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*Supplement of*

## **Comprehensive isoprene and terpene gas-phase chemistry improves simulated surface ozone in the southeastern US**

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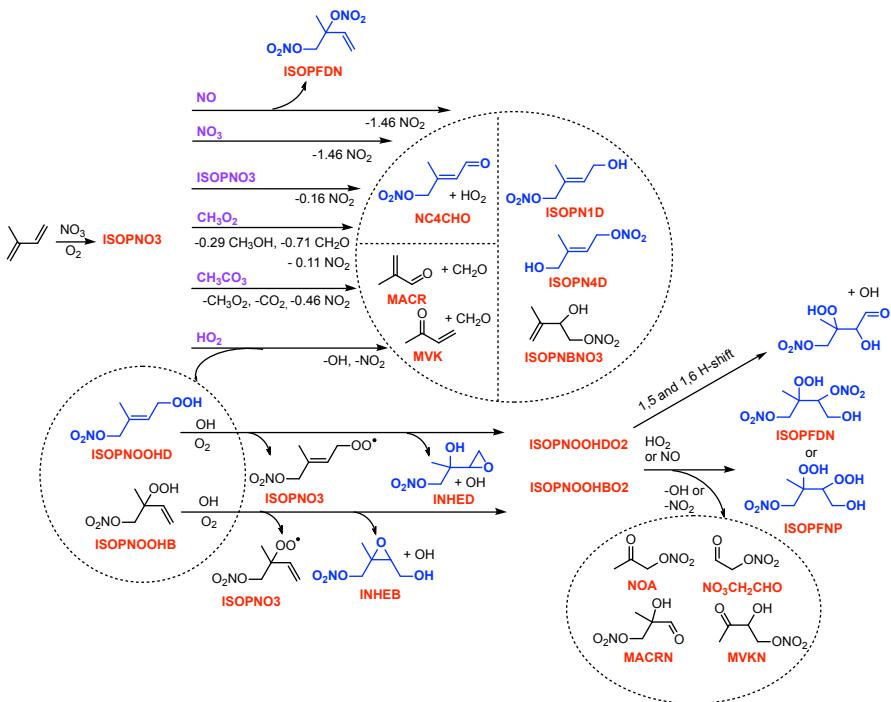
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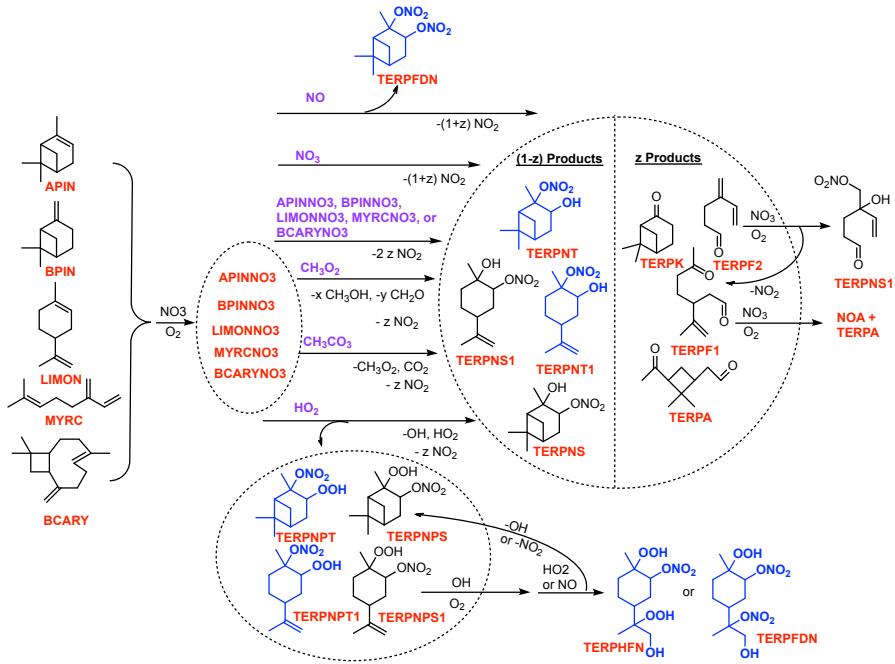
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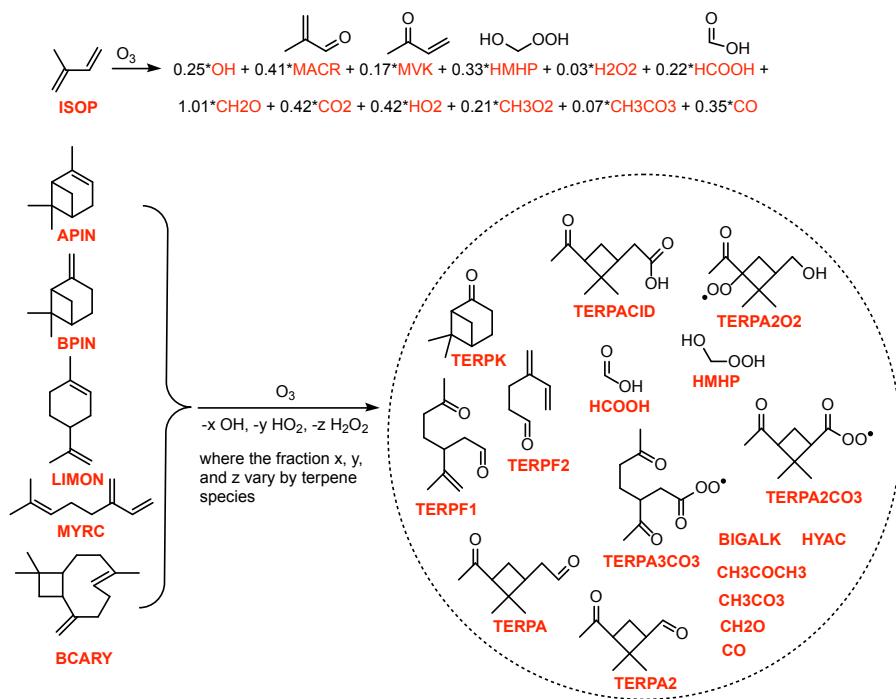
## S1 Schematics of NO<sub>3</sub> oxidation



**Figure S1.** Simplified schematic of the MOZART-TS2 chemical mechanism for isoprene NO<sub>3</sub>-initiated oxidation. Blue compounds undergo aerosol uptake.

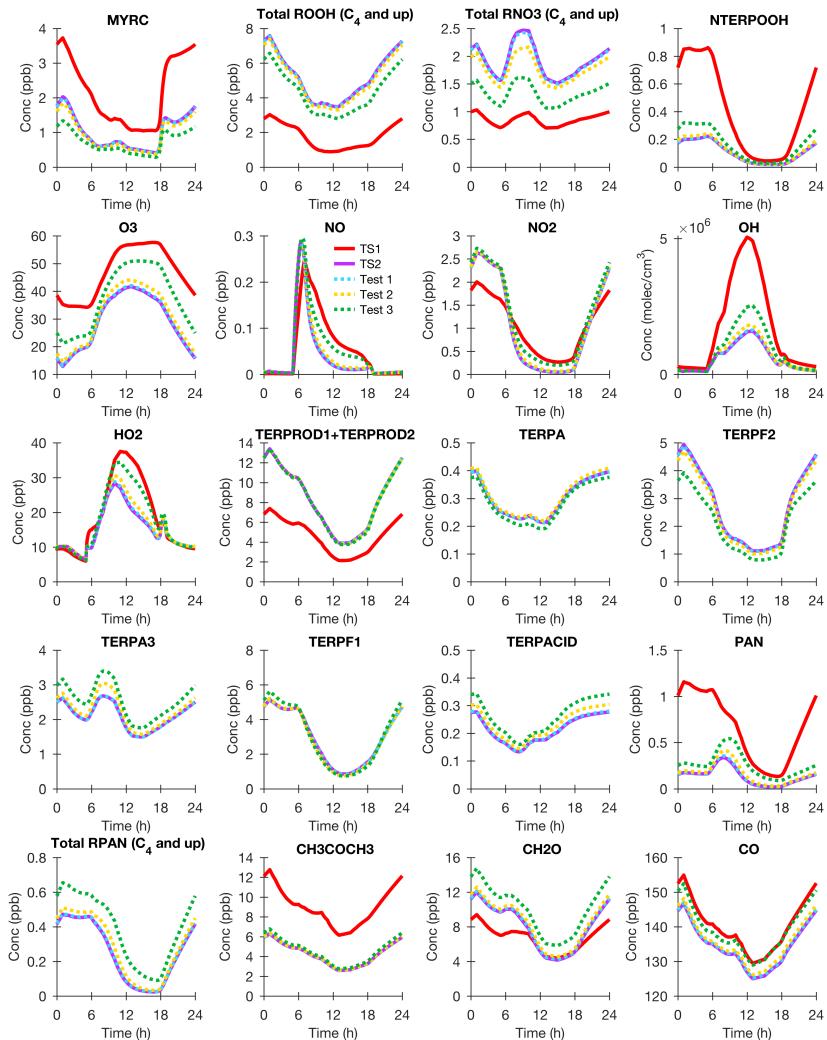


**Figure S2.** Simplified schematic of the MOZART-TS2 chemical mechanism for terpene  $\text{NO}_3$ -initiated oxidation. Blue compounds undergo aerosol uptake.

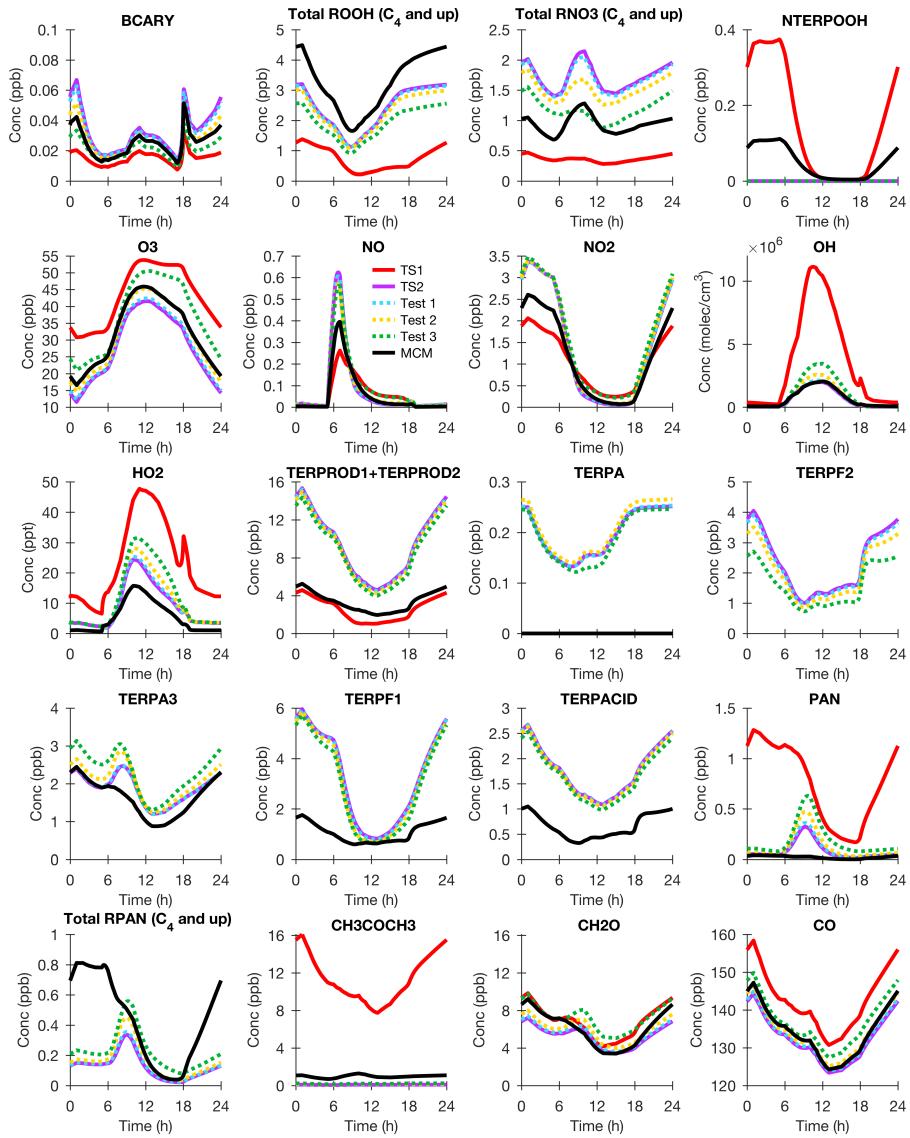


**Figure S3.** Simplified schematic of the MOZART-TS2 chemical mechanism for isoprene and terpene  $\text{O}_3$ -initiated oxidation.

## S2 Evaluation Against More Explicit Chemical Schemes for Myrcene and $\beta$ -caryophyllene



**Figure S4.** BOXMOX results for myrcene (MYRC) oxidation using TS1 (red), TS2 (purple), TS2 with MCM pinonaldehyde nitrate yield - Test 1 (blue), 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 (green). MYRC (myrcene surrogate), TERPOOH (terpene hydroxy hydroperoxide), Total ROOH (all terpene hydroperoxides  $C_4$  and up), TERPNIT (terpene hydroxy nitrate), Total RNO<sub>3</sub> (all terpene derived nitrates  $C_4$  and up), O<sub>3</sub> (ozone), NO (nitrogen oxide), NO<sub>2</sub> (nitrogen dioxide), OH (hydroxyl radical), HO<sub>2</sub> (hydroperoxy radical), CH<sub>3</sub>COCH<sub>3</sub> (acetone), TERPROD1 + TERPROD2 (all terpene 1<sup>st</sup>- and 2<sup>nd</sup>-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).



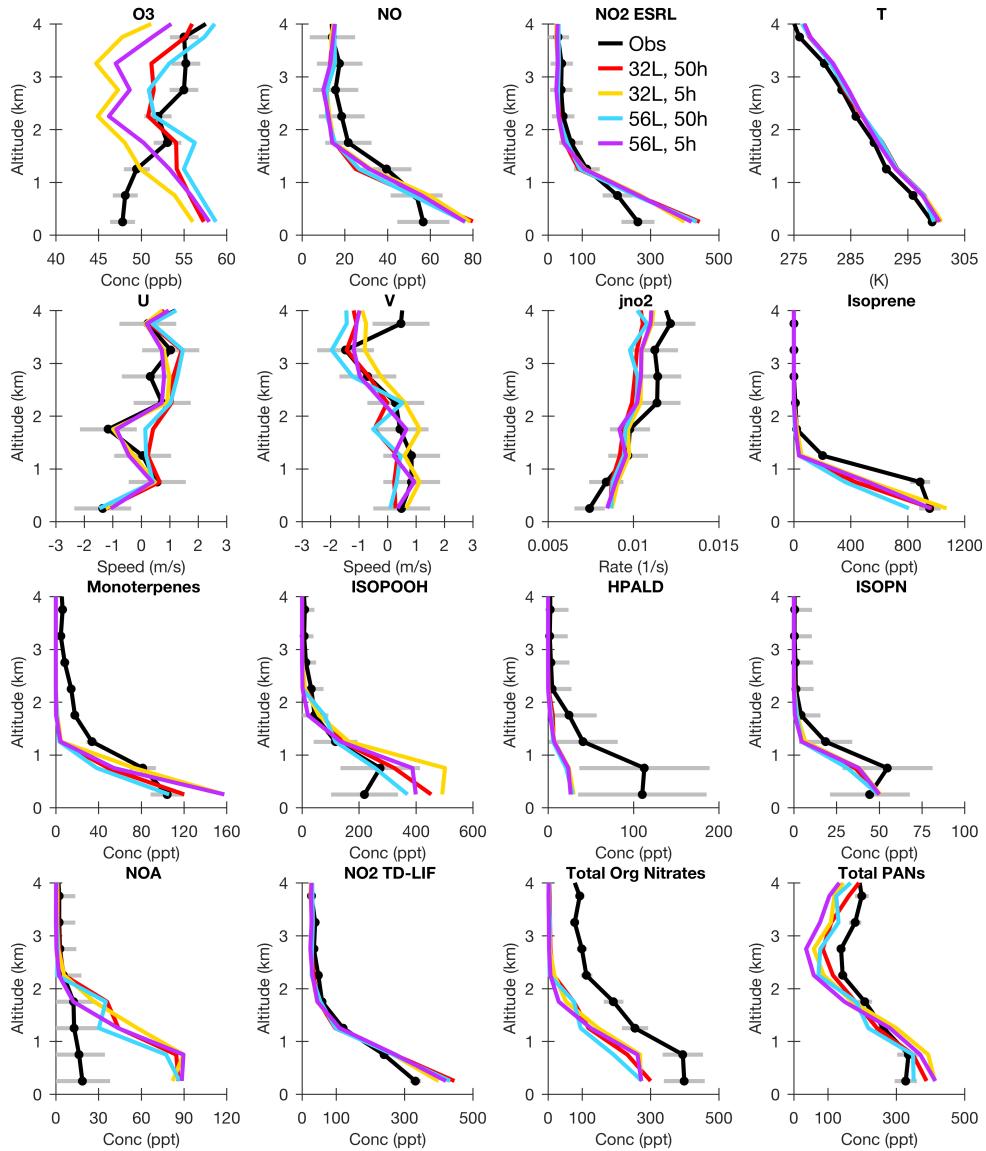
**Figure S5.** BOXMOX results for  $\beta$ -caryophyllene (BCARY) oxidation using TS1 (red), TS2 (purple), MCM (black), TS2 with MCM pinonaldehyde nitrate yield - Test 1 (blue), TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield - Test 2 (gold), and TS2 with MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield and assumptions for oxidation of unsaturated hydroxy nitrates - Test 3 (green). All species are identical to Figure S4.

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

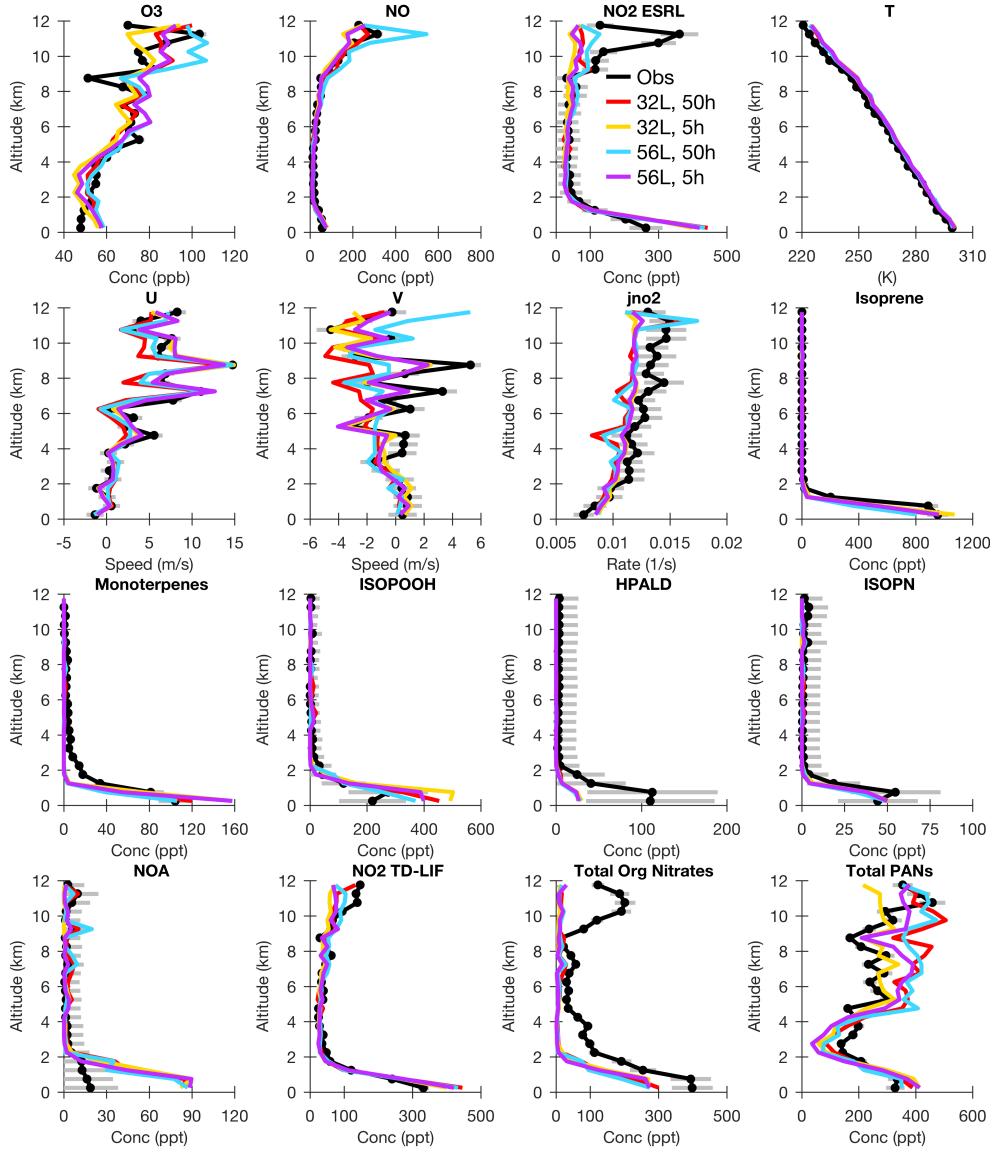
As shown in Figure S6 and S7, nudging at 50 h versus 5 h relaxation times increases the biogenic emissions likely because of increased surface temperatures, improves the representation of winds compared to observations, but also increases biases in the ozone vertical profile. There are some small differences in ozone and other compounds when using 32 levels versus 56 levels.

- 5 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.

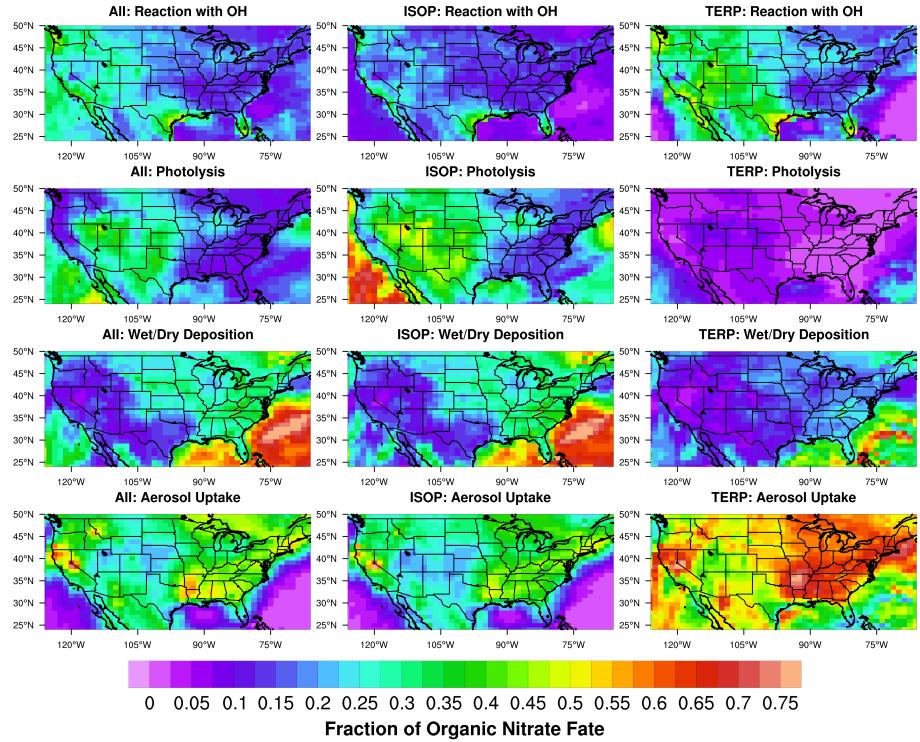


**Figure S6.** Median vertical profile plots up to 4 km over the SEAC<sup>4</sup>Rs flight tracks for observations (black), MOZART-TS1 with 32 vertical levels and 50 h relaxation time (red), MOZART-TS1 with 32 vertical levels and 5 h relaxation time (gold), MOZART-TS1 with 56 vertical levels and 50 h relaxation time (blue), and MOZART-TS1 with 56 vertical levels and 5 h relaxation time (purple). Acronyms are defined in Figure S4. Data are grouped into 0.5 km bins and exclude urban plumes ( $\text{NO}_2 > 4 \text{ ppb}$ ), fire plumes (acetonitrile  $> 0.2 \text{ ppb}$ ), and stratospheric air ( $\text{O}_3/\text{CO} > 1.25$ ) as done in previous work (Travis et al., 2016). Domain includes the Southeast U.S. ( $29.5\text{--}40^\circ\text{N}$ ,  $75\text{--}94.5^\circ\text{W}$ ), and local sun time 9 am to 5 pm. Observational uncertainty is shown in gray bars.



**Figure S7.** Median vertical profile plots over the SEAC<sup>4</sup>Rs flight tracks identical to Figure S6 except up to 12 km altitude instead of 4 km.

#### S4 Organic Nitrate Fate in MOZART-TS1



**Figure S8.** 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<sub>3</sub> to form another organic nitrate is omitted from this calculation.

## S5 Tables Defining Chemical Compounds and Reactions in MOZART-TS2

Table S1: General peroxy ( $\text{RO}_2$ ) and peroxyacetyl ( $\text{RCO}_3$ ) reaction rate constant sources used in MOZART-TS2 for isoprene and terpene chemistry

<b>Reaction</b>	<b>Source of rate constant</b>
$\text{RO}_2 + \text{CH}_3\text{O}_2$	Either isoprene general rate (Jenkin et al., 1998) or geometric mean of $\text{RO}_2 + \text{RO}_2$ and $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2$ from IUPAC (Atkinson et al., 2006)
$\text{RO}_2 + \text{CH}_3\text{CO}_3$	JPL ( $\text{CH}_3\text{O}_2 + \text{CH}_3\text{CO}_3$ ), Burkholder et al. (2015)
$\text{RO}_2 + \text{RCO}_3$	JPL ( $\text{CH}_3\text{O}_2 + \text{CH}_3\text{CO}_3$ ), Burkholder et al. (2015)
$\text{RO}_2 + \text{HO}_2$	Wennberg et al. (2018) parameterization based on n (# of C + O + N - 2 atoms in the peroxy radical)
$\text{RO}_2 + \text{NO}$	MCM v3.3.1, Jenkin et al. (2015)
$\text{RO}_2 + \text{NO}_3$	MCM v3.3.1, Jenkin et al. (2015)
$\text{RCO}_3 + \text{CH}_3\text{CO}_3$	JPL ( $\text{CH}_3\text{CO}_3 + \text{CH}_3\text{CO}_3$ ), Burkholder et al. (2015)
$\text{RCO}_3 + \text{RCO}_3$	JPL ( $\text{CH}_3\text{CO}_3 + \text{CH}_3\text{CO}_3$ ), Burkholder et al. (2015)
$\text{RCO}_3 + \text{CH}_3\text{O}_2$	JPL ( $\text{CH}_3\text{O}_2 + \text{CH}_3\text{CO}_3$ ), Burkholder et al. (2015)
$\text{RCO}_3 + \text{HO}_2$	JPL ( $\text{CH}_3\text{CO}_3 + \text{HO}_2$ ), Burkholder et al. (2015)
$\text{RCO}_3 + \text{NO}$	JPL ( $\text{CH}_3\text{CO}_3 + \text{NO}$ ), Burkholder et al. (2015)
$\text{RCO}_3 + \text{NO}_3$	IUPAC ( $\text{CH}_3\text{CO}_3 + \text{NO}_3$ ), Atkinson et al. (2006)
$\text{RCO}_3 + \text{NO}_2$	JPL ( $\text{CH}_3\text{CO}_3 + \text{NO}_2$ ), 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 <sub>7</sub> H <sub>5</sub> O <sub>3</sub>	acylperoxy radical from benzaldehyde
ALKNIT	C <sub>5</sub> H <sub>11</sub> ONO <sub>2</sub>	standard alkyl nitrate from BIGALK+OH
ALKO2	C <sub>5</sub> H <sub>11</sub> O <sub>2</sub>	lumped alkane peroxy radical from BIGALK
ALKOOH	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	lumped alkane hydroperoxide
AOA_NH	CO	age of air tracer
APIN	C <sub>10</sub> H <sub>16</sub>	$\alpha$ -pinene surrogate monoterpene
APINNO3	C <sub>10</sub> H <sub>16</sub> NO <sub>5</sub>	peroxy radical from NO <sub>3</sub> + $\alpha$ -pinene
APINO2	C <sub>10</sub> H <sub>17</sub> O <sub>3</sub>	peroxy radical from OH + $\alpha$ -pinene reaction
BCARY	C <sub>15</sub> H <sub>24</sub>	$\beta$ -caryophyllene surrogate sesquiterpene
BCARYNO3	C <sub>15</sub> H <sub>24</sub> NO <sub>5</sub>	peroxy radical from NO <sub>3</sub> + sesquiterpenes
BCARYO2	C <sub>15</sub> H <sub>25</sub> O <sub>3</sub>	peroxy radical from OH + sesquiterpenes
BENZENE	C <sub>6</sub> H <sub>6</sub>	benzene
BENZO2	C <sub>6</sub> H <sub>7</sub> O <sub>5</sub>	bicyclic peroxy radical from OH + benzene
BENZOOH	C <sub>6</sub> H <sub>8</sub> O <sub>5</sub>	bicyclic hydroperoxide from OH + benzene
BEPOMUC	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	unsaturated dialdehydic epoxide from OH + benzene
BIGALD1	C <sub>4</sub> H <sub>4</sub> O <sub>2</sub>	butenedial, a product of aromatic oxidation
BIGALD2	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	4-oxy-2-pentenal, a product of aromatic oxidation
BIGALD3	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	2-methyl butenedial, a product of aromatic oxidation
BIGALD4	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	2-methyl-4-oxo-2-pentenal, a product of aromatic oxidation
BIGALD	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	lumped aldehyde from terpene ozonolysis
BIGALK	C <sub>5</sub> H <sub>12</sub>	lumped alkanes C>3
BIGENE	C <sub>4</sub> H <sub>8</sub>	lumped alkenes C>3
BPIN	C <sub>10</sub> H <sub>16</sub>	$\beta$ -pinene
BPINNO3	C <sub>10</sub> H <sub>16</sub> NO <sub>5</sub>	peroxy radical from NO <sub>3</sub> + $\beta$ -pinene
BPINO2	C <sub>10</sub> H <sub>17</sub> O <sub>3</sub>	peroxy radical from OH + $\beta$ -pinene
BR	Br	bromine radical
BRCL	BrCl	bromine monochloride
BRO	BrO	bromine monooxide radical
BRONO2	BrONO <sub>2</sub>	bromine nitrate
BRY	BrY	total reactive bromine
BZALD	C <sub>7</sub> H <sub>6</sub> O	benzaldehyde
BZOO	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	peroxy radical from toluene oxidation
BZOOH	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	hydroperoxide from toluene oxidation
C2H2	C <sub>2</sub> H <sub>2</sub>	ethyne (acetylene)
C2H4	C <sub>2</sub> H <sub>4</sub>	ethene
C2H5O2	C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	ethylperoxy radical
C2H5OH	C <sub>2</sub> H <sub>5</sub> OH	ethanol
C2H5OOH	C <sub>2</sub> H <sub>5</sub> OOH	ethyl hydroperoxide
C2H6	C <sub>2</sub> H <sub>6</sub>	ethane
C3H6	C <sub>3</sub> H <sub>6</sub>	propene
C3H7O2	C <sub>3</sub> H <sub>7</sub> O <sub>2</sub>	propylperoxy radical
C3H7OOH	C <sub>3</sub> H <sub>7</sub> OOH	propyl hydrogen peroxide
C3H8	C <sub>3</sub> H <sub>8</sub>	propane
C6H5O2	C <sub>6</sub> H <sub>5</sub> O <sub>2</sub>	phenylperoxy radical
C6H5OOH	C <sub>6</sub> H <sub>5</sub> OOH	phenyl hydroperoxide
CCL4	CCl <sub>4</sub>	carbon tetrachloride (LBC)
CF2CLBR	CF <sub>2</sub> ClBr	bromochlorodifluoromethane (LBC)
CF3BR	CF <sub>3</sub> Br	Bromotrifluoromethane (LBC)
CFC113	CCl <sub>2</sub> FCClF <sub>2</sub>	1,1,2-trichlorotrifluoroethane (LBC)
CFC114	CClF <sub>2</sub> CClF <sub>2</sub>	1,2-dichlorotetrafluoroethane (LBC)

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
CFC115	CClF <sub>2</sub> CF <sub>3</sub>	chloropentafluoroethane (LBC)
CFC11	CFCl <sub>3</sub>	trichlorofluoromethane (LBC)
CFC12	CF <sub>2</sub> Cl <sub>2</sub>	difluorodichloromethane (LBC)
CH2BR2	CH <sub>2</sub> Br <sub>2</sub>	dibromomethane (LBC)
CH2O	CH <sub>2</sub> O	formaldehyde
CH3BR	CH <sub>3</sub> Br	bromomethane (methyl bromide) (LBC)
CH3CCL3	CH <sub>3</sub> CCl <sub>3</sub>	1,1,1-trichloroethane (methylchloroform) (LBC)
CH3CHO	CH <sub>3</sub> CHO	acetaldehyde
CH3CL	CH <sub>3</sub> Cl	chloromethane (methyl chloride) (LBC)
CH3CN	CH <sub>3</sub> CN	acetonitrile
CH3CO3	CH <sub>3</sub> CO <sub>3</sub>	acetylperoxy radical
CH3COCH3	CH <sub>3</sub> COCH <sub>3</sub>	acetone
CH3COCHO	CH <sub>3</sub> COCHO	methyl glyoxal
CH3COOH	CH <sub>3</sub> COOH	acetic acid
CH3COOOH	CH <sub>3</sub> COOOH	peracetic acid
CH3O2	CH <sub>3</sub> O <sub>2</sub>	methylperoxy radical
CH3OH	CH <sub>3</sub> OH	methanol
CH3OOH	CH <sub>3</sub> OOH	methyl hydroperoxide
CH4	CH <sub>4</sub>	methane (LBC)
CHBR3	CHBr <sub>3</sub>	tribromomethane (bromoform) (LBC)
CL2	Cl <sub>2</sub>	chlorine
CL2O2	Cl <sub>2</sub> O <sub>2</sub>	dichlorine dioxide
CL	Cl	chlorine radical
CLO	CLO	chlorine monoxide radical
CLONO2	ClONO <sub>2</sub>	chlorine nitrate
CLY	Cl <sub>Y</sub>	total reactive chlorine
CO2	CO <sub>2</sub>	carbon dioxide (LBC)
CO	CO	carbon monoxide
COF2	COF <sub>2</sub>	carbonyl fluoride
COFCL	COFCl	carbonyl chloride fluoride
CRESOL	C <sub>7</sub> H <sub>8</sub> O	lumped cresols (hydroxymethylbenzenes)
<b>DHPMPAL</b>	C <sub>4</sub> H <sub>8</sub> O <sub>5</sub>	C4 dihydroperoxy carbonyl derived from isoprene
DICARBO2	C <sub>5</sub> H <sub>5</sub> O <sub>4</sub>	acylperoxy radical formed from aromatic oxidation, via unsaturated dicarbonyl chemistry
DMS	CH <sub>3</sub> SCH <sub>3</sub>	dimethyl sulfide
E90	CO	artificial tracer with 90-day lifetime emitted from surface
ENE02	C <sub>4</sub> H <sub>9</sub> O <sub>3</sub>	lumped hydroxyperoxy radical from OH + large alkenes
EO2	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub>	hydroxyperoxy radical from OH + ethene
EO	HOCH <sub>2</sub> CH <sub>2</sub> O	hydroxyalkoxy radical from OH + ethene
EOOH	HOCH <sub>2</sub> CH <sub>2</sub> OOH	hydroxyhydroperoxide from OH + ethene
F	F	fluorine radical
GLYALD	HOCH <sub>2</sub> CHO	glycolaldehyde
GLYOXAL	C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>	glyoxal
H2402	CBrF <sub>2</sub> CBrF <sub>2</sub>	dibromotetrafluoroethane (LBC)
H2	H <sub>2</sub>	hydrogen (LBC)
H2O2	H <sub>2</sub> O <sub>2</sub>	hydrogen peroxide
H2SO4	H <sub>2</sub> SO <sub>4</sub>	sulfuric acid
H	H	hydrogen radical
HBR	HBr	hydrogen bromide
HCFC141B	CH <sub>3</sub> CCl <sub>2</sub> F	1,1-dichoro-1-fluoroethane (LBC)

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
HCFC142B	CH <sub>3</sub> CClF <sub>2</sub>	1-choro-1,1-difluoroethane (LBC)
HCFC22	CHF <sub>2</sub> Cl	difluorochloromethane (LBC)
HCL	HCl	hydrogen chloride
HCN	HCN	hydrogen cyanide
<b>HCOCH2OOH</b>	C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>	hydroperoxy acetaldehyde
HCOOH	HCOOH	formic acid
HF	HF	hydrogen fluoride
<b>HMHP</b>	CH <sub>4</sub> O <sub>3</sub>	hydroxy methyl hydroperoxide
HNO <sub>3</sub>	HNO <sub>3</sub>	nitric acid
HO <sub>2</sub>	HO <sub>2</sub>	hydroperoxyl radical
HO <sub>2</sub> NO <sub>2</sub>	HO <sub>2</sub> NO <sub>2</sub>	pernitric acid
HOBr	HOBr	hypobromous acid
HOCH <sub>2</sub> OO	HOCH <sub>2</sub> OO	hydroxy-methyl-peroxy radical
HOCl	HOCl	hypochlorous acid
HONITR	C <sub>4</sub> H <sub>9</sub> NO <sub>4</sub>	lumped hydroxynitrates from various compounds
<b>HPALD1</b>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	hydroperoxy aldehyde from ISOPZD1O2
<b>HPALD4</b>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	hydroperoxy aldehyde from ISOPZD4O2
<b>HPALDB1C</b>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	$\beta$ -2-hydroperoxy-1-aldehyde
<b>HPALDB4C</b>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	$\beta$ -3-hydroperoxy-4-aldehyde
HYAC	CH <sub>3</sub> COCH <sub>2</sub> OH	hydroxyacetone
HYDRALD	HOCH <sub>2</sub> CCH <sub>3</sub> CHCHO	lumped unsaturated hydroxycarbonyl
<b>HYPERACET</b>	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	hydroperoxy acetone
<b>ICHE</b>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	C <sub>5</sub> carbonyl hydroxy epoxide
IEPOX	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	isoprene dihydroxy epoxide
<b>IEPOXOO</b>	C <sub>5</sub> H <sub>9</sub> O <sub>5</sub>	peroxy radical from IEPOX + OH
<b>INHEB</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>5</sub>	$\beta$ -isoprene nitrooxy hydroxy epoxide
<b>INHED</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>5</sub>	$\delta$ -isoprene nitrooxy hydroxy epoxide
ISOP	C <sub>5</sub> H <sub>8</sub>	isoprene
<b>ISOPB1O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-1-O <sub>2</sub> -2- $\beta$ -isoprene hydroxy peroxy radical
<b>ISOPB4O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-4-O <sub>2</sub> -3- $\beta$ -isoprene hydroxy peroxy radical
<b>ISOPC1C</b>	C <sub>5</sub> H <sub>9</sub> O	OH-1- <i>cis</i> -isoprene allylic radical
<b>ISOPC1T</b>	C <sub>5</sub> H <sub>9</sub> O	OH-1- <i>trans</i> -isoprene allylic radical
<b>ISOPC4C</b>	C <sub>5</sub> H <sub>9</sub> O	OH-4- <i>cis</i> -isoprene allylic radical
<b>ISOPC4T</b>	C <sub>5</sub> H <sub>9</sub> O	OH-4- <i>trans</i> -isoprene allylic radical
<b>ISOPED1O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-1-O <sub>2</sub> -4-E- $\delta$ -isoprene hydroxy peroxy radical
<b>ISOPED4O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-4-O <sub>2</sub> -1-E- $\delta$ -isoprene hydroxy peroxy radical
<b>ISOPFDN</b>	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>8</sub>	isoprene functionalized dinitrates
<b>ISOPFDNC</b>	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>8</sub>	C <sub>5</sub> carbonyl hydroxy dinitrate
<b>ISOPFNC</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>7</sub>	C <sub>5</sub> carbonyl hydroxy hydroperoxy nitrate
<b>ISOPFNP</b>	C <sub>5</sub> H <sub>11</sub> NO <sub>7</sub>	isoprene highly functionalized nitrates
<b>ISOPHFP</b>	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	isoprene highly functionalized hydroperoxide
<b>ISOPN1D</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$\delta$ -isoprene hydroxy nitrate (nitrooxy in 1 position)
<b>ISOPN1DO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>7</sub>	peroxy radical from ISOPN1D + OH
<b>ISOPN2B</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$\beta$ -isoprene hydroxy nitrate (nitrooxy in 2 position)
<b>ISOPN2BO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>7</sub>	peroxy radical from ISOPN2B + OH
<b>ISOPN3B</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$\beta$ -isoprene hydroxy nitrate (nitrooxy in 3 position)
<b>ISOPN3BO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>7</sub>	peroxy radical from ISOPN3B + OH
<b>ISOPN4D</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$\delta$ -isoprene hydroxy nitrate (nitrooxy in 4 position)
<b>ISOPN4DO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>7</sub>	peroxy radical from ISOPN4D + OH

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
<b>ISOPNBNO3</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$\beta$ -isoprene hydroxy nitrate from isoprene NO <sub>3</sub> oxidation (combined isomers)
<b>ISOPNBNO3O2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>7</sub>	peroxy radical from ISOPNBNO3 + OH
<b>ISOPNO3</b>	CH <sub>2</sub> CHCCH <sub>3</sub> OOCH <sub>2</sub> ONO <sub>2</sub>	peroxy radical from isoprene NO <sub>3</sub> oxidation
<b>ISOPNOOHB</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>5</sub>	$\beta$ -isoprene hydroperoxy nitrate
<b>ISOPNOOHBO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>8</sub>	peroxy radical from ISOPNOOHB + OH
<b>ISOPNOOHD</b>	C <sub>5</sub> H <sub>9</sub> NO <sub>5</sub>	$\delta$ -isoprene hydroperoxy nitrate
<b>ISOPNOOHDO2</b>	C <sub>5</sub> H <sub>10</sub> NO <sub>8</sub>	peroxy radical from ISOPNOOHD + OH
<b>ISOPOH</b>	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	isoprene diol from RO <sub>2</sub> + RO <sub>2</sub> reactions
<b>ISOPOOH</b>	HOCH <sub>2</sub> C(OOH)(CH <sub>3</sub> )CHCH <sub>2</sub>	unsaturated hydroxyhydroperoxide
<b>ISOPZD1O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-1-O <sub>2</sub> -4-Z- $\delta$ -isoprene hydroxy peroxy radical
<b>ISOPZD4O2</b>	C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>	OH-4-O <sub>2</sub> -1-Z- $\delta$ -isoprene hydroxy peroxy radical
<b>IVOC</b>	C <sub>13</sub> H <sub>28</sub>	intermediate volatility organic precursor of VBS SOA
<b>LIMON</b>	C <sub>10</sub> H <sub>16</sub>	limonene
<b>LIMONNO3</b>	C <sub>10</sub> H <sub>16</sub> NO <sub>5</sub>	peroxy radical from NO <sub>3</sub> + limonene
<b>LIMONO2</b>	C <sub>10</sub> H <sub>17</sub> O <sub>3</sub>	peroxy radical from OH + limonene
<b>MACR</b>	CH <sub>2</sub> CCH <sub>3</sub> CHO	methacrolein
<b>MACRN</b>	C <sub>4</sub> H <sub>7</sub> NO <sub>5</sub>	hydroxy nitrate from MACR
<b>MACRO2</b>	CH <sub>3</sub> COCHO <sub>2</sub> CH <sub>2</sub> OH	peroxy radical from methacrolein oxidation
<b>MACROOH</b>	CH <sub>3</sub> COCHOOHCH <sub>2</sub> OH	hydroxyhydroperoxide from methacrolein
<b>MALO2</b>	C <sub>4</sub> H <sub>3</sub> O <sub>4</sub>	acylperoxy radical from OH reaction with BIGALD1
<b>MCO3</b>	CH <sub>2</sub> CCH <sub>3</sub> CO <sub>3</sub>	peroxy radical from OH abstraction reaction with MACR
<b>MDIALO2</b>	C <sub>4</sub> H <sub>5</sub> O <sub>4</sub>	peroxy radical from OH addition to BIGALD1
<b>MEK</b>	C <sub>4</sub> H <sub>8</sub> O	methyl ethyl ketone
<b>MEKO2</b>	C <sub>4</sub> H <sub>7</sub> O <sub>3</sub>	peroxy radical formed from MEK oxidation
<b>MEKOOH</b>	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	hydroperoxide from MEK oxidation
<b>MPAN</b>	CH <sub>2</sub> CCH <sub>3</sub> CO <sub>3</sub> NO <sub>2</sub>	methacryloyl peroxy nitrate
<b>MVK</b>	CH <sub>2</sub> CHCOCH <sub>3</sub>	methyl vinyl ketone
<b>MVKN</b>	C <sub>4</sub> H <sub>7</sub> NO <sub>5</sub>	hydroxy nitrate from MVK
<b>MVKO2</b>	C <sub>4</sub> H <sub>7</sub> O <sub>4</sub>	MVK hydroxy peroxy radical
<b>MVKOOH</b>	C <sub>4</sub> H <sub>8</sub> O <sub>4</sub>	C <sub>4</sub> hydroxy hydroperoxide ketone from MVK
<b>MYRC</b>	C <sub>10</sub> H <sub>16</sub>	myrcene
<b>MYRCNO3</b>	C <sub>10</sub> H <sub>16</sub> NO <sub>5</sub>	peroxy radical from NO <sub>3</sub> + myrcene
<b>MYRCO2</b>	C <sub>10</sub> H <sub>17</sub> O <sub>3</sub>	peroxy radical from OH + myrcene
<b>N2O5</b>	N <sub>2</sub> O <sub>5</sub>	dinitrogen pentoxide
<b>N2O</b>	N <sub>2</sub> O	nitrous oxide (LBC)
<b>N</b>	N	nitrogen radical
<b>NC4CHO</b>	C <sub>5</sub> H <sub>7</sub> NO <sub>4</sub>	nitrooxy-aldehyde from NO <sub>3</sub> + isoprene
<b>NC4CHOO2</b>	C <sub>5</sub> H <sub>8</sub> NO <sub>7</sub>	peroxy radical from NC4CHO + OH
<b>NDEP</b>	N	diagnostic of nitrogen deposition
<b>NH3</b>	NH <sub>3</sub>	ammonia
<b>NH4</b>	NH <sub>4</sub>	ammonium ion aerosol
<b>NHDEP</b>	N	diagnostic of ammonia deposition
<b>NH_50</b>	CO	idealized tracer with 50-day loss rate
<b>NH_5</b>	CO	idealized tracer with 5 day loss rate
<b>NO2</b>	NO <sub>2</sub>	nitrogen dioxide
<b>NO3</b>	NO <sub>3</sub>	nitrate radical
<b>NO3CH2CHO</b>	C <sub>2</sub> H <sub>3</sub> O <sub>4</sub> N	ethanal nitrate
<b>NO</b>	NO	nitric oxide
<b>NOA</b>	CH <sub>3</sub> COCH <sub>2</sub> ONO <sub>2</sub>	nitrooxyacetone (propanone nitrate)

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
O1D	O	excited state atomic oxygen
O3	O <sub>3</sub>	ozone
O	O	ground state atomic oxygen
OCLO	OCLO	chlorine dioxide
OCS	OCS	carbonyl sulfide (LBC)
OH	OH	hydroxyl radical
ONITR	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	lumped hydroxynitrates
PAN	CH <sub>3</sub> CO <sub>3</sub> NO <sub>2</sub>	peroxy acetyl nitrate
PBZNIT	C <sub>7</sub> H <sub>5</sub> NO <sub>5</sub>	peroxy benzoyl nitrate
PHENO2	C <sub>6</sub> H <sub>7</sub> O <sub>6</sub>	bicyclic peroxy radical from phenol
PHENO	C <sub>6</sub> H <sub>5</sub> O	phenoxy radical
PHENOL	C <sub>6</sub> H <sub>5</sub> OH	phenol, product of benzene chemistry
PHENOOH	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	bicyclic hydroperoxide from phenol
PO2	C <sub>3</sub> H <sub>6</sub> (OH)O <sub>2</sub>	propene-derived peroxy radical
POOH	C <sub>3</sub> H <sub>6</sub> (OH)OOH	propene-derived hydroxy hydroperoxide
RO2	CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub>	peroxy radical from acetone
ROOH	CH <sub>3</sub> COCH <sub>2</sub> OOH	acetone hydroperoxide
S	S	sulfur radical
SF6	SF <sub>6</sub>	sulfur hexafluoride (LBC)
SO2	SO <sub>2</sub>	sulfur dioxide
SO3	SO <sub>3</sub>	sulfur trioxide
SO	SO	sulfur monoxide
SOAG0	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA gas-phase precursor VBS bin 0
SOAG1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA gas-phase precursor VBS bin 1
SOAG2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA gas-phase precursor VBS bin 2
SOAG3	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA gas-phase precursor VBS bin 3
SOAG4	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA gas-phase precursor VBS bin 4
<b>SQTN</b>	C <sub>15</sub> H <sub>25</sub> NO <sub>4</sub>	nitrate from sesquiterpene oxidation
ST80_25	CO	stratospheric loss tracer
SVOC	C <sub>22</sub> H <sub>46</sub>	semi-volatile organic precursor of VBS SOA
TEPOMUC	C <sub>7</sub> H <sub>8</sub> O <sub>3</sub>	toluene, xylenes product
<b>TERP1OOH</b>	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>	terpene-derived hydroxy hydroperoxide with 1 double bond
<b>TERP1OOHO2</b>	C <sub>10</sub> H <sub>19</sub> O <sub>6</sub>	peroxy radical from OH + TERP1OOH
<b>TERP2AOOH</b>	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>	terpene-derived hydroxy hydroperoxide with 2 double bonds
<b>TERP2OOHO2</b>	C <sub>10</sub> H <sub>19</sub> O <sub>6</sub>	peroxy radical from OH + TERP2AOOH
<b>TERPA1O2</b>	C <sub>9</sub> H <sub>15</sub> O <sub>3</sub>	TERPA peroxy radical 1st step
<b>TERPA2</b>	C <sub>9</sub> H <sub>14</sub> O <sub>2</sub>	TERPA oxidation product with no double bonds that contains an aldehydic group
<b>TERPA2CO3</b>	C <sub>9</sub> H <sub>13</sub> O <sub>4</sub>	acyl peroxy radical from TERPA2
<b>TERPA2O2</b>	C <sub>9</sub> H <sub>15</sub> O <sub>4</sub>	TERPA peroxy radical 2nd step
<b>TERPA2PAN</b>	C <sub>9</sub> H <sub>13</sub> NO <sub>6</sub>	PAN from TERPA2
<b>TERPA3</b>	C <sub>9</sub> H <sub>14</sub> O <sub>3</sub>	aldehyde terpene product with no ring like limonaldehyde
<b>TERPA3CO3</b>	C <sub>9</sub> H <sub>13</sub> O <sub>5</sub>	acyl peroxy radical from TERPA3
<b>TERPA3O2</b>	C <sub>9</sub> H <sub>15</sub> O <sub>5</sub>	TERPA peroxy radical 3rd step
<b>TERPA3PAN</b>	C <sub>9</sub> H <sub>13</sub> NO <sub>7</sub>	PAN from TERPA3
<b>TERPA4O2</b>	C <sub>6</sub> H <sub>9</sub> O <sub>5</sub>	TERPA peroxy radical 4th step
<b>TERPA</b>	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>	aldehyde terpene product with no double bonds that contains a ring like pinonaldehyde
<b>TERPACID2</b>	C <sub>9</sub> H <sub>14</sub> O <sub>4</sub>	carboxylic acid/peracid from TERPA2
<b>TERPACID3</b>	C <sub>9</sub> H <sub>14</sub> O <sub>5</sub>	carboxylic acid/peracid from TERPA3

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
<b>TERPACID</b>	C <sub>10</sub> H <sub>16</sub> O <sub>4</sub>	carboxylic acid/peracid from TERPA
<b>TERPACO3</b>	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub>	TERPA acyl peroxy radical
<b>TERPAPAN</b>	C <sub>10</sub> H <sub>15</sub> NO <sub>6</sub>	PAN from TERPA
<b>TERPDHDP</b>	C <sub>10</sub> H <sub>20</sub> O <sub>6</sub>	terpene oxidation product, dihydroxy dihydroperoxy
<b>TERPF1</b>	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>	functionalized terpene product with 1 double bond typically containing carbonyl groups
<b>TERPF1O2</b>	C <sub>10</sub> H <sub>17</sub> O <sub>5</sub>	peroxy radical from OH + TERPF1
<b>TERPF2</b>	C <sub>7</sub> H <sub>10</sub> O	functionalized terpene product with 2 double bonds typically containing carbonyl groups
<b>TERPF2O2</b>	C <sub>7</sub> H <sub>11</sub> O <sub>4</sub>	peroxy radical from OH + TERPF2
<b>TERPFDN</b>	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>8</sub>	terpene highly functionalized organic dinitrate
<b>TERPHFN</b>	C <sub>10</sub> H <sub>19</sub> NO <sub>7</sub>	terpene highly functionalized nitrate
<b>TERPK</b>	C <sub>9</sub> H <sub>14</sub> O	terpene product containing a ketone group
<b>TERPNPS1</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>5</sub>	terpene-derived unsaturated secondary or primary hydroperoxy nitrate
<b>TERPNPS1O2</b>	C <sub>10</sub> H <sub>18</sub> NO <sub>8</sub>	peroxy radical from OH + TERPNPS1
<b>TERPNPS</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>5</sub>	terpene-derived saturated secondary or primary hydroperoxy nitrate
<b>TERPNPT1</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>5</sub>	terpene-derived unsaturated tertiary hydroperoxy nitrate
<b>TERPNPT1O2</b>	C <sub>10</sub> H <sub>18</sub> NO <sub>8</sub>	peroxy radical from OH + TERPNPT1
<b>TERPNPT</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>5</sub>	terpene-derived saturated tertiary hydroperoxy nitrate
<b>TERPNS1</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub>	terpene-derived unsaturated secondary or primary nitrate
<b>TERPNS1O2</b>	C <sub>10</sub> H <sub>18</sub> NO <sub>7</sub>	peroxy radical from OH + TERPNS1
<b>TERPNS</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub>	terpene-derived saturated secondary or primary nitrate
<b>TERPNT1</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub>	terpene-derived unsaturated tertiary nitrate
<b>TERPNT1O2</b>	C <sub>10</sub> H <sub>18</sub> NO <sub>7</sub>	peroxy radical from OH + TERPNT1
<b>TERPNT</b>	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub>	terpene-derived saturated tertiary nitrate
<b>TERPOOH</b>	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>	terpene-derived saturated hydroperoxide with ring
<b>TERPOOHL</b>	C <sub>10</sub> H <sub>18</sub> O <sub>5</sub>	terpene-derived saturated hydroperoxide with no ring
<b>TOLO2</b>	C <sub>7</sub> H <sub>9</sub> O <sub>5</sub>	bicyclic peroxy radical from toluene
<b>TOLOOH</b>	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub>	bicyclic hydroperoxide from toluene
<b>TOLUENE</b>	C <sub>7</sub> H <sub>8</sub>	toluene
<b>XYLENES</b>	C <sub>8</sub> H <sub>10</sub>	lumped xylenes
<b>XYLENO2</b>	C <sub>8</sub> H <sub>11</sub> O <sub>5</sub>	bicyclic peroxy radical from OH + XYLENES
<b>XYLENOOH</b>	C <sub>8</sub> H <sub>12</sub> O <sub>5</sub>	bicyclic hydroperoxide from OH+ XYLENES
<b>XYLOL</b>	C <sub>8</sub> H <sub>10</sub> O	dimethyl phenol from xylenes oxidation
<b>XYLOLO2</b>	C <sub>8</sub> H <sub>11</sub> O <sub>6</sub>	bicyclic peroxy radical from OH + XYLOL
<b>XYLOLOOH</b>	C <sub>8</sub> H <sub>12</sub> O <sub>6</sub>	bicyclic hydroperoxide from OH+XYLOL
<b>bc_a1</b>	C	black carbon, MAM accumulation mode
<b>bc_a4</b>	C	black carbon, MAM primary carbon mode
<b>dst_a1</b>	AlSiO <sub>5</sub>	dust, MAM accumulation mode
<b>dst_a2</b>	AlSiO <sub>5</sub>	dust, MAM Aitken mode
<b>dst_a3</b>	AlSiO <sub>5</sub>	dust, MAM coarse mode
<b>ncl_a1</b>	NaCl	sea salt, MAM accumulation mode
<b>ncl_a2</b>	NaCl	sea salt, MAM Aitken mode
<b>ncl_a3</b>	NaCl	sea salt, MAM coarse mode
<b>num_a1</b>	H	aerosol number concentration, MAM accumulation mode
<b>num_a2</b>	H	aerosol number concentration, MAM Aitken mode
<b>num_a3</b>	H	aerosol number concentration, MAM coarse mode
<b>num_a4</b>	H	aerosol number concentration, MAM primary carbon mode
<b>pom_a1</b>	C	primary organic matter, MAM accumulation mode

Table S2: MOZART-TS2 chemical Species

Species name	Chemical Formula	Description
pom_a4	C	primary organic matter, MAM primary carbon mode
so4_a1	NH <sub>4</sub> HSO <sub>4</sub>	sulfate aerosol, MAM accumulation mode
so4_a2	NH <sub>4</sub> HSO <sub>4</sub>	sulfate aerosol, MAM Aitken mode
so4_a3	NH <sub>4</sub> HSO <sub>4</sub>	sulfate aerosol, MAM coarse mode
soa1_a1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 1, MAM accumulation mode
soa1_a2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 1, MAM Aitken mode
soa2_a1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 2, MAM accumulation mode
soa2_a2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 2, MAM Aitken mode
soa3_a1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 3, MAM accumulation mode
soa3_a2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 3, MAM Aitken mode
soa4_a1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 4, MAM accumulation mode
soa4_a2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 4, MAM Aitken mode
soa5_a1	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	SOA bin 5, MAM accumulation mode
soa5_a2	C <sub>15</sub> H <sub>38</sub> O <sub>2</sub>	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. (2020))

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	$\alpha$ -pinene, <b>myrtenal</b>
MTERP	BPIN	3-carene, $\alpha$ -thujene, bornene, $\alpha$ -fenchene, $\beta$ -pinene, sabinene, camphene, <b>4-terpineol, <math>\alpha</math>-terpineol, <math>\alpha</math>-terpinyl acetate</b>
MTERP	LIMON	terpinolene, limonene, $\alpha$ -phellandrene, $\gamma$ -terpinene, $\alpha$ -terpinene, $\beta$ -phellandrene, <b>linalool, <math>\beta</math>-ionone, geranyl acetone, neryl acetone, jasmone, verbenene, ipsenol</b>
MTERP	MYRC	allo-ocimene, myrcene, $t$ - $\beta$ -ocimene, $c$ - $\beta$ -ocimene, <b>dimethyl-nonatriene</b>
BCARY	BCARY	$\alpha$ - <b>farnescene, <math>\beta</math>-caryophyllene, <b>acoradiene, aromadendrene, <math>\alpha</math>-bergamotene, <math>\beta</math>-bergamotene, <math>\alpha</math>-bisabolene, <math>\beta</math>-bisabolene, <math>\beta</math>-bourbonene, <math>\delta</math>-cadinene, <math>\gamma</math>-cadinene, <math>\alpha</math>-cedrene, <math>\alpha</math>-copaene, <math>\alpha</math>-cubebene, <math>\beta</math>-cubebene, <math>\beta</math>-elemene, <math>\beta</math>-farnescene, germacrene B, germacrene D, <math>\beta</math>-gurjunene, <math>\alpha</math>-humulene, <math>\gamma</math>-humulene, isolongifolene, longifolene, longipinene, <math>\alpha</math>-muurolene, <math>\gamma</math>-muurolene, <math>\beta</math>-selinene, <math>\delta</math>-selinene, <math>c</math>-nerolidol, <math>t</math>-nerolidol</b></b>
BIGALK	BIGALK	tricyclene, <b>camphor, fenchone, <math>\alpha</math>-thujone, <math>\beta</math>-thujone, 1,8-cineole, borneol, bornyl acetate, cedrol, decanal, heptanal, heptane, hexane, nonanal, octanal, octanol, oxopentanal, pentane, hexanal, 1-hexanol, pentanal, heptanone</b>
BIGENE	BIGENE	dimethyl styrene, estragole, piperitone, $c$ -linalool oxide, $t$ -linalool oxide, <b>1-dodecene, methyl heptenone, nonenal, 1,3-octenol, 1-tetradecene, butene, diallyl disulfide, methyl propenyl disulfide, methyl jasmonate, <math>c</math>-3-hexenal, <math>t</math>-2-hexenal, <math>c</math>-3-hexenol, <math>c</math>-3-hexenyl acetate</b>
TOLUENE	TOLUENE	toluene, <b>methyl benzoate, phenylacetaldehyde, methyl salicylate, indole, anisole, benzyl acetate, benzyl alcohol, naphthalene</b>
N/A	XYLENES	<i>p</i> -cymene, <i>o</i> -cymene, <b>homosalate, <i>m</i>-cymenene</b>
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	<b>benzaldehyde</b>
N/A	MEK	<b>2-butanone</b>
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 <sup>-1</sup> )	$\Delta H/R$ (K)	$K1_{298}$	$\Delta H1/R$ (K)	$K2_{298}$	$\Delta H2/R$ (K)	$F_0$	Sources
<b>MOZART-TS1 Species</b>								
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), Re- ichl(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)
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)

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

Species	$KH_{298}$ (M atm <sup>-1</sup> )	$\Delta H/R$ (K)	$K1_{298}$	$\Delta H1/R$ (K)	$K2_{298}$	$\Delta H2/R$ (K)	$F_0$	Sources
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), Gold- stein(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
HYRALD	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
MEK	1.80E+01	5740	0	0	0	0	1	JPL(2015)
MEKOHH	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)
PHENOHH	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), Mc- Neil(2012)

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

Species	$KH_{298}$ (M atm <sup>-1</sup> )	$\Delta H/R$ (K)	$K1_{298}$	$\Delta H1/R$ (K)	$K2_{298}$	$\Delta H2/R$ (K)	$F_0$	Sources
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
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)
XYLOOHOH	1.9E+06	5995	0	0	0	0	1	Note B
<b>New MOZART-TS2 Species</b>								
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
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

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

Species	$KH_{298}$ (M atm <sup>-1</sup> )	$\Delta H/R$ (K)	$K1_{298}$	$\Delta H1/R$ (K)	$K2_{298}$	$\Delta H2/R$ (K)	$F_0$	Sources
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
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

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

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

Where:  $K_H = KH_{298} \exp \left( \Delta H/R \left( \frac{1}{T} - \frac{1}{298} \right) \right)$ ,  $K_1 = K1_{298} \exp \left( \Delta H1/R \left( \frac{1}{T} - \frac{1}{298} \right) \right)$ ,

$K_2 = K2_{298} \exp \left( \Delta H2/R \left( \frac{1}{T} - \frac{1}{298} \right) \right)$ , 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
<b>Odd Oxygen</b>		
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
<b>Odd Nitrogen</b>		
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
<b>Organics</b>		
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
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

Table S5: MOZART-TS2 Photolysis Reactions

Reactant	Products	Rate
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
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
ISOPHFNP + hν	→ OH + HO2 + 0.72*CH3COCHO + 0.72*GLYALD + 0.28*GLY-OXAL + 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
MEKO OH + 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

Table S5: MOZART-TS2 Photolysis Reactions

Reactant	Products	Rate
MVKN + h $\nu$	$\rightarrow 0.75*\text{NO}_2 + 0.25*\text{NO}_3\text{CH}_2\text{CHO} + 0.75*\text{CH}_3\text{CO}_3 + 0.5*\text{GLYALD} + 0.5*\text{HO}_2 + 0.25*\text{CH}_2\text{O} + 0.25*\text{CH}_3\text{COCHO}$	1.26*jch2o_a
MVKOOH + h $\nu$	$\rightarrow \text{OH} + 0.56*\text{GLYALD} + 0.56*\text{CH}_3\text{CO}_3 + 0.44*\text{CH}_2\text{O} + 0.44*\text{HO}_2 + 0.44*\text{CH}_3\text{COCHO}$	jch3ooh
NC4CHO + h $\nu$	$\rightarrow \text{NO}_2 + \text{HO}_2 + \text{HYDRALD}$	9.2*jch2o_a
NO3CH2CHO + h $\nu$	$\rightarrow \text{NO}_2 + \text{CH}_2\text{O} + \text{CO} + \text{HO}_2$	4.3*jch2o_a
NOA + h $\nu$	$\rightarrow \text{NO}_2 + \text{CH}_2\text{O} + \text{CH}_3\text{CO}_3$	jch2o_a
ONITR + h $\nu$	$\rightarrow \text{NO}_2$	jch3cho
PAN + h $\nu$	$\rightarrow 0.6*\text{CH}_3\text{CO}_3 + 0.6*\text{NO}_2 + 0.4*\text{CH}_3\text{O}_2 + 0.4*\text{NO}_3 + 0.4*\text{CO}_2$	jpan
PHENOOH + h $\nu$	$\rightarrow \text{OH} + \text{HO}_2 + 0.7*\text{GLYOXAL}$	jch3ooh
POOH + h $\nu$	$\rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{O} + \text{HO}_2 + \text{OH}$	jch3ooh
ROOH + h $\nu$	$\rightarrow \text{CH}_3\text{CO}_3 + \text{CH}_2\text{O} + \text{OH}$	jch3ooh
TEPOMUC + h $\nu$	$\rightarrow 0.5*\text{CH}_3\text{CO}_3 + \text{HO}_2 + 1.5*\text{CO}$	0.10*jno2
TERP1OOH + h $\nu$	$\rightarrow \text{OH} + \text{TERPF1} + \text{HO}_2$	jch3ooh
TERP2AOOH + h $\nu$	$\rightarrow \text{OH} + \text{TERPF2} + \text{HO}_2$	jch3ooh
TERPA + h $\nu$	$\rightarrow \text{CO} + \text{HO}_2 + \text{TERPA1O}_2$	jch3cho
TERPA2 + h $\nu$	$\rightarrow \text{CO} + \text{HO}_2 + \text{TERPA2O}_2$	jch3cho
TERPA2PAN + h $\nu$	$\rightarrow \text{TERPA2CO}_3 + \text{NO}_2$	jpan
TERPA3 + h $\nu$	$\rightarrow \text{CO} + \text{HO}_2 + \text{TERPA4O}_2$	jch3cho
TERPA3PAN + h $\nu$	$\rightarrow \text{TERPA3CO}_3 + \text{NO}_2$	jpan
TERPACID + h $\nu$	$\rightarrow \text{OH} + \text{CO}_2 + \text{TERPA1O}_2$	0.71*jch3ooh
TERPACID2 + h $\nu$	$\rightarrow \text{OH} + \text{CO}_2 + \text{TERPA2O}_2$	0.71*jch3ooh
TERPACID3 + h $\nu$	$\rightarrow \text{OH} + \text{CO}_2 + \text{TERPA4O}_2$	0.71*jch3ooh
TERPAPAN + h $\nu$	$\rightarrow \text{TERPACO}_3 + \text{NO}_2$	jpan
TERPDHDP + h $\nu$	$\rightarrow \text{TERPOOH} + \text{OH} + \text{HO}_2$	2.0*jch3ooh
TERPFDN + h $\nu$	$\rightarrow \text{TERPNS} + \text{HO}_2 + \text{NO}_2$	jch3ooh
TERPHFN + h $\nu$	$\rightarrow \text{TERPNS} + \text{OH} + \text{HO}_2$	jch3ooh
TERPNPS + h $\nu$	$\rightarrow \text{OH} + 0.5*\text{TERPNS} + 0.5*\text{HO}_2 + 0.5*\text{TERPA} + 0.5*\text{NO}_2$	jch3ooh
TERPNPS1 + h $\nu$	$\rightarrow \text{OH} + 0.54*\text{TERPNS1} + 0.54*\text{HO}_2 + 0.46*\text{TERPF1} + 0.46*\text{NO}_2$	jch3ooh
TERPNPT + h $\nu$	$\rightarrow \text{TERPA} + \text{NO}_2 + \text{OH}$	jch3ooh
TERPNPT1 + h $\nu$	$\rightarrow \text{OH} + 0.54*\text{TERPNPT1} + 0.54*\text{HO}_2 + 0.46*\text{TERPF1} + 0.46*\text{NO}_2$	jch3ooh
TERPNS + h $\nu$	$\rightarrow \text{NO}_2 + \text{HO}_2 + \text{TERPA}$	jch3ooh
TERPNS1 + h $\nu$	$\rightarrow \text{NO}_2 + \text{HO}_2 + \text{TERPF1}$	jch3ooh
TERPNPT + h $\nu$	$\rightarrow \text{NO}_2 + \text{HO}_2 + \text{TERPA}$	jch3ooh
TERPNPT1 + h $\nu$	$\rightarrow \text{NO}_2 + \text{HO}_2 + \text{TERPF1}$	jch3ooh
TERPOOH + h $\nu$	$\rightarrow \text{OH} + \text{TERPA} + \text{HO}_2$	jch3ooh
TERPOOHL + h $\nu$	$\rightarrow \text{OH} + \text{TERPA3} + \text{HO}_2$	jch3ooh
TOLOOH + h $\nu$	$\rightarrow \text{OH} + 0.6*\text{GLYOXAL} + 0.4*\text{CH}_3\text{COCHO} + \text{HO}_2 + 0.2*\text{BIGALD1} + 0.2*\text{BIGALD2} + 0.2*\text{BIGALD3}$	jch3ooh
XYLENOOH + h $\nu$	$\rightarrow \text{OH} + \text{HO}_2 + 0.34*\text{GLYOXAL} + 0.54*\text{CH}_3\text{COCHO} + 0.06*\text{BIGALD1} + 0.2*\text{BIGALD2} + 0.15*\text{BIGALD3} + 0.21*\text{BIGALD4}$	jch3ooh
XYLOLOOH + h $\nu$	$\rightarrow \text{OH} + 0.17*\text{GLYOXAL} + 0.51*\text{CH}_3\text{COCHO} + \text{HO}_2$	jch3ooh
<b>Halogens</b>		
BRCL + h $\nu$	$\rightarrow \text{BR} + \text{CL}$	jbrcl
BRO + h $\nu$	$\rightarrow \text{BR} + \text{O}$	jbro
BRONO2 + h $\nu$	$\rightarrow \text{BRO} + \text{NO}_2$	jbrono2_b
BRONO2 + h $\nu$	$\rightarrow \text{BR} + \text{NO}_3$	jbrono2_a
CCL4 + h $\nu$	$\rightarrow 4*\text{CL}$	jccl4
CF2CLBR + h $\nu$	$\rightarrow \text{BR} + \text{CL} + \text{COF2}$	jcf2clbr
CF3BR + h $\nu$	$\rightarrow \text{BR} + \text{F} + \text{COF2}$	jcf3br

Table S5: MOZART-TS2 Photolysis Reactions

Reactant	Products	Rate
CFC11 + hν	→ 2*CL + COFCL	jfccl3
CFC113 + hν	→ 2*CL + COFCL + COF2	jfc113
CFC114 + hν	→ 2*CL + 2*COF2	jfc114
CFC115 + hν	→ CL + F + 2*COF2	jfc115
CFC12 + hν	→ 2*CL + COF2	jfc2cl2
CH2BR2 + hν	→ 2*BR	jch2br2
CH3BR + hν	→ BR + CH3O2	jch3br
CH3CCL3 + hν	→ 3*CL	jch3ccl3
CH3CL + hν	→ CL + CH3O2	jch3cl
CHBR3 + hν	→ 3*BR	jchbr3
CL2 + hν	→ 2*CL	jcl2
CL2O2 + hν	→ 2*CL	jcl2o2
CLO + hν	→ CL + O	jclo
CLONO2 + hν	→ CL + NO3	jclono2_a
CLONO2 + hν	→ CLO + NO2	jclono2_b
COF2 + hν	→ 2*F	jcof2
COFCL + hν	→ F + CL	jcofcl
H2402 + hν	→ 2*BR + 2*COF2	jh2402
HBR + hν	→ BR + H	jhbr
HCFC141B + hν	→ CL + COFCL	jhcfc141b
HCFC142B + hν	→ CL + COF2	jhcfc142b
HCFC22 + hν	→ CL + COF2	jhcfc22
HCL + hν	→ H + CL	jhcl
HF + hν	→ H + F	jhf
HOBR + hν	→ BR + OH	jhobr
HOCL + hν	→ OH + CL	jhocl
OCLO + hν	→ O + CLO	joclo
SF6 + hν	→ sink	jsf6
<b>Sulfur compounds</b>		
H2SO4 + hν	→ SO3 + H2O	jh2so4
OCS + hν	→ S + CO	jocs
SO + hν	→ S + O	jso
SO2 + hν	→ SO + O	js02
SO3 + hν	→ SO2 + O	js03
<b>Secondary organic aerosol tracers</b>		
soa1_a1 + hν	→	0.0004*jno2
soa1_a2 + hν	→	0.0004*jno2
soa2_a1 + hν	→	0.0004*jno2
soa2_a2 + hν	→	0.0004*jno2
soa3_a1 + hν	→	0.0004*jno2
soa3_a2 + hν	→	0.0004*jno2
soa4_a1 + hν	→	0.0004*jno2
soa4_a2 + hν	→	0.0004*jno2
soa5_a1 + hν	→	0.0004*jno2
soa5_a2 + hν	→	0.0004*jno2

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
<b>Odd-Oxygen</b>		
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 ) <sup>2,4</sup>
<b>Odd-Hydrogen</b>		
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 ))
<b>Odd-Nitrogen</b>		
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 )
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 )

Table S6: MOZART-TS2 Kinetic Reactions

<b>Reactant</b>	<b>Products</b>	<b>Rate</b>
NO + O + M	→ NO2 + M	TROEE(9.00e-32, 3.000000e-11, 0.00, 0.60) 1.50,
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, 4.000000e-12, 0.30, 0.60) 3.40,
NO2 + NO3 + M	→ N2O5 + M	TROEE(2.40e-30, 1.600000e-12, -0.10, 0.60) 3.00,
NO2 + OH + M	→ HNO3 + M	TROEE(1.80e-30, 2.800000e-11, 0.00, 0.60) 3.00,
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 )
<b>Odd-Chlorine</b>		
CL + CH2O	→ HCL + HO2 + CO	8.10e-11 exp( -30.00 / t )
CL + CH4	→ CH3O2 + HCL	7.10e-12 exp( -1270.00 / t )
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 )
CLONO2 + NO2 + M	→ CLONO2 + M	TROEE(1.80e-31, 1.500000e-11, 1.90, 0.60) 3.40,
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

Table S6: MOZART-TS2 Kinetic Reactions

<b>Reactant</b>	<b>Products</b>	<b>Rate</b>
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) usr_CL2O2_M
CL2O2 + M	→ CLO + CLO + M	
<b>Odd-Bromine</b>		
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
<b>Odd-Fluorine</b>		
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
<b>Organic Halogens</b>		
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 )
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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
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
<b>C1 Organics</b>		
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
<b>HMHP + OH</b>	→ <b>0.5*CH2O + 0.5*HO2 + 0.5*HCOOH + 0.5*OH + H2O</b>	<b>1.30e-12 exp( 500.00 / t )</b>
HOCH2OO + HO2	→ <b>0.5*HMHP + 0.5*HCOOH + 0.3*H2O + 0.2*HO2 + 0.2*OH</b>	<b>5.60e-15 exp( 2300.00 / t )</b>
HOCH2OO	→ CH2O + HO2	2.40e+12 exp( -7000.00 / t )
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 ) <sup>6.1</sup> , k = (k0/(1+k0/(ki/M))) * (0.6^(1/(1+(log(k0/(ki/M))^2))))
<b>C2 Organics</b>		
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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
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	→ <b>0.36*CH3COOOH + 0.15*CH3COOH + 0.15*O3 + 0.49*OH + 0.49*CH3O2 + 0.49*CO2</b>	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
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
<b>HCOCH2OOH + OH</b>	→ <b>0.89*GLYOXAL + 0.89*OH + 0.11*CH2O + 0.11*HO2 + 0.11*CO</b>	<b>3.300e-11</b>
<b>NO3CH2CHO + OH</b>	→ <b>CO2 + CH2O + NO2</b>	<b>3.400e-12</b>
PAN + OH	→ CH2O + NO3	4.000e-14
C2H4 + OH + M	→ EO2 + M	TROEE(8.60e-29, 9.000000e-12, 0.85, 0.48)
CH3CO3 + NO2 + M	→ PAN + M	TROEE(9.70e-29, 9.300000e-12, 1.50, 0.60)
PAN + M	→ CH3CO3 + NO2 + M	k(CH3CO3+NO2+M) * 1.111e28 exp( -14000 / t )
<b>C3 Organics</b>		
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
<b>HYPERACET + OH</b>	→ <b>0.3*CH3CO3 + 0.3*CH2O + 0.7*CH3COCHO + 0.7*OH</b>	<b>1.200e-11</b>
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 )
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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
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
<b>C4 Organics</b>		
BIGENE + NO3	→ NO2 + CH3CHO + 0.5*CH2O + 0.5*CH3COCH3	3.500e-13
BIGENE + OH	→ ENEO2	5.400e-11
DHPMPAL + OH	→ HYPERACET + CO + OH	<b>3.770e-11</b>
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	<b>1.290e-11</b>
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	<b>2.90e+7 exp( -5297.00 / t )</b>
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	<b>3.770e-11</b>
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 )
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 )
MEKOHH + 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	<b>1.780e-12</b>
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

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
MVKO2 + HO2	$\rightarrow 0.46*\text{MVKOOH} + 0.54*\text{OH} + 0.36*\text{GLYALD} + 0.49*\text{CH}_3\text{CO}_3 + 0.26*\text{CO} + 0.18*\text{HO}_2 + 0.05*\text{CH}_3\text{COCHO} + 0.05*\text{CH}_2\text{O}$	$2.11\text{e-13 exp}(1300.00 / t)$
MVK + O3	$\rightarrow 0.6*\text{CH}_2\text{O} + 0.56*\text{CO} + 0.1*\text{CH}_3\text{CHO} + 0.1*\text{CO}_2 + 0.28*\text{CH}_3\text{CO}_3 + 0.5*\text{CH}_3\text{COCHO} + 0.28*\text{HO}_2 + 0.36*\text{OH} + 0.12*\text{HCOOH}$	$8.50\text{e-16 exp}(-1520.00 / t)$
MVK + OH	$\rightarrow \text{MVKO2}$	$2.70\text{e-12 exp}(580.00 / t)$
MVKOOH + OH	$\rightarrow 1.56*\text{CO} + 0.44*\text{HO}_2 + 0.44*\text{CH}_3\text{COCHO} + 0.56*\text{CH}_3\text{CO}_3$	$4.800\text{e-11}$
MCO3 + NO2 + M	$\rightarrow \text{MPAN} + \text{M}$	TROEE(9.70e-29, 5.60, 9.300000e-12, 1.50, 0.60)
MPAN + M	$\rightarrow \text{MCO3} + \text{NO2} + \text{M}$	$k(\text{MCO3+NO2+M}) * 1.111\text{e}28 \exp(-14000 / t)$
<b>C5 Organics</b>		
ALKNIT + OH	$\rightarrow 0.4*\text{CH}_2\text{O} + 0.8*\text{CH}_3\text{CHO} + 0.8*\text{CH}_3\text{COCH}_3 + \text{NO}_2$	$1.600\text{e-12}$
ALKO2 + HO2	$\rightarrow \text{ALKOOH}$	$7.50\text{e-13 exp}(700.00 / t)$
ALKO2 + NO	$\rightarrow 0.4*\text{CH}_3\text{CHO} + 0.1*\text{CH}_2\text{O} + 0.25*\text{CH}_3\text{COCH}_3 + \text{HO}_2 + 0.8*\text{MEK} + \text{NO}_2$	$6.700\text{e-12}$
ALKO2 + NO	$\rightarrow \text{ALKNIT}$	$5.40\text{e-14 exp}(870.00 / t)$
ALKOOH + OH	$\rightarrow \text{ALKO2}$	$3.80\text{e-12 exp}(200.00 / t)$
BIGALK + OH	$\rightarrow \text{ALKO2}$	$3.500\text{e-12}$
HPALD1 + OH	$\rightarrow 0.51*\text{HO}_2 + 1.06*\text{CO} + 0.38*\text{CH}_3\text{COCHO} + 0.54*\text{CO}_2 + 0.06*\text{CH}_3\text{O}_2 + 0.06*\text{CH}_3\text{CO}_3 + 0.08*\text{ICHE} + 0.07*\text{DH-PMPAL} + 0.43*\text{OH} + 0.35*\text{MVK}$	$1.17\text{e-11 exp}(450.00 / t)$
HPALD4 + OH	$\rightarrow 0.41*\text{HO}_2 + 0.76*\text{CO} + 0.03*\text{CH}_3\text{COCHO} + 0.54*\text{CO}_2 + 0.06*\text{CH}_3\text{O}_2 + 0.06*\text{CH}_3\text{CO}_3 + 0.15*\text{HYPERACET} + 0.18*\text{ICHE} + 0.17*\text{DHPMPAL} + 0.35*\text{MACR} + 0.53*\text{OH}$	$1.17\text{e-11 exp}(450.00 / t)$
HPALDB1C + OH	$\rightarrow 0.58*\text{ICHE} + \text{OH} + 0.42*\text{CO} + 0.23*\text{MVK} + 0.19*\text{MVKOOH}$	$2.20\text{e-11 exp}(390.00 / t)$
HPALDB4C + OH	$\rightarrow 0.77*\text{ICHE} + \text{OH} + 0.23*\text{CO} + 0.14*\text{MACR} + 0.09*\text{MACROOH}$	$3.50\text{e-11 exp}(390.00 / t)$
HYDRALD + OH	$\rightarrow 1.08*\text{OH} + \text{CO} + 0.36*\text{CO}_2 + 0.46*\text{CH}_3\text{COCHO} + 0.32*\text{IEPOXOO} + 0.22*\text{HYAC} + 0.32*\text{HO}_2$	$6.420\text{e-11}$
ICHE + OH	$\rightarrow \text{OH} + 1.5*\text{CO} + 0.5*\text{HYAC} + 0.5*\text{CH}_3\text{COCHO} + 0.5*\text{CH}_2\text{O}$	$9.85\text{e-12 exp}(410.00 / t)$
IEPOX + OH	$\rightarrow 0.19*\text{ICHE} + 0.19*\text{HO}_2 + 0.81*\text{IEPOXOO}$	$4.43\text{e-11 exp}(-400.00 / t)$
IEPOXOO + HO2	$\rightarrow 0.35*\text{ISOPHFP} + 0.65*\text{OH} + 0.65*\text{HO}_2 + 0.26*\text{CO} + 0.37*\text{GLYALD} + 0.46*\text{CH}_3\text{COCHO} + 0.15*\text{GLYOXAL} + 0.19*\text{HYAC}$	$2.38\text{e-13 exp}(1300.00 / t)$
INHEB + OH	$\rightarrow 0.2*\text{INHEB} + 0.4*\text{NC4CHOO}_2 + 0.4*\text{CH}_3\text{COCHO} + 0.4*\text{HCOOH} + 0.4*\text{CH}_2\text{O} + 0.4*\text{NO}_2$	$4.43\text{e-11 exp}(-400.00 / t)$
INHED + OH	$\rightarrow 0.35*\text{NOA} + 0.35*\text{CO} + 0.4*\text{HO}_2 + 0.59*\text{CH}_2\text{O} + 0.35*\text{NC4CHOO}_2 + 0.06*\text{INHED} + 0.19*\text{HYAC} + 0.19*\text{CO}_2 + 0.19*\text{NO}_2 + 0.05*\text{MVKN}$	$3.22\text{e-11 exp}(-400.00 / t)$
ISOPB1O2 + CH3CO3	$\rightarrow \text{MVK} + \text{CH}_2\text{O} + \text{HO}_2 + \text{CO}_2 + \text{CH}_3\text{O}_2$	$2.00\text{e-12 exp}(500.00 / t)$
ISOPB1O2 + CH3O2	$\rightarrow 1.75*\text{CH}_2\text{O} + 0.25*\text{ISOPOH} + 0.75*\text{MVK} + 1.5*\text{HO}_2$	$1.600\text{e-13}$
ISOPB1O2 + HO2	$\rightarrow 0.06*\text{MVK} + 0.06*\text{CH}_2\text{O} + 0.06*\text{OH} + 0.06*\text{HO}_2 + 0.94*\text{ISOPOOH}$	$2.12\text{e-13 exp}(1300.00 / t)$
ISOPB1O2	$\rightarrow \text{MVK} + \text{CH}_2\text{O} + \text{OH}$	$1.04\text{e}11 \exp(-9746.00 / t)$

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
ISOPB1O2	→	ISOPC1C + O2	2.24e+15 exp( -10865.00 / t )
ISOPB1O2	→	ISOPC1T + O2	2.22e+15 exp( -10355.00 / t )
ISOPB4O2	+	MACR + CH2O + HO2 + CO2 + CH3O2	2.00e-12 exp( 500.00 / t )
CH3CO3			
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*ISOOPOH	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	+	0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MVKOOH + CO2 + CH3O2	2.00e-12 exp( 500.00 / t )
CH3CO3			
ISOPED1O2	+	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	→	ISOOPOH	2.12e-13 exp( 1300.00 / t )
ISOPED1O2	→	ISOPC1T + O2	1.83e+14 exp( -8930.00 / t )
ISOPED4O2	+	0.45*HO2 + 0.45*HYDRALD + 0.55*CO + 0.55*OH + 0.55*MACROOH + CO2 + CH3O2	2.00e-12 exp( 500.00 / t )
CH3CO3			
ISOPED4O2	+	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	→	ISOOPOH	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
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
ISOPHFNP + 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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
ISOPN2B + OH	→ 0.15*IEPOX + 0.15*NO2 + 0.85*ISOPN2BO2	3.000e-11
ISOPN3BO2 + HO2	→ 0.4*ISOPFNP + 0.6*OH + 0.6*MVK + 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*MVK + 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*MVK + 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*MVK + 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 )
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 +	+ → 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
ISOPNOOHB02 + HO2	+ → 0.49*ISOPFNP + 0.85*OH + 0.17*CH2O + 0.17*HO2 + 0.15*MACRN + 0.02*MVK + 0.28*NOA + 0.28*GLYALD + 0.06*HYAC + 0.06*NO3CH2CHO	2.64e-13 exp( 1300.00 / t )
ISOPNOOHB02	→ 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*ISOPNOOHB02	3.900e-11
ISOPNOOHD02 + HO2	+ → 0.17*ISOPFNP + 0.86*OH + 0.03*CH2O + 0.02*MACRN + 0.01*MVK + 0.68*NOA + 0.68*HCOCH2OOH + 0.12*HYPERACET + 0.12*NO3CH2CHO + 0.8*HO2	2.64e-13 exp( 1300.00 / t )
ISOPNOOHD02	→ 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*INHEB + 0.07*IEPOX + 0.07*NO2 + 0.57*ISOPNOOHD02	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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
ISOP + OH	$\rightarrow 0.315*\text{ISOPC1T} + 0.315*\text{ISOPC1C} + 0.111*\text{ISOPC4T} + 0.259*\text{ISOPC4C}$	2.70e-11 exp( 390.00 / t )
ISOPOH + OH	$\rightarrow \text{HYAC} + \text{GLYALD} + \text{HO2}$	3.850e-11
ISOPOOH + OH	$\rightarrow 0.53*\text{ISOPB1O2} + 0.16*\text{ISOPB4O2} + 0.13*\text{HYDRALD} + 0.13*\text{OH} + 0.09*\text{HPALDB1C} + 0.09*\text{HPALDB4C} + 0.18*\text{HO2}$	5.53e-12 exp( 200.00 / t )
ISOPOOH + OH	$\rightarrow 0.85*\text{IEPOX} + 0.92*\text{OH} + 0.07*\text{GLYALD} + 0.07*\text{HYAC} + 0.08*\text{ISOPHFP}$	2.08e-11 exp( 390.00 / t )
ISOPZD1O2 CH3CO3	$\rightarrow 0.45*\text{HO2} + 0.45*\text{HYDRALD} + 0.55*\text{CO} + 0.55*\text{OH} + 0.55*\text{MVKOOH} + \text{CO2} + \text{CH3O2}$	2.00e-12 exp( 500.00 / t )
ISOPZD1O2 CH3O2	$\rightarrow 0.25*\text{CH3OH} + 0.25*\text{ISOPOH} + 0.75*\text{CH2O} + 0.72*\text{HO2} + 0.28*\text{CO} + 0.28*\text{OH} + 0.28*\text{MVKOOH} + 0.47*\text{HYDRALD}$	1.200e-12
ISOPZD1O2 + HO2	$\rightarrow \text{ISOPOOH}$	2.12e-13 exp( 1300.00 / t )
ISOPZD1O2	$\rightarrow \text{ISOPC1C} + \text{O2}$	1.79e+14 exp( -8830.00 / t )
ISOPZD4O2 CH3CO3	$\rightarrow 0.45*\text{HO2} + 0.45*\text{HYDRALD} + 0.55*\text{CO} + 0.55*\text{OH} + 0.55*\text{MACROOH} + \text{CO2} + \text{CH3O2}$	2.00e-12 exp( 500.00 / t )
ISOPZD4O2 CH3O2	$\rightarrow 0.25*\text{CH3OH} + 0.25*\text{ISOPOH} + 0.75*\text{CH2O} + 0.72*\text{HO2} + 0.28*\text{CO} + 0.28*\text{OH} + 0.28*\text{MACROOH} + 0.47*\text{HYDRALD}$	9.800e-13
ISOPZD4O2 + HO2	$\rightarrow \text{ISOPOOH}$	2.12e-13 exp( 1300.00 / t )
ISOPZD4O2	$\rightarrow \text{ISOPC4C} + \text{O2}$	1.75e+14 exp( -9054.00 / t )
NC4CHOO2 + HO2	$\rightarrow 0.2*\text{ISOPFNP} + 0.8*\text{OH} + 0.8*\text{HO2} + 0.1*\text{NOA} + 0.1*\text{GLYOXAL} + 0.1*\text{CH3COCHO} + 0.1*\text{NO3CH2CHO} + 0.29*\text{MACRN} + 0.31*\text{MVKN} + 0.6*\text{CO}$	2.60e-13 exp( 1300.00 / t )
NC4CHOO2	$\rightarrow 0.51*\text{MACRN} + 0.49*\text{MVKN} + \text{CO} + \text{OH}$	1.00e+7 exp( -5000.00 / t )
NC4CHO + O3	$\rightarrow 0.66*\text{H2O2} + 0.66*\text{GLYOXAL} + 0.34*\text{CH3COCHO} + 0.61*\text{NOA} + 0.22*\text{NO3CH2CHO} + 0.34*\text{OH} + 0.17*\text{NO2} + 0.3*\text{CO} + 0.13*\text{HO2} + 0.04*\text{CH3CO3}$	4.400e-18
NC4CHO + OH	$\rightarrow 0.45*\text{CO2} + 0.1*\text{CH3CO3} + 0.1*\text{NO3CH2CHO} + 0.35*\text{NOA} + 0.04*\text{NO2} + 0.04*\text{ICHE} + 0.24*\text{MACRN} + 0.04*\text{MVKN} + 0.63*\text{CO} + 0.63*\text{HO2} + 0.23*\text{NC4CHOO2}$	3.600e-11
IEPOXOO + NO	$\rightarrow \text{NO2} + \text{HO2} + 0.57*\text{GLYALD} + 0.71*\text{CH3COCHO} + 0.4*\text{CO} + 0.23*\text{GLYOXAL} + 0.29*\text{HYAC}$	see notes <sup>a</sup> : $\alpha = 0.025$ , n = 8
IEPOXOO + NO	$\rightarrow \text{ISOPFNC}$	see notes <sup>a</sup> : $\alpha = 0.025$ , n = 8
ISOPB1O2 + NO	$\rightarrow \text{NO2} + \text{MVK} + \text{CH2O} + \text{HO2}$	see notes <sup>a</sup> : $\alpha = 0.14$ , n = 6
ISOPB1O2 + NO	$\rightarrow \text{ISOPN2B}$	see notes <sup>a</sup> : $\alpha = 0.14$ , n = 6
ISOPB4O2 + NO	$\rightarrow \text{NO2} + \text{MACR} + \text{CH2O} + \text{HO2}$	see notes <sup>a</sup> : $\alpha = 0.13$ , n = 6
ISOPB4O2 + NO	$\rightarrow \text{ISOPN3B}$	see notes <sup>a</sup> : $\alpha = 0.13$ , n = 6
ISOPED1O2 + NO	$\rightarrow \text{NO2} + 0.45*\text{HYDRALD} + 0.45*\text{HO2} + 0.55*\text{MVKOOH} + 0.55*\text{CO} + 0.55*\text{OH}$	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPED1O2 + NO	$\rightarrow \text{ISOPN4D}$	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPED4O2 + NO	$\rightarrow \text{NO2} + 0.45*\text{HYDRALD} + 0.45*\text{HO2} + 0.55*\text{MACROOH} + 0.55*\text{CO} + 0.55*\text{OH}$	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPED4O2 + NO	$\rightarrow \text{ISOPN1D}$	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPN1DO2 + NO	$\rightarrow \text{NO2} + \text{HO2} + 0.94*\text{NOA} + 0.94*\text{GLYALD} + 0.06*\text{MACRN} + 0.06*\text{CH2O}$	see notes <sup>a</sup> : $\alpha = 0.084$ , n = 11
ISOPN1DO2 + NO	$\rightarrow \text{ISOPFDN}$	see notes <sup>a</sup> : $\alpha = 0.084$ , n = 11
ISOPN2BO2 + NO	$\rightarrow 1.73*\text{NO2} + 0.27*\text{MACRN} + 0.27*\text{CH2O} + 0.27*\text{HO2} + 0.73*\text{HYAC} + 0.73*\text{GLYALD}$	see notes <sup>a</sup> : $\alpha = 0.065$ , n = 11

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
ISOPN2BO2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.065$ , n = 11
ISOPN3BO2 + NO	→ NO2 + MVKN + CH2O + HO2	see notes <sup>a</sup> : $\alpha = 0.053$ , n = 11
ISOPN3BO2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.053$ , n = 11
ISOPN4DO2 + NO	→ NO2 + HO2 + 0.13*MVKN + 0.13*CH2O + 0.87*HYAC + 0.87*NO3CH2CHO	see notes <sup>a</sup> : $\alpha = 0.165$ , n = 11
ISOPN4DO2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.165$ , 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	see notes <sup>a</sup> : $\alpha = 0.203$ , n = 11
ISOPNBNO3O2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.203$ , n = 11
ISOPNO3 + NO	→ 1.46*NO2 + 0.46*CH2O + 0.54*NC4CHO + 0.54*HO2 + 0.42*MVK + 0.04*MACR	see notes <sup>a</sup> : $\alpha = 0.135$ , n = 9
ISOPNO3 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.135$ , 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	see notes <sup>a</sup> : $\alpha = 0.141$ , n = 12
ISOPNOOHBO2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.141$ , 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	see notes <sup>a</sup> : $\alpha = 0.045$ , n = 12
ISOPNOOHDO2 + NO	→ ISOPFDN	see notes <sup>a</sup> : $\alpha = 0.045$ , n = 12
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 <sup>3</sup> )
ISOPZD1O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPZD1O2 + NO	→ ISOPN4D	see notes <sup>a</sup> : $\alpha = 0.12$ , 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 <sup>3</sup> )
ISOPZD4O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
ISOPZD4O2 + NO	→ ISOPN1D	see notes <sup>a</sup> : $\alpha = 0.12$ , n = 6
MACRO2 + NO	→ NO2 + HO2 + 0.86*HYAC + 0.86*CO + 0.14*CH2O + 0.14*CH3COCHO	see notes <sup>a</sup> : $\alpha = 0.06$ , n = 6
MACRO2 + NO	→ MACRN	see notes <sup>a</sup> : $\alpha = 0.06$ , n = 6
MVKO2 + NO	→ NO2 + 0.24*HO2 + 0.24*CH2O + 0.76*CH3CO3 + 0.76*GLYALD + 0.24*CH3COCHO	see notes <sup>a</sup> : $\alpha = 0.04$ , n = 6
MVKO2 + NO	→ MVKN	see notes <sup>a</sup> : $\alpha = 0.04$ , n = 6
NC4CHO02 + NO	→ NO2 + HO2 + 0.13*NOA + 0.13*GLYOXAL + 0.12*CH3COCHO + 0.12*NO3CH2CHO + 0.39*MACRN + 0.36*MVKN + 0.75*CO	see notes <sup>a</sup> : $\alpha = 0.021$ , n = 11
NC4CHO02 + NO	→ ISOPFDNC	see notes <sup>a</sup> : $\alpha = 0.021$ , n = 11
<b>C7 Organics</b>		
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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
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 )
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, 9.300000e-12, 1.50, 0.60) 5.60,
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, 9.300000e-12, 1.50, 0.60) 5.60,
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, 9.300000e-12, 1.50, 0.60) 5.60,
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, 9.300000e-12, 1.50, 0.60) 5.60,
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 )
XYLEMES + OH	→ 0.15*XYLOL + 0.23*TEPOMUC + 0.06*BZOO + 0.56*XYLENO2 + 0.38*HO2	1.700e-11
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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
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 + AP-	→	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 +	→	NO2 + TERPA + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
APINNO3 +	→	NO2 + TERPA + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
APINNO3 + TER-	→	NO2 + TERPA + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
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 )
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 +	→	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 )
TERPA2CO3			
APINO2 +	→	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 )
TERPA3CO3			
APINO2 + TER-	→	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 )
PACO3			
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 +	→	0.36*SQTN + 1.64*NO2 + 1.64*TERPF2	5.300e-13
BCARYNO3			

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
BCARYNO3	+	→ CH3O2 + CO2 + NO2 + TERPF2	2.00e-12 exp( 500.00 / t )
CH3CO3			
BCARYNO3	+	→ 0.18*SQTN + 0.95*CH2O + 0.82*TERPF2 + 0.82*NO2 + 0.82*HO2 + 0.05*CH3OH	2.000e-12
CH3O2			
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	+	→ TERPA2O2 + CO2 + NO2 + TERPF2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
BCARYNO3	+	→ TERPA4O2 + CO2 + NO2 + TERPF2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
BCARYNO3 + TER-	→	TERPA1O2 + CO2 + NO2 + TERPF2	2.00e-12 exp( 500.00 / t )
PACO3			
BCARYO2	+	→ TERPF2 + HO2 + CH3O2 + CO2	2.00e-12 exp( 500.00 / t )
CH3CO3			
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	+	→ TERPF2 + HO2 + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
BCARYO2	+	→ TERPF2 + HO2 + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
BCARYO2 + TER-	→	TERPF2 + HO2 + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
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	+	→ 0.94*NO2 + 0.92*TERPNS + 0.9*TERPA3 + 0.04*TERPK + 0.04*CH2O + 0.14*TERPNPT + 0.94*HO2	5.300e-13
BPINNO3	→	CH3O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNPT + 0.5*HO2	2.00e-12 exp( 500.00 / t )
BPINNO3 + CH3CO3	→	0.56*TERPNS + 0.08*TERPNPT + 0.02*TERPK + 0.34*TERPA3 + 0.36*NO2 + 1.1*HO2 + 0.99*CH2O + 0.03*CH3OH	2.000e-12
BPINNO3 + CH3O2	→	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 + HO2	→	0.07*TERPFDN + 1.39*NO2 + 0.42*TERPNS + 0.44*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNPT + 0.47*HO2	2.70e-12 exp( 360.00 / t )
BPINNO3 + NO	→	1.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNPT + 0.5*HO2	2.300e-12
BPINNO3 + NO3	→	TERPA2O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNPT + 0.5*HO2	2.00e-12 exp( 500.00 / t )
BPINNO3	+	→ TERPA2O2 + CO2 + 0.5*NO2 + 0.45*TERPNS + 0.48*TERPA3 + 0.02*TERPK + 0.02*CH2O + 0.05*TERPNPT + 0.5*HO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
BPINNO3	+	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 )
TERPA3CO3			
BPINNO3 + TER-PACO3	+	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 + TER-PACO3	+	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 )
LIMON + NO3	→	LIMONNO3	1.200e-11
LIMONNO3	+	CH3O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp( 500.00 / t )
CH3CO3			
LIMONNO3	+	0.27*TERPNT1 + 0.91*CH2O + 0.09*CH3OH + 1.01*HO2 + 0.31*TERPF1 + 0.31*NO2 + 0.42*TERPNS1	2.000e-12
CH3O2			
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	+	0.42*TERPNT1 + 0.99*HO2 + 0.86*TERPF1 + 0.86*NO2 + 0.72*TERPNS1	5.300e-13
LIMONNO3			
LIMONNO3 + NO	→	0.07*TERPDFN + 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	+	TERPA2O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
LIMONNO3	+	TERPA4O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
LIMONNO3 + TER-	→	TERPA1O2 + CO2 + 0.46*NO2 + 0.46*TERPF1 + 0.19*TERPNT1 + 0.35*TERPNS1 + 0.54*HO2	2.00e-12 exp( 500.00 / t )
PACO3			
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 + TER-PACO3	→	TERPF1 + 0.56*CH2O + HO2 + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
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 + MYR-CNO3	→	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 + TER-PACO3	→	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 )

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
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 )
MYRCO2 + NO3	→	NO2 + TERPF2 + 0.46*CH3COCH3 + 0.42*CH2O + HO2	2.300e-12
MYRCO2 +	+	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
MYRCO2 +	+	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
MYRCO2 + TER-	→	TERPF2 + HO2 + 0.46*CH3COCH3 + 0.42*CH2O + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
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, 9.300000e-12, 1.50, 0.60) 5.60,
TERPA3CO3 + NO2 + M	→	TERPA3PAN + M	TROEE(9.70e-29, 9.300000e-12, 1.50, 0.60) 5.60,
TERPACO3 + NO2 + M	→	TERPAPAN + M	TROEE(9.70e-29, 9.300000e-12, 1.50, 0.60) 5.60,
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 +	+	2*TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA1O2 +	+	TERPA2O2 + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
TERPA1O2 + TER-	→	TERPA2O2 + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
TERPA2CO3 +	+	2*CO2 + TERPA2O2 + CH3O2	2.90e-12 exp( 500.00 / t )
CH3CO3			
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

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPA2CO3	+	→ 2*CO2 + 2*TERPA2O2	2.90e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA2CO3 + TER-	→	2*CO2 + TERPA2O2 + TERPA1O2	2.90e-12 exp( 500.00 / t )
PACO3			
TERPA2 + NO3	→	HNO3 + TERPA2CO3	2.000e-14
TERPA2O2	+	→ TERPA3O2 + CH3O2 + CO2	2.00e-12 exp( 500.00 / t )
CH3CO3			
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*TERPN + 0.83*NO2 + 0.83*TERPA3O2	2.70e-12 exp( 360.00 / t )
TERPA2O2 + NO3	→	NO2 + TERPA3O2	2.300e-12
TERPA2O2	+	→ TERPA3O2 + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA2O2	+	→ TERPA3O2 + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
TERPA2O2 + TER-	→	TERPA3O2 + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
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	+	→ 2*CO2 + TERPA4O2 + CH3O2	2.90e-12 exp( 500.00 / t )
CH3CO3			
TERPA3CO3	+	→ CO2 + TERPA4O2 + CH2O + HO2	2.00e-12 exp( 500.00 / t )
CH3O2			
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	+	→ 2*CO2 + TERPA4O2 + TERPA2O2	2.90e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA3CO3	+	→ 2*CO2 + 2*TERPA4O2	2.90e-12 exp( 500.00 / t )
TERPA3CO3			
TERPA3CO3 + TER-	→	2*CO2 + TERPA4O2 + TERPA1O2	2.90e-12 exp( 500.00 / t )
PACO3			
TERPA3 + NO3	→	HNO3 + TERPA3CO3	2.000e-14
TERPA3O2	+	→ TERPA4O2 + CH3COCH3 + CH3O2 + CO2	2.00e-12 exp( 500.00 / t )
CH3CO3			
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*TERPN + 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	+	→ TERPA4O2 + CH3COCH3 + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA3O2	+	→ 2*TERPA4O2 + CH3COCH3 + CO2	2.00e-12 exp( 500.00 / t )
TERPA3CO3			
TERPA3O2 + TER-	→	TERPA4O2 + CH3COCH3 + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
PACO3			
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

Table S6: MOZART-TS2 Kinetic Reactions

Reactant		Products	Rate
TERPA4O2 + CH3CO3	+	$\rightarrow$ CH3CO3 + HO2 + 2*CH2O + CO + CH3O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA4O2 + CH3O2	$\rightarrow$	CH3CO3 + 2*HO2 + 3*CH2O + CO	2.000e-12
TERPA4O2 + HO2	$\rightarrow$	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	$\rightarrow$	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	$\rightarrow$	NO2 + CH3CO3 + HO2 + 2*CH2O + CO	2.300e-12
TERPA4O2 +	+	$\rightarrow$ CH3CO3 + HO2 + 2*CH2O + CO + TERPA2O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA2CO3			
TERPA4O2 + TERPA3CO3	$\rightarrow$	CH3CO3 + HO2 + 2*CH2O + CO + TERPA4O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPA4O2 + TERPACO3	$\rightarrow$	CH3CO3 + HO2 + 2*CH2O + CO + TERPA1O2 + CO2	2.00e-12 exp( 500.00 / t )
TERPACID2 + OH	$\rightarrow$	0.71*TERPA2CO3 + 0.29*CO2 + 0.29*TERPA2O2	8.800e-12
TERPACID3 + OH	$\rightarrow$	0.71*TERPA3CO3 + 0.29*CO2 + 0.29*TERPA4O2	8.800e-12
TERPACID + OH	$\rightarrow$	0.71*TERPACO3 + 0.29*CO2 + 0.29*TERPA1O2	8.800e-12
TERPACO3 + CH3CO3	$\rightarrow$	2*CO2 + TERPA1O2 + CH3O2	2.90e-12 exp( 500.00 / t )
TERPACO3 + CH3O2	$\rightarrow$	CO2 + TERPA1O2 + CH2O + HO2	2.00e-12 exp( 500.00 / t )
TERPACO3 + HO2	$\rightarrow$	0.15*O3 + 0.51*TERPACID + 0.49*OH + 0.49*CO2 + 0.49*TERPA1O2	4.30e-13 exp( 1040.00 / t )
TERPACO3 + NO	$\rightarrow$	NO2 + CO2 + TERPA1O2	8.10e-12 exp( 270.00 / t )
TERPACO3 + NO3	$\rightarrow$	NO2 + CO2 + TERPA1O2	4.000e-12
TERPACO3 + TERPACO3	$\rightarrow$	2*CO2 + 2*TERPA1O2	2.90e-12 exp( 500.00 / t )
TERPA + NO3	$\rightarrow$	HNO3 + TERPACO3	2.000e-14
TERPA + OH	$\rightarrow$	0.77*TERPACO3 + 0.23*TERPA2O2	5.20e-12 exp( 600.00 / t )
TERPAPAN + OH	$\rightarrow$	TERPA2 + NO2 + CO	3.660e-12
TERPDHDP + OH	$\rightarrow$	TERPOOH + OH	2.800e-11
TERPF1 + NO3	$\rightarrow$	NO2 + 0.44*CH2O + TERPA3	2.600e-13
TERPF1O2 + HO2	$\rightarrow$	0.9*TERPOOHL + 0.1*OH + 0.1*HO2 + 0.1*TERPA3 + 0.04*CH2O	2.68e-13 exp( 1300.00 / t )
TERPF1O2 + NO	$\rightarrow$	0.3*TERPHFN + 0.7*NO2 + 0.7*HO2 + 0.7*TERPA3 + 0.31*CH2O	2.70e-12 exp( 360.00 / t )
TERPF1 + O3	$\rightarrow$	0.09*OH + TERPA3 + 0.62*CH2O + 0.23*HMHP + 0.02*H2O2 + 0.15*HCOOH	8.300e-18
TERPF1 + OH	$\rightarrow$	0.83*TERPF1O2 + 0.17*TERPA3CO3	1.100e-10
TERPF2 + NO3	$\rightarrow$	0.5*TERPNS1 + 0.5*HO2 + 0.5*TERPF1 + 0.5*CH2O + 0.5*NO2	2.95e-12 exp( -450.00 / t )
TERPF2O2 + HO2	$\rightarrow$	0.9*TERP1OOH + 0.1*OH + 0.1*HO2 + 0.1*TERPF1	2.47e-13 exp( 1300.00 / t )
TERPF2O2 + NO	$\rightarrow$	0.18*TERPN1 + 0.12*TERPNS1 + 0.7*NO2 + 0.7*HO2 + 0.7*TERPF1	2.70e-12 exp( 360.00 / t )
TERPF2 + O3	$\rightarrow$	TERPF1 + 0.34*CH2O + 0.4*HMHP + 0.04*H2O2 + 0.26*HCOOH	1.100e-16
TERPF2 + OH	$\rightarrow$	TERPF2O2	2.70e-11 exp( 390.00 / t )
TERPFDN + OH	$\rightarrow$	NO2 + TERPNS	3.640e-12
TERPHFN + OH	$\rightarrow$	TERPNS + OH	2.800e-11
TERPK + OH	$\rightarrow$	0.14*TERPA2CO3 + 0.86*TERPA1O2	1.700e-11

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
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	→ TERPNPT + 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	
<b>Sulfur Compounds</b>		
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
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 ) <sup>3.3</sup> , ki = 1.5e-12, f=0.6
SO3 + H2O	→ H2SO4	8.5e-21*[H2O]* exp( 6540 / t ) * 1.0e-20
<b>Tropospheric Aerosol<sup>b</sup></b>		
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	$\gamma = 0.0002$
HO2	→ 0.5*H2O2	$\gamma = 0.2$
HONITR	→ HNO3	$\gamma = 0.005$
ICHE	→ M	$\gamma = \textbf{0.0042}$
IEPOX	→ M	$\gamma = \textbf{0.0042}$

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
INHEB	→ HNO3	$\gamma = 0.02$
INHED	→ HNO3	$\gamma = 0.02$
ISOPNNOHD	→ HNO3	$\gamma = 0.02$
ISOPFDN	→ HNO3	$\gamma = 0.1$
ISOPFDNC	→ HNO3	$\gamma = 0.1$
ISOPFNC	→ M	$\gamma = 0.1$
ISOPFNP	→ M	$\gamma = 0.1$
ISOPHFP	→ M	$\gamma = 0.1$
ISOPN1D	→ HNO3	$\gamma = 0.02$
ISOPN2B	→ HNO3	$\gamma = 0.02$
ISOPN4D	→ HNO3	$\gamma = 0.02$
N2O5	→ 2*HNO3	$\gamma = 0.1$
NC4CHO	→ HNO3	$\gamma = 0.005$
NH4	→ M	6.340e-8
NO2	→ 0.5*OH + 0.5*NO + 0.5*HNO3	$\gamma = 0.0001$
NO3	→ HNO3	$\gamma = 0.001$
ONITR	→ HNO3	$\gamma = 0.005$
SQTN	→ M	$\gamma = 0.1$
TERPDHDP	→ M	$\gamma = 0.1$
TERPFDN	→ HNO3	$\gamma = 0.1$
TERPHFN	→ M	$\gamma = 0.1$
TERPNPT1	→ HNO3	$\gamma = 0.02$
TERPNPT	→ HNO3	$\gamma = 0.02$
TERPN1	→ HNO3	$\gamma = 0.02$
TERPN	→ HNO3	$\gamma = 0.02$
<b>Secondary Organic Aerosol<sup>c</sup></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 )
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

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
LIMON + O3	$\rightarrow$ 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	$\rightarrow$ 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	$\rightarrow$ MYRC + NO3 + 0.17493*SOAG3 + 0.59019*SOAG4	1.100e-11
MYRC + O3	$\rightarrow$ 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	$\rightarrow$ MYRC + OH + 0.0508*SOAG0 + 0.1149*SOAG1 + 0.0348*SOAG2 + 0.0554*SOAG3 + 0.1278*SOAG4	2.100e-10
SVOC + OH	$\rightarrow$ OH + 0.5931*SOAG0 + 0.1534*SOAG1 + 0.0459*SOAG2 + 0.0085*SOAG3 + 0.0128*SOAG4	1.340e-11
TOLUENE + OH	$\rightarrow$ TOLUENE + OH + 0.1364*SOAG0 + 0.0101*SOAG1 + 0.0763*SOAG2 + 0.2157*SOAG3 + 0.0232*SOAG4	1.70e-12 exp( 352.00 / t )
XYLEMES + OH	$\rightarrow$ XYLEMES + OH + 0.1677*SOAG0 + 0.0174*SOAG1 + 0.086*SOAG2 + 0.0512*SOAG3 + 0.1598*SOAG4	1.700e-11
<b>Stratospheric Heterogeneous Uptake Reactions</b>		
Sulfate aerosol reactions		
N2O5 + H2O(l)	$\rightarrow$ 2*HNO3	$\gamma = f(\text{wt}\%)$
CLONO2 + H2O(l)	$\rightarrow$ HOCL + HNO3	$\gamma = f(T,P,\text{HCl},\text{H}_2\text{O},r)$
BRONO2 + H2O(l)	$\rightarrow$ HOBr + HNO3	$\gamma = f(T,P,\text{H}_2\text{O},r)$
CLONO2 + HCl(l)	$\rightarrow$ CL2 + HNO3	$\gamma = f(T,P,\text{HCl},\text{H}_2\text{O},r)$
HOCL + HCl(l)	$\rightarrow$ CL2 + H2O	$\gamma = f(T,P,\text{HCl},\text{HOCl},\text{H}_2\text{O},r)$
HOBr + HCl(l)	$\rightarrow$ BRCL + H2O	$\gamma = f(T,P,\text{HCl},\text{HOBr},\text{H}_2\text{O},r)$
Nitric Acid Tri-hydrate Reactions		
N2O5 + H2O(s)	$\rightarrow$ 2*HNO3	$\gamma = 4e-4$
CLONO2 + H2O(s)	$\rightarrow$ HOCL + HNO3	$\gamma = 4e-3$
CLONO2 + HCl(s)	$\rightarrow$ CL2 + HNO3	$\gamma = 0.2$
HOCL + HCl(s)	$\rightarrow$ CL2 + H2O	$\gamma = 0.1$
BRONO2 + H2O(s)	$\rightarrow$ HOBr + HNO3	$\gamma = 0.006$
Water-Ice Aerosol Reactions		
N2O5 + H2O(s)	$\rightarrow$ 2*HNO3	$\gamma = 0.02$
CLONO2 + H2O(s)	$\rightarrow$ HOCL + HNO3	$\gamma = 0.3$
BRONO2 + H2O(s)	$\rightarrow$ HOBr + HNO3	$\gamma = 0.3$
CLONO2 + HCl(s)	$\rightarrow$ CL2 + HNO3	$\gamma = 0.3$
HOCL + HCl(s)	$\rightarrow$ CL2 + H2O	$\gamma = 0.2$
HOBr + HCl(s)	$\rightarrow$ BRCL + H2O	$\gamma = 0.3$
<b>Synthetic Tracers</b>		
AOA_NH	$\rightarrow$ AOA_NH	1.000e+0
E90	$\rightarrow$ sink	1.290e-7
NH_50	$\rightarrow$ M	2.310e-7
NH_5	$\rightarrow$ M	2.310e-6
ST80_25	$\rightarrow$ M	4.630e-7

•<sup>a</sup> For all isoprene peroxy radicals, the RO<sub>2</sub> + NO general reaction rate constant (2.7e-12 exp(360/T)) from MCM v3.3.1 is used with the pressure and temperature dependent organic nitrate yield recommended by Wennberg et al. (2018), which is based on Arey et al. (2001). The organic nitrate yield ( $\alpha$ ) at T = 293 K and M = 2.45e19 molecules cm<sup>-3</sup> and the number of heavy atoms excluding the peroxy group (n) are reported above.  $\alpha$  and n are used in the following equation to calculate the temperature and pressure dependent organic nitrate branching ratio ( $\alpha_{\text{RONO}2}$ ):

$$\alpha_{\text{RONO}2} = \frac{A(T,M,n)}{A(T,M,n) + A_0(n) * \frac{1-\alpha(n)}{\alpha(n)}}, \text{ where } A_0(n) = A(T=293K, M=2.45e19, n),$$

$\gamma = 2e-22 \text{ cm}^3 \text{ molecule}^{-1}$ , T = temperature (K), [M] is the number density of air in molecules cm<sup>-3</sup>,

Table S6: MOZART-TS2 Kinetic Reactions

Reactant	Products	Rate
and $A(T, M, n) = \frac{\gamma e^n[M]}{1 + \frac{\gamma e^n[M]}{0.43(T(K)/298)^{-8}}}$	$*0.41^{(1 + [\log(\gamma e^n[M]/0.43(T(K)/298)^{-8})]^2)^{-1}}$	

- <sup>b</sup> For new gas-phase species undergoing aerosol uptake, the aerosol uptake coefficient ( $\gamma$ ) value is reported.
- <sup>c</sup> 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
<b>Caltech assumptions for PAN and C<sub>4</sub> dihydroperoxy carbonyls</b>		
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 <sup>3</sup> )
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 <sup>3</sup> )
<b>Caltech assumptions for PAN, C<sub>4</sub> dihydroperoxy carbonyls, and carbonyl nitrates</b>		
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 <sup>3</sup> )
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 <sup>3</sup> )
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
<b>MCM v3.3.1 assumptions for pinonaldehyde nitrate yield</b>		
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

<b>Reactant</b>	<b>Products</b>	<b>Rate</b>
TERPA3O2 + NO	$\rightarrow 0.12^*\text{TERPNT} + 0.88^*\text{NO}_2 + 0.88^*\text{TERPA4O}_2 + 0.88^*\text{CH}_3\text{COCH}_3$	2.70e-12 exp( 360.00 / t )
TERPA4O2 + NO	$\rightarrow 0.05^*\text{TERPNS} + 0.95^*\text{NO}_2 + 0.95^*\text{CH}_3\text{CO}_3 + 0.95^*\text{HO}_2 + 1.9^*\text{CH}_2\text{O} + 0.95^*\text{CO}$	2.70e-12 exp( 360.00 / t )
<b>MCM v3.3.1 assumptions for pinonaldehyde and limonaldehyde/limaketone nitrate yield</b>		
Changed the following reactions:		
TERPA1O2 + NO	$\rightarrow 0.16^*\text{TERPNS} + 0.84^*\text{NO}_2 + 0.84^*\text{TERPA2O}_2$	2.70e-12 exp( 360.00 / t )
TERPA2O2 + NO	$\rightarrow 0.03^*\text{TERPNT} + 0.97^*\text{NO}_2 + 0.97^*\text{TERPA3O}_2$	2.70e-12 exp( 360.00 / t )
TERPA3O2 + NO	$\rightarrow 0.12^*\text{TERPNT} + 0.88^*\text{NO}_2 + 0.88^*\text{TERPA4O}_2 + 0.88^*\text{CH}_3\text{COCH}_3$	2.70e-12 exp( 360.00 / t )
TERPA4O2 + NO	$\rightarrow 0.05^*\text{TERPNS} + 0.95^*\text{NO}_2 + 0.95^*\text{CH}_3\text{CO}_3 + 0.95^*\text{HO}_2 + 1.9^*\text{CH}_2\text{O} + 0.95^*\text{CO}$	2.70e-12 exp( 360.00 / t )
TERPF1O2 + NO	$\rightarrow 0.15^*\text{TERPHFN} + 0.85^*\text{NO}_2 + 0.85^*\text{HO}_2 + 0.85^*\text{TERPA3} + 0.31^*\text{CH}_2\text{O}$	2.70e-12 exp( 360.00 / t )
<b>MCM pinonaldehyde and limonaldehyde/limaketone nitrate yield and oxidation of unsaturated hydroxy nitrates</b>		
Changed the following reactions:		
TERPA1O2 + NO	$\rightarrow 0.16^*\text{TERPNS} + 0.84^*\text{NO}_2 + 0.84^*\text{TERPA2O}_2$	2.70e-12 exp( 360.00 / t )
TERPA2O2 + NO	$\rightarrow 0.03^*\text{TERPNT} + 0.97^*\text{NO}_2 + 0.97^*\text{TERPA3O}_2$	2.70e-12 exp( 360.00 / t )
TERPA3O2 + NO	$\rightarrow 0.12^*\text{TERPNT} + 0.88^*\text{NO}_2 + 0.88^*\text{TERPA4O}_2 + 0.88^*\text{CH}_3\text{COCH}_3$	2.70e-12 exp( 360.00 / t )
TERPA4O2 + NO	$\rightarrow 0.05^*\text{TERPNS} + 0.95^*\text{NO}_2 + 0.95^*\text{CH}_3\text{CO}_3 + 0.95^*\text{HO}_2 + 1.9^*\text{CH}_2\text{O} + 0.95^*\text{CO}$	2.70e-12 exp( 360.00 / t )
TERPF1O2 + NO	$\rightarrow 0.15^*\text{TERPHFN} + 0.85^*\text{NO}_2 + 0.85^*\text{HO}_2 + 0.85^*\text{TERPA3} + 0.31^*\text{CH}_2\text{O}$	2.70e-12 exp( 360.00 / t )
TERPNS1 + OH	$\rightarrow \text{TERPF1+NO}_2$	1.100e-10
TERPNT1 + OH	$\rightarrow \text{TERPF1+NO}_2$	1.100e-10

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

Reactant	Products	Rate
<b>I_TEST1 Sensitivity Test</b>		
Updated the following reactions:		
ISOPB1O2 + NO	→ NO2 + MVK + CH2O + HO2	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPB1O2 + NO	→ ISOPN2B	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPB4O2 + NO	→ NO2 + MACR + CH2O + HO2	In code, $\alpha = \mathbf{0.13}$ , n = 6
ISOPB4O2 + NO	→ ISOPN3B	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPED1O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPED1O2 + NO	→ ISOPN4D	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPED4O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPED4O2 + NO	→ ISOPN1D	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPZD1O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MVKOOH + 0.55*CO + 0.55*OH	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPZD1O2 + NO	→ ISOPN4D	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPZD4O2 + NO	→ NO2 + 0.45*HYDRALD + 0.45*HO2 + 0.55*MACROOH + 0.55*CO + 0.55*OH	In code, $\alpha = \mathbf{0.09}$ , n = 6
ISOPZD4O2 + NO	→ ISOPN1D	In code, $\alpha = \mathbf{0.09}$ , n = 6
<b>I_TEST2 Sensitivity Test</b>		
Updated the following reactions:		
ISOPN1DO2 + NO	→ NO2 + HO2 + 0.94*NOA + 0.94*GLYALD + 0.06*MACRN + 0.06*CH2O	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN1DO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN2BO2 + NO	→ 1.73*NO2 + 0.27*MACRN + 0.27*CH2O + 0.27*HO2 + 0.73*HYAC + 0.73*GLYALD	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN2BO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN3BO2 + NO	→ NO2 + MVKN + CH2O + HO2	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN3BO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN4DO2 + NO	→ NO2 + HO2 + 0.13*MVKN + 0.13*CH2O + 0.87*HYAC + 0.87*NO3CH2CHO	In code, $\alpha = \mathbf{0.3}$ , n = 11
ISOPN4DO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , 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, $\alpha = \mathbf{0.3}$ , n = 11
ISOPNBNO3O2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , n = 11
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, $\alpha = \mathbf{0.3}$ , n = 12
ISOPNOOHBO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , 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, $\alpha = \mathbf{0.3}$ , n = 12
ISOPNOOHDO2 + NO	→ ISOPFDN	In code, $\alpha = \mathbf{0.3}$ , n = 12
NC4CHO02 + 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, $\alpha = \mathbf{0.3}$ , n = 11
NC4CHO02 + NO	→ ISOPFDNC	In code, $\alpha = \mathbf{0.3}$ , n = 11
<b>I_TEST3 Sensitivity Test</b>		
Removed the following reactions:		
ISOPN1DO2	→ ISOPFNP + HO2	$1.26e+13 \exp(-10000.00/t)$

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

Reactant	Products	Rate
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 )
ISOPNOOHD2	→ OH + ISOPFNP	6.55e+12 exp( -10000.00 / t )
<b>T_TEST1 Sensitivity Test</b>		
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 )
<b>T_TEST2 Sensitivity Test</b>		
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 )
<b>T_TEST3 Sensitivity Test</b>		
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 )

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

Reactant		Products	Rate	
APINO2	+	$\rightarrow 0.1*\text{TERPF1} + 0.32*\text{TERPA} + 0.36*\text{TERPA3}$	$+ 2e-12 \exp(500/t)$	
TERPA3CO3		$\rightarrow 0.22*\text{TERP1OOH} + \text{HO2} + \text{TERPA4O2} + \text{CO2}$		
APINO2 + TERPACO3	$\rightarrow$	$0.1*\text{TERPF1} + 0.32*\text{TERPA} + 0.36*\text{TERPA3}$	$+ 2e-12 \exp(500/t)$	
		$\rightarrow 0.22*\text{TERP1OOH} + \text{HO2} + \text{TERPA1O2} + \text{CO2}$		
APIN + OH	$\rightarrow$	$0.06*\text{TERP1OOH} + 0.06*\text{HO2} + 0.94*\text{APINO2}$	$1.34e-11 \exp(410/t)$	
BPINO2 + CH3CO3	$\rightarrow$	$0.1*\text{TERPF1} + 0.35*\text{TERPK} + 0.35*\text{CH2O} + 0.28*\text{TERPA3}$	$+ 2e-12 \exp(500/t)$	
		$+ 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 0.81*\text{HO2} + \text{CH3O2} + \text{CO2}$		
BPINO2 + CH3O2	$\rightarrow$	$1.26*\text{CH2O} + 0.06*\text{CH3OH} + 0.1*\text{TERPF1} + 0.32*\text{TERPK}$	$+ 0.31*\text{TERPA3} + 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 1.57*\text{HO2}$	$2e-12$
BPINO2 + HO2	$\rightarrow$	$0.18*\text{TERP1OOH} + 0.65*\text{TERPOOH} + 0.03*\text{TERPK}$	$+ 0.03*\text{CH2O} + 0.03*\text{TERPA3} + 0.11*\text{TERPA3CO3} + 0.18*\text{OH} + 0.07*\text{HO2}$	$2.6e-13 \exp(1300/t)$
BPINO2 + NO	$\rightarrow$	$0.03*\text{TERPNS} + 0.09*\text{TERPNT} + 0.01*\text{TERPNS1}$	$+ 2.7e-12 \exp(360/t)$	
		$+ 0.87*\text{NO2} + 0.72*\text{HO2} + 0.08*\text{TERPF1} + 0.31*\text{TERPK}$		
		$+ 0.31*\text{CH2O} + 0.26*\text{TERPA3} + 0.15*\text{TERPA3CO3} + 0.07*\text{TERP1OOH}$		
BPINO2 + NO3	$\rightarrow$	$0.1*\text{TERPF1} + 0.35*\text{TERPK} + 0.35*\text{CH2O} + 0.28*\text{TERPA3}$	$+ 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 0.81*\text{HO2} + \text{NO2}$	$2.3e-12$
BPINO2	+	$\rightarrow 0.1*\text{TERPF1} + 0.35*\text{TERPK} + 0.35*\text{CH2O} + 0.28*\text{TERPA3}$	$+ 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 0.81*\text{HO2} + \text{TERPA2O2} + \text{CO2}$	$2e-12 \exp(500/t)$
TERPA2CO3				
BPINO2	+	$\rightarrow 0.1*\text{TERPF1} + 0.35*\text{TERPK} + 0.35*\text{CH2O} + 0.28*\text{TERPA3}$	$+ 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 0.81*\text{HO2} + \text{TERPA4O2} + \text{CO2}$	$2e-12 \exp(500/t)$
TERPA3CO3				
BPINO2 + TERPACO3	$\rightarrow$	$0.1*\text{TERPF1} + 0.35*\text{TERPK} + 0.35*\text{CH2O} + 0.28*\text{TERPA3}$	$+ 0.19*\text{TERPA3CO3} + 0.08*\text{TERP1OOH} + 0.81*\text{HO2} + \text{TERPA1O2} + \text{CO2}$	$2e-12 \exp(500/t)$

#### T\_TEST4 Sensitivity Test

Updated the following reactions:

TERPA1O2 + NO	$\rightarrow$	$0.16*\text{TERPNS} + 0.84*\text{NO2} + 0.84*\text{TERPA2O2}$	$2.70e-12 \exp(360.00/t)$
TERPA2O2 + NO	$\rightarrow$	$0.03*\text{TERPNT} + 0.97*\text{NO2} + 0.97*\text{TERPA3O2}$	$2.70e-12 \exp(360.00/t)$
TERPA3O2 + NO	$\rightarrow$	$0.12*\text{TERPNT} + 0.88*\text{NO2} + 0.88*\text{TERPA4O2} + 0.88*\text{CH3COCH3}$	$2.70e-12 \exp(360.00/t)$
TERPA4O2 + NO	$\rightarrow$	$0.05*\text{TERPNS} + 0.95*\text{NO2} + 0.95*\text{CH3CO3} + 0.95*\text{HO2} + 1.9*\text{CH2O} + 0.95*\text{CO}$	$2.70e-12 \exp(360.00/t)$
TERPF1O2 + NO	$\rightarrow$	$0.15*\text{TERPHFN} + 0.85*\text{NO2} + 0.85*\text{HO2} + 0.85*\text{TERPA3} + 0.31*\text{CH2O}$	$2.70e-12 \exp(360.00/t)$

#### A\_TEST1 Sensitivity Test

Removed the following reactions:

HONITR	$\rightarrow$	HNO3	In code
INHEB	$\rightarrow$	HNO3	In code, $\gamma = 0.02$
INHED	$\rightarrow$	HNO3	In code, $\gamma = 0.02$
ISOPNOOHD	$\rightarrow$	HNO3	In code, $\gamma = 0.02$
ISOPFDN	$\rightarrow$	HNO3	In code, $\gamma = 0.1$
ISOPFDNC	$\rightarrow$	HNO3	In code, $\gamma = 0.1$
ISOPFNC	$\rightarrow$	M	In code, $\gamma = 0.1$
ISOPFNP	$\rightarrow$	M	In code, $\gamma = 0.1$

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

Reactant	Products	Rate
ISOPN1D	→ HNO3	In code, $\gamma = 0.02$
ISOPN2B	→ HNO3	In code, $\gamma = 0.02$
ISOPN4D	→ HNO3	In code, $\gamma = 0.02$
NC4CHO	→ HNO3	In code
ONITR	→ HNO3	In code
SQTN	→ M	In code, $\gamma = 0.1$
TERPFDN	→ HNO3	In code, $\gamma = 0.1$
TERPHFN	→ M	In code, $\gamma = 0.1$
TERPNPT1	→ HNO3	In code, $\gamma = 0.02$
TERPNPT	→ HNO3	In code, $\gamma = 0.02$
TERPNT1	→ HNO3	In code, $\gamma = 0.02$
TERPNT	→ HNO3	In code, $\gamma = 0.02$
<b>A_TEST2 Sensitivity Test</b>		
Removed the following reactions:		
INHEB	→ HNO3	In code, $\gamma = 0.02$
INHED	→ HNO3	In code, $\gamma = 0.02$
ISOPNOOHD	→ HNO3	In code, $\gamma = 0.02$
Added the following reactions:		
ISOPN3B	→ HNO3	In code, $\gamma = 0.005$
ISOPNBNO3	→ HNO3	In code, $\gamma = 0.005$
MVKN	→ HNO3	In code, $\gamma = 0.005$
MACRN	→ HNO3	In code, $\gamma = 0.005$
TERPNPS1	→ HNO3	In code, $\gamma = 0.01$
TERPNPS	→ HNO3	In code, $\gamma = 0.01$
TERPNS	→ HNO3	In code, $\gamma = 0.01$
TERPNS1	→ HNO3	In code, $\gamma = 0.01$
Updated the following reactions:		
NC4CHO	→ HNO3	In code, $\gamma = 0.005$
ISOPFDN	→ HNO3	In code, $\gamma = 0.005$
ISOPFNP	→ M	In code, $\gamma = 0.005$
ISOPN1D	→ HNO3	In code, $\gamma = 0.005$
ISOPN2B	→ HNO3	In code, $\gamma = 0.005$
ISOPN4D	→ HNO3	In code, $\gamma = 0.005$
ISOPFNC	→ M	In code, $\gamma = 0.005$
ISOPFDNC	→ HNO3	In code, $\gamma = 0.005$
TERPNT1	→ HNO3	In code, $\gamma = 0.01$
TERPNT	→ HNO3	In code, $\gamma = 0.01$
TERPNPT1	→ HNO3	In code, $\gamma = 0.01$
TERPNPT	→ HNO3	In code, $\gamma = 0.01$
TERPFDN	→ HNO3	In code, $\gamma = 0.01$
SQTN	→ M	In code, $\gamma = 0.01$
TERPHFN	→ M	In code, $\gamma = 0.01$
<b>A_TEST3 Sensitivity Test</b>		
Added the following reactions:		
ISOPNOOHB	→ HNO3	In code, $\gamma = 0.02$
ISOPN3B	→ HNO3	In code, $\gamma = 0.02$
ISOPNBNO3	→ HNO3	In code, $\gamma = 0.02$
MVKN	→ HNO3	In code, $\gamma = 0.02$
MACRN	→ HNO3	In code, $\gamma = 0.02$
TERPNPS1	→ HNO3	In code, $\gamma = 0.02$

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

Reactant	Products	Rate
TERPNPS	→ HNO3	In code, $\gamma = 0.02$
TERPNS	→ HNO3	In code, $\gamma = 0.02$
TERPNS1	→ HNO3	In code, $\gamma = 0.02$

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