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Supporting Information for

The GFDL Global Atmospheric Chemistry-Climate Model AM4.1: Model Description and Simulation Characteristics

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Introduction

The tables contained in this electronic supplement describe the chemical tracers, photolysis reactions, and kinetic reactions included in AM4.1.

Figure S1 shows an evaluation of lightning flash frequency in AM3 and AM4.1 against spaceborne Optical Transient Detector (OTD) and Lightning Imaging Sensor (LIS) retrievals. Figures S2–S5 show evaluations of mean surface MDA8 O_3 concentrations for 2005–2014 from model simulations and observations for MAM, JJA, SON, and DJF seasons. Figure S6 shows an evaluation of the monthly regional climatology of aerosol optical depth simulated by AM3, AM4.0, and AM4.1 with retrievals from MODIS and MISR satellite instruments. Bars denote the speciated aerosol optical depth in AM4.1.

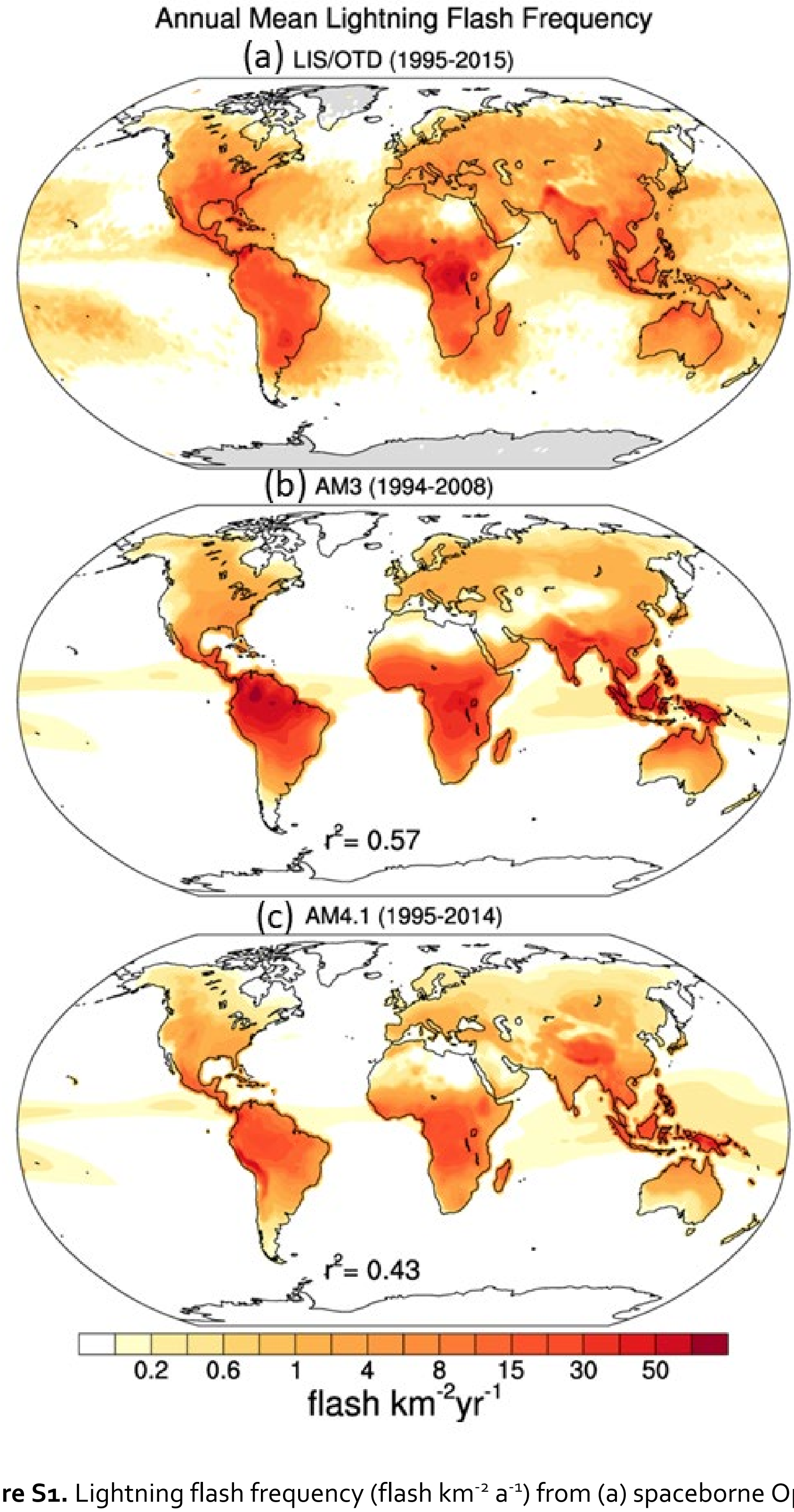

Figure S1. Lightning flash frequency (flash km^{-2} a^{-1}) from (a) spaceborne Optical Transient Detector (OTD) and Lightning Imaging Sensor (LIS) retrievals (Cecil et al., 2014) and parameterized in (b) AM3 and (c) AM4.1.

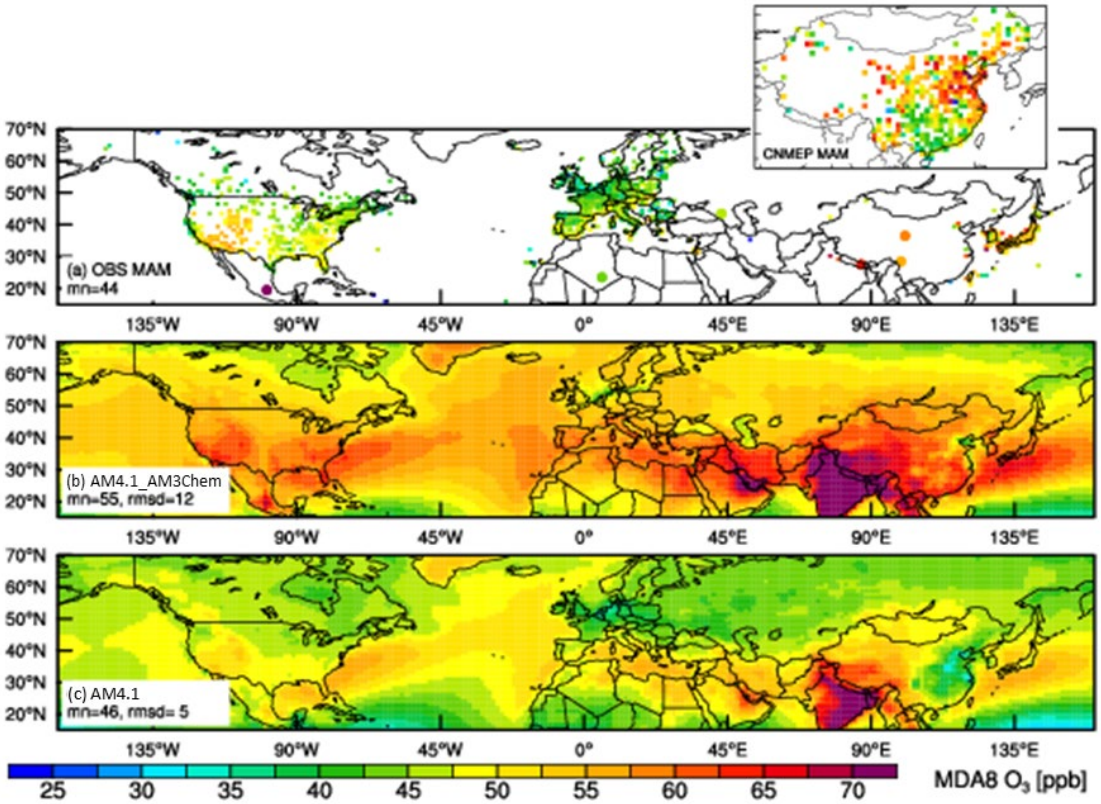

Figure S2. MAM mean surface MDA8 O3 concentrations for 2005-2014 from: (a) TOAR (inset map for CNMEP 2013-2017) observations on the same 1° x 1° grid used for AM4.1, (b) AM4.1 simulation with AM3-like chemistry, (c) standard AM4.1 simulation. Here, mn is the mean and rmsd is the root-mean-square deviation between observations and simulations.

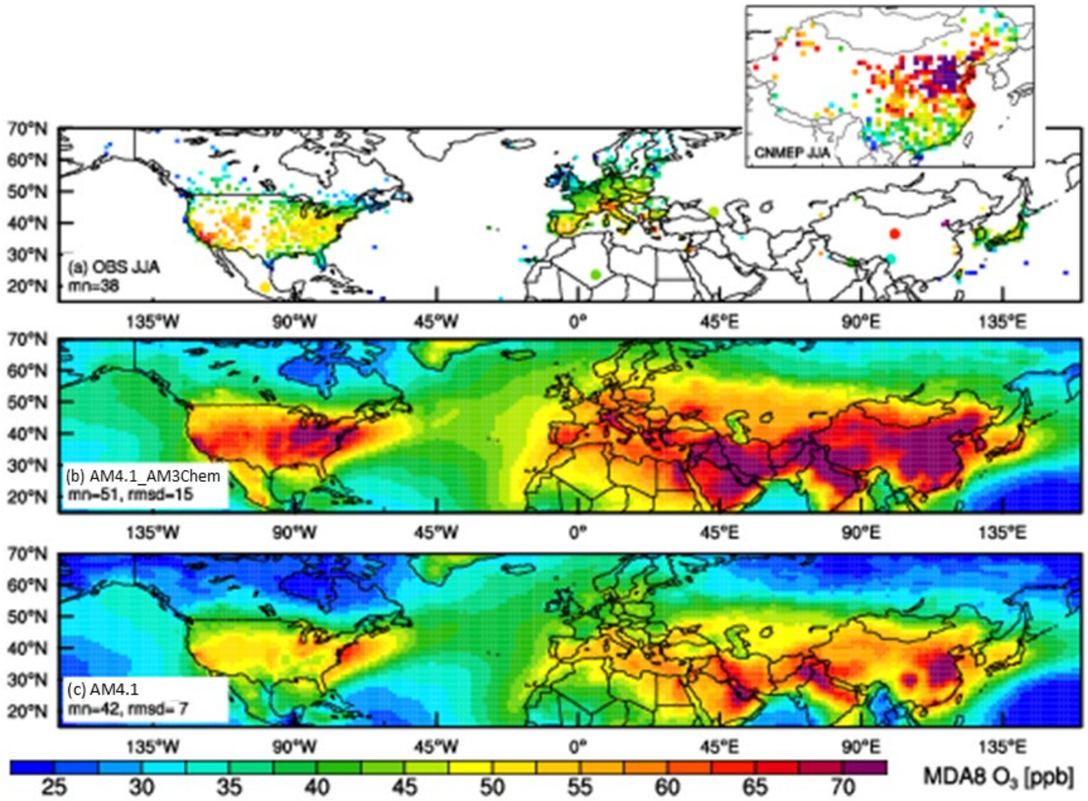

Figure S3. Same as Figure S2, but for JJA.

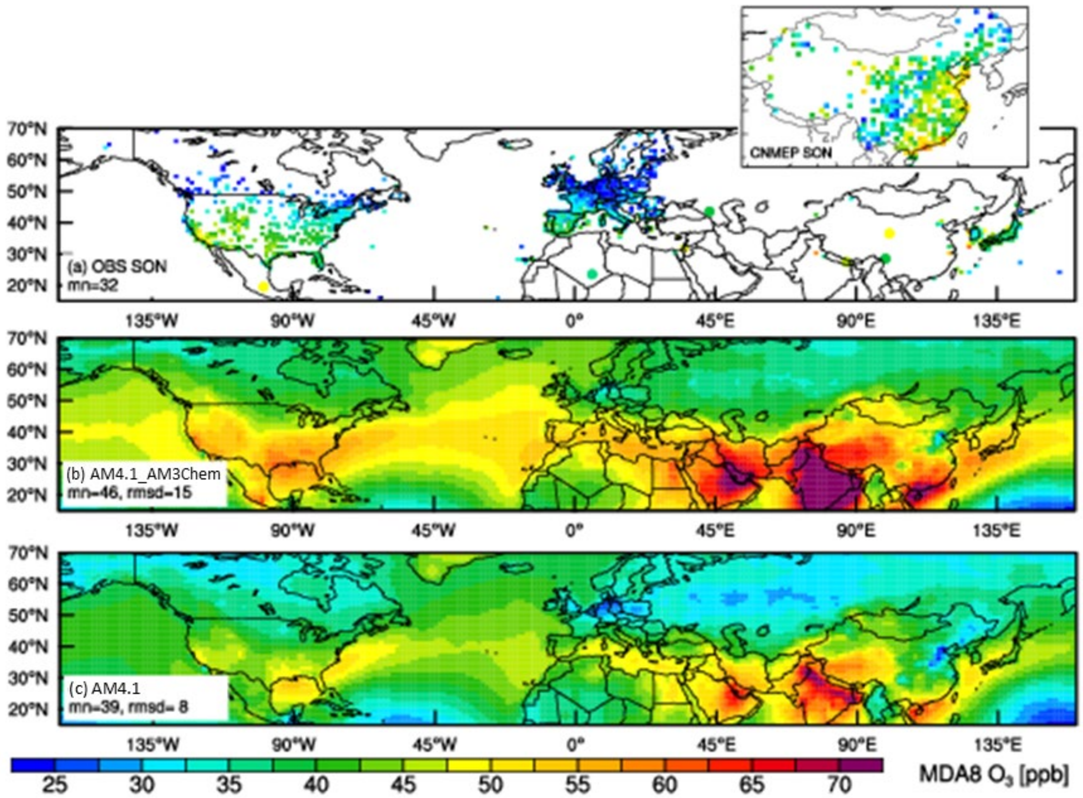

Figure S4. Same as Figure S2, but for SON.

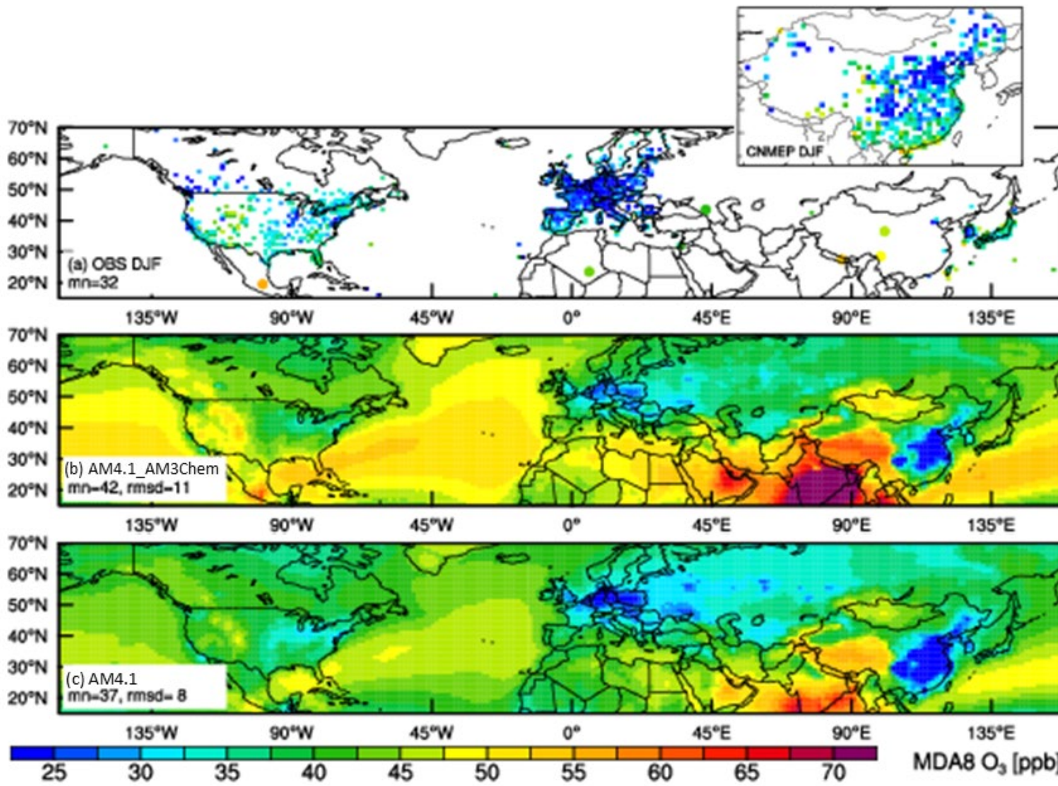

Figure S5. Same as Figure S2, but for DJF.

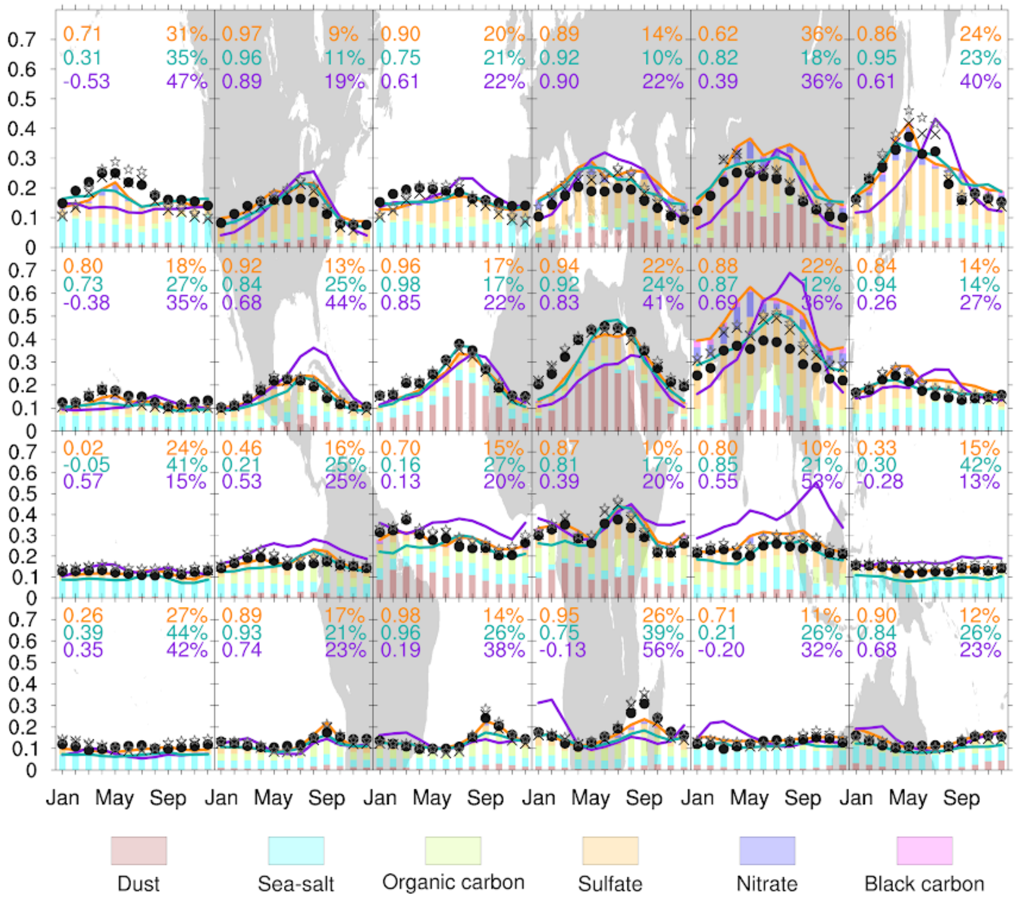

Figure S6. Monthly climatology (2003–2014) of aerosol optical depth simulated by AM3 (purple line), AM4.0 (green line) and AM4.1 (orange line) and measured by MODIS (TERRA: star, AQUA: cross) and MISR (filled circles) satellite instruments. Each panel represents a spatial average over the corresponding region on the background map. The numbers in each box show the correlation coefficients (left) and normalized root mean square error(right) compared to MODIS-TERRA (purple: AM3, green: AM4.0, orange: AM4.1). Bars denote the speciated aerosol optical depth in AM4.1 (species indicated by shading, with colors indicated below).

Table S1. Chemical species represented in AM4.1.

Table S2. Photolysis reactions represented in AM4.1.

Table S3. Kinetic reactions represented in AM4.1.

Name	Description
Aerosol tracers	
SO4	Sulfate aerosol
BCPHOB	Hydrophobic black carbon aerosol
BCPHIL	Hydrophilic black carbon aerosol
OMPHOB	Hydrophobic organic aerosol
OMPHIL	Hydrophilic organic aerosol
SOA	Secondary organic aerosol
DUST1	Mineral dust aerosol (r=0.1-1.0μm)
DUST2	Mineral dust aerosol (r=1.0-2.0μm)
DUST3	Mineral dust aerosol (r=2.0-3.0μm)
DUST4	Mineral dust aerosol (r=3.0-6.0μm)
DUST5	Mineral dust aerosol (r=6.0-10.0μm)
SSALT1	Sea salt aerosol (r=0.1-0.5μm)
SSALT2	Sea salt aerosol (r=0.5-1.0μm)
SSALT3	Sea salt aerosol (r=1.0-2.5μm)
SSALT4	Sea salt aerosol (r=2.5-5.0μm)
SSALT5	Sea salt aerosol (r=5.0-10.0μm)
Gas-phase tracers	
O3	Ozone
O (d)	Atomic oxygen
O1D (d)	$O(^1D)$
N2O	Nitrous oxide
N (d)	Atomic nitrogen
NO	Nitric oxide
NO2	Nitrogen dioxide
NO3	Nitrate radical
HNO3	Nitric acid
HO2NO2	Pernitric acid
N2O5	Dinitrogen pentoxide

CH4	Methane
CH3O2 (d)	Methylperoxy radical
CH3OOH	Methylhydroperoxide
CH2O	Formaldehyde
CO	Carbon monoxide
OH (d)	Hydroxyl radical
HO2 (d)	Hydroperoxy radical
H2O2	Hydrogen peroxide
C3H6	Propane
ISOP	Isoprene (C_5H_8)
PO2 (d)	$C_3H_6OHO_2$
CH3CHO	Acetaldehyde (CH_3CHO)
POOH (d)	C_3H_6OHOOH
CH3CO3 (d)	Acetylperoxy radical
CH3COOOH (d)	Peroxyacetic acid
PAN	Peroxyacetyl nitrate ($CH_3CO_3NO_2$)
C2H6	Ethane
C2H4	Ethene
C4H10	Butane
MPAN	$CH_2CCH_3CO_3NO_2$
ISOPO2 (d)	$HOCH_2COOCH_3CHCH_2$
MVK	$CH_2CHCOCH_3$
MACR	CH_2CCH_3CHO
MACRO2 (d)	$CH_3COCHO_2CH_2OH$
MACROOH (d)	$CH_3COCHOOHCH_2OH$
C2H5O2 (d)	Ethylperoxy radical
C2H5OOH (d)	Ethylhydroperoxide
C10H16	Terpene
C3H8	Propane
C3H7O2 (d)	Propylperoxy radical
C3H7OOH (d)	Propylhydroperoxide

CH3COCH3	Acetone
CH3OH	Methanol
C2H5OH	Ethanol
GLYALD	$HOCH_2CHO$
HYAC	CH_3COCH_2OH
EO2 (d)	$HOCH_2CH_2O_2$
EO (d)	$HOCH_2CH2O$
ISOPOOH	$HOCH_2COOHCH_3CHCH_2$
H2	Molecular hydrogen
SO2	Sulfur dioxide
DMS	Dimethyl sulfide (CH_3SCH_3)
NH3	Ammonia
NH4NO3	Nitrate aerosol
NH4	Ammonium aeorsol
HCl	Hydrochloric acid
HOCl	Hypochlorous acid
ClONO2	Chlorine nitrate
Cl	Atomic chlorine
ClO	Chlorine monoxide
Cl2O2	Dichlorine dioxide
Cl2	Molecular chlorine
HOBr	Hypobromous acid
HBr	Hydrobromic acid
BrONO2	Bromine nitrate
Br	Atomic bromine
BrO	Bromine monoxide
BrCl	Bromine chloride
H (d)	Atomic hydrogen
H2O	Water vapor
ROH (d)	C_3H_7OH
RCHO (d)	C_2H_5CHO

ISOPNB	$HOCH_2C(CH_3)=CHCH_2ONO_2$
ISOPNBO2 (d)	$HOC_5H_7(OH)(O_2)ONO_2$
MACRN	$HC(O)C(CH_3)=CHCOOH$
MVKN	$HC(O)C(CH_3)=CHCOOH$
R4N2	$RONO_2$
MEK (d)	$C_2H_5C(O)CH_3$
R4N1	RO_2 from R4N2
IEPOX	$C_5H_{10}O_3$
IEPOXOO (d)	RO_2 from IEPOX
GLYX	CHOCHO
MGLY	CH_3COCHO
MVKO2 (d)	$HOCH_2CH(O_2)C(O)CH_3$
MVKOOH (d)	$HOCH_2CH(OOH)C(O)CH_3$
MACRNO2 (d)	RO_2 from MACRN
MAO3 (d)	$CH_2=C(CH_3)C(O)OO$
MAOP (d)	$CH_2=C(CH_3)C(O)OOH$
MAOPO2 (d)	RO_2 from MAOP
ATO2 (d)	$CH_3C(O)CH_2O_2$
ATOOH	$CH_3C(O)CH_2OOH$
INO2 (d)	$O_2NOCH_2C(OO)(CH_3)CH=CH_2$
INPN (d)	$O_2NOCH_2C(OOH)(CH_3)CH=CH_2$
ISNOOA (d)	Peroxy radical from ISN1
ISN1 (d)	$CH_2CHCCH_3OOCH_2ONO_2$
Idealized tracers	
LCH4 (d)	Loss of CH_4 by reaction with OH
O3S	Stratospheric O_3
O3S_E90	Stratospheric O_3 (tagged by E90)
E90	Tropopause tracer
AOANH	Northern hemisphere tracer lifetime
NH50	Northern hemisphere transport tracer
NOy (d)	Total reactive nitrogen

Cly (d)	Total reactive chlorine
Bry (d)	Total reactive bromine

Tracers marked with (d) are diagnostic (i.e., not transported).

Reaction
O2 + hv → 2*O
O3 + hv → O1D + O2
O3 + hv → O + O2
N2O + hv → O1D + N2
NO + hv → N + O
NO2 + hv → NO + O
N2O5 + hv → NO2 + NO3
HNO3 + hv → NO2 + OH
NO3 + hv → .89*NO2 + .11*NO + .89*O
HO2NO2 + hv → NO2 + HO2
CH3OOH + hv → CH2O + HO2 + OH
CH2O + hv → CO + HO2 + H
CH2O + hv → CO + H2
H2O + hv → OH + H
H2O2 + hv → 2*OH
CH3CHO + hv → CH3O2 + CO + HO2
POOH + hv → CH3CHO + CH2O + HO2 + OH
CH3COOOH + hv → CH3O2 + OH + {CO2}
PAN + hv → .6*CH3CO3 + .6*NO2 + .4*CH3O2 + .4*NO3
MPAN + hv → MAO3 + NO2
MACR → 1.34*HO2 + .66*MAO3 + 1.34*CH2O + 1.34*CH3CO3
MACR → .66*OH + 1.34*CO
MVK + hv → .7*C3H6 + .7*CO + .3*CH3O2 + .3*CH3CO3
C2H5OOH + hv → CH3CHO + HO2 + OH
C3H7OOH + hv → 0.82*CH3COCH3 + OH + HO2
CH3COCH3 + hv → CH3CO3 + CH3O2
MGLY + hv → CH3CO3 + CO + HO2
GLYX + hv → 2.0*CO + 2.0*HO2
ISOPOOH + hv → .402*MVK + .288*MACR + .69*CH2O + HO2

HYAC + hv → CH3CO3 + HO2 + CH2O
GLYALD + hv → 2*HO2 + CO + CH2O
ISOPNB + hv → RCHO + NO2 + HO2
MACRN + hv → NO2 + HYAC + MGLY + .5*CH2O + HO2 + .5*CO
MVKN + hv → GLYALD + NO2 + CH3CO3
R4N2 + hv → NO2 + .32*CH3COCH3 + .19*MEK + .18*CH3O2 + .27*HO2 + .32*CH3CHO + .13*RCHO
ClONO2 + hv → Cl + NO3
HOCl + hv → OH + Cl
Cl2O2 + hv → 2*Cl + O2
BrONO2 + hv → Br + NO3
HOBr + hv → OH + Br
BrCl + hv → Br + Cl
BrO + hv → Br + O
Cl2 + hv → 2*Cl

Reaction	**Rate Constant**
O + O2 + M → O3 + M	6.00e-34*(300/T)**2.4
O + O3 → 2*O2	8.00E-12*exp(-2060/T)
N + O2 → NO + O	1.50E-11*exp(-3600/T)
N + NO → N2 + O	2.10E-11*exp(100/T)
CO + OH + M → {CO2} + HO2	k0=5.90E-33*(300/T)**1.4 ki=1.10E-12*(300/T)**-1.3 f=0.6
CO + OH → {CO2} + H	k0=1.50E-13*(300/T)**-0.6 ki=2.10E+09*(300/T)**-6.1 f=0.6
H2 + O1D → HO2 + OH	1.20E-10
O + OH → H + O2	1.80E-11*exp(180/T)
HO2 + O → OH + O2	3.00E-11*exp(200/T)
OH + O3 → HO2 + O2	1.70E-12*exp(-940/T)
HO2 + O3 → OH + 2*O2	1.00E-14*exp(-490/T)
HO2 + HO2 → H2O2	k1 = 3.0E-13*exp(460/T) k2 = 2.1E-33*exp(920/T) k3 = 1.4E-21*exp(2200/T) k = (k1 + k2*[M]) * (1 + k3*[H2O])
H2O2 + OH → H2O + HO2	1.80E-12
OH + HO2 → H2O + O2	4.8E-11*exp(250/T)
OH + OH → H2O + O	1.80E-12
H2 + OH → H2O + HO2	2.8E-12*exp(-1800/T)
O1D + N2 → O + N2	2.15E-11*exp(110/T)
O1D + O2 → O + O2	3.3E-11*exp(55/T)
O1D + H2O → 2*OH	1.63E-10*exp(60/T)
N2O + O1D → 2*NO	7.25E-11*exp(20/T)
N2O + O1D → N2 + O2	4.63E-11*exp(20/T)
NO + HO2 → NO2 + OH	3.3E-12*exp(270/T)
NO + O3 → NO2 + O2	3E-12*exp(-1500/T)
NO2 + O → NO + O2	5.1E-12*exp(210/T)
NO2 + O3 → NO3 + O2	1.2E-13*exp(-2450/T)

NO3 + HO2 → OH + NO2	3.50E-12
NO2 + NO3 + M → N2O5 + M	k0=2.00E-30*(300/T)**4.0 ki=1.40E-12*(300/T)**0.7 f=0.6
N2O5 + M → NO2 + NO3 + M	K_{eq} = 2.70E-27*exp(11000/T)
N2O5 + H2O → 2*HNO3	0
NO2 + OH + M → HNO3 + M	k0=1.80E-30*(300/T)**3.0 ki=2.80E-11 f=0.6
HNO3 + OH → NO3 + H2O	k1=2.4E-14*exp(460/T) k2=2.7E-17*exp(2199/T) k3=6.5E-34*exp(1335/T) k = k1 + k3*[M] / (1 + k3*[M] / k2)
NO3 + NO → 2*NO2	1.5E-11*exp(170/T)
NO2 + HO2 + M → HO2NO2 + M	k0=2.00E-31*(300/T)**3.4 ki=2.90E-12*(300/T)**1.1 f=0.6
HO2NO2 + OH → H2O + NO2 + O2	1.3E-12*exp(380/T)
HO2NO2 + M → HO2 + NO2 + M	K_{eq} = 2.10E-27*exp(10900/T)
CH4 + OH → CH3O2 + H2O + LCH4	2.45E-12*exp(-1775/T)
CH4 + O1D → .75*CH3O2 + .75*OH + .25*CH2O + .2*HO2 + .2*H + .05*H2	1.50E-10
CH3O2 + NO → CH2O + NO2 + HO2	2.8E-12*exp(300/T)
CH3O2 + CH3O2 → 2*CH2O + 2*HO2	6.03E-13*exp(-453/T)
CH3O2 + CH3O2 → CH2O + CH3OH	2.3E-14*exp(677/T)
CH3O2 + HO2 → CH3OOH + O2	4.1E-13*exp(750/T)
CH3OOH + OH → .7*CH3O2 + .3*OH + .3*CH2O + H2O	3.8E-12*exp(200/T)
CH2O + NO3 → CO + HO2 + HNO3	3.4E-13*exp(-1900/T)
CH2O + OH → CO + H2O + HO2	5.5E-12*exp(125/T)
OH + C2H4 + M → .75*EO2 + .5*CH2O + .25*HO2 + M	k0=1.00E-28*(300/T)**4.50 ki=7.50E-12*(300/T)**0.85 f=0.6
EO2 + NO → EO + NO2	4.2E-12*exp(180/T)

EO + O2 → GLYALD + HO2	1.00E-14
EO → 2*CH2O + HO2	1.60E+11*exp(-4150/T)
C2H4 + O3 → CH2O + .12*HO2 + .5*CO + .12*OH	1.2E-14*exp(-2630/T)
C3H6 + OH + M → PO2 + M	k0=8.00E-27*(300/T)**3.5 ki=3.00E-11 f=0.5
C3H6 + O3 → .4*CH3CHO + .244*OH + .244*HO2 + .42*CO + .58*CH2O + .036*CH3OH	5.5E-15*exp(-1880/T)
C3H6 + NO3 → R4N2	4.6E-13*exp(-1156/T)
PO2 + NO → CH3CHO + CH2O + HO2 + NO2	2.7E-12*exp(350/T)
PO2 + HO2 → POOH + O2	7.5E-13*exp(700/T)
POOH + OH → .791*OH + .209*PO2 + .791*RCHO	8.78E-12*exp(200/T)
CH3CHO + OH → H2O + .95*CH3CO3 + .05*CH2O + .05*CO + .05*HO2	4.63E-12*exp(350/T)
CH3CHO + NO3 → CH3CO3 + HNO3	1.4E-12*exp(-1900/T)
CH3CO3 + NO → CH3O2 + {CO2} + NO2	8.1E-12*exp(270/T)
CH3CO3 + NO2 + M → PAN + M	k0=9.70E-29*(300/T)**5.6 ki=9.30E-12*(300/T)**1.5 f=0.6
CH3CO3 + HO2 → .15*O3 + .44*OH + .44*CH3O2 + .41*CH3COOOH	5.2E-13*exp(980/T)
CH3CO3 + CH3O2 → .9*CH3O2 + CH2O + .9*HO2 + .9*{CO2}	2E-12*exp(500/T)
CH3COOOH + OH → .5*CH3CO3 + .5*CH2O + .5*OH	3.8E-12*exp(200/T)
PAN + M → CH3CO3 + NO2 + M	K_{eq} = 9.00E-29*exp(14000/T)
CH3CO3 + CH3CO3 → 2*CH3O2 + 2*{CO2}	2.5E-12*exp(500/T)
C2H6 + OH → C2H5O2 + H2O	7.66E-12*exp(-1020/T)
C2H5O2 + NO → CH3CHO + HO2 + NO2	2.6E-12*exp(365/T)
C2H5O2 + HO2 → C2H5OOH + O2	7.5E-13*exp(700/T)
C2H5O2 + CH3O2 → .75*CH2O + .75*CH3CHO + HO2 + .25*CH3OH + .25*C2H5OH	3.00E-13

C2H5O2 + C2H5O2 → 2*CH3CHO + 2*HO2	4.10E-14
C2H5OOH + OH → .36*C2H5O2 + .64*CH3CHO + .64*OH	5.18E-12*exp(200/T)
C4H10 + OH → C3H7O2	1.55E-11*exp(-540/T)
C3H8 + OH → C3H7O2 + H2O	8.7E-12*exp(-615/T)
C3H7O2 + NO → .82*CH3COCH3 + NO2 + HO2 + .27*CH3CHO	4.2E-12*exp(180/T)
C3H7O2 + HO2 → C3H7OOH + O2	7.5E-13*exp(700/T)
C3H7O2 + CH3O2 → CH2O + HO2 + .82*CH3COCH3	3.75E-13*exp(-40/T)
C3H7OOH + OH → H2O + C3H7O2	3.8E-12*exp(200/T)
CH3COCH3 + OH → ATO2 + H2O	3.82e-11*exp(-2000/T) + 1.33e-13
OH + CH3OH → HO2 + CH2O	2.9E-12*exp(-345/T)
OH + C2H5OH → HO2 + CH3CHO	6.9E-12*exp(-230/T)
ISOP + OH → ISOPO2	3.1E-11*exp(350/T)
ISOPO2 → HO2 + CH2O + .25*MGLY + .5*GLYALD + 0.25*GLYX + .5*HYAC + OH	4.07E+08*exp(-7694/T)
ISOP + O3 → .325*MACR + .244*MVK + .845*CH2O + .11*H2O2 + .522*CO + .199*CH3CO3 + .026*HO2 + .27*OH + .128*C3H6 + .051*CH3O2	1E-14*exp(-1970/T)
ISOPO2 + NO → .90*NO2 + .90*HO2 + .90*CH2O + .55*MVK + .35*MACR + .10*ISOPNB	2.7E-12*exp(350/T)
ISOPO2 + HO2 → .937*ISOPOOH + .063*OH + .025*MACR + .038*MVK + .063*HO2 + .063*CH2O	2.06E-13*exp(1300/T)
ISOPO2 + CH3O2 → 1.1*HO2 + 1.22*CH2O + .28*MVK + .18*MACR + .3*RCHO + .24*CH3OH + .24*ROH	8.37E-14
ISOPO2 + ISOPO2 → 1.28*HO2 + .92*CH2O + .56*MVK + .36*MACR + .48*ROH + .5*RCHO	1.54E-13
ISOPNB + OH → ISOPNBO2	3.61E-12*exp(380/T)

ISOPNBO2 + NO → .09*GLYALD + .09*HYAC + .69*CH2O + 0.88*NO2 + .44*MACRN + .69*HO2 + .26*MVKN + 0.42*HNO3	2.4E-12*exp(360/T)
ISOPNBO2 + HO2 → .06*GLYALD + .06*HYAC + .44*CH2O + .28*MACRN + .16*MVKN + .06*NO2 + .44*HO2 + .5*OH + .5*HNO3	8.7E-14*exp(1650/T)
ISOPNB + O3 → .61*MVKN + .39*MACRN + .27*OH + CH2O	3.70E-19
ISOPOOH + OH → .387*ISOPO2 + .613*OH + .613*RCHO	4.75E-12*exp(200/T)
ISOPOOH + OH → OH + IEPOX	1.9E-11*exp(390/T)
IEPOX + OH → IEPOXOO	5.78E-11*exp(-400/T)
IEPOXOO + HO2 → .725*HYAC + .275*GLYALD + .275*GLYX + .275*MGLY + 1.125*OH + .825*HO2 + .375*CH2O + .251*CO	2.06E-13*exp(1300/T)
IEPOXOO + NO → .725*HYAC + .275*GLYALD + .275*GLYX + .275*MGLY + .125*OH + .825*HO2 + .375*CH2O + .251*CO + NO2	2.7E-12*exp(350/T)
MVK + OH → MVKO2	2.6E-12*exp(610/T)
MVK + O3 → .202*OH + .202*HO2 + .535*CO + .05*CH3CHO + .95*MGLY + .05*CH2O	8.5E-16*exp(-1520/T)
MVKO2 + NO → .965*NO2 + .249*HO2 + .249*CH2O + .716*CH3CO3 + .716*GLYALD + .249*MGLY + .035*MVKN	2.7E-12*exp(350/T)
MVKO2 + HO2 → .38*MVKOOH + .62*OH + .37*GLYALD + .37*CH3CO3 + .13*MEK + .25*HO2 + .12*CH2O + .12*MGLY + .033*RCHO	1.82E-13*exp(1300/T)
MVKO2 + CH3O2 → .14*HO2 + .14*CH2O + .36*CH3CO3 + .36*GLYALD + .14*MGLY + .25*MEK + .75*CH2O + .25*CH3OH + .25*ROH + .5*HO2	8.37E-14
MVKOOH + OH → .791*OH + .791*MEK + .209*MVKO2	8.78E-12*exp(200/T)
MVKN + OH → NO3 + .65*MGLY + .35*CH2O	1.60E-12
MACR + OH → .45*MAO3 + .55*MACRO2	8E-12*exp(380/T)

MACRO2 → CO + HYAC + OH	2.90E+07*exp(-5297/T)
MACR + O3 → .261*OH + .202*HO2 + .569*CO + .88*MGLY + 0.12*CH2O	1.4E-15*exp(-2100/T)
MACR + NO3 → MAO3 + HNO3	3.40E-15
MACRO2 + NO → .97*NO2 + .97*HO2 + .97*HYAC + .97*CO + .03*MACRN	2.7E-12*exp(350/T)
MACRO2 + HO2 → .42*MACROOH + .58*OH + .58*HYAC + .58*CO + .58*HO2	1.82E-13*exp(1300/T)
MACRO2 + CH3O2 → .595*HYAC + .255*MGLY + .595*CO + 1.255*CH2O + 1.7*HO2 + .15*ROH	8.37E-14
MACROOH + OH → MACRO2	1.84E-12*exp(200/T)
MACROOH + OH → HYAC + OH	4.4E-12*exp(380/T)
MACRN + OH → MACRNO2	3.20E-12
MACRNO2 + NO → .08*CH2O + .15*NO3 + .07*MGLY + .85*HYAC + 1.85*NO2	2.7E-12*exp(350/T)
MACRNO2 + HO2 → .08*CH2O + .15*NO3 + .07*MGLY + .85*HYAC + .85*NO2 + OH	1.82E-13*exp(1300/T)
MAO3 + NO → NO2 + .5*CH2O + .5*CO + .5*CH3O2 + .5*CH3CO3	6.7E-12*exp(340/T)
MAO3 + HO2 → .44*OH + .15*O3 + .59*CH2O + .39*CH3O2 + .41*MAOP + .39*CO	4.3E-13*exp(1040/T)
MAO3 + CH3O2 → CH2O + HO2 + CH2O + CH3CO3	1.68E-12*exp(500/T)
MAO3 + CH3O2 → CH2O	1.87E-13*exp(500/T)
MAO3 + NO2 + M → MPAN + M	k0=9.00E-28*(300/T)**8.90 ki=7.70E-12*(300/T)**0.20 f=0.6
MPAN → MAO3 + NO2	K_{eq} = 9.00E-29*exp(14000/T)
MAOP + OH → MAO3	6.13E-13*exp(200/T)
MAOP + OH → MAOPO2	3.6E-12*exp(380/T)
MAOPO2 + HO2 → HYAC + 2*OH	1.82E-13*exp(1300/T)
MAOPO2 + CH3O2 → .7*HYAC + .7*OH + CH2O + .7*HO2 + .3*C2H5OH	8.37E-14

MAOPO2 + NO → HYAC + OH + NO2	2.35E-12*exp(350/T)
MAOPO2 + NO → HNO3	3.5E-13*exp(350/T)
ATO2 + NO → .96*NO2 + .96*CH2O + .96*CH3CO3 + .04*R4N2	2.8E-12*exp(300/T)
ATO2 + HO2 → .15*CH3CO3 + .15*OH + .15*CH2O + .85*ATOOH	8.6E-13*exp(700/T)
ATOOH + OH → ATO2 + H2O	2.66E-12*exp(200/T)
ATOOH + OH → MGLY + OH + H2O	1.14E-12*exp(200/T)
MPAN + OH → HYAC + CO + NO2	2.90E-11
GLYALD + OH → .8*CH2O + .8*CO + HO2 + .2*GLYX	1.00E-11
GLYX + OH → HO2 + 2*CO	3.1E-12*exp(340/T)
GLYX + NO3 → HNO3 + HO2 + 2*CO	4.00E-16
MGLY + OH → CH3CO3 + CO	1.50E-11
MGLY + NO3 → HNO3 + CO + CH3CO3	1.4E-12*exp(-1860/T)
HYAC + OH → MGLY + HO2	1.6E-12*exp(305/T)
ISOP + NO3 → INO2	3.3E-12*exp(-450/T)
INO2 + NO → .7*ISN1 + .035*MVK + .035*MACR + .07*CH2O + .8*HO2 + 1.3*NO2 + .23*RCHO	2.7E-12*exp(350/T)
INO2 + NO3 → .7*ISN1 + .035*MVK + .035*MACR + .07*CH2O + .8*HO2 + 1.3*NO2 + .23*RCHO	2.30E-12
INO2 + HO2 → .22*MVK + .015*MACR + .235*OH + .235*NO2 + .235*CH2O + .765*INPN	2.06E-13*exp(1300/T)
INPN + OH → OH + NO2 + MEK	1.9E-11*exp(390/T)
INPN + OH → .36*INO2 + .64*R4N2 + .64*OH	5.18E-12*exp(200/T)
ISN1 + NO3 → ISNOOA + HNO3	3.15E-13*exp(-448/T)
ISNOOA + NO3 → NO2 + R4N2 + CO + HO2	4.00E-12
ISNOOA + NO → NO2 + R4N2 + CO + HO2	6.7E-12*exp(340/T)

ISNOOA + HO2 → .25*{RCOOH} + .25*O3 + HNO3	5.2E-13*exp(980/T)
ISN1 + O3 → .3*R4N2 + .45*CO + .15*OH + .45*HO2 + .7*GLYX + .7*OH + .7*NO2 + .7*MGLY	4.15E-15*exp(-1520/T)
ISN1 + OH → ISNOOA	7.48E-12*exp(410/T)
R4N2 + OH → R4N1 + H2O	1.60E-12
C10H16 + OH → 1.64*ISOPO2 + 0.1*CH3COCH3	1.2E-11*exp(440/T)
C10H16 + O3 → 1.122*MACR + .442*MVK + .765*O + 1.156*OH	5.3E-16*exp(-530/T)
C10H16 + NO3 → 1.7*ISOPO2 + NO2	1.2E-12*exp(490/T)
N2O5 → 2*HNO3	aerosol (γ=0.02)
NO3 → HNO3	aerosol (γ=0.02)
HO2 → H2O	aerosol (γ=0.2)
NO2 → 0.5*HNO3 + 0.5*OH + 0.5*NO	aerosol (γ=1e-5)
SO2 → SO4	aerosol (γ from Zheng et al. 2015)
SO2 + OH + M → SO4 + M	k0=3.30E-31*(300/T)**4.30 ki=1.60E-12 f=0.6
SO2 + H2O2 → SO4	in-cloud (Paulot et al. 2017)
SO2 + O3 → SO4	in-cloud (Paulot et al. 2017)
DMS + OH → SO2 + CH2O	1.2E-11*exp(-280/T)
DMS + OH → 0.75*SO2 + CH2O	k1=8.2E-39*exp(5376/T) k2=1.05E-5*exp(3644/T) k=k1*[O2]/(1+k2*[O2]/[M])
DMS + NO3 → SO2 + HNO3 + CH2O	1.9E-13*exp(530/T)
NH3 → NH4	aerosol (γ=0)
NH3 + OH → H2O + HNO3	1.7E-12*exp(-710/T)
H + O3 → OH + O2	1.40E-10*exp(-470/T)
H + O2 + M → HO2 + M	k0=4.40E-32*(300/T)**1.30 ki=4.70E-11*(300/T)**0.20 f=0.6

Cl + O3 → ClO + O2	2.3E-11*exp(-200/T)
O + ClO → Cl + O2	2.8E-11*exp(85/T)
ClO + NO → NO2 + Cl	6.4E-12*exp(290/T)
ClO + NO2 + M → ClONO2 + M	k0=1.80E-31*(300/T)**3.40 ki=1.50E-11*(300/T)**1.90 f=0.6
O + ClONO2 → ClO + NO3	2.9E-12*exp(-800/T)
Cl + CH4 → HCl + CH3O2	7.3E-12*exp(-1280/T)
OH + HCl → H2O + Cl	2.6E-12*exp(-350/T)
Cl + HO2 → HCl + O2	1.8E-11*exp(170/T)
ClO + HO2 → HOCl + O2	2.7E-12*exp(220/T)
ClO + OH → HO2 + Cl	7.4E-12*exp(270/T)
CH2O + Cl → HCl + HO2 + CO	8.1E-11*exp(-30/T)
OH + OH + M → H2O2 + M	k0=6.90E-31*(300/T)**1.00 ki=2.60E-11 f=0.6
ClO + ClO + M → Cl2O2 + M	k0=1.60E-32*(300/T)**4.50 ki=2.00E-12*(300/T)**2.40 f=0.6
Cl2O2 + M → 2*ClO + M	K_{eq} = 9.30E-28*exp(8835/T)
Br + O3 → BrO + O2	1.7E-11*exp(-800/T)
BrO + NO2 + M → BrONO2 + M	k0=5.20E-31*(300/T)**3.20 ki=6.90E-12*(300/T)**2.90 f=0.6
BrO + ClO → Br + Cl + O2	2.3E-12*exp(260/T)
BrO + HO2 → HOBr + O2	4.5E-12*exp(460/T)
BrO + NO → Br + NO2	8.8E-12*exp(260/T)
HOBr + O → BrO + OH	1.20E-10*exp(-430/T)
Br + HO2 → HBr + O2	4.8E-12*exp(-310/T)
Br + CH2O → HBr + HO2 + CO	1.7E-11*exp(-800/T)
HBr + OH → Br + H2O	5.5E-12*exp(200/T)
BrO + ClO → BrCl + O2	4.1E-13*exp(290/T)
ClO + OH → HCl + O2	6E-13*exp(230/T)

NO2 + NO3 → NO + NO2 + O2	4.5E-14*exp(-1260/T)
NO3 + NO3 → 2*NO2 + O2	8.5E-13*exp(-2450/T)
NO + O + M → NO2 + M	k0=9.00E-32*(300/T)**1.50 ki=3.00E-11 f=0.6
N + NO2 → N2O + O	5.8E-12*exp(220/T)
HOCl + HCl → H2O + Cl2	heterogeneous (Austin and Wilson, 2006)
N2O5 + HCl → HNO3 + Cl + NO2	heterogeneous (Austin and Wilson, 2006)
N2O5 + H2O → 2*HNO3	heterogeneous (Austin and Wilson, 2006)
ClONO2 + H2O → HOCl + HNO3	heterogeneous (Austin and Wilson, 2006)
ClONO2 + HCl → Cl2 + HNO3	heterogeneous (Austin and Wilson, 2006)
HOBr + HCl → BrCl + H2O	heterogeneous (Austin and Wilson, 2006)
HOCl + HBr → BrCl + H2O	heterogeneous (Austin and Wilson, 2006)
HOBr + HBr → 2*Br + H2O	heterogeneous (Austin and Wilson, 2006)
BrONO2 + H2O → HOBr + HNO3	heterogeneous (Austin and Wilson, 2006)

Notes:
Read 6.00E-34 as 6.00×10^{-34}.
T = temperature (K);
[M] = atmospheric density (molecules cm^{-3});
[O2] = molecular oxygen density (molecules cm^{-3});
[H2O] = water vapor density (molecules cm^{-3}).
a) Rate constants are given in units of s^{-1} for first-order reactions, cm^3 $molec^{-1}$ s^{-1} for second order reactions, and cm^6 $molec^{-2}$ s^{-1} for third-order reactions.
b) Three-body reaction rate constants are defined by: a = 1 + [$\log_{10}$(k0 * [M] / ki)]^2,
k = [(k0 * [M]) / (1 + k0 * [M] / ki)] * $f^{(1/a)}$.
c) Rate constants for dissociation reactions are calculated based on the rate constant (k_f) for the corresponding association ("forward") reaction and the equilibrium constant (K_{eq}) using: k = k_f / K_{eq}.