THE GEOS-CHEM

CHEMICAL MECHANISM

Version 5-07-8

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Table of Contents

List of species in GEOS-CHEM mechanism.....3

Format of the globchem.dat input file.....6

Kinetic Reactions.....10

Explanation of lettered flags in globchem.dat.....23

Notes on special kinetic reactions.....26

Photolysis Reactions.....27

Explanation of lettered flags for photolysis reactions.....29

Fast-J photolysis code input files.....30

Ratj.d.....30

Jv_spec.dat.....32

Species emitted and deposited in GEOS-CHEM.....40

Acknowledgments.....40

References.....41

List of Species in the GEOS-CHEM Chemical Mechanism

Species are listed in the same order as in the globchem.dat input file.

Symbol	Formula (a sample is given for lumped species)	Description
A3O2	CH3CH2CH2OO	primary RO2 from C3H8
ACET	CH3C(O)CH3	acetone
ACTA	CH3C(O)OH	acetic acid
ALD2	CH3CHO	acetaldehyde
ALK4	RH	≥C4 alkanes
ATO2	CH3C(O)CH2O2	RO2 from acetone
B3O2	CH3CH(OO)CH3	secondary RO2 from C3H8
C2H6	C2H6	ethane
C3H8	C3H8	propane
CH2O	CH2O	formaldehyde
CH4	CH4	methane
CO	CO	carbon monoxide
CO2	CO2	carbon dioxide
DRYDEP		generic entry for dry dep
EMISSION		generic entry to do emissions
EOH	C2H5OH	ethanol
ETO2	CH3CH2OO	ethylperoxy radical
ETP	CH3CH2OOH	ethylhydroperoxide
GCO3	HOCH2C(O)OO	hydroxy peroxyacetyl radical
GLCO3	HCOHC(O)OO	peroxyacyl from GLYX
GLP	HCOHC(O)OOH	peroxide from GLCO3
GLPAN	HCOHC(O)OONO2	peroxyacylnitrate from GLCO3
GLYC	HOCH2CHO	glycoaldehyde (hydroxyacetaldehyde)
GLYX	CHOCHO	glyoxal
GP	HOCH2C(O)OOH	peroxide from GCO3
GPAN	HOCH2C(O)OONO2	peroxyacylnitrate from GCO3
H	H	hydrogen atom
H2	H2	hydrogen molecule
H2O	H2O	water vapor
H2O2	H2O2	hydrogen peroxide
HAC	HOCH2C(O)CH3	hydroxyacetone
HCOOH	HCOOH	formic acid
HNO2	HONO	nitrous acid

HNO3	HNO3	nitric acid
HNO4	HNO4	pernitric acid
HO2	HO2	hydroperoxyl radical
IALD	HOCH2C(CH3)=CHCHO	hydroxy carbonyl alkenes from isoprene
IAO2	HOCH2C(CH3)(OO)CH(OH)CHO	RO2 from isoprene oxidation products
IAP	HOCH2C(CH3)(OOH)CH(OH)CHO	peroxide from IAO2
INO2	O2NOCH2C(OO)(CH3)CH=CH2	RO2 from ISOP+NO3
INPN	O2NOCH2C(OOH)(CH3)CH=CH2	peroxide from INO2
ISN1	HOCH2C(OO)(CH3)CH(ONO2)CH2OH	RO2 from ISN2
ISN2	CH2=C(CH3)CH(ONO2)CH2OH	isoprene nitrate
ISNO3	RONO2	stable organic nitrate
ISNP	HOCH2C(OOH)(CH3)CH(ONO2)CH2OH	peroxide from ISN1
ISOP	CH2=C(CH3)CH=CH2	isoprene
KO2	RO2 from >3 ketones	RO2 from >3 ketones
M		for three body reactions
MACR	CH2=C(CH3)CHO	methacrolein
MAN2	HOCH2C(ONO2)(CH3)CHO	RO2 from MACR+NO3
MAO3	CH2=C(CH3)C(O)OO	peroxyacyl from MVK and MACR
MAOP	CH2=C(CH3)C(O)OOH	peroxide from MAO3
MAP	CH3C(O)OOH	peroxyacetic acid
MCO3	CH3C(O)OO	peroxyacetyl radical
MEK	RC(O)R	>C3 ketones
MGLY	CH3COCHO	methylglyoxal
MNO3	CH3ONO2	methylnitrate
MO2	CH3OO	methylperoxy radical
MOH	CH3OH	methanol
MP	CH3OOH	methylhydroperoxide
MRO2	HOCH2C(OO)(CH3)CHO	RO2 from MACR+OH
MRP	HOCH2C(OOH)(CH3)CHO	peroxide from MRO2
MVK	CH2=CHC(O)CH3	methylvinylketone
MVN2	O2NOCH2CH(OO)C(O)CH3	RO2 from MVK+NO3
N2	N2	nitrogen
N2O	N2O	nitrous oxide
N2O5	N2O5	dinitrogen pentoxide
NH2	NH2	ammonia radical
NH3	NH3	ammonia
NO	NO	nitric oxide

NO2	NO2	nitrogen dioxide
NO3	NO3	nitrate radical
O	O	oxygen atom (3P)
O1D	O1D	oxygen atom (1D)
O2	O2	molecular oxygen
O2CH2OH	O2CH2OH	produced by CH2O+HO2
O3	O3	ozone
OH	OH	hydroxyl radical
PAN	CH3C(O)OONO2	peroxyacetylnitrate
PMN	CH2=C(CH3)C(O)OONO2	peroxymethacryloyl nitrate (MPAN)
PO2	HOCH2CH(OO)CH3	RO2 from propene
PP	HOCH2CH(OOH)CH3	peroxide from PO2
PPN	CH3CH2C(O)OONO2	peroxypropionylnitrate
PRN1	O2NOCH2CH(OO)CH3	RO2 from propene + NO3
PRPE	C3H6	≥C4 alkenes
PRPN	O2NOCH2CH(OOH)CH3	peroxide from PRN1
R4N1	RO2 from R4N2	RO2 from R4N2
R4N2	RO2NO	≥C4 alkylnitrates
R4O2	RO2 from ALK4	RO2 from ALK4
R4P	peroxide from R4O2	peroxide from R4O2
RA3P	peroxide from A3O2	peroxide from A3O2
RB3P	peroxide from B3O2	peroxide from B3O2
RCHO	CH3CH2CHO	>C2 aldehydes
RCO3	CH3CH2C(O)OO	peroxypropionyl radical
RCOOH	C2H5C(O)OH	>C2 organic acids
RIO1	HOCH2C(OO)(CH3)CH=CHOH	RO2 from isoprene oxidation products
RIO2	HOCH2C(OO)(CH3)CH=CH2	RO2 from isoprene
RIP	HOCH2C(OOH)(CH3)CH=CH2	peroxide from RIO2
ROH	C3H7OH	>C2 alcohols
RP	CH3CH2C(O)OOH	peroxide from RCO3
VRO2	HOCH2CH(OO)C(O)CH3	RO2 from MVK+OH
VRP	HOCH2CH(OOH)C(O)CH3	peroxide from VRO2
DMS	(CH3)2S	dimethylsulfide
SO2	SO2	sulfur dioxide
SO4	SO4	sulfate radical
MSA	CH4SO3	methylsulfonic acid

Format of the globchem.dat input file

The format for how to read the globchem.dat input file is provided below as comments cut and pasted from readchem.f by Mark Jacobson. GEOS-CHEM uses his smvgear solvers [*Jacobson*, 1994]; the current GEOS-CHEM model version includes the recent smvgear II solver.

Note that although different types of chemistry (e.g. urban, stratospheric, free tropospheric) are available in smvgear II, we currently run the same chemistry everywhere in the troposphere; stratospheric influence on troposphere is currently parameterized (in subroutine upbdflx_mod.f). As a result, the initial concentrations for different types of chemistry are all identical (first line of initial block of information, see comments directly below READCHEM header).

We do not use the mass balance capability of smvgearII, which is why the second line of the intial block of information (see below READCHEM header) in globchem.dat is all zeroes.

We do not use the "AB" parameter (all set to 1.0 in globchem.dat) which tells whether a species absorbs radiation – see FAST-J code and later in this document for the radiative transfer calculations in GEOS-CHEM. Photolysis reactions are the last set of reactions to be read in from globchem.dat; rates are calculated by FAST-J.

Arlene's comments below are labeled as "AF:".

```
C
C ******************************************************************
C ************        WRITTEN BY MARK JACOBSON (1990-4)    ************
C ***                        (650) 723-6836                       ***
C ******************************************************************
C
C  RRRRRR   EEEEEEE     A     DDDDDD  CCCCCCC  H     H  EEEEEEE M     M
C  R     R  E          A A    D     D C        H     H  E       M M M M
C  RRRRRR   EEEE      A   A   D     D C        HHHHHHH  EEEEEEE M  M  M
C  R  R     E        AAAAAAA  D     D C        H     H  E       M     M
C  R   R    EEEEEEE A       A DDDDDD  CCCCCCC  H     H  EEEEEEE M     M
C
C ******************************************************************
C *  THIS IS THE SETUP ROUTINE FOR GAS-PHASE CHEMISTRY. IT READS      *
C *  SPECIES NAMES, CHEMICAL REACTIONS, AND PHOTOPROCESSES FROM AN    *
C *  INPUT DATA SET. IT THEN PLACES ALL NECESSARY INFORMATION INTO    *
C *  ARRAYS AND PRINTS OUT THE INPUT INFORMATION.                     *
C ******************************************************************
```

AF: The comments below describe how to read the first block of information in globchem.dat. A sample line being read looks like:

```
A A302                1.00 1.000E-20 1.000E-20 1.000E-20 1.000E-20
                      0   0   0   0   0   0   0   0   0
```

```
C ******************************************************************
C * READ IN THE SPECIES AND OTHER DATA FOR THIS RUN FROM INPUT DATA   *
C ******************************************************************
C
```

```
C                    ITEMS IN THE FIRST READ STATEMENT
C                    ---------------------------------
C
C A/I/D
C         D = SPECIES IS DEAD AND NOT USED
C         I = INACTIVE BUT USED (THESE SPECIES MUST ALSO BE INITIALIZED)
C         A = SPECIES USED WHEN IFURBAN, IFTROP, OR IFSTRAT > 0
C             (URBAN, TROPSOSPHERIC AND STRATOSPHERIC SETS)
C         U = SPECIES USED WHEN IFURBAN > 0
C         S = SPECIES USED WHEN IFSTRAT > 0
C         T = SPECIES USED WHEN IFTROP  > 0
C         R = SPECIES USED WHEN IFURBAN OR IFTROP  > 0
C         H = SPECIES USED WHEN IFTROP  OR IFSTRAT > 0
C SPEC      = NAME OF THE SPECIES,
C AB          TELLS WHETHER SPECIES ABSORBS RADIATION (THE SPECIES
C             DOES NOT NECESSARILY PHOTOLYZE)
C MW        = ATOMIC MASS IN AMU;
C IFSTRAT   = 1: SOLVE STRATOSPHERIC CHEMISTRY
C IFTROP    = 1: SOLVE FREE TROPOSPHERIC CHEMISTRY
C IFURBAN   = 1: SOLVE URBAN CHEMISTRY
C INITCONC  = DEF'T BACKGROUND CONC. AT LOWEST LEVEL (VOL MIXING RATIO);
C CSTRAT    = DEFAULT VOL MIX RATIO (FRACTION) IN STRATOSPHERE (25 KM)
C CTROPL    = DEFAULT VOL MIX RATIO (FRACTION) IN FREE TROP OVER LAND (0 KM)
C CTROPS    = DEFAULT VOL MIX RATIO (FRACTION) IN FREE TROP OVER SEA  (0 KM)
C CURBAN    = DEFAULT VOL MIX RATIO (FRACTION) IN URBAN REGIONS (0 KM)
C
C ********************************************************************
C ******************** READ IN SPECIES INFORMATION ********************
C ********************************************************************
C
C            FORMAT OF ITEMS IN THE SPECIES-LIST READ STATEMENT
C
C A/I/D SPEC   AB   MW  CSTRAT CTROPL CTROPS  CURBAN
C A1,1X, A14,A2,1X,F6.0,E9.2,  E9.2,  E9.2    E9.2
C
C        S     NO3  NH4     C    CL    BR    F     H     O
C 20X,   I2,2X,I2,2X,I2,2X,I2,2X,I2,2X,I2,2X,I2,2X,I2,2X,I2
C*************************************************************************
```

AF: the comments below describe how to read the reaction rates (second block of information) in globchem.dat. A sample line is:

```
A   21 2.00E-12  0.0E+00  -1400 0     0.00     0.     0.
      O3            +     NO
=1.000NO2           +1.000O2            +                   +
+                   +                   +                   +
+                   +                   +                   +
+                   +                   +                   +
```

```
C
C ********************************************************************
C *****************    READ IN REACTION RATES   **********************
C ********************************************************************
C
C HERE, WE CAN HAVE 3 REACTANTS (EACH WITH COEFFICIENT OF 1) AND 12
C             PRODUCTS [EACH WITH ANY REAL COEFFICIENT].
C FOR A 3-BODY M REACTION, PLACE AN M IN THE THIRD REACTANT POSITION
C             [NO [+] BEFORE IT]
```

```
C FOR A 3-BODY OTHER SPECIES REACTION, PLACE THE SPECIES NAME IN THE THIRD
C             REACTANT POSITION [NO [+] BEFORE IT]
C FOR A 3RD REACTANT, PLACE THE SPECIES NAME IN THE THIRD REACTANT POSITION
C             WITH A PLUS BEFORE IT.
C FOR A REACTANT NOT INCLUDED IN THE REACTION RATE [I.E.02] PLACE THE
C             SPECIES NAME IN THE FOURTH REACTANT POSITION [NO [+]
C             BEFORE IT]. THE SPECIES MAY HAVE A COEFFICIENT PRECEDING IT.
C A PRODUCT MAY EITHER BE LISTED TWICE [OR MORE TIMES] OR
C             HAVE A COEFFICIENT [I.E. 2 OR 3, 0.34] IMMEDIATELY BEFORE IT.
C N COLUMN:   NUMBER OF RATE COEFFICIENT LINES FOLLOWING TOP LINE
C P COLUMN:
C   P         = REACTION IS PRESSURE DEPENDENT 3-BODY REACTION.
C               THE FIRST COEFFICIENT IS A 3-BODY COEF. THE SECOND IS 2-BODY.
C   S         = IDENTIFIES A ONE-BODY SURFACE REACTION
C   E         = IDENTIFIES REVERSE EQUILIBRIUM REACTION
C   V         = IDENTIFIES CH3SCH3 + OH --> CH3S(OH)CH3
C   W         = IDENTIFIES O(1D) + N2 OR O2
C   X         = IDENTIFIES OH  + HNO3
C   Y         = IDENDIFIES OH  + CO
C   Z         = IDENDIFIES HO2 + HO2
C
C Fc COLUMN   = VALUE OF Fc FOR THREE-BODY RATE REACTIONS (SEE REF 9, P.1145)
C Fc(T)       = Fc CALCULATED AS EXP(-T(K)/Fc(T))
C
C REACTION RATES HAVE THE FORM K = A * (300 / T)**B * EXP(C / T)
C
C ********************************************************************
C *                     READ PRELIMINARY COMMENTS                    *
C ********************************************************************
C
C                   ----- REACTION RATE FORMAT -----
C
C A/D ORD AR BR CR N P Fc FcT COM    X  +Y  +Z  IV  =aA  +bB  +cC  +dD  +...
C
C A/D
C   D       = REACTION IS DEAD. SKIP THIS REACTION.
C   A       = REACTION ACTIVE AND INCLUDED IN ALL CHEMISTRY SETS
C             (URBAN, TROPSOSPHERIC AND STRATOSPHERIC SETS)
C   U       = REACTION IN URBAN CHEMISTRY SET
C   S       = REACTION IN STRATOSPHERIC CHEMISTRY SET
C   T       = REACTION IN TROPOSPHERIC CHEMISTRY SET
C   R       = REACTION IN TROPOSPHERIC AND URBAN CHEMISTRY SETS
C   H       = REACTION IN TROPOSPHERIC AND STRATOSPHERIC CHEMISTRY SETS
C ORD       = ORDINAL NUMBER OF REACTION
C AR,BR,CR  = RATE COEFFICIENTS: K = AR * (300/T) * BR * EXP( CR / T)
```

AF: note typo above - should actually be K = AR * (300/T) BR * EXP(CR / T)**

```
C AR        = DEFAULT PHOTORATE (S-1) FOR PHOTOPROCESSES
C NCOF      = DESCRIBED IN 'N COLUMN' ABOVE
C P         = DESCRIBED IN 'P COLUMN' ABOVE
C FCVT       = CHARACTERIZES FALLOFF CURVE IN PRESSURE-DEPENDENT REACTION
C FCT1T,2T  = EXPONENTS GIVING TEMPERATURE DEPENDENCE OF FCVT
C             FCVT = EXP(-T/FCT1)     OR
C             FCVT = EXP(-T/FCT1) + EXP(-FCT2/T)
C COM       = A9 AT THE END IS CURRENTLY FOR COMMENTS.
C X,Y,Z     = REACTANTS
```

```
C Z          = REACTANT OR 3RD BODY 'M' OR OTHER THIRD BODY
C I          = COEFFICIENT (INTEGER) FOR V
C V          = REACT NOT INCLUDED IN REACT. RATE, BUT WHICH IS LOST IN
REACTION.
C a,b,c,d.   = COEFFICIENTS FOR PRODUCTS (1,2,3,0.45,1.32, ETC (>=0.))
C A,B,C,D.. = PRODUCTS
C
C*********************************************************************
```

Kinetic Reactions in the GEOS-CHEM Mechanism

Reactions are in the order in which they are presented in the globchem.dat input file.

Reactions are read in by readchem.f. Rate constants are calculated in calcrate.f which then calls the smvgear chemistry solver.

Lettered flags (in the Flag column) specify reactions that are hard-wired to be treated explicitly in the code.

Numbered notes (in the reference column) provide explanations for how the specified reaction rate is determined.

HPL = High Pressure Limit; LPL = low pressure limit

Reaction	Rate constant	Reference	Date updated	Flag	
O3+NO = NO2+O2	~~2.00E-12 exp(-1400/T)~~	~~JPL97~~			X
	3.00E-12 exp(-1500/T)	JPL00	7/2003		X
O3+OH = HO2+O2	~~1.60E-12 exp(-940/T)~~	~~JPL97~~			~~X~~
	~~1.50E-12 exp(-880/T)~~	~~JPL00~~	~~7/2003~~		~~X~~
	1.70E-12 exp(-940/T)	JPL02	7/2003		X
O3+HO2 = OH+2O2	~~1.10E-14 exp(-500/T)~~	~~JPL97~~			X
	~~2.00E-14 exp(-680/T)~~	~~JPL00~~	~~7/2003~~		X
	1.00E-14 exp(-490/T)	JPL02	7/2003		X
O3+NO2 = O2+NO3	1.20E-13 exp(-2450/T)	JPL97			X
O3+MO2 = CH2O+HO2+2O2	~~3.00E-16 exp(-1000/T)~~	~~New reaction added: Tyndall~~	~~8/2001~~		X
	2.90E-16 exp(-1000/T)	JPL02	7/03		X
OH+OH = H2O+O3	4.20E-12 exp (-240/T)	JPL97			X
OH+OH+M = H2O2	~~LPL: 6.2E-31 (300/T)~~ ~~HPL:2.60E-11~~ ~~Fc: 0.6~~	~~JPL97~~		P	X
	LPL: 6.9E-31(300/T) HPL: 2.60E-11 Fc:0.6	JPL02	07/2003		X
OH+HO2 = H2O + O2	4.80E-11 exp (250/T)	JPL97			X
OH+H2O2 = H2O + HO2	2.90E-12 exp (-160/T)	JPL97			X
HO2+NO = OH + NO2	3.50E-12 exp(250/T)	JPL97			X
HO2+HO2 = H2O2 HO2+HO2+M=H2O2	K1=2.30E-13 exp(600/T) K2=1.70E-33 exp(1000/T) K = (K1 + K2)*(1+1.4E-21*[H2O]*EXP(2200/T)	JPL97		Z	X

	)				
OH+H2 = H2O + HO2	5.50E-12 exp(-2000/T)	JPL97			X
CO+OH = HO2 + CO2	K0=1.50E-13 K = K0(1+0.6 Patm)	JPL97		Y	X
OH+ CH4 = MO2+H2O	1.26E-12 (300/T)^ (-6.7E-01) exp(-1575/T)	JPL97			X
MO2+NO = CH2O+HO2+NO2	~~3.00E-12 exp(280/T~~	~~JPL97~~			X
	2.80E-12 exp(300/T)	Tyndall; see note 1.	8/2001		~~X~~
MO2+HO2 = MP+O2	~~3.80E-13 exp (800/T)~~	~~JPL92~~		~~V~~	~~X~~
	K1=4.10E-13 exp(750/T) K2=2.00E-03 exp(1160/T) K=K1 / (1+K2)	Tyndall & Elrod et al. [2001] Added 2nd rxn branch	8/2001	V	X ? B R
MO2+HO2 = CH2O + O2	K1=4.10E-13 exp(750/T) K2=4.98E+2 exp(- 1160/T) K=K1 / (1+K2)	Tyndall, Elrod et al. [2001]	8/2001	V	X
MO2+MO2 = MOH+CH2O+O2	K=K1 / (1+K2) ~~K1=2.50E-13 exp~~ ~~(190/T)~~ ~~K2=1.9E+1 exp(-1130/T)~~	~~JPL97~~		V	X
	K1=9.5E-14 exp(390/T) K2=2.62E+1 exp(- 1130/T)	Tyndall	8/2001		X
MO2+MO2 = 2CH2O + 2HO2	K1=9.5E-14 exp(390/T) K2=4.00E-02 exp(1130/T) K=K1 / (1+K2)	Tyndall	8/2001	V	X
MP+OH = MO2+H2O	2.66E-12 exp(200/T)	JPL97			X
MP+OH = CH2O+OH+H2O	1.14E-12 exp(200/T)	JPL97			X
CH2O+OH = CO+HO2+H2O	~~1.00E-11~~	~~JPL97~~			~~X~~
	9.00E-12	JPL 02	7/2003		X
NO2+OH+M = HNO3+M	~~LPL: 2.47E-30(300/T)^3~~ ~~HPL:1.45E-~~ ~~11(300/T)^2.8~~ ~~Fc: 0.6~~	~~Dransfield et al., 1999.~~		P	X
	LPL: 2.00E-30(300/T)^3 HPL:2.50E-11(300/T)^0 Fc: 0.6	JPL 02	7/2003		X
HNO3+OH = H2O+NO3	K0=2.41E-14 exp(460/T) K2=2.69E-17 exp(2199/T)	Brown 98; see note X.		X	X

	K3=6.51E-34 exp(1335/T)				
NO+OH+M = HNO2+M	LPL: 7.00E-31(300/T)^2.6 HPL:3.60E-11(300/T)^0.1 Fc: 0.6	JPL97		P	X
HNO2+OH = H2O+NO2	1.80E-11 exp(-390/T)	JPL97			X
HO2+NO2+M = HNO4+M	LPL: 1.80E-31(300/T)^3.2 HPL:4.7E-12(300/T)^1.4 Fc= 0.6	JPL97		P	X
HNO4+M = HO2+NO2	LPL: 8.64E-5(300/T)^3.2* exp(-10900/T) HPL:2.24E+15*(300/T)^1.4*exp(-10900/T); Fc= 0.6	K=forward rxn/Keq Keq=2.1E-27 exp (10900/T) JPL97		P	X
HNO4+OH = H2O+NO2+O2	1.30E-12 exp(380/T)	JPL97			X
HO2+NO3 = OH+NO2+O2	3.50E-12	JPL97 (k 298; T-dep unknown)			X
NO+NO3 = 2NO2	1.50E-11 exp(170/T)	JPL97			X
OH+NO3 = HO2+NO2	2.20E-11	JPL97 (k298; T-dep unknown			X
NO2+NO3+M = N2O5+M	~~LPL: 2.2E-30(300/T)^3.9 HPL:1.5E-12(300/T)^0.7 Fc=0.6~~	~~JPL97~~		~~P~~	~~X~~
	LPL: 2.0E-30(300/T)^4.4 HPL:1.4E-12(300/T)^0.7 Fc=0.6	JPL00	7/2003	P	X
N2O5+M = NO2+NO3	~~LPL: 8.15E-4(300/T)^3.9* exp(-11000/T) HPL:5.56E+14*(300/T)^0.7*exp(-11000/T); Fc= 0.6~~	~~K=forward rxn/ Keq Keq = 2.70E-27exp (11000/T) JPL97~~		~~P~~	~~X~~
	LPL: 6.67E-4(300/T)^4.4* exp(-10990/T) HPL:4.67E+14*(300/T)^0.7*exp(-10990/T); Fc= 0.6	K=forward rxn/ Keq Keq = 3.00E-27exp (10990/T) JPL00	7/2003	P	X

HCOOH+OH = H2O+CO2+HO2	4.00E-13	JPL97			X
MOH+OH = HO2+CH2O	~~6.70E-12 exp(-600/T)~~	~~JPL97~~			X
	7.30E-12 exp(-620/T)	JPL02			X
NO2+NO3 = NO+NO2+O2	4.50E-14 exp(-1260/T)	JPL97			X
NO3+CH2O = HNO3+HO2+CO	5.80E-16	JPL97 k298			X
ALD2+OH = MCO3+H2O	5.60E-12 exp(270/T)	JPL97			X
ALD2+NO3 = HNO3+MCO3	1.40E-12 exp(-1860/T)	IUPAC 02			X
MCO3+NO2+M = PAN	~~LPL: 9.70E-29(300/T)^5.6~~ ~~HPL:9.30E-12(300/T)^1.5~~ ~~Fc: 0.6~~	~~JPL97~~		~~P~~	~~?~~
	LPL: 8.50E-29(300/T)^6.5 HPL:1.10E-11(300/T) Fc: 0.6	Tyndall	8/2001	P	?
PAN = MCO3+NO2	1.10E-11 (300/T)	Atkinson92, Tyndall, see note 13	8/2001	E	X
	9.30E-29 exp(14000/T)	Tyndall	8/2001	E	X
MCO3+NO = MO2+NO2+CO2	~~5.30E-12 exp(360/T)~~	~~JPL97~~			X
	8.10E-12 exp(270/T)	Tyndall; see note 6.	8/2001		X
C2H6+OH = ETO2+H2O	8.7E-12 exp(-1070/T)	JPL97			X
ETO2+NO = ALD2+NO2+HO2	~~2.60E-12 exp(365/T)~~	~~JPL97~~			?
	2.70E-12 exp(350/T)	Tyndall (notes 4 & 5)	8/2001		X
C3H8+OH = B3O2	~~6.30E-12 exp(-580/T)~~	~~JPL97~~			~~X~~
	K1=7.60e-12 exp(-585/T) K2= 5.87*(300/T)^0.64exp(-816/T) K=K1 / (1+K2)	IUPAC02 See appendix mje_1	7/2003		X
C3H8+OH = A3O2	~~6.30E-12 exp(-1050/T)~~	~~JPL97~~			~~X~~
	K1=7.60E-12 exp(-585/T) K2= 0.17*(300/T)^-0.64exp(816/T) K=K1 / (1+K2)	IUPAC02 See appendix mje_1	7/2003		X

A3O2+NO = NO2 + HO2 + RCHO	2.70E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		
PO2+NO = NO2+HO2+CH2O+ALD2	2.70E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
ALK4+OH = R4O2	~~8.20E-12 exp(-300/T)~~	~~Atkinson 92~~			X
	9.10E-12 exp(-405/T)	IUPAC02	7/2003		X
R4O2+NO = NO2 + 0.32ACET + 0.19MEK + 0.18MO2 + 0.27HO2 + 0.32ALD2 + 0.13RCHO + 0.50A3O2 + 0.18B3O2 + 0.32ETO2	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.50E00)	Atkinson 97		B	?
R4O2+NO = R4N2	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.50E00)	Atkinson 97		A	?
R4N1+NO = 2NO2 + 0.39CH2O + 0.75ALD2 + 0.57RCHO + 0.30R4O2	2.70E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
ATO2+NO = 0.96NO2 + 0.960CH2O +0.960MCO3 + 0.04R4N2	~~2.70E-12 exp (360/T)~~	~~(see note 9)~~ ~~Atkinson 92~~			~~X~~
	2.80E-12 exp(300/T)	Tyndall	8/2001		X
KO2+NO = 0.93NO2+ 0.93NO + 0.93ALD2 + 0.93MCO3 + 0.07R4N2	2.70E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
RIO2+NO = NO2+ 0.864HO2+0.690CH2O+ 0.402MVK+0.288MACR +0.136RIO1+0.127IALD	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	Atkinson 97		B	?
RIO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	Atkinson 97		A	?
RIO1+NO = NO2+IALD +HO2+0.75CH2O	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	Atkinson 97		B	?
RIO1+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=5.00E00)	Atkinson 97		A	?
IAO2+NO = 0.92HO2+ 0.61CO+0.17H2+	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X

0.33HAC+0.24GLYC + 0.53MGLY+0.92NO2 + 0.35CH2O+0.08HNO3					
ISN1+NO = 1.9NO2+ 0.95GLYC+0.95HAC + 0.05HNO3+0.05NO2	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
VRO2+NO = NO2+ 0.28HO2+0.28CH2O+ 0.72MCO3+0.72GLYC+ 0.28MGLY	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97		B	?
VRO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97		A	?
MRO2+NO = NO2+HO2 + 0.17MGLY+0.83HAC + 0.83CO+0.17CH2O	K* (1-YN) where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97		B	?
MRO2+NO = HNO3	K* YN where YN is returned from fyrno3.f K=2.7E-12 exp(350/T) (Xcarbn=4.00E00)	Atkinson 97		A	?
MVN2+NO = 1.90NO2 + 0.30HO2+0.30CH2O+ 0.60MCO3+0.60GLYC+ 0.30MGLY+0.10HNO3	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
MAN2+NO = 2NO2+ CH2O+MGLY	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
B3O2+NO = NO2+HO2+ ACET	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
INO2+NO = 1.10NO2+ 0.80HO2+0.85HNO3+ 0.05NO2+0.10MACR+ 0.15CH2O+0.05MVK	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
PRN1+NO = 2NO2+ CH2O+ALD2	2.7E-12 exp(350/T)	Tyndall ETO2+NO	8/2001		X
ALK4+NO3 = HNO3 + R4O2	~~6.00E-17~~	~~Atkinson 92~~			X
	2.8E-12 exp(-3280/T)	IUPAC02	7/2003		X
R4N2+OH = R4N1+H2O	1.30E-12	Atkinson 92	? Can't find		
ACTA+OH = MO2+CO2 +H2O	4.00E-13 exp(200/T)	DeMore et al., 1994			X
OH+RCHO= RCO3+H2O	~~2.00E-11~~	~~Atkinson92,9~~ 4			X

	5.10E-12 exp(405/T)	IUPAC02	7/2003		X
RCO3+NO2 = PPN	~~1.10E-11 (300/T)~~	~~Atkinson92, Tyndall, see note 13~~	~~8/2001~~		X
	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02	7/2003	P	X
PPN = RCO3+NO2	~~2.80E+16 exp (-13850/T)~~	~~Tyndall PAN high pressure decomp. rate~~	~~8/2001~~		~~X~~
	9e-29*exp(14000)	JPL02	7/2003	E	X
MAO3+NO2 = PMN	~~1.10E-11 (300/T)~~	~~Ibid.~~	~~8/2001~~		
	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same as PPN	7/2003	P	X
PMN = MAO3+NO2	~~2.80E16 exp (-13580/T)~~	~~Tyndall PAN high pressure decomp. rate~~	~~8/2001~~		X
	9e-29*exp(14000)	JPL02	7/2003	E	X
GLCO3+NO2 = GLPAN	~~1.10E-11 (300/T)~~	~~Ibid.~~	~~8/2001~~		
	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same as PPN	7/2003	P	X
GLPAN = GLCO3+NO2	~~2.80E+16 exp (-13850/T)~~	~~Tyndall PAN high pressure decomp. rate~~	~~8/2001~~		~~X~~
	9e-29*exp(14000)	JPL02 PPN	7/2003	E	X
GCO3+NO2 = GPAN	~~1.10E-11 (300/T)~~	~~Ibid.~~	~~8/2001~~		
	LPL: 9.00E-28(300/T)^8.9 HPL:7.70E-12(300/T)^0.2 Fc: 0.6	JPL02 Same as PPN	7/2003	P	X
GPAN = GCO3+NO2N	~~2.80E+16 exp (-13850/T)~~	~~Tyndall PAN high pressure decomp. rate~~	~~8/2001~~		~~X~~
	9e-29*exp(14000)	JPL02 PPN	7/2003	E	X
RCO3+NO = NO2+ETO2	~~8.10E-12 exp(270/T)~~	~~Tyndall MCO3+NO~~	~~8/2001~~		X
	6.70E-12 exp(340/T)	IUPAC02	7/2003		X

		$C_2H_5CO_3$+NO			
GCO3+NO = NO2+HO2 + CH2O	~~8.10E-12 exp(270/T)~~	~~Tyndall MCO3+NO~~	~~8/2001~~		X
	6.70E-12 exp(340/T)	IUPAC02 $C_2H_5CO_3$+NO	7/2003		X
GLCO3+NO = NO2+HO2 +CO	~~8.10E-12 exp(270/T)~~	~~Tyndall MCO3+NO~~	~~8/2001~~		~~X~~
	6.70E-12 exp(340/T)	IUPAC02 $C_2H_5CO_3$+NO	7/2003		X
RCHO+NO3 = HNO3 + RCO3	~~1.40E-12 exp(-1860/T)~~	~~Atkinson92,94 (ALD2)~~			~~X~~
	1.82E-12exp(-1680/T)	IUPAC02 Mean of CH3CHO+NO3 and C3H7CH+NO3			X
ACET+OH = ATO2 + H2O	~~2.20E-12 exp(-685/T)~~	~~JPL97~~			X
	1.33E-13+ 3.82E-11 exp(-2000/T)	JPL 02 Implemented as 2 reactions	7/2003		X
A3O2+MO2 = HO2 + 0.75CH2O+0.75RCHO+ 0.25MOH + 0.25ROH	5.92E-13	Tyndall Rate MO2+MO2 Atkinson97 RO2+RO2 (see note10 below)	8/2001		?
PO2+MO2 = HO2 + 0.5ALD2+1.25CH2O + 0.16HAC + 0.09RCHO + 0.25MOH + 0.25ROH	5.92E-13	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (see note 10 below)	8/2001		?
R4O2+HO2 = R4P	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
R4N1+HO2 = R4N2	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
ATO2+HO2 = MCO3 + MO2	~~1.90E-13 exp (1300/T)~~	~~Atkinson 97~~			X
	8.60E-13 exp(700/T)	Tyndall; see note 7	8/2001		X
KO2+HO2 = MO2 + MGLY	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
RIO2+HO2 = RIP	7.40E-13 exp(700/T)	Tyndall	8/2001		X

		ETO2+HO2			
RIO1+HO2 = RIP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
IAO2 + HO2 = IAP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
ISN1+HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
VRO2+HO2 = VRP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
MRO2+HO2 = MRP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
MVN2 + HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
MAN2 + HO2 = ISNP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
B3O2+HO2 = RB3P	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
INO2 + HO2 = INPN	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
PRN1 + HO2 = PRPN	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
MEK+OH = KO2+H2O	~~2.92E-13 * (300/T)^-2 * exp(414/T)~~	~~Atkinson 90~~			~~X~~
	2.28E-13 * (300/T)^-2 * exp(503/T)	IUPAC02	7/2003		X
MO2+ETO2 = 0.75CH2O +0.75ALD2+HO2+ 0.25MOH+0.25EOH	3.00E-13	Horowitz 98, Atkinson 92 & 94			?
MEK+NO3 = HNO3+ KO2	8.00E-16	Lurmann et al., 1986.			?
R4O2+MO2 = 0.16ACET +0.10MEK+0.09MO2+ 0.14HO2+0.16ALD2 + 0.07RCHO+0.03A3O2 + 0.09B3O2+0.16ETO2+ 0.25MEK+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
R4N1+MO2 = NO2+ 0.20CH2O+0.38ALD2 + 0.29RCHO+0.15R4O2+ 0.25RCHO+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
ATO2+MO2 = 0.30HO2+ 0.30CH20+0.30MCO3+	~~9.70E-14~~	~~secondaryRO2+MO2~~			X

0.20HAC+0.20CH2O+ 0.50MGLY+0.50MOH		~~(note 11)~~	~~8/2001~~		
	7.5E-13 exp(500/T)	Tyndall, 2001	8/2001		X
KO2+MO2 = 0.5ALD2 + 0.50MCO3+0.25MEK+ 0.75CH2O+0.25MOH+ 0.25ROH+0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
RIO2+MO2 = 0.42HO2 + 0.35CH2O+0.2MVK + 0.14MACR + 0.07RIO1 + 0.06IALD+0.25MEK+ 0.75CH2O+0.25MOH+ 0.25ROH + 0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
RIO1+MO2 = 0.50IALD+ 0.50HO2+0.38CH2O+ 0.25MEK+0.75CH2O+ 0.25MOH+0.25ROH+ 0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
IAO2+MO2 = 0.50HO2+ 0.33CO+0.09H2+ 0.18HAC+0.13GLYC+ 0.29MGLY+0.25MEK+ 0.95CH2O+0.25MOH+ 0.25ROH+0.5HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
ISN1+MO2 = NO2+ 0.50GLYC+0.50HAC+ 0.25RCHO+0.75CH2O+ 0.25MOH+ 0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
VRO2+MO2 = 0.14HO2+ 0.14CH2O+0.36MCO3+ 0.36GLYC+0.14MGLY+ 0.25MEK+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
MRO2+MO2 = 0.50HO2 +0.09MGLY+0.42HAC+ 0.42CO+0.09CH2O+ 0.25MEK+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?

MVN2+MO2 = NO2+ 0.50CH2O+0.25MCO3 + 0.25MGLY+0.25HO2+ 0.25RCHO+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
MAN2+MO2= NO2+ 0.50CH2O+0.50MGLY+ 0.25RCHO+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
B3O2+MO2 = 0.50HO2+ 0.50ACET+0.25ACET + 0.75CH2O+0.25MOH+ 0.25ROH+0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
INO2+MO2 = 0.55NO2+ 0.40HO2+0.425HNO3+ 0.025NO2+0.05MACR+ 0.08CH2O+0.03MVK+ 0.25RCHO+0.75CH2O+ 0.25MOH+0.25ROH+ 0.05HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
PRN1+MO2 = NO2+ 0.50CH2O+ 0.50ALD2+ 0.25RCHO+0.75CH2O+ 0.25MOH+0.25ROH+ 0.50HO2	8.37E-14	Tyndall MO2+MO2 Atkinson97 RO2+RO2 (See note 11 below)	8/2001		?
EOH+OH = HO2+ALD2	~~7.00E-12 exp(-235/T)~~	~~JPL97~~			~~X~~
	6.90E-12 exp(-230/T)	JPL02	7/2003		X
ROH+OH = HO2+RCHO	~~5.50E-12~~	~~Atk92,94(1-butanol)~~			X
	4.6E-12 exp(70/T)	IUPAC ? Products	7/2003		X
ETO2+ETO2 = 2ALD2 + 2HO2	4.10E-14	JPL97 ? B Ratio			X
ETO2+ETO2 = EOH + ALD2	2.70E-14	JPL97 ? B Ratio			X
PAN = MNO3 + CO2	~~2.10E12 exp (-12525/T)~~	~~This reaction is of uncertain pedigree but should be~~			X

		~~removed upon next revision as per JPL97 recommendation~~			
	Removed	7/03			X
HO2+ETO2 = ETP	~~7.50E-13 exp(700/T)~~	~~JPL97~~			X
	7.40E-13 exp(700/T)	Tyndall (see note 4) Not JPL 03	8/2001		X
A3O2+HO2 = RA3P	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
PO2+HO2 = PP	7.40E-13 exp(700/T)	Tyndall ETO2+HO2	8/2001		X
HO2+MCO3 =ACTA+O3	K=K1 / (1+K2) ~~K1=4.50E-13 exp(1000/T)~~ ~~K2=3.30E+2 exp(-1430/T)~~	~~See note 6.~~ ~~JPL97~~		~~V~~	~~X~~
	K1=4.30E-13 exp(1040/T) K2=3.70E+1 exp(-660/T)	RateTyndall: br crawford & moortgart	8/2001		X
HO2+MCO3 = MAP	K=K1 / (1+K2) ~~K1=4.50E-13 exp(1000/T)~~ ~~K2=3.03E-3 exp(1430/T)~~	~~See note 6.~~ ~~JPL97~~		~~V~~	X
	K1=4.30E-13 exp(1040/T) K2=2.70E-2 exp(660/T)	RateTyndall: br crawford & moortgart	8/2001		X
RCO3+HO2=0.3RCOOH +0.3O3+ 0.7RP	4.30E-13 exp(1040/T)	Tyndall ETO2+HO2	8/2001		X
GCO3+HO2=0.3RCOOH +0.3O3+0.7GP	4.30E-13 exp(1040/T)	Tyndall ETO2+HO2	8/2001		X
MAO3+HO2=0.3RCOOH +0.3O3 + 0.7MAOP	4.30E-13 exp(1040/T)	Tyndall ETO2+HO2	8/2001		X
GLCO3+HO2=0.3RCOOH +0.3O3+0.7GLP	4.30E-13 exp(1040/T)	Tyndall ETO2+HO2	8/2001		X
PRPE+OH+M = PO2	LPL: 8.00E-27(300/T)^3.5 HPL:3.00E-11 Fc: 0.5	Atkinson 92 & IUPAC 03 for Fc.		P	X
PRPE+O3 = 0.535CH2O+ 0.500ALD2+0.420CO+	6.50E-15 exp(-1880/T)	Paulson & Seinfeld 92			X

0.300HO2+0.135OH+ 0.065H2+0.305MO2					
PMN+OH = NO2+ 0.59HAC+2HO2+ 2.23CH2O	~~3.60E-12~~	~~Grosjean 93ab~~			X
	3.20E-11	Orlando et al. 2002	Jul 2003		X
PMN+O3 = NO2+ 0.6CH2O+HO2	8.20E-18	Grosjean 93ab			X
GLYC+OH = 0.8GCO3 + 0.4CO+0.2H2+0.2HO2	1.00E-11	Atkinson 92, 94			?
PRPE+NO3 = PRN1	4.59E-13 exp(-1156/T)	Atkinson 92,94			X
GLYX+OH = HO2+2CO	K1=1.10E-11 K = K1*([O2]+3.5D18)/ (2*[O2]+3.5D18)	Atkinson 92, 94		C	?
MGLY+OH = MCO3+CO	1.70E-11	Atkinson 92, 94			?
GLYX+NO3 = HNO3 + HO2 + 2CO	K1=1.40E-12exp(-1860/T) K = K1*([O2]+3.5D18)/ (2*[O2]+3.5D18)	Atkinson92& 94, (ALD2)		C	?
MGLY+NO3 = HNO3 + CO + MCO3	1.40E-12 exp(-1860/T)	Atkinson92& 94, (ALD2)			?
ISOP+OH = RIO2	~~2.54E-11 exp(410/T)~~	~~Atkinson 92 & 94~~			X
	2.70E-11 exp(390/T)	IUPAC02			X
MVK+OH = VRO2	4.13E-12 exp(452/T)	Atkinson92,94; Tuazon & Atkinson 89, 90			?
MACR+OH = 0.5MAO3 + 0.5MRO2	1.86E-11 exp(175/T)	Atkinson92,94; Tuazon & Atkinson 89,90			?
HAC+OH = MGLY+HO2	3.00E-12	Atkinson 92, 94			?
MCO3+A3O2 = MO2+ RCHO+HO2	1.68E-12 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
MCO3+PO2 = MO2 + ALD2+CH2O+HO2	1.68E-12 exp(500/T)	T dep & B.R. Tyndall	8/2001		X

		K298 Villenave 98 See note 12			
MCO3+A3O2 = ACTA + RCHO	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
MCO3+PO2 = ACTA + 0.35RCHO+0.65HAC	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
ISOP+O3 = 0.387MACR + 0.159MVK+0.100O3+ 0.270OH+0.070PRPE+ 0.900CH2O+0.060HO2+ 0.150CO2+0.050CO	1.05E-14 exp(-2000/T)	Paulson & Seinfeld, 92 Aschmann & Atkinson, 94			?
MVK+O3 = 0.82MGLY+ 0.80CH2O+0.20O2+ 0.05CO+0.06HO2+ 0.04ALD2	4.00E-15 exp(-2000/T)	Paulson & Seinfeld 92			?
MACR+O3 = 0.800MGLY + 0.700CH2O+0.200O3+ 0.200CO+0.275HO2+ 0.215OH+0.160CO2	4.40E-15 exp(-2500/T)	Paulson & Seinfeld 92			?
ISOP+NO3 = INO2	3.03E-12 exp(-446/T)	Atkinson 92, 94			X
MVK+NO3 = MVN2	2.00E-14	Horowitz et al., 1998, Lurmann et al., 1986			?
MACR+NO3 = MAN2	6.70E-15	Lurmann et al., 1986			?
MACR+NO3 = MAO3+ HNO3	3.30E-15	Lurmann et al., 1986			?
RCO3+MO2 = CH2O+ HO2+ETO2	1.68E-12 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12			X
GCO3+MO2 = 2CH2O + 2HO2	1.68E-12 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12			X
MAO3+MO2 = CH2O +	1.68E-12 exp(500/T)	T dep & B.R.			X

HO2+CH2O+MCO3		Tyndall K298 Villenave 98 See note 12			
GLCO3+MO2 = CH2O + 2HO2+CO	1.68E-12 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12			X
RCO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
GCO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
MAO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
GLCO3+MO2 = RCOOH + CH2O	1.87E-13 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X
INPN+OH = INO2	3.80E-12 exp(200/T)	DeMore, reported in Horowitz as MP+OH			X
PRPN+OH = PRN1	3.80E-12 exp(200/T)	JPL97 MP+OH			X
ETP+OH = 0.50OH+ 0.50ETO2+0.50ALD2	3.80E-12 exp(200/T)	JPL97 MP+OH			X
RA3P+OH = 0.50OH + 0.50A3O2+0.50RCHO	3.80E-12 exp(200/T)	JPL97 MP+OH			X
RB3P+OH = 0.50OH+ 0.50B3O2+0.50RCHO	3.80E-12 exp(200/T)	JPL97 MP+OH			X
R4P+OH = 0.50OH+ 0.50R4O2 + 0.50RCHO	3.80E-12 exp(200/T)	JPL97 MP+OH			X
RP+OH = 0.50OH+ 0.50RCO3+0.50ALD2	3.80E-12 exp(200/T)	JPL97 MP+OH			X
PP+OH = 0.50OH+	3.80E-12 exp(200/T)	JPL97			X

0.50PO2+0.50RCHO		MP+OH			
GP+OH = 0.50OH+ 0.50GCO3+0.50CH2O	3.80E-12 exp(200/T)	JPL97 MP+OH			X
GLP+OH = 0.50OH+ 0.50GLCO3+0.50CO	3.80E-12 exp(200/T)	JPL97 MP+OH			X
RIP+OH = 0.50IAO2 + 0.40RIO2 + 0.20RIO1	3.80E-12 exp(200/T)	JPL97 MP+OH			X
IAP+OH = 0.50OH + 0.50RCHO+0.50IAO2	3.80E-12 exp(200/T)	JPL97 MP+OH			X
ISNP+OH = 0.50OH+ 0.50RCHO+0.50NO2+ 0.50ISN1	3.80E-12 exp(200/T)	JPL97 MP+OH			X
VRP+OH = 0.50OH+ 0.50RCHO+0.50VRO2	3.80E-12 exp(200/T)	JPL97 MP+OH			X
MRP+OH = 0.50OH + 0.50RCHO + 0.50MRO2	3.80E-12 exp(200/T)	JPL97 MP+OH			X
MAOP+OH = 0.50OH+ 0.50RCHO + 0.50MAO3	3.80E-12 exp(200/T)	JPL97 MP+OH			X
OH+MAP = 0.50OH+ 0,50CH2O + 0.50MCO3	3.80E-12 exp(200/T)	JPL97 MP+OH			X
C2H6+NO3 = ETO2+HNO3	1.40E-18	Atkinson 1992			X
MNO3+OH = CH2O+NOMNO32	~~5.00E-13 exp(-890/T)~~	~~JPL97~~			X
	5.00E-13 exp(-810/T)	JPL02	07/03		X
IALD+OH = 0.44IAO2 + 0.41MAO3+0.15HO2	3.70E-11	Paulson & Seinfeld, 92			?
IALD+O3 = 0.60MGLY+ 0.10OH+0.12CH2O+ 0.28GLYC+0.30O3+ 0.40CO+0.20H2+ 0.20HAC+0.20HCOOH	6.16E-15 exp(-1814/T)	Paulson & Seinfeld 92			?
MCO3+MCO3 = 2MO2	~~2.90E-12 exp(500/T)~~	~~JPL97~~			
	2.50E-12 exp(500/T)	Tyndall; See note 6.	8/2001		~~X~~
MCO3+MO2 = CH2O+ MO2+HO2	~~8.45E-13 exp(640/T)~~	~~JPL97~~			~~X~~
	1.80E-12 exp(500/T)	Tyndall	8/2001		X
MCO3+MO2 = ACTA + CH2O	~~4.55E-13 exp(640/T)~~	~~JPL97~~			X
	2.00E-13 exp(500/T)	Tyndall	8/2001		X
R4O2+MCO3 = MO2 + 0.32ACET+0.19MEK+ 0.18MO2+0.27HO2+ 0.32ALD2+0.13RCHO+ 0.05A3O2+0.18B3O2+	1.68E-12 exp(500/T)	T dep & B.R. Tyndall K298 Villenave 98 See note 12	8/2001		X

0.32ETO2					
ATO2+MCO3 = MO2 + 0.8HO2+0.2CH2O+ 0.2MCO3+0.8MGLY	1.68E-12 exp(500/T)	Ibid.	8/2001		X
KO2+MCO3 = MO2 + ALD2+MCO3	1.68E-12 exp(500/T)	Ibid.	8/2001		X
RIO2+MCO3 = MO2+ 0.864HO2+0.690CH2O + 0.402MVK+0.288MACR+ 0.136RIO1+0.127IALD	1.68E-12 exp(500/T)	Ibid.	8/2001		X
RIO1+MCO3 = MO2 + IALD+HO2+0.75CH2O	1.68E-12 exp(500/T)	Ibid.	8/2001		X
IAO2+MCO3 = MO2 + HO2+0.65CO+0.18H2+ 0.36HAC+0.26GLYC+ 0.58MGLY+0.4CH2O	1.68E-12 exp(500/T)	Ibid.	8/2001		X
ISN1+MCO3 = MO2+ NO2+GLYC+HAC	1.68E-12 exp(500/T)	Ibid.	8/2001		X
VRO2+MCO3 = MO2+ 0.28HO2+0.28CH2O+ 0.72MCO3+0.72GLYC+ 0.28MGLY	1.68E-12 exp(500/T)	Ibid.	8/2001		X
MRO2+MCO3 = MO2+ HO2+0.17MGLY+ 0.83HAC+0.83CO+ 0.17CH2O	1.68E-12 exp(500/T)	Ibid.	8/2001		X
B3O2+MCO3 = MO2+ HO2+ACET	1.68E-12 exp(500/T)	Ibid.	8/2001		X
R4N1+MCO3 = MO2+ NO2+0.39CH2O+ 0.75ALD2+0.57RCHO+ 0.30R4O2	1.68E-12 exp(500/T)	Ibid.	8/2001		X
MVN2+MCO3 = MO2 + NO2+CH2O+0.5MCO3+ 0.5MGLY+0.5HO2	1.68E-12 exp(500/T)	Ibid.	8/2001		X
MAN2+MCO3 = MO2 + NO2+CH2O+MGLY	1.68E-12 exp(500/T)	Ibid.	8/2001		X
INO2+MCO3 = MO2 + 0.10NO2 + 0.80HO2 + 0.85HNO3 + 0.05NO2 + 0.10MACR + 0.15CH2O + 0.05MVK	1.68E-12 exp(500/T)	Ibid.	8/2001		X
PRN1+MCO3 = MO2 + NO2+CH2O+ALD2	1.68E-12 exp(500/T)	Ibid.	8/2001		X
R4O2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X

ATO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
KO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
RIO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
RIO1+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
IAO2+MCO3 = MEK+ ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
VRO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
MRO2+MCO3 = MEK + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
R4N1+MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
ISN1+MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
MVN2+MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
MAN2+MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
INO2+MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
PRN1 + MCO3 = RCHO + ACTA + NO2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
B3O2+MCO3 = ACET + ACTA	1.87E-13 exp(500/T)	Ibid.	8/2001		X
MCO3+ETO2 = MO2+ ALD2+HO2	1.68E-12 exp(500/T)	Ibid.	8/2001		X
MCO3+ETO2 = ACTA + ALD2	1.87E-13 exp(500/T)	Ibid.	8/2001		X
RCO3+MCO3 = MO2 + ETO2	2.50E-12 exp(500/T)	Tyndall MCO3+MCO3	8/2001		X
GCO3+MCO3 = MO2 + HO2 + CH2O	2.50E-12 exp(500/T)	Tyndall MCO3+MCO3	8/2001		X
MAO3+MCO3 = MO2 + CH2O + MCO3	2.50E-12 exp(500/T)	Tyndall MCO3+MCO3	8/2001		X
GLCO3+MCO3 = MO2+ HO2 + CO	2.50E-12 exp(500/T)	Tyndall MCO3+MCO3	8/2001		X
NO3+NO3 = 2NO2 + O2	8.50E-13 exp(-2450/T)	JPL 97			X
HO2 = 0.50H2O2	gamma=2E-1	Jacob, 2000		K	X
NO2 = 0.50HNO3 + 0.50HNO2	gamma=1E-4	Jacob, 2000		K	X

NO3 = HNO3	gamma=1E-3	Jacob, 2000		K	X
N2O5 = 2HNO3	~~gamma=1E-1~~	~~Jacob, 2000~~		~~K~~	~~X~~
	gamma= fct(aerosol type, rh, temp)	See Appendix	10/2003	K	X
DMS+OH = SO2+MO2+ CH2O	1.20E-11 exp(-260/T)	JPL 2003	4/2003		X
DMS+OH+O2 = 0.75SO2+ 0.25MSA+MO2	K1 = 1.7E-42 exp(7810/T) K2 = 5.5E-31 exp(7460/T) K = K1/(1.0+K2*[O2])	Atkinson 89, yields from Chatfield and Crutzen 90, as reported by Chin et al., 1996.	4/2003	G	?
DMS+NO3 = SO2+HNO3 + MO2+CH2O	1.90E-13 exp(500/T)	JPL2003	4/2003		X
SO2+OH+M = SO4+HO2	LPL: 3.00E-31(300/T)^3.3 HPL:1.50E-12 Fc: 0.6	JPL97	4/2003	P	X

Explanation of lettered flags in globchem.dat for kinetic reactions

These flags specify reactions that are treated specially (hard-wired) in the code (calcrate.f).
Arlene's comments are listed as *AF note*

P IDENTIFIES IF REACTION IS PRESSURE DEPENDENT 3-BODY REACTION.
From calcrate.f:
FCV = CHARACTERIZES FALLOFF CURVE (SEE ATKINSON ET. AL (1992 J. PHYS. CHEM. REF. DATA 21, P. 1145). USUALLY = 0.6 for NASA rate expressions)
(*AF note*: Fc is the 3rd entry in globchem.dat)
HOWEVER, TWO TEMPERATURE-DEPENDENT EXPRESSIONS ARE ALSO USED: FCV = EXP(-T/FCT1) OR
FCV = EXP(-T/FCT1)+EXP(-FCT2/T)
RATE(NK) = K(0,T)[M], WHERE K(0,T) = 3-BODY, LOW PRESSURE LIMIT COEF
(*AF note*: 1st entry in globchem.dat)
RATE(NK+1) = K(INF,T) = 2-BODY, HIGH PRESSURE LIMIT COEF.
(*AF note:* 2nd entry in globchem.dat)

E IDENTIFIES REVERSE EQUILIBRIUM REACTION
From calcrate.f:
****
SET THE RATES OF ALL THERMALLY DISSOCIATING SPECIES. SEE DEMORE ET AL. (1990). CHEMICAL KINETICS AND PHOTOCHEMICAL DATA FOR USE IN STRATOSPHERIC MODELING. JPL. 90-1, P. 93. THE RATE HAS THE FORM Kf / [A EXP (C / T)], WHERE Kf IS THE REACTION IN THE REVERSE DIRECTION (previous equation read in must be pressure dependent)
****

X IDENTIFIES OH + HNO3
OH + HNO3: K = K0 + K3[M] / (1 + K3[M]/K2) rates from Brown, 1998
K0=2.41E-14 exp(460/T)
K2=2.69E-17 exp(2199/T)
K3=6.51E-34 exp(1335/T)

Y IDENTIFIES OH + CO
OH + CO: K = K0(1+0.6 Patm) ----------
CONSTC includes a factor to convert PRESS3 from (dyn cm-2) to (atm)
CONSTC = 0.6D0 * 9.871D-07

Z IDENTIFIES HO2 + HO2
HO2 + HO2: K = (K1 + K2)*(1+1.4E-21*[H2O]*EXP(2200/T)) ---
dependence of HO2 + HO2 on water vapor

A IDENTIFIES ADDITION BRANCH OF RO2+NO (forms organic nitrate)
reaction rate for this branch = total rate * YN
Calcrate.f calls fyrno3.f :
! Function FYRNO3 returns organic nitrate yields YN = RKA/(RKA+RKB)
! from RO2+NO reactions as a function of the number N of carbon atoms.
! Arguments as Input:
! (1) XCARBN (REAL*8) : Number of C atoms in RO2
(*AF note*: read in on second line of globchem.dat)
! (2) ZDNUM (REAL*8) : Air density [molec/cm3]
! (3) TT (REAL*8) : Temperature [K]
! (2) Updated following Atkinson 1990.
! (3) yield from Isoprene Nitrate (ISN2) ~ 12%,
! according to Sprengnether et al., 2002.

B IDENTIFIES ABSTRACTION BRANCH OF RO2+NO (forms RO+NO2)
Reaction rate for this branch = total rate * (1-YN)
See notes A for fyrno3.f

C IDENTIFIES BRANCH OF GLYX+OH/NO3 forming HO2,CO
K = K1*([O2]+3.5D18)/(2*[O2]+3.5D18)
AF note: K1 is specified in input file

D IDENTIFIES BRANCH OF GLYX+OH/NO3 forming GLCO3
K = K1*[O2]/(2*[O2]+3.5D18)
AF note: K1 is specified in input file; we no longer include this reaction since we ignore the GLCO3 branch. The assumption is that GLYX is water soluble so loss via GLCO3 is not important. We treat GLCO3 as an inactive species since this product only comes from GLYX and this saves us a few reactions. The existence of GLCO3 in the mechanism can be traced to the 1986 Lurmann mechanism (it was included in the Horowitz 98 mechanism).

K IDENTIFIES REACTION ON AEROSOL SURFACE
1st entry is molecular weight; second entry is gamma (sticking coefficient)
! Subroutine ARSL1K calculates the 1st-order loss rate of species on
! wet aerosol surface. (lwh, jyl, gmg, djj, 7/1/94; bmy, 4/1/03)
! Arguments as Input:
! (1) AREA (REAL*8) : sfc area of wet aerosols/volume of air [cm2/cm3]
! (2) RADIUS (REAL*8) : radius of wet aerosol [cm], order of 0.01-10 um;
! note that radius here is Rd, not Ro
! (3) DENAIR (REAL*8) : Density of air [#/cm3]
! (4) STKCF (REAL*8) : Sticking coefficient [unitless], order of 0.1
! (5) STK (REAL*8) : Square root of temperature [K]
! (6) SQM (REAL*8) : Square root of molecular weight [g/mole]
! References:
! The 1st-order loss rate on wet aerosol (Dentener's Thesis, p. 14)
! is computed as ARSL1K [1/s] = area / [radius/dfkg + 4./(stkcf * xmms)]

! where XMMS = Mean molecular speed [cm/s] = sqrt(8R*TK/pi/M) for Maxwell;
DFKG = Gas phase diffusion coeff [cm2/s] (order of 0.1)

V TEMPERATURE DEPENDENT BRANCHING RATIO: e.g. MCO3+MO2
K = K1 / (1+K2)

G IDENTIFIES DMS + OH
K = K1/(1.0+K2*[O2]

Notes on special kinetic reactions

1. MO2+NO: nitrate path assumed not important (Tyndall recommends <.005formation).

2. MO2+NO2: forms methyl peroxynitrate, which is apparently themally unstable so it is not included in the mechanism

3. ETO2+NO2: forms ethyl peroxynitrate which is also thermally unstable, not included

4. ETO2+NO,HO2: apply these rates to all higher peroxy radicals for which we do not have measured rates

5. ETO2+NO: our mechanism considers that there is a 0% yield of ethyl nitrate. Tyndall actually recommends a 1.4% yield.

6.MCO3+NO,MCO3,HO2,RCO3,GCO3,MAO3,GLCO3 rates are used for other radicals. RCO3+HO2 same as MCO3+HO2, RCO3+NO same as MCO3+NO, RCO3+MCO3 same as MCO3+MCO3.

7.ATO2+HO2: Tyndall forms CH3C(O)CH2OOH → this must then split and go to MCO3+MO2, the products in chem..dat ??

8.ATO2+NO2: forms acetonyl peroxynitrate which is much less stable than PAN, (weak 00-NO2 bond) and is not an imp NOy reservoir in the free trop [Tyndall, 2001] – this is not included in our mechanism.

9.ATO2+NO assumes a 4% yield of alkyl nitrates – no recommendation was made by Tyndall except that Sehested had reported substantial yields of nitrate. 4% R4N2 yield is from Lurmann et al., 1986.

10.RO2 primary+MO2: following madronich & calvert:

K(RO2+MO2) = 2*sqrt(k(MO2+MO2)*k(RO2+RO2)).

11.RO2 secondary+MO2: same calculation as in note 10, but with the updated MO2+MO2 rate.

12.MCO3+RO2: k 298 = 1e-11cm^3 molec^{-1}. Use T dep. From MCO3+MO2 according to Tyndall, and apply branching ratio from Tyndall. Keeping rate constant at 298K equal to 1E-11, means that A factor is 1.87E-12. Branching ratio from Tyndall sends 90% to the radical branch (A = 0.9*1.87E-12 = 1.68E-12), and 10% to molecular branch (A = 0.1* 1.87E-12 =1.87E-13).

13. RCO3+NO2: these PANs use the reaction rate of the high pressure limit of MCO3+NO2 as recommended by Atkinson 92.

Photolysis Reactions

Photolysis reactions are listed below. They are calculated by Fast-J [*Wild et al.*, 2000]. The master rate file (ratj.d) must include the reactions given in globchem.dat -- it specifies which cross sections to use for the reactions. The cross sections are given in jv_spec.dat. Both of these input files are reproduced below the photolysis reaction table and accompanying notes. All reaction data is from JPL97 and Atkinson97 (IUPAC) as reported by Wild et al. [2000] unless otherwise specified.

Photolysis reaction	reference	Date updated	Flag
O3 = 2OH	JPL97 and Atkinson97 as reported by Wild et al., 2000; See also notes with Q flag	1/2002	Q
NO2 = NO + O3	As in Wild et al., 2000		
H2O2 = 2OH	As in Wild et al., 2000		
MP = CH2O + HO2 + OH	As in Wild et al., 2000.		
CH2O = 2HO2 + CO	As in Wild et al., 2000.		
CH2O = H2 + CO	As in Wild et al., 2000.		
HNO3 = OH+NO2	As in Wild et al., 2000.		
HNO2 = OH+NO	As in Wild et al., 2000.		
HNO4 = OH+NO3	As in Wild et al., 2000.		
NO3 = NO2 + O3	As in Wild et al., 2000.		
NO3 = NO + O2	As in Wild et al., 2000.		
N2O5 = NO2 + NO2	As in Wild et al., 2000.		
N2O5 = NO3 + NO + O3	As in Wild et al., 2000.		
HNO4 = HO2 + NO2	As in Wild et al., 2000.; See also T flag notes [Roehl, 2002]	1/2002	T
ALD2 = MO2 + HO2 + CO	As in Wild et al., 2000.		
ALD2 = CH4 + CO	As in Wild et al., 2000.		
PAN = MCO3 + NO2	As in Wild et al.		
RCHO = ETO2 + HO2 + CO	As in Wild et al.		
ACET = MCO3 + MO2	Pressure dependent cross-sections from Cameron-Smith et al., 2000		
MEK = MCO3 + ETO2	As in Wild et al., 2000.		
MNO3 = CH2O + H2O + NO2	As in Wild et al., 2000.		
GLYC = CH2O + HO2 + CO	As in Wild et al.		
GLYX = H2 + 2CO	As in Wild et al.		
GLYX = 2CO + 2HO2	As in Wild et al.		
GLYX = CH2O + CO	As in Wild et al.		
MGLY = MCO3 + CO + HO2	As in Wild et al.		
MGLY = ALD2 + CO	As in Wild et al.		
MVK = PRPE + CO	As in Wild et al.		
MVK = MCO3+CH2O+CO+ HO2	As in Wild et al.		

MVK = MO2+MAO3	As in Wild et al.		
MACR = MAO3 + HO2	As in Wild et al.		
MACR = CO + HO2 +0.8MGLY +0.8HO2 +0.2MCO3+0.2CH2O	As in Wild et al.		
HAC = MCO3 + CH2O + HO2	Uses pressure-dependent acetone cross-section; Cameron-Smith et al., 2000.		
INPN = OH + HO2 + RCHO + NO2	Uses MP cross-section		
PRPN = OH + HO2 + RCHO + NO2	Uses MP cross-section		
ETP = OH + HO2 + ALD2	Uses MP cross-section		
RA3P = OH + HO2 + RCHO	Uses MP cross-section		
RB3P = OH + HO2 + RCHO	Uses MP cross-section		
R4P = OH + HO2 + RCHO	Uses MP cross-section		
PP = OH + HO2 + RCHO	Uses MP cross-section		
RP = OH + HO2 + ALD2	Uses MP cross-section		
GP = OH + HO2 + CH2O	Uses MP cross-section		
GLP = OH + HO2 + CO	Uses MP cross-section		
RIP = OH +0.864HO2 + 0.69CH2O + 0.402MVK + 0.288MACR + 0.136RIO1 + 0.127IALD	Uses MP cross-section		
IAP = OH + HO2 + 0.67CO +0.19H2 + 0.36HAC+0.26GLYC+ 0.58MGLY	Uses MP cross-section		
ISNP = OH + HO2 + RCHO + NO2	Uses MP cross-section		
VRP = OH + 0.28HO2 + 0.28CH2O +0.72MCO3+0.72GLYC+0.28MGLY	Uses MP cross-section		
MRP = OH + HO2 + 0.17MGLY + 0.83HAC+0.83CO+0.17CH2O	Uses MP cross-section		
MAOP = OH + HO2 + RCHO	Uses MP cross-section		
R4N2 = NO2 + 0.32ACET + 0.19MEK + 0.18MO2 + 0.27HO2 + 0.32ALD2+0.13RCHO+0.05A3O2+ 0.18B3O2+0.32ETO2	Uses MNO3 cross-section		
MAP = OH + MO2	Uses MP cross-section		

Explanation of Lettered flags in globchem.dat for photolysis reactions

Q IDENTIFIES O3 PHOTOLYSIS

This reaction is picked up by the NKO3PHOT variable in readchem and handled specially in calcrate.f : [O1D] at steady state = J[O3] / (k[H2O]+k[N2]+k[O2]) the effective J-value is then: J* k[H2O]/(k[H2O]+k[N2]+k[O2]). Current J is:
2.2E-10[H2O] /
(2.2E-10[H2O] + 2.14E-11 exp (110*T) [N2] + 3.2E-11 exp (70*T) [O2])
The N2 rate constant is from Ravishankara et al., 2002.
(Old N2 rate was $1.8e^{-11}$exp(110/T) from JPL97)
The O2 and H2O rates and N2 temperature dependence are from JPL97.

T IDENTIFIES HNO4 PHOTOLYSIS IN THE near-IR

This reaction is handled similarly to the O3 + hv → 2OH reaction. The 'T' flag is picked up by the NKHNO4 variable in readchem.f and passed to calcrate.f where the near-IR J-value of $1e^{-5}s^{-1}$ is added to that previously calculated by FAST-J.

Fast-J Photolysis code input files

Below is the master rate file, ratj.d [*Wild et al.*, 2000].

```
# PHOTOLYSIS REACTIONS - MASTER RATEFILE - Paul Brown, Oliver Wild & David
Rowley
# Centre for Atmospheric Science, Cambridge, U.K.  Release date:  22 November
1993
# SCCS version information: @(#)photol.d  1.2 5/11/94
#
# Modified for Harvard chemistry: several reactions added, re-ordered per
chem.dat
# Also putting in the Harvard names in col 1, the UCI x-sec names in last col
!!!
#                              -Prashant Murti [4/13/98]
#
# The new peroxide recycling now activates the following photolysis species:
#   GP,IAP,INPN,ISN1,ISNP,MAOP,MRP,PP,PRPN,RIP,VRP.
# Also be sure to set parameter JPMAX = 55 in "cmn_fj.h".
#                                       - Randall Martin & Bob Yantosca
[12/20/00]
#
#
# Harvard species    Products - UCI notation        UCI xsec
================================                      ========
    1 H2O      PHOTON    OH    HO2     0.00E+00  0.00      0.0
    2 HO2      PHOTON    OH    O(3P)   0.00E+00  0.00      0.0
    3 O2       PHOTON    O(3P) O(3P)   0.00E+00  0.00    100.0  O2
    4 O3_P     PHOTON    O2    O(3P)   0.00E+00  0.00    100.0  O3
    5 O3       PHOTON    O2    O(1D)   0.00E+00  0.00    100.0  O3_1d
    6 NO2      PHOTON    NO    O(3P)   0.00E+00  0.00    100.0  NO2
    7 H2O2     PHOTON    OH    OH      0.00E+00  0.00    100.0  H2O2
    8 MP       PHOTON    HCHO OH HO2   0.00E+00  0.00    100.0  ROOH
    9 CH2O     PHOTON    CO   HO2 HO2  0.00E+00  0.00    100.0  HCHO=H+
   10 CH2O     PHOTON    CO   H2       0.00E+00  0.00    100.0  HCHO=H2
   11 HNO3     PHOTON    OH   NO2      0.00E+00  0.00    100.0  HONO2
   12 HNO2     PHOTON    OH   NO       0.00E+00  0.00    100.0  HONO
   13 HNO4     PHOTON    OH   NO3      0.00E+00  0.00     33.3  HO2NO2
   14 HNO4     PHOTON    HO2  N        0.00E+00  0.00     66.7  HO2NO2
   15 NO3      PHOTON    NO   O2       0.00E+00  0.00    100.0  NO3=O2+
   16 NO3      PHOTON    NO2  O(3P)    0.00E+00  0.00    100.0  NO3=O+
   17 N2O5     PHOTON    NO3  NO O(3P) 0.00E+00  0.00      0.0  N2O5
   18 N2O      PHOTON    NO3  NO2      0.00E+00  0.00    100.0  N2O5
   19 ALD2     PHOTON    CH4  CO       0.00E+00  0.00    100.0  Acet=R+
   20 ALD2     PHOTON    MeOO HO2 CO   0.00E+00  0.00    100.0  Acet=RO
   21 PAN      PHOTON    MeCO3 NO2     0.00E+00  0.00    100.0  PAN
   22 RCHO     PHOTON    EtO2 HO2  CO  0.00E+00  0.00    100.0  RCHO
   23 ACET     PHOTON    MeCO3 MeOO    0.00E+00  0.00    100.0  Acetone
   24 MEK      PHOTON    MeCO3 EtOO    0.00E+00  0.00    100.0  EtCOMe
   25 MNO3     PHOTON    HCHO H2O  NO2 0.00E+00  0.00    100.0  MeNO3
   26 GLYC     PHOTON    HCHO  HO2 CO  0.00E+00  0.00    100.0  HOMeCHO
   27 GLYX     PHOTON    H2 CO         0.00E+00  0.00     33.3  HCOCHO
   28 GLYX     PHOTON    CO HO2        0.00E+00  0.00     33.3  HCOCHO
   29 GLYX     PHOTON    HCHO CO       0.00E+00  0.00     33.3  HCOCHO
   30 MGLY     PHOTON    MeCO3 CO HO2  0.00E+00  0.00     50.0  MeCOCHO
   31 MGLY     PHOTON    Acet CO       0.00E+00  0.00     50.0  MeCOCHO
```

```
   32 MVK      PHOTON    PRPE CO       0.00E+00  0.00     60.0  MeCOVi
   33 MVK      PHOTON MeCO3 HCHO CO HO2 0.00E+00  0.00     20.0  MeCOVi
   34 MVK      PHOTON    MeOO MAO3     0.00E+00  0.00     20.0  MeCOVi
   35 MACR     PHOTON     MAO3 HO2     0.00E+00  0.00     50.0  MACR
   36 MACR PHOTON CO HO2 MGLY HO2 MeCO3 HCHO 0.00E+00  0.00  50.0  MACR
   37 HAC      PHOTON   MeCO3 HCHO HO2 0.00E+00  0.00    100.0  Acetone
   38 ETP      PHOTON OH HO2 Acet      0.00E+00  0.00    100.0  ROOH
   39 RA3P     PHOTON    OH HO2 RCHO   0.00E+00  0.00    100.0  ROOH
   40 RB3P     PHOTON    OH HO2 RCHO   0.00E+00  0.00    100.0  ROOH
   41 R4P      PHOTON    OH HO2 RCHO   0.00E+00  0.00    100.0  ROOH
   42 RP       PHOTON    OH HO2 Acet   0.00E+00  0.00    100.0  ROOH
   43 R4N2 PHOTON NO2 MeCOMe MEK MO2 HO2ALD2 ... 0.00 0.00 100.0 MeNO3
   44 MAP      PHOTON    OH  MO2       0.00E+00  0.00    100.0  ROOH
   45 INPN     PHOTON OH HO2 RCHO NO2  0.00E+00  0.00    100.0  ROOH
   46 PRPN     PHOTON OH HO2 RCHO NO2  0.00E+00  0.00    100.0  ROOH
   47 PP       PHOTON OH HO2 RCHO      0.00E+00  0.00    100.0  ROOH
   48 GP       PHOTON OH HO2 RCHO      0.00E+00  0.00    100.0  ROOH
   49 GLP      PHOTON OH HO2 RCHO      0.00E+00  0.00    100.0  ROOH
   50 RIP PHOTON OH HO2 CH2O MVK MACR RIO1 IALD  0.00  0.00 100.0  ROOH
   51 IAP PHOTON OH HO2 CO  H2  HAC  GLYC  MGLY 0.00 0.00 100.0  ROOH
   52 ISNP     PHOTON OH HO2 RCHO NO2  0.00E+00  0.00    100.0  ROOH
   53 VRP  PHOTON OH HO2 CH2O MCO3 GLYC MGLY 0.00E+00  0.00 100.0  ROOH
   54 MRP  PHOTON OH HO2 MGLY HAC CO CH2O    0.00E+00  0.00 100.0  ROOH
   55 MAOP     PHOTON OH HO2 RCHO      0.00E+00  0.00    100.0  ROOH
 9999                                 0.00E-00  0.00      0.0
```

NOTES:

[4/15/98]
Oliver Wild: All reaction data from JPL '97, IUPAC IV. IUPAC V is soon expected. - ppm

All reaction data taken from IUPAC supplement IV unless otherwise indicated.

JPL - data from JPL (latest assessment as far as possible)

? - reaction products unknown
* - user strongly advised to consult source material
B - branching ratio assumed equal for all channels in the absence of more information
U - upper limit for rate coefficient

Changes since 08/3/93 release:
O now written as O(3P)

(Note that the second of the acetaldehyde channels above occurs at wavelengths
less than 289 nm, and therefore doesn't appear in the Fast-J region at all - I've simply included it here for completeness) - [from Oliver, 3/7/98]

Below is the jv_spec.dat input file for the FAST-J photolysis code [*Wild et al*., 2000].

```
jv_spec.dat:  FAST-J, std JPL 00 (mje 4/02) -- aerosol & mineral dust (rvm, 3/02)
NW-JValues   27    7    1    7     NJVAL, NWWW, NW1:NW2
w-beg (nm)    289.00    298.25    307.45    312.45    320.30    345.00    412.45
w-end (nm)    298.25    307.45    312.45    320.30    345.00    412.45    850.00
w-eff (nm)      294.      303.      310.      316.      333.      380.      574.
SOL#/cm2/s 7.352E+14 7.332E+14 5.022E+14 8.709E+14 3.786E+15 1.544E+16 2.110E+17
Raylay cm2  6.18E-26  5.43E-26  4.92E-26  4.54E-26  3.63E-26  2.09E-26  3.83E-27
BCarb m2/g     10.08      9.96      9.87      9.79      9.58      9.00      6.50
O2     180
O2     260
O2     300
O3     180 8.693E-19 2.365E-19 8.722E-20 3.694E-20 4.295E-21 1.804E-23 1.630E-21
O3     260 9.189E-19 2.571E-19 9.673E-20 4.141E-20 5.457E-21 2.775E-23 1.630E-21
O3     300 9.574E-19 2.777E-19 1.075E-19 4.725E-20 6.782E-21 4.824E-23 1.630E-21
O3_1d  180 9.500E-01 9.330E-01 4.270E-01 6.930E-02 6.060E-02       0.0       0.0
O3_1d  260 9.500E-01 9.420E-01 4.890E-01 1.360E-01 7.110E-02       0.0       0.0
O3_1d  300 9.500E-01 9.550E-01 5.870E-01 2.370E-01 8.570E-02       0.0       0.0
NO2    200 1.048E-19 1.494E-19 1.898E-19 2.295E-19 3.391E-19 4.230E-19 4.047E-22
NO2    300 1.039E-19 1.462E-19 1.845E-19 2.223E-19 3.256E-19 4.150E-19 4.020E-22
H2O2   200 8.838E-21 4.991E-21 3.190E-21 2.099E-21 7.716E-22 1.707E-23       0.0
H2O2   300 9.801E-21 5.718E-21 3.773E-21 2.568E-21 1.020E-21 2.287E-23       0.0
ROOH   300 5.883E-21 3.573E-21 2.437E-21 1.756E-21 7.428E-22 4.194E-23       0.0
ROOH   300 5.883E-21 3.573E-21 2.437E-21 1.756E-21 7.428E-22 4.194E-23       0.0
HCHO=H+223       0.0 1.969E-20 1.274E-20 1.971E-20 4.354E-21       0.0       0.0
HCHO=H+293       0.0 1.873E-20 1.304E-20 1.896E-20 3.949E-21       0.0       0.0
HCHO=H2223       0.0 6.475E-21 4.392E-21 9.027E-21 1.041E-20 1.946E-22       0.0
HCHO=H2293       0.0 6.163E-21 4.500E-21 8.715E-21 9.434E-21 1.883E-22       0.0
HONO2  200 3.706E-21 1.377E-21 5.451E-22 2.102E-22 2.154E-23 8.105E-26       0.0
HONO2  300 4.747E-21 1.923E-21 8.314E-22 3.589E-22 4.764E-23 2.499E-25       0.0
HONO   300       0.0       0.0 1.265E-20 3.469E-20 1.090E-19 8.644E-20 0.000E+00
HONO   300       0.0       0.0 1.265E-20 3.469E-20 1.090E-19 8.644E-20 0.000E+00
HO2NO2 300 2.869E-20 1.102E-20 5.222E-21 2.794E-21 3.255E-22       0.0       0.0
HO2NO2 300 2.869E-20 1.102E-20 5.222E-21 2.794E-21 3.255E-22       0.0       0.0
NO3=O+ 298       0.0       0.0       0.0       0.0       0.0       0.0 7.428E-19
NO3=O+ 298       0.0       0.0       0.0       0.0       0.0       0.0 7.428E-19
NO3=O2+298       0.0       0.0       0.0       0.0       0.0       0.0 9.569E-20
NO3=O2+298       0.0       0.0       0.0       0.0       0.0       0.0 9.569E-20
N2O5   225 4.130E-20 1.998E-20 1.167E-20 7.250E-21 2.296E-21 1.161E-22       0.0
N2O5   300 5.718E-20 3.317E-20 2.223E-20 1.552E-20 6.409E-21 5.415E-22       0.0
Acet=RO298 4.008E-20 2.869E-20 1.840E-20 3.626E-21       0.0       0.0       0.0
Acet=RO298 4.008E-20 2.869E-20 1.840E-20 3.626E-21       0.0       0.0       0.0
Acet=R+298       0.0       0.0       0.0       0.0       0.0       0.0       0.0
Acet=R+298       0.0       0.0       0.0       0.0       0.0       0.0       0.0
PAN    250 2.714E-21 9.251E-22 4.342E-22 2.290E-22 5.508E-23 6.551E-25       0.0
PAN    298 3.931E-21 1.399E-21 6.730E-22 3.630E-22 9.301E-23 1.193E-24       0.0
RCHO   298 5.203E-20 3.671E-20 2.220E-20 1.170E-20 1.569E-21       0.0       0.0
RCHO   298 5.203E-20 3.671E-20 2.220E-20 1.170E-20 1.569E-21       0.0       0.0
Acetone235 2.982E-20 1.301E-20 4.321E-21 1.038E-21 5.878E-23 1.529E-25 0.000E+00
Acetone298 3.255E-20 1.476E-20 5.179E-21 1.304E-21 9.619E-23 2.671E-25 0.000E+00
EtCOMe 298 1.432E-20 4.217E-21 1.150E-21 3.394E-22 4.706E-23       0.0       0.0
EtCOMe 298 1.432E-20 4.217E-21 1.150E-21 3.394E-22 4.706E-23       0.0       0.0
MeNO3  298 2.871E-20 1.080E-20 5.497E-21 3.460E-21 2.919E-22       0.0       0.0
MeNO3  298 2.871E-20 1.080E-20 5.497E-21 3.460E-21 2.919E-22       0.0       0.0
```

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HOMeCHO296 2.322E-20 1.773E-20 1.139E-20 5.584E-21 3.639E-22       0.0       0.0
HOMeCHO296 2.322E-20 1.773E-20 1.139E-20 5.584E-21 3.639E-22       0.0       0.0
HCOCHO 298 9.701E-22 1.498E-21 8.257E-21 1.434E-21 2.078E-22 6.393E-22 3.277E-22
HCOCHO 298 9.701E-22 1.498E-21 8.257E-21 1.434E-21 2.078E-22 6.393E-22 3.277E-22
MeCOCHO298 2.381E-21 1.853E-21 1.296E-21 9.572E-22 3.327E-22 2.004E-21 4.255E-22
MeCOCHO298 2.381E-21 1.853E-21 1.296E-21 9.572E-22 3.327E-22 2.004E-21 4.255E-22
MeCOVi 298 1.388E-21 1.985E-21 2.587E-21 2.837E-21 3.115E-21 6.627E-22       0.0
MeCOVi 298 1.388E-21 1.985E-21 2.587E-21 2.837E-21 3.115E-21 6.627E-22       0.0
MACR   298 7.862E-22 1.215E-21 1.645E-21 1.804E-21 1.998E-21 3.654E-22       0.0
MACR   298 7.862E-22 1.215E-21 1.645E-21 1.804E-21 1.998E-21 3.654E-22       0.0
CH3I   225 3.289E-20 9.071E-21 4.037E-21 2.073E-21 3.577E-22 1.551E-24 0.000E+00
CH3I   298 5.024E-20 1.479E-20 6.296E-21 3.199E-21 6.783E-22 6.121E-24 0.000E+00
===================Pressure Dependencies=========================================
Pressure Dep: 1
Acetone    5.651E-20 1.595E-19 2.134E-19 1.262E-19 1.306E-19 1.548E-19 0.000E+00
==================================================================================
NW-SCATTER   56  ! Scattering phase fns, scale extinct @ 999 nm    (mjp 99/07)
 w(nm)    Q    r-eff  ss-alb  pi(0) pi(1) pi(2) pi(3) pi(4) pi(5) pi(6) pi(7)
01 RAYLE  = Rayleigh phase
  300   123.5  0.001  1.0000  1.000   0.0 0.500   0.0   0.0   0.0   0.0   0.0
  400    39.1  0.001  1.0000  1.000   0.0 0.500   0.0   0.0   0.0   0.0   0.0
  600     7.7  0.001  1.0000  1.000   0.0 0.500   0.0   0.0   0.0   0.0   0.0
  999     1.0  0.001  1.0000  1.000   0.0 0.500   0.0   0.0   0.0   0.0   0.0
02 ISOTR  = isotropic
  300     1.0  0.001  1.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  400     1.0  0.001  1.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  600     1.0  0.001  1.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  999     1.0  0.001  1.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
03 ABSRB  = fully absorbing 'soot', wavelength indep.
  300     1.0  0.039  0.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  400     1.0  0.039  0.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  600     1.0  0.039  0.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
  999     1.0  0.039  0.0000  1.000   0.0   0.0   0.0   0.0   0.0   0.0   0.0
04 S_Bkg = backgrnd stratospheric sulfate (n=1.46, log-norm: r=.09um/sigma=.6)
  300  2.7541  0.221  1.0000  1.000 2.157 2.767 2.627 2.457 2.098 1.792 1.518
  400  2.4017  0.221  1.0000  1.000 2.146 2.641 2.422 2.122 1.709 1.357 1.070
  600  1.6454  0.221  1.0000  1.000 2.076 2.377 2.023 1.608 1.177 0.846 0.599
  999  0.7449  0.221  1.0000  1.000 1.877 1.920 1.412 0.970 0.614 0.388 0.238
05 S_Vol = volcanic stratospheric sulfate (n=1.46, log-norm: r=.08um/sigma=.8)
  300  2.6437  0.386  1.0000  1.000 2.152 2.901 2.856 2.971 2.772 2.709 2.587
  400  2.5603  0.386  1.0000  1.000 2.142 2.810 2.706 2.691 2.421 2.254 2.066
  600  2.2221  0.386  1.0000  1.000 2.127 2.673 2.488 2.308 1.963 1.698 1.461
  999  1.5319  0.386  1.0000  1.000 2.076 2.458 2.165 1.841 1.449 1.142 0.898
06 W_H01 = water haze (H1/Deirm.) (n=1.335, gamma:  r-mode=0.1um / alpha=2)
  300  2.8438   0.25  1.0000  1.000 2.454 3.376 3.624 3.608 3.300 2.911 2.526
  400  2.3497   0.25  1.0000  1.000 2.431 3.235 3.355 3.108 2.686 2.180 1.690
  600  1.4037   0.25  1.0000  1.000 2.328 2.789 2.593 2.062 1.492 1.013 0.632
  999  0.5034   0.25  1.0000  1.000 1.916 1.870 1.233 0.704 0.338 0.154 0.062
07 W_H04 = water haze (H1/Deirm.) (n=1.335, gamma:  r-mode=0.4um / alpha=2)
  300  2.2995   1.00  1.0000  1.000 2.433 3.625 4.104 4.645 5.020 5.409 5.802
  400  2.4743   1.00  1.0000  1.000 2.341 3.475 3.863 4.330 4.589 4.878 5.125
  600  2.6719   1.00  1.0000  1.000 2.325 3.334 3.624 3.896 3.939 3.968 3.964
  999  2.9565   1.00  1.0000  1.000 2.434 3.393 3.685 3.709 3.528 3.213 2.903
08 W_C02 = water cloud (C1/Deirm.) (n=1.335, gamma:  r-mode=2.0um / alpha=6)
  300  2.1410   3.00  1.0000  1.000 2.544 3.886 4.572 5.256 5.933 6.530 7.291
  400  2.1778   3.00  1.0000  1.000 2.513 3.834 4.480 5.160 5.785 6.356 7.044
  600  2.2287   3.00  1.0000  1.000 2.483 3.767 4.359 4.998 5.542 6.054 6.639
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  999  2.3071   3.00  1.0000  1.000 2.395 3.597 4.063 4.648 5.052 5.478 5.857
09 W_C04 = water cloud (C1/Deirm.) (n=1.335, gamma:  r-mode=4.0um / alpha=6)
  300  2.0835   6.00  1.0000  1.000 2.596 3.973 4.725 5.406 6.129 6.751 7.607
  400  2.1064   6.00  1.0000  1.000 2.571 3.936 4.660 5.345 6.056 6.670 7.492
  600  2.1345   6.00  1.0000  1.000 2.557 3.902 4.596 5.263 5.923 6.507 7.267
  999  2.1922   6.00  1.0000  1.000 2.499 3.799 4.418 5.081 5.667 6.213 6.851
10 W_C08 = water cloud (C1/Deirm.) (n=1.335, gamma:  r-mode=8.0um / alpha=6)
  300  2.0539  12.00  1.0000  1.000 2.619 4.013 4.798 5.476 6.232 6.870 7.780
  400  2.0643  12.00  1.0000  1.000 2.611 3.999 4.773 5.451 6.194 6.826 7.716
  600  2.0883  12.00  1.0000  1.000 2.589 3.965 4.712 5.394 6.121 6.744 7.599
  999  2.1236  12.00  1.0000  1.000 2.563 3.917 4.625 5.302 5.992 6.593 7.385
11 W_C13 = water cloud (C1/Deirm.) (n=1.335, gamma:  r-mode=13.3um / alpha=6)
  300  2.0440  20.00  1.0000  1.000 2.627 4.026 4.822 5.499 6.264 6.907 7.833
  400  2.0529  20.00  1.0000  1.000 2.620 4.014 4.800 5.477 6.234 6.872 7.783
  600  2.0716  20.00  1.0000  1.000 2.604 3.990 4.755 5.435 6.178 6.807 7.690
  999  2.0978  20.00  1.0000  1.000 2.585 3.955 4.691 5.368 6.077 6.688 7.520
12 W_L06 = water cloud (Lacis) (n=1.335, r-mode=5.5um / alpha=11/3)
  300  2.0616  10.00  1.0000  1.000 2.613 4.002 4.779 5.458 6.205 6.839 7.735
  400  2.0747  10.00  1.0000  1.000 2.601 3.984 4.745 5.425 6.158 6.785 7.657
  600  2.1005  10.00  1.0000  1.000 2.580 3.947 4.679 5.359 6.070 6.684 7.514
  999  2.1423  10.00  1.0000  1.000 2.545 3.884 4.568 5.244 5.909 6.496 7.250
13 Ice-H = hexagonal ice cloud (Mishchenko)
  300  2.0000    67.  1.0000  1.000 2.435 3.712 4.756 5.960 6.908 7.865 8.954
  400  2.0000    67.  1.0000  1.000 2.435 3.712 4.756 5.960 6.908 7.865 8.954
  600  2.0000    67.  1.0000  1.000 2.435 3.712 4.756 5.960 6.908 7.865 8.954
  999  2.0000    67.  1.0000  1.000 2.435 3.712 4.756 5.960 6.908 7.865 8.954
14 Ice-I = irregular ice cloud (Mishchenko)
  300  2.0000    50.  1.0000  1.000 2.257 3.164 4.096 5.088 6.018 6.897 7.794
  400  2.0000    50.  1.0000  1.000 2.257 3.164 4.096 5.088 6.018 6.897 7.794
  600  2.0000    50.  1.0000  1.000 2.257 3.164 4.096 5.088 6.018 6.897 7.794
  999  2.0000    50.  1.0000  1.000 2.257 3.164 4.096 5.088 6.018 6.897 7.794
15 Mdust 0.15 = mineral dust (R.V.Martin)
  300  3.0039  0.150  0.884 1.000 2.030 2.363 2.082 1.710 1.290  0.941  0.638
  400  2.4763  0.150  0.937 1.000 1.988 2.151 1.735 1.248 0.809  0.503  0.279
  600  1.2768  0.150  0.979 1.000 1.816 1.675 1.075 0.604 0.281  0.132  0.049
  999  0.3595  0.150  0.958 1.000 1.320 0.994 0.377 0.126 0.031  0.008  0.001
16 Mdust 0.25 = mineral dust (R.V.Martin)
  300  2.9406  0.250  0.820 1.000 2.046 2.643 2.593 2.634 2.406  2.244  1.944
  400  3.1046  0.250  0.913 1.000 2.021 2.486 2.264 2.047 1.671  1.362  1.039
  600  2.6144  0.250  0.980 1.000 2.026 2.296 1.926 1.470 1.013  0.668  0.403
  999  1.2426  0.250  0.974 1.000 1.824 1.689 1.087 0.611 0.286  0.134  0.050
17 Mdust 0.4 = mineral dust (R.V.Martin)
  300  2.6069  0.400  0.739 1.000 2.192 3.070 3.393 3.903 4.021  4.248  4.168
  400  2.8244  0.400  0.860 1.000 2.027 2.711 2.679 2.900 2.734  2.723  2.478
  600  3.1156  0.400  0.971 1.000 2.017 2.537 2.306 2.136 1.761  1.466  1.151
  999  2.4773  0.400  0.975 1.000 2.036 2.286 1.903 1.428 0.966  0.623  0.368
18 Mdust 0.8 = mineral dust (R.V.Martin)
  300  2.3457  0.800  0.640 1.000 2.517 3.780 4.729 5.755 6.524  7.339  7.903
  400  2.4344  0.800  0.763 1.000 2.295 3.320 3.800 4.578 4.913  5.482  5.662
  600  2.6416  0.800  0.936 1.000 2.023 2.830 2.805 3.279 3.178  3.418  3.275
  999  3.0396  0.800  0.957 1.000 2.019 2.618 2.441 2.414 2.106  1.895  1.610
19 Mdust 1.5 = mineral dust (R.V.Martin)
  300  2.2228  1.500  0.579 1.000 2.705 4.250 5.641 7.023 8.293  9.539 10.662
  400  2.2732  1.500  0.676 1.000 2.539 3.821 4.771 5.881 6.738  7.733  8.463
  600  2.3707  1.500  0.890 1.000 2.240 3.259 3.544 4.375 4.592  5.292  5.471
  999  2.5751  1.500  0.913 1.000 2.083 2.944 3.008 3.555 3.538  3.852  3.789
20 Mdust 2.5 = mineral dust (R.V.Martin)
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  300  2.1579  2.500  0.556 1.000 2.780 4.476 6.085 7.664 9.186 10.673 12.096
  400  2.1923  2.500  0.616 1.000 2.678 4.164 5.458 6.813 8.046  9.325 10.461
  600  2.2560  2.500  0.842 1.000 2.391 3.526 4.044 5.035 5.527  6.483  6.961
  999  2.3716  2.500  0.869 1.000 2.268 3.300 3.634 4.458 4.720  5.401  5.624
21 Mdust 4.0 = mineral dust (R.V.Martin)
  300  2.1154  4.000  0.550 1.000 2.809 4.574 6.281 7.960 9.607 11.224 12.806
  400  2.1402  4.000  0.577 1.000 2.761 4.405 5.941 7.485 8.974 10.462 11.878
  600  2.1852  4.000  0.786 1.000 2.505 3.744 4.488 5.599 6.354  7.485  8.238
  999  2.2637  4.000  0.819 1.000 2.413 3.563 4.133 5.118 5.652  6.582  7.097
22 S00(rvm) Trop sulfate at RH=00 (n@400=1.44 log-norm: r=.05um/sigma=2.0)
  300  2.1411  0.159  1.0000  1.000 2.107 2.570 2.325 2.050 1.662 1.353 1.095
  400  1.5786  0.159  1.0000  1.000 2.116 2.510 2.228 1.873 1.461 1.126 0.865
  600  0.9088  0.159  1.0000  1.000 2.027 2.269 1.885 1.470 1.067 0.765 0.544
 1000  0.3537  0.159  1.0000  1.000 1.815 1.865 1.368 0.952 0.619 0.404 0.260
23 S50(rvm) Trop sulfate at RH=50 (n@400=1.38 log-norm: r=.06um/sigma=2.0)
  300  2.3057  0.217  1.0000  1.000 2.274 2.963 2.935 2.768 2.430 2.099 1.812
  400  1.8327  0.217  1.0000  1.000 2.279 2.900 2.823 2.563 2.172 1.797 1.477
  600  1.1573  0.217  1.0000  1.000 2.212 2.679 2.473 2.112 1.683 1.309 1.006
 1000  0.5062  0.217  1.0000  1.000 2.033 2.273 1.894 1.469 1.065 0.762 0.536
24 S70(rvm) Trop sulfate at RH=70 (n@400=1.36 log-norm: r=.07um/sigma=2.0)
  300  2.3816  0.241  1.0000  1.000 2.302 3.044 3.070 2.945 2.635 2.318 2.034
  400  1.9462  0.241  1.0000  1.000 2.310 2.986 2.964 2.743 2.371 1.998 1.673
  600  1.2726  0.241  1.0000  1.000 2.254 2.782 2.632 2.298 1.874 1.488 1.167
 1000  0.5840  0.241  1.0000  1.000 2.089 2.388 2.053 1.635 1.218 0.891 0.642
25 S80(rvm) Trop sulfate at RH=80 (n@400=1.36 log-norm: r=.07um/sigma=2.0)
  300  2.4415  0.260  1.0000  1.000 2.317 3.092 3.153 3.060 2.773 2.471 2.196
  400  2.0391  0.260  1.0000  1.000 2.328 3.040 3.054 2.862 2.508 2.142 1.816
  600  1.3726  0.260  1.0000  1.000 2.280 2.851 2.740 2.429 2.011 1.620 1.289
 1000  0.6501  0.260  1.0000  1.000 2.130 2.473 2.173 1.765 1.340 0.997 0.730
26 S90(rvm) Trop sulfate at RH=90 (n@400=1.35 log-norm: r=.08um/sigma=2.0)
  300  2.5294  0.297  1.0000  1.000 2.337 3.166 3.281 3.244 3.002 2.733 2.479
  400  2.1924  0.297  1.0000  1.000 2.352 3.121 3.194 3.053 2.733 2.386 2.067
  600  1.5527  0.297  1.0000  1.000 2.319 2.958 2.912 2.643 2.243 1.850 1.506
 1000  0.7869  0.297  1.0000  1.000 2.189 2.606 2.366 1.979 1.547 1.181 0.887
27 S95(rvm) Trop sulfate at RH=95 (n@400=1.35 log-norm: r=.10um/sigma=2.0)
  300  2.6088  0.347  1.0000  1.000 2.349 3.227 3.392 3.420 3.232 3.012 2.796
  400  2.3545  0.347  1.0000  1.000 2.370 3.194 3.323 3.242 2.967 2.652 2.353
  600  1.7709  0.347  1.0000  1.000 2.352 3.060 3.083 2.866 2.494 2.107 1.759
 1000  0.9688  0.347  1.0000  1.000 2.248 2.746 2.577 2.222 1.791 1.405 1.085
28 S99(rvm) Trop sulfate at RH=99 (n@400=1.34 log-norm: r=.14um/sigma=2.0)
  300  2.6638  0.498  1.0000  1.000 2.355 3.326 3.577 3.760 3.717 3.648 3.566
  400  2.6086  0.498  1.0000  1.000 2.384 3.311 3.540 3.603 3.454 3.252 3.045
  600  2.2570  0.498  1.0000  1.000 2.395 3.233 3.387 3.301 3.021 2.691 2.372
 1000  1.4906  0.498  1.0000  1.000 2.346 3.015 3.005 2.751 2.356 1.957 1.601
29 BC00(rvm) Black C, RH=00 (n@400=1.75-.46i log-norm: r=.01um/sigma=2.0)
  300  1.0643  0.039  0.3128  1.000 1.361 1.201 0.710 0.410 0.231 0.135 0.080
  400  0.7563  0.039  0.2672  1.000 1.189 1.018 0.514 0.262 0.131 0.069 0.037
  600  0.4289  0.039  0.1920  1.000 0.961 0.828 0.324 0.135 0.056 0.024 0.011
 1000  0.2166  0.039  0.0964  1.000 0.672 0.661 0.167 0.048 0.013 0.003 0.001
30 BC50(rvm) Black C, RH=50 (n@400=1.75-.46i log-norm: r=.01um/sigma=2.0)
  300  1.0643  0.039  0.3128  1.000 1.361 1.201 0.710 0.410 0.231 0.135 0.080
  400  0.7563  0.039  0.2672  1.000 1.189 1.018 0.514 0.262 0.131 0.069 0.037
  600  0.4289  0.039  0.1920  1.000 0.961 0.828 0.324 0.135 0.056 0.024 0.011
 1000  0.2166  0.039  0.0964  1.000 0.672 0.661 0.167 0.048 0.013 0.003 0.001
31 BC70(rvm) Black C, RH=70 (n@400=1.75-.46i log-norm: r=.01um/sigma=2.0)
  300  1.0643  0.039  0.3128  1.000 1.361 1.201 0.710 0.410 0.231 0.135 0.080
  400  0.7563  0.039  0.2672  1.000 1.189 1.018 0.514 0.262 0.131 0.069 0.037
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  600  0.4289  0.039  0.1920  1.000 0.961 0.828 0.324 0.135 0.056 0.024 0.011
 1000  0.2166  0.039  0.0964  1.000 0.672 0.661 0.167 0.048 0.013 0.003 0.001
32 BC80(rvm) Black C, RH=80 (n@400=1.57-.27i log-norm: r=.01um/sigma=2.0)
  300  0.9310  0.047  0.3604  1.000 1.626 1.530 1.035 0.659 0.407 0.255 0.160
  400  0.6525  0.047  0.3131  1.000 1.438 1.291 0.768 0.439 0.245 0.140 0.081
  600  0.3640  0.047  0.2331  1.000 1.171 1.022 0.490 0.236 0.112 0.055 0.028
 1000  0.1808  0.047  0.1220  1.000 0.827 0.768 0.254 0.089 0.030 0.010 0.003
33 BC90(rvm) Black C, RH=90 (n@400=1.48-.17i log-norm: r=.02um/sigma=2.0)
  300  0.8554  0.055  0.4318  1.000 1.811 1.807 1.338 0.919 0.608 0.402 0.266
  400  0.5876  0.055  0.3839  1.000 1.623 1.535 1.017 0.635 0.384 0.234 0.144
  600  0.3186  0.055  0.2989  1.000 1.341 1.206 0.664 0.356 0.187 0.101 0.054
 1000  0.1518  0.055  0.1666  1.000 0.966 0.879 0.350 0.143 0.057 0.023 0.008
34 BC95(rvm) Black C, RH=95 (n@400=1.45-.14i log-norm: r=.02um/sigma=2.0)
  300  0.8369  0.059  0.4723  1.000 1.882 1.925 1.476 1.046 0.712 0.481 0.325
  400  0.5692  0.059  0.4251  1.000 1.697 1.644 1.136 0.735 0.459 0.288 0.181
  600  0.3039  0.059  0.3389  1.000 1.414 1.293 0.750 0.420 0.229 0.128 0.071
 1000  0.1411  0.059  0.1961  1.000 1.029 0.935 0.399 0.174 0.074 0.032 0.013
35 BC99(rvm) Black C, RH=99 (n@400=1.39-.07i log-norm: r=.02um/sigma=2.0)
  300  0.8533  0.075  0.6328  1.000 2.076 2.294 1.941 1.506 1.109 0.802 0.576
  400  0.5647  0.075  0.5956  1.000 1.914 2.001 1.554 1.117 0.765 0.519 0.350
  600  0.2860  0.075  0.5187  1.000 1.643 1.599 1.074 0.682 0.416 0.256 0.157
 1000  0.1184  0.075  0.3536  1.000 1.248 1.150 0.602 0.311 0.157 0.081 0.041
36 OC00(rvm) Organic C, RH=00 (n@400=1.53-.005i log-norm: r=.02um/sigma=2.0)
  300  1.0162  0.070  0.9530  1.000 1.871 1.938 1.467 1.056 0.706 0.480 0.316
  400  0.6261  0.070  0.9673  1.000 1.759 1.732 1.211 0.811 0.503 0.321 0.196
  600  0.2733  0.070  0.9493  1.000 1.559 1.436 0.876 0.522 0.290 0.168 0.093
 1000  0.0833  0.070  0.7901  1.000 1.234 1.089 0.528 0.262 0.125 0.064 0.031
37 OC50(rvm) Organic C, RH=50 (n@400=1.44-.003i log-norm: r=.03um/sigma=2.0)
  300  1.1021  0.087  0.9716  1.000 2.040 2.288 1.914 1.500 1.095 0.789 0.565
  400  0.6904  0.087  0.9803  1.000 1.939 2.074 1.626 1.198 0.822 0.561 0.378
  600  0.3114  0.087  0.9696  1.000 1.739 1.732 1.207 0.802 0.498 0.313 0.193
 1000  0.0955  0.087  0.8711  1.000 1.402 1.301 0.740 0.417 0.224 0.126 0.069
38 OC70(rvm) Organic C, RH=70 (n@400=1.42-.002i log-norm: r=.03um/sigma=2.0)
  300  1.1602  0.095  0.9771  1.000 2.095 2.408 2.079 1.675 1.258 0.928 0.680
  400  0.7380  0.095  0.9843  1.000 1.998 2.194 1.783 1.354 0.959 0.671 0.464
  600  0.3373  0.095  0.9759  1.000 1.805 1.845 1.342 0.924 0.596 0.385 0.245
 1000  0.1047  0.095  0.8982  1.000 1.470 1.390 0.834 0.490 0.275 0.159 0.090
39 OC80(rvm) Organic C, RH=80 (n@400=1.40-.002i log-norm: r=.03um/sigma=2.0)
  300  1.2225  0.102  0.9811  1.000 2.134 2.499 2.208 1.817 1.393 1.047 0.781
  400  0.7864  0.102  0.9871  1.000 2.045 2.289 1.912 1.487 1.078 0.770 0.543
  600  0.3664  0.102  0.9805  1.000 1.858 1.937 1.455 1.030 0.682 0.451 0.294
 1000  0.1150  0.102  0.9180  1.000 1.527 1.466 0.916 0.556 0.322 0.191 0.111
40 OC90(rvm) Organic C, RH=90 (n@400=1.38-.001i log-norm: r=.03um/sigma=2.0)
  300  1.3563  0.116  0.9867  1.000 2.196 2.646 2.424 2.062 1.634 1.265 0.972
  400  0.8922  0.116  0.9911  1.000 2.119 2.451 2.137 1.727 1.301 0.961 0.701
  600  0.4317  0.116  0.9869  1.000 1.946 2.099 1.661 1.229 0.850 0.583 0.394
 1000  0.1401  0.116  0.9462  1.000 1.629 1.607 1.073 0.688 0.418 0.258 0.157
41 OC95(rvm) Organic C, RH=95 (n@400=1.37-.001i log-norm: r=.04um/sigma=2.0)
  300  1.5220  0.133  0.9909  1.000 2.248 2.781 2.631 2.306 1.885 1.502 1.186
  400  1.0365  0.133  0.9941  1.000 2.184 2.601 2.355 1.969 1.535 1.169 0.879
  600  0.5230  0.133  0.9915  1.000 2.031 2.262 1.877 1.446 1.042 0.740 0.517
 1000  0.1771  0.133  0.9665  1.000 1.734 1.761 1.251 0.844 0.538 0.345 0.219
42 OC99(rvm) Organic C, RH=99 (n@400=1.350.000i log-norm: r=.05um/sigma=2.0)
  300  1.9223  0.177  0.9958  1.000 2.322 3.000 2.985 2.758 2.380 1.999 1.664
  400  1.4182  0.177  0.9975  1.000 2.288 2.866 2.763 2.452 2.032 1.637 1.301
  600  0.7958  0.177  0.9967  1.000 2.178 2.576 2.318 1.921 1.487 1.124 0.836
 1000  0.3046  0.177  0.9883  1.000 1.935 2.089 1.655 1.224 0.851 0.586 0.398
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43 SSa00(rvm) Sea Salt (accum), RH=00 (n@400=1.50 log-norm: r=.21um/sigma=2.0)
  300  2.4998  0.732  0.9999  1.000 2.122 3.044 3.083 3.688 3.676 4.110 4.155
  400  2.6308  0.732  1.0000  1.000 2.096 2.938 2.916 3.332 3.234 3.455 3.412
  600  2.7565  0.732  1.0000  1.000 2.092 2.812 2.714 2.854 2.633 2.591 2.435
 1000  2.5373  0.732  0.9987  1.000 2.125 2.701 2.530 2.378 2.037 1.776 1.533
44 SSa50(rvm) Sea Salt (accum), RH=50 (n@400=1.38 log-norm: r=.34um/sigma=2.0)
  300  2.3632  1.177  1.0000  1.000 2.337 3.457 3.796 4.390 4.661 5.083 5.455
  400  2.4743  1.177  1.0000  1.000 2.318 3.383 3.677 4.144 4.320 4.586 4.814
  600  2.6330  1.177  1.0000  1.000 2.316 3.297 3.529 3.799 3.814 3.849 3.864
 1000  2.6210  1.177  0.9995  1.000 2.345 3.224 3.387 3.422 3.241 3.028 2.821
45 SSa70(rvm) Sea Salt (accum), RH=70 (n@400=1.37 log-norm: r=.38um/sigma=2.0)
  300  2.3305  1.324  1.0000  1.000 2.368 3.522 3.911 4.518 4.845 5.290 5.712
  400  2.4328  1.324  1.0000  1.000 2.347 3.450 3.796 4.289 4.526 4.828 5.109
  600  2.5958  1.324  1.0000  1.000 2.338 3.359 3.640 3.953 4.027 4.111 4.175
 1000  2.6449  1.324  0.9996  1.000 2.364 3.287 3.502 3.588 3.456 3.284 3.107
46 SSa80(rvm) Sea Salt (accum), RH=80 (n@400=1.36 log-norm: r=.42um/sigma=2.0)
  300  2.3054  1.457  1.0000  1.000 2.389 3.568 3.993 4.612 4.977 5.442 5.901
  400  2.3997  1.457  1.0000  1.000 2.367 3.498 3.881 4.395 4.678 5.011 5.334
  600  2.5625  1.457  1.0000  1.000 2.353 3.404 3.720 4.068 4.188 4.313 4.420
 1000  2.6557  1.457  0.9997  1.000 2.374 3.329 3.579 3.705 3.615 3.479 3.334
47 SSa90(rvm) Sea Salt (accum), RH=90 (n@400=1.35 log-norm: r=.50um/sigma=2.0)
  300  2.2634  1.740  1.0000  1.000 2.423 3.640 4.121 4.759 5.193 5.694 6.222
  400  2.3437  1.740  1.0000  1.000 2.396 3.571 4.012 4.568 4.926 5.317 5.717
  600  2.4954  1.740  1.0000  1.000 2.373 3.471 3.843 4.253 4.458 4.662 4.853
 1000  2.6519  1.740  0.9998  1.000 2.384 3.387 3.688 3.887 3.875 3.816 3.740
48 SSa95(rvm) Sea Salt (accum), RH=95 (n@400=1.35 log-norm: r=.60um/sigma=2.0)
  300  2.2247  2.119  1.0000  1.000 2.454 3.705 4.237 4.898 5.388 5.925 6.518
  400  2.2881  2.119  1.0000  1.000 2.428 3.644 4.141 4.734 5.166 5.612 6.093
  600  2.4211  2.119  1.0000  1.000 2.393 3.538 3.962 4.436 4.729 5.017 5.304
 1000  2.6125  2.119  0.9998  1.000 2.390 3.440 3.787 4.064 4.140 4.174 4.187
49 SSa99(rvm) Sea Salt (accum), RH=99 (n@400=1.34 log-norm: r=.99um/sigma=2.0)
  300  2.1540  3.484  1.0000  1.000 2.518 3.828 4.455 5.141 5.742 6.338 7.067
  400  2.1920  3.484  1.0000  1.000 2.497 3.790 4.399 5.052 5.620 6.162 6.806
  600  2.2683  3.484  1.0000  1.000 2.455 3.700 4.248 4.841 5.318 5.769 6.271
 1000  2.4312  3.484  0.9998  1.000 2.410 3.565 4.015 4.471 4.770 5.037 5.303
50 SSc00(rvm) Sea Salt (coarse), RH=00 (n@400=1.50 log-norm: r=1.8um/sigma=2.0)
  300  2.1044  5.674  0.9995  1.000 2.411 3.610 3.964 4.970 5.369 6.477 7.058
  400  2.1270  5.674  1.0000  1.000 2.399 3.592 3.941 4.926 5.304 6.354 6.926
  600  2.1674  5.674  1.0000  1.000 2.372 3.544 3.872 4.823 5.158 6.119 6.644
 1000  2.2422  5.674  0.9901  1.000 2.331 3.466 3.770 4.632 4.916 5.701 6.153
51 SSc50(rvm) Sea Salt (coarse), RH=50 (n@400=1.38 log-norm: r=2.8um/sigma=2.0)
  300  2.0767  9.024  0.9998  1.000 2.547 3.870 4.492 5.262 5.886 6.637 7.545
  400  2.0932  9.024  1.0000  1.000 2.543 3.867 4.496 5.245 5.870 6.583 7.456
  600  2.1231  9.024  1.0000  1.000 2.525 3.836 4.449 5.182 5.783 6.455 7.262
 1000  2.1768  9.024  0.9962  1.000 2.490 3.773 4.351 5.052 5.603 6.206 6.899
52 SSc70(rvm) Sea Salt (coarse), RH=70 (n@400=1.37 log-norm: r=3.2um/sigma=2.0)
  300  2.0710 10.107  0.9999  1.000 2.563 3.901 4.555 5.300 5.955 6.677 7.597
  400  2.0863 10.107  1.0000  1.000 2.560 3.900 4.564 5.290 5.949 6.635 7.519
  600  2.1139 10.107  1.0000  1.000 2.544 3.873 4.524 5.237 5.875 6.526 7.347
 1000  2.1631 10.107  0.9969  1.000 2.512 3.816 4.433 5.122 5.713 6.307 7.022
53 SSc80(rvm) Sea Salt (coarse), RH=80 (n@400=1.36 log-norm: r=3.5um/sigma=2.0)
  300  2.0671 10.879  0.9999  1.000 2.573 3.920 4.597 5.326 6.002 6.706 7.631
  400  2.0815 10.879  1.0000  1.000 2.571 3.921 4.609 5.322 6.001 6.673 7.562
  600  2.1075 10.879  1.0000  1.000 2.557 3.898 4.575 5.276 5.937 6.577 7.406
 1000  2.1534 10.879  0.9974  1.000 2.526 3.844 4.488 5.170 5.786 6.377 7.106
54 SSc90(rvm) Sea Salt (coarse), RH=90 (n@400=1.35 log-norm: r=4.2um/sigma=2.0)
  300  2.0604 12.372  0.9999  1.000 2.586 3.946 4.651 5.363 6.063 6.750 7.681
```

```
  400  2.0734 12.372  1.0000  1.000 2.586 3.950 4.668 5.366 6.072 6.729 7.626
  600  2.0967 12.372  1.0000  1.000 2.574 3.932 4.642 5.332 6.023 6.653 7.496
 1000  2.1377 12.372  0.9981  1.000 2.548 3.886 4.569 5.244 5.898 6.487 7.240
55 SSc95(rvm) Sea Salt (coarse), RH=95 (n@400=1.34 log-norm: r=5.1um/sigma=2.0)
  300  2.0542 14.057  0.9999  1.000 2.597 3.967 4.694 5.395 6.113 6.788 7.724
  400  2.0658 14.057  1.0000  1.000 2.598 3.973 4.716 5.405 6.130 6.778 7.681
  600  2.0866 14.057  1.0000  1.000 2.589 3.960 4.699 5.380 6.096 6.720 7.574
 1000  2.1230 14.057  0.9986  1.000 2.564 3.918 4.629 5.303 5.983 6.576 7.354
56 SSc99(rvm) Sea Salt (coarse), RH=99 (n@400=1.34 log-norm: r=8.6um/sigma=2.0)
  300  2.0431 18.159  1.0000  1.000 2.611 3.992 4.743 5.433 6.171 6.839 7.788
  400  2.0523 18.159  1.0000  1.000 2.614 4.002 4.773 5.454 6.201 6.846 7.764
  600  2.0688 18.159  1.0000  1.000 2.609 3.997 4.770 5.447 6.190 6.816 7.695
 1000  2.0973 18.159  0.9991  1.000 2.591 3.968 4.725 5.397 6.120 6.724 7.545
C===this section not read!===alternate O(1D) yields===can replace above data
OLD MJP Q'S
O3_1d X180     0.950     0.868     0.112     0.004       0.0       0.0       0.0
O3_1d X260     0.950     0.926     0.470     0.065       0.0       0.0       0.0
O3_1d X300     0.950     0.938     0.605     0.130       0.0       0.0       0.0
MICHELSEN Q'S
O3_1d M180     0.953     0.960     0.308     0.020     0.001       0.0       0.0
O3_1d M260     0.953     0.974     0.492     0.146     0.011       0.0       0.0
O3_1d M300     0.953     0.973     0.567     0.267     0.024       0.0       0.0
C====channel in Herzberg Contiuum to be added======(*caveat - not fully tested)=
photolysis in the Herzberg continuum:  198-209 nm is core, 195-212 nm covers all
J at top-of-atmosphere and X-sect for O2 and O3 (computing J at 12-14-16-18 km)
QO2: HerzC  8.15E-24
QO3: HerzC  4.40E-19
O2    Jtoa  1.67E-10
H1211 Jtoa  2.76E-05
H2402 Jtoa  2.75E-05
CCl4  Jtoa  1.31E-05
F11   Jtoa  7.24E-06
H1301 Jtoa  2.82E-06
N2O   Jtoa  3.36E-07
================================================================================
                        Spare Stuff - all from JPL 1997

    Note:  in code, assume that lower temperature is given first.
    Probably worth setting temperatures the same if only one x-section

HONO   300       0.0       0.0 1.265E-20 3.469E-20 1.090E-19 8.644E-20 0.000E+00
HONO   300       0.0       0.0 1.265E-20 3.469E-20 1.090E-19 8.644E-20 0.000E+00
HCOCHO 298 9.701E-22 1.498E-21 8.257E-21 1.434E-21 2.078E-22 6.393E-22 3.277E-22
HCOCHO 298 9.701E-22 1.498E-21 8.257E-21 1.434E-21 2.078E-22 6.393E-22 3.277E-22
MeCOCHO298 2.381E-21 1.853E-21 1.296E-21 9.572E-22 3.327E-22 2.004E-21 4.255E-22
MeCOCHO298 2.381E-21 1.853E-21 1.296E-21 9.572E-22 3.327E-22 2.004E-21 4.255E-22
EtCOMe 298 1.432E-20 4.217E-21 1.150E-21 3.394E-22 4.706E-23       0.0       0.0
EtCOMe 298 1.432E-20 4.217E-21 1.150E-21 3.394E-22 4.706E-23       0.0       0.0
MeNO3  298 2.871E-20 1.080E-20 5.497E-21 3.460E-21 2.919E-22       0.0       0.0
MeNO3  298 2.871E-20 1.080E-20 5.497E-21 3.460E-21 2.919E-22       0.0       0.0

ClONO2 200 3.707E-20 1.816E-20 1.084E-20 6.951E-21 3.040E-21 9.423E-22 6.852E-24
ClONO2 300 5.025E-20 2.610E-20 1.633E-20 1.079E-20 4.473E-21 1.204E-21 9.733E-24
Cl2    200 7.653E-20 1.387E-19 1.882E-19 2.283E-19 2.549E-19 6.209E-20 6.456E-22
Cl2    300 8.191E-20 1.403E-19 1.851E-19 2.204E-19 2.436E-19 6.467E-20 6.806E-22
HOCl   300 5.573E-20 6.018E-20 5.862E-20 5.304E-20 3.178E-20 5.051E-21 0.000E+00
HOCl   300 5.573E-20 6.018E-20 5.862E-20 5.304E-20 3.178E-20 5.051E-21 0.000E+00
```

```
OClO   204 1.145E-18 1.946E-18 2.806E-18 3.170E-18 4.798E-18 3.213E-18 4.112E-20
OClO   298 1.046E-18 1.664E-18 2.319E-18 2.925E-18 4.599E-18 3.407E-18 3.925E-20
Cl2O2  230 9.769E-19 6.254E-19 4.331E-19 3.064E-19 1.572E-19 2.698E-20 1.615E-22
Cl2O2  230 9.769E-19 6.254E-19 4.331E-19 3.064E-19 1.572E-19 2.698E-20 1.615E-22
ClO    300 1.324E-18 4.496E-19 1.499E-19 5.197E-20 2.410E-21 0.000E+00 0.000E+00
ClO    300 1.324E-18 4.496E-19 1.499E-19 5.197E-20 2.410E-21 0.000E+00 0.000E+00
BrO    300 0.000E+00 1.932E-18 3.681E-18 4.221E-18 6.179E-18 6.431E-19 0.000E+00
BrO    300 0.000E+00 1.932E-18 3.681E-18 4.221E-18 6.179E-18 6.431E-19 0.000E+00
BrONO2 300 2.042E-19 1.575E-19 1.311E-19 1.134E-19 8.127E-20 3.397E-20 1.286E-21
BrONO2 300 2.042E-19 1.575E-19 1.311E-19 1.134E-19 8.127E-20 3.397E-20 1.286E-21
HOBr   300 2.604E-19 1.837E-19 1.390E-19 1.159E-19 1.137E-19 6.710E-20 1.146E-21
HOBr   300 2.604E-19 1.837E-19 1.390E-19 1.159E-19 1.137E-19 6.710E-20 1.146E-21
CHBr3  210 9.247E-21 1.877E-21 5.752E-22 2.123E-22 2.564E-23 9.540E-25 0.000E+00
CHBr3  300 1.928E-20 5.034E-21 1.819E-21 7.631E-22 1.072E-22 9.540E-25 0.000E+00
CF3I   210 1.297E-19 4.093E-20 1.624E-20 7.639E-21 1.297E-21 0.000E+00 0.000E+00
CF3I   300 1.748E-19 6.652E-20 2.985E-20 1.476E-20 2.625E-21 0.000E+00 0.000E+00
(and from Calvert 1967:
 CH3I  300 4.194E-20 8.986E-21 4.210E-21 2.035E-21 2.943E-22 1.193E-24 0.000E+00
 CH3I  300 4.194E-20 8.986E-21 4.210E-21 2.035E-21 2.943E-22 1.193E-24 0.000E+00
)
# To shut off Rayleigh scattering
Raylay cm2  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
# To turn on Rayleigh scattering
Raylay cm2  6.18E-26  5.43E-26  4.92E-26  4.54E-26  3.63E-26  2.09E-26  3.83E-27
# Original cross section
O3     180 8.693E-19 2.365E-19 8.722E-20 3.694E-20 4.295E-21 1.804E-23 1.630E-21
O3     260 9.189E-19 2.571E-19 9.673E-20 4.141E-20 5.457E-21 2.775E-23 1.630E-21
O3     300 9.574E-19 2.777E-19 1.075E-19 4.725E-20 6.782E-21 4.824E-23 1.630E-21
# Original quantum yield
O3_1d  180 9.500E-01 9.303E-01 3.089E-01 2.293E-02 8.747E-04       0.0       0.0
O3_1d  260 9.500E-01 9.366E-01 4.618E-01 1.380E-01 9.857E-03       0.0       0.0
O3_1d  300 9.500E-01 9.387E-01 5.385E-01 2.524E-01 2.138E-02       0.0       0.0
# JPL 1997, replaced by Mat Evans 4/16/2002 for GEOS-CHEM version 4.32
O3_1d  180 9.500E-01 9.303E-01 3.089E-01 2.293E-02 8.747E-04       0.0       0.0
O3_1d  260 9.500E-01 9.366E-01 4.618E-01 1.380E-01 9.857E-03       0.0       0.0
O3_1d  300 9.500E-01 9.387E-01 5.385E-01 2.524E-01 2.138E-02       0.0       0.0
```

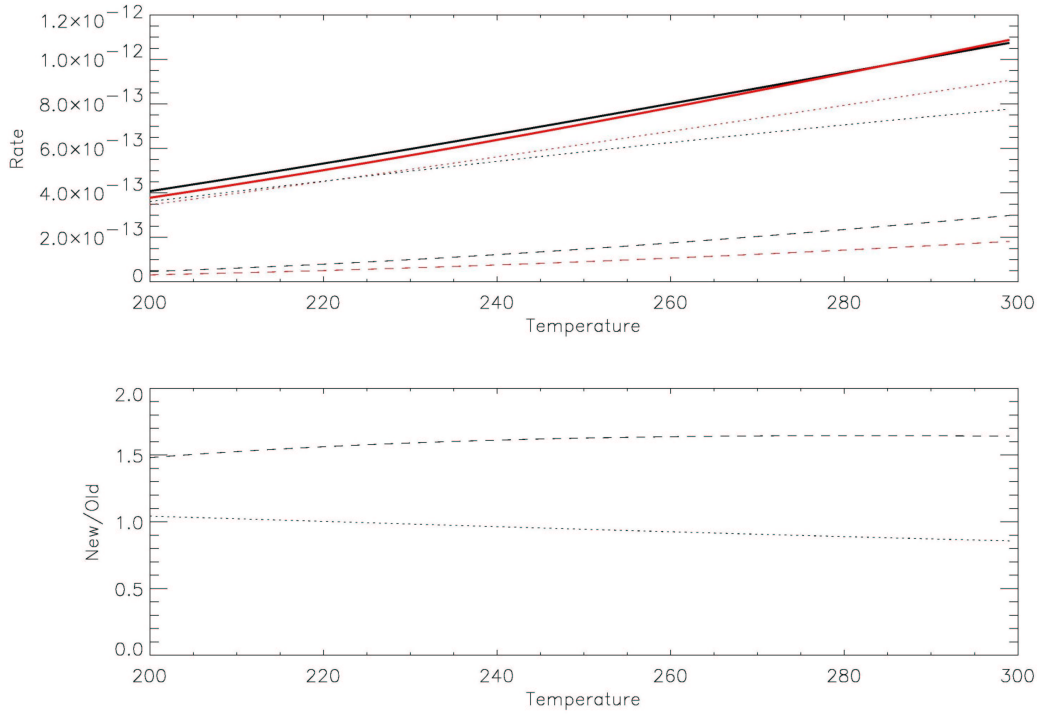
Species emitted and deposited in the GEOS-CHEM model

(entered in globchem.dat)

Species emitted	Species deposited
NO	NO2
NO2	O3
CO	PAN
ALK4	HNO3
ISOP	CH2O
ACET	H2O2
PRPE	PMN
C3H8	PPN
C2H6	R4N2
MEK	
ALD2	
CH2O	

Appendix mje_1

Branching ratio of C_3H_8+OH has been implemented from IUPAC-02



Top panel. Thick lines represent the total rate constant for the loss of propane by OH. Black is IUPAC recommendation; red is previous GEOS-CHEM rate. Little change in the overall loss rate. Dashed lines show the rate constant for the production of the primary radical (A3O2 or CH3CH2CH2O2) with the black showing the IUPAC and the red the previous GEOS-CHEM value. Dotted line is the production of the secondary radical (B3O2 or CH3C(O2)HCH3) with black being IUPAC and red the previous GEOS-CHEM value.

Bottom panel. Dashed line shows ratio of new to old for primary radical production, dotted line for the secondary radical production. So secondary radical production has not changed very much but primary radical production has increased by around 50%.

Appendix – N_2O_5 hydrolysis on aerosol – mje Oct 2003

The hydrolysis of N_2O_5 had previously been described with a single γ for all aerosol types and for all conditions. More recent laboratory studies have started to provide information on the impact of aerosol type, relative humidity and temperature on the reaction probability. The representation of aerosol chemistry in GEOS-CHEM is a work in progress. This describes the situation as of October 2003.

GEOS-CHEM considers 12 different types of aerosols. 7 dust size distributions, sulfate, black carbon, organic carbon, and 2 different sea salt components. We ignore any difference due to size and therefore consider uptake onto dust, sulfate, black carbon, organic carbon and sea salt.

Dust

This value is based on unpublished work of John Crowley's group from the web. This is highly uncertain.

```
      GAMMA = 0.01d0
```

Sulfate

We assume independent impacts from temperature and relative humidity. For temperature we use work of Kane et al. [2001] and for temperature we use Hallquist et al. [2003]. We also assume that the aerosol is made up of ammonium sulfate (ie it is completely neutralized).

Kane et al. [2001] give the relationship between reaction probability and relative humidity as a cubic. This has been rearranged here for numerical expediency. The relationship between reaction probability and temperature has been defined as a log function fitted to the data presented in Hallquist et al. [2003].

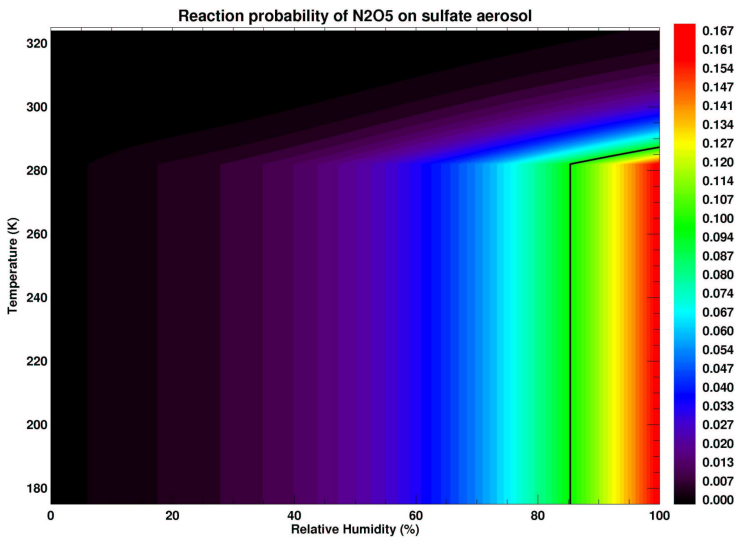
```
      GAMMA = 2.79d-4 + RH_P*(  1.30d-4 +
     &                  RH_P*( -3.43d-6 +
     &                  RH_P*(  7.52d-8 ) ) )

      TTEMP = MAX( TEMP, 282d0 )
      FACT  = 10.d0**( -2d0 - 4d-2*( TTEMP - 294.d0 ) ) / 1d-2

      GAMMA = GAMMA * FACT
```

Where TEMP is temperature in K and RH_P is relative humidity as a percentage.

Passing this function through the likely temperatures and relative humidities found in the atmosphere gives values that range from essentially 0 (warm dry conditions) to 1.7 (cold wet conditions). The range of values is shown in the figure below. The continuous dark line shows the 0.1 contour which was the previous recommendations for all conditions. This change to the model has let the γ which are higher for the cold wet conditions and γ which lower for the dry warm atmosphere.



Black carbon

Based on the IUPAC recommendation we use

```
GAMMA = 0.005d0
```

Organic Carbon

This is based on a fitting of data presented in Thornton et al. [2003].

```
IF ( RH_P >= 57d0 ) THEN
   GAMMA = 0.03d0
ELSE
   GAMMA = RH_P*5.2d-4
ENDIF
```

Where RH_P is the relative humidity as a percentage

Sea salt

The IUPAC recommendation has one value for wet and another value for dry sea-salt. Deciding upon whether sea-salt is wet or dry is complicated as it depends upon the hysteresis of deliquescence and efflorescence [Martin, 2000]. We use a mean value of these points from to define whether the salt is wet or dry.

```
IF ( RH_P >= 62 ) THEN
   GAMMA = 0.03d0
ELSE
   GAMMA = 0.005d0
ENDIF
```

Where RH_P is the relative humidity as a percentage.

Acknowledgments
This document draws heavily from Table 2b. in Horowitz et al., 1998, and previous documentation on updates to the chemical mechanism from Isabelle Bey. Thanks to Mat Evans for his help. We acknowledge all who contributed to compiling the master "listospecies" over the years.

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