Supplement to Comprehensive isoprene and terpene chemistry improves simulated surface ozone in the southeastern U.S.

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Contents

List of Figures

List of Tables

S1 Schematics of NO_3 oxidation

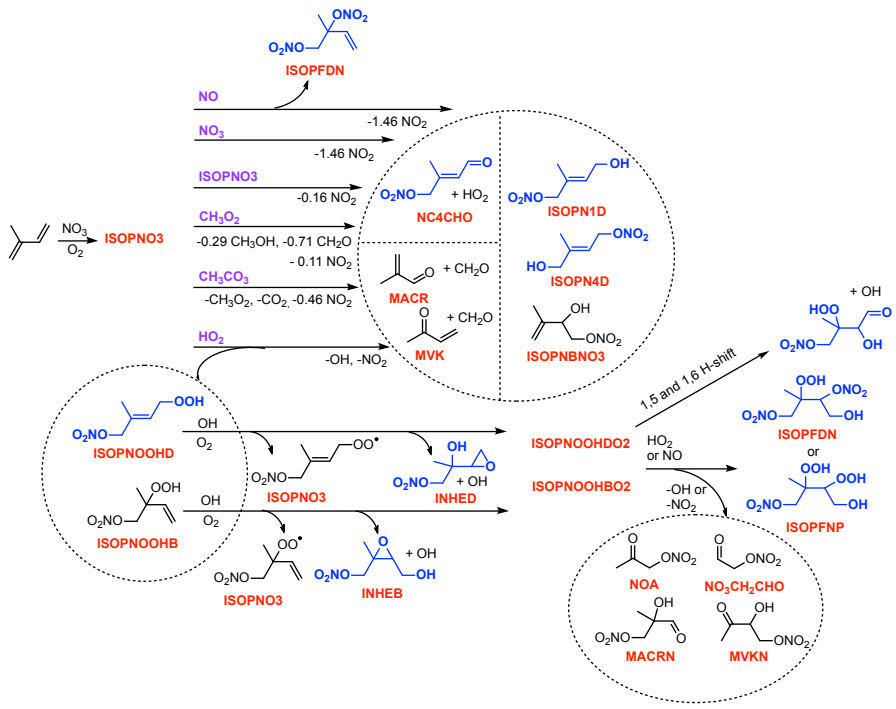

Figure S1. Simplified schematic of the MOZART-TS2 chemical mechanism for isoprene NO_3-initiated oxidation. Blue compounds undergo aerosol uptake.

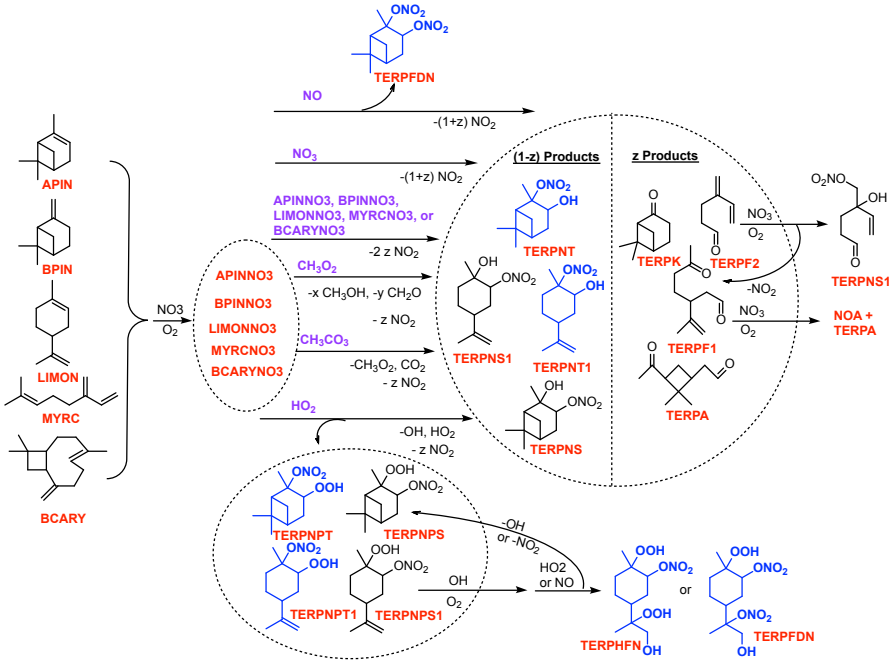

Figure S2. Simplified schematic of the MOZART-TS2 chemical mechanism for terpene NO_3-initiated oxidation. Blue compounds undergo aerosol uptake.

S2 Evaluation Against More Explicit Chemical Schemes for Myrcene and β-caryophyllene

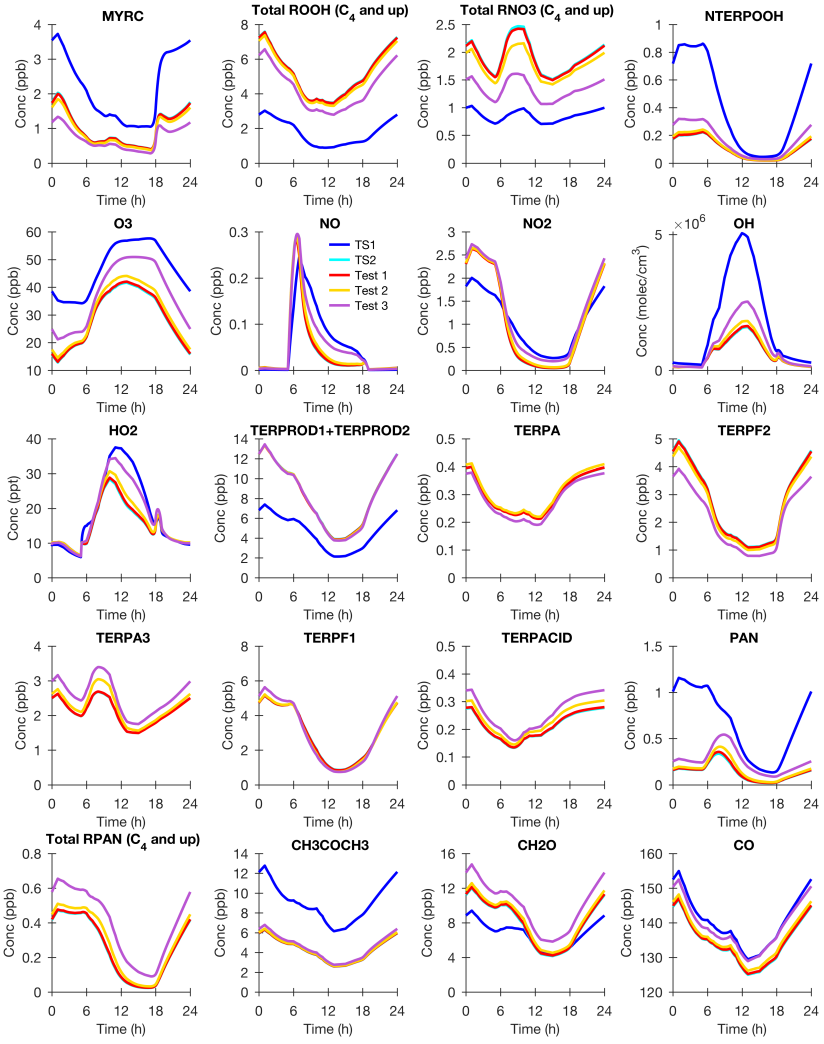

Figure S3. BOXMOX results for myrcene (MYRC) oxidation using TS1 (blue), TS2 (cyan), TS2 with MCM pinonaldehyde nitrate yield - Test 1 (red), TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield - Test 2 (gold), and TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield and assumptions for oxidation of unsaturated hydroxy nitrates - Test 3 (purple). MYRC (myrcene surrogate), TERPOOH (terpene hydroxy hydroperoxide), Total ROOH (all terpene hydroperoxides C_4 and up), TERPNIT (terpene hydroxy nitrate), Total RNO3 (all terpene derived nitrates C_4 and up), O3 (ozone), NO (nitrogen oxide), NO2 (nitrogen dioxide), OH (hydroxyl radical), HO2 (hydroperoxy radical), CH3COCH3 (acetone), TERPROD1 + TERPROD2 (all terpene 1st- and 2nd-gen products except hydroperoxides, nitrates and PANs), TERPA (terpene aldehyde like pinonaldehyde), TERPF2 (terpene product - 2 double bonds), TERPA3 (terpene aldehyde like limonaldehyde), TERPF1 (terpene product - 1 double bond), TERPACID (terpene acid), PAN (peroxy acyl nitrate), and Total RPAN (all terpene PANs C_4 and up), and CO (carbon monoxide).

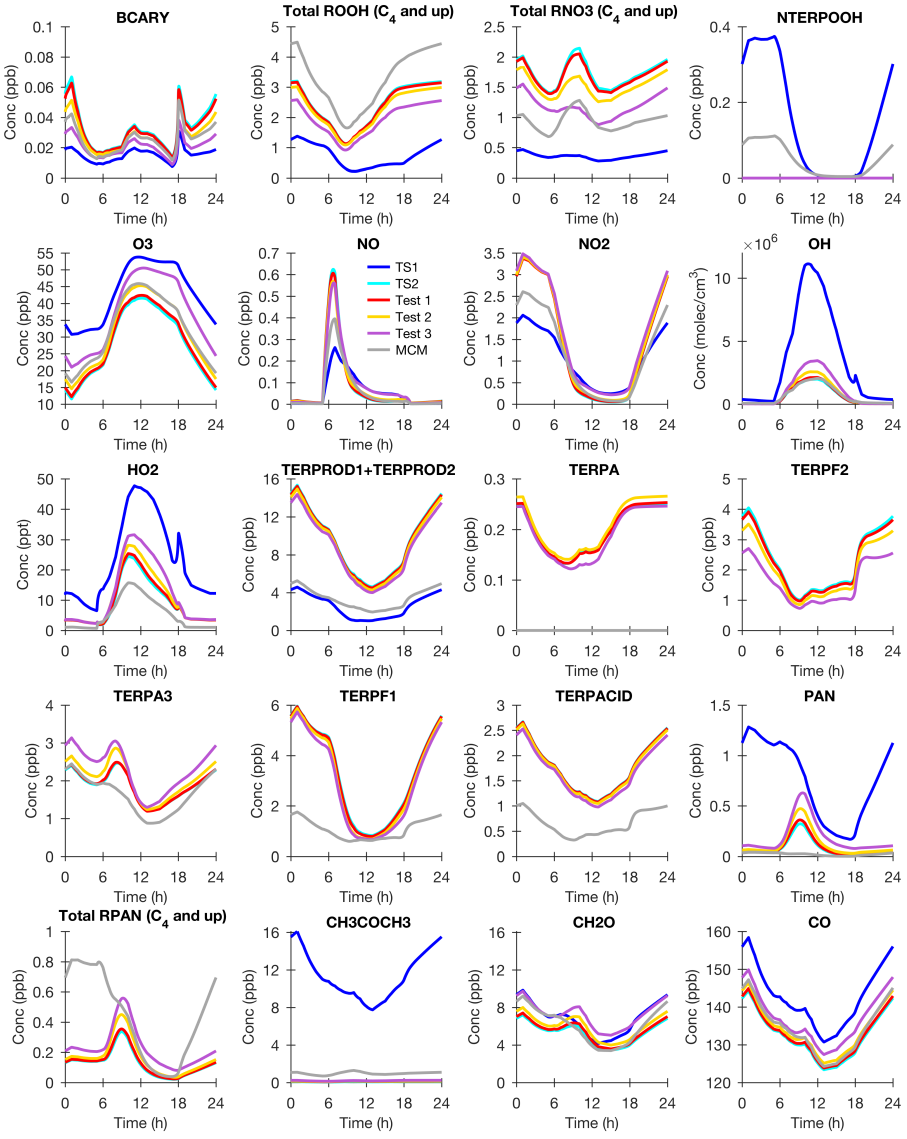

Figure S4. BOXMOX results for β-caryophyllene (BCARY) oxidation using TS1 (blue), TS2 (cyan), MCM (gray), TS2 with MCM pinonaldehyde nitrate yield - Test 1 (red), TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield - Test 2 (gold), and TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield and assumptions for oxidation of unsaturated hydroxy nitrates - Test 3 (purple). All species are identical to Figure S3.

S3 Nudging and Vertical Level Resolution in CESM/CAM-Chem

As shown in Figure S5 and S6, nudging at 50 h versus 5 h relaxation times increases the biogenic emissions likely because of increased surface temperatures, improves the representation of winds compared to observations, but also increases biases in the

ozone vertical profile. There are some small differences in ozone and other compounds when using 32 levels versus 56 levels. Given that CESM/CAM-Chem is tuned using 32 levels and nudging with a 50 h relaxation time appears to add less biases into the ozone vertical profile, 32 levels with a 50 h nudging relaxation time were used in all simulations for this work. The model results do appear to be quite sensitive to the choice of the nudging relaxation time, which will be explored more completely in future work.

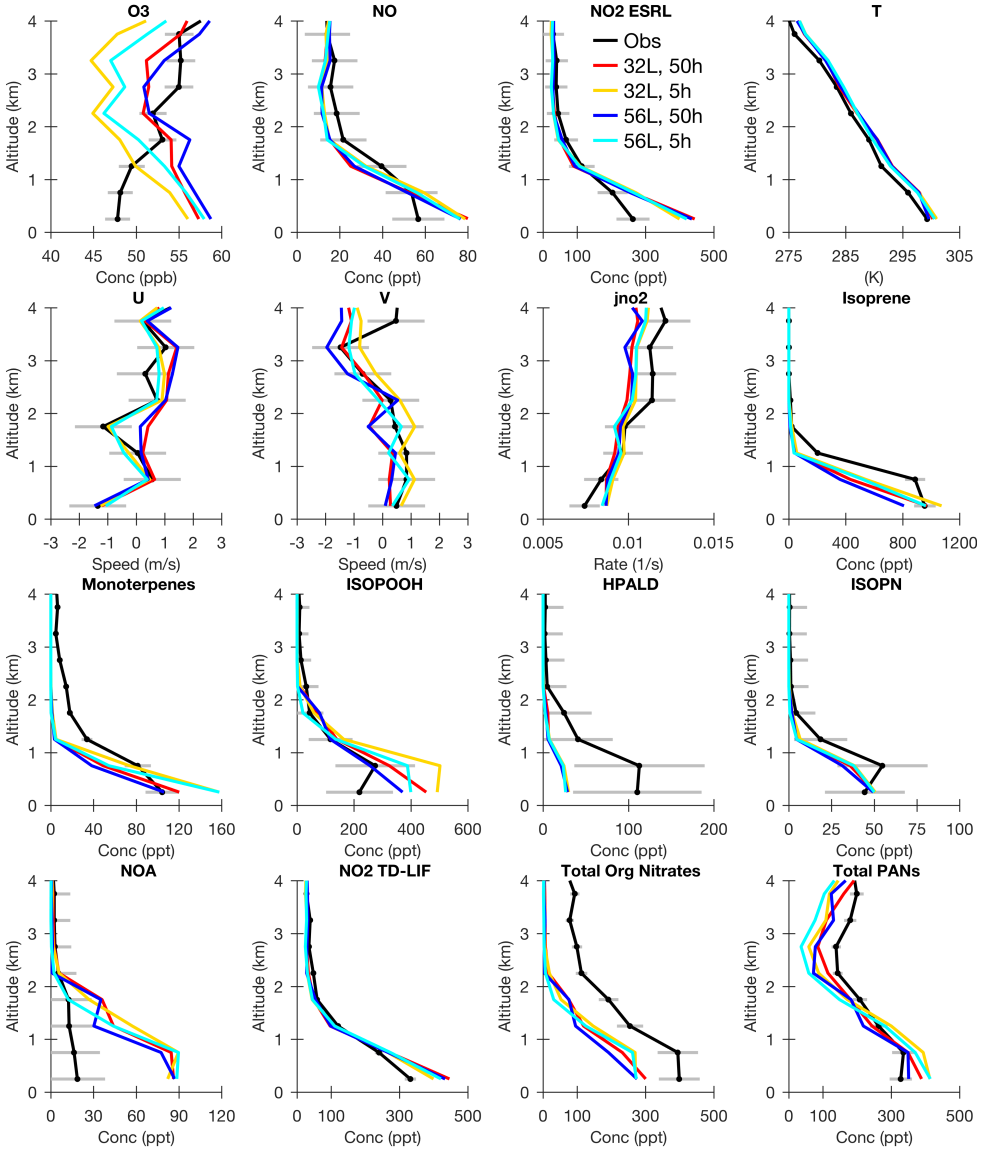

Figure S5. Median vertical profile plots up to 4 km over the SEAC^{4}Rs flight tracks for observations (black), MOZART-TS1 with 32 vertical levels and 50 h relaxation time (red), MOZART-TS1 with 32 vertical levels and 5 h relaxation time (gold), MOZART-TS1 with 56 vertical levels and 50 h relaxation time (blue), and MOZART-TS1 with 56 vertical levels and 5 h relaxation time (cyan). Acronyms are defined in Figure S3. Data are grouped into 0.5 km bins and exclude urban plumes (NO_2> 4 ppb), fire plumes (acetonitrile > 0.2 ppb), and stratospheric air (O_3/CO > 1.25) as done in previous work (Travis et al., 2016). Domain includes the Southeast U.S. (29.5-40°N, 75-94.5°W), and local sun time 9 am to 5 pm. Observational uncertainty is shown in gray bars.

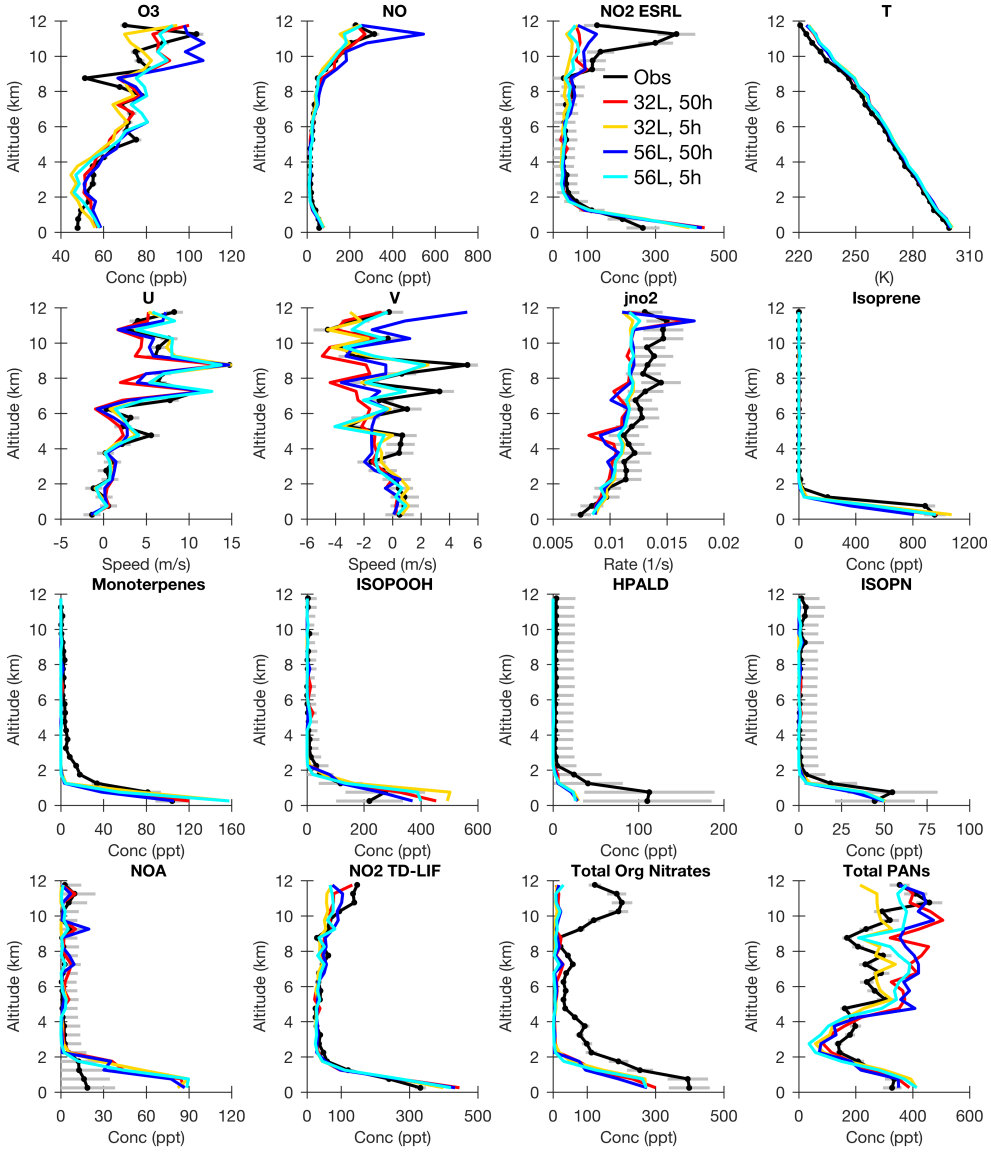

Figure S6. Median vertical profile plots over the SEAC[4]Rs flight tracks identical to Figure S5 except up to 12 km altitude instead of 4 km.

S4 Organic Nitrate Fate in MOZART-TS1

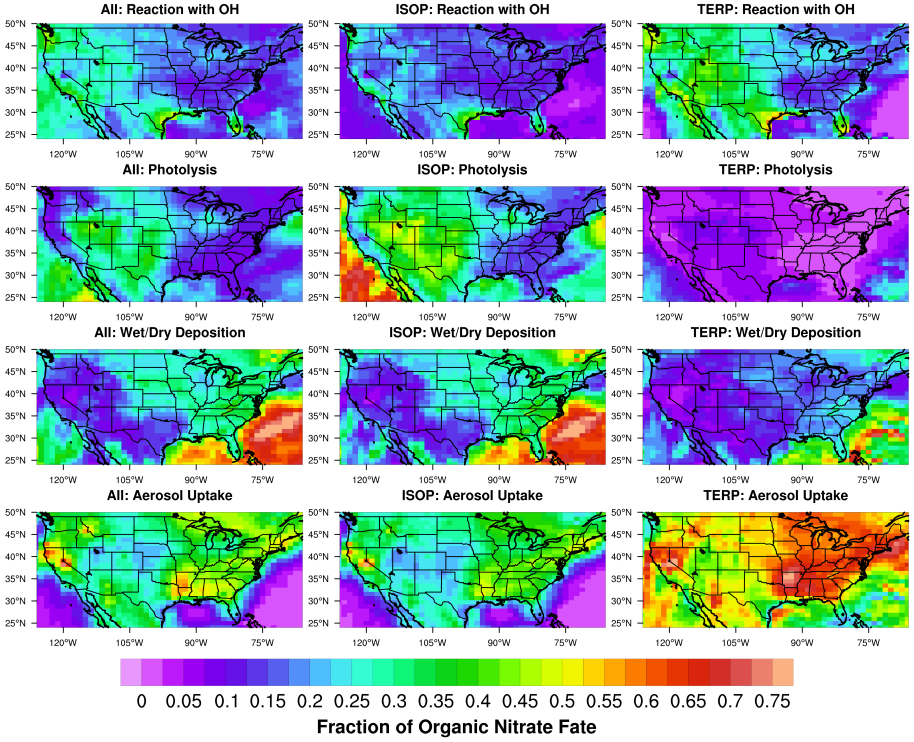

Figure S7. 2013 August average organic nitrate fate below 2 km using MOZART-TS1 for all organic nitrates (left), isoprene organic nitrates (middle), and terpene organic nitrates (right). To avoid double counting, only the final fate is included, so reaction with OH/O_3 to form another organic nitrate is omitted from this calculation.

S5 Tables Defining Chemical Compounds and Reactions in MOZART-TS2

Table S1: General peroxy (RO_2) and peroxyacyl (RCO_3) reaction rate constant sources used in MOZART-TS2 for isoprene and terpene chemistry

Reaction	**Source of rate constant**
RO_2 + CH_3O_2	Either isoprene general rate (Jenkin et al., 1998) or geometric mean of RO_2 + RO_2 and CH_3O_2 + CH_3O_2 from IUPAC (Atkinson et al., 2006)
RO_2 + CH_3CO_3	JPL (CH_3O_2 + CH_3CO_3), Burkholder et al. (2015)
RO_2 + RCO_3	JPL (CH_3O_2 + CH_3CO_3), Burkholder et al. (2015)
RO_2 + HO_2	Wennberg et al. (2018) parameterization based on n (# of C + O + N - 2 atoms in the peroxy radical)
RO_2 + NO	MCM v3.3.1, Jenkin et al. (2015)
RO_2 + NO_3	MCM v3.3.1, Jenkin et al. (2015)
RCO_3 + CH_3CO_3	JPL (CH_3CO_3 + CH_3CO_3), Burkholder et al. (2015)
RCO_3 + RCO_3	JPL (CH_3CO_3 + CH_3CO_3), Burkholder et al. (2015)
RCO_3 + CH_3O_2	JPL (CH_3O_2 + CH_3CO_3), Burkholder et al. (2015)
RCO_3 + HO_2	JPL (CH_3CO_3 + HO_2), Burkholder et al. (2015)
RCO_3 + NO	JPL (CH_3CO_3 + NO), Burkholder et al. (2015)
RCO_3 + NO_3	IUPAC (CH_3CO_3 + NO_3), Atkinson et al. (2006)
RCO_3 + NO_2	JPL (CH_3CO_3 + NO_2), Burkholder et al. (2015)
RPAN + M	JPL (PAN + M), Burkholder et al. (2015)

Table S2: MOZART-TS2 chemical species

Species name	Chemical Formula	Description
ACBZO2	$C_7H_5O_3$	acylperoxy radical from benzaldehyde
ALKNIT	$C_5H_{11}ONO_2$	standard alkyl nitrate from BIGALK+OH
ALKO2	$C_5H_{11}O_2$	lumped alkane peroxy radical from BIGALK
ALKOOH	$C_5H_{12}O_2$	lumped alkane hydroperoxide
AOA_NH	CO	age of air tracer
APIN	$C_{10}H_{16}$	α-pinene surrogate monoterpene
APINNO3	$C_{10}H_{16}NO_5$	peroxy radical from NO_3 + α-pinene
APINO2	$C_{10}H_{17}O_3$	peroxy radical from OH + α-pinene reaction
BCARY	$C_{15}H_{24}$	β-caryophyllene surrogate sesquiterpene
BCARYNO3	$C_{15}H_{24}NO_5$	peroxy radical from NO_3 + sesquiterpenes
BCARYO2	$C_{15}H_{25}O_3$	peroxy radical from OH + sesquiterpenes
BENZENE	C_6H_6	benzene
BENZO2	$C_6H_7O_5$	bicyclic peroxy radical from OH + benzene
BENZOOH	$C_6H_8O_5$	bicyclic hydroperoxide from OH + benzene
BEPOMUC	$C_6H_6O_3$	unsaturated dialdehydic epoxide from OH + benzene
BIGALD1	$C_4H_4O_2$	butenedial, a product of aromatic oxidation
BIGALD2	$C_5H_6O_2$	4-oxy-2-pentenal, a product of aromatic oxidation
BIGALD3	$C_5H_6O_2$	2-methyl butenedial, a product of aromatic oxidation
BIGALD4	$C_6H_8O_2$	2-methyl-4-oxo-2-pentenal, a product of aromatic oxidation
BIGALD	$C_5H_6O_2$	lumped aldehyde from terpene ozonolysis
BIGALK	C_5H_{12}	lumped alkanes C>3
BIGENE	C_4H_8	lumped alkenes C>3
BPIN	$C_{10}H_{16}$	β-pinene
BPINNO3	$C_{10}H_{16}NO_5$	peroxy radical from NO_3 + β-pinene
BPINO2	$C_{10}H_{17}O_3$	peroxy radical from OH + $beta$-pinene
BR	Br	bromine radical
BRCL	BrCl	bromine monochloride
BRO	BrO	bromine monooxide radical
BRONO2	$BrONO_2$	bromine nitrate
BRY	Br_Y	total reactive bromine
BZALD	C_7H_6O	benzaldehyde
BZOO	$C_7H_7O_2$	peroxy radical from toluene oxidation
BZOOH	$C_7H_8O_2$	hydroperoxide from toluene oxidation
C2H2	C_2H_2	ethyne (acetylene)
C2H4	C_2H_4	ethene

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
C2H5O2	$C_2H_5O_2$	ethylperoxy radical
C2H5OH	C_2H_5OH	ethanol
C2H5OOH	C_2H_5OOH	ethyl hydroperoxide
C2H6	C_2H_6	ethane
C3H6	C_3H_6	propene
C3H7O2	$C_3H_7O_2$	propylperoxy radical
C3H7OOH	C_3H_7OOH	propyl hydrogen peroxide
C3H8	C_3H_8	propane
C6H5O2	$C_6H_5O_2$	phenylperoxy radical
C6H5OOH	C_6H_5OOH	phenyl hydroperoxide
CCL4	CCl_4	carbon tetrachloride (LBC)
CF2CLBR	CF_2ClBr	bromochlorodifluoromethane (LBC)
CF3BR	CF_3Br	Bromotrifluoromethane (LBC)
CFC113	CCl_2FCClF_2	1,1,2-trichlorotrifluoroethane (LBC)
CFC114	$CClF_2CClF_2$	1,2-dichlorotetrafluoroethane (LBC)
CFC115	$CClF_2CF_3$	chloropentafluoroethane (LBC)
CFC11	$CFCl_3$	trichlorofluoromethane (LBC)
CFC12	CF_2Cl_2	difluorodichloromethane (LBC)
CH2BR2	CH_2Br_2	dibromomethane (LBC)
CH2O	CH_2O	formaldehyde
CH3BR	CH_3Br	bromomethane (methyl bromide) (LBC)
CH3CCL3	CH_3CCl_3	1,1,1-trichloroethane (methylchloroform) (LBC)
CH3CHO	CH_3CHO	acetaldehyde
CH3CL	CH_3Cl	chloromethane (methyl chloride) (LBC)
CH3CN	CH_3CN	acetonitrile
CH3CO3	CH_3CO_3	acetylperoxy radical
CH3COCH3	CH_3COCH_3	acetone
CH3COCHO	CH_3COCHO	methyl glyoxal
CH3COOH	CH_3COOH	acetic acid
CH3COOOH	CH_3COOOH	peracetic acid
CH3O2	CH_3O_2	methylperoxy radical
CH3OH	CH_3OH	methanol
CH3OOH	CH_3OOH	methyl hydroperoxide
CH4	CH_4	methane (LBC)
CHBR3	$CHBr_3$	tribromomethane (bromoform) (LBC)

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
CL2	Cl_2	chlorine
CL2O2	Cl_2O_2	dichlorine dioxide
CL	Cl	chlorine radical
CLO	ClO	chlorine monoxide radical
CLONO2	$ClONO_2$	chlorine nitrate
CLY	Cl_Y	total reactive chlorine
CO2	CO_2	carbon dioxide (LBC)
CO	CO	carbon monoxide
COF2	COF_2	carbonyl fluoride
COFCL	COFCl	carbonyl chloride fluoride
CRESOL	C_7H_8O	lumped cresols (hydroxymethylbenzenes)
DHPMPAL	$C_4H_8O_5$	C4 dihydroperoxy carbonyl derived from isoprene
DICARBO2	$C_5H_5O_4$	acylperoxy radical formed from aromatic oxidation, via unsaturated dicarbonyl chemistry
DMS	CH_3SCH_3	dimethyl sulfide
E90	CO	artificial tracer with 90-day lifetime emitted from surface
ENEO2	$C_4H_9O_3$	lumped hydroxyperoxy radical from OH + large alkenes
EO2	$HOCH_2CH_2O_2$	hydroxyperoxy radical from OH + ethene
EO	$HOCH_2CH_2O$	hydroxyalkoxy radical from OH + ethene
EOOH	$HOCH_2CH_2OOH$	hydroxyhydroperoxide from OH + ethene
F	F	fluorine radical
GLYALD	$HOCH_2CHO$	glycolaldehyde
GLYOXAL	$C_2H_2O_2$	glyoxal
H2402	$CBrF_2CBrF_2$	dibromotetrafluoroethane (LBC)
H2	H_2	hydrogen (LBC)
H2O2	H_2O_2	hydrogen peroxide
H2SO4	H_2SO_4	sulfuric acid
H	H	hydrogen radical
HBR	HBr	hydrogen bromide
HCFC141B	CH_3CCl_2F	1,1-dichoro-1-fluoroethane (LBC)
HCFC142B	CH_3CClF_2	1-choro-1,1-difluoroethane (LBC)
HCFC22	CHF_2Cl	difluorochloromethane (LBC)
HCL	HCl	hydrogen chloride
HCN	HCN	hydrogen cyanide
HCOCH2OOH	$C_2H_4O_3$	hydroperoxy acetaldehyde

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
HCOOH	HCOOH	formic acid
HF	HF	hydrogen fluoride
HMHP	CH_4O_3	hydroxy methyl hydroperoxide
HNO3	HNO_3	nitric acid
HO2	HO_2	hydroperoxyl radical
HO2NO2	HO_2NO_2	pernitric acid
HOBR	HOBr	hypobromous acid
HOCH2OO	$HOCH_2OO$	hydroxy-methyl-peroxy radical
HOCL	HOCl	hypochlorous acid
HONITR	$C_4H_9NO_4$	lumped hydroxynitrates from various compounds
HPALD1	$C_5H_8O_3$	hydroperoxy aldehyde from ISOPZD1O2
HPALD4	$C_5H_8O_3$	hydroperoxy aldehyde from ISOPZD4O2
HPALDB1C	$C_5H_8O_3$	β-2-hydroperoxy-1-aldehyde
HPALDB4C	$C_5H_8O_3$	β-3-hydroperoxy-4-aldehyde
HYAC	CH_3COCH_2OH	hydroxyacetone
HYDRALD	$HOCH_2CCH_3CHCHO$	lumped unsaturated hydroxycarbonyl
HYPERACET	$C_3H_6O_3$	hydroperoxy acetone
ICHE	$C_5H_8O_3$	C5 carbonyl hydroxy epoxide
IEPOX	$C_5H_{10}O_3$	isoprene dihydroxy epoxide
IEPOXOO	$C_5H_9O_5$	peroxy radical from IEPOX + OH
INHEB	$C_5H_9NO_5$	β-isoprene nitrooxy hydroxy epoxide
INHED	$C_5H_9NO_5$	δ-isoprene nitrooxy hydroxy epoxide
ISOP	C_5H_8	isoprene
ISOPB1O2	$C_5H_9O_3$	OH-1-O_2-2-β-isoprene hydroxy peroxy radical
ISOPB4O2	$C_5H_9O_3$	OH-4-O_2-3-β-isoprene hydroxy peroxy radical
ISOPC1C	C_5H_9O	OH-1-*cis*-isoprene allylic radical
ISOPC1T	C_5H_9O	OH-1-*trans*-isoprene allylic radical
ISOPC4C	C_5H_9O	OH-4-*cis*-isoprene allylic radical
ISOPC4T	C_5H_9O	OH-4-*trans*-isoprene allylic radical
ISOPED1O2	$C_5H_9O_3$	OH-1-O_2-4-E-δ-isoprene hydroxy peroxy radical
ISOPED4O2	$C_5H_9O_3$	OH-4-O_2-1-E-δ-isoprene hydroxy peroxy radical
ISOPFDN	$C_5H_{10}N_2O_8$	isoprene functionalized dinitrates
ISOPFDNC	$C_5H_8N_2O_8$	C5 carbonyl hydroxy dinitrate
ISOPFNC	$C_5H_9NO_7$	C5 carbonyl hydroxy hydroperoxy nitrate
ISOPFNP	$C_5H_{11}NO_7$	isoprene highly functionalized nitrates

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
ISOPHFP	$C_5H_{10}O_5$	isoprene highly functionalized hydroperoxide
ISOPN1D	$C_5H_9NO_4$	δ-isoprene hydroxy nitrate (nitrooxy in 1 position)
ISOPN1DO2	$C_5H_{10}NO_7$	peroxy radical from ISOPN1D + OH
ISOPN2B	$C_5H_9NO_4$	β-isoprene hydroxy nitrate (nitrooxy in 2 position)
ISOPN2BO2	$C_5H_{10}NO_7$	peroxy radical from ISOPN2B + OH
ISOPN3B	$C_5H_9NO_4$	β-isoprene hydroxy nitrate (nitrooxy in 3 position)
ISOPN3BO2	$C_5H_{10}NO_7$	peroxy radical from ISOPN3B + OH
ISOPN4D	$C_5H_9NO_4$	δ-isoprene hydroxy nitrate (nitrooxy in 4 position)
ISOPN4DO2	$C_5H_{10}NO_7$	peroxy radical from ISOPN4D + OH
ISOPNBNO3	$C_5H_9NO_4$	β-isoprene hydroxy nitrate from isoprene NO_3 oxidation (combined isomers)
ISOPNBNO3O2	$C_5H_{10}NO_7$	peroxy radical from ISOPNBNO3 + OH
ISOPNO3	$CH_2CHCCH_3OOCH_2ONO_2$	peroxy radical from isoprene NO_3 oxidation
ISOPNOOHB	$C_5H_9NO_5$	β-isoprene hydroperoxy nitrate
ISOPNOOHBO2	$C_5H_{10}NO_8$	peroxy radical from ISOPNOOHB + OH
ISOPNOOHD	$C_5H_9NO_5$	δ-isoprene hydroperoxy nitrate
ISOPNOOHDO2	$C_5H_{10}NO_8$	peroxy radical from ISOPNOOHD + OH
ISOPOH	$C_5H_{10}O_2$	isoprene diol from RO_2 + RO_2 reactions
ISOPOOH	$HOCH_2C(OOH)(CH_3)CHCH_2$	unsaturated hydroxyhydroperoxide
ISOPZD1O2	$C_5H_9O_3$	OH-1-O_2-4-Z-δ-isoprene hydroxy peroxy radical
ISOPZD4O2	$C_5H_9O_3$	OH-4-O_2-1-Z-δ-isoprene hydroxy peroxy radical
IVOC	$C_{13}H_{28}$	intermediate volatility organic precursor of VBS SOA
LIMON	$C_{10}H_{16}$	limonene
LIMONNO3	$C_{10}H_{16}NO_5$	peroxy radical from NO_3 + limonene
LIMONO2	$C_{10}H_{17}O_3$	peroxy radical from OH + limonene
MACR	CH_2CCH_3CHO	methacrolein
MACRN	$C_4H_7NO_5$	hydroxy nitrate from MACR
MACRO2	$CH_3COCHO_2CH_2OH$	peroxy radical from methacrolein oxidation
MACROOH	$CH_3COCHOOHCH_2OH$	hydroxyhydroperoxide from methacrolein
MALO2	$C_4H_3O_4$	acylperoxy radical from OH reaction with BIGALD1
MCO3	$CH_2CCH_3CO_3$	peroxy radical from OH abstraction reaction with MACR
MDIALO2	$C_4H_5O_4$	peroxy radical from OH addition to BIGALD1
MEK	C_4H_8O	methyl ethyl ketone
MEKO2	$C_4H_7O_3$	peroxy radical formed from MEK oxidation
MEKOOH	$C_4H_8O_3$	hydroperoxide from MEK oxidation

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
MPAN	$CH_2CCH_3CO_3NO_2$	methacryloyl peroxynitrate
MVK	$CH_2CHCOCH_3$	methyl vinyl ketone
MVKN	$C_4H_7NO_5$	hydroxy nitrate from MVK
MVKO2	$C_4H_7O_4$	MVK hydroxy peroxy radical
MVKOOH	$C_4H_8O_4$	C_4 hydroxy hydroperoxide ketone from MVK
MYRC	$C_{10}H_{16}$	myrcene
MYRCNO3	$C_{10}H_{16}NO_5$	peroxy radical from NO_3 + myrcene
MYRCO2	$C_{10}H_{17}O_3$	peroxy radical from OH + myrcene
N2O5	N_2O_5	dinitrogen pentoxide
N2O	N_2O	nitrous oxide (LBC)
N	N	nitrogen radical
NC4CHO	$C_5H_7NO_4$	nitrooxy-aldehyde from NO_3 + isoprene
NC4CHOO2	$C_5H_8NO_7$	peroxy radical from NC4CHO + OH
NDEP	N	diagnostic of nitrogen deposition
NH3	NH_3	ammonia
NH4	NH_4	ammonium ion aerosol
NHDEP	N	diagnostic of ammonia deposition
NH_50	CO	idealized tracer with 50-day loss rate
NH_5	CO	idealized tracer with 5 day loss rate
NO2	NO_2	nitrogen dioxide
NO3	NO_3	nitrate radical
NO3CH2CHO	$C_2H_3O_4N$	ethanal nitrate
NO	NO	nitric oxide
NOA	$CH_3COCH_2ONO_2$	nitrooxyacetone (propanone nitrate)
O1D	O	excited state atomic oxygen
O3	O_3	ozone
O	O	ground state atomic oxygen
OCLO	OClO	chlorine dioxide
OCS	OCS	carbonyl sulfide (LBC)
OH	OH	hydroxyl radical
ONITR	$C_4H_7NO_4$	lumped hydroxynitrates
PAN	$CH_3CO_3NO_2$	peroxy acetyl nitrate
PBZNIT	$C_7H_5NO_5$	peroxy benzoyl nitrate
PHENO2	$C_6H_7O_6$	bicyclic peroxy radical from phenol
PHENO	C_6H_5O	phenoxy radical

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
PHENOL	C_6H_5OH	phenol, product of benzene chemistry
PHENOOH	$C_6H_8O_6$	bicyclic hydroperoxide from phenol
PO2	$C_3H_6(OH)O_2$	propene-derived peroxy radical
POOH	$C_3H_6(OH)OOH$	propene-derived hydroxy hydroperoxide
RO2	$CH_3COCH_2O_2$	peroxy radical from acetone
ROOH	CH_3COCH_2OOH	acetone hydroperoxide
S	S	sulfur radical
SF6	SF_6	sulfur hexafluoride (LBC)
SO2	SO_2	sulfur dioxide
SO3	SO_3	sulfur trioxide
SO	SO	sulfur monoxide
SOAG0	$C_{15}H_{38}O_2$	SOA gas-phase precursor VBS bin 0
SOAG1	$C_{15}H_{38}O_2$	SOA gas-phase precursor VBS bin 1
SOAG2	$C_{15}H_{38}O_2$	SOA gas-phase precursor VBS bin 2
SOAG3	$C_{15}H_{38}O_2$	SOA gas-phase precursor VBS bin 3
SOAG4	$C_{15}H_{38}O_2$	SOA gas-phase precursor VBS bin 4
SQTN	$C_{15}H_{25}NO_4$	nitrate from sesquiterpene oxidation
ST80_25	CO	stratospheric loss tracer
SVOC	$C_{22}H_{46}$	semi-volatile organic precursor of VBS SOA
TEPOMUC	$C_7H_8O_3$	toluene, xylenes product
TERP1OOH	$C_{10}H_{18}O_3$	terpene-derived hydroxy hydroperoxide with 1 double bond
TERP1OOHO2	$C_{10}H_{19}O_6$	peroxy radical from OH + TERP1OOH
TERP2AOOH	$C_{10}H_{18}O_3$	terpene-derived hydroxy hydroperoxide with 2 double bonds
TERP2OOHO2	$C_{10}H_{19}O_6$	peroxy radical from OH + TERP2AOOH
TERPA1O2	$C_9H_{15}O_3$	TERPA peroxy radical 1st step
TERPA2	$C_9H_{14}O_2$	TERPA oxidation product with no double bonds that contains an aldehydic group
TERPA2CO3	$C_9H_{13}O_4$	acyl peroxy radical from TERPA2
TERPA2O2	$C_9H_{15}O_4$	TERPA peroxy radical 2nd step
TERPA2PAN	$C_9H_{13}NO_6$	PAN from TERPA2
TERPA3	$C_9H_{14}O_3$	aldehyde terpene product with no ring like limonaldehyde
TERPA3CO3	$C_9H_{13}O_5$	acyl peroxy radical from TERPA3
TERPA3O2	$C_9H_{15}O_5$	TERPA peroxy radical 3rd step
TERPA3PAN	$C_9H_{13}NO_7$	PAN from TERPA3
TERPA4O2	$C_6H_9O_5$	TERPA peroxy radical 4th step

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
TERPA	$C_{10}H_{16}O_2$	aldehyde terpene product with no double bonds that contains a ring like pinonaldehyde
TERPACID2	$C_9H_{14}O_4$	carboxylic acid/peracid from TERPA2
TERPACID3	$C_9H_{14}O_5$	carboxylic acid/peracid from TERPA3
TERPACID	$C_{10}H_{16}O_4$	carboxylic acid/peracid from TERPA
TERPACO3	$C_{10}H_{15}O_4$	TERPA acyl peroxy radical
TERPAPAN	$C_{10}H_{15}NO_6$	PAN from TERPA
TERPDHDP	$C_{10}H_{20}O_6$	terpene oxidation product, dihydroxy dihydroperoxy
TERPF1	$C_{10}H_{16}O_2$	functionalized terpene product with 1 double bond typically containing carbonyl groups
TERPF1O2	$C_{10}H_{17}O_5$	peroxy radical from OH + TERPF1
TERPF2	$C_7H_{10}O$	functionalized terpene product with 2 double bonds typically containing carbonyl groups
TERPF2O2	$C_7H_{11}O_4$	peroxy radical from OH + TERPF2
TERPFDN	$C_{10}H_{18}N_2O_8$	terpene highly functionalized organic dinitrate
TERPHFN	$C_{10}H_{19}NO_7$	terpene highly functionalized nitrate
TERPK	$C_9H_{14}O$	terpene product containing a ketone group
TERPNPS1	$C_{10}H_{17}NO_5$	terpene-derived unsaturated secondary or primary hydroperoxy nitrate
TERPNPS1O2	$C_{10}H_{18}NO_8$	peroxy radical from OH + TERPNPS1
TERPNPS	$C_{10}H_{17}NO_5$	terpene-derived saturated secondary or primary hydroperoxy nitrate
TERPNPT1	$C_{10}H_{17}NO_5$	terpene-derived unsaturated tertiary hydroperoxy nitrate
TERPNPT1O2	$C_{10}H_{18}NO_8$	peroxy radical from OH + TERPNPT1
TERPNPT	$C_{10}H_{17}NO_5$	terpene-derived saturated tertiary hydroperoxy nitrate
TERPNS1	$C_{10}H_{17}NO_4$	terpene-derived unsaturated secondary or primary nitrate
TERPNS1O2	$C_{10}H_{18}NO_7$	peroxy radical from OH + TERPNS1
TERPNS	$C_{10}H_{17}NO_4$	terpene-derived saturated secondary or primary nitrate
TERPNT1	$C_{10}H_{17}NO_4$	terpene-derived unsaturated tertiary nitrate
TERPNT1O2	$C_{10}H_{18}NO_7$	peroxy radical from OH + TERPNT1
TERPNT	$C_{10}H_{17}NO_4$	terpene-derived saturated tertiary nitrate
TERPOOH	$C_{10}H_{18}O_3$	terpene-derived saturated hydroperoxide with ring
TERPOOHL	$C_{10}H_{18}O_5$	terpene-derived saturated hydroperoxide with no ring
TOLO2	$C_7H_9O_5$	bicyclic peroxy radical from toluene
TOLOOH	$C_7H_{10}O_5$	bicyclic hydroperoxide from toluene
TOLUENE	C_7H_8	toluene

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
XYLENES	C_8H_{10}	lumped xylenes
XYLENO2	$C_8H_{11}O_5$	bicyclic peroxy radical from OH + XYLENES
XYLENOOH	$C_8H_{12}O_5$	bicyclic hydroperoxide from OH+ XYLENES
XYLOL	$C_8H_{10}O$	dimethyl phenol from xylenes oxidation
XYLOLO2	$C_8H_{11}O_6$	bicyclic peroxy radical from OH + XYLOL
XYLOLOOH	$C_8H_{12}O_6$	bicyclic hydroperoxide from OH+XYLOL
bc_a1	C	black carbon, MAM accumulation mode
bc_a4	C	black carbon, MAM primary carbon mode
dst_a1	$AlSiO_5$	dust, MAM accumulation mode
dst_a2	$AlSiO_5$	dust, MAM Aitken mode
dst_a3	$AlSiO_5$	dust, MAM coarse mode
ncl_a1	NaCl	sea salt, MAM accumulation mode
ncl_a2	NaCl	sea salt, MAM Aitken mode
ncl_a3	NaCl	sea salt, MAM coarse mode
num_a1	H	aerosol number concentration, MAM accumulation mode
num_a2	H	aerosol number concentration, MAM Aitken mode
num_a3	H	aerosol number concentration, MAM coarse mode
num_a4	H	aerosol number concentration, MAM primary carbon mode
pom_a1	C	primary organic matter, MAM accumulation mode
pom_a4	C	primary organic matter, MAM primary carbon mode
so4_a1	NH_4HSO_4	sulfate aerosol, MAM accumulation mode
so4_a2	NH_4HSO_4	sulfate aerosol, MAM Aitken mode
so4_a3	NH_4HSO_4	sulfate aerosol, MAM coarse mode
soa1_a1	$C_{15}H_{38}O_2$	SOA bin 1, MAM accumulation mode
soa1_a2	$C_{15}H_{38}O_2$	SOA bin 1, MAM Aitken mode
soa2_a1	$C_{15}H_{38}O_2$	SOA bin 2, MAM accumulation mode
soa2_a2	$C_{15}H_{38}O_2$	SOA bin 2, MAM Aitken mode
soa3_a1	$C_{15}H_{38}O_2$	SOA bin 3, MAM accumulation mode
soa3_a2	$C_{15}H_{38}O_2$	SOA bin 3, MAM Aitken mode
soa4_a1	$C_{15}H_{38}O_2$	SOA bin 4, MAM accumulation mode
soa4_a2	$C_{15}H_{38}O_2$	SOA bin 4, MAM Aitken mode
soa5_a1	$C_{15}H_{38}O_2$	SOA bin 5, MAM accumulation mode
soa5_a2	$C_{15}H_{38}O_2$	SOA bin 5, MAM Aitken mode

Compounds with the species name in **bold** are new compounds added to the MOZART-TS2 chemical mechanism. Non-bolded compounds are unchanged from the MOZART-TS1 chemical mechanism Emmons et al. (2019))

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description

LBC = lower boundary conditions are specified for this species.

Table S3: Biogenic VOCs from MEGAN assignments to MOZART-TS1 and MOZART-TS2 surrogate species

TS1 Surrogate Species	**TS2 Surrogate Species**	**Biogenic VOC**
ISOP	ISOP	isoprene
MTERP	APIN	α-pinene, **myrtenal**
MTERP	BPIN	3-carene, α-thujene, bornene, α-fenchene, β-pinene, sabinene, camphene, **4-terpineol**, **α-terpineol**, **α-terpinyl acetate**
MTERP	LIMON	terpinolene, limonene, α-phellandrene, γ-terpinene, α-terpinene, β-phellandrene, **linalool**, **β-ionone**, **geranyl acetone**, **neryl acetone**, **jasmone**, **verbenene**, **ipsenol**
MTERP	MYRC	allo-ocimene, myrcene, *t*-β-ocimene, *c*-β-ocimene, **dimethyl-nonatriene**
BCARY	BCARY	**α-farnescene**, β-caryophyllene, **acoradiene**, **aromadendrene**, α-bergamotene, **β-bergamotene**, **α-bisabolene**, β-bisabolene, **β-bourbonene**, **δ-cadinene**, **γ-cadinene**, **α-cedrene**, **α-copaene**, **α-cubebene**, **β-cubebene**, **β-elemene**, β-farnescene, **germacrene B**, **germacrene D**, **β-gurjunene**, α-humulene, **γ-humulene**, **isolongifolene**, **longifolene**, **longipinene**, **α-muurolene**, **γ-muurolene**, **β-selinene**, **δ-selinene**, ***c*-nerolidol**, ***t*-nerolidol**
BIGALK	BIGALK	tricyclene, **camphor**, **fenchone**, **α-thujone**, **β-thujone**, **1,8-cineole**, **borneol**, **bornyl acetate**, **cedrol**, **decanal**, **heptanal**, heptane, hexane, **nonanal**, **octanal**, **octanol**, **oxopentanal**, pentane, **hexanal**, **1-hexanol**, **pentanal**, **heptanone**
BIGENE	BIGENE	dimethyl styrene, **estragole**, **piperitone**, ***c*-linalool oxide**, ***t*-linalool oxide**, **1-dodecene**, **methyl heptenone**, **nonenal**, **1,3-octenol**, **1-tetradecene**, butene, **diallyl disulfide**, **methyl propenyl disulfide**, **methyl jasmonate**, ***c*-3-hexenal**, ***t*-2-hexenal**, ***c*-3-hexenol**, ***c*-3-hexenyl acetate**
TOLUENE	TOLUENE	toluene, **methyl benzoate**, **phenylacetaldehyde**, **methyl salicylate**, **indole**, **anisole**, **benzyl acetate**, **benzyl alcohol**, **napthalene**
N/A	XYLENES	*p*-cymene, *o*-cymene, **homosalate**, ***m*-cymenene**
CH3OH	CH3OH	methanol
CH3COCH3	CH3COCH3	acetone
CH3CHO	CH3CHO	acetaldehyde
C2H5OH	C2H5OH	ethanol
HCOOH	HCOOH	formic acid
CH2O	CH2O	formaldehyde
CH3COOH	CH3COOH	acetic acid
N/A	BZALD	**benzaldehyde**
N/A	MEK	**2-butanone**

Table S3: Biogenic VOCs from MEGAN assignments to MOZART-TS1 and MOZART-TS2 surrogate species

TS1 Surrogate Species	**TS2 Surrogate Species**	**Biogenic VOC**
CO	CO	carbon monoxide
C2H6	C2H6	ethane
C2H4	C2H4	ethene
HCN	HCN	hydrogen cyanide
C3H8	C3H8	propane
C3H6	C3H6	propene

Compounds in **bold** are not included in the default version of CESM 2.1. N/A = not applicable.

Compounds underlined are moved from MTERP (default) to BIGALK or XYLENES

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** ($M\ atm^{-1}$)	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
MOZART-TS1 Species								
ALKNIT	1.01	5790	0	0	0	0	1	JPL(2015)
ALKOOH	3.36E+02	5995	0	0	0	0	1	S:C2H5OOH
BCARY	5.57E-03	2800	0	0	0	0	1E-36	S:C3H6
BENZENE	1.8E-01	3800	0	0	0	0	1E-36	Sander(2015), Hiatt(2013)
BENZOOH	2.3E+03	5995	0	0	0	0	1	T
BEPOMUC	3.0E+07	6014	0	0	0	0	1	S:IEPOX
BIGALD	9.6	6220	0	0	0	0	1	JPL(2015)
BIGALD1	1.0E+05	5890	0	0	0	0	1	T
BIGALD2	2.9E+04	5890	0	0	0	0	1	T
BIGALD3	2.2E+04	5890	0	0	0	0	1	T
BIGALD4	2.2E+04	5890	0	0	0	0	1	T
BIGALK	1.24E-03	3010	0	0	0	0	1E-36	JPL(2015)
BIGENE	5.96E-03	2365	0	0	0	0	1E-36	S:C2H4
BZALD	3.24E+01	6300	0	0	0	0	1	Sander(2015), Allou(2011)
BZOOH	3.36E+02	5995	0	0	0	0	1	S:C2H5OOH
C2H2	4.14E-02	1890	0	0	0	0	1E-36	JPL(2015)
C2H4	5.96E-03	2200	0	0	0	0	1E-36	JPL(2015)
C2H5OH	1.90E+02	6500	0	0	0	0	1	JPL(2015)
C2H5OOH	3.36E+02	5995	0	0	0	0	1	JPL(2015)
C2H6	1.88E-03	2750	0	0	0	0	1E-36	JPL(2015)
C3H6	5.57E-03	2800	0	0	0	0	1E-36	Sander(2015), Reichl(1995)
C3H7OOH	3.36E+02	5995	0	0	0	0	1	S:C2H5OOH
C3H8	1.51E-03	3120	0	0	0	0	1E-36	JPL(2015)
C6H5OOH	3.36E+02	5995	0	0	0	0	1	S:C2H5OOH
CH2O	3.23E+03	7100	0	0	0	0	1	JPL(2015)
CH3CHO	1.29E+01	5890	0	0	0	0	1	JPL(2015)
CH3CN	5.28e+01	3970	0	0	0	0	1E-36	JPL(2015)
CH3COCH3	2.78E+01	5530	0	0	0	0	1	JPL(2015)
CH3COCHO	3.50E+03	7545	0	0	0	0	1	JPL(2015)
CH3COOH	4.1E+03	6200	0	0	0	0	1	JPL(2015)

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** ($M\ atm^{-1}$)	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
CH3COOOH	8.37E+02	5310	1.8E-04	-20	0	0	1	JPL(2015), S:HCOOH
CH3OH	2.03E+02	5645	0	0	0	0	1	JPL(2015)
CH3OOH	3.00E+02	5280	0	0	0	0	1	JPL(2015)
CO	9.81E-04	1650	0	0	0	0	1E-36	JPL(2015)
CRESOL	5.67E+02	5800	0	0	0	0	1	Sander(2015), Dohnal(1995)
DMS	5.4E-01	3460	0	0	0	0	1E-36	JPL(2015)
EOOH	1.9E+06	6014	0	0	0	0	1	T
GLYALD	4.00E+04	4630	0	0	0	0	1	JPL(2015)
GLYOXAL	4.19e+05	7480	0	0	0	0	1	JPL(2015)
H2O2	8.70E+04	7320	2.2e-12	-3730	0	0	1	JPL(2015)
H2SO4	1.0E+11	6014	0	0	0	0	1E-36	Note A
HCN	9.02	8258	0	0	0	0	1E-36	JPL(2015)
HCOOH	8.90E+03	6100	1.8E-04	-20	0	0	1	JPL(2015), Chameides(1984)
HNO3	2.10E+05	8700	2.2e+01	0	0	0	1E-36	Schwartz(1981)
HO2NO2	4.00E+01	8400	1.3E-06	0	0	0	0.1	Sander(2015), Leu(1999), Goldstein(1997)
HONITR	2.64E+03	6014	0	0	0	0	1	T
HPALD	2.30E+05	6014	0	0	0	0	1	T
HYAC	1.46E+03	6014	0	0	0	0	1	T
HYDRALD	1.10E+05	6000	0	0	0	0	1	T
IEPOX	3.0E+07	6014	0	0	0	0	1	Sander(2015), Chan(2010)
ISOP	3.45E-02	4400	0	0	0	0	1E-36	Sander(2015), Leng(2013)
ISOPNITA	8.34E+03	6014	0	0	0	0	1	T
ISOPNITB	4.82E+04	6014	0	0	0	0	1	T
ISOPNOOH	8.75E+04	6014	0	0	0	0	1	T
ISOPOOH	3.5E+06	5995	0	0	0	0	1	T
MACR	6.50	6014	0	0	0	0	1	JPL(2015)
MACROOH	4.4E+06	6014	0	0	0	0	1	T

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** ($M\ atm^{-1}$)	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
MEK	1.80E+01	5740	0	0	0	0	1	JPL(2015)
MEKOOH	6.4E+04	6014	0	0	0	0	1	T
MPAN	1.72	5700	0	0	0	0	1	Sander(2015), Kames(1995)
MTERP	2.94E-02	1800	0	0	0	0	1E-36	S: APIN
MVK	4.10E+01	6014	0	0	0	0	1	JPL(2015)
N2O5	2.14	3362	0	0	0	0	0.1	Sander(2015), Fried(1994)
NC4CH2OH	4.02E+04	9500	0	0	0	0	1	T
NC4CHO	1.46E+03	6014	0	0	0	0	1	T
NH3	6.02E+01	4160	1.7E-05	-4325	1.0E-14	-6716	1E-36	JPL(2015), Chameides(1984)
NO	1.92E-03	1762	0	0	0	0	0	JPL(2015)
NO2	1.20E-02	2440	0	0	0	0	0.1	JPL(2015)
NOA	1.0E+03	6014	0	0	0	0	1	JPL(2015)
NTERPOOH	6.67E+04	6014	0	0	0	0	1	T
O3	1.03E-02	2830	0	0	0	0	1	JPL(2015)
ONITR	1.44E+03	6014	0	0	0	0	1	T
PAN	2.80E+00	5730	0	0	0	0	0.1	JPL(2015)
PBZNIT	2.8	5730	0	0	0	0	1	S: PAN
PHENOL	2.84E+03	2700	0	0	0	0	1	Sander(2015), Guo(2007)
PHENOOH	1.5E+06	5995	0	0	0	0	1	T
POOH	1.50E+06	6014	0	0	0	0	1	T
ROOH	3.36E+02	5995	0	0	0	0	1	S: C2H5OOH
SO2	1.36	3100	1.30E-02	1960	6.6E-08	1500	1E-36	JPL(2015), Smith(1976)
TEPOMUC	2.5E+05	6014	0	0	0	0	1	Sander(2015), McNeil(2012)
TERP2OOH	3.36E+02	5995	0	0	0	0	1	S: C2H5OOH
TERPNIT	8.41E+03	6014	0	0	0	0	1	T
TERPOOH	1.9E+06	5995	0	0	0	0	1	Note B
TERPROD1	3.92E+04	6014	0	0	0	0	1	T
TERPROD2	7.20E+04	6014	0	0	0	0	1	T

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** ($M\ atm^{-1}$)	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
TOLOOH	2.30E+04	5995	0	0	0	0	1	T
TOLUENE	1.5E-01	4300	0	0	0	0	1E-36	Sander(2015), Staudinger(2001)
XOOH	1.0E+11	5995	0	0	0	0	1	Note C
XYLENES	2.0E-01	4300	0	0	0	0	1E-36	Sander(2015), Sieg(2009)
XYLENOOH	3.36E+02	5995	0	0	0	0	1	S: C2H5OOH
XYLOL	1.01E+03	6800	0	0	0	0	1	Sander(2015), Dohnal(1995)
XYLOLOOH	1.9E+06	5995	0	0	0	0	1	Note B
New MOZART-TS2 Species								
APIN	2.94E-02	1800	0	0	0	0	1E-36	Sander(2015), Leng(2013)
BPIN	1.52E-02	4500	0	0	0	0	1E-36	Sander(2015), Copolovici(2005)
DHPMPAL	9.37E+07	6014	0	0	0	0	1	T
HCOCH2OOH	2.99E+04	6014	0	0	0	0	1	T
HMHP	1.70E+06	9870	0	0	0	0	1	T
HPALD1	2.30E+05	6014	0	0	0	0	1	T
HPALD4	2.30E+05	6014	0	0	0	0	1	T
HPALDB1C	5.43E+04	6014	0	0	0	0	1	T
HPALDB4C	5.43E+04	6014	0	0	0	0	1	T
HYPERACET	1.16E+04	6014	0	0	0	0	1	T
ICHE	2.09E+06	6014	0	0	0	0	1	T
INHEB	1.05E+05	6014	0	0	0	0	1	T
INHED	1.51E+05	6014	0	0	0	0	1	T
ISOPFDN	5.02E+08	6014	0	0	0	0	1	T
ISOPFDNC	7.16E+09	6014	0	0	0	0	1	T
ISOPFNC	1.41E+11	6014	0	0	0	0	1	T
ISOPFNP	2.97E+11	6014	0	0	0	0	1	T
ISOPHFP	7.60E+09	6014	0	0	0	0	1	T
ISOPN1D	4.82E+04	6014	0	0	0	0	1	T
ISOPN2B	8.34E+03	6014	0	0	0	0	1	T
ISOPN3B	8.34E+03	6014	0	0	0	0	1	T

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** ($M\ atm^{-1}$)	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
ISOPN4D	4.82E+04	6014	0	0	0	0	1	T
ISOPNBNO3	8.34E+03	6014	0	0	0	0	1	T
ISOPNOOHB	6.61E+04	6014	0	0	0	0	1	T
ISOPNOOHD	9.67E+04	6014	0	0	0	0	1	T
ISOPOH	8.77E+06	6014	0	0	0	0	1	T
LIMON	4.86E-02	4600	0	0	0	0	1E-36	Sander(2015), Leng(2013)
MACRN	4.14E+06	6014	0	0	0	0	1	T
MVKN	1.84E+05	6014	0	0	0	0	1	T
MVKOOH	1.24E+06	6014	0	0	0	0	1	T
MYRC	7.30E-02	2800	0	0	0	0	1E-36	Sander(2015), van Roon(2005)
NO3CH2CHO	3.39E+04	6014	0	0	0	0	1	T
SQTN	9.04E+03	6014	0	0	0	0	1	T
TERPOOH	3.6E+06	6014	0	0	0	0	1	T
TERP1OOH	3.64E+06	6014	0	0	0	0	1	T
TERP2AOOH	3.67E+06	6014	0	0	0	0	1	T
TERPA	3.92E+04	6014	0	0	0	0	1	T
TERPA2	7.20E+04	6014	0	0	0	0	1	T
TERPA2PAN	9.59E+03	6014	0	0	0	0	1	T
TERPA3	1.04E+08	6014	0	0	0	0	1	T
TERPA3PAN	1.23E+07	6014	0	0	0	0	1	T
TERPACID	5.63E+06	6014	0	0	0	0	1	T
TERPACID2	2.64E+06	6014	0	0	0	0	1	T
TERPACID3	3.38E+09	6014	0	0	0	0	1	T
TERPAPAN	7.94E+03	6014	0	0	0	0	1	T
TERPDHDP	3.41E+14	6014	0	0	0	0	1	T
TERPF1	4.05E+04	6014	0	0	0	0	1	T
TERPF2	6.54E+01	6014	0	0	0	0	1	T
TERPFDN	1.65E+09	6014	0	0	0	0	1	T
TERPHFN	7.53E+11	6014	0	0	0	0	1	T
TERPK	6.39E+01	6014	0	0	0	0	1	T
TERPNPS	6.67E+04	6014	0	0	0	0	1	T
TERPNPS1	6.78E+04	6014	0	0	0	0	1	T

Table S4: Effective Henry's law constants and reactivity factors for all species

Species	**KH_{298}** (M atm^{-1})	**dH/R** (K)	**$K1_{298}$**	**dH1/R** (K)	**$K2_{298}$**	**dH2/R** (K)	**F_0**	**Sources**
TERPNPT	6.67E+04	6014	0	0	0	0	1	T
TERPNPT1	6.78E+04	6014	0	0	0	0	1	T
TERPNS	8.41E+03	6014	0	0	0	0	1	T
TERPNS1	8.55E+03	6014	0	0	0	0	1	T
TERPNT	8.41E+03	6014	0	0	0	0	1	T
TERPNT1	8.55E+03	6014	0	0	0	0	1	T
TERPOOHL	4.41E+12	6014	0	0	0	0	1	T

For acids: $H_{eff} = K_H \left(1 + \frac{K_1}{[H+]} \left(1 + \frac{K_2}{[H+]} \right) \right)$

For bases: $H_{eff} = K_H \left(1 + \frac{K_1}{K_2} [H+] \right)$

Where: $K_H = KH_{298} \exp\left(dH/R \left(\frac{1}{T} - \frac{1}{298} \right) \right)$, $K_1 = K1_{298} \exp\left(dH1/R \left(\frac{1}{T} - \frac{1}{298} \right) \right)$,

$K_2 = K2_{298} \exp\left(dH2/R \left(\frac{1}{T} - \frac{1}{298} \right) \right)$, and $[H+] = 10^{-pH}$

F_0 is the reactivity factor. S = surrogate. T = Theoretically estimated using GROMHE (Raventos-Duran et al., 2010).

Note A: Henry's law constant set high to ensure all H_2SO_4 is in water.

Note B: KH(C2H5OOH) * (KH(HMHP) / KH(MHP)).

Note C: Henry's law constant set high due to large number of multifunctional groups.

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		Products	Rate
Odd Oxygen			
H2O + hν	→	H2 + O1D	jh2o_b
H2O + hν	→	OH + H	jh2o_a
H2O + hν	→	2*H + O	jh2o_c
H2O2 + hν	→	2*OH	jh2o2
O2 + hν	→	O + O1D	jo2_a
O2 + hν	→	2*O	jo2_b
O3 + hν	→	O1D + O2	jo3_a
O3 + hν	→	O + O2	jo3_b
Odd Nitrogen			
HNO3 + hν	→	NO2 + OH	jhno3
HO2NO2 + hν	→	OH + NO3	jho2no2_a
HO2NO2 + hν	→	NO2 + HO2	jho2no2_b
N2O + hν	→	O1D + N2	jn2o
N2O5 + hν	→	NO2 + NO3	jn2o5_a
N2O5 + hν	→	NO + O + NO3	jn2o5_b
NO + hν	→	N + O	jno
NO2 + hν	→	NO + O	jno2
NO3 + hν	→	NO + O2	jno3_b
NO3 + hν	→	NO2 + O	jno3_a
Organics			
ALKNIT + hν	→	NO2 + 0.4*CH3CHO + 0.1*CH2O + 0.25*CH3COCH3 + HO2 + 0.8*MEK	jch3ooh
ALKOOH + hν	→	0.4*CH3CHO + 0.1*CH2O + 0.25*CH3COCH3 + 0.9*HO2 + 0.8*MEK + OH	jch3ooh
BENZOOH + hν	→	OH + GLYOXAL + 0.5*BIGALD1 + HO2	jch3ooh
BEPOMUC + hν	→	BIGALD1 + 1.5*HO2 + 1.5*CO	0.10*jno2
BIGALD + hν	→	0.45*CO + 0.13*GLYOXAL + 0.56*HO2 + 0.13*CH3CO3 + 0.18*CH3COCHO	0.2*jno2
BIGALD1 + hν	→	0.6*MALO2 + HO2	0.14*jno2
BIGALD2 + hν	→	0.6*HO2 + 0.6*DICARBO2	0.20*jno2
BIGALD3 + hν	→	0.6*HO2 + 0.6*CO + 0.6*MDIALO2	0.20*jno2
BIGALD4 + hν	→	HO2 + CO + CH3COCHO + CH3CO3	0.006*jno2
BZOOH + hν	→	BZALD + OH + HO2	jch3ooh
C2H5OOH + hν	→	CH3CHO + HO2 + OH	jch3ooh

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		Products	Rate
C3H7OOH + hν	→	0.82*CH3COCH3 + OH + HO2	jch3ooh
C6H5OOH + hν	→	PHENO + OH	jch3ooh
CH2O + hν	→	CO + 2*H	jch2o_a
CH2O + hν	→	CO + H2	jch2o_b
CH3CHO + hν	→	CH3O2 + CO + HO2	jch3cho
CH3COCH3 + hν	→	CH3CO3 + CH3O2	jacet
CH3COCHO + hν	→	CH3CO3 + CO + HO2	jmgly
CH3COOOH + hν	→	CH3O2 + OH + CO2	0.28*jh2o2
CH3OOH + hν	→	CH2O + H + OH	jch3ooh
CH4 + hν	→	1.44*H2 + 0.18*CH2O + 0.18*O + 0.33*OH + 0.33*H + 0.44*CO2 + 0.38*CO + 0.05*H2O	jch4_b
CH4 + hν	→	H + CH3O2	jch4_a
CO2 + hν	→	CO + O	jco2
DHPMPAL + hν	→	**0.5*CH3COCHO + 1.5*OH + 0.5*CH2O + 0.5*HYPERACET + 0.5*HO2 + 0.5*CO**	**4.62*jch3ooh**
EOOH + hν	→	EO + OH	jch3ooh
GLYALD + hν	→	2*HO2 + CO + CH2O	jglyald
GLYOXAL + hν	→	2*CO + 2*HO2	jmgly
HCOCH2OOH + hν	→	**CH2O + HO2 + CO + OH**	**jch3ooh**
HMHP + hν	→	**2*OH + CH2O**	**0.75*jch3ooh**
HONITR + hν	→	NO2 + 0.67*HO2 + 0.33*CH3CHO + 0.33*CH2O + 0.33*CO + 0.33*GLYALD + 0.33*CH3CO3 + 0.17*HYAC + 0.17*CH3COCH3	jch2o_a
HPALD1 + hν	→	**0.62*HO2 + 1.32*CO + 0.68*CH3COCHO + 0.17*CO2 + 0.04*CH3O2 + 0.05*CH3CO3 + 1.11*OH + 0.23*MVKO2 + 0.41*HCOOH**	**110.0*jmacr_a**
HPALD4 + hν	→	**0.56*HO2 + 1.74*CO + 0.67*CH3COCHO + 0.28*CO2 + 0.07*CH3O2 + 0.07*CH3CO3 + 1.18*OH + 0.19*MACRO2**	**110.0*jmacr_a**
HPALDB1C + hν	→	**OH + MVK + CO + HO2**	**4.62*jch3ooh**
HPALDB4C + hν	→	**OH + HO2 + CO + MACR**	**4.62*jch3ooh**
HYAC + hν	→	CH3CO3 + HO2 + CH2O	jhyac
HYDRALD + hν	→	**3*OH + HO2 + CO + CO2 + CH3COCHO**	**jmacr_a**
HYDRALD + hν	→	**1.5*HO2 + 1.5*CO + 0.5*HYAC + 0.5*CH3CO3 + 0.5*GLYALD**	**jmacr_b**
HYPERACET + hν	→	**CH3CO3 + CH2O + OH**	**jacet**
HYPERACET + hν	→	**CH3CO3 + CH2O + OH**	**jch3ooh**
INHEB + hν	→	**NO2 + ICHE + HO2**	**jch3ooh**

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		Products	Rate
INHED + hν	→	**NO2 + ICHE + HO2**	**jch3ooh**
ISOPFDN + hν	→	**HYAC + 2*NO2 + GLYALD**	**jch3ooh**
ISOPFDNC + hν	→	**2*NO2 + 0.5*CH3COCHO + 0.5*GLYALD + 0.5*HYAC + 0.5*GLYOXAL**	**10.0*jch2o_a**
ISOPFNC + hν	→	**OH + NO2 + 0.5*GLYALD + 0.5*CH3COCHO + 0.5*HYAC + 0.5*GLYOXAL**	**10.0*jch2o_a**
ISOPFNP + hν	→	**OH + NO2 + GLYALD + HYAC**	**jch3ooh**
ISOPHFP + hν	→	**OH + HO2 + 0.72*CH3COCHO + 0.72*GLYALD + 0.28*GLYOXAL + 0.28*HYAC**	**jch3ooh**
ISOPN1D + hν	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH**	**jch3ooh**
ISOPN2B + hν	→	**NO2 + MVK + CH2O + HO2**	**jch3ooh**
ISOPN3B + hν	→	**NO2 + MACR + CH2O + HO2**	**jch3ooh**
ISOPN4D + hν	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH**	**jch3ooh**
ISOPNBNO3 + hν	→	**NO2 + HO2 + CH2O + 0.5*MVK + 0.5*MACR**	**jch3ooh**
ISOPNOOHB + hν	→	**OH + CH2O + NO2 + 0.88*MVK + 0.12*MACR**	**jch3ooh**
ISOPNOOHD + hν	→	**OH + HO2 + NC4CHO**	**jch3ooh**
ISOPOOH + hν	→	**0.7*MVK + 0.3*MACR + OH + CH2O + HO2**	jch3ooh
MACR + hν	→	**HO2 + CO + CH2O + 0.35*CH3CO3 + 0.65*CH3O2 + 0.65*CO**	jmacr_b
MACR + hν	→	**HO2 + MCO3**	jmacr_a
MACRN + hν	→	**0.75*CO + 0.75*NO2 + 0.5*HYAC + 1.25*HO2 + 0.25*CH3COCHO + 0.25*CH2O + 0.25*NOA**	**5.8*jch2o_a**
MACROOH + hν	→	**OH + HO2 + 0.86*HYAC + 0.86*CO + 0.14*CH2O + 0.14*CH3COCHO**	**jch3ooh**
MEK + hν	→	CH3CO3 + C2H5O2	jacet
MEKOOH + hν	→	OH + CH3CO3 + CH3CHO	jch3ooh
MPAN + hν	→	MCO3 + NO2	jpan
MVK + hν	→	0.7*C3H6 + 0.7*CO + 0.3*CH3O2 + 0.3*CH3CO3	jmvk
MVKN + hν	→	**0.75*NO2 + 0.25*NO3CH2CHO + 0.75*CH3CO3 + 0.5*GLYALD + 0.5*HO2 + 0.25*CH2O + 0.25*CH3COCHO**	**1.26*jch2o_a**
MVKOOH + hν	→	**OH + 0.56*GLYALD + 0.56*CH3CO3 + 0.44*CH2O + 0.44*HO2 + 0.44*CH3COCHO**	**jch3ooh**
NC4CHO + hν	→	**NO2 + HO2 + HYDRALD**	**9.2*jch2o_a**
NO3CH2CHO + hν	→	**NO2 + CH2O + CO + HO2**	**4.3*jch2o_a**

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		Products	Rate
NOA + hν	→	NO2 + CH2O + CH3CO3	jch2o_a
ONITR + hν	→	NO2	jch3cho
PAN + hν	→	0.6*CH3CO3 + 0.6*NO2 + 0.4*CH3O2 + 0.4*NO3 + 0.4*CO2	jpan
PHENOOH + hν	→	OH + HO2 + 0.7*GLYOXAL	jch3ooh
POOH + hν	→	CH3CHO + CH2O + HO2 + OH	jch3ooh
ROOH + hν	→	CH3CO3 + CH2O + OH	jch3ooh
TEPOMUC + hν	→	0.5*CH3CO3 + HO2 + 1.5*CO	0.10*jno2
TERP1OOH + hν	→	**OH + TERPF1 + HO2**	**jch3ooh**
TERP2AOOH + hν	→	**OH + TERPF2 + HO2**	**jch3ooh**
TERPA + hν	→	**CO + HO2 + TERPA1O2**	**jch3cho**
TERPA2 + hν	→	**CO + HO2 + TERPA2O2**	**jch3cho**
TERPA2PAN + hν	→	**TERPA2CO3 + NO2**	**jpan**
TERPA3 + hν	→	**CO + HO2 + TERPA4O2**	**jch3cho**
TERPA3PAN + hν	→	**TERPA3CO3 + NO2**	**jpan**
TERPACID + hν	→	**OH + CO2 + TERPA1O2**	**0.71*jch3ooh**
TERPACID2 + hν	→	**OH + CO2 + TERPA2O2**	**0.71*jch3ooh**
TERPACID3 + hν	→	**OH + CO2 + TERPA4O2**	**0.71*jch3ooh**
TERPAPAN + hν	→	**TERPACO3 + NO2**	**jpan**
TERPDHDP + hν	→	**TERPOOH + OH + HO2**	**2.0*jch3ooh**
TERPFDN + hν	→	**TERPNS + HO2 + NO2**	**jch3ooh**
TERPHFN + hν	→	**TERPNS + OH + HO2**	**jch3ooh**
TERPNPS + hν	→	**OH + 0.5*TERPNS + 0.5*HO2 + 0.5*TERPA + 0.5*NO2**	**jch3ooh**
TERPNPS1 + hν	→	**OH + 0.54*TERPNS1 + 0.54*HO2 + 0.46*TERPF1 + 0.46*NO2**	**jch3ooh**
TERPNPT + hν	→	**TERPA + NO2 + OH**	**jch3ooh**
TERPNPT1 + hν	→	**OH + 0.54*TERPNT1 + 0.54*HO2 + 0.46*TERPF1 + 0.46*NO2**	**jch3ooh**
TERPNS + hν	→	**NO2 + HO2 + TERPA**	**jch3ooh**
TERPNS1 + hν	→	**NO2 + HO2 + TERPF1**	**jch3ooh**
TERPNT + hν	→	**NO2 + HO2 + TERPA**	**jch3ooh**
TERPNT1 + hν	→	**NO2 + HO2 + TERPF1**	**jch3ooh**
TERPOOH + hν	→	**OH + TERPA + HO2**	jch3ooh
TERPOOHL + hν	→	**OH + TERPA3 + HO2**	**jch3ooh**
TOLOOH + hν	→	OH + 0.6*GLYOXAL + 0.4*CH3COCHO + HO2 + 0.2*BIGALD1 + 0.2*BIGALD2 + 0.2*BIGALD3	jch3ooh
XYLENOOH + hν	→	OH + HO2 + 0.34*GLYOXAL + 0.54*CH3COCHO + 0.06*BIGALD1 + 0.2*BIGALD2 + 0.15*BIGALD3 + 0.21*BIGALD4	jch3ooh

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		Products	Rate
XYLOLOOH + hν	$\rightarrow$	OH + 0.17*GLYOXAL + 0.51*CH3COCHO + HO2	jch3ooh
Halogens			
BRCL + hν	$\rightarrow$	BR + CL	jbrcl
BRO + hν	$\rightarrow$	BR + O	jbro
BRONO2 + hν	$\rightarrow$	BRO + NO2	jbrono2_b
BRONO2 + hν	$\rightarrow$	BR + NO3	jbrono2_a
CCL4 + hν	$\rightarrow$	4*CL	jccl4
CF2CLBR + hν	$\rightarrow$	BR + CL + COF2	jcf2clbr
CF3BR + hν	$\rightarrow$	BR + F + COF2	jcf3br
CFC11 + hν	$\rightarrow$	2*CL + COFCL	jcfcl3
CFC113 + hν	$\rightarrow$	2*CL + COFCL + COF2	jcfc113
CFC114 + hν	$\rightarrow$	2*CL + 2*COF2	jcfc114
CFC115 + hν	$\rightarrow$	CL + F + 2*COF2	jcfc115
CFC12 + hν	$\rightarrow$	2*CL + COF2	jcf2cl2
CH2BR2 + hν	$\rightarrow$	2*BR	jch2br2
CH3BR + hν	$\rightarrow$	BR + CH3O2	jch3br
CH3CCL3 + hν	$\rightarrow$	3*CL	jch3ccl3
CH3CL + hν	$\rightarrow$	CL + CH3O2	jch3cl
CHBR3 + hν	$\rightarrow$	3*BR	jchbr3
CL2 + hν	$\rightarrow$	2*CL	jcl2
CL2O2 + hν	$\rightarrow$	2*CL	jcl2o2
CLO + hν	$\rightarrow$	CL + O	jclo
CLONO2 + hν	$\rightarrow$	CL + NO3	jclono2_a
CLONO2 + hν	$\rightarrow$	CLO + NO2	jclono2_b
COF2 + hν	$\rightarrow$	2*F	jcof2
COFCL + hν	$\rightarrow$	F + CL	jcofcl
H2402 + hν	$\rightarrow$	2*BR + 2*COF2	jh2402
HBR + hν	$\rightarrow$	BR + H	jhbr
HCFC141B + hν	$\rightarrow$	CL + COFCL	jhcfc141b
HCFC142B + hν	$\rightarrow$	CL + COF2	jhcfc142b
HCFC22 + hν	$\rightarrow$	CL + COF2	jhcfc22
HCL + hν	$\rightarrow$	H + CL	jhcl
HF + hν	$\rightarrow$	H + F	jhf
HOBR + hν	$\rightarrow$	BR + OH	jhobr
HOCL + hν	$\rightarrow$	OH + CL	jhocl

Table S5: MOZART-TS2 Photolysis Reactions

Reactant		**Products**	**Rate**
OCLO + hν	$\rightarrow$	O + CLO	joclo
SF6 + hν	$\rightarrow$	sink	jsf6
Sulfur compounds			
H2SO4 + hν	$\rightarrow$	SO3 + H2O	jh2so4
OCS + hν	$\rightarrow$	S + CO	jocs
SO + hν	$\rightarrow$	S + O	jso
SO2 + hν	$\rightarrow$	SO + O	jso2
SO3 + hν	$\rightarrow$	SO2 + O	jso3
Secondary organic aerosol tracers			
soa1_a1 + hν	$\rightarrow$		0.0004*jno2
soa1_a2 + hν	$\rightarrow$		0.0004*jno2
soa2_a1 + hν	$\rightarrow$		0.0004*jno2
soa2_a2 + hν	$\rightarrow$		0.0004*jno2
soa3_a1 + hν	$\rightarrow$		0.0004*jno2
soa3_a2 + hν	$\rightarrow$		0.0004*jno2
soa4_a1 + hν	$\rightarrow$		0.0004*jno2
soa4_a2 + hν	$\rightarrow$		0.0004*jno2
soa5_a1 + hν	$\rightarrow$		0.0004*jno2
soa5_a2 + hν	$\rightarrow$		0.0004*jno2

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
Odd-Oxygen			
O1D + H2	→	H + OH	1.200e-10
O1D + H2O	→	2*OH	1.63e-10 exp(60.00 / t)
O1D + N2	→	O + N2	2.15e-11 exp(110.00 / t)
O1D + O2	→	O + O2	3.30e-11 exp(55.00 / t)
O1D + O3	→	O2 + O2	1.200e-10
O + O3	→	2*O2	8.00e-12 exp(-2060.00 / t)
O + O + M	→	O2 + M	2.76e-34 exp(720 / t)
O + O2 + M	→	O3 + M	6e-34 (300 / t)$^{2.4}$
Odd-Hydrogen			
H2 + O	→	OH + H	1.60e-11 exp(-4570.00 / t)
H2O2 + O	→	OH + HO2	1.40e-12 exp(-2000.00 / t)
H + HO2	→	H2 + O2	6.900e-12
H + HO2	→	2*OH	7.200e-11
H + HO2	→	H2O + O	1.600e-12
H + O2 + M	→	HO2 + M	TROEE(4.40e-32, 1.30, 7.500000e-11, -0.20, 0.60)
HO2 + O	→	OH + O2	3.00e-11 exp(200.00 / t)
HO2 + O3	→	OH + 2*O2	1.00e-14 exp(-490.00 / t)
H + O3	→	OH + O2	1.40e-10 exp(-470.00 / t)
OH + H2	→	H2O + H	2.80e-12 exp(-1800.00 / t)
OH + H2O2	→	H2O + HO2	1.800e-12
OH + HO2	→	H2O + O2	4.80e-11 exp(250.00 / t)
OH + O	→	H + O2	1.80e-11 exp(180.00 / t)
OH + O3	→	HO2 + O2	1.70e-12 exp(-940.00 / t)
OH + OH	→	H2O + O	1.800e-12
OH + OH + M	→	H2O2 + M	TROEE(6.90e-31, 1.00, 2.600000e-11, 0.00, 0.60)
HO2 + HO2	→	H2O2 + O2	(3.0e-13 exp(460 / t) + 2.1e-33 [M] exp(920 / t)) (1+1.4e-21[H2O] exp(2200 / t))
Odd-Nitrogen			
HO2NO2 + OH	→	H2O + NO2 + O2	1.30e-12 exp(380.00 / t)
N + NO	→	N2 + O	2.10e-11 exp(100.00 / t)
N + NO2	→	N2O + O	2.90e-12 exp(220.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
N + NO2	→	2*NO	1.45e-12 exp(220.00 / t)
N + NO2	→	N2 + O2	1.45e-12 exp(220.00 / t)
N + O2	→	NO + O	1.50e-11 exp(-3600.00 / t)
NO2 + O	→	NO + O2	5.10e-12 exp(210.00 / t)
NO2 + O3	→	NO3 + O2	1.20e-13 exp(-2450.00 / t)
NO2 + O + M	→	NO3 + M	TROEE(2.50e-31, 1.80, 2.200000e-11, 0.70, 0.60)
NO3 + HO2	→	OH + NO2 + O2	3.500e-12
NO3 + NO	→	2*NO2	1.50e-11 exp(170.00 / t)
NO3 + O	→	NO2 + O2	1.000e-11
NO3 + OH	→	HO2 + NO2	2.200e-11
N + OH	→	NO + H	5.000e-11
NO + HO2	→	NO2 + OH	3.30e-12 exp(270.00 / t)
NO + O3	→	NO2 + O2	3.00e-12 exp(-1500.00 / t)
NO + O + M	→	NO2 + M	TROEE(9.00e-32, 1.50, 3.000000e-11, 0.00, 0.60)
O1D + N2O	→	2*NO	7.26e-11 exp(20.00 / t)
O1D + N2O	→	N2 + O2	4.64e-11 exp(20.00 / t)
NO2 + HO2 + M	→	HO2NO2 + M	TROEE(1.90e-31, 3.40, 4.000000e-12, 0.30, 0.60)
NO2 + NO3 + M	→	N2O5 + M	TROEE(2.40e-30, 3.00, 1.600000e-12, -0.10, 0.60)
NO2 + OH + M	→	HNO3 + M	TROEE(1.80e-30, 3.00, 2.800000e-11, 0.00, 0.60)
HNO3 + OH	→	NO3 + H2O	k0 + k3[M] / (1+k3[M]/k2): k0 = 2.4e-14 exp(460 / t), k2 = 2.7e-17 exp(2199 / t), k3 = 6.5e-34 exp(1335 / t)
HO2NO2 + M	→	HO2 + NO2 + M	k(NO2+HO2+M) * exp(- 10900 / t) / 2.1e-27)
N2O5 + M	→	NO2 + NO3 + M	k(NO2+NO3) * 2.724138e26 exp(-10840 / t)
Odd-Chlorine			
CL + CH2O	→	HCL + HO2 + CO	8.10e-11 exp(-30.00 / t)
CL + CH4	→	CH3O2 + HCL	7.10e-12 exp(-1270.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
CL + H2	→	HCL + H	3.05e-11 exp(-2270.00 / t)
CL + H2O2	→	HCL + HO2	1.10e-11 exp(-980.00 / t)
CL + HO2	→	HCL + O2	1.40e-11 exp(270.00 / t)
CL + HO2	→	OH + CLO	3.60e-11 exp(-375.00 / t)
CL + O3	→	CLO + O2	2.30e-11 exp(-200.00 / t)
CLO + CH3O2	→	CL + HO2 + CH2O	3.30e-12 exp(-115.00 / t)
CLO + CLO	→	2*CL + O2	3.00e-11 exp(-2450.00 / t)
CLO + CLO	→	CL2 + O2	1.00e-12 exp(-1590.00 / t)
CLO + CLO	→	CL + OCLO	3.50e-13 exp(-1370.00 / t)
CLO + HO2	→	O2 + HOCL	2.60e-12 exp(290.00 / t)
CLO + NO	→	NO2 + CL	6.40e-12 exp(290.00 / t)
CLONO2 + CL	→	CL2 + NO3	6.50e-12 exp(135.00 / t)
CLO + NO2 + M	→	CLONO2 + M	TROEE(1.80e-31, 3.40, 1.500000e-11, 1.90, 0.60)
CLONO2 + O	→	CLO + NO3	3.60e-12 exp(-840.00 / t)
CLONO2 + OH	→	HOCL + NO3	1.20e-12 exp(-330.00 / t)
CLO + O	→	CL + O2	2.80e-11 exp(85.00 / t)
CLO + OH	→	CL + HO2	7.40e-12 exp(270.00 / t)
CLO + OH	→	HCL + O2	6.00e-13 exp(230.00 / t)
HCL + O	→	CL + OH	1.00e-11 exp(-3300.00 / t)
HCL + OH	→	H2O + CL	1.80e-12 exp(-250.00 / t)
HOCL + CL	→	HCL + CLO	3.40e-12 exp(-130.00 / t)
HOCL + O	→	CLO + OH	1.700e-13
HOCL + OH	→	H2O + CLO	3.00e-12 exp(-500.00 / t)
O1D + CCL4	→	4*CL	2.607e-10
O1D + CF2CLBR	→	CL + BR + COF2	9.750e-11
O1D + CFC11	→	2*CL + COFCL	2.070e-10
O1D + CFC113	→	2*CL + COFCL + COF2	2.088e-10
O1D + CFC114	→	2*CL + 2*COF2	1.170e-10
O1D + CFC115	→	CL + F + 2*COF2	4.644e-11
O1D + CFC12	→	2*CL + COF2	1.204e-10
O1D + HCL	→	CL + OH	9.900e-11
O1D + HCL	→	CLO + H	3.300e-12
CLO + CLO + M	→	CL2O2 + M	TROEE(1.90e-32, 3.60, 3.700000e-12, 1.60, 0.60)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
CL2O2 + M	→	CLO + CLO + M	usr_CL2O2_M
Odd-Bromine			
BR + CH2O	→	HBR + HO2 + CO	1.70e-11 exp(-800.00 / t)
BR + HO2	→	HBR + O2	4.80e-12 exp(-310.00 / t)
BR + O3	→	BRO + O2	1.60e-11 exp(-780.00 / t)
BRO + BRO	→	2*BR + O2	1.50e-12 exp(230.00 / t)
BRO + CLO	→	BR + OCLO	9.50e-13 exp(550.00 / t)
BRO + CLO	→	BR + CL + O2	2.30e-12 exp(260.00 / t)
BRO + CLO	→	BRCL + O2	4.10e-13 exp(290.00 / t)
BRO + HO2	→	HOBR + O2	4.50e-12 exp(460.00 / t)
BRO + NO	→	BR + NO2	8.80e-12 exp(260.00 / t)
BRO + NO2 + M	→	BRONO2 + M	TROEE(5.20e-31, 3.20, 6.900000e-12, 2.90, 0.60)
BRONO2 + O	→	BRO + NO3	1.90e-11 exp(215.00 / t)
BRO + O	→	BR + O2	1.90e-11 exp(230.00 / t)
BRO + OH	→	BR + HO2	1.70e-11 exp(250.00 / t)
HBR + O	→	BR + OH	5.80e-12 exp(-1500.00 / t)
HBR + OH	→	BR + H2O	5.50e-12 exp(200.00 / t)
HOBR + O	→	BRO + OH	1.20e-10 exp(-430.00 / t)
O1D + CF3BR	→	BR + F + COF2	4.500e-11
O1D + CHBR3	→	3*BR	4.620e-10
O1D + H2402	→	2*BR + 2*COF2	1.200e-10
O1D + HBR	→	BR + OH	9.000e-11
O1D + HBR	→	BRO + H	3.000e-11
Odd-Fluorine			
F + CH4	→	HF + CH3O2	1.60e-10 exp(-260.00 / t)
F + H2	→	HF + H	1.40e-10 exp(-500.00 / t)
F + H2O	→	HF + OH	1.40e-11 exp(0.00 / t)
F + HNO3	→	HF + NO3	6.00e-12 exp(400.00 / t)
O1D + COF2	→	2*F	2.140e-11
O1D + COFCL	→	F + CL	1.900e-10
Organic Halogens			
CH2BR2 + CL	→	2*BR + HCL	6.30e-12 exp(-800.00 / t)
CH2BR2 + OH	→	2*BR + H2O	2.00e-12 exp(-840.00 / t)
CH3BR + CL	→	HCL + HO2 + BR	1.46e-11 exp(-1040.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
CH3BR + OH	→	BR + H2O + HO2	1.42e-12 exp(-1150.00 / t)
CH3CCL3 + OH	→	H2O + 3*CL	1.64e-12 exp(-1520.00 / t)
CH3CL + CL	→	HO2 + CO + 2*HCL	2.03e-11 exp(-1100.00 / t)
CH3CL + OH	→	CL + H2O + HO2	1.96e-12 exp(-1200.00 / t)
CHBR3 + CL	→	3*BR + HCL	4.85e-12 exp(-850.00 / t)
CHBR3 + OH	→	3*BR	9.00e-13 exp(-360.00 / t)
HCFC141B + OH	→	CL + COFCL	1.25e-12 exp(-1600.00 / t)
HCFC142B + OH	→	CL + COF2	1.30e-12 exp(-1770.00 / t)
HCFC22 + OH	→	H2O + CL + COF2	9.20e-13 exp(-1560.00 / t)
O1D + CH2BR2	→	2*BR	2.570e-10
O1D + CH3BR	→	BR	1.800e-10
O1D + HCFC141B	→	CL + COFCL	1.794e-10
O1D + HCFC142B	→	CL + COF2	1.300e-10
O1D + HCFC22	→	CL + COF2	7.650e-11
C1 Organics			
CH2O + HO2	→	HOCH2OO	9.70e-15 exp(625.00 / t)
CH2O + NO3	→	CO + HO2 + HNO3	6.00e-13 exp(-2058.00 / t)
CH2O + O	→	HO2 + OH + CO	3.40e-11 exp(-1600.00 / t)
CH2O + OH	→	CO + H2O + H	5.50e-12 exp(125.00 / t)
CH3O2 + CH3O2	→	2*CH2O + 2*HO2	5.00e-13 exp(-424.00 / t)
CH3O2 + CH3O2	→	CH2O + CH3OH	1.90e-14 exp(706.00 / t)
CH3O2 + HO2	→	CH3OOH + O2	4.10e-13 exp(750.00 / t)
CH3O2 + NO	→	CH2O + NO2 + HO2	2.80e-12 exp(300.00 / t)
CH3OH + OH	→	HO2 + CH2O	2.90e-12 exp(-345.00 / t)
CH3OOH + OH	→	0.7*CH3O2 + 0.3*OH + 0.3*CH2O + H2O	3.80e-12 exp(200.00 / t)
CH4 + OH	→	CH3O2 + H2O	2.45e-12 exp(-1775.00 / t)
CO + OH + M	→	CO2 + HO2 + M	TROEE(5.90e-33, 1.00, 1.100000e-12, -1.30, 0.60)
HCN + OH + M	→	HO2 + M	TROEE(4.28e-33, 0.00, 9.300000e-15, -4.42, 0.80)
HCOOH + OH	→	HO2 + CO2 + H2O	4.000e-13
HMHP + OH	→	**0.5*CH2O + 0.5*HO2 + 0.5*HCOOH + 0.5*OH + H2O**	**1.30e-12 exp(500.00 / t)**
HOCH2OO + HO2	→	**0.5*HMHP + 0.5*HCOOH + 0.3*H2O + 0.2*HO2 + 0.2*OH**	**5.60e-15 exp(2300.00 / t)**
HOCH2OO	→	CH2O + HO2	2.40e+12 exp(-7000.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
HOCH2OO + NO	→	HCOOH + NO2 + HO2	2.60e-12 exp(265.00 / t)
O1D + CH4	→	CH3O2 + OH	1.310e-10
O1D + CH4	→	CH2O + H + HO2	3.500e-11
O1D + CH4	→	CH2O + H2	9.000e-12
O1D + HCN	→	OH	1.08e-10 exp(105.00 / t)
CO + OH	→	CO2 + H	k0 = 1.5e-13 , ki = 2.1e9 (t / 300)$^{6.1}$, k = (k0/(1+k0/(ki/M))) * (0.6^(1/(1+(log(k0/(ki/M)))^2)))
C2 Organics			
C2H2 + CL + M	→	CL + M	TROEE(5.20e-30, 2.40, 2.200000e-10, 0.70, 0.60)
C2H2 + OH + M	→	0.65*GLYOXAL + 0.65*OH + 0.35*HCOOH + 0.35*HO2 + 0.35*CO + M	TROEE(5.50e-30, 0.00, 8.300000e-13, -2.00, 0.60)
C2H4 + CL + M	→	CL + M	TROEE(1.60e-29, 3.30, 3.100000e-10, 1.00, 0.60)
C2H4 + O3	→	0.63*CO + 0.13*OH + 0.13*HO2 + 0.37*HCOOH + CH2O	1.20e-14 exp(-2630.00 / t)
C2H5O2 + C2H5O2	→	1.6*CH3CHO + 1.2*HO2 + 0.4*C2H5OH	6.800e-14
C2H5O2 + CH3O2	→	0.7*CH2O + 0.8*CH3CHO + HO2 + 0.3*CH3OH + 0.2*C2H5OH	2.000e-13
C2H5O2 + HO2	→	C2H5OOH + O2	7.50e-13 exp(700.00 / t)
C2H5O2 + NO	→	CH3CHO + HO2 + NO2	2.60e-12 exp(365.00 / t)
C2H5OH + OH	→	HO2 + CH3CHO	6.90e-12 exp(-230.00 / t)
C2H5OOH + OH	→	0.5*C2H5O2 + 0.5*CH3CHO + 0.5*OH	3.80e-12 exp(200.00 / t)
C2H6 + CL	→	HCL + C2H5O2	7.20e-11 exp(-70.00 / t)
C2H6 + OH	→	C2H5O2 + H2O	7.66e-12 exp(-1020.00 / t)
CH3CHO + NO3	→	CH3CO3 + HNO3	1.40e-12 exp(-1900.00 / t)
CH3CHO + OH	→	CH3CO3 + H2O	4.63e-12 exp(350.00 / t)
CH3CN + OH	→	HO2	7.80e-13 exp(-1050.00 / t)
CH3CO3 + CH3CO3	→	2*CH3O2 + 2*CO2	2.90e-12 exp(500.00 / t)
CH3CO3 + CH3O2	→	0.9*CH3O2 + CH2O + 0.9*HO2 + 0.9*CO2 + 0.1*CH3COOH	2.00e-12 exp(500.00 / t)
CH3CO3 + HO2	→	**0.36*CH3COOOH + 0.15*CH3COOH + 0.15*O3 + 0.49*OH + 0.49*CH3O2 + 0.49*CO2**	4.30e-13 exp(1040.00 / t)
CH3CO3 + NO	→	CH3O2 + CO2 + NO2	8.10e-12 exp(270.00 / t)
CH3COOH + OH	→	CH3O2 + CO2 + H2O	7.000e-13

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
CH3COOOH + OH	→	0.5*CH3CO3 + 0.5*CH2O + 0.5*CO2 + H2O	1.000e-12
EO2 + HO2	→	EOOH	7.50e-13 exp(700.00 / t)
EO2 + NO	→	0.5*CH2O + 0.25*HO2 + 0.75*EO + NO2	4.20e-12 exp(180.00 / t)
EO	→	2*CH2O + HO2	1.60e+11 exp(-4150.00 / t)
EO + O2	→	GLYALD + HO2	1.000e-14
GLYALD + OH	→	HO2 + 0.2*GLYOXAL + 0.8*CH2O + 0.8*CO2	1.000e-11
GLYOXAL + OH	→	HO2 + CO + CO2	1.150e-11
HCOCH2OOH + OH	→	**0.89*GLYOXAL + 0.89*OH + 0.11*CH2O + 0.11*HO2 + 0.11*CO**	**3.300e-11**
NO3CH2CHO + OH	→	**CO2 + CH2O + NO2**	**3.400e-12**
PAN + OH	→	CH2O + NO3	4.000e-14
C2H4 + OH + M	→	EO2 + M	TROEE(8.60e-29, 3.10, 9.000000e-12, 0.85, 0.48)
CH3CO3 + NO2 + M	→	PAN + M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
PAN + M	→	CH3CO3 + NO2 + M	k(CH3CO3+NO2+M) * 1.111e28 exp(-14000 / t)
C3 Organics			
C3H6 + NO3	→	NOA	4.60e-13 exp(-1156.00 / t)
C3H6 + O3	→	0.5*CH2O + 0.12*HCOOH + 0.12*CH3COOH + 0.5*CH3CHO + 0.56*CO + 0.28*CH3O2 + 0.1*CH4 + 0.2*CO2 + 0.28*HO2 + 0.36*OH	6.50e-15 exp(-1900.00 / t)
C3H7O2 + CH3O2	→	CH2O + HO2 + 0.82*CH3COCH3	3.75e-13 exp(-40.00 / t)
C3H7O2 + HO2	→	C3H7OOH + O2	7.50e-13 exp(700.00 / t)
C3H7O2 + NO	→	0.82*CH3COCH3 + NO2 + HO2 + 0.27*CH3CHO	4.20e-12 exp(180.00 / t)
C3H7OOH + OH	→	H2O + C3H7O2	3.80e-12 exp(200.00 / t)
C3H8 + OH	→	C3H7O2 + H2O	8.70e-12 exp(-615.00 / t)
CH3COCHO + NO3	→	HNO3 + CO + CH3CO3	1.40e-12 exp(-1860.00 / t)
CH3COCHO + OH	→	CH3CO3 + CO + H2O	8.40e-13 exp(830.00 / t)
HYAC + OH	→	CH3COCHO + HO2	3.000e-12
HYPERACET + OH	→	**0.3*CH3CO3 + 0.3*CH2O + 0.7*CH3COCHO + 0.7*OH**	**1.200e-11**
NOA + OH	→	NO2 + CH3COCHO	6.700e-13
PO2 + HO2	→	POOH + O2	7.50e-13 exp(700.00 / t)
PO2 + NO	→	CH3CHO + CH2O + HO2 + NO2	4.20e-12 exp(180.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
POOH + OH	→	0.5*PO2 + 0.5*OH + 0.5*HYAC + H2O	3.80e-12 exp(200.00 / t)
RO2 + CH3O2	→	0.3*CH3CO3 + 0.8*CH2O + 0.3*HO2 + 0.2*HYAC + 0.5*CH3COCHO + 0.5*CH3OH	7.10e-13 exp(500.00 / t)
RO2 + HO2	→	0.85*ROOH + 0.15*OH + 0.15*CH2O + 0.15*CH3CO3	8.60e-13 exp(700.00 / t)
RO2 + NO	→	CH3CO3 + CH2O + NO2	2.90e-12 exp(300.00 / t)
ROOH + OH	→	RO2 + H2O	3.80e-12 exp(200.00 / t)
C3H6 + OH + M	→	PO2 + M	TROEE(8.00e-27, 3.50, 3.000000e-11, 0.00, 0.50)
CH3COCH3 + OH	→	RO2 + H2O	3.82e-11 exp(-2000 / t) + 1.33e-13
C4 Organics			
BIGENE + NO3	→	NO2 + CH3CHO + 0.5*CH2O + 0.5*CH3COCH3	3.500e-13
BIGENE + OH	→	ENEO2	5.400e-11
DHPMPAL + OH	→	**HYPERACET + CO + OH**	**3.770e-11**
ENEO2 + NO	→	CH3CHO + 0.5*CH2O + 0.5*CH3COCH3 + HO2 + NO2	4.80e-12 exp(120.00 / t)
ENEO2 + NO	→	HONITR	5.10e-14 exp(693.00 / t)
HONITR + OH	→	ONITR + HO2	2.000e-12
MACRN + OH	→	**CO + 0.5*HO2 + 0.5*NOA + 0.5*NO2 + 0.5*HYAC**	**1.290e-11**
MACRO2 + CH3CO3	→	**HO2 + 0.86*HYAC + 0.86*CO + 0.14*CH2O + 0.14*CH3COCHO + CO2 + CH3O2**	**2.00e-12 exp(500.00 / t)**
MACRO2 + CH3O2	→	**0.9*HYAC + 0.9*CO + 1.5*HO2 + 0.1*CH3COCH3 + 1.1*CH2O**	**4.500e-14**
MACRO2 + HO2	→	**0.41*MACROOH + 0.59*OH + 0.59*HO2 + 0.51*HYAC + 0.51*CO + 0.08*CH3COCHO + 0.08*CH2O**	**2.11e-13 exp(1300.00 / t)**
MACRO2	→	**HYAC + CO + OH**	**2.90e+7 exp(-5297.00 / t)**
MACR + O3	→	0.12*CH2O + 0.24*OH + 0.65*CO + 0.1*CH3CO3 + 0.88*CH3COCHO + 0.33*HCOOH + 0.14*HO2	1.50e-15 exp(-2100.00 / t)
MACR + OH	→	**0.55*MACRO2 + 0.45*H2O + 0.45*MCO3**	9.60e-12 exp(360.00 / t)
MACROOH + OH	→	**HYAC + CO + OH**	**3.770e-11**
MCO3 + CH3CO3	→	**2*CO2 + 0.35*CH3CO3 + CH2O + 1.65*CH3O2 + 0.65*CO**	**2.90e-12 exp(500.00 / t)**
MCO3 + CH3O2	→	**CO2 + 0.35*CH3CO3 + 2*CH2O + 0.65*CH3O2 + 0.65*CO + HO2**	2.00e-12 exp(500.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
MCO3 + HO2	→	**0.49*CH2O + 0.49*OH + 0.49*CO2 + 0.17*CH3CO3 + 0.32*CH3O2 + 0.32*CO + 0.15*O3 + 0.15*CH3COOH + 0.36*CH3COOOH**	4.30e-13 exp(1040.00 / t)
MCO3 + MCO3	→	**2*CO2 + 0.7*CH3CO3 + 2*CH2O + 1.3*CH3O2 + 1.3*CO**	**2.90e-12 exp(500.00 / t)**
MCO3 + NO	→	**NO2 + CO2 + 0.35*CH3CO3 + CH2O + 0.65*CH3O2 + 0.65*CO**	**8.10e-12 exp(270.00 / t)**
MCO3 + NO3	→	**NO2 + CO2 + 0.35*CH3CO3 + CH2O + 0.65*CH3O2 + 0.65*CO**	**4.000e-12**
MEKO2 + HO2	→	0.8*MEKOOH + 0.2*OH + 0.2*CH3CHO + 0.2*CH3CO3	7.50e-13 exp(700.00 / t)
MEKO2 + NO	→	CH3CO3 + CH3CHO + NO2	4.20e-12 exp(180.00 / t)
MEK + OH	→	MEKO2	2.30e-12 exp(-170.00 / t)
MEKOOH + OH	→	MEKO2	3.80e-12 exp(200.00 / t)
MPAN + OH + M	→	**0.25*HYAC + NO3 + 0.25*CO + M**	TROEE(8.00e-27, 3.50, 3.000000e-11, 0.00, 0.50)
MVKN + OH	→	**HO2 + 0.5*ONITR + 0.5*CO + 0.5*NOA**	**1.780e-12**
MVKO2 + CH3CO3	→	**CH3O2 + CO2 + 0.75*GLYALD + 0.75*CH3CO3 + 0.25*CH2O + 0.25*HO2 + 0.25*CH3COCHO**	**2.00e-12 exp(500.00 / t)**
MVKO2 + CH3O2	→	**0.25*CH3OH + 1*CO + 0.87*CH2O + 0.62*HO2 + 0.38*GLYALD + 0.88*CH3CO3 + 0.12*CH3COCHO**	**6.100e-13**
MVKO2 + HO2	→	**0.46*MVKOOH + 0.54*OH + 0.36*GLYALD + 0.49*CH3CO3 + 0.26*CO + 0.18*HO2 + 0.05*CH3COCHO + 0.05*CH2O**	**2.11e-13 exp(1300.00 / t)**
MVK + O3	→	0.6*CH2O + 0.56*CO + 0.1*CH3CHO + 0.1*CO2 + 0.28*CH3CO3 + 0.5*CH3COCHO + 0.28*HO2 + 0.36*OH + 0.12*HCOOH	8.50e-16 exp(-1520.00 / t)
MVK + OH	→	**MVKO2**	**2.70e-12 exp(580.00 / t)**
MVKOOH + OH	→	**1.56*CO + 0.44*HO2 + 0.44*CH3COCHO + 0.56*CH3CO3**	**4.800e-11**
MCO3 + NO2 + M	→	MPAN + M	**TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)**
MPAN + M	→	MCO3 + NO2 + M	k(MCO3+NO2+M) * 1.111e28 exp(-14000 / t)
C5 Organics			
ALKNIT + OH	→	0.4*CH2O + 0.8*CH3CHO + 0.8*CH3COCH3 + NO2	1.600e-12
ALKO2 + HO2	→	ALKOOH	7.50e-13 exp(700.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ALKO2 + NO	→	0.4*CH3CHO + 0.1*CH2O + 0.25*CH3COCH3 + HO2 + 0.8*MEK + NO2	6.700e-12
ALKO2 + NO	→	ALKNIT	5.40e-14 exp(870.00 / t)
ALKOOH + OH	→	ALKO2	3.80e-12 exp(200.00 / t)
BIGALK + OH	→	ALKO2	3.500e-12
HPALD1 + OH	→	**0.51*HO2 + 1.06*CO + 0.38*CH3COCHO + 0.54*CO2 + 0.06*CH3O2 + 0.06*CH3CO3 + 0.08*ICHE + 0.07*DHPMPAL + 0.43*OH + 0.35*MVK**	**1.17e-11 exp(450.00 / t)**
HPALD4 + OH	→	**0.41*HO2 + 0.76*CO + 0.03*CH3COCHO + 0.54*CO2 + 0.06*CH3O2 + 0.06*CH3CO3 + 0.15*HYPERACET + 0.18*ICHE + 0.17*DHPMPAL + 0.35*MACR + 0.53*OH**	**1.17e-11 exp(450.00 / t)**
HPALDB1C + OH	→	**0.58*ICHE + OH + 0.42*CO + 0.23*MVK + 0.19*MVKOOH**	**2.20e-11 exp(390.00 / t)**
HPALDB4C + OH	→	**0.77*ICHE + OH + 0.23*CO + 0.14*MACR + 0.09*MACROOH**	**3.50e-11 exp(390.00 / t)**
HYDRALD + OH	→	**1.08*OH + CO + 0.36*CO2 + 0.46*CH3COCHO + 0.32*IEPOXOO + 0.22*HYAC + 0.32*HO2**	**6.420e-11**
ICHE + OH	→	**OH + 1.5*CO + 0.5*HYAC + 0.5*CH3COCHO + 0.5*CH2O**	**9.85e-12 exp(410.00 / t)**
IEPOX + OH	→	**0.19*ICHE + 0.19*HO2 + 0.81*IEPOXOO**	**4.43e-11 exp(-400.00 / t)**
IEPOXOO + HO2	→	**0.35*ISOPHFP + 0.65*OH + 0.65*HO2 + 0.26*CO + 0.37*GLYALD + 0.46*CH3COCHO + 0.15*GLYOXAL + 0.19*HYAC**	**2.38e-13 exp(1300.00 / t)**
INHEB + OH	→	**0.2*INHEB + 0.4*NC4CHOO2 + 0.4*CH3COCHO + 0.4*HCOOH + 0.4*CH2O + 0.4*NO2**	**4.43e-11 exp(-400.00 / t)**
INHED + OH	→	**0.35*NOA + 0.35*CO + 0.4*HO2 + 0.59*CH2O + 0.35*NC4CHOO2 + 0.06*INHED + 0.19*HYAC + 0.19*CO2 + 0.19*NO2 + 0.05*MVKN**	**3.22e-11 exp(-400.00 / t)**
ISOPB1O2 + CH3CO3	→	**MVK + CH2O + HO2 + CO2 + CH3O2**	**2.00e-12 exp(500.00 / t)**
ISOPB1O2 + CH3O2	→	**1.75*CH2O + 0.25*ISOPOH + 0.75*MVK + 1.5*HO2**	**1.600e-13**
ISOPB1O2 + HO2	→	**0.06*MVK + 0.06*CH2O + 0.06*OH + 0.06*HO2 + 0.94*ISOPOOH**	**2.12e-13 exp(1300.00 / t)**
ISOPB1O2	→	**MVK + CH2O + OH**	**1.04e+11 exp(-9746.00 / t)**
ISOPB1O2	→	**ISOPC1C + O2**	**2.24e+15 exp(-10865.00 / t)**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPB1O2	→	ISOPC1T + O2	2.22e+15 exp(-10355.00 / t)
ISOPB4O2 + CH3CO3	→	MACR + CH2O + HO2 + CO2 + CH3O2	2.00e-12 exp(500.00 / t)
ISOPB4O2 + CH3O2	→	0.25*CH3OH + 0.25*HYDRALD + 0.25*ISOPOH + 1.25*CH2O + HO2 + 0.5*MACR	1.400e-12
ISOPB4O2 + HO2	→	0.06*MACR + 0.06*CH2O + 0.06*OH + 0.06*HO2 + 0.94*ISOPOOH	2.12e-13 exp(1300.00 / t)
ISOPB4O2	→	MACR + CH2O + OH	1.88e+11 exp(-9752.00 / t)
ISOPB4O2	→	ISOPC4C + O2	2.49e+15 exp(-11112.00 / t)
ISOPB4O2	→	ISOPC4T + O2	2.49e+15 exp(-10890.00 / t)
O2 + ISOPC1C	→	ISOPB1O2	7.500e-13
ISOPC1C + O2	→	ISOPZD1O2	1.400e-13
ISOPC1T + O2	→	ISOPB1O2	7.500e-13
ISOPC1T + O2	→	ISOPED1O2	3.600e-13
ISOPC4C + O2	→	ISOPB4O2	6.500e-13
ISOPC4C + O2	→	ISOPZD4O2	2.100e-13
ISOPC4T + O2	→	ISOPB4O2	6.500e-13
ISOPC4T + O2	→	ISOPED4O2	4.900e-13
ISOPED1O2 + CH3CO3	→	0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MVKOOH + CO2 + CH3O2	2.00e-12 exp(500.00 / t)
ISOPED1O2 + CH3O2	→	0.25*CH3OH + 0.25*ISOPOH + 0.75*CH2O + 0.72*HO2 + 0.28*CO + 0.28*OH + 0.28*MVKOOH + 0.47*HYDRALD	1.200e-12
ISOPED1O2 + HO2	→	ISOPOOH	2.12e-13 exp(1300.00 / t)
ISOPED1O2	→	ISOPC1T + O2	1.83e+14 exp(-8930.00 / t)
ISOPED4O2 + CH3CO3	→	0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MACROOH + CO2 + CH3O2	2.00e-12 exp(500.00 / t)
ISOPED4O2 + CH3O2	→	0.25*CH3OH + 0.25*ISOPOH + 0.75*CH2O + 0.72*HO2 + 0.28*CO + 0.28*OH + 0.28*MACROOH + 0.47*HYDRALD	9.800e-13
ISOPED4O2 + HO2	→	ISOPOOH	2.12e-13 exp(1300.00 / t)
ISOPED4O2	→	ISOPC4T + O2	2.08e+14 exp(-9400.00 / t)
ISOPFDNC + OH	→	CO + NO2 + 0.5*MACRN + 0.5*MVKN	1.850e-11
ISOPFDN + OH	→	ISOPFDNC + HO2	1.630e-12

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPFNC + OH	→	**CO + 0.5*NO2 + 0.5*OH + 0.25*MACRN + 0.25*MVKN + 0.25*MACROOH + 0.25*MVKOOH**	**2.500e-11**
ISOPFNP + OH	→	**ISOPFNC + HO2**	**1.100e-11**
ISOPHFP + OH	→	**2*CO + OH + 0.72*CH3COCHO + 0.28*HYAC**	**3.300e-11**
ISOPN1DO2 + HO2	→	**0.42*ISOPFNP + 0.58*OH + 0.58*HO2 + 0.55*NOA + 0.55*GLYALD + 0.03*MACRN + 0.03*CH2O**	**2.60e-13 exp(1300.00 / t)**
ISOPN1DO2	→	**ISOPFNP + HO2**	**1.26e+13 exp(-10000.00 / t)**
ISOPN1D + O3	→	**0.66*H2O2 + 0.83*GLYALD + 0.83*NOA + 0.34*OH + 0.17*NO2 + 0.17*CH3COCHO + 0.17*GLYOXAL + 0.17*HO2**	**2.800e-17**
ISOPN1D + OH	→	**0.08*IEPOX + 0.08*NO2 + 0.04*NC4CHO + 0.04*HO2 + 0.06*MACRN + 0.06*OH + 0.06*CO + 0.82*ISOPN1DO2**	**8.000e-11**
ISOPN2BO2 + HO2	→	**0.48*ISOPFNP + 0.52*OH + 0.06*MACRN + 0.06*CH2O + 0.06*HO2 + 0.46*HYAC + 0.46*NO2 + 0.46*GLYALD**	**2.60e-13 exp(1300.00 / t)**
ISOPN2BO2	→	**ISOPFNC + HO2**	**1.88e+13 exp(-10000.00 / t)**
ISOPN2B + OH	→	**0.15*IEPOX + 0.15*NO2 + 0.85*ISOPN2BO2**	**3.000e-11**
ISOPN3BO2 + HO2	→	**0.4*ISOPFNP + 0.6*OH + 0.6*MVKN + 0.6*CH2O + 0.6*HO2**	**2.60e-13 exp(1300.00 / t)**
ISOPN3BO2	→	**ISOPFNC + HO2**	**1.88e+13 exp(-10000.00 / t)**
ISOPN3B + OH	→	**0.13*IEPOX + 0.13*NO2 + 0.87*ISOPN3BO2**	**4.200e-11**
ISOPN4DO2 + HO2	→	**0.5*ISOPFNP + 0.5*OH + 0.5*HO2 + 0.06*MVKN + 0.06*CH2O + 0.44*HYAC + 0.44*NO3CH2CHO**	**2.60e-13 exp(1300.00 / t)**
ISOPN4DO2	→	**ISOPFNP + HO2**	**5.09e+12 exp(-10000.00 / t)**
ISOPN4D + O3	→	**0.66*H2O2 + 0.83*NO3CH2CHO + 0.83*HYAC + 0.34*OH + 0.17*NO2 + 0.17*GLYOXAL + 0.17*CH3COCHO + 0.17*HO2**	**2.800e-17**
ISOPN4D + OH	→	**0.04*IEPOX + 0.04*NO2 + 0.03*NC4CHO + 0.03*HO2 + 0.04*MVKN + 0.04*CO + 0.04*OH + 0.89*ISOPN4DO2**	**1.100e-10**
ISOPNBNO3O2 + HO2	→	**0.6*ISOPFNP + 0.4*OH + 0.4*HO2 + 0.06*MACRN + 0.04*MVKN + 0.1*CH2O + 0.15*NOA + 0.15*GLYALD + 0.15*HYAC + 0.15*NO3CH2CHO**	**2.60e-13 exp(1300.00 / t)**
ISOPNBNO3 + OH	→	**0.03*INHED + 0.03*OH + 0.05*NC4CHO + 0.05*HO2 + 0.92*ISOPNBNO3O2**	**3.900e-11**
ISOP + NO3	→	ISOPNO3	**2.95e-12 exp(-450.00 / t)**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPNO3 + CH3CO3	→	**CH3O2 + CO2 + 0.46*NO2 + 0.46*CH2O + 0.54*NC4CHO + 0.54*HO2 + 0.42*MVK + 0.04*MACR**	**2.00e-12 exp(500.00 / t)**
ISOPNO3 + CH3O2	→	**0.07*ISOPNBNO3 + 0.71*CH2O + 0.05*MVK + 0.07*NO2 + 0.4*HO2 + 0.02*MACR + 0.53*NC4CHO + 0.36*CH3OH + 0.28*ISOPN1D + 0.05*ISOPN4D**	**1.300e-12**
ISOPNO3 + HO2	→	**0.23*ISOPNOOHB + 0.53*ISOPNOOHD + 0.22*MVK + 0.02*MACR + 0.24*CH2O + 0.24*OH + 0.24*NO2**	**2.47e-13 exp(1300.00 / t)**
ISOPNO3 + ISOPNO3	→	**1.07*NC4CHO + 0.4*HO2 + 0.16*MACR + 0.16*CH2O + 0.16*NO2 + 0.53*ISOPN1D + 0.09*ISOPN4D + 0.15*ISOPNBNO3**	**5.000e-12**
ISOPNO3 + NO3	→	**1.46*NO2 + 0.46*CH2O + 0.54*NC4CHO + 0.54*HO2 + 0.42*MVK + 0.04*MACR**	**2.300e-12**
ISOPNOOHBO2 + HO2	→	**0.49*ISOPFNP + 0.85*OH + 0.17*CH2O + 0.17*HO2 + 0.15*MACRN + 0.02*MVKN + 0.28*NOA + 0.28*GLYALD + 0.06*HYAC + 0.06*NO3CH2CHO**	**2.64e-13 exp(1300.00 / t)**
ISOPNOOHBO2	→	**OH + ISOPFNP**	**8.72e+12 exp(-10000.00 / t)**
ISOPNOOHB + OH	→	**0.17*ISOPNO3 + 0.02*NC4CHO + 0.4*INHEB + 0.42*OH + 0.41*ISOPNOOHBO2**	**3.900e-11**
ISOPNOOHDO2 + HO2	→	**0.17*ISOPFNP + 0.86*OH + 0.03*CH2O + 0.02*MACRN + 0.01*MVKN + 0.68*NOA + 0.68*HCOCH2OOH + 0.12*HYPERACET + 0.12*NO3CH2CHO + 0.8*HO2**	**2.64e-13 exp(1300.00 / t)**
ISOPNOOHDO2	→	**OH + ISOPFNP**	**6.55e+12 exp(-10000.00 / t)**
ISOPNOOHD + O3	→	**0.66*H2O2 + 0.7*HCOCH2OOH + 0.13*HYPERACET + 0.7*NOA + 0.13*NO3CH2CHO + 0.51*OH + 0.17*NO2 + 0.17*CH3COCHO + 0.17*GLYOXAL**	**2.800e-17**
ISOPNOOHD + OH	→	**0.07*ISOPNO3 + 0.09*NC4CHO + 0.29*OH + 0.2*INHED + 0.07*IEPOX + 0.07*NO2 + 0.57*ISOPNOOHDO2**	**9.200e-11**
ISOP + O3	→	**0.25*OH + 0.41*MACR + 0.17*MVK + 0.33*HMHP + 0.03*H2O2 + 0.22*HCOOH + 1.01*CH2O + 0.42*CO2 + 0.42*HO2 + 0.21*CH3O2 + 0.07*CH3CO3 + 0.35*CO**	**1.03e-14 exp(-1995.00 / t)**
ISOP + OH	→	**0.315*ISOPC1T + 0.315*ISOPC1C + 0.111*ISOPC4T + 0.259*ISOPC4C**	**2.70e-11 exp(390.00 / t)**
ISOPOH + OH	→	**HYAC + GLYALD + HO2**	**3.850e-11**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPOOH + OH	→	**0.53*ISOPB1O2 + 0.16*ISOPB4O2 + 0.13*HYDRALD + 0.13*OH + 0.09*HPALDB1C + 0.09*HPALDB4C + 0.18*HO2**	**5.53e-12 exp(200.00 / t)**
ISOPOOH + OH	→	**0.85*IEPOX + 0.92*OH + 0.07*GLYALD + 0.07*HYAC + 0.08*ISOPHFP**	**2.08e-11 exp(390.00 / t)**
ISOPZD1O2 + CH3CO3	→	**0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MVKOOH + CO2 + CH3O2**	**2.00e-12 exp(500.00 / t)**
ISOPZD1O2 + CH3O2	→	**0.25*CH3OH + 0.25*ISOPOH + 0.75*CH2O + 0.72*HO2 + 0.28*CO + 0.28*OH + 0.28*MVKOOH + 0.47*HYDRALD**	**1.200e-12**
ISOPZD1O2 + HO2	→	**ISOPOOH**	**2.12e-13 exp(1300.00 / t)**
ISOPZD1O2	→	**ISOPC1C + O2**	**1.79e+14 exp(-8830.00 / t)**
ISOPZD4O2 + CH3CO3	→	**0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MACROOH + CO2 + CH3O2**	**2.00e-12 exp(500.00 / t)**
ISOPZD4O2 + CH3O2	→	**0.25*CH3OH + 0.25*ISOPOH + 0.75*CH2O + 0.72*HO2 + 0.28*CO + 0.28*OH + 0.28*MACROOH + 0.47*HYDRALD**	**9.800e-13**
ISOPZD4O2 + HO2	→	**ISOPOOH**	**2.12e-13 exp(1300.00 / t)**
ISOPZD4O2	→	**ISOPC4C + O2**	**1.75e+14 exp(-9054.00 / t)**
NC4CHOO2 + HO2	→	**0.2*ISOPFNP + 0.8*OH + 0.8*HO2 + 0.1*NOA + 0.1*GLYOXAL + 0.1*CH3COCHO + 0.1*NO3CH2CHO + 0.29*MACRN + 0.31*MVKN + 0.6*CO**	**2.60e-13 exp(1300.00 / t)**
NC4CHOO2	→	**0.51*MACRN + 0.49*MVKN + CO + OH**	**1.00e+7 exp(-5000.00 / t)**
NC4CHO + O3	→	**0.66*H2O2 + 0.66*GLYOXAL + 0.34*CH3COCHO + 0.61*NOA + 0.22*NO3CH2CHO + 0.34*OH + 0.17*NO2 + 0.3*CO + 0.13*HO2 + 0.04*CH3CO3**	**4.400e-18**
NC4CHO + OH	→	**0.45*CO2 + 0.1*CH3CO3 + 0.1*NO3CH2CHO + 0.35*NOA + 0.04*NO2 + 0.04*ICHE + 0.24*MACRN + 0.04*MVKN + 0.63*CO + 0.63*HO2 + 0.23*NC4CHOO2**	**3.600e-11**
IEPOXOO + NO	→	**NO2 + HO2 + 0.57*GLYALD + 0.71*CH3COCHO + 0.4*CO + 0.23*GLYOXAL + 0.29*HYAC**	**α = 0.025, n = 8**
IEPOXOO + NO	→	**ISOPFNC**	**α = 0.025, n = 8**
ISOPB1O2 + NO	→	**NO2 + MVK + CH2O + HO2**	**α = 0.14, n = 6**
ISOPB1O2 + NO	→	**ISOPN2B**	**α = 0.14, n = 6**
ISOPB4O2 + NO	→	**NO2 + MACR + CH2O + HO2**	**α = 0.13, n = 6**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPB4O2 + NO	→	**ISOPN3B**	**α = 0.13, n = 6**
ISOPED1O2 + NO	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH**	**α = 0.12, n = 6**
ISOPED1O2 + NO	→	**ISOPN4D**	**α = 0.12, n = 6**
ISOPED4O2 + NO	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH**	**α = 0.12, n = 6**
ISOPED4O2 + NO	→	**ISOPN1D**	**α = 0.12, n = 6**
ISOPN1DO2 + NO	→	**NO2 + HO2 + 0.94*NOA + 0.94*GLYALD + 0.06*MACRN + 0.06*CH2O**	**α = 0.084, n = 11**
ISOPN1DO2 + NO	→	**ISOPFDN**	**α = 0.084, n = 11**
ISOPN2BO2 + NO	→	**1.73*NO2 + 0.27*MACRN + 0.27*CH2O + 0.27*HO2 + 0.73*HYAC + 0.73*GLYALD**	**α = 0.065, n = 11**
ISOPN2BO2 + NO	→	**ISOPFDN**	**α = 0.065, n = 11**
ISOPN3BO2 + NO	→	**NO2 + MVKN + CH2O + HO2**	**α = 0.053, n = 11**
ISOPN3BO2 + NO	→	**ISOPFDN**	**α = 0.053, n = 11**
ISOPN4DO2 + NO	→	**NO2 + HO2 + 0.13*MVKN + 0.13*CH2O + 0.87*HYAC + 0.87*NO3CH2CHO**	**α = 0.165, n = 11**
ISOPN4DO2 + NO	→	**ISOPFDN**	**α = 0.165, n = 11**
ISOPNBNO3O2 + NO	→	**NO2 + HO2 + 0.21*MACRN + 0.12*MVKN + 0.33*CH2O + 0.34*NOA + 0.34*GLYALD + 0.33*HYAC + 0.33*NO3CH2CHO**	**α = 0.203, n = 11**
ISOPNBNO3O2 + NO	→	**ISOPFDN**	**α = 0.203, n = 11**
ISOPNO3 + NO	→	**1.46*NO2 + 0.46*CH2O + 0.54*NC4CHO + 0.54*HO2 + 0.42*MVK + 0.04*MACR**	**α = 0.135, n = 9**
ISOPNO3 + NO	→	**ISOPFDN**	**α = 0.135, n = 9**
ISOPNOOHBO2 + NO	→	**NO2 + 0.53*CH2O + 0.53*HO2 + 0.49*MACRN + 0.04*MVKN + 0.4*NOA + 0.4*GLYALD + 0.07*HYAC + 0.07*NO3CH2CHO + 0.47*OH**	**α = 0.141, n = 12**
ISOPNOOHBO2 + NO	→	**ISOPFDN**	**α = 0.141, n = 12**
ISOPNOOHDO2 + NO	→	**NO2 + 0.04*CH2O + 0.04*OH + 0.02*MACRN + 0.02*MVKN + 0.81*NOA + 0.81*HCOCH2OOH + 0.15*HYPERACET + 0.15*NO3CH2CHO + 0.96*HO2**	**α = 0.045, n = 12**
ISOPNOOHDO2 + NO	→	**ISOPFDN**	**α = 0.045, n = 12**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPZD1O2	→	**0.15*HPALDB1C + 0.25*HPALD1 + 0.4*HO2 + 0.6*OH + 0.6*DHPMPAL + 0.6*CO**	**5.05e15 exp(-12200.00 / t) exp(1e8 / t^3)**
ISOPZD1O2 + NO	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH**	**α = 0.12, n = 6**
ISOPZD1O2 + NO	→	**ISOPN4D**	**α = 0.12, n = 6**
ISOPZD4O2	→	**0.15*HPALDB4C + 0.25*HPALD4 + 0.4*HO2 + 0.6*OH + 0.6*DHPMPAL + 0.6*CO**	**2.22e9 exp(-7160.00 / t) exp(1e8 / t^3)**
ISOPZD4O2 + NO	→	**NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH**	**α = 0.12, n = 6**
ISOPZD4O2 + NO	→	**ISOPN1D**	**α = 0.12, n = 6**
MACRO2 + NO	→	**NO2 + HO2 + 0.86*HYAC + 0.86*CO + 0.14*CH2O + 0.14*CH3COCHO**	**α = 0.06, n = 6**
MACRO2 + NO	→	**MACRN**	**α = 0.06, n = 6**
MVKO2 + NO	→	**NO2 + 0.24*HO2 + 0.24*CH2O + 0.76*CH3CO3 + 0.76*GLYALD + 0.24*CH3COCHO**	**α = 0.04, n = 6**
MVKO2 + NO	→	**MVKN**	**α = 0.04, n = 6**
NC4CHOO2 + NO	→	**NO2 + HO2 + 0.13*NOA + 0.13*GLYOXAL + 0.12*CH3COCHO + 0.12*NO3CH2CHO + 0.39*MACRN + 0.36*MVKN + 0.75*CO**	**α = 0.021, n = 11**
NC4CHOO2 + NO	→	**ISOPFDNC**	**α = 0.021, n = 11**
C7 Organics			
ACBZO2 + HO2	→	0.4*C6H5O2 + 0.4*OH	4.30e-13 exp(1040.00 / t)
ACBZO2 + NO	→	C6H5O2 + NO2	7.50e-12 exp(290.00 / t)
BENZENE + OH	→	0.53*PHENOL + 0.12*BEPOMUC + 0.65*HO2 + 0.35*BENZO2	2.30e-12 exp(-193.00 / t)
BENZO2 + HO2	→	BENZOOH	7.50e-13 exp(700.00 / t)
BENZO2 + NO	→	NO2 + GLYOXAL + 0.5*BIGALD1 + HO2	2.60e-12 exp(365.00 / t)
BENZOOH + OH	→	BENZO2	3.80e-12 exp(200.00 / t)
BZALD + OH	→	ACBZO2	5.90e-12 exp(225.00 / t)
BZOO + HO2	→	BZOOH	7.50e-13 exp(700.00 / t)
BZOOH + OH	→	BZOO	3.80e-12 exp(200.00 / t)
BZOO + NO	→	BZALD + NO2 + HO2	2.60e-12 exp(365.00 / t)
C6H5O2 + HO2	→	C6H5OOH	7.50e-13 exp(700.00 / t)
C6H5O2 + NO	→	PHENO + NO2	2.60e-12 exp(365.00 / t)
C6H5OOH + OH	→	C6H5O2	3.80e-12 exp(200.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
CRESOL + OH	→	0.2*PHENO2 + 0.73*HO2 + 0.07*PHENO	4.700e-11
DICARBO2 + HO2	→	0.4*OH + 0.07*HO2 + 0.07*CH3COCHO + 0.07*CO + 0.33*CH3O2	4.30e-13 exp(1040.00 / t)
DICARBO2 + NO	→	NO2 + 0.17*HO2 + 0.17*CH3COCHO + 0.17*CO + 0.83*CH3O2	7.50e-12 exp(290.00 / t)
DICARBO2 + NO2 + M	→	M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
MALO2 + HO2	→	0.16*GLYOXAL + 0.16*HO2 + 0.16*CO	4.30e-13 exp(1040.00 / t)
MALO2 + NO	→	0.4*GLYOXAL + 0.4*HO2 + 0.4*CO + NO2	7.50e-12 exp(290.00 / t)
MALO2 + NO2 + M	→	M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
MDIALO2 + HO2	→	0.4*OH + 0.33*HO2 + 0.07*CH3COCHO + 0.14*CO + 0.07*CH3O2 + 0.07*GLYOXAL	4.30e-13 exp(1040.00 / t)
MDIALO2 + NO	→	NO2 + 0.83*HO2 + 0.17*CH3COCHO + 0.35*CO + 0.17*CH3O2 + 0.17*GLYOXAL	7.50e-12 exp(290.00 / t)
MDIALO2 + NO2 + M	→	M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
PHENO2 + HO2	→	PHENOOH	7.50e-13 exp(700.00 / t)
PHENO2 + NO	→	HO2 + 0.7*GLYOXAL + NO2	2.60e-12 exp(365.00 / t)
PHENOL + OH	→	0.14*PHENO2 + 0.8*HO2 + 0.06*PHENO	4.70e-13 exp(1220.00 / t)
PHENO + NO2	→	M	2.100e-12
PHENO + O3	→	C6H5O2	2.800e-13
PHENOOH + OH	→	PHENO2	3.80e-12 exp(200.00 / t)
ACBZO2 + NO2 + M	→	PBZNIT + M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
TOLO2 + HO2	→	TOLOOH	7.50e-13 exp(700.00 / t)
TOLO2 + NO	→	NO2 + 0.6*GLYOXAL + 0.4*CH3COCHO + HO2 + 0.2*BIGALD1 + 0.2*BIGALD2 + 0.2*BIGALD3	2.60e-12 exp(365.00 / t)
TOLOOH + OH	→	TOLO2	3.80e-12 exp(200.00 / t)
TOLUENE + OH	→	0.18*CRESOL + 0.1*TEPOMUC + 0.07*BZOO + 0.65*TOLO2 + 0.28*HO2	1.70e-12 exp(352.00 / t)
PBZNIT + M	→	ACBZO2 + NO2 + M	k(ACBZO2+NO2) * 1.111e28 exp(-14000 / t)
XYLENES + OH	→	0.15*XYLOL + 0.23*TEPOMUC + 0.06*BZOO + 0.56*XYLENO2 + 0.38*HO2	1.700e-11

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
XYLENO2 + HO2	→	XYLENOOH	7.50e-13 exp(700.00 / t)
XYLENO2 + NO	→	NO2 + HO2 + 0.34*GLYOXAL + 0.54*CH3COCHO + 0.06*BIGALD1 + 0.2*BIGALD2 + 0.15*BIGALD3 + 0.21*BIGALD4	2.60e-12 exp(365.00 / t)
XYLENOOH + OH	→	XYLENO2	3.80e-12 exp(200.00 / t)
XYLOLO2 + HO2	→	XYLOLOOH	7.50e-13 exp(700.00 / t)
XYLOLO2 + NO	→	HO2 + NO2 + 0.17*GLYOXAL + 0.51*CH3COCHO	2.60e-12 exp(365.00 / t)
XYLOL + OH	→	0.3*XYLOLO2 + 0.63*HO2 + 0.07*PHENO	8.400e-11
XYLOLOOH + OH	→	XYLOLO2	3.80e-12 exp(200.00 / t)
C10 Organics			
APIN + NO3	→	**APINNO3**	**1.20e-12 exp(490.00 / t)**
APINNO3 + APINNO3	→	**0.27*TERPNT + 0.09*TERPNS + 1.64*NO2 + 1.64*TERPA**	**5.300e-13**
APINNO3 + CH3CO3	→	**NO2 + TERPA + CH3O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINNO3 + CH3O2	→	**0.09*TERPNT + 0.09*TERPNS + 0.95*CH2O + 0.05*CH3OH + 0.82*HO2 + 0.82*NO2 + 0.82*TERPA**	**2.000e-12**
APINNO3 + HO2	→	**0.3*TERPNPT + 0.7*TERPA + 0.7*NO2 + 0.7*OH**	**2.71e-13 exp(1300.00 / t)**
APINNO3 + NO	→	**1.86*NO2 + 0.07*TERPFDN + 0.93*TERPA**	**2.70e-12 exp(360.00 / t)**
APINNO3 + NO3	→	**2*NO2 + TERPA**	**2.300e-12**
APINNO3 + TERPA2CO3	→	**NO2 + TERPA + TERPA2O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINNO3 + TERPA3CO3	→	**NO2 + TERPA + TERPA4O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINNO3 + TERPACO3	→	**NO2 + TERPA + TERPA1O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINO2 + CH3CO3	→	**0.39*TERPA + 0.35*TERPA3 + 0.14*TERP1OOH + 0.12*CH3COCH3 + 0.12*TERPF1 + 0.27*CH2O + HO2 + CH3O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINO2 + CH3O2	→	**0.83*CH2O + 0.14*TERPF1 + 0.42*TERPA + 0.2*TERPA3 + 0.13*TERP1OOH + 0.17*CH3OH + 0.11*TERPK + 0.06*CH3COCH3 + 1.16*HO2**	**2.000e-12**
APINO2 + HO2	→	**0.06*CH3COCH3 + 0.06*TERPF1 + 0.08*CH2O + 0.25*TERP1OOH + 0.48*HO2 + 0.4*TERPOOH + 0.29*TERPA + 0.35*OH**	**2.60e-13 exp(1300.00 / t)**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
APINO2 + NO	→	**0.01*TERPHFN + 0.02*TERPNS1 + 0.1*TERPNS + 0.05*TERPNT + 0.05*TERPNT1 + 0.77*NO2 + 0.77*HO2 + 0.3*TERPA + 0.27*TERPA3 + 0.09*CH3COCH3 + 0.09*TERPF1 + 0.21*CH2O + 0.11*TERP1OOH**	**2.70e-12 exp(360.00 / t)**
APINO2 + NO3	→	**NO2 + HO2 + 0.39*TERPA + 0.35*TERPA3 + 0.12*CH3COCH3 + 0.12*TERPF1 + 0.27*CH2O + 0.14*TERP1OOH**	**2.300e-12**
APINO2 + TERPA2CO3	→	**0.39*TERPA + 0.35*TERPA3 + 0.14*TERP1OOH + 0.12*CH3COCH3 + 0.12*TERPF1 + 0.27*CH2O + HO2 + TERPA2O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINO2 + TERPA3CO3	→	**0.39*TERPA + 0.35*TERPA3 + 0.14*TERP1OOH + 0.12*CH3COCH3 + 0.12*TERPF1 + 0.27*CH2O + HO2 + TERPA4O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APINO2 + TERPACO3	→	**0.39*TERPA + 0.35*TERPA3 + 0.14*TERP1OOH + 0.12*CH3COCH3 + 0.12*TERPF1 + 0.27*CH2O + HO2 + TERPA1O2 + CO2**	**2.00e-12 exp(500.00 / t)**
APIN + O3	→	**0.77*OH + 0.33*TERPA2O2 + 0.22*H2O2 + 0.22*TERPA + 0.01*TERPACID + 0.17*TERPA2 + 0.17*HO2 + 0.17*CO + 0.27*CH2O + 0.27*TERPA2CO3**	**8.05e-16 exp(-640.00 / t)**
APIN + OH	→	**APINO2**	**1.34e-11 exp(410.00 / t)**
BCARY + NO3	→	**BCARYNO3**	1.900e-11
BCARYNO3 + BCARYNO3	→	**0.36*SQTN + 1.64*NO2 + 1.64*TERPF2**	**5.300e-13**
BCARYNO3 + CH3CO3	→	**CH3O2 + CO2 + NO2 + TERPF2**	**2.00e-12 exp(500.00 / t)**
BCARYNO3 + CH3O2	→	**0.18*SQTN + 0.95*CH2O + 0.82*TERPF2 + 0.82*NO2 + 0.82*HO2 + 0.05*CH3OH**	**2.000e-12**
BCARYNO3 + HO2	→	**0.5*SQTN + 0.5*OH + 0.5*NO2 + 0.5*TERPF2**	**2.78e-13 exp(1300.00 / t)**
BCARYNO3 + NO	→	**0.07*SQTN + 1.86*NO2 + 0.93*TERPF2**	**2.70e-12 exp(360.00 / t)**
BCARYNO3 + NO3	→	**2*NO2 + TERPF2**	**2.300e-12**
BCARYNO3 + TERPA2CO3	→	**TERPA2O2 + CO2 + NO2 + TERPF2**	**2.00e-12 exp(500.00 / t)**
BCARYNO3 + TERPA3CO3	→	**TERPA4O2 + CO2 + NO2 + TERPF2**	**2.00e-12 exp(500.00 / t)**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
BCARYNO3 + TERPACO3	→	**TERPA1O2 + CO2 + NO2 + TERPF2**	**2.00e-12 exp(500.00 / t)**
BCARYO2 + CH3CO3	→	**TERPF2 + HO2 + CH3O2 + CO2**	**2.00e-12 exp(500.00 / t)**
BCARYO2 + CH3O2	→	**0.25*CH3OH + TERPF2 + 0.75*CH2O + HO2**	**2.000e-12**
BCARYO2 + HO2	→	**0.9*TERP2AOOH + 0.1*OH + 0.1*HO2 + 0.1*TERPF2**	**2.75e-13 exp(1300.00 / t)**
BCARYO2 + NO	→	**0.3*SQTN + 0.7*NO2 + 0.7*HO2 + 0.7*TERPF2**	**2.70e-12 exp(360.00 / t)**
BCARYO2 + NO3	→	**NO2 + HO2 + TERPF2**	**2.300e-12**
BCARYO2 + TERPA2CO3	→	**TERPF2 + HO2 + TERPA2O2 + CO2**	**2.00e-12 exp(500.00 / t)**
BCARYO2 + TERPA3CO3	→	**TERPF2 + HO2 + TERPA4O2 + CO2**	**2.00e-12 exp(500.00 / t)**
BCARYO2 + TERPACO3	→	**TERPF2 + HO2 + TERPA1O2 + CO2**	**2.00e-12 exp(500.00 / t)**
BCARY + O3	→	**0.13*TERPACID + 0.17*H2O2 + 0.08*OH + 0.08*HO2 + 0.08*CH2O + 0.87*TERPF2**	1.200e-14
BCARY + OH	→	**BCARYO2**	2.000e-10
BPIN + NO3	→	**BPINNO3**	**2.500e-12**
BPINNO3 + BPINNO3	→	**0.94*NO2 + 0.92*TERPNS + 0.9*TERPA3 + 0.04*TERPK + 0.04*CH2O + 0.14*TERPNT + 0.94*HO2**	**5.300e-13**
BPINNO3 + CH3CO3	→	**CH3O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.5*HO2**	**2.00e-12 exp(500.00 / t)**
BPINNO3 + CH3O2	→	**0.56*TERPNS + 0.08*TERPNT + 0.02*TERPK + 0.34*TERPA3 + 0.36*NO2 + 1.1*HO2 + 0.99*CH2O + 0.03*CH3OH**	**2.000e-12**
BPINNO3 + HO2	→	**0.47*OH + 0.45*TERPNPS + 0.22*TERPA3 + 0.02*TERPK + 0.08*TERPNPT + 0.24*NO2 + 0.02*CH2O + 0.23*TERPNS**	**2.71e-13 exp(1300.00 / t)**
BPINNO3 + NO	→	**0.07*TERPFDN + 1.39*NO2 + 0.42*TERPNS + 0.44*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.47*HO2**	**2.70e-12 exp(360.00 / t)**
BPINNO3 + NO3	→	**1.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.5*HO2**	**2.300e-12**

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
BPINNO3 + TERPA2CO3	→	TERPA2O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.5*HO2	2.00e-12 exp(500.00 / t)
BPINNO3 + TERPA3CO3	→	TERPA4O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.5*HO2	2.00e-12 exp(500.00 / t)
BPINNO3 + TERPACO3	→	TERPA1O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNT + 0.5*HO2	2.00e-12 exp(500.00 / t)
BPINO2 + CH3CO3	→	0.32*TERPK + 0.27*TERPF1 + 0.41*TERPA3 + 0.11*CH3COCH3 + 0.65*CH2O + HO2 + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
BPINO2 + CH3O2	→	1.4*CH2O + 0.37*TERPF1 + 0.32*TERPK + 1.5*HO2 + 0.08*CH3COCH3 + 0.31*TERPA3	2.000e-12
BPINO2 + HO2	→	0.68*TERP1OOH + 0.03*OH + 0.03*TERPK + 0.03*CH2O + 0.03*HO2 + 0.29*TERPOOH	2.60e-13 exp(1300.00 / t)
BPINO2 + NO	→	0.08*CH3COCH3 + 0.49*CH2O + 0.2*TERPF1 + 0.24*TERPK + 0.04*TERPNS1 + 0.02*TERPNS + 0.06*TERPNT + 0.13*TERPNT1 + 0.31*TERPA3 + 0.75*HO2 + 0.75*NO2	2.70e-12 exp(360.00 / t)
BPINO2 + NO3	→	0.11*CH3COCH3 + 0.65*CH2O + 0.27*TERPF1 + 0.32*TERPK + 0.41*TERPA3 + HO2 + NO2	2.300e-12
BPINO2 + TERPA2CO3	→	0.32*TERPK + 0.27*TERPF1 + 0.41*TERPA3 + 0.11*CH3COCH3 + 0.65*CH2O + HO2 + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
BPINO2 + TERPA3CO3	→	0.32*TERPK + 0.27*TERPF1 + 0.41*TERPA3 + 0.11*CH3COCH3 + 0.65*CH2O + HO2 + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
BPINO2 + TERPACO3	→	0.32*TERPK + 0.27*TERPF1 + 0.41*TERPA3 + 0.11*CH3COCH3 + 0.65*CH2O + HO2 + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
BPIN + O3	→	0.51*TERPK + 0.3*OH + 0.3*TERPA2CO3 + 0.32*H2O2 + 0.19*BIGALK + 0.19*CO2 + 0.81*CH2O + 0.11*HMHP + 0.08*HCOOH	1.35e-15 exp(-1270.00 / t)
BPIN + OH	→	BPINO2	1.62e-11 exp(460.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
LIMON + NO3	→	LIMONNO3	1.200e-11
LIMONNO3 + CH3CO3	→	CH3O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp(500.00 / t)
LIMONNO3 + CH3O2	→	0.27*TERPNT1 + 0.91*CH2O + 0.09*CH3OH + 1.01*HO2 + 0.31*TERPF1 + 0.31*NO2 + 0.42*TERPNS1	2.000e-12
LIMONNO3 + HO2	→	0.18*TERPNPT1 + 0.32*TERPNPS1 + 0.5*OH + 0.23*TERPF1 + 0.23*NO2 + 0.18*TERPNS1 + 0.09*TERPNT1 + 0.27*HO2	2.71e-13 exp(1300.00 / t)
LIMONNO3 + LIMONNO3	→	0.42*TERPNT1 + 0.99*HO2 + 0.86*TERPF1 + 0.86*NO2 + 0.72*TERPNS1	5.300e-13
LIMONNO3 + NO	→	0.07*TERPFDN + 1.36*NO2 + 0.43*TERPF1 + 0.17*TERPNT1 + 0.33*TERPNS1 + 0.5*HO2	2.70e-12 exp(360.00 / t)
LIMONNO3 + NO3	→	1.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.300e-12
LIMONNO3 + TERPA2CO3	→	TERPA2O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp(500.00 / t)
LIMONNO3 + TERPA3CO3	→	TERPA4O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp(500.00 / t)
LIMONNO3 + TERPACO3	→	TERPA1O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp(500.00 / t)
LIMONO2 + CH3CO3	→	TERPF1 + 0.56*CH2O + HO2 + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
LIMONO2 + CH3O2	→	0.25*CH3OH + TERPF1 + 1.03*CH2O + HO2	2.000e-12
LIMONO2 + HO2	→	0.9*TERP1OOH + 0.1*TERPF1 + 0.1*OH + 0.1*HO2 + 0.06*CH2O	2.60e-13 exp(1300.00 / t)
LIMONO2 + NO	→	0.17*TERPNT1 + 0.06*TERPNS1 + 0.77*NO2 + 0.77*TERPF1 + 0.77*HO2 + 0.43*CH2O	2.70e-12 exp(360.00 / t)
LIMONO2 + NO3	→	NO2 + TERPF1 + HO2 + 0.56*CH2O	2.300e-12
LIMONO2 + TERPA2CO3	→	TERPF1 + 0.56*CH2O + HO2 + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
LIMONO2 + TERPA3CO3	→	TERPF1 + 0.56*CH2O + HO2 + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
LIMONO2 + TERPACO3	→	TERPF1 + 0.56*CH2O + HO2 + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
LIMON + O3	→	0.66*OH + 0.66*TERPF1 + 0.33*CH3CO3 + 0.33*CH2O + 0.33*TERPA3CO3 + 0.33*H2O2 + 0.01*TERPACID	2.80e-15 exp(-770.00 / t)
LIMON + OH	→	LIMONO2	3.41e-11 exp(470.00 / t)
MYRC + NO3	→	MYRCNO3	1.100e-11
MYRCNO3 + CH3CO3	→	CH3O2 + CO2 + 0.95*NO2 + 0.95*TERPF2 + 0.04*CH2O + 0.05*TERPNS1 + 0.05*HO2 + 0.91*CH3COCH3	2.00e-12 exp(500.00 / t)
MYRCNO3 + CH3O2	→	0.14*TERPNS1 + 0.98*CH2O + 0.77*TERPF2 + 0.77*NO2 + 0.87*HO2 + 0.74*CH3COCH3 + 0.09*TERPNT1 + 0.05*CH3OH	2.000e-12
MYRCNO3 + HO2	→	0.48*OH + 0.48*TERPF2 + 0.02*CH2O + 0.48*NO2 + 0.46*CH3COCH3 + 0.36*TERPNPS1 + 0.16*TERPNPT1	2.71e-13 exp(1300.00 / t)
MYRCNO3 + MYRCNO3	→	0.19*TERPNS1 + 0.27*TERPNT1 + 1.54*NO2 + 1.54*TERPF2 + 1.48*CH3COCH3 + 0.06*CH2O	5.300e-13
MYRCNO3 + NO	→	0.07*TERPFDN + 1.82*NO2 + 0.89*TERPF2 + 0.04*CH2O + 0.04*TERPNS1 + 0.04*HO2 + 0.85*CH3COCH3	2.70e-12 exp(360.00 / t)
MYRCNO3 + NO3	→	1.95*NO2 + 0.95*TERPF2 + 0.04*CH2O + 0.05*TERPNS1 + 0.05*HO2 + 0.91*CH3COCH3	2.300e-12
MYRCNO3 + TERPA2CO3	→	TERPA2O2 + CO2 + 0.95*NO2 + 0.95*TERPF2 + 0.04*CH2O + 0.05*TERPNS1 + 0.05*HO2 + 0.91*CH3COCH3	2.00e-12 exp(500.00 / t)
MYRCNO3 + TERPA3CO3	→	TERPA4O2 + CO2 + 0.95*NO2 + 0.95*TERPF2 + 0.04*CH2O + 0.05*TERPNS1 + 0.05*HO2 + 0.91*CH3COCH3	2.00e-12 exp(500.00 / t)
MYRCNO3 + TERPACO3	→	TERPA1O2 + CO2 + 0.95*NO2 + 0.95*TERPF2 + 0.04*CH2O + 0.05*TERPNS1 + 0.05*HO2 + 0.91*CH3COCH3	2.00e-12 exp(500.00 / t)
MYRCO2 + CH3CO3	→	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
MYRCO2 + CH3O2	→	0.25*CH3OH + TERPF2 + 0.75*CH2O + HO2	2.000e-12
MYRCO2 + HO2	→	0.9*TERP2AOOH + 0.1*TERPF2 + 0.1*OH + 0.1*HO2 + 0.05*CH3COCH3 + 0.04*CH2O	2.60e-13 exp(1300.00 / t)
MYRCO2 + NO	→	0.1*TERPNS1 + 0.19*TERPNT1 + 0.71*NO2 + 0.71*TERPF2 + 0.33*CH3COCH3 + 0.3*CH2O + 0.71*HO2	2.70e-12 exp(360.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
MYRCO2 + NO3	→	NO2 + TERPF2 + 0.46*CH3COCH3 + 0.42*CH2O + HO2	2.300e-12
MYRCO2 + TERPA2CO3	→	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
MYRCO2 + TERPA3CO3	→	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
MYRCO2 + TERPACO3	→	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
MYRC + O3	→	TERPF2 + 0.63*OH + 0.63*HO2 + 0.25*CH3COCH3 + 0.39*CH2O + 0.18*HYAC	2.65e-15 exp(-520.00 / t)
MYRC + OH	→	MYRCO2	2.100e-10
TERPA2CO3 + NO2 + M	→	TERPA2PAN + M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
TERPA3CO3 + NO2 + M	→	TERPA3PAN + M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
TERPACO3 + NO2 + M	→	TERPAPAN + M	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
TERP1OOHO2 + HO2	→	0.82*TERPDHDP + 0.18*TERPOOHL + 0.18*OH + 0.18*HO2 + 0.08*CH2O	2.71e-13 exp(1300.00 / t)
TERP1OOHO2 + NO	→	0.3*TERPHFN + 0.7*NO2 + 0.7*TERPOOHL + 0.31*CH2O + 0.7*HO2	2.70e-12 exp(360.00 / t)
TERP1OOH + OH	→	TERP1OOHO2	8.900e-11
TERP2AOOH + OH	→	TERP2OOHO2	8.900e-11
TERP2OOHO2 + HO2	→	0.82*TERPDHDP + 0.18*TERP1OOH + 0.18*OH + 0.18*HO2	2.71e-13 exp(1300.00 / t)
TERP2OOHO2 + NO	→	0.3*TERPHFN + 0.7*NO2 + 0.7*TERP1OOH + 0.7*HO2	2.70e-12 exp(360.00 / t)
TERPA1O2 + CH3CO3	→	TERPA2O2 + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA1O2 + CH3O2	→	0.25*CH3OH + 0.75*CH2O + 0.5*HO2 + 0.5*TERPA2 + 0.5*TERPA2O2	2.000e-12
TERPA1O2 + HO2	→	TERPOOH	2.54e-13 exp(1300.00 / t)
TERPA1O2 + NO	→	0.3*TERPNS + 0.7*NO2 + 0.7*TERPA2O2	2.70e-12 exp(360.00 / t)
TERPA1O2 + NO3	→	NO2 + TERPA2O2	2.300e-12
TERPA1O2 + TERPA2CO3	→	2*TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPA1O2 + TERPA3CO3	→	TERPA2O2 + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA1O2 + TERPACO3	→	TERPA2O2 + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA2CO3 + CH3CO3	→	2*CO2 + TERPA2O2 + CH3O2	2.90e-12 exp(500.00 / t)
TERPA2CO3 + CH3O2	→	CO2 + TERPA2O2 + CH2O + HO2	2.00e-12 exp(500.00 / t)
TERPA2CO3 + HO2	→	0.15*O3 + 0.51*TERPACID2 + 0.49*OH + 0.49*CO2 + 0.49*TERPA2O2	4.30e-13 exp(1040.00 / t)
TERPA2CO3 + NO	→	NO2 + CO2 + TERPA2O2	8.10e-12 exp(270.00 / t)
TERPA2CO3 + NO3	→	NO2 + CO2 + TERPA2O2	4.000e-12
TERPA2CO3 + TERPA2CO3	→	2*CO2 + 2*TERPA2O2	2.90e-12 exp(500.00 / t)
TERPA2CO3 + TERPACO3	→	2*CO2 + TERPA2O2 + TERPA1O2	2.90e-12 exp(500.00 / t)
TERPA2 + NO3	→	HNO3 + TERPA2CO3	2.000e-14
TERPA2O2 + CH3CO3	→	TERPA3O2 + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA2O2 + CH3O2	→	TERPA3O2 + CH2O + HO2	2.000e-12
TERPA2O2 + HO2	→	0.62*TERPOOH + 0.38*TERPA3O2 + 0.38*OH	2.62e-13 exp(1300.00 / t)
TERPA2O2 + NO	→	0.17*TERPNT + 0.83*NO2 + 0.83*TERPA3O2	2.70e-12 exp(360.00 / t)
TERPA2O2 + NO3	→	NO2 + TERPA3O2	2.300e-12
TERPA2O2 + TERPA2CO3	→	TERPA3O2 + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA2O2 + TERPA3CO3	→	TERPA3O2 + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA2O2 + TERPACO3	→	TERPA3O2 + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA2 + OH	→	TERPA2CO3	5.20e-12 exp(600.00 / t)
TERPA2PAN + OH	→	CH3COCH3 + 2*CO2 + 2*CH2O + NO2 + 2*CO + HO2	2.520e-11
TERPA3CO3 + CH3CO3	→	2*CO2 + TERPA4O2 + CH3O2	2.90e-12 exp(500.00 / t)
TERPA3CO3 + CH3O2	→	CO2 + TERPA4O2 + CH2O + HO2	2.00e-12 exp(500.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPA3CO3 + HO2	→	0.15*O3 + 0.51*TERPACID3 + 0.49*OH + 0.49*CO2 + 0.49*TERPA4O2	4.30e-13 exp(1040.00 / t)
TERPA3CO3 + NO	→	NO2 + CO2 + TERPA4O2	8.10e-12 exp(270.00 / t)
TERPA3CO3 + NO3	→	NO2 + CO2 + TERPA4O2	4.000e-12
TERPA3CO3 + TERPA2CO3	→	2*CO2 + TERPA4O2 + TERPA2O2	2.90e-12 exp(500.00 / t)
TERPA3CO3 + TERPA3CO3	→	2*CO2 + 2*TERPA4O2	2.90e-12 exp(500.00 / t)
TERPA3CO3 + TERPACO3	→	2*CO2 + TERPA4O2 + TERPA1O2	2.90e-12 exp(500.00 / t)
TERPA3 + NO3	→	HNO3 + TERPA3CO3	2.000e-14
TERPA3O2 + CH3CO3	→	TERPA4O2 + CH3COCH3 + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA3O2 + CH3O2	→	TERPA4O2 + CH3COCH3 + CH2O + HO2	2.000e-12
TERPA3O2 + HO2	→	0.85*TERPOOHL + 0.15*TERPA4O2 + 0.15*OH + 0.15*CH3COCH3	2.66e-13 exp(1300.00 / t)
TERPA3O2 + NO	→	0.3*TERPNT + 0.7*NO2 + 0.7*TERPA4O2 + 0.7*CH3COCH3	2.70e-12 exp(360.00 / t)
TERPA3O2 + NO3	→	NO2 + TERPA4O2 + CH3COCH3	2.300e-12
TERPA3O2 + TERPA2CO3	→	TERPA4O2 + CH3COCH3 + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA3O2 + TERPA3CO3	→	2*TERPA4O2 + CH3COCH3 + CO2	2.00e-12 exp(500.00 / t)
TERPA3O2 + TERPACO3	→	TERPA4O2 + CH3COCH3 + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA3 + OH	→	0.75*TERPA3CO3 + 0.25*TERPA4O2	5.20e-12 exp(600.00 / t)
TERPA3PAN + OH	→	CO + NO2 + 3*CO2 + 2*CH3CO3 + CH2O + HO2	1.920e-11
TERPA4O2 + CH3CO3	→	CH3CO3 + HO2 + 2*CH2O + CO + CH3O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA4O2 + CH3O2	→	CH3CO3 + 2*HO2 + 3*CH2O + CO	2.000e-12
TERPA4O2 + HO2	→	0.47*TERPOOHL + 0.53*CH3CO3 + 0.53*HO2 + 1.06*CH2O + 0.53*CO + 0.53*OH	2.51e-13 exp(1300.00 / t)
TERPA4O2 + NO	→	0.09*TERPNS + 0.91*NO2 + 0.91*CH3CO3 + 0.91*HO2 + 1.82*CH2O + 0.91*CO	2.70e-12 exp(360.00 / t)
TERPA4O2 + NO3	→	NO2 + CH3CO3 + HO2 + 2*CH2O + CO	2.300e-12

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPA4O2 + TERPA2CO3	→	CH3CO3 + HO2 + 2*CH2O + CO + TERPA2O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA4O2 + TERPA3CO3	→	CH3CO3 + HO2 + 2*CH2O + CO + TERPA4O2 + CO2	2.00e-12 exp(500.00 / t)
TERPA4O2 + TERPACO3	→	CH3CO3 + HO2 + 2*CH2O + CO + TERPA1O2 + CO2	2.00e-12 exp(500.00 / t)
TERPACID2 + OH	→	0.71*TERPA2CO3 + 0.29*CO2 + 0.29*TERPA2O2	8.800e-12
TERPACID3 + OH	→	0.71*TERPA3CO3 + 0.29*CO2 + 0.29*TERPA4O2	8.800e-12
TERPACID + OH	→	0.71*TERPACO3 + 0.29*CO2 + 0.29*TERPA1O2	8.800e-12
TERPACO3 + CH3CO3	→	2*CO2 + TERPA1O2 + CH3O2	2.90e-12 exp(500.00 / t)
TERPACO3 + CH3O2	→	CO2 + TERPA1O2 + CH2O + HO2	2.00e-12 exp(500.00 / t)
TERPACO3 + HO2	→	0.15*O3 + 0.51*TERPACID + 0.49*OH + 0.49*CO2 + 0.49*TERPA1O2	4.30e-13 exp(1040.00 / t)
TERPACO3 + NO	→	NO2 + CO2 + TERPA1O2	8.10e-12 exp(270.00 / t)
TERPACO3 + NO3	→	NO2 + CO2 + TERPA1O2	4.000e-12
TERPACO3 + TERPACO3	→	2*CO2 + 2*TERPA1O2	2.90e-12 exp(500.00 / t)
TERPA + NO3	→	HNO3 + TERPACO3	2.000e-14
TERPA + OH	→	0.77*TERPACO3 + 0.23*TERPA2O2	5.20e-12 exp(600.00 / t)
TERPAPAN + OH	→	TERPA2 + NO2 + CO	3.660e-12
TERPDHDP + OH	→	TERPOOH + OH	2.800e-11
TERPF1 + NO3	→	NO2 + 0.44*CH2O + TERPA3	2.600e-13
TERPF1O2 + HO2	→	0.9*TERPOOHL + 0.1*OH + 0.1*HO2 + 0.1*TERPA3 + 0.04*CH2O	2.68e-13 exp(1300.00 / t)
TERPF1O2 + NO	→	0.3*TERPHFN + 0.7*NO2 + 0.7*HO2 + 0.7*TERPA3 + 0.31*CH2O	2.70e-12 exp(360.00 / t)
TERPF1 + O3	→	0.09*OH + TERPA3 + 0.62*CH2O + 0.23*HMHP + 0.02*H2O2 + 0.15*HCOOH	8.300e-18
TERPF1 + OH	→	0.83*TERPF1O2 + 0.17*TERPA3CO3	1.100e-10
TERPF2 + NO3	→	0.5*TERPNS1 + 0.5*HO2 + 0.5*TERPF1 + 0.5*CH2O + 0.5*NO2	2.95e-12 exp(-450.00 / t)
TERPF2O2 + HO2	→	0.9*TERP1OOH + 0.1*OH + 0.1*HO2 + 0.1*TERPF1	2.47e-13 exp(1300.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPF2O2 + NO	→	**0.18*TERPNT1 + 0.12*TERPNS1 + 0.7*NO2 + 0.7*HO2 + 0.7*TERPF1**	**2.70e-12 exp(360.00 / t)**
TERPF2 + O3	→	**TERPF1 + 0.34*CH2O + 0.4*HMHP + 0.04*H2O2 + 0.26*HCOOH**	**1.100e-16**
TERPF2 + OH	→	**TERPF2O2**	**2.70e-11 exp(390.00 / t)**
TERPFDN + OH	→	**NO2 + TERPNS**	**3.640e-12**
TERPHFN + OH	→	**TERPNS + OH**	**2.800e-11**
TERPK + OH	→	**0.14*TERPA2CO3 + 0.86*TERPA1O2**	**1.700e-11**
TERPNPS1O2 + HO2	→	**0.9*TERPHFN + 0.1*OH + 0.1*TERPNPS + 0.1*HO2**	**2.76e-13 exp(1300.00 / t)**
TERPNPS1O2 + NO	→	**0.3*TERPFDN + 0.7*NO2 + 0.7*TERPNPS + 0.7*HO2**	**2.70e-12 exp(360.00 / t)**
TERPNPS1 + OH	→	**TERPNPS1O2**	**1.100e-10**
TERPNPS + OH	→	**H2O + BPINNO3**	**9.580e-12**
TERPNPT1O2 + HO2	→	**0.9*TERPHFN + 0.1*OH + 0.1*TERPNPT + 0.1*HO2**	**2.76e-13 exp(1300.00 / t)**
TERPNPT1O2 + NO	→	**0.3*TERPFDN + 0.7*NO2 + 0.7*TERPNPT + 0.7*HO2**	**2.70e-12 exp(360.00 / t)**
TERPNPT1 + OH	→	**TERPNPT1O2**	**1.100e-10**
TERPNPT + OH	→	**TERPNT + H2O + OH**	**1.230e-11**
TERPNS1O2 + HO2	→	**0.9*TERPHFN + 0.1*OH + 0.1*TERPNS + 0.1*HO2**	**2.75e-13 exp(1300.00 / t)**
TERPNS1O2 + NO	→	**0.3*TERPFDN + 0.7*NO2 + 0.7*TERPNS + 0.7*HO2**	**2.70e-12 exp(360.00 / t)**
TERPNS1 + OH	→	**TERPNS1O2**	**1.100e-10**
TERPNS + OH	→	**TERPA + NO2**	**3.640e-12**
TERPNT1O2 + HO2	→	**0.9*TERPHFN + 0.1*OH + 0.1*TERPNT + 0.1*HO2**	**2.75e-13 exp(1300.00 / t)**
TERPNT1O2 + NO	→	**0.3*TERPFDN + 0.7*NO2 + 0.7*TERPNT + 0.7*HO2**	**2.70e-12 exp(360.00 / t)**
TERPNT1 + OH	→	**TERPNT1O2**	**1.100e-10**
TERPNT + OH	→	**TERPA + NO2**	**5.500e-12**
TERPOOHL + OH	→	**TERPA3 + OH**	**4.650e-11**
TERPOOH + OH	→	**TERPA + OH**	**2.800e-11**
TERPA2PAN + M	→	**M + TERPA2CO3 + NO2**	
TERPA3PAN + M	→	**TERPA3CO3 + NO2 + M**	
TERPAPAN + M	→	**TERPACO3 + NO2 + M**	
Sulfur Compounds			
OCS + O	→	SO + CO	2.10e-11 exp(-2200.00 / t)
OCS + OH	→	SO2 + CO + H	7.20e-14 exp(-1070.00 / t)
S + O2	→	SO + O	2.300e-12
S + O3	→	SO + O2	1.200e-11
SO + BRO	→	SO2 + BR	5.700e-11

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
SO + CLO	→	SO2 + CL	2.800e-11
S + OH	→	SO + H	6.600e-11
SO + NO2	→	SO2 + NO	1.400e-11
SO + O2	→	SO2 + O	1.60e-13 exp(-2280.00 / t)
SO + O3	→	SO2 + O2	3.40e-12 exp(-1100.00 / t)
SO + OCLO	→	SO2 + CLO	1.900e-12
SO + OH	→	SO2 + H	2.70e-11 exp(335.00 / t)
SO2 + OH	→	SO3 + HO2	ko = 3.0e-31 (300 / t)$^{3.3}$, ki = 1.5e-12, f=0.6
SO3 + H2O	→	H2SO4	8.5e-21*[H2O]* exp(6540 / t) * 1.0e-20
Tropospheric Aerosol [a]			
DMS + NO3	→	SO2 + HNO3	1.90e-13 exp(520.00 / t)
DMS + OH	→	SO2	9.60e-12 exp(-234.00 / t)
NH3 + OH	→	H2O	1.70e-12 exp(-710.00 / t)
DMS + OH	→	0.5*SO2 + 0.5*HO2	1.7e-42 exp(7810 / t) * [M] * 0.21 / (1+5.5e-31 exp(7460 / t) * [M] * 0.21)
GLYOXAL	→	SOAG0	γ = 0.0002
HO2	→	0.5*H2O2	γ = 0.2
HONITR	→	HNO3	γ = 0.005
ICHE	→	**M**	γ **= 0.0042**
IEPOX	→	**M**	γ **= 0.0042**
INHEB	→	**HNO3**	γ **= 0.02**
INHED	→	**HNO3**	γ **= 0.02**
ISOPNOOHD	→	**HNO3**	γ **= 0.02**
ISOPFDN	→	**HNO3**	γ **= 0.1**
ISOPFDNC	→	**HNO3**	γ **= 0.1**
ISOPFNC	→	**M**	γ **= 0.1**
ISOPFNP	→	**M**	γ **= 0.1**
ISOPHFP	→	**M**	γ **= 0.1**
ISOPN1D	→	**HNO3**	γ **= 0.02**
ISOPN2B	→	**HNO3**	γ **= 0.02**
ISOPN4D	→	**HNO3**	γ **= 0.02**
N2O5	→	2*HNO3	γ = 0.1

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
NC4CHO	→	HNO3	γ = 0.005
NH4	→	M	6.340e-8
NO2	→	0.5*OH + 0.5*NO + 0.5*HNO3	γ = 0.0001
NO3	→	HNO3	γ = 0.001
ONITR	→	HNO3	γ = 0.005
SQTN	→	**M**	**γ = 0.1**
TERPDHDP	→	**M**	**γ = 0.1**
TERPFDN	→	**HNO3**	**γ = 0.1**
TERPHFN	→	**M**	**γ = 0.1**
TERPNPT1	→	**HNO3**	**γ = 0.02**
TERPNPT	→	**HNO3**	**γ = 0.02**
TERPNT1	→	**HNO3**	**γ = 0.02**
TERPNT	→	**HNO3**	**γ = 0.02**
Secondary Organic Aerosol [b]			
APIN + NO3	→	**APIN + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4**	**1.20e-12 exp(490.00 / t)**
APIN + O3	→	**APIN + O3 + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**8.05e-16 exp(-640.00 / t)**
APIN + OH	→	**APIN + OH + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**1.34e-11 exp(410.00 / t)**
BCARY + NO3	→	BCARY + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4	1.900e-11
BCARY + O3	→	BCARY + O3 + 0.2202*SOAG0 + 0.2067*SOAG1 + 0.0653*SOAG2 + 0.1284*SOAG3 + 0.114*SOAG4	1.200e-14
BCARY + OH	→	BCARY + OH + 0.2202*SOAG0 + 0.2067*SOAG1 + 0.0653*SOAG2 + 0.1284*SOAG3 + 0.114*SOAG4	2.000e-10
BENZENE + OH	→	BENZENE + OH + 0.0023*SOAG0 + 0.0008*SOAG1 + 0.0843*SOAG2 + 0.0443*SOAG3 + 0.1621*SOAG4	2.30e-12 exp(-193.00 / t)
BPIN + NO3	→	**BPIN + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4**	**2.500e-12**
BPIN + O3	→	**BPIN + O3 + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**1.35e-15 exp(-1270.00 / t)**
BPIN + OH	→	**BPIN + OH + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**1.62e-11 exp(460.00 / t)**
ISOP + NO3	→	ISOP + NO3 + 0.059024*SOAG3 + 0.025024*SOAG4	3.03e-12 exp(-446.00 / t)
ISOP + O3	→	ISOP + O3 + 0.0033*SOAG3	1.05e-14 exp(-2000.00 / t)
ISOP + OH	→	ISOP + OH + 0.0031*SOAG0 + 0.0035*SOAG1 + 0.0003*SOAG2 + 0.0271*SOAG3 + 0.0474*SOAG4	2.54e-11 exp(410.00 / t)

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
IVOC + OH	→	OH + 0.2381*SOAG0 + 0.1308*SOAG1 + 0.0348*SOAG2 + 0.0076*SOAG3 + 0.0113*SOAG4	1.340e-11
LIMON + NO3	→	**LIMON + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4**	**1.200e-11**
LIMON + O3	→	**LIMON + O3 + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**2.80e-15 exp(-770.00 / t)**
LIMON + OH	→	**LIMON + OH + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**3.41e-11 exp(470.00 / t)**
MYRC + NO3	→	**MYRC + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4**	**1.100e-11**
MYRC + O3	→	**MYRC + O3 + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**2.65e-15 exp(-520.00 / t)**
MYRC + OH	→	**MYRC + OH + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4**	**2.100e-10**
SVOC + OH	→	OH + 0.5931*SOAG0 + 0.1534*SOAG1 + 0.0459*SOAG2 + 0.0085*SOAG3 + 0.0128*SOAG4	1.340e-11
TOLUENE + OH	→	TOLUENE + OH + 0.1364*SOAG0 + 0.0101*SOAG1 + 0.0763*SOAG2 + 0.2157*SOAG3 + 0.0232*SOAG4	1.70e-12 exp(352.00 / t)
XYLENES + OH	→	XYLENES + OH + 0.1677*SOAG0 + 0.0174*SOAG1 + 0.086*SOAG2 + 0.0512*SOAG3 + 0.1598*SOAG4	1.700e-11
Stratospheric Heterogeneous Uptake Reactions			
Sulfate aerosol reactions			
N2O5 + H2O(l)	→	2*HNO3	γ = f(wt%)
CLONO2 + H2O(l)	→	HOCL + HNO3	γ = f(T,P,HCl,H2O,r)
BRONO2 + H2O(l)	→	HOBR + HNO3	γ = f(T,P,H2O,r)
CLONO2 + HCL(l)	→	CL2 + HNO3	γ = f(T,P,HCl,H2O,r)
HOCL + HCL(l)	→	CL2 + H2O	γ = f(T,P,HCl,HOCl,H2O,r)
HOBR + HCL(l)	→	BRCL + H2O	γ = f(T,P,HCl,HOBr,H2O,r)
Nitric Acid Tri-hydrate Reactions			
N2O5 + H2O(s)	→	2*HNO3	γ = 4e-4
CLONO2 + H2O(s)	→	HOCL + HNO3	γ = 4e-3
CLONO2 + HCL(s)	→	CL2 + HNO3	γ = 0.2
HOCL + HCL(s)	→	CL2 + H2O	γ = 0.1
BRONO2 + H2O(s)	→	HOBR + HNO3	γ = 0.006
Water-Ice Aerosol Reactions			
N2O5 + H2O(s)	→	2*HNO3	γ = 0.02
CLONO2 + H2O(s)	→	HOCL + HNO3	γ = 0.3

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		**Products**	**Rate**
BRONO2 + H2O(s)	→	HOBR + HNO3	γ = 0.3
CLONO2 + HCL(s)	→	CL2 + HNO3	γ = 0.3
HOCL + HCL(s)	→	CL2 + H2O	γ = 0.2
HOBR + HCL(s)	→	BRCL + H2O	γ = 0.3
Synthetic Tracers			
AOA_NH	→	AOA_NH	1.000e+0
E90	→	sink	1.290e-7
NH_50	→	M	2.310e-7
NH_5	→	M	2.310e-6
ST80_25	→	M	4.630e-7

• The pressure and temperature dependence for all isoprene derived organic nitrates yields are included as recommended by Wennberg et al. (2018). The organic nitrate yield (α) at T = 293 K, M= 2.45E19 molecules cm^{-3} and the number of heavy atoms excluding the peroxy group (n) are reported.

• [a] For new gas-phase species undergoing aerosol uptake, the aerosol uptake coefficient (γ) value is reported.

• [b] Secondary organic aerosol reactions in bold were added only to treat the new tracers (APIN, BPIN, LIMON, and. MYRC) separately. No changes are made to the yields of the SOA gas-phase tracers.

Table S7: MOZART-TS2 Kinetic Reactions Changed For Box-Model Sensitivity Tests

Reactant		Products	Rate
Caltech assumptions for PAN and C_4 dihydroperoxy carbonyls			
Removed the following reactions:			
PAN + hν	→	**0.6*CH3CO3 + 0.6*NO2 + 0.4*CH3O2 + 0.4*NO3 + 0.4*CO2**	**jpan**
CH3CO3 + CH3CO3	→	**2*CH3O2 + 2*CO2**	**2.90e-12 exp(500.00 / t)**
Changed the following reactions:			
PAN + OH	→	**CH2O + CO + NO2**	**3.000e-14**
CH3CO3 + NO2	→	**PAN**	**TROE_I(2.591E-28,0.,-6.87,1.125E-11,0.,-1.105,0.3)**
PAN	→	**CH3CO3 + NO2**	**TROE_I(3.871E-3,-12100.,0.,5.4E16,-13830.,0.,0.3)**
ISOPZD1O2	→	0.15*HPALDB1C + 0.25*HPALD1 + 0.4*HO2 + **1.5*OH + 0.3*CH3COCHO + 0.3*CH2O + 0.3*HCOCH2OOH + 0.3*CH3CO3** + 0.6*CO	5.05e15 exp(-12200.00 / t) exp(1e8 / t^3)
ISOPZD4O2	→	0.15*HPALDB4C + 0.25*HPALD4 + 0.4*HO2 + **1.5*OH + 0.3*CH3COCHO + 0.3*CH2O + 0.3*HYPERACET + 0.9*CO**	2.22e9 exp(-7160.00 / t) exp(1e8 / t^3)
Caltech assumptions for PAN, C_4 dihydroperoxy carbonyls, and carbonyl nitrates			
Removed the following reactions:			
PAN + hν	→	**0.6*CH3CO3 + 0.6*NO2 + 0.4*CH3O2 + 0.4*NO3 + 0.4*CO2**	**jpan**
CH3CO3 + CH3CO3	→	**2*CH3O2 + 2*CO2**	**2.90e-12 exp(500.00 / t)**
Changed the following reactions:			
PAN + OH	→	**CH2O + CO + NO2**	**3.000e-14**
CH3CO3 + NO2	→	**PAN**	**TROE_I(2.591E-28,0.,-6.87,1.125E-11,0.,-1.105,0.3)**
PAN	→	**CH3CO3 + NO2**	**TROE_I(3.871E-3,-12100.,0.,5.4E16,-13830.,0.,0.3)**
ISOPZD1O2	→	0.15*HPALDB1C + 0.25*HPALD1 + 0.4*HO2 + **1.5*OH + 0.3*CH3COCHO + 0.3*CH2O + 0.3*HCOCH2OOH + 0.3*CH3CO3** + 0.6*CO	5.05e15 exp(-12200.00 / t) exp(1e8 / t^3)
ISOPZD4O2	→	0.15*HPALDB4C + 0.25*HPALD4 + 0.4*HO2 + **1.5*OH + 0.3*CH3COCHO + 0.3*CH2O + 0.3*HYPERACET + 0.9*CO**	2.22e9 exp(-7160.00 / t) exp(1e8 / t^3)

Table S7: MOZART-TS2 Kinetic Reactions Changed For Box-Model Sensitivity Tests

Reactant		Products	Rate
ISOPFDNC + hν	→	2*NO2 + 0.5*CH3COCHO + 0.5*GLYALD + 0.5*HYAC + 0.5*GLYOXAL	**0.86***jch2o_a
ISOPFNC + hν	→	OH + NO2 + 0.5*GLYALD + 0.5*CH3COCHO + 0.5*HYAC + 0.5*GLYOXAL	**0.89***jch2o_a
MACRN + hν	→	0.75*CO + 0.75*NO2 + 0.5*HYAC + 1.25*HO2 + 0.25*CH3COCHO + 0.25*CH2O + 0.25*NOA	**0.70***jch2o_a
MVKN + hν	→	0.75*NO2 + 0.25*NO3CH2CHO + 0.75*CH3CO3 + 0.5*GLYALD + 0.5*HO2 + 0.25*CH2O + 0.25*CH3COCHO	**1.15***jch2o_a
NC4CHO + hν	→	NO2 + HO2 + HYDRALD	**4.86***jch2o_a
NO3CH2CHO + hν	→	NO2 + CH2O + CO + HO2	**1.39***jch2o_a
NOA + hν	→	NO2 + CH2O + CH3CO3	**0.18***jch2o_a
MCM v3.3.1 assumptions for pinonaldehyde nitrate yield			
Changed the following reactions:			
TERPA1O2 + NO	→	**0.16***TERPNS + **0.84***NO2 + **0.84***TERPA2O2	2.70e-12 exp(360.00 / t)
TERPA2O2 + NO	→	**0.03***TERPNT + **0.97***NO2 + **0.97***TERPA3O2	2.70e-12 exp(360.00 / t)
TERPA3O2 + NO	→	**0.12***TERPNT + **0.88***NO2 + **0.88***TERPA4O2 + **0.88***CH3COCH3	2.70e-12 exp(360.00 / t)
TERPA4O2 + NO	→	**0.05***TERPNS + **0.95***NO2 + **0.95***CH3CO3 + **0.95***HO2 + **1.9***CH2O + **0.95***CO	2.70e-12 exp(360.00 / t)
MCM v3.3.1 assumptions for pinonaldehyde and limonaldehyde/limaketone nitrate yield			
Changed the following reactions:			
TERPA1O2 + NO	→	**0.16***TERPNS + **0.84***NO2 + **0.84***TERPA2O2	2.70e-12 exp(360.00 / t)
TERPA2O2 + NO	→	**0.03***TERPNT + **0.97***NO2 + **0.97***TERPA3O2	2.70e-12 exp(360.00 / t)
TERPA3O2 + NO	→	**0.12***TERPNT + **0.88***NO2 + **0.88***TERPA4O2 + **0.88***CH3COCH3	2.70e-12 exp(360.00 / t)
TERPA4O2 + NO	→	**0.05***TERPNS + **0.95***NO2 + **0.95***CH3CO3 + **0.95***HO2 + **1.9***CH2O + **0.95***CO	2.70e-12 exp(360.00 / t)
TERPF1O2 + NO	→	**0.15***TERPHFN + **0.85***NO2 + **0.85***HO2 + **0.85***TERPA3 + 0.31*CH2O	2.70e-12 exp(360.00 / t)
MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield and oxidation of unsaturated hydroxy nitrates			
Changed the following reactions:			
TERPA1O2 + NO	→	**0.16***TERPNS + **0.84***NO2 + **0.84***TERPA2O2	2.70e-12 exp(360.00 / t)
TERPA2O2 + NO	→	**0.03***TERPNT + **0.97***NO2 + **0.97***TERPA3O2	2.70e-12 exp(360.00 / t)

Table S7: MOZART-TS2 Kinetic Reactions Changed For Box-Model Sensitivity Tests

Reactant		**Products**	**Rate**
TERPA3O2 + NO	→	**0.12***TERPNT + **0.88***NO2 + **0.88***TERPA4O2 + **0.88***CH3COCH3	2.70e-12 exp(360.00 / t)
TERPA4O2 + NO	→	**0.05***TERPNS + **0.95***NO2 + **0.95***CH3CO3 + **0.95***HO2 + **1.9***CH2O + **0.95***CO	2.70e-12 exp(360.00 / t)
TERPF1O2 + NO	→	**0.15***TERPHFN + **0.85***NO2 + **0.85***HO2 + **0.85***TERPA3 + 0.31*CH2O	2.70e-12 exp(360.00 / t)
TERPNS1 + OH	→	**TERPF1+NO2**	1.100e-10
TERPNT1 + OH	→	**TERPF1+NO2**	1.100e-10

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		Products	Rate
I_TEST1 Sensitivity Test			
Updated the following reactions:			
ISOPB1O2 + NO	→	NO2 + MVK + CH2O + HO2	In code, α **= 0.09**, n = 6
ISOPB1O2 + NO	→	ISOPN2B	In code, α **= 0.09**, n = 6
ISOPB4O2 + NO	→	NO2 + MACR + CH2O + HO2	In code, α **= 0.13**, n = 6
ISOPB4O2 + NO	→	ISOPN3B	In code, α **= 0.09**, n = 6
ISOPED1O2 + NO	→	NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH	In code, α **= 0.09**, n = 6
ISOPED1O2 + NO	→	ISOPN4D	In code, α **= 0.09**, n = 6
ISOPED4O2 + NO	→	NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH	In code, α **= 0.09**, n = 6
ISOPED4O2 + NO	→	ISOPN1D	In code, α **= 0.09**, n = 6
ISOPZD1O2 + NO	→	NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH	In code, α **= 0.09**, n = 6
ISOPZD1O2 + NO	→	ISOPN4D	In code, α **= 0.09**, n = 6
ISOPZD4O2 + NO	→	NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH	In code, α **= 0.09**, n = 6
ISOPZD4O2 + NO	→	ISOPN1D	In code, α **= 0.09**, n = 6
I_TEST2 Sensitivity Test			
Updated the following reactions:			
ISOPN1DO2 + NO	→	NO2 + HO2 + 0.94*NOA + 0.94*GLYALD + 0.06*MACRN + 0.06*CH2O	In code, α **= 0.3**, n = 11
ISOPN1DO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 11
ISOPN2BO2 + NO	→	1.73*NO2 + 0.27*MACRN + 0.27*CH2O + 0.27*HO2 + 0.73*HYAC + 0.73*GLYALD	In code, α **= 0.3**, n = 11
ISOPN2BO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 11
ISOPN3BO2 + NO	→	NO2 + MVKN + CH2O + HO2	In code, α **= 0.3**, n = 11
ISOPN3BO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 11
ISOPN4DO2 + NO	→	NO2 + HO2 + 0.13*MVKN + 0.13*CH2O + 0.87*HYAC + 0.87*NO3CH2CHO	In code, α **= 0.3**, n = 11
ISOPN4DO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 11
ISOPNBNO3O2 + NO	→	NO2 + HO2 + 0.21*MACRN + 0.12*MVKN + 0.33*CH2O + 0.34*NOA + 0.34*GLYALD + 0.33*HYAC + 0.33*NO3CH2CHO	In code, α **= 0.3**, n = 11
ISOPNBNO3O2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 11

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		**Products**	**Rate**
ISOPNOOHBO2 + NO	→	NO2 + 0.53*CH2O + 0.53*HO2 + 0.49*MACRN + 0.04*MVKN + 0.4*NOA + 0.4*GLYALD + 0.07*HYAC + 0.07*NO3CH2CHO + 0.47*OH	In code, α **= 0.3**, n = 12
ISOPNOOHBO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 12
ISOPNOOHDO2 + NO	→	NO2 + 0.04*CH2O + 0.04*OH + 0.02*MACRN + 0.02*MVKN + 0.81*NOA + 0.81*HCOCH2OOH + 0.15*HYPERACET + 0.15*NO3CH2CHO + 0.96*HO2	In code, α **= 0.3**, n = 12
ISOPNOOHDO2 + NO	→	ISOPFDN	In code, α **= 0.3**, n = 12
NC4CHOO2 + NO	→	NO2 + HO2 + 0.13*NOA + 0.13*GLYOXAL + 0.12*CH3COCHO + 0.12*NO3CH2CHO + 0.39*MACRN + 0.36*MVKN + 0.75*CO	In code, α **= 0.3**, n = 11
NC4CHOO2 + NO	→	ISOPFDNC	In code, α **= 0.3**, n = 11
I_TEST3 Sensitivity Test			
Removed the following reactions:			
ISOPN1DO2	→	**ISOPFNP + HO2**	**1.26e+13 exp(-10000.00 / t)**
ISOPN2BO2	→	**ISOPFNC + HO2**	**1.88e+13 exp(-10000.00 / t)**
ISOPN3BO2	→	**ISOPFNC + HO2**	**1.88e+13 exp(-10000.00 / t)**
ISOPN4DO2	→	**ISOPFNP + HO2**	**5.09e+12 exp(-10000.00 / t)**
ISOPNOOHBO2	→	**OH + ISOPFNP**	**8.72e+12 exp(-10000.00 / t)**
ISOPNOOHDO2	→	**OH + ISOPFNP**	**6.55e+12 exp(-10000.00 / t)**
T_TEST1 Sensitivity Test			
Updated the following reactions:			
APINO2 + NO	→	0.01*TERPHFN + **0.04***TERPNS1 + **0.13***TERPNS + **0.06***TERPNT + **0.06***TERPNT1 + **0.7*NO2** + **0.7***HO2 + **0.26***TERPA + **0.24***TERPA3 + 0.09*CH3COCH3 + 0.09*TERPF1 + 0.21*CH2O + 0.11*TERP1OOH	2.70e-12 exp(360.00 / t)
BPINO2 + NO	→	0.08*CH3COCH3 + 0.49*CH2O + 0.2*TERPF1 + 0.24*TERPK + **0.05***TERPNS1 + 0.02*TERPNS + **0.07***TERPNT + **0.16***TERPNT1 + **0.26***TERPA3 + **0.7***HO2 + **0.7***NO2	2.70e-12 exp(360.00 / t)
LIMONO2 + NO	→	**0.22***TERPNT1 + **0.08***TERPNS1 + **0.7***NO2 + **0.7***TERPF1 + **0.7***HO2 + 0.43*CH2O	2.70e-12 exp(360.00 / t)
MYRCO2 + NO	→	0.1*TERPNS1 + **0.2***TERPNT1 + **0.7***NO2 + **0.7***TERPF2 + 0.33*CH3COCH3 + 0.3*CH2O + **0.7***HO2	2.70e-12 exp(360.00 / t)
T_TEST2 Sensitivity Test			

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		Products	Rate
Updated the following reactions:			
APINO2 + NO	→	0.01*TERPHFN + 0.02*TERPNS1 + **0.06***TERPNS + **0.03***TERPNT + **0.03***TERPNT1 + **0.85***NO2 + **0.85***HO2 + **0.34***TERPA + **0.31***TERPA3 + 0.09*CH3COCH3 + 0.09*TERPF1 + 0.21*CH2O + 0.11*TERP1OOH	2.70e-12 exp(360.00 / t)
BCARYO2 + NO	→	**0.15***SQTN + **0.85***NO2 + **0.85***HO2 + **0.85***TERPF2	2.70e-12 exp(360.00 / t)
BPINO2 + NO	→	0.08*CH3COCH3 + 0.49*CH2O + 0.2*TERPF1 + 0.24*TERPK + **0.02***TERPNS1 + **0.01***TERPNS + **0.04***TERPNT + **0.08***TERPNT1 + **0.41***TERPA3 + **0.85***HO2 + **0.85***NO2	2.70e-12 exp(360.00 / t)
LIMONO2 + NO	→	**0.11***TERPNT1 + **0.04***TERPNS1 + **0.85***NO2 + **0.85***TERPF1 + **0.85***HO2 + 0.43*CH2O	2.70e-12 exp(360.00 / t)
MYRCO2 + NO	→	**0.05***TERPNS1 + **0.1***TERPNT1 + **0.85***NO2 + **0.85***TERPF2 + 0.33*CH3COCH3 + 0.3*CH2O + **0.85***HO2	2.70e-12 exp(360.00 / t)
T_TEST3 Sensitivity Test			
Updated the following reactions:			
APINO2 + CH3CO3	→	**0.1***TERPF1 + **0.32***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH + HO2 + CH3O2 + CO2	2e-12 exp (500.00 / t)
APINO2 + CH3O2	→	**0.87***CH2O + **0.13***CH3OH + **1.49***HO2 + **0.1***TERPF1 + **0.15***TERPK + **0.17***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH	2e-12
APINO2 + HO2	→	**0.32***TERP1OOH + **0.43***TERPOOH + **0.03***TERPA + **0.22*TERPA3** + **0.26***OH + **0.26***HO2	2.6e-13 exp(1300.00 / t)
APINO2 + NO	→	**0.04***TERPNS + 0.05*TERPNT + **0.015***TERPNS1 + **0.015***TERPNT1 + **0.88***NO2 + **0.88***HO2 + **0.08***TERPF1 + 0.3*TERPA + **0.31***TERPA3 + **0.19***TERP1OOH	2.7e-12 exp(360.00 / t)
APINO2 + NO3	→	NO2 + HO2 + **0.1***TERPF1 + **0.32***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH	2.3e-12
APINO2 + TERPA2CO3	→	**0.1***TERPF1 + **0.32***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH + HO2 + TERPA2O2 + CO2	2e-12 exp(500 / t)
APINO2 + TERPA3CO3	→	**0.1***TERPF1 + **0.32***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH + HO2 + TERPA4O2 + CO2	2e-12 exp(500 / t)
APINO2 + TERPACO3	→	**0.1***TERPF1 + **0.32***TERPA + **0.36***TERPA3 + **0.22***TERP1OOH + HO2 + TERPA1O2 + CO2	2e-12 exp(500 / t)
APIN + OH	→	**0.06*TERP1OOH** + **0.06*HO2** + **0.94***APINO2	1.34e-11 exp(410 / t)

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		Products	Rate
BPINO2 + CH3CO3	→	**0.1***TERPF1 + **0.35***TERPK + **0.35***CH2O + **0.28***TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **0.81***HO2 + CH3O2 + CO2	2e-12 exp(500 / t)
BPINO2 + CH3O2	→	**1.26***CH2O + **0.06*CH3OH** + **0.1***TERPF1 + 0.32*TERPK + 0.31*TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **1.57***HO2	2e-12
BPINO2 + HO2	→	**0.18***TERP1OOH + **0.65***TERPOOH + 0.03*TERPK + 0.03*CH2O + **0.03*TERPA3** + **0.11*TERPA3CO3** + **0.18***OH + **0.07***HO2	2.6e-13 exp(1300 / t)
BPINO2 + NO	→	**0.03***TERPNS + **0.09***TERPNT + **0.01***TERPNS1 + **0.87***NO2 + **0.72***HO2 + **0.08***TERPF1 + **0.31***TERPK + **0.31***CH2O + **0.26***TERPA3 + **0.15*TERPA3CO3** + **0.07*TERP1OOH**	2.7e-12 exp(360 / t)
BPINO2 + NO3	→	**0.1***TERPF1 + **0.35***TERPK + **0.35***CH2O + **0.28***TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **0.81***HO2 + NO2	2.3e-12
BPINO2 + TERPA2CO3	→	**0.1***TERPF1 + **0.35***TERPK + **0.35***CH2O + **0.28***TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **0.81***HO2 + TERPA2O2 + CO2	2e-12 exp(500 / t)
BPINO2 + TERPA3CO3	→	**0.1***TERPF1 + **0.35***TERPK + **0.35***CH2O + **0.28***TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **0.81***HO2 + TERPA4O2 + CO2	2e-12 exp(500 / t)
BPINO2 + TERPACO3	→	**0.1***TERPF1 + **0.35***TERPK + **0.35***CH2O + **0.28***TERPA3 + **0.19*TERPA3CO3** + **0.08*TERP1OOH** + **0.81***HO2 + TERPA1O2 + CO2	2e-12 exp(500 / t)
T_TEST4 Sensitivity Test			
Updated the following reactions:			
TERPA1O2 + NO	→	**0.16***TERPNS + **0.84***NO2 + **0.84***TERPA2O2	2.70e-12 exp(360.00 / t)
TERPA2O2 + NO	→	**0.03***TERPNT + **0.97***NO2 + **0.97***TERPA3O2	2.70e-12 exp(360.00 / t)
TERPA3O2 + NO	→	**0.12***TERPNT + **0.88***NO2 + **0.88***TERPA4O2 + **0.88***CH3COCH3	2.70e-12 exp(360.00 / t)
TERPA4O2 + NO	→	**0.05***TERPNS + **0.95***NO2 + **0.95***CH3CO3 + **0.95***HO2 + **1.9***CH2O + **0.95***CO	2.70e-12 exp(360.00 / t)
TERPF1O2 + NO	→	**0.15***TERPHFN + **0.85***NO2 + **0.85***HO2 + **0.85***TERPA3 + 0.31*CH2O	2.70e-12 exp(360.00 / t)

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		Products	Rate
A_TEST1 Sensitivity Test			
Removed the following reactions:			
HONITR	→	**HNO3**	**In code**
INHEB	→	**HNO3**	**In code, γ = 0.02**
INHED	→	**HNO3**	**In code, γ = 0.02**
ISOPNOOHD	→	**HNO3**	**In code, γ = 0.02**
ISOPFDN	→	**HNO3**	**In code, γ = 0.1**
ISOPFDNC	→	**HNO3**	**In code, γ = 0.1**
ISOPFNC	→	**M**	**In code, γ = 0.1**
ISOPFNP	→	**M**	**In code, γ = 0.1**
ISOPN1D	→	**HNO3**	**In code, γ = 0.02**
ISOPN2B	→	**HNO3**	**In code, γ = 0.02**
ISOPN4D	→	**HNO3**	**In code, γ = 0.02**
NC4CHO	→	**HNO3**	**In code**
ONITR	→	**HNO3**	**In code**
SQTN	→	**M**	**In code, γ = 0.1**
TERPFDN	→	**HNO3**	**In code, γ = 0.1**
TERPHFN	→	**M**	**In code, γ = 0.1**
TERPNPT1	→	**HNO3**	**In code, γ = 0.02**
TERPNPT	→	**HNO3**	**In code, γ = 0.02**
TERPNT1	→	**HNO3**	**In code, γ = 0.02**
TERPNT	→	**HNO3**	**In code, γ = 0.02**
A_TEST2 Sensitivity Test			
Removed the following reactions:			
INHEB	→	**HNO3**	**In code, γ = 0.02**
INHED	→	**HNO3**	**In code, γ = 0.02**
ISOPNOOHD	→	**HNO3**	**In code, γ = 0.02**
Added the following reactions:			
ISOPN3B	→	**HNO3**	**In code, γ = 0.005**
ISOPNBNO3	→	**HNO3**	**In code, γ = 0.005**
MVKN	→	**HNO3**	**In code, γ = 0.005**
MACRN	→	**HNO3**	**In code, γ = 0.005**
TERPNPS1	→	**HNO3**	**In code, γ = 0.01**
TERPNPS	→	**HNO3**	**In code, γ = 0.01**
TERPNS	→	**HNO3**	**In code, γ = 0.01**

Table S8: MOZART-TS2 Kinetic Reactions Changed For CESM/CAM-Chem Sensitivity Tests

Reactant		**Products**	**Rate**
TERPNS1	→	**HNO3**	**In code, γ = 0.01**
Updated the following reactions:			
NC4CHO	→	HNO3	**In code, γ = 0.005**
ISOPFDN	→	HNO3	**In code, γ = 0.005**
ISOPFNP	→	M	**In code, γ = 0.005**
ISOPN1D	→	HNO3	**In code, γ = 0.005**
ISOPN2B	→	HNO3	**In code, γ = 0.005**
ISOPN4D	→	HNO3	**In code, γ = 0.005**
ISOPFNC	→	M	**In code, γ = 0.005**
ISOPFDNC	→	HNO3	**In code, γ = 0.005**
TERPNT1	→	HNO3	**In code, γ = 0.01**
TERPNT	→	HNO3	**In code, γ = 0.01**
TERPNPT1	→	HNO3	**In code, γ = 0.01**
TERPNPT	→	HNO3	**In code, γ = 0.01**
TERPFDN	→	HNO3	**In code, γ = 0.01**
SQTN	→	M	**In code, γ = 0.01**
TERPHFN	→	M	**In code, γ = 0.01**
A_TEST3 Sensitivity Test			
Added the following reactions:			
ISOPNOOHB	→	**HNO3**	**In code, γ = 0.02**
ISOPN3B	→	**HNO3**	**In code, γ = 0.02**
ISOPNBNO3	→	**HNO3**	**In code, γ = 0.02**
MVKN	→	**HNO3**	**In code, γ = 0.02**
MACRN	→	**HNO3**	**In code, γ = 0.02**
TERPNPS1	→	**HNO3**	**In code, γ = 0.02**
TERPNPS	→	**HNO3**	**In code, γ = 0.02**
TERPNS	→	**HNO3**	**In code, γ = 0.02**
TERPNS1	→	**HNO3**	**In code, γ = 0.02**

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