaction probability	reference
$O_3 \longrightarrow HO_2$	$\gamma = 10^{-6}$	Stadtler et al. (2017)
$HO_2 \longrightarrow 0.5 \cdot H_2O_2$	$\gamma = 0.2$	Stadtler et al. (2017)
$NO_3 \longrightarrow$	$\gamma = 0.001$	Stadtler et al. (2017)
$NO_2 \longrightarrow 0.5 \cdot HONO$	$\gamma = 10^{-4}$	Stadtler et al. (2017)
$HNO_3 \longrightarrow$	$\gamma_{SS} = 0.01$, $\gamma_{DU} = 0.1$	Stadtler et al. (2017)
$N_2O_5 \longrightarrow$	$\gamma = f(T, RH)$	Stadtler et al. (2017)

Table S21: Stratospheric Sulfate aerosol reactions

reaction	reaction probability	reference
$N_2O_5 \longrightarrow 2 \cdot HNO_3$	$\gamma = 0.04$	Lamarque et al. (2012)
$CLONO_2 \longrightarrow HOCL + HNO_3$	$f(sulfuricacidwt\%)$	Lamarque et al. (2012)
$BRONO_2 \longrightarrow HOBR + HNO_3$	$f(T, P, HCl, H_2O, r)$	Lamarque et al. (2012)
$CLONO_2 + HCL \longrightarrow CL_2 + HNO_3$	$f(T, P, H_2O, r)$	Lamarque et al. (2012)
$HOCL + HCL \longrightarrow CL_2 + H_2O$	$f(T, P, HCl, H_2O, r)$	Lamarque et al. (2012)
$HOBR + HCL \longrightarrow BRCL + H_2O$	$f(T, P, HCl, HOBr, H_2O, r)$	Lamarque et al. (2012)

Table S22: Stratospheric Nitric acid dihydrate reactions

reaction	reaction probability	reference
$N_2O_5 \longrightarrow 2 \cdot HNO_3$	$\gamma = 0.0004$	Lamarque et al. (2012)
$CLONO_2 \longrightarrow HOCL + HNO_3$	$\gamma = 0.004$	Lamarque et al. (2012)
$CLONO_2 + HCL \longrightarrow CL_2 + HNO_3$	$\gamma = 0.2$	Lamarque et al. (2012)
$HOCL + HCL \longrightarrow CL_2 + H_2O$	$\gamma = 0.1$	Lamarque et al. (2012)
$BRONO_2 \longrightarrow HOBR + HNO_3$	$\gamma = 0.3$	Lamarque et al. (2012)

Table S23: Stratospheric Ice aerosol reactions

reaction	reaction probability	reference
$N_2O_5 \longrightarrow 2 \cdot HNO_3$	$\gamma = 0.02$	Lamarque et al. (2012)
$CLONO_2 \longrightarrow HOCL + HNO_3$	$\gamma = 0.3$	Lamarque et al. (2012)
$BRONO_2 \longrightarrow HOBR + HNO_3$	$\gamma = 0.3$	Lamarque et al. (2012)
$CLONO_2 + HCL \longrightarrow CL_2 + HNO_3$	$\gamma = 0.3$	Lamarque et al. (2012)
$HOCL + HCL \longrightarrow CL_2 + H_2O$	$\gamma = 0.2$	Lamarque et al. (2012)
$HOBR + HCL \longrightarrow BRCL + H_2O$	$\gamma = 0.3$	Lamarque et al. (2012)

Table S24: Henry coefficients (H_0 and temperature factor) and dry deposition reactivities for gas-phase species in ECHAM-HAMMOZ.

Species	H	Reactivity coefficient	Source
CO	$9.81 \cdot 10^{-4}$, 1720.	0.	JPL (2011)
H_2	$7.8 \cdot 10^{-4}$, 500.	0.	Sander (1999)
H_2O_2	$8.44 \cdot 10^{4}$, 7600.	1	JPL (2011)
HCN	12., 5000.	1	Sander (1999)
HNO_3	$3.2 \cdot 10^{11}$, 8700.	1	$H = 2.1 \cdot 10^5$ M/atm and $Ka = 15.4$ M (Schwartz and White, 1981). At an average cloud droplet pH=5 $\Rightarrow$ H* $= H \cdot (1 + Ka/[H+]) = 2.1 \cdot 10^5 \cdot (1 + 15.4/1 \cdot 10^{-5}) = 3.2 \cdot 10^{11}$
HO_2	690., 0.	1	JPL (2006)
HO_2NO_2	$1.2 \cdot 10^{4}$, 6900.	1	Sander (1999)
HONO	$5.05 \cdot 10^{3}$, 4800.	0.1	Sander (1999): H=49 and $Ka = 5.1 \cdot 10^{-4} \Rightarrow$ H* $= 49(1 + 5.1 \cdot 10^{-4} * 1 \cdot 10^7) = 5.05 \cdot 10^3$
N_2O_5	2.1, 3400.	1	Sander (1999): 2 ref. give it as infinite and one as 2.1 M/atm
N_2O_5	$3.2 \cdot 10^{11}$, 8700.	1	HNO_3 as proxy as done in GEOS-Chem
NH_3	$1.02 \cdot 10^{4}$, 4200.	0.	Sander (2015): $H(298) = 58$ M/atm and H*(298) calculated at pH=7 with $Kb = 1.75 \cdot 10^5$ M
NO	$1.92 \cdot 10^{-3}$, 1790.	1	JPL (2006), comment
NO_2	$12. \cdot 10^{-2}$, 2360.	1	JPL (2011)
NO_3	$3.8 \cdot 10^{-2}$, 0.	1	JPL (2006)
O_3	$1.03 \cdot 10^{-2}$, 2830.	1	JPL (2006)
SO_2	$2.45 \cdot 10^{5}$, 3100.	0.	Sander (2015): $H(298) = 1.2$ M/atm and H*(298) calculated at pH=7 with $K1a = 1.23 \cdot 10^{-2}$ M and $K2a = 6.61 \cdot 10^{-8}$ M
H_2SO_4	$1.3 \cdot 10^{15}$, 20000.	0.	Sander (2015)
CH_4	$1.41 \cdot 10^{-3}$, 2040.	0.	JPL (2011)
CH_2O	$3.23 \cdot 10^{3}$, 7100.	0.1	JPL (2011)
CH_3OH	203., 5640.	0.	JPL (2011)
CH_3OOH	300., 5280.	0.1	JPL (2011)
HCOOH	$8.9 \cdot 10^{3}$, 6100.	0.	Sander (1999): measured value by Johnson et al. (1996)??, surface reactivity as in Nguyen et al. (2015)
$CH_3O_2NO_2$	2.0, 4700.	0.1	Sander (1999): methyl nitrate as proxy species
C_2H_5OH	190., 6660.	0.	JPL (2011)
C_2H_5OOH	336., 5995.	1	JPL (2011)
CH_3CHO	12.9, 5890.	0.1	JPL (2011)
CH_3CN	52.8, 3970.	0.	JPL (2011)
PAN	2.8, 5730.	0.1	JPL (2011)
CH_3COOH	$4.1 \cdot 10^{3}$, 6200.	0.	JPL (2011)

Table S24: Henry coefficients (... continued)

Species	H	Reactivity coefficient	Source
CH_3COOOH	837., 5310.	0.1	JPL (2011)
GLYALD	$4.1 \cdot 10^4$, 4600.	0.1	Sander (1999)
GLYOXAL	$4.19 \cdot 10^5$, 7480.	0.1	JPL (2011)
$HCOCO_2H$	$1.1 \cdot 10^4$, 4800.	0.1	Sander (2015)
$HCOCO_3H$	$1.1 \cdot 10^4$, 4800.	0.1	Sander (2015)
$HOCH_2CO_2H$	$2.8 \cdot 10^4$, 4000.	0.1	Sander (2015)
$HOCH_2CO_3H$	$2.8 \cdot 10^4$, 4000.	0.1	Sander (2015)
C_3H_7OOH	336., 5995.	1	
CH_3COCH_3	27.8, 5530.	0.	JPL (2011)
CH_3COCHO	$3.7 \cdot 10^3$, 7500.	0.1	Sander (1999)
HYAC	$7.7 \cdot 10^3$, 0.	0.1	Sander (2015)
NOA	$1. \cdot 10^3$, 0.	0.1	Sander (2015)
MACR	6.5, 5300.	0.1	Sander (1999)
MACROOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
MACROH	$2.1 \cdot 10^5$, 9900.	0.	Sander (2015)
MEK	37., 8200.	0.1	Sander (2015)
MEKOOH	$1.1 \cdot 10^3$, 7300.	1	Sander (2015)
MPAN	1.7, 0.	0.1	Sander (1999)
MVK	$4.1 \cdot 10^1$, 7800.	0.1	Sander (1999)
$MACO_2H$	$1.5 \cdot 10^3$, 6800.	0.1	Sander (2015)
$MACO_3H$	$1.5 \cdot 10^3$, 6800.	1	Sander (2015)
$BIGALD_1$	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
CO_2H_3CHO	$4.1 \cdot 10^4$, 4600.	0.1	Sander (1999)
$CO_2H_3CO_3H$	$4.1 \cdot 10^4$, 4600.	1	Sander (1999)
BIACETOH	$4.1 \cdot 10^4$, 4600.	0.1	Sander (1999)
IBUTALOH	$4.1{\cdot}10^4$, 4600.	0.1	Sander (1999)
IBUTALOHOOH	$4.1 \cdot 10^4$, 4600.	1	Sander (1999)
LHMVKABOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
MVKN	$5. \cdot 10^3$, 0.	0.1	like for ISOPNO3 from Nguyen et al. (2015)
MACRN	$5. \cdot 10^3$, 0.	0.1	like for ISOPNO3 from Nguyen et al. (2015)
MBO	64., 0.	0.1	Sander (2015)
HPALD	$4.1 \cdot 10^4$, 4600.	1	Sander (1999)
PACALD	$4.1 \cdot 10^4$, 4600.	1	Sander (1999)
$ISOPBNO_3$	$5. \cdot 10^3$, 0.	0.1	Nguyen et al. (2015)

Table S24: Henry coefficients (... continued)

Species	H	Reactivity coefficient	Source
$ISOPDNO_3$	$5. \cdot 10^3$, 0.	0.1	Nguyen et al. (2015)
$LISOPACNO_3$	$5. \cdot 10^3$, 0.	0.1	Nguyen et al. (2015)
LC_5PAN_{1719}	$5. \cdot 10^3$, 0.	0.1	Nguyen et al. (2015)
LHC_4ACCO_2H	$2.1 \cdot 10^5$, 9900.	0.1	Sander (2015)
LHC_4ACCO_3H	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
LIECHO	$4.1 \cdot 10^4$, 4600.	0.1	Sander (1999)
$LIECO_3H$	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
LIEPOX	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
LNISOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
MBOOOH	$3. \cdot 10^{11}$, 0.	1	Sander (2015)
NC_4CHO	2.3, 0.	0.1	Sander (2015)
NISOPOOH	$3.6 \cdot 10^4$, 0.	1	Sander (2015)
LHC_4ACCHO	$4.1 \cdot 10^4$, 4600.	0.1	Sander (1999)
$HCOC_5$	$4.1 \cdot 10^4$, 4600.	1	Sander (1999)
ISOPBOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
ISOPDOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
LISOPACOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
ISOPBOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
ISOPDOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
ISOPAOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
LISOPOOHOOH	$2. \cdot 10^{16}$, 0.	1	Sander (2015)
$LISOPNO_3OOH$	$3. \cdot 10^{11}$, 0.	1	Sander (2015)
$LISOPNO_3NO_3$	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
$LC_{578}OOH$	$3. \cdot 10^{11}$, 0.	1	Sander (2015)
$C_{59}OOH$	$3. \cdot 10^{11}$, 0.	1	Sander (2015)
$BIGALD_2$	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
$BIGALD_3$	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
BZALD	38., 5500.	0.1	Sander (2015)
BZOOH	$2.9 \cdot 10^3$, 0.	1	Sander (2015)
PHENOOH	$3. \cdot 10^{11}$, 0.	1	Sander (2015)
C_6H_5OOH	$3. \cdot 10^3$, 5900.	1	Sander (2015)
PHENOL	$3. \cdot 10^3$, 5900.	0.1	Sander (2015)
CATECHOL	$4.6 \cdot 10^3$, 0.	0.1	Sander (2015)
$CATEC_1OOH$	$4.6 \cdot 10^3$, 0.	1	Sander (2015)

Table S24: Henry coefficients (... continued)

Species	H	Reactivity coefficient	Source
BEPOMUC	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
BENZOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
PBZNIT	2.8, 5730.	0.1	PAN as proxy MCM3.2 name PBZN
$BIGALD_4$	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
TOLOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
CRESOL	$1.1 \cdot 10^3$, 6700.	0.1	Sander (2015)
TEPOMUC	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
$TERPROD_2$	$2.5 \cdot 10^5$, 0.	0.1	Sander (2015)
XYLENOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
XYLOL	$1.1 \cdot 10^3$, 6700.	0.1	cresol as proxy MCM3.2 name OXYLOL
XYLOLOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
TERPOOH	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
$TERP_2OOH$	$2.1 \cdot 10^5$, 9900.	1	Sander (2015)
$TERPNO_3$	$5. \cdot 10^3$, 0.	0.1	like an isoprene nitrate MCM3.2 name APINANO3
$TERPROD_1$	$2.5 \cdot 10^5$, 0.	1	Sander (2015)
$NTERPNO_3$	$5. \cdot 10^3$, 0.	0.1	like an isoprene nitrate MCM3.2 name NAPINAOOH
MTHOM	$2. \cdot 10^9$, 0.	1	Sander (2015)
ALKOH	336., 5995.	0.1	
ALKOOH	336., 5995.	1	
POOH	300., 5280.	0.1	
ROOH	300., 5280.	1	
EOOH	300., 5280.	0.1	
$ALKNO_3$	$5. \cdot 10^3$, 0.	0.1	like for $ISOPNO_3$ from Nguyen et al. (2015) MCM3.2
HF	$1.3 \cdot 10^4$, 0.	0.	Sander (2015)
HCL	$2.0 \cdot 10^{11}$, 600.	0.	Fernandez et al. (2014)
HOCL	$6.6 \cdot 10^2$, 5900.	0.	Sander (1999)
CL_2	$9.2 \cdot 10^{-2}$, 2000.	0.	Sander (1999)
$CLONO_2$	$2. \cdot 10^{13}$, 0.	1	Sander (1999) : listed as ”infinite”
BR_2	$7.2 \cdot 10^{-1}$, 0.	0.	Sander (2015)
HBR	$7.2 \cdot 10^{13}$, 6100.	0.	Fernandez et al. (2014)
HOBR	$6.1 \cdot 10^3$, 0.	0.	Sander (1999)
$BRONO_2$	$2. \cdot 10^{13}$, 0.	1	Sander (1999) : listed as ”infinite”
BRONO	$3. \cdot 10^{-1}$, 0.	0.	Sander (2015)
$BRNO_2$	$3. \cdot 10^{-1}$, 0.	0.	Sander (2015)

Table S24: Henry coefficients (... continued)

Species	H	Reactivity coefficient	Source
BRCL	$9.7 \cdot 10^{-1}$, 5600.	0.	Sander (2015)
DMS	0.54, 3460.	0.	JPL (2011)
DMSO	$9.8 \cdot 10^{4}$, 0.	0.1	JPL (2011)
CH_3SO_3H	$1. \cdot 10^{30}$, 0.	1	Jöckel et al. (2006)

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