The Chemical Mechanism of MECCA

KPP version: `2.2.3_rs3`

MECCA version: `4.4.0.m1`

Date: March 1, 2021

Batch file: `CCMI2-base-01.bat`

Integrator: `rosenbrock_mz`

Gas equation file: `gas.eqn`

Replacement file: `mim1-CCMI2-base-01`

Selected reactions:
“`(((Tr && (G || Het) && !I) || St) && !Hg)`”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	158
Aqueous phase:	0
All species:	158

Number of reactions in selected mechanism:

Gas phase (Gnnn):	261
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	80
Aqueous phase photolysis (PHnnn):	0
Heterogeneous (HETnnn):	12
Equilibria (EQnn):	0
Isotope exchange (IEXnnn):	0
Tagging equations (TAGnnn):	0
Dummy (Dnn):	0
All equations:	353

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	O_2 + O(^{1}D) → O(^{3}P) + O_2	3.3E-11*EXP(55./temp)	Burkholder et al. (2015)
G1001	UpStTrG	O_2 + O(^{3}P) → O_3	6.0E-34*((temp/300.)**(-2.4)) *cair	Burkholder et al. (2015)
G1002a	UpStG	O_3 + O(^{1}D) → 2.0 LossO3O + 2.0 LossO3 + 2 O_2	1.2E-10	Burkholder et al. (2015)*
G1003	UpStG	O_3 + O(^{3}P) → 2.0 LossO3O + 2.0 LossO3 + 2 O_2	8.0E-12*EXP(-2060./temp)	Burkholder et al. (2015)
G2100	UpStTrG	H + O_2 → HO_2	k_3rd(temp,cair,4.4E-32,1.3, 7.5E-11,-0.2,0.6)	Burkholder et al. (2015)
G2101	UpStG	H + O_3 → 1.0 LossO3H + 1.0 LossO3 + OH + O_2	1.4E-10*EXP(-470./temp)	Burkholder et al. (2015)
G2102	UpStG	H_2 + O(^{1}D) → 1.0 LossO3H + 1.0 LossO3 + H + OH	1.2E-10	Burkholder et al. (2015)
G2103	UpStG	OH + O(^{3}P) → 1.0 LossO3H + 1.0 LossO3 + H + O_2	1.8E-11*EXP(180./temp)	Burkholder et al. (2015)
G2104	UpStTrG	OH + O_3 → 1.0 LossO3H + LossOH + 1.0 LossO3 + HO_2 + O_2	1.7E-12*EXP(-940./temp)	Burkholder et al. (2015)
G2105	UpStTrG	OH + H_2 → ProdH2O + H_2O + H	2.8E-12*EXP(-1800./temp)	Burkholder et al. (2015)
G2106	UpStG	HO_2 + O(^{3}P) → 1.0 LossO3H + 1.0 LossO3 + OH + O_2	3.E-11*EXP(200./temp)	Burkholder et al. (2015)
G2107	UpStTrG	HO_2 + O_3 → 1.0 LossO3H + LossHO2 + 1.0 LossO3 + OH + 2 O_2	1.E-14*EXP(-490./temp)	Burkholder et al. (2015)
G2108a	UpStG	HO_2 + H → 2 OH	7.2E-11	Burkholder et al. (2015)
G2108b	UpStG	HO_2 + H → H_2 + O_2	6.9E-12	Burkholder et al. (2015)
G2108c	UpStG	HO_2 + H → ProdH2O + 1.0 ProdO3 + O(^{3}P) + H_2O	1.6E-12	Burkholder et al. (2015)
G2109	UpStTrG	HO_2 + OH → ProdH2O + H_2O + O_2	4.8E-11*EXP(250./temp)	Burkholder et al. (2015)
G2110	UpStTrG	HO_2 + HO_2 → H_2O_2 + O_2	k_HO2_HO2	Burkholder et al. (2015)*
G2111	UpStTrG	H_2O + O(^{1}D) → LossH2O + 1.0 LossO3O + LossO1D + 1.0 LossO3 + 2 OH	1.63E-10*EXP(60./temp)	Burkholder et al. (2015)
G2112	UpStTrG	H_2O_2 + OH → ProdH2O + H_2O + HO_2	1.8E-12	Burkholder et al. (2015)
G3100	UpStGN	N + O_2 → 1.0 ProdO3 + NO + O(^{3}P)	1.5E-11*EXP(-3600./temp)	Burkholder et al. (2015)
G3101	UpStTrGN	N_2 + O(^{1}D) → O(^{3}P) + N_2	2.15E-11*EXP(110./temp)	Burkholder et al. (2015)
G3102a	UpStGN	N_2O + O(^{1}D) → 1.0 LossO3O + 1.0 LossO3 + 2 NO	7.259E-11*EXP(20./temp)	Burkholder et al. (2015)
G3102b	StGN	N_2O + O(^{1}D) → 1.0 LossO3O + 1.0 LossO3 + N_2 + O_2	4.641E-11*EXP(20./temp)	Burkholder et al. (2015)
G3103	UpStTrGN	NO + O_3 → NO_2 + O_2	3.0E-12*EXP(-1500./temp)	Burkholder et al. (2015)
G3104	UpStGN	NO + N → 1.0 ProdO3 + O(^{3}P) + N_2	2.1E-11*EXP(100./temp)	Burkholder et al. (2015)
G3105	UpStGN	NO_2 + O(^{3}P) → 2.0 LossO3N + 2.0 LossO3 + NO + O_2	5.1E-12*EXP(210./temp)	Burkholder et al. (2015)
G3106	StTrGN	NO_2 + O_3 → NO_3 + O_2	1.2E-13*EXP(-2450./temp)	Burkholder et al. (2015)
G3107	UpStGN	NO_2 + N → N_2O + O(^{3}P)	5.8E-12*EXP(220./temp)	Burkholder et al. (2015)
G3108	StTrGN	NO_3 + NO → 2 NO_2	1.5E-11*EXP(170./temp)	Burkholder et al. (2015)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(5.8E-27*EXP(10840./temp))`	Burkholder et al. (2015)*
G3200	TrGN	$NO + OH \rightarrow HONO$	`k_3rd(temp,cair,7.0E-31,2.6,3.6E-11,0.1,0.6)`	Burkholder et al. (2015)
G3201	UpStTrGN	$NO + HO_2 \rightarrow$ ProdHO2 + 1.0 ProdO3 + NO_2 + OH	`3.3E-12*EXP(270./temp)`	Burkholder et al. (2015)
G3202	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	`k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0.,0.6)`	Burkholder et al. (2015)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Burkholder et al. (2015)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow$ 1.0 LossO3N + 1.0 LossO3 + NO_2 + OH + O_2	`3.5E-12`	Burkholder et al. (2015)
G3205	TrGN	HONO + OH $\rightarrow$ ProdH2O + 1.0 ProdO3 + NO_2 + H_2O	`1.8E-11*EXP(-390./temp)`	Burkholder et al. (2015)
G3206	StTrGN	HNO_3 + OH $\rightarrow$ ProdH2O + 1.0 ProdO3 + H_2O + NO_3	`k_HNO3_OH`	Dulitz et al. (2018)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Burkholder et al. (2015)*
G3208	StTrGN	HNO_4 + OH $\rightarrow$ ProdH2O + NO_2 + H_2O	`1.3E-12*EXP(380./temp)`	Burkholder et al. (2015)
G3209	TrGN	NH_3 + OH $\rightarrow$ ProdH2O + NH_2 + H_2O	`1.7E-12*EXP(-710./temp)`	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow$ 1.0 LossO3N + 1.0 LossO3 + NH_2O + O_2	`4.3E-12*EXP(-930./temp)`	Kohlmann and Poppe (1999)
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	`4.8E-07*EXP(-628./temp)*(temp)**(-1.32)`	Kohlmann and Poppe (1999)
G3212	TrGN	$NH_2 + HO_2 \rightarrow$ ProdH2O + HNO + H_2O	`9.4E-09*EXP(-356./temp)*(temp)**(-1.12)`	Kohlmann and Poppe (1999)
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	`1.92E-12*((temp/298.)**(-1.5))`	Kohlmann and Poppe (1999)
G3214	TrGN	NH_2 + NO $\rightarrow$ ProdH2O + N_2 + H_2O	`1.41E-11*((temp/298.)**(-1.5))`	Kohlmann and Poppe (1999)
G3215	TrGN	$NH_2 + NO_2 \rightarrow$ ProdH2O + 1.0 LossO3N + 1.0 LossO3 + N_2O + H_2O	`1.2E-11*((temp/298.)**(-2.0))`	Kohlmann and Poppe (1999)
G3216	TrGN	$NH_2 + NO_2 \rightarrow$ 1.0 LossO3N + 1.0 LossO3 + NH_2O + NO	`0.8E-11*((temp/298.)**(-2.0))`	Kohlmann and Poppe (1999)
G3217	TrGN	$NH_2O + O_3 \rightarrow$ 1.0 LossO3N + 1.0 LossO3 + NH_2 + O_2	`1.2E-14`	Kohlmann and Poppe (1999)
G3218	TrGN	$NH_2O \rightarrow NHOH$	`1.3E3`	Kohlmann and Poppe (1999)
G3219	TrGN	HNO + OH $\rightarrow$ ProdH2O + NO + H_2O	`8.0E-11*EXP(-500./temp)`	Kohlmann and Poppe (1999)
G3220	TrGN	HNO + NHOH $\rightarrow$ NH_2OH + NO	`1.66E-12*EXP(-1500./temp)`	Kohlmann and Poppe (1999)
G3221	TrGN	HNO + NO_2 $\rightarrow$ 1.0 LossO3N + 1.0 LossO3 + HONO + NO	`1.0E-12*EXP(-1000./temp)`	Kohlmann and Poppe (1999)
G3222	TrGN	NHOH + OH $\rightarrow$ ProdH2O + HNO + H_2O	`1.66E-12`	Kohlmann and Poppe (1999)
G3223	TrGN	NH_2OH + OH $\rightarrow$ ProdH2O + NHOH + H_2O	`4.13E-11*EXP(-2138./temp)`	Kohlmann and Poppe (1999)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G3224	TrGN	$HNO + O_2 \rightarrow HO_2 + NO$	3.65E-14*EXP(-4600./temp)	Kohlmann and Poppe (1999)
G4100	UpStG	$CH_4 + O(^1D) \rightarrow$ 1.0 LossO3O + 1.0 LossO3 + .75 CH_3O_2 + .75 OH + .25 HCHO + .4 H + .05 H_2	1.75E-10	Sander et al. (2011)
G4101	StTrG	$CH_4 + OH \rightarrow$ ProdH2O + $CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*LOG(temp) -987./temp)	Atkinson (2003)
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	2.9E-12*EXP(-345./temp)	Sander et al. (2011)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	4.1E-13*EXP(750./temp)	Sander et al. (2011)*
G4104	UpStTrGN	$CH_3O_2 + NO \rightarrow$ ProdMeO2 + 1.0 ProdO3 + HCHO + $NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2011)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow$ 1.0 LossO3R + 1.0 LossO3 + HCHO + $HO_2 + NO_2$	1.3E-12	Atkinson et al. (2006)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow$ 2 HCHO + 2 HO_2	9.5E-14*EXP(390./temp)/(1.+1./ 26.2*EXP(1130./temp))	Sander et al. (2011)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2011)
G4107	StTrG	$CH_3OOH + OH \rightarrow$ ProdH2O + .7 CH_3O_2 + .3 HCHO + .3 OH + H_2O	k_CH3OOH_OH	Wallington et al. (2018)
G4108	StTrG	$HCHO + OH \rightarrow$ ProdH2O + CO + $H_2O + HO_2$	9.52E-18*EXP(2.03*LOG(temp) +636./temp)	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow$ 1.0 LossO3R + 1.0 LossO3 + HNO_3 + CO + HO_2	3.4E-13*EXP(-1900./temp)	Sander et al. (2011)*
G4110	UpStTrG	$CO + OH \rightarrow H + CO_2$	(1.57E-13+cair*3.54E-33)	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow$ ProdH2O + $CO_2 + HO_2 + H_2O$	4.0E-13	Sander et al. (2011)
G4200	TrGC	$C_2H_6 + OH \rightarrow$ ProdH2O + $C_2H_5O_2 + H_2O$	1.49E-17*temp*temp*EXP(-499./ temp)	Atkinson (2003)
G4201	TrGC	$C_2H_4 + O_3 \rightarrow$ 1.0 LossO3R + 1.0 LossO3 + HCHO + .63 CO + .13 HO_2 + 0.23125 HCOOH + 0.13875 HCHO + 0.13875 H_2O_2 + .13 OH	1.2E-14*EXP(-2630./temp)	Sander et al. (2011)*
G4202	TrGC	$C_2H_4 + OH \rightarrow$ .6666667 $CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,1.0E-28,4.5, 7.5E-12,0.85,0.6)	Sander et al. (2011)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*EXP(700./temp)	Sander et al. (2011)
G4204	TrGCN	$C_2H_5O_2 + NO \rightarrow$ ProdRO2 + 1.0 ProdO3 + CH_3CHO + $HO_2 + NO_2$	2.6E-12*EXP(365./temp)	Sander et al. (2011)
G4205	TrGCN	$C_2H_5O_2 + NO_3 \rightarrow$ 1.0 LossO3R + 1.0 LossO3 + CH_3CHO + $HO_2 + NO_2$	2.3E-12	Wallington et al. (2018)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4206	TrGC	$C_2H_5O_2$ + CH_3O_2 → .75 HCHO + HO_2 + .75 CH_3CHO + .25 CH_3OH	`1.6E-13*EXP(195./temp)`	see note*
G4207	TrGC	C_2H_5OOH + OH → .3 $C_2H_5O_2$ + .7 CH_3CHO + .7 OH	`k_CH3OOH_OH`	see note*
G4208	TrGC	CH_3CHO + OH → ProdH2O + $CH_3C(O)OO$ + H_2O	`4.4E-12*EXP(365./temp)`	Atkinson et al. (2006)
G4209	TrGCN	CH_3CHO + NO_3 → 1.0 LossO3R + 1.0 LossO3 + $CH_3C(O)OO$ + HNO_3	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2011)
G4210	TrGC	CH_3COOH + OH → ProdH2O + CH_3O_2 + CO_2 + H_2O	`4.2E-14*EXP(855./temp)`	Atkinson et al. (2006)
G4211a	TrGC	$CH_3C(O)OO$ + HO_2 → $CH_3C(O)OOH$	`4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))`	Tyndall et al. (2001a)
G4211b	TrGC	$CH_3C(O)OO$ + HO_2 → 1.0 ProdO3 + CH_3COOH + O_3	`4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))`	Tyndall et al. (2001a)
G4212	TrGCN	$CH_3C(O)OO$ + NO → ProdRO2 + 1.0 ProdO3 + CH_3O_2 + CO_2 + NO_2	`8.1E-12*EXP(270./temp)`	Tyndall et al. (2001a)
G4213	TrGCN	$CH_3C(O)OO$ + NO_2 → PAN	`k_CH3CO3_NO2`	Sander et al. (2011)*
G4214	TrGCN	$CH_3C(O)OO$ + NO_3 → 1.0 LossO3R + 1.0 LossO3 + CH_3O_2 + NO_2 + CO_2	`4.E-12`	Canosa-Mas et al. (1996)
G4215a	TrGC	$CH_3C(O)OO$ + CH_3O_2 → HCHO + HO_2 + CH_3O_2 + CO_2	`0.9*2.0E-12*EXP(500./temp)`	Sander et al. (2011)
G4215b	TrGC	$CH_3C(O)OO$ + CH_3O_2 → CH_3COOH + HCHO	`0.1*2.0E-12*EXP(500./temp)`	Sander et al. (2011)
G4216	TrGC	$CH_3C(O)OO$ + $C_2H_5O_2$ → .82 CH_3O_2 + CH_3CHO + .82 HO_2 + .18 CH_3COOH	`4.9E-12*EXP(211./temp)`	Wallington et al. (2018), Kirchner and Stockwell (1996)
G4217	TrGC	$CH_3C(O)OO$ + $CH_3C(O)OO$ → 2 CH_3O_2 + 2 CO_2 + O_2	`2.5E-12*EXP(500./temp)`	Tyndall et al. (2001a)
G4218	TrGC	$CH_3C(O)OOH$ + OH → ProdH2O + $CH_3C(O)OO$ + H_2O	`0.6*k_CH3OOH_OH`	Rickard and Pascoe (2009)
G4219	TrGCN	NACA + OH → NO_2 + HCHO + CO	`5.6E-12*EXP(270./temp)`	Pöschl et al. (2000)
G4220	TrGCN	PAN + OH → ProdH2O + HCHO + CO + NO_2 + H_2O	`9.50E-13*EXP(-650./temp)`	Rickard and Pascoe (2009)
G4221	TrGCN	PAN → $CH_3C(O)OO$ + NO_2	`k_PAN_M`	Sander et al. (2011)*
G4222	TrGC	C_2H_2 + OH → CH_3O_2	`k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,-2.,0.6)`	Sander et al. (2011)
G4300	TrGC	C_3H_8 + OH → ProdH2O + .82 $iC_3H_7O_2$ + .18 $C_2H_5O_2$ + H_2O	`1.65E-17*temp*temp*EXP(-87./temp)`	Atkinson (2003)
G4301	TrGC	C_3H_6 + O_3 → 1.0 LossO3R + 1.0 LossO3 + .57 HCHO + .47 CH_3CHO + .33 OH + .26 HO_2 + .07 CH_3O_2 + .06 $C_2H_5O_2$ + .23 $CH_3C(O)OO$ + .04 MGLYOX + .06 CH_4 + .31 CO + .22 HCOOH + .03 CH_3OH	`6.5E-15*EXP(-1900./temp)`	Sander et al. (2011)
G4302	TrGC	C_3H_6 + OH → $CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)`	Wallington et al. (2018)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4303	TrGCN	C_3H_6 + NO_3 → 1.0 LossO3R + 1.0 LossO3 + LC4H9NO3	`4.6E-13*EXP(-1155./temp)`	Wallington et al. (2018)
G4304	TrGC	$iC_3H_7O_2$ + HO_2 → iC_3H_7OOH	`k_PrO2_HO2`	Atkinson (1997)
G4305	TrGCN	$iC_3H_7O_2$ + NO → ProdRO2 + 1.0 ProdO3 + .96 CH_3COCH_3 + .96 HO_2 + .96 NO_2 + .04 $iC_3H_7ONO_2$	`k_PrO2_NO`	Wallington et al. (2018)
G4306	TrGC	$iC_3H_7O_2$ + CH_3O_2 → CH_3COCH_3 + .8 HCHO + .8 HO_2 + .2 CH_3OH	`k_PrO2_CH3O2`	Kirchner and Stockwell (1996)
G4307	TrGC	iC_3H_7OOH + OH → .3 $iC_3H_7O_2$ + .7 CH_3COCH_3 + .7 OH	`k_CH3OOH_OH`	see note*
G4308	TrGC	$CH_3CH(O_2)CH_2OH$ + HO_2 → $CH_3CH(OOH)CH_2OH$	`6.5E-13*EXP(650./temp)`	Müller and Brasseur (1995)
G4309	TrGCN	$CH_3CH(O_2)CH_2OH$ + NO → ProdRO2 + 1.0 ProdO3 + .98 CH_3CHO + .98 HCHO + .98 HO_2 + .98 NO_2 + .02 LC4H9NO3	`4.2E-12*EXP(180./temp)`	Müller and Brasseur (1995)
G4310	TrGC	$CH_3CH(OOH)CH_2OH$ + OH → ProdH2O + .5 $CH_3CH(O_2)CH_2OH$ + .5 CH_3COCH_2OH + .5 OH + H_2O	`3.8E-12*EXP(200./temp)`	Müller and Brasseur (1995)
G4311	TrGC	CH_3COCH_3 + OH → ProdH2O + $CH_3COCH_2O_2$ + H_2O	`1.33E-13+3.82E-11*EXP(-2000./temp)`	Sander et al. (2011)
G4312	TrGC	$CH_3COCH_2O_2$ + HO_2 → $CH_3COCH_2O_2H$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001a)
G4313	TrGCN	$CH_3COCH_2O_2$ + NO → ProdRO2 + 1.0 ProdO3 + $CH_3C(O)OO$ + HCHO + NO_2	`2.9E-12*EXP(300./temp)`	Sander et al. (2011)
G4314	TrGC	$CH_3COCH_2O_2$ + CH_3O_2 → .5 MGLYOX + .5 CH_3OH + .3 $CH_3C(O)OO$ + .8 HCHO + .3 HO_2 + .2 CH_3COCH_2OH	`7.5E-13*EXP(500./temp)`	Tyndall et al. (2001a)
G4315	TrGC	$CH_3COCH_2O_2H$ + OH → .3 $CH_3COCH_2O_2$ + .7 MGLYOX + .7 OH	`k_CH3OOH_OH`	see note*
G4316	TrGC	CH_3COCH_2OH + OH → MGLYOX + HO_2	`2.15E-12*EXP(305./temp)`	Dillon et al. (2006)
G4317	TrGC	MGLYOX + OH → $CH_3C(O)OO$ + CO	`8.4E-13*EXP(830./temp)`	Tyndall et al. (1995)
G4320	TrGCN	$iC_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	`6.2E-13*EXP(-230./temp)`	Wallington et al. (2018)
G4400	TrGC	C_4H_{10} + OH → ProdH2O + $LC_4H_9O_2$ + H_2O	`1.81E-17*temp*temp*EXP(114./temp)`	Atkinson (2003)
G4401	TrGC	$LC_4H_9O_2$ + CH_3O_2 → .88 MEK + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	`k_PrO2_CH3O2`	see note*
G4402	TrGC	$LC_4H_9O_2$ + HO_2 → LC_4H_9OOH	`k_PrO2_HO2`	see note*
G4403	TrGCN	$LC_4H_9O_2$ + NO → ProdRO2 + 1.0 ProdO3 + .84 NO_2 + .56 MEK + .56 HO_2 + .28 $C_2H_5O_2$ + .28 CH_3CHO + .16 LC4H9NO3	`k_PrO2_NO`	see note*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4404	TrGC	$LC_4H_9OOH + OH \rightarrow 0.85\ ProdH2O + .15\ LC_4H_9O_2 + .85\ MEK + .85\ OH + .85\ H_2O$	`k_CH3OOH_OH`	see note*
G4405	TrGC	$MVK + O_3 \rightarrow 1.0\ LossO3R + 1.0\ LossO3 + .45\ HCOOH + .9\ MGLYOX + .1\ CH_3C(O)OO + .19\ OH + .22\ CO + .32\ HO_2$	`.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))`	Pöschl et al. (2000)
G4406	TrGC	$MVK + OH \rightarrow MVKO2$	`.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))`	Pöschl et al. (2000)
G4407	TrGC	$MVKO2 + HO_2 \rightarrow MVKOOH$	`1.82E-13*EXP(1300./temp)`	Pöschl et al. (2000)
G4408	TrGCN	$MVKO2 + NO \rightarrow ProdRO2 + 1.0\ ProdO3 + NO_2 + .25\ CH_3C(O)OO + .25\ CH_3COCH_2OH + .75\ HCHO + .25\ CO + .75\ HO_2 + .5\ MGLYOX$	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)
G4409	TrGCN	$MVKO2 + NO_2 \rightarrow MPAN$	`.25*k_3rd(temp,cair,9.7E-29,5.6, 9.3E-12,1.5,0.6)`	Pöschl et al. (2000)
G4410	TrGC	$MVKO2 + CH_3O_2 \rightarrow .5\ MGLYOX + .375\ CH_3COCH_2OH + .125\ CH_3C(O)OO + 1.125\ HCHO + .875\ HO_2 + .125\ CO + .25\ CH_3OH$	`2.E-12`	von Kuhlmann (2001)
G4411	TrGC	$MVKO2 + MVKO2 \rightarrow CH_3COCH_2OH + MGLYOX + .5\ CO + .5\ HCHO + HO_2$	`2.E-12`	Pöschl et al. (2000)
G4412	TrGC	$MVKOOH + OH \rightarrow MVKO2$	`3.E-11`	Pöschl et al. (2000)
G4413	TrGC	$MEK + OH \rightarrow LMEKO2$	`1.3E-12*EXP(-25./temp)`	Wallington et al. (2018)
G4414	TrGC	$LMEKO2 + HO_2 \rightarrow LMEKOOH$	`k_PrO2_HO2`	see note*
G4415	TrGCN	$LMEKO2 + NO \rightarrow ProdRO2 + 1.0\ ProdO3 + .985\ CH_3CHO + .985\ CH_3C(O)OO + .985\ NO_2 + .015\ LC4H9NO3$	`k_PrO2_NO`	see note*
G4416	TrGC	$LMEKOOH + OH \rightarrow .8\ BIACET + .8\ OH + .2\ LMEKO2$	`k_CH3OOH_OH`	see note*
G4417	TrGCN	$LC4H9NO3 + OH \rightarrow ProdH2O + MEK + NO_2 + H_2O$	`1.7E-12`	Wallington et al. (2018)
G4418	TrGCN	$MPAN + OH \rightarrow CH_3COCH_2OH + NO_2$	`3.2E-11`	Orlando et al. (2002)
G4419	TrGCN	$MPAN \rightarrow MVKO2 + NO_2$	`k_PAN_M`	see note*
G4500	TrGC	$C_5H_8 + O_3 \rightarrow 1.0\ LossO3R + 1.0\ LossO3 + .28\ HCOOH + .65\ MVK + .1\ MVKO2 + .1\ CH_3C(O)OO + .14\ CO + .58\ HCHO + .09\ H_2O_2 + .08\ CH_3O_2 + .25\ OH + .25\ HO_2$	`7.86E-15*EXP(-1913./temp)`	Pöschl et al. (2000)
G4501	TrGC	$C_5H_8 + OH \rightarrow ISO2$	`2.54E-11*EXP(410./temp)`	Pöschl et al. (2000)
G4502	TrGCN	$C_5H_8 + NO_3 \rightarrow 1.0\ LossO3R + 1.0\ LossO3 + ISON$	`3.03E-12*EXP(-446./temp)`	Pöschl et al. (2000)
G4503	TrGC	$ISO2 + HO_2 \rightarrow ISOOH$	`2.22E-13*EXP(1300./temp)`	Boyd et al. (2003)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4504	TrGCN	ISO2 + NO → ProdRO2 + 1.0 ProdO3 + .956 NO_2 + .956 MVK + .956 HCHO + .956 HO_2 + .044 ISON	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)
G4505	TrGC	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 MGLYOX + .25 CH_3COCH_2OH + .25 CH_3OH	`2.E-12`	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	`2.E-12`	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH	`1.E-10`	Pöschl et al. (2000)
G4508	TrGCN	ISON + OH → CH_3COCH_2OH + NACA	`1.3E-11`	Pöschl et al. (2000)
G6100	UpStTrGCl	Cl + O_3 → ClO + O_2	`2.8E-11*EXP(-250./temp)`	Atkinson et al. (2007)
G6101	UpStGCl	ClO + $O(^3P)$ → 2.0 LossO3Cl + 2.0 LossO3 + Cl + O_2	`2.5E-11*EXP(110./temp)`	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → 2.0 LossO3Cl + 2.0 LossO3 + Cl_2 + O_2	`1.0E-12*EXP(-1590./temp)`	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2.0 LossO3Cl + 2.0 LossO3 + 2 Cl + O_2	`3.0E-11*EXP(-2450./temp)`	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → 1.0 LossO3Cl + 1.0 LossO3 + Cl + OClO	`3.5E-13*EXP(-1370./temp)`	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	`k_ClO_ClO`	Burkholder et al. (2015)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	`k_ClO_ClO/(2.16E-27*EXP(8537./temp))`	Burkholder et al. (2015)*
G6200	StGCl	Cl + H_2 → HCl + H	`3.9E-11*EXP(-2310./temp)`	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO_2 → HCl + O_2	`4.4E-11-7.5E-11*EXP(-620./temp)`	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO_2 → 1.0 ProdO3 + ClO + OH	`7.5E-11*EXP(-620./temp)`	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	`1.1E-11*EXP(-980./temp)`	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → 1.0 LossO3Cl + 1.0 LossO3 + .94 Cl + .94 HO_2 + .06 HCl + .06 O_2	`7.3E-12*EXP(300./temp)`	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO_2 → HOCl + O_2	`2.2E-12*EXP(340./temp)`	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH → ProdH2O + Cl + H_2O	`1.7E-12*EXP(-230./temp)`	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH → ProdH2O + ClO + H_2O	`3.0E-12*EXP(-500./temp)`	Burkholder et al. (2015)
G6300	UpStTrGClN	ClO + NO → NO_2 + Cl	`6.2E-12*EXP(295./temp)`	Atkinson et al. (2007)
G6301	StTrGClN	ClO + NO_2 → $ClNO_3$	`k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4)`	Atkinson et al. (2007)
G6302	TrGClN	$ClNO_3$ → ClO + NO_2	`6.918E-7*EXP(-10909./temp)*cair`	Anderson and Fahey (1990)
G6303	StGClN	$ClNO_3$ + $O(^3P)$ → ClO + NO_3	`4.5E-12*EXP(-900./temp)`	Atkinson et al. (2007)
G6304	StTrGClN	$ClNO_3$ + Cl → Cl_2 + NO_3	`6.2E-12*EXP(145./temp)`	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH_4 → HCl + CH_3O_2	`6.6E-12*EXP(-1240./temp)`	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO_2	`8.1E-11*EXP(-34./temp)`	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH_3OOH → HCHO + HCl + OH	`5.9E-11`	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH_3O_2 → 1.0 LossO3Cl + 1.0 LossO3 + HO_2 + Cl + HCHO	`1.8E-12*EXP(-600./temp)`	Burkholder et al. (2015)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G6404	StGCl	CCl_4 + $O(^1D)$ → 4.0 ProdLCl + LCARBON + ClO + 3 Cl	`3.3E-10`	Burkholder et al. (2015)
G6405	StGCl	CH_3Cl + $O(^1D)$ → 1.0 ProdLCl + 1.0 LossO3Cl + 1.0 LossO3 + OH + Cl	`1.65E-10`	see note*
G6406	StGCl	CH_3Cl + OH → ProdH2O + 1.0 ProdLCl + LCARBON + H_2O + Cl	`1.96E-12*EXP(-1200./temp)`	Burkholder et al. (2015)
G6407	StGCCl	CH_3CCl_3 + $O(^1D)$ → 3.0 ProdLCl + 1.0 LossO3Cl + 1.0 LossO3 + 2 LCARBON + OH + 3 Cl	`3.25E-10`	Burkholder et al. (2015)
G6408	StTrGCCl	CH_3CCl_3 + OH → ProdH2O + 3.0 ProdLCl + 2 LCARBON + H_2O + 3 Cl	`1.64E-12*EXP(-1520./temp)`	Burkholder et al. (2015)
G6409	TrGCCl	Cl + C_2H_4 → .6666667 $CH_3CH(O_2)CH_2OH$ + HCl	`k_3rd_iupac(temp,cair,1.85E-29, 3.3,6.0E-10,0.0,0.4)`	Atkinson et al. (2006)
G6410	TrGCCl	Cl + CH_3CHO → HCl + $CH_3C(O)OO$	`8.0e-11`	Atkinson et al. (2006)
G6411	TrGCCl	C_2H_2 + Cl → LCARBON + CH_3 + HCl	`k_3rd_iupac(temp,cair,6.1e-30, 3.0,2.0e-10,0.,0.6)`	Atkinson et al. (2006)
G6412	TrGCCl	C_2H_6 + Cl → $C_2H_5O_2$ + HCl	`8.3E-11*EXP(-100./temp)`	Atkinson et al. (2006)
G6500	StGClF	CF_2Cl_2 + $O(^1D)$ → 2.0 ProdLCl + LCARBON + 2 LFLUORINE + ClO + Cl	`1.4E-10`	Burkholder et al. (2015)
G6501	StGClF	$CFCl_3$ + $O(^1D)$ → 3.0 ProdLCl + LCARBON + LFLUORINE + ClO + 2 Cl	`2.3E-10`	Burkholder et al. (2015)
G7100	StTrGBr	Br + O_3 → BrO + O_2	`1.7E-11*EXP(-800./temp)`	Atkinson et al. (2007)
G7101	StGBr	BrO + $O(^3P)$ → 2.0 LossO3Br + 2.0 LossO3 + Br + O_2	`1.9E-11*EXP(230./temp)`	Atkinson et al. (2007)
G7102a	StTrGBr	BrO + BrO → 2.0 LossO3Br + 2.0 LossO3 + 2 Br + O_2	`2.7E-12`	Atkinson et al. (2007)
G7102b	StTrGBr	BrO + BrO → 2.0 LossO3Br + 2.0 LossO3 + Br_2 + O_2	`2.9E-14*EXP(840./temp)`	Atkinson et al. (2007)
G7200	StTrGBr	Br + HO_2 → HBr + O_2	`7.7E-12*EXP(-450./temp)`	Atkinson et al. (2007)
G7201	StTrGBr	BrO + HO_2 → HOBr + O_2	`4.5E-12*EXP(500./temp)`	Atkinson et al. (2007)
G7202	StTrGBr	HBr + OH → ProdH2O + Br + H_2O	`6.7E-12*EXP(155./temp)`	Atkinson et al. (2007)
G7203	StGBr	HOBr + $O(^3P)$ → 1.0 LossO3Br + 1.0 LossO3 + OH + BrO	`1.2E-10*EXP(-430./temp)`	Atkinson et al. (2007)
G7204	StTrGBr	Br_2 + OH → 1.0 ProdO3 + HOBr + Br	`2.0E-11*EXP(240./temp)`	Atkinson et al. (2007)
G7300	TrGBrN	Br + $BrNO_3$ → Br_2 + NO_3	`4.9E-11`	Orlando and Tyndall (1996)
G7301	StTrGBrN	BrO + NO → Br + NO_2	`8.7E-12*EXP(260./temp)`	Atkinson et al. (2007)
G7302	StTrGBrN	BrO + NO_2 → $BrNO_3$	`k_BrO_NO2`	Atkinson et al. (2007)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G7303	TrGBrN	$BrNO_3 \rightarrow BrO + NO_2$	`k_BrO_NO2/(5.44E-9*EXP(14192./temp)*1.E6*R_gas*temp/(atm2Pa*N_A))`	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	`7.7E-12*EXP(-580./temp)`	Atkinson et al. (2006)
G7401	TrGBr	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	`2.6E-12*EXP(-1600./temp)`	Kondo and Benson (1984)
G7402a	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + HCHO$	`f_BrO_CH3O2*5.7E-12`	Aranda et al. (1997)
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow$ 1.0 LossO3Br + 1.0 LossO3 + Br + HCHO + HO_2	`(1.-f_BrO_CH3O2)*5.7E-12`	Aranda et al. (1997)
G7403	StTrGBr	$CH_3Br + OH \rightarrow$ ProdH2O + 1.0 ProdLBr + LCARBON + H_2O + Br	`1.42E-12*EXP(-1150./temp)`	Burkholder et al. (2015)
G7404	TrGBrC	$Br + C_2H_4 \rightarrow .6666667\ CH_3CH(O_2)CH_2OH + HBr$	`2.8E-13*EXP(224./temp)/(1.+1.13E24*EXP(-3200./temp)/C(ind_O2))`	Atkinson et al. (2006)
G7405	TrGBrC	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)OO$	`1.8e-11*EXP(-460./temp)`	Atkinson et al. (2006)
G7406	TrGBrC	$Br + C_2H_2 \rightarrow$ LCARBON + CH_3O_2 + HBr	`6.35e-15*EXP(440./temp)`	Atkinson et al. (2006)
G7407	TrGBr	$CHBr_3 + OH \rightarrow$ ProdH2O + 3.0 ProdSBr + LCARBON + H_2O + 3 Br	`9.0E-13*EXP(-360./temp)`	Burkholder et al. (2015)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow$ ProdH2O + 2.0 ProdSBr + LCARBON + H_2O + 2 Br	`2.0E-12*EXP(-840./temp)`	Burkholder et al. (2015)*
G7600	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	`3.32E-15`	Manion et al. (2015)
G7601	TrGBrCl	$Br + Cl_2 \rightarrow BrCl + Cl$	`1.10E-15`	Dolson and Leone (1987)
G7602	TrGBrCl	$Br_2 + Cl \rightarrow BrCl + Br$	`2.3E-10*EXP(135./temp)`	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$BrO + ClO \rightarrow$ 0.5 LossO3Br + 0.5 LossO3Cl + 1.0 LossO3 + Br + OClO	`1.6E-12*EXP(430./temp)`	Atkinson et al. (2007)
G7603b	StTrGBrCl	$BrO + ClO \rightarrow$ 1.0 LossO3Br + 1.0 LossO3Cl + 2.0 LossO3 + Br + Cl + O_2	`2.9E-12*EXP(220./temp)`	Atkinson et al. (2007)
G7603c	StTrGBrCl	$BrO + ClO \rightarrow$ 1.0 LossO3Br + 1.0 LossO3Cl + 2.0 LossO3 + BrCl + O_2	`5.8E-13*EXP(170./temp)`	Atkinson et al. (2007)
G7604	TrGBrCl	$BrCl + Cl \rightarrow Br + Cl_2$	`1.45E-11`	Clyne and Cruse (1972)
G7605	TrGBrCl	$CHCl_2Br + OH \rightarrow$ ProdH2O + 1.0 ProdSBr + 2.0 ProdSCl + LCARBON + 2 Cl + H_2O + Br	`2.0E-12*EXP(-840./temp)`	see note*
G7606	TrGBrCl	$CHClBr_2 + OH \rightarrow$ ProdH2O + 2.0 ProdSBr + 1.0 ProdSCl + LCARBON + Cl + H_2O + 2 Br	`2.0E-12*EXP(-840./temp)`	see note*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G7607	TrGBrCl	CH_2ClBr + OH → ProdH2O + 1.0 ProdSBr + 1.0 ProdSCl + LCARBON + Cl + H_2O + Br	`2.1E-12*EXP(-880./temp)`	Burkholder et al. (2015)*
G9200a	StTrGS	SO_2 + OH → 1.0 ProdO3 + SO_3 + HO_2	`k_3rd(temp,cair,3.3E-31,4.3, 1.6E-12,0.,0.6)`	Sander et al. (2011)
G9400a	TrGCS	DMS + OH → 1.0 ProdO3 + CH_3SO_2 + HCHO	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2004)*
G9400b	TrGCS	DMS + OH → 1.0 ProdO3 + DMSO + HO_2	`k_DMS_OH`	Atkinson et al. (2004)*
G9401	TrGCNS	DMS + NO_3 → CH_3SO_2 + HNO_3 + HCHO	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2004)
G9402	TrGCS	DMSO + OH → 0.40 ProdO3 + .6 SO_2 + HCHO + .6 CH_3O_2 + .4 HO_2 + .4 CH_3SO_3H	`1.E-10`	Hynes and Wine (1996)
G9403	TrGS	CH_3SO_2 → SO_2 + CH_3O_2	`1.8E13*EXP(-8661./temp)`	Barone et al. (1995)
G9404	TrGS	CH_3SO_2 + O_3 → CH_3SO_3	`3.E-13`	Barone et al. (1995)
G9405	TrGS	CH_3SO_3 + HO_2 → CH_3SO_3H	`5.E-11`	Barone et al. (1995)
G9600	TrGCClS	DMS + Cl → 1.0 ProdO3 + CH_3SO_2 + HCl + HCHO	`3.3E-10`	Atkinson et al. (2004)
G9700	TrGBrCS	DMS + Br → 1.0 ProdO3 + CH_3SO_2 + HBr + HCHO	`9.E-11*EXP(-2386./temp)`	Jefferson et al. (1994)
G9701	TrGBrCS	DMS + BrO → DMSO + Br	`4.4E-13`	Ingham et al. (1999)
G01Diag	StTrG	O_3(s) → LO_3(s)	`k_O3s`	Roelofs and Lelieveld (1997)
G42085abS	TrGCN	CH_3CN + OH → OH	`8.1E-13*EXP(-1080./temp)`	Atkinson et al. (2006), Tyndall et al. (2001b)
G42086bcS	TrGCN	CH_3CN + $O(^1D)$ → $O(^1D)$	`2.54E-10*EXP(-24./temp) *(1.-0.0269*EXP(137./temp))`	Strekowski et al. (2010)
G6416S	TrGCClN	Cl + CH_3CN → Cl	`1.6E-11*EXP(-2104./temp)`	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019)
G6500dc01	StGClF	CHF_2Cl + $O(^1D)$ → 0.72 ProdLCl + 0.17 LossO3O + 0.17 LossO3 + 0.55 ClO + 0.05 OH + 0.28 $O(^3P)$ + 0.28 CHF_2Cl +0.72 LCARBON + 0.17 Cl	`1.0E-10`	Sander et al. (2011)
G6500dc02	StG	CHF_2Cl + OH → ProdH2O + LCARBON + H_2O	`1.05e-12*EXP(-1600./temp)`	Sander et al. (2011)
G6500dc03	StG	CHF_2Cl + Cl → HCl + LCARBON	`1.05e-12*EXP(-2430./temp)`	Sander et al. (2011)
G5300dc01	StGCF	CH_2FCF_3 + $O(^1D)$ → 0.35 LossO3O + 0.35 LossO3 + 0.65 $O(^3P)$ + 0.65 CH_2FCF_3 + 0.24 OH + 0.70 LCARBON	`4.9E-11`	Sander et al. (2011)*
G5300dc02	StG	CH_2FCF_3 + OH → ProdH2O + 2 LCARBON + H_2O	`1.05e-12*EXP(-1630./temp)`	Sander et al. (2011)
G5300dc03	StG	CH_2FCF_3 + Cl → HCl + 2 LCARBON	`2.4e-12*EXP(-2200./temp)`	Sander et al. (2011)
G6500dc04	StG	$CF_2ClCFCl_2$ + $O(^1D)$ → 2.4 ProdLCl + 0.2 $O(^3P)$ + 0.2 $CF_2ClCFCl_2$ + 0.8 ClO + 1.6 LCARBON + 1.6 Cl	`2.0E-10`	Sander et al. (2011)
G6400dc01	StG	CH_2Cl_2 + OH → ProdH2O + LCARBON + H_2O	`1.09e-12*EXP(-870./temp)`	Sander et al. (2011)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G6400dc02	StG	CH_2Cl_2 + Cl → LCARBON + HCl	.4e-12*EXP(-910./temp)	Sander et al. (2011)
G5300dc04	StG	CHF_3 + $O(^1D)$ → 0.23 LossO3O + 0.23 LossO3 + 0.77 $O(^3P)$ + 0.77 CHF_3 + 0.23 LCARBON	9.1E-12	Sander et al. (2011)*
G5300dc05	StG	CHF_3 + OH → ProdH2O + LCARBON + H_2O	5.2e-13*EXP(-2210./temp)	Sander et al. (2011)
G6500dc05	StG	CH_3CFCl_2 + $O(^1D)$ → 0.69 LossO3O + 0.69 LossO3 + 0.31 $O(^3P)$ + 0.31 CH_3CFCl_2 + 0.69 LCARBON + 0.69 Cl	2.6E-10	Sander et al. (2011)*
G6500dc06	StG	CH_3CFCl_2 + OH → ProdH2O + H_2O + 2 LCARBON	1.25e-12*EXP(-1600./temp)	Sander et al. (2011)
G6500dc07	StG	CH_3CFCl_2 + Cl → HCl + 2 LCARBON	3.4e-12*EXP(-2200./temp)	Sander et al. (2011)
G6500dc08	StG	CF_2ClCF_2Cl + $O(^1D)$ → 0.75 LossO3O + 0.75 LossO3 + 0.25 $O(^3P)$ + 0.25 CF_2ClCF_2Cl + 0.75 LCARBON	1.3E-10	Sander et al. (2011)
G5300dc06	StG	CHF_2CF_3 + $O(^1D)$ → 0.76 LossO3O + 0.76 LossO3 + 0.24 $O(^3P)$ + 0.24 CHF_2CF_3 + 0.6 OH + 1.52 LCARBON	1.2E-10	Sander et al. (2011)*
G5300dc07	StG	CHF_2CF_3 + OH → ProdH2O + H_2O + 2 LCARBON	6.0e-13*EXP(-1700./temp)	Sander et al. (2011)
G6500dc09	StG	CHF_2CF_3 + Cl → HCl + 2 LCARBON	1.8e-12*EXP(-2600./temp)	Sander et al. (2011)
G5300dc08	StG	CH_3CF_3 + $O(^1D)$ → 0.82 LossO3O + 0.82 LossO3 + 0.18 $O(^3P)$ + 0.18 CH_3CF_3 + 0.38 OH + 0.8 LCARBON	4.4E-11	Sander et al. (2011)*
G5300dc09	StG	CH_3CF_3 + OH → ProdH2O + H_2O + 2 LCARBON	1.1e-12*EXP(-2010./temp)	Sander et al. (2011)
G6500dc10	StG	CH_3CF_3 + Cl → HCl + 2 LCARBON	1.44e-11*EXP(-3940./temp)	Sander et al. (2011)
G6400dc03	StG	$CHCl_3$ + OH → ProdH2O + H_2O + LCARBON + 3 Cl	2.2e-12*EXP(-920./temp)	Sander et al. (2011)
G6400dc04	StG	$CHCl_3$ + Cl → HCl + LCARBON + 3 Cl	3.31e-12*EXP(-990./temp)	Sander et al. (2011)
G6500dc11	StG	CF_3CF_2Cl + $O(^1D)$ → 0.30 LossO3O + 0.30 LossO3 + 0.7 $O(^3P)$ + 0.7 CF_3CF_2Cl + 0.6 LCARBON	5.0E-11	Sander et al. (2011)
G5300dc10	StG	CH_2F_2 + $O(^1D)$ → 0.30 LossO3O + 0.30 LossO3 + 0.7 $O(^3P)$ + 0.7 CH_2F_2 + 0.3 LCARBON	5.1e-11	Sander et al. (2011)
G5300dc11	StG	CH_2F_2 + OH → ProdH2O + H_2O + LCARBON	1.7e-12*EXP(-1500./temp)	Sander et al. (2011)
G5300dc12	StG	CH_3CHF_2 + $O(^1D)$ → 0.66 LossO3O + 0.66 LossO3 + 0.34 $O(^1D)$ + 0.34 CH_3CHF_2 + 0.15 OH + LCARBON	1.75e-10	Sander et al. (2011)
G5300dc13	StG	CH_3CHF_2 + OH → 2 LCARBON	8.7e-13*EXP(-975./temp)	Sander et al. (2011)
G6500dc12	StG	CH_3CHF_2 + Cl → HCl + 2 LCARBON	6.0e-12*EXP(-960./temp)	Sander et al. (2011)
G9100	TrStGS	SO + O_2 → 2.0 ProdO3 + SO_2 + $O(^3P)$	1.25e-13*exp(-2190/temp)	Sander et al. (2011)
G9101	TrStGS	SO + O_3 → SO_2 + O_2	3.4e-12*exp(-1100/temp)	Sander et al. (2011)
G9102	TrStGS	S + O_2 → 1.0 ProdO3 + SO + $O(^3P)$	2.3e-12	Sander et al. (2011)
G9201	TrStGS	SH + O_2 → OH + SO	4.e-19	Sander et al. (2011)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G9202	TrStGS	SO_3 + H_2O → LossH2O + H_2SO_4	8.5e-41*exp(6540./temp)*C(ind_H2O)	Sander et al. (2003)
G9406	TrStGS	OCS + OH → SH + CO_2	1.1e-13*exp(-1200./temp)	Sander et al. (2011)
G9407	TrStGS	OCS + O(^{3}P) → 1.0 LossO3Su + 1.0 LossO3 + CO + SO	2.1e-11*exp(-2200./temp)	Sander et al. (2011)

General notes

Three-body reactions

Rate coefficients for three-body reactions are defined via the function k_3rd(T, M, k_0^{300}, n, k_{inf}^{300}, m, f_c). In the code, the temperature T is called temp and the concentration of "air molecules" M is called cair. Using the auxiliary variables $k_0(T)$, $k_{\text{inf}}(T)$, and k_{ratio}, k_3rd is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \tag{1}$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \tag{2}$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \tag{3}$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1+(\log_{10}(k_{\text{ratio}}))^2}\right)} \tag{4}$$

A similar function, called k_3rd_iupac here, is used by Wallington et al. (2018) for three-body reactions. It has the same function parameters as k_3rd and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \tag{5}$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \tag{6}$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \tag{7}$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \tag{8}$$

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1+(\log_{10}(k_{\text{ratio}})/N)^2}\right)} \tag{9}$$

Structure-Activity Relationships (SAR)

Some unmeasured rate coefficients are estimated with structure-activity relationships, using the following parameters and substituent factors:

k for H-abstraction by OH in $\text{cm}^{-3}\text{s}^{-1}$	
k_p	$4.49 \times 10^{-18} \times (T/\text{K})^2 \exp(-320\,\text{K}/T)$
k_s	$4.50 \times 10^{-18} \times (T/\text{K})^2 \exp(253\,\text{K}/T)$
k_t	$2.12 \times 10^{-18} \times (T/\text{K})^2 \exp(696\,\text{K}/T)$
k_ROHRO	$2.1 \times 10^{-18} \times (T/\text{K})^2 \exp(-85\,\text{K}/T)$
k_CO2H	$0.7 \times k_{CH_3CO_2H+OH}$
k_ROOHRO	$0.6 \times k_{CH_3OOH+OH}$
f_alk	1.23
f_sOH	3.44
f_tOH	2.68
f_sOOH	8.
f_tOOH	8.
f_ONO2	0.04
f_CH2ONO2	0.20
f_cpan	0.25
f_allyl	3.6
f_CHO	0.55
f_CO2H	1.67
f_CO	0.73
f_O	8.15
f_pCH2OH	1.29
f_tCH2OH	0.53

k for OH-addition to double bonds in $\text{cm}^{-3}\text{s}^{-1}$	
k_adp	$4.5 \times 10^{-12} \times (T/300\,\text{K})^{-0.85}$
k_ads	$1/4 \times (1.1 \times 10^{-11} \times \exp(485\,\text{K}/T) + 1.0 \times 10^{-11} \times \exp(553\,\text{K}/T))$
k_adt	$1.922 \times 10^{-11} \times \exp(450\,\text{K}/T) - k_{\text{ads}}$
k_adsecprim	3.0×10^{-11}
k_adtertprim	5.7×10^{-11}
a_PAN	0.56
a_CHO	0.31
a_COCH3	0.76
a_CH2OH	1.7
a_CH2OOH	1.7
a_COH	2.2
a_COOH	2.2
a_CO2H	0.25
a_CH2ONO2	0.64

RO_2 self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as decribed by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{1\text{st}} = 2 \times \sqrt{k_{\text{self}} \times \texttt{k\_CH3O2}} \times [RO_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH3O2 = second-order rate coefficient of the self reaction of CH_3O_2, and $[RO_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

`G1002a`: The path leading to 2 $O(^3P) + O_2$ results in a null cycle regarding odd oxygen and is neglected.

`G2110`: The rate coefficient is: `k_HO2_HO2 = (3.0E-13*EXP(460./temp)+2.1E-33*EXP(920./temp) *cair)*(1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`.

`G3109`: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.4E-30,3.0,1.6E-12,-0.1,0.6)`.

`G3110`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G3203`: The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.9E-31,3.4,4.0E-12,0.3,0.6)`.

`G3206`: The rate coefficient is: `k_HNO3_OH = 1.32E-14 * EXP(527/temp) + 1 / ( 1 / (7.39E-32 * EXP(453/temp)*cair) + 1 / (9.73E-17 * EXP(1910/temp)) )`

`G3207`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G4103`: Sander et al. (2006) recommend a zero product yield for HCHO.

`G4109`: The same temperature dependence assumed as for CH_3CHO+NO_3. At 298 K, $k = 5.8 \times 10^{-16}$.

`G4201`: The product distribution is from Rickard and Pascoe (2009), after substitution of the Criegee intermediate by its decomposition products.

`G4206`: The product C_2H_5OH, which reacts only with OH, is substituted by its degradation products $\approx$ 0.1 $HOCH_2CH_2O_2$ + 0.9 CH_3CHO + 0.9 HO_2.

`G4207`: Same value as for G4107

`G4213`: The rate coefficient is: `k_CH3CO3_NO2 = k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)`.

`G4221`: The rate coefficient is`k_PAN_M = k_CH3CO3_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

`G4307`: Same value as for G4107

`G4315`: Same value as for G4107

`G4401`: Same value as for G4306

`G4402`: Same value as for G4304

`G4403`: Same value as for G4305

`G4404`: Same value as for G4107

`G4414`: Same value as for G4304

`G4415`: Same value as for G4305

`G4416`: Same value as for G4107

`G4419`: Same value as for G4221

`G6103`: The rate coefficient is defined as backward reaction divided by equilibrium constant.

`G6204`: At low temperatures, there may be a minor reaction channel leading to O_3+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

`G6402`: The initial products are probably HCl and CH_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

`G6405`: Sander et al. (2006), but simplified shortcut to release all Cl

`G7302`: The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

`G7303`: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (Orlando and Tyndall, 1996).

`G7407`: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

`G7408`: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

`G7605`: Same value as for G7408: CH_2Br_2+OH assumed. It is assumed that the reaction liberates all Br and all Cl. The fate of the carbon atom is currently not considered.

`G7606`: Same value as for G7408: CH_2Br_2+OH assumed. It is assumed that the reaction liberates all Br atoms and also Cl. The fate of the carbon atom is currently not considered.

`G7607`: It is assumed that the reaction liberates all Br atoms and also Cl. The fate of the carbon atom is currently not considered.

`G9400a`: For the abstraction path, the assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

$$\begin{array}{rcl}
\mathrm{DMS + OH} & \rightarrow & \mathrm{CH_3SCH_2} \\
\mathrm{CH_3SCH_2 + O_2} & \rightarrow & \mathrm{CH_3SCH_2OO} \\
\mathrm{CH_3SCH_2OO + NO} & \rightarrow & \mathrm{CH_3SCH_2O + NO_2} \\
\mathrm{CH_3SCH_2O} & \rightarrow & \mathrm{CH_3S + HCHO} \\
\mathrm{CH_3S + O_3} & \rightarrow & \mathrm{CH_3SO} \\
\mathrm{CH_3SO + O_3} & \rightarrow & \mathrm{CH_3SO_2} \\
\hline
\mathrm{DMS + OH + NO + 2O_3} & \rightarrow & \mathrm{CH_3SO_2 + HCHO + NO_2}
\end{array}$$

Neglecting the effect on O_3 and NO_x, the remaining reaction is:

$$\mathrm{DMS + OH + O_3 \rightarrow CH_3SO_2 + HCHO}$$

.

`G9400b`: For the addition path, the rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

`G5300dc01`: Kono and Matsumi 2001

`G5300dc04`: force and wiesenfeld 1981

`G6500dc05`: physical quenching (O1D-¿O3P) Warren 1991

`G5300dc06`: Kono and Matsumi

`G5300dc08`: Kono and Matsumi

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
J1000a	UpStTrGJ	O_2 + hν → 2.0 ProdO3 + O(^{3}P) + O(^{3}P)	`jx(ip_O2)`	Sander et al. (2014)
J1001a	UpStTrGJ	O_3 + hν → O(^{1}D) + O_2	`jx(ip_O1D)`	Sander et al. (2014)
J1001b	UpStTrGJ	O_3 + hν → O(^{3}P) + O_2	`jx(ip_O3P)`	Sander et al. (2014)
J2100a	UpStGJ	H_2O + hν → LossH2O + H + OH	`jx(ip_H2O)`	Sander et al. (2014)
J2101	UpStTrGJ	H_2O_2 + hν → 2 OH	`jx(ip_H2O2)`	Sander et al. (2014)
J3100	UpStGJN	N_2O + hν → 1.0 ProdO3 + O(^{1}D) + N_2	`jx(ip_N2O)`	Sander et al. (2014)
J3101	UpStTrGJN	NO_2 + hν → NO + O(^{3}P)	`jx(ip_NO2)`	Sander et al. (2014)
J3102a	UpStGJN	NO + hν → 1.0 ProdO3 + N + O(^{3}P)	`jx(ip_NO)`	Sander et al. (2014)
J3103a	UpStTrGJN	NO_3 + hν → NO_2 + O(^{3}P)	`jx(ip_NO2O)`	Sander et al. (2014)
J3103b	UpStTrGJN	NO_3 + hν → 2.0 LossO3N + 2.0 LossO3 + NO + O_2	`jx(ip_NOO2)`	Sander et al. (2014)
J3104	StTrGJN	N_2O_5 + hν → NO_2 + NO_3	`jx(ip_N2O5)`	Sander et al. (2014)
J3200	TrGJN	HONO + hν → NO + OH	`jx(ip_HONO)`	Sander et al. (2014)
J3201	StTrGJN	HNO_3 + hν → NO_2 + OH	`jx(ip_HNO3)`	Sander et al. (2014)
J3202	StTrGJN	HNO_4 + hν → 0.333 ProdO3 + .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH	`jx(ip_HNO4)`	Sander et al. (2014)
J4100	StTrGJ	CH_3OOH + hν → HCHO + OH + HO_2	`jx(ip_CH3OOH)`	Sander et al. (2014)
J4101a	StTrGJ	HCHO + hν → H_2 + CO	`jx(ip_COH2)`	Sander et al. (2014)
J4101b	StTrGJ	HCHO + hν → H + CO + HO_2	`jx(ip_CHOH)`	Sander et al. (2014)
J4102	StGJ	CO_2 + hν → 1.0 ProdO3 + CO + O(^{3}P)	`jx(ip_CO2)`	Sander et al. (2014)
J4103	StGJ	CH_4 + hν → 1.155 ProdH2O + CO + 0.31 H + 0.69 H_2 + 1.155 H_2O	`jx(ip_CH4)`	Sander et al. (2014)
J4200	TrGJC	C_2H_5OOH + hν → CH_3CHO + HO_2 + OH	`jx(ip_CH3OOH)`	von Kuhlmann (2001)
J4201	TrGJC	CH_3CHO + hν → CH_3O_2 + HO_2 + CO	`jx(ip_CH3CHO)`	Sander et al. (2014)
J4202	TrGJC	$CH_3C(O)OOH$ + hν → CH_3O_2 + OH + CO_2	`jx(ip_CH3CO3H)`	Sander et al. (2014)
J4203	TrGJCN	NACA + hν → NO_2 + HCHO + CO	`0.19*jx(ip_CHOH)`	von Kuhlmann (2001)
J4204	TrGJCN	PAN + hν → $CH_3C(O)OO$ + NO_2	`jx(ip_PAN)`	Sander et al. (2014)
J4300	TrGJC	iC_3H_7OOH + hν → CH_3COCH_3 + HO_2 + OH	`jx(ip_CH3OOH)`	von Kuhlmann (2001)
J4301	TrGJC	CH_3COCH_3 + hν → $CH_3C(O)OO$ + CH_3O_2	`jx(ip_CH3COCH3)`	Sander et al. (2014)
J4302	TrGJC	CH_3COCH_2OH + hν → $CH_3C(O)OO$ + HCHO + HO_2	`0.074*jx(ip_CHOH)`	see note*
J4303	TrGJC	MGLYOX + hν → $CH_3C(O)OO$ + CO + HO_2	`jx(ip_MGLYOX)`	Sander et al. (2014)
J4304	TrGJC	$CH_3COCH_2O_2H$ + hν → $CH_3C(O)OO$ + HCHO + OH	`jx(ip_CH3OOH)`	see note*
J4306	TrGJCN	$iC_3H_7ONO_2$ + hν → CH_3COCH_3 + NO_2 + HO_2	`3.7*jx(ip_PAN)`	von Kuhlmann et al. (2003)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4400	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + .67\ MEK + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J4401	TrGJC	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	`0.019*jx(ip_COH2)+.015*jx(ip_MGLYOX)`	Sander et al. (2014)
J4402	TrGJC	$MVKOOH + h\nu \rightarrow OH + .5\ MGLYOX + .25\ CH_3COCH_2OH + .75\ HCHO + .75\ HO_2 + .25\ CH_3C(O)OO + .25\ CO$	`jx(ip_CH3OOH)`	see note*
J4403	TrGJC	$MEK + h\nu \rightarrow CH_3C(O)OO + C_2H_5O_2$	`0.42*jx(ip_CHOH)`	von Kuhlmann et al. (2003)
J4404	TrGJC	$LMEKOOH + h\nu \rightarrow CH_3C(O)OO + CH_3CHO + OH$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J4405	TrGJC	$BIACET + h\nu \rightarrow 2\ CH_3C(O)OO$	`2.15*jx(ip_MGLYOX)`	see note*
J4406	TrGJCN	$LC4H9NO3 + h\nu \rightarrow NO_2 + .67\ MEK + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	`3.7*jx(ip_PAN)`	von Kuhlmann (2001)
J4407	TrGJCN	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	`jx(ip_PAN)`	see note*
J4500	TrGJC	$ISOOH + h\nu \rightarrow MVK + HCHO + HO_2 + OH$	`jx(ip_CH3OOH)`	see note*
J4501	TrGJCN	$ISON + h\nu \rightarrow MVK + HCHO + NO_2 + HO_2$	`3.7*jx(ip_PAN)`	von Kuhlmann (2001)
J6000	StTrGJCl	$Cl_2 + h\nu \rightarrow Cl + Cl$	`jx(ip_Cl2)`	Sander et al. (2014)
J6100	StTrGJCl	$Cl_2O_2 + h\nu \rightarrow 2.0\ LossO3Cl + 2.0\ LossO3 + 2\ Cl$	`jx(ip_Cl2O2)`	Sander et al. (2014)
J6101	StTrGJCl	$OClO + h\nu \rightarrow 1.0\ ProdO3 + ClO + O(^3P)$	`jx(ip_OClO)`	Sander et al. (2014)
J6200	StGJCl	$HCl + h\nu \rightarrow Cl + H$	`jx(ip_HCl)`	Sander et al. (2014)
J6201	StTrGJCl	$HOCl + h\nu \rightarrow 1.0\ LossO3Cl + 1.0\ LossO3 + OH + Cl$	`jx(ip_HOCl)`	Sander et al. (2014)
J6300	TrGJClN	$ClNO_2 + h\nu \rightarrow 1.0\ ProdO3 + Cl + NO_2$	`jx(ip_ClNO2)`	Sander et al. (2014)
J6301a	StTrGJClN	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	`jx(ip_ClNO3)`	Sander et al. (2014)
J6301b	StTrGJClN	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	`jx(ip_ClONO2)`	Sander et al. (2014)
J6400	StGJCl	$CH_3Cl + h\nu \rightarrow 1.0\ ProdLCl + Cl + CH_3O_2$	`jx(ip_CH3Cl)`	Sander et al. (2014)
J6401	StGJCl	$CCl_4 + h\nu \rightarrow 4.0\ ProdLCl + LCARBON + 4\ Cl$	`jx(ip_CCl4)`	Sander et al. (2014)
J6402	StGJCCl	$CH_3CCl_3 + h\nu \rightarrow 3.0\ ProdLCl + 2\ LCARBON + 3\ Cl$	`jx(ip_CH3CCl3)`	Sander et al. (2014)
J6500	StGJClF	$CFCl_3 + h\nu \rightarrow 3.0\ ProdLCl + 3\ Cl + LCARBON + LFLUORINE$	`jx(ip_CFCl3)`	Sander et al. (2014)
J6501	StGJClF	$CF_2Cl_2 + h\nu \rightarrow 2.0\ ProdLCl + 2\ Cl + LCARBON + 2\ LFLUORINE$	`jx(ip_CF2Cl2)`	Sander et al. (2014)
J7000	StTrGJBr	$Br_2 + h\nu \rightarrow Br + Br$	`jx(ip_Br2)`	Sander et al. (2014)
J7100	StTrGJBr	$BrO + h\nu \rightarrow Br + O(^3P)$	`jx(ip_BrO)`	Sander et al. (2014)
J7200	StTrGJBr	$HOBr + h\nu \rightarrow 1.0\ LossO3Br + 1.0\ LossO3 + Br + OH$	`jx(ip_HOBr)`	Sander et al. (2014)
J7300	TrGJBrN	$BrNO_2 + h\nu \rightarrow 1.0\ ProdO3 + Br + NO_2$	`jx(ip_BrNO2)`	Sander et al. (2014)
J7301	StTrGJBrN	$BrNO_3 + h\nu \rightarrow .85\ Br + .85\ NO_3 + .15\ BrO + .15\ NO_2$	`jx(ip_BrNO3)`	Sander et al. (2014)*
J7400	StGJBr	$CH_3Br + h\nu \rightarrow 1.0\ ProdLBr + Br + CH_3O_2$	`jx(ip_CH3Br)`	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7401	TrGJBr	CH_2Br_2 + hν $\rightarrow$ 2.0 ProdSBr + LCARBON + 2 Br	`jx(ip_CH2Br2)`	Sander et al. (2014)
J7402	TrGJBr	$CHBr_3$ + hν $\rightarrow$ 3.0 ProdSBr + LCARBON + 3 Br	`jx(ip_CHBr3)`	Sander et al. (2014)
J7500	StGJBrF	CF_3Br + hν $\rightarrow$ 1.0 ProdLBr + LCARBON + 3 LFLUORINE + Br	`jx(ip_CF3Br)`	Sander et al. (2014)
J7600	StTrGJBrCl	BrCl + hν $\rightarrow$ Br + Cl	`jx(ip_BrCl)`	Sander et al. (2014)
J7601	StGJBrClF	CF_2ClBr + hν $\rightarrow$ 1.0 ProdLBr + 1.0 ProdLCl + LCARBON + 2 LFLUORINE + Br + Cl	`jx(ip_CF2ClBr)`	Sander et al. (2014)
J7602	TrGJBrCl	CH_2ClBr + hν $\rightarrow$ 1.0 ProdSBr + 1.0 ProdSCl + LCARBON + Br + Cl	`jx(ip_CH2ClBr)`	Sander et al. (2014)
J7603	TrGJBrCl	$CHCl_2Br$ + hν $\rightarrow$ 1.0 ProdSBr + 2.0 ProdSCl + LCARBON + Br + 2 Cl	`jx(ip_CHCl2Br)`	Sander et al. (2014)
J7604	TrGJBrCl	$CHClBr_2$ + hν $\rightarrow$ 2.0 ProdSBr + 1.0 ProdSCl + LCARBON + 2 Br + Cl	`jx(ip_CHClBr2)`	Sander et al. (2014)
J8401	StTrGJI	CH_3I + hν $\rightarrow$ CH_3O_2	`JX(ip_CH3I)`	Sander et al. (2014)
J6500dc01	StGJClF	CHF_2Cl + hν $\rightarrow$ 1.0 ProdLCl + Cl + LCARBON + 2 LFLUORINE	`jx(ip_CHF2Cl)`	Sander et al. (2011)*
J6500dc02	StGJCClF	$CF_2ClCFCl_2$ + hν $\rightarrow$ 3.0 ProdLCl + 3 Cl + 2 LCARBON	`jx(ip_CF2ClCFCl2)`	Sander et al. (2011)
J6400dc01	StGJCl	CH_2Cl_2 + hν $\rightarrow$ 2.0 ProdLCl + 2 Cl + LCARBON	`jx(ip_CH2Cl2)`	Sander et al. (2011)
J6500dc03	StGJCClF	CH_3CFCl_2 + hν $\rightarrow$ 2.0 ProdLCl + 2 Cl + 2 LCARBON	`jx(ip_CH3CFCl2)`	Sander et al. (2011)
J6500dc04	StGJCClF	CF_2ClCF_2Cl + hν $\rightarrow$ 2.0 ProdLCl + 2 Cl + 2 LCARBON	`jx(ip_CF2ClCF2Cl)`	Sander et al. (2011)
J6400dc02	StGJCl	$CHCl_3$ + hν $\rightarrow$ 3.0 ProdLCl + 3 Cl + LCARBON	`jx(ip_CHCl3)`	Sander et al. (2011)
J6500dc05	StGJCClF	CF_3CF_2Cl + hν $\rightarrow$ 1.0 ProdLCl + Cl + 2 LCARBON	`jx(ip_CF3CF2Cl)`	Sander et al. (2011)
J6500dc06	StG	CH_2F_2 + Cl $\rightarrow$ HCl + LCARBON	`4.9e-12*EXP(-1500./temp)`	Sander et al. (2011)
J9000	TrStGJS	OCS + hν $\rightarrow$ CO + S	`JX(ip_OCS)`	[redacted]
J9001	TrStGJS	SO_2 + hν $\rightarrow$ SO + $O(^3P)$	`60.*JX(ip_OCS)`	[redacted]
J9002	TrStGJS	SO_3 + hν $\rightarrow$ SO_2 + $O(^3P)$	`JX(ip_SO3)`	[redacted]
J9003	TrStGJS	H_2SO_4 + hν $\rightarrow$ ProdH2O + SO_3 + H_2O	`JX(ip_H2SO4)`	[redacted]
PH (aqueous)				

General notes

j-values are calculated with an external module (e.g., JVAL) and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:

j(11) $\rightarrow$ `jx(ip_COH2)`
j(12) $\rightarrow$ `jx(ip_CHOH)`
j(15) $\rightarrow$ `jx(ip_HOCH2CHO)`
j(18) $\rightarrow$ `jx(ip_MACR)`
j(22) $\rightarrow$ `jx(ip_ACETOL)`
j(23)+j(24) $\rightarrow$ `jx(ip_MVK)`
j(31)+j(32)+j(33) $\rightarrow$ `jx(ip_GLYOX)`
j(34) $\rightarrow$ `jx(ip_MGLYOX)`

j(41) → `jx(ip_CH3OOH)`
j(53) → j(isopropyl nitrate)
j(54) → j(isopropyl nitrate)
j(55) → j(isopropyl nitrate)
j(56)+j(57) → `jx(ip_NOA)`

Specific notes

`J4302`: It is assumed that J(CH_3COCH_2OH) is 0.074 times that of J4101b.

`J4304`: It is assumed that J($CH_3COCH_2O_2H$) is the same as J(CH_3OOH).

`J4306`: Following von Kuhlmann et al. (2003), we use J($iC_3H_7ONO_2$) = `3.7*jx(ip_PAN)`.

`J4402`: It is assumed that J(MVKOOH) is the same as J(CH_3OOH).

`J4405`: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

`J4407`: It is assumed that J(MPAN) is the same as J(PAN).

`J4500`: It is assumed that J(ISOOH) is the same as J(CH_3OOH).

`J7301`: The quantum yields are recommended by Burkholder et al. (2015) for $\lambda > 300$nm and used here for the entire spectrum.

`J6500dc01`: OKAY!

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference

General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry's law constants from chemprop (see `chemprop.pdf`).

For uptake of X (X = N_2O_5, $ClNO_3$, or $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\mathrm{exf}}(\mathrm{X})=\frac{k_{\mathrm{mt}}(\mathrm{X}) \times \mathrm{LWC}}{[\mathrm{H_2O}] + 5 \times 10^2[\mathrm{Cl}^-] + 3 \times 10^5[\mathrm{Br}^-]}$$

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt}. The factors only affect the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[Cl^-] > 0.1$ M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[H_2O]/[Cl^-]$ is less than 5×10^2. The ratio $5\times10^2/3\times10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N_2O_5. Here, they are also used for $ClNO_3$ and $BrNO_3$.

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	N_2O_5 + H_2O → LossH2O + 1.0 LossO3N + 1.0 LossO3 + 2 HNO_3	`khet_St(ihs_N2O5_H2O)`	see general notes*
HET201	TrHetN	N_2O_5 → 3.0 LossO3N + 3.0 LossO3 + 2 NO_3^-(cs) + 2 H^+(cs)	`khet_Tr(iht_N2O5)`	see general notes*
HET410	StHetCl	HOCl + HCl → ProdH2O + 1.0 LossO3Cl + 1.0 LossO3 + Cl_2 + H_2O	`khet_St(ihs_HOCl_HCl)`	see general notes*
HET420	StHetClN	$ClNO_3$ + HCl → 0.5 LossO3Cl + 0.5 LossO3N + 1.0 LossO3 + Cl_2 + HNO_3	`khet_St(ihs_ClNO3_HCl)`	see general notes*
HET421	StHetClN	$ClNO_3$ + H_2O → LossH2O + HOCl + HNO_3	`khet_St(ihs_ClNO3_H2O)`	see general notes*
HET422	StHetClN	N_2O_5 + HCl → 1.0 LossO3Cl + 1.0 LossO3N + 2.0 LossO3 + $ClNO_2$ + HNO_3	`khet_St(ihs_N2O5_HCl)`	see general notes*
HET510	StHetBr	HOBr + HBr → ProdH2O + 1.0 LossO3Br + 1.0 LossO3 + Br_2 + H_2O	`khet_St(ihs_HOBr_HBr)`	see general notes*
HET520	StHetBrN	$BrNO_3$ + H_2O → LossH2O + HOBr + HNO_3	`khet_St(ihs_BrNO3_H2O)`	see general notes*
HET540	StHetBrClN	$ClNO_3$ + HBr → 0.333333 LossO3Br + 0.333333 LossO3Cl + 0.333333 LossO3N + 1.0 LossO3 + BrCl + HNO_3	`khet_St(ihs_ClNO3_HBr)`	see general notes*
HET541	StHetBrClN	$BrNO_3$ + HCl → 0.333333 LossO3Br + 0.333333 LossO3Cl + 0.333333 LossO3N + 1.0 LossO3 + BrCl + HNO_3	`khet_St(ihs_BrNO3_HCl)`	see general notes*
HET542	StHetBrCl	HOCl + HBr → ProdH2O + 0.5 LossO3Br + 0.5 LossO3Cl + 1.0 LossO3 + BrCl + H_2O	`khet_St(ihs_HOCl_HBr)`	see general notes*
HET543	StHetBrCl	HOBr + HCl → ProdH2O + 0.5 LossO3Br + 0.5 LossO3Cl + 1.0 LossO3 + BrCl + H_2O	`khet_St(ihs_HOBr_HCl)`	see general notes*

General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA_KHET) and then supplied to the MECCA chemistry (see `www.messy-interface.org` for details)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$	reference

Specific notes

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference

Specific notes

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