The Chemical Mechanism of MECCA

KPP version: `2.2.3_rs`

MECCA version: `3.8f`

Date: March 23, 2017.

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

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	253
Aqueous phase:	0
All species:	253

Number of reactions in selected mechanism:

Gas phase (Gnnn):	304
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	73
Aqueous phase photolysis (PHnnn):	0
Heterogeneous (HETnnn):	12
Equilibria (EQnn):	0
Isotope exchange (IEXnnn):	0
Tagging equations (TAGnnn):	410
Dummy (Dnn):	1
All equations:	800

This document is part of the electronic supplement to our article
"The atmospheric chemistry box model CAABA/MECCA-3.0"
in Geosci. Model Dev. (2011), available at:
`http://www.geosci-model-dev.net`

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.3E-11*EXP(55./temp)	Sander et al. (2011)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4))*cair	Sander et al. (2011)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow$ 2. LossO3O + 2. LossO3 + 2 O_2	1.2E-10	Sander et al. (2011)*
G1003	UpStG	$O_3 + O(^3P) \rightarrow$ 2. LossO3O + 2. LossO3 + 2 O_2	8.E-12*EXP(-2060./temp)	Sander et al. (2011)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	tag_kG2100	Sander et al. (2011)
	tag: FHM	$^{FHM}H + O_2 \rightarrow O_2 + {}^{FHM}HO_2$	tag_kG2100	
	tag: FHM	$^{FHMr}H + O_2 \rightarrow O_2 + {}^{FHMr}HO_2$	tag_kG2100	
G2101	UpStG	$H + O_3 \rightarrow$ LossO3H + LossO3 + OH + O_2	tag_kG2101	Sander et al. (2011)
	tag: FHM	$^{FHM}H + O_3 \rightarrow O_3 + {}^{FHM}OH$ + PTPFHMOH	tag_kG2101	
	tag: FHM	$^{FHMr}H + O_3 \rightarrow O_3 + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG2101	
G2102	UpStG	$H_2 + O(^1D) \rightarrow$ LossO3H + LossO3 + H + OH	tag_kG2102	Sander et al. (2011)
	tag: FHM	$^{FHM}H_2 + O(^1D) \rightarrow O(^1D) + {}^{FHM}H + {}^{FHM}OH$ + PTPFHMOH + PTLFHMH2	tag_kG2102	
	tag: FHM	$^{FHMr}H_2 + O(^1D) \rightarrow O(^1D) + {}^{FHMr}H + {}^{FHMr}OH$ + PTPFHMrOH + PTLFHMrH2	tag_kG2102	
G2103	UpStG	$OH + O(^3P) \rightarrow$ LossO3H + LossO3 + H + O_2	tag_kG2103	Sander et al. (2011)
	tag: FHM	$^{FHM}OH + O(^3P) \rightarrow O(^3P) + {}^{FHM}H$ + PTLFHMOH	tag_kG2103	
	tag: FHM	$^{FHMr}OH + O(^3P) \rightarrow O(^3P) + {}^{FHMr}H$ + PTLFHMrOH	tag_kG2103	
G2104	UpStTrG	$OH + O_3 \rightarrow$ LossO3H + LossO3 + $HO_2 + O_2$	tag_kG2104	Sander et al. (2011)
	tag: FHM	$^{FHM}OH + O_3 \rightarrow O_3 + {}^{FHM}HO_2$ + PTLFHMOH	tag_kG2104	
	tag: FHM	$^{FHMr}OH + O_3 \rightarrow O_3 + {}^{FHMr}HO_2$ + PTLFHMrOH	tag_kG2104	
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	tag_kG2105	Sander et al. (2011)
	transfer:	$OH \rightarrow 0.5\ H_2O$		
	tag: FHM	$H_2 + {}^{FHM}OH \rightarrow H_2 + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG2105	
	tag: FHM	$H_2 + {}^{FHMr}OH \rightarrow H_2 + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG2105	
	transfer:	$H_2 \rightarrow 0.5\ H_2O + H$		
	tag: FHM	$OH + {}^{FHM}H_2 \rightarrow OH + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O + ^{FHM}H + PTLFHMH2	tag_kG2105	
	tag: FHM	$OH + {}^{FHMr}H_2 \rightarrow OH + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + ^{FHMr}H + PTLFHMrH2	tag_kG2105	
G2106	UpStG	$HO_2 + O(^3P) \rightarrow$ LossO3H + LossO3 + OH + O_2	tag_kG2106	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + O(^3P) \rightarrow O(^3P) + {}^{FHM}OH$ + PTPFHMOH	tag_kG2106	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}HO_2 + O(^3P) \rightarrow O(^3P) + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG2106	
G2107	UpStTrG	$HO_2 + O_3 \rightarrow$ LossO3H + LossO3 + OH + 2 O_2	tag_kG2107	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + O_3 \rightarrow O_3 + {}^{FHM}OH$ + PTPFHMOH	tag_kG2107	
	tag: FHM	$^{FHMr}HO_2 + O_3 \rightarrow O_3 + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG2107	
G2108a	UpStG	$HO_2 + H \rightarrow 2$ OH	tag_kG2108a	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + H \rightarrow H + {}^{FHM}OH$ + PTPFHMOH	tag_kG2108a	
	tag: FHM	$^{FHMr}HO_2 + H \rightarrow H + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG2108a	
	tag: FHM	$^{FHM}H + HO_2 \rightarrow HO_2 + {}^{FHM}OH$ + PTPFHMOH	tag_kG2108a	
	tag: FHM	$^{FHMr}H + HO_2 \rightarrow HO_2 + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG2108a	
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	tag_kG2108b	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + H \rightarrow H + 0.5\ {}^{FHM}H_2$ + 0.5 PTPFHMH2	tag_kG2108b	
	tag: FHM	$^{FHMr}HO_2 + H \rightarrow H + 0.5\ {}^{FHMr}H_2$ + 0.5 PTPFHMrH2	tag_kG2108b	
	tag: FHM	$^{FHM}H + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHM}H_2$ + 0.5 PTPFHMH2	tag_kG2108b	
	tag: FHM	$^{FHMr}H + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHMr}H_2$ + 0.5 PTPFHMrH2	tag_kG2108b	
G2108c	UpStG	$HO_2 + H \rightarrow$ ProdO3H + ProdO3 + $O(^3P) + H_2O$	tag_kG2108c	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + H \rightarrow H + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG2108c	
	tag: FHM	$^{FHMr}HO_2 + H \rightarrow H + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG2108c	
	tag: FHM	$^{FHM}H + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG2108c	
	tag: FHM	$^{FHMr}H + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG2108c	
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	tag_kG2109	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + OH \rightarrow OH + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG2109	
	tag: FHM	$^{FHMr}HO_2 + OH \rightarrow OH + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG2109	
	tag: FHM	$^{FHM}OH + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG2109	
	tag: FHM	$^{FHMr}OH + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG2109	
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	tag_kG2110	Burkholder et al. (2015), Kircher and Sander (1984)
	tag: FHM	$^{FHM}HO_2 + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHM}H_2O_2$	tag_kG2110*(2.0)	
	tag: FHM	$^{FHMr}HO_2 + HO_2 \rightarrow HO_2 + 0.5\ {}^{FHMr}H_2O_2$	tag_kG2110*(2.0)	
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow$ LossO3O + LossO3 + 2 OH	tag_kG2111	Sander et al. (2011)
	tag: FHM	$^{FHM}H_2O + O(^1D) \rightarrow O(^1D) + 2.0\ {}^{FHMr}OH$ + 2.0 PTPFHMrOH + PTLFHMH2O	tag_kG2111	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}H_2O + O(^1D) \rightarrow O(^1D) + 2.0\ ^{FHMr}OH + 2.0$ PTPFHMrOH + PTLFHMrH2O	tag_kG2111	
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	tag_kG2112	Sander et al. (2011)
	transfer:	$OH \rightarrow 0.5\ H_2O$		
	tag: FHM	$H_2O_2 + {}^{FHM}OH \rightarrow H_2O_2 + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG2112	
	tag: FHM	$H_2O_2 + {}^{FHMr}OH \rightarrow H_2O_2 + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG2112	
	transfer:	$H_2O_2 \rightarrow 0.5\ H_2O + HO_2$		
	tag: FHM	$OH + {}^{FHM}H_2O_2 \rightarrow OH + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O + $^{FHM}HO_2$	tag_kG2112	
	tag: FHM	$OH + {}^{FHMr}H_2O_2 \rightarrow OH + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O + $^{FHMr}HO_2$	tag_kG2112	
G3100	UpStGN	$N + O_2 \rightarrow$ 1. ProdO3N + 1. ProdO3 + NO + $O(^3P)$	1.5E-11*EXP(-3600./temp)	Sander et al. (2011)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	2.15E-11*EXP(110./temp)	Sander et al. (2011)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow$ 1. LossO3O + 1. LossO3 + 2 NO	7.25E-11*EXP(20./temp)	Sander et al. (2011)
G3102b	StGN	$N_2O + O(^1D) \rightarrow$ 1. LossO3O + 1. LossO3 + $N_2 + O_2$	4.63E-11*EXP(20./temp)	Sander et al. (2011)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2011)
G3104	UpStGN	NO + N $\rightarrow$ 1. ProdO3N + 1. ProdO3 + $O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Sander et al. (2011)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow$ 2. LossO3N + 2. LossO3 + NO + O_2	5.1E-12*EXP(210./temp)	Sander et al. (2011)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2011)
G3107	UpStGN	NO_2 + N $\rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./temp)	Sander et al. (2011)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2011)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2011)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(2.7E-27*EXP(11000./temp))	Sander et al. (2011)*
G3200	TrGN	NO + OH $\rightarrow$ HONO	tag_kG3200	Sander et al. (2011)
	tag: FHM	^{FHM}OH + NO $\rightarrow$ NO + ^{FHM}HONO + PTLFHMOH	tag_kG3200	
	tag: FHM	^{FHMr}OH + NO $\rightarrow$ NO + ^{FHMr}HONO + PTLFHMrOH	tag_kG3200	
G3201	UpStTrGN	$NO + HO_2 \rightarrow$ ProdO3N + ProdO3 + NO_2 + OH	tag_kG3201	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2$ + NO $\rightarrow$ NO + ^{FHM}OH + PTPFHMOH	tag_kG3201	
	tag: FHM	$^{FHMr}HO_2$ + NO $\rightarrow$ NO + ^{FHMr}OH + PTPFHMrOH	tag_kG3201	
G3202	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	tag_kG3202	Sander et al. (2011)
	tag: FHM	$^{FHM}OH + NO_2 \rightarrow NO_2 + {}^{FHM}HNO_3$ + PTLFHMOH	tag_kG3202	
	tag: FHM	$^{FHMr}OH + NO_2 \rightarrow NO_2 + {}^{FHMr}HNO_3$ + PTLFHMrOH	tag_kG3202	

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

#	labels	reaction	rate coefficient	reference
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	tag_kG3203	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + NO_2 \rightarrow NO_2 + {}^{FHM}HNO_4$	tag_kG3203	
	tag: FHM	$^{FHMr}HO_2 + NO_2 \rightarrow NO_2 + {}^{FHMr}HNO_4$	tag_kG3203	
G3204	TrGN	$NO_3 + HO_2 \rightarrow$ LossO3N + LossO3 + $NO_2 + OH + O_2$	tag_kG3204	Sander et al. (2011)
	tag: FHM	$^{FHM}HO_2 + NO_3 \rightarrow NO_3 + {}^{FHM}OH$ + PTPFHMOH	tag_kG3204	
	tag: FHM	$^{FHMr}HO_2 + NO_3 \rightarrow NO_3 + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG3204	
G3205	TrGN	HONO + OH → ProdO3N + ProdO3 + $NO_2 + H_2O$	tag_kG3205	Sander et al. (2011)
	tag: FHM	^{FHM}HONO + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3205	
	tag: FHM	^{FHMr}HONO + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3205	
	tag: FHM	^{FHM}OH + HONO → HONO + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3205	
	tag: FHM	^{FHMr}OH + HONO → HONO + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG3205	
G3206	StTrGN	$HNO_3 + OH \rightarrow$ ProdO3N + ProdO3 + $H_2O + NO_3$	tag_kG3206	Sander et al. (2011)
	tag: FHM	$^{FHM}HNO_3$ + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3206	
	tag: FHM	$^{FHMr}HNO_3$ + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3206	
	tag: FHM	^{FHM}OH + $HNO_3 \rightarrow HNO_3$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3206	
	tag: FHM	^{FHMr}OH + $HNO_3 \rightarrow HNO_3$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG3206	
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	tag_kG3207	Sander et al. (2011)
	tag: FHM	$^{FHM}HNO_4 \rightarrow {}^{FHM}HO_2$	tag_kG3207	
	tag: FHM	$^{FHMr}HNO_4 \rightarrow {}^{FHMr}HO_2$	tag_kG3207	
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	tag_kG3208	Sander et al. (2011)
	tag: FHM	$^{FHM}HNO_4$ + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3208	
	tag: FHM	$^{FHMr}HNO_4$ + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3208	
	tag: FHM	^{FHM}OH + $HNO_4 \rightarrow HNO_4$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3208	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}OH + HNO_4 \rightarrow HNO_4 + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG3208	
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	tag_kG3209	Kohlmann and Poppe (1999)
	transfer:	$NH_3 \rightarrow NH_2 + 0.5\ H_2O$		
	tag: FHM	$OH + {}^{FHM}NH_3 \rightarrow OH + {}^{FHM}NH_2 + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG3209	
	tag: FHM	$OH + {}^{FHMr}NH_3 \rightarrow OH + {}^{FHMr}NH_2 + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kG3209	
	transfer:	$OH \rightarrow 0.5\ H_2O$		
	tag: FHM	$NH_3 + {}^{FHM}OH \rightarrow NH_3 + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG3209	
	tag: FHM	$NH_3 + {}^{FHMr}OH \rightarrow NH_3 + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG3209	
G3210	TrGN	$NH_2 + O_3 \rightarrow$ LossO3N + LossO3 + $NH_2O + O_2$	tag_kG3210	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2 + O_3 \rightarrow O_3 + {}^{FHM}NH_2O$	tag_kG3210	
	tag: FHM	$^{FHMr}NH_2 + O_3 \rightarrow O_3 + {}^{FHMr}NH_2O$	tag_kG3210	
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	tag_kG3211	Kohlmann and Poppe (1999)
	transfer:	$NH_2 \rightarrow NH_2O$		
	tag: FHM	$HO_2 + {}^{FHM}NH_2 \rightarrow HO_2 + {}^{FHM}NH_2O$	tag_kG3211	
	tag: FHM	$HO_2 + {}^{FHMr}NH_2 \rightarrow HO_2 + {}^{FHMr}NH_2O$	tag_kG3211	
	transfer:	$HO_2 \rightarrow OH$		
	tag: FHM	$NH_2 + {}^{FHM}HO_2 \rightarrow NH_2 + {}^{FHM}OH$ + PTPFHMOH	tag_kG3211	
	tag: FHM	$NH_2 + {}^{FHMr}HO_2 \rightarrow NH_2 + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG3211	
G3212	TrGN	$NH_2 + HO_2 \rightarrow HNO + H_2O$	tag_kG3212	Kohlmann and Poppe (1999)
	transfer:	$NH_2 \rightarrow HNO + 0.5\ H_2O$		
	tag: FHM	$HO_2 + {}^{FHM}NH_2 \rightarrow HO_2 + {}^{FHM}HNO + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG3212	
	tag: FHM	$HO_2 + {}^{FHMr}NH_2 \rightarrow HO_2 + {}^{FHMr}HNO + 0.5\ {}^{FHMr}H_2O +$ 0.5 PTPFHMrH2O	tag_kG3212	
	transfer:	$HO_2 \rightarrow 0.5\ H_2O$		
	tag: FHM	$NH_2 + {}^{FHM}HO_2 \rightarrow NH_2 + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG3212	
	tag: FHM	$NH_2 + {}^{FHMr}HO_2 \rightarrow NH_2 + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kG3212	
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	tag_kG3213	Kohlmann and Poppe (1999)

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHM}NH_2$ + NO → NO + $^{FHM}HO_2$ + ^{FHM}OH + PTPFHMOH	tag_kG3213	
	tag: FHM	$^{FHMr}NH_2$ + NO → NO + $^{FHMr}HO_2$ + ^{FHMr}OH + PTPFHMrOH	tag_kG3213	
G3214	TrGN	NH_2 + NO → N_2 + H_2O	tag_kG3214	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2$ + NO → NO + $^{FHM}H_2O$ + PTPFHMH2O	tag_kG3214	
	tag: FHM	$^{FHMr}NH_2$ + NO → NO + $^{FHMr}H_2O$ + PTPFHMrH2O	tag_kG3214	
G3215	TrGN	NH_2 + NO_2 → LossO3N + LossO3 + N_2O + H_2O	tag_kG3215	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2$ + NO_2 → NO_2 + $^{FHM}H_2O$ + PTPFHMH2O	tag_kG3215	
	tag: FHM	$^{FHMr}NH_2$ + NO_2 → NO_2 + $^{FHMr}H_2O$ + PTPFHMrH2O	tag_kG3215	
G3216	TrGN	NH_2 + NO_2 → LossO3N + LossO3 + NH_2O + NO	tag_kG3216	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2$ + NO_2 → NO_2 + $^{FHM}NH_2O$	tag_kG3216	
	tag: FHM	$^{FHMr}NH_2$ + NO_2 → NO_2 + $^{FHMr}NH_2O$	tag_kG3216	
G3217	TrGN	NH_2O + O_3 → LossO3N + LossO3 + NH_2 + O_2	tag_kG3217	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2O$ + O_3 → O_3 + $^{FHM}NH_2$	tag_kG3217	
	tag: FHM	$^{FHMr}NH_2O$ + O_3 → O_3 + $^{FHMr}NH_2$	tag_kG3217	
G3218	TrGN	NH_2O → NHOH	tag_kG3218	Kohlmann and Poppe (1999)
	tag: FHM	$^{FHM}NH_2O$ → ^{FHM}NHOH	tag_kG3218	
	tag: FHM	$^{FHMr}NH_2O$ → ^{FHMr}NHOH	tag_kG3218	
G3219	TrGN	HNO + OH → NO + H_2O	tag_kG3219	Kohlmann and Poppe (1999)
	tag: FHM	^{FHM}HNO + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3219	
	tag: FHM	^{FHMr}HNO + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3219	
	tag: FHM	^{FHM}OH + HNO → HNO + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3219	
	tag: FHM	^{FHMr}OH + HNO → HNO + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG3219	
G3220	TrGN	HNO + NHOH → NH_2OH + NO	tag_kG3220	Kohlmann and Poppe (1999)
	tag: FHM	^{FHM}HNO + NHOH → NHOH + 0.3333333 $^{FHM}NH_2OH$	tag_kG3220	
	tag: FHM	^{FHMr}HNO + NHOH → NHOH + 0.3333333 $^{FHMr}NH_2OH$	tag_kG3220	
	tag: FHM	^{FHM}NHOH + HNO → HNO + 0.6666667 $^{FHM}NH_2OH$	tag_kG3220	
	tag: FHM	^{FHMr}NHOH + HNO → HNO + 0.6666667 $^{FHMr}NH_2OH$	tag_kG3220	
G3221	TrGN	HNO + NO_2 → LossO3N + LossO3 + HONO + NO	tag_kG3221	Kohlmann and Poppe (1999)
	tag: FHM	^{FHM}HNO + NO_2 → NO_2 + ^{FHM}HONO	tag_kG3221	
	tag: FHM	^{FHMr}HNO + NO_2 → NO_2 + ^{FHMr}HONO	tag_kG3221	

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

#	labels	reaction	rate coefficient	reference
G3222	TrGN	NHOH + OH → HNO + H_2O	tag_kG3222	Kohlmann and Poppe (1999)
	transfer:	NHOH → HNO + 0.5 H_2O		
	tag: FHM	OH + ^{FHM}NHOH → OH + ^{FHM}HNO + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3222	
	tag: FHM	OH + ^{FHMr}NHOH → OH + ^{FHMr}HNO + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3222	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	NHOH + ^{FHM}OH → NHOH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3222	
	tag: FHM	NHOH + ^{FHMr}OH → NHOH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG3222	
G3223	TrGN	NH_2OH + OH → NHOH + H_2O	tag_kG3223	Kohlmann and Poppe (1999)
	transfer:	NH_2OH → NHOH + 0.5 H_2O		
	tag: FHM	OH + $^{FHM}NH_2OH$ → OH + ^{FHM}NHOH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG3223	
	tag: FHM	OH + $^{FHMr}NH_2OH$ → OH + ^{FHMr}NHOH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG3223	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	NH_2OH + ^{FHM}OH → NH_2OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG3223	
	tag: FHM	NH_2OH + ^{FHMr}OH → NH_2OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG3223	
G3224	TrGN	HNO + O_2 → HO_2 + NO	tag_kG3224	Kohlmann and Poppe (1999)
	tag: FHM	^{FHM}HNO + O_2 → O_2 + $^{FHM}HO_2$	tag_kG3224	
	tag: FHM	^{FHMr}HNO + O_2 → O_2 + $^{FHMr}HO_2$	tag_kG3224	
G4100	UpStG	CH_4 + $O(^1D)$ → LossO3C + LossO3 + 0.75 CH_3 + 0.75 OH + 0.2 CH_3O + 0.2 H + 0.05 HCHO + 0.05 H_2	tag_kG4100	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_4$ + $O(^1D)$ → $O(^1D)$ + 0.75 $^{FHM}CH_3$ + 0.75 ^{FHM}OH + 0.75 PTPFHMOH + 0.2 $^{FHM}CH_3O$ + 0.2 ^{FHM}H + 0.05 ^{FHM}HCHO + 0.05 $^{FHM}H_2$ + 0.05 PTPFHMH2 + PTLFHMCH4	tag_kG4100	
	tag: FHM	$^{FHMr}CH_4$ + $O(^1D)$ → $O(^1D)$ + 0.75 $^{FHMr}CH_3$ + 0.75 ^{FHMr}OH + 0.75 PTPFHMrOH + 0.2 $^{FHMr}CH_3O$ + 0.2 ^{FHMr}H + 0.05 ^{FHMr}HCHO + 0.05 $^{FHMr}H_2$ + 0.05 PTPFHMrH2 + PTLFHMrCH4	tag_kG4100	

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

#	labels	reaction	rate coefficient	reference
G4101	StTrG	$CH_4 + OH \rightarrow CH_3 + H_2O$	tag_kG4101	Atkinson (2003)
	transfer:	$CH_4 \rightarrow CH_3 + 0.5\ H_2O + CH_3O_2$		
	tag: FHM	$OH + {}^{FHM}CH_4 \rightarrow OH + {}^{FHM}CH_3 + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMCH4	tag_kG4101	
	tag: FHM	$OH + {}^{FHMr}CH_4 \rightarrow OH + {}^{FHMr}CH_3 + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrCH4	tag_kG4101	
	transfer:	$OH \rightarrow 0.5\ H_2O$		
	tag: FHM	$CH_4 + {}^{FHM}OH \rightarrow CH_4 + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG4101	
	tag: FHM	$CH_4 + {}^{FHMr}OH \rightarrow CH_4 + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG4101	
G4102	TrG	$CH_3OH + OH \rightarrow 0.85\ HCHO + 0.85\ HO_2 + 0.15\ CH_3O + H_2O$	tag_kG4102	Atkinson et al. (2006)
	transfer:	$CH_3OH \rightarrow HCHO + HO_2 + CH_3O + 0.5\ H_2O + CH_3O_2$		
	tag: FHM	$OH + {}^{FHM}CH_3OH \rightarrow OH + 0.85\ {}^{FHM}HCHO + 0.85\ {}^{FHM}HO_2 + 0.15\ {}^{FHM}CH_3O + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG4102	
	tag: FHM	$OH + {}^{FHMr}CH_3OH \rightarrow OH + 0.85\ {}^{FHMr}HCHO + 0.85\ {}^{FHMr}HO_2 + 0.15\ {}^{FHMr}CH_3O + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kG4102	
	transfer:	$OH \rightarrow 0.5\ H_2O$		
	tag: FHM	$CH_3OH + {}^{FHM}OH \rightarrow CH_3OH + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG4102	
	tag: FHM	$CH_3OH + {}^{FHMr}OH \rightarrow CH_3OH + 0.5\ {}^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG4102	
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	tag_kG4103a	Atkinson et al. (2006)
	tag: FHM	${}^{FHM}CH_3O_2 + HO_2 \rightarrow HO_2 + 0.75\ {}^{FHM}CH_3OOH$	tag_kG4103a	
	tag: FHM	${}^{FHMr}CH_3O_2 + HO_2 \rightarrow HO_2 + 0.75\ {}^{FHMr}CH_3OOH$	tag_kG4103a	
	tag: FHM	${}^{FHM}HO_2 + CH_3O_2 \rightarrow CH_3O_2 + 0.25\ {}^{FHM}CH_3OOH$	tag_kG4103a	
	tag: FHM	${}^{FHMr}HO_2 + CH_3O_2 \rightarrow CH_3O_2 + 0.25\ {}^{FHMr}CH_3OOH$	tag_kG4103a	
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	tag_kG4103b	Atkinson et al. (2006)
	transfer:	$CH_3O_2 \rightarrow 0.5\ H_2O + HCHO$		
	tag: FHM	$HO_2 + {}^{FHM}CH_3O_2 \rightarrow HO_2 + {}^{FHM}HCHO + 0.5\ {}^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG4103b	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	HO_2 + $^{FHMr}CH_3O_2$ → HO_2 + $^{FHMr}HCHO$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG4103b	
	transfer:	HO_2 → 0.5 H_2O		
	tag: FHM	CH_3O_2 + $^{FHM}HO_2$ → CH_3O_2 + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG4103b	
	tag: FHM	CH_3O_2 + $^{FHMr}HO_2$ → CH_3O_2 + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG4103b	
G4104a	StTrGN	CH_3O_2 + NO → ProdO3C + ProdO3 + CH_3O + NO_2	tag_kG4104a	Atkinson et al. (2006), ?, ?
	tag: FHM	$^{FHM}CH_3O_2$ + NO → NO + $^{FHM}CH_3O$	tag_kG4104a	
	tag: FHM	$^{FHMr}CH_3O_2$ + NO → NO + $^{FHMr}CH_3O$	tag_kG4104a	
G4104b	StTrGN	CH_3O_2 + NO → CH_3ONO_2	tag_kG4104b	Atkinson et al. (2006), ?, ?
	tag: FHM	$^{FHM}CH_3O_2$ + NO → NO + $^{FHM}CH_3ONO_2$	tag_kG4104b	
	tag: FHM	$^{FHMr}CH_3O_2$ + NO → NO + $^{FHMr}CH_3ONO_2$	tag_kG4104b	
G4105	TrGN	CH_3O_2 + NO_3 → LossO3C + LossO3 + CH_3O + NO_2 + O_2	tag_kG4105	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O_2$ + NO_3 → NO_3 + $^{FHM}CH_3O$	tag_kG4105	
	tag: FHM	$^{FHMr}CH_3O_2$ + NO_3 → NO_3 + $^{FHMr}CH_3O$	tag_kG4105	
G4106a	StTrG	CH_3O_2 → CH_3O + 0.5 O_2	tag_kG4106a	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O_2$ → $^{FHM}CH_3O$	tag_kG4106a	
	tag: FHM	$^{FHMr}CH_3O_2$ → $^{FHMr}CH_3O$	tag_kG4106a	
G4106b	StTrG	CH_3O_2 → 0.5 HCHO + 0.5 CH_3OH + 0.5 O_2	tag_kG4106b	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O_2$ → 0.5 $^{FHM}HCHO$ + 0.5 $^{FHM}CH_3OH$	tag_kG4106b	
	tag: FHM	$^{FHMr}CH_3O_2$ → 0.5 $^{FHMr}HCHO$ + 0.5 $^{FHMr}CH_3OH$	tag_kG4106b	
G4107	StTrG	CH_3OOH + OH → 0.6 CH_3O_2 + 0.4 HCHO + 0.4 OH + H_2O	tag_kG4107	Wallington et al.
	transfer:	CH_3OOH → 0.5 H_2O + CH_3O_2 + HCHO + OH		
	tag: FHM	OH + $^{FHM}CH_3OOH$ → OH + 0.6 $^{FHM}CH_3O_2$ + 0.4 $^{FHM}HCHO$ + 0.4 ^{FHM}OH + 0.4 PTPFHMOH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG4107	
	tag: FHM	OH + $^{FHMr}CH_3OOH$ → OH + 0.6 $^{FHMr}CH_3O_2$ + 0.4 $^{FHMr}HCHO$ + 0.4 ^{FHMr}OH + 0.4 PTPFHMrOH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG4107	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	CH_3OOH + ^{FHM}OH → CH_3OOH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG4107	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	CH_3OOH + ^{FHMr}OH → CH_3OOH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG4107	
G4108	StTrG	HCHO + OH → CO + H_2O + HO_2	tag_kG4108	Sivakumaran et al. (2003)
	transfer:	HCHO → 0.5 H_2O + HO_2		
	tag: FHM	OH + ^{FHM}HCHO → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + $^{FHM}HO_2$	tag_kG4108	
	tag: FHM	OH + ^{FHMr}HCHO → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + $^{FHMr}HO_2$	tag_kG4108	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	HCHO + ^{FHM}OH → HCHO + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG4108	
	tag: FHM	HCHO + ^{FHMr}OH → HCHO + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG4108	
G4109	TrGN	HCHO + NO_3 → LossO3C + LossO3 + HNO_3 + CO + HO_2	tag_kG4109	Sander et al. (2011)
	tag: FHM	^{FHM}HCHO + NO_3 → NO_3 + $^{FHM}HNO_3$ + $^{FHM}HO_2$	tag_kG4109	
	tag: FHM	^{FHMr}HCHO + NO_3 → NO_3 + $^{FHMr}HNO_3$ + $^{FHMr}HO_2$	tag_kG4109	
G4110	UpStTrG	CO + OH → H + CO_2	tag_kG4110	McCabe et al. (2001)
	tag: FHM	^{FHM}OH + CO → CO + ^{FHM}H + PTLFHMOH	tag_kG4110	
	tag: FHM	^{FHMr}OH + CO → CO + ^{FHMr}H + PTLFHMrOH	tag_kG4110	
G4111	TrG	HCOOH + OH → CO_2 + HO_2 + H_2O	tag_kG4111	Paulot et al. (2011)
	transfer:	HCOOH → 0.5 H_2O + HO_2		
	tag: FHM	OH + ^{FHM}HCOOH → OH + $^{FHM}HO_2$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG4111	
	tag: FHM	OH + ^{FHMr}HCOOH → OH + $^{FHMr}HO_2$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG4111	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	HCOOH + ^{FHM}OH → HCOOH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG4111	
	tag: FHM	HCOOH + ^{FHMr}OH → HCOOH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG4111	
G4112	UpStG	CO + O(^{3}P) → 1. LossO3C + 1. LossO3 + CO_2	6.60E-33*EXP(-1103./temp)	Roble (1995)
G4113	UpStG	CH_4 + O(^{3}P) → LossO3C + LossO3 + 0.51 CH_3 + 0.51 OH + 0.49 CH_3O + 0.49 H	tag_kG4113	Roble (1995), **?**, **?**

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHM}CH_4 + O(^3P) \rightarrow O(^3P) + 0.51\ ^{FHM}CH_3 + 0.51\ ^{FHM}OH$ + 0.51 PTPFHMOH + 0.49 $^{FHM}CH_3O$ + 0.49 ^{FHM}H + PTLFHMCH4	tag_kG4113	
	tag: FHM	$^{FHMr}CH_4 + O(^3P) \rightarrow O(^3P) + 0.51\ ^{FHMr}CH_3 + 0.51\ ^{FHMr}OH$ + 0.51 PTPFHMrOH + 0.49 $^{FHMr}CH_3O$ + 0.49 ^{FHMr}H + PTLFHMrCH4	tag_kG4113	
G4114	StTrGN	$CH_3O_2 + NO_2 \rightarrow$ LossO3C + LossO3 + $CH_3O_2NO_2$	tag_kG4114	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3O_2 + NO_2 \rightarrow NO_2 + {}^{FHM}CH_3O_2NO_2$	tag_kG4114	
	tag: FHM	$^{FHMr}CH_3O_2 + NO_2 \rightarrow NO_2 + {}^{FHMr}CH_3O_2NO_2$	tag_kG4114	
G4115	StTrGN	$CH_3O_2NO_2 \rightarrow$ ProdO3C + ProdO3 + $CH_3O_2 + NO_2$	tag_kG4115	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3O_2NO_2 \rightarrow {}^{FHM}CH_3O_2$	tag_kG4115	
	tag: FHM	$^{FHMr}CH_3O_2NO_2 \rightarrow {}^{FHMr}CH_3O_2$	tag_kG4115	
G4116	StTrGN	$CH_3O_2NO_2 + OH \rightarrow 2$ ProdO3C + 2 ProdO3 + HCHO + $NO_3 + H_2O$	tag_kG4116	
	transfer:	$CH_3O_2NO_2 \rightarrow$ HCHO		
	tag: FHM	$OH + {}^{FHM}CH_3O_2NO_2 \rightarrow OH + {}^{FHM}$HCHO	tag_kG4116	
	tag: FHM	$OH + {}^{FHMr}CH_3O_2NO_2 \rightarrow OH + {}^{FHMr}$HCHO	tag_kG4116	
	transfer:	$OH \rightarrow H_2O$		
	tag: FHM	$CH_3O_2NO_2 + {}^{FHM}OH \rightarrow CH_3O_2NO_2 + {}^{FHM}H_2O$ + PTPFHMH2O + PTLFHMOH	tag_kG4116	
	tag: FHM	$CH_3O_2NO_2 + {}^{FHMr}OH \rightarrow CH_3O_2NO_2 + {}^{FHMr}H_2O$ + PTPFHMrH2O + PTLFHMrOH	tag_kG4116	
G4117	StTrGN	$CH_3ONO_2 + OH \rightarrow$ ProdO3C + ProdO3 + H_2O + HCHO + NO_2	tag_kG4117	Atkinson et al. (2006)
	transfer:	$CH_3ONO_2 \rightarrow$ HCHO		
	tag: FHM	$OH + {}^{FHM}CH_3ONO_2 \rightarrow OH + {}^{FHM}$HCHO	tag_kG4117	
	tag: FHM	$OH + {}^{FHMr}CH_3ONO_2 \rightarrow OH + {}^{FHMr}$HCHO	tag_kG4117	
	transfer:	$OH \rightarrow H_2O$		
	tag: FHM	$CH_3ONO_2 + {}^{FHM}OH \rightarrow CH_3ONO_2 + {}^{FHM}H_2O$ + PTPFHMH2O + PTLFHMOH	tag_kG4117	
	tag: FHM	$CH_3ONO_2 + {}^{FHMr}OH \rightarrow CH_3ONO_2 + {}^{FHMr}H_2O$ + PTPFHMrH2O + PTLFHMrOH	tag_kG4117	
G4118	StTrG	$CH_3O \rightarrow HO_2 +$ HCHO	tag_kG4118	Chai et al. (2014)
	transfer:	$CH_3O \rightarrow HO_2 +$ HCHO		
	tag: FHM	$^{FHM}CH_3O \rightarrow + {}^{FHM}HO_2 + {}^{FHM}$HCHO	tag_kG4118	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}CH_3O \rightarrow + \ ^{FHMr}HO_2 + \ ^{FHMr}HCHO$	tag_kG4118	
G4119a	StTrGN	$CH_3O + NO_2 \rightarrow$ LossO3C + LossO3 + CH_3ONO_2	tag_kG4119a	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O + NO_2 \rightarrow NO_2 + \ ^{FHM}CH_3ONO_2$	tag_kG4119a	
	tag: FHM	$^{FHMr}CH_3O + NO_2 \rightarrow NO_2 + \ ^{FHMr}CH_3ONO_2$	tag_kG4119a	
G4119b	StTrGN	$CH_3O + NO_2 \rightarrow$ LossO3C + LossO3 + HCHO + HONO	tag_kG4119b	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O + NO_2 \rightarrow NO_2 + \ ^{FHM}HCHO + \ ^{FHM}HONO$	tag_kG4119b	
	tag: FHM	$^{FHMr}CH_3O + NO_2 \rightarrow NO_2 + \ ^{FHMr}HCHO + \ ^{FHMr}HONO$	tag_kG4119b	
G4120a	StTrGN	$CH_3O + NO \rightarrow CH_3ONO$	tag_kG4120a	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O + NO \rightarrow NO + \ ^{FHM}CH_3ONO$	tag_kG4120a	
	tag: FHM	$^{FHMr}CH_3O + NO \rightarrow NO + \ ^{FHMr}CH_3ONO$	tag_kG4120a	
G4120b	StTrGN	$CH_3O + NO \rightarrow HCHO + HNO$	tag_kG4120b	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3O + NO \rightarrow NO + \ ^{FHM}HCHO + \ ^{FHM}HNO$	tag_kG4120b	
	tag: FHM	$^{FHMr}CH_3O + NO \rightarrow NO + \ ^{FHMr}HCHO + \ ^{FHMr}HNO$	tag_kG4120b	
G4121	StTrG	$CH_3O_2 + O_3 \rightarrow$ LossO3C + LossO3 + CH_3O + 2 O_2	tag_kG4121	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3O_2 + O_3 \rightarrow O_3 + \ ^{FHM}CH_3O$	tag_kG4121	
	tag: FHM	$^{FHMr}CH_3O_2 + O_3 \rightarrow O_3 + \ ^{FHMr}CH_3O$	tag_kG4121	
G4122	StTrGN	$CH_3ONO + OH \rightarrow H_2O + HCHO + NO$	tag_kG4122	Nielsen et al. (1991)
	transfer:	$CH_3ONO \rightarrow HCHO$		
	tag: FHM	$OH + \ ^{FHM}CH_3ONO \rightarrow OH + \ ^{FHM}HCHO$	tag_kG4122	
	tag: FHM	$OH + \ ^{FHMr}CH_3ONO \rightarrow OH + \ ^{FHMr}HCHO$	tag_kG4122	
	transfer:	$OH \rightarrow H_2O$		
	tag: FHM	$CH_3ONO + \ ^{FHM}OH \rightarrow CH_3ONO + \ ^{FHM}H_2O +$ PTPFHMH2O + PTLFHMOH	tag_kG4122	
	tag: FHM	$CH_3ONO + \ ^{FHMr}OH \rightarrow CH_3ONO + \ ^{FHMr}H_2O +$ PTPFHMrH2O + PTLFHMrOH	tag_kG4122	
G4133	StTrG	$CH_3O_2 + OH \rightarrow CH_3O + HO_2$	tag_kG4133	Bossolasco et al. (2014)
	transfer:	$CH_3O_2 \rightarrow CH_3O$		
	tag: FHM	$OH + \ ^{FHM}CH_3O_2 \rightarrow OH + \ ^{FHM}CH_3O$	tag_kG4133	
	tag: FHM	$OH + \ ^{FHMr}CH_3O_2 \rightarrow OH + \ ^{FHMr}CH_3O$	tag_kG4133	
	transfer:	$OH \rightarrow HO_2$		
	tag: FHM	$CH_3O_2 + \ ^{FHM}OH \rightarrow CH_3O_2 + \ ^{FHM}HO_2 +$ PTLFHMOH	tag_kG4133	
	tag: FHM	$CH_3O_2 + \ ^{FHMr}OH \rightarrow CH_3O_2 + \ ^{FHMr}HO_2 +$ PTLFHMrOH	tag_kG4133	
G4151	StTrG	$CH_3 + O_2 \rightarrow CH_3O_2$	tag_kG4151	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3 + O_2 \rightarrow O_2 + \ ^{FHM}CH_3O_2$	tag_kG4151	
	tag: FHM	$^{FHMr}CH_3 + O_2 \rightarrow O_2 + \ ^{FHMr}CH_3O_2$	tag_kG4151	

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

#	labels	reaction	rate coefficient	reference
G4152	StTrG	$CH_3 + O_3 \rightarrow$ LossO3C + LossO3 + 0.956 HCHO + 0.956 H + 0.044 CH_3O + O_2	tag_kG4152	Albaladejo et al. (2002), **?**
	tag: FHM	$^{FHM}CH_3 + O_3 \rightarrow O_3 + 0.956\ ^{FHM}HCHO + 0.956\ ^{FHM}H + 0.044\ ^{FHM}CH_3O$	tag_kG4152	
	tag: FHM	$^{FHMr}CH_3 + O_3 \rightarrow O_3 + 0.956\ ^{FHMr}HCHO + 0.956\ ^{FHMr}H + 0.044\ ^{FHMr}CH_3O$	tag_kG4152	
G4153	StTrG	$CH_3 + O(^3P) \rightarrow$ LossO3C + LossO3 + 0.83 HCHO + 0.83 H + 0.17 CO + 0.17 H_2 + 0.17 H	tag_kG4153	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3 + O(^3P) \rightarrow O(^3P) + 0.83\ ^{FHM}HCHO + 0.83\ ^{FHM}H + 0.17\ ^{FHM}H_2$ + 0.17 PTPFHMH2 + 0.17 ^{FHM}H	tag_kG4153	
	tag: FHM	$^{FHMr}CH_3 + O(^3P) \rightarrow O(^3P) + 0.83\ ^{FHMr}HCHO + 0.83\ ^{FHMr}H + 0.17\ ^{FHMr}H_2$ + 0.17 PTPFHMrH2 + 0.17 ^{FHMr}H	tag_kG4153	
G4154	StTrG	$CH_3O + O_3 \rightarrow$ LossO3C + LossO3 + CH_3O_2 + O_2	tag_kG4154	Albaladejo et al. (2002)
	tag: FHM	$^{FHM}CH_3O + O_3 \rightarrow O_3 + {}^{FHM}CH_3O_2$	tag_kG4154	
	tag: FHM	$^{FHMr}CH_3O + O_3 \rightarrow O_3 + {}^{FHMr}CH_3O_2$	tag_kG4154	
G4155	StTrG	$CH_3O + O(^3P) \rightarrow$ LossO3C + LossO3 + 0.75 CH_3 + 0.75 O_2 + 0.25 HCHO + 0.25 OH	tag_kG4155	Baulch et al. (2005)
	tag: FHM	$^{FHM}CH_3O + O(^3P) \rightarrow O(^3P) + 0.75\ ^{FHM}CH_3 + 0.25\ ^{FHM}HCHO + 0.25\ ^{FHM}OH$ + 0.25 PTPFHMOH	tag_kG4155	
	tag: FHM	$^{FHMr}CH_3O + O(^3P) \rightarrow O(^3P) + 0.75\ ^{FHMr}CH_3 + 0.25\ ^{FHMr}HCHO + 0.25\ ^{FHMr}OH$ + 0.25 PTPFHMrOH	tag_kG4155	
G4156	StTrG	$CH_3O_2 + O(^3P) \rightarrow$ LossO3C + LossO3 + CH_3O + O_2	tag_kG4156	Zellner et al. (1988)
	tag: FHM	$^{FHM}CH_3O_2 + O(^3P) \rightarrow O(^3P) + {}^{FHM}CH_3O$	tag_kG4156	
	tag: FHM	$^{FHMr}CH_3O_2 + O(^3P) \rightarrow O(^3P) + {}^{FHMr}CH_3O$	tag_kG4156	
G4157	StTrG	$HCHO + O(^3P) \rightarrow$ LossO3C + LossO3 + 0.7 OH + 0.7 CO + 0.3 H + 0.3 CO_2 + HO_2	tag_kG4157	Sander et al. (2011)
	tag: FHM	$^{FHM}HCHO + O(^3P) \rightarrow O(^3P) + 0.7\ ^{FHM}OH$ + 0.7 PTPFHMOH + 0.3 $^{FHM}H + {}^{FHM}HO_2$	tag_kG4157	
	tag: FHM	$^{FHMr}HCHO + O(^3P) \rightarrow O(^3P) + 0.7\ ^{FHMr}OH$ + 0.7 PTPFHMrOH + 0.3 $^{FHMr}H + {}^{FHMr}HO_2$	tag_kG4157	
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	1.49E-17*temp*temp*EXP(-499./temp)	Atkinson (2003)
G4201	TrGC	$C_2H_4 + O_3 \rightarrow$ 1. LossO3R + 1. 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)*

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

#	labels	reaction	rate coefficient	reference
G4202	TrGC	C_2H_4 + OH → .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 → C_2H_5OOH	7.5E-13*EXP(700./temp)	Sander et al. (2011)
G4204	TrGCN	$C_2H_5O_2$ + NO → 1. ProdO3R + 1. 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 → 1. LossO3R + 1. LossO3 + CH_3CHO + HO_2 + NO_2	2.3E-12	Wallington et al.
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 → $CH_3C(O)OO$ + H_2O	4.4E-12*EXP(365./temp)	Atkinson et al. (2006)
G4209	TrGCN	CH_3CHO + NO_3 → 1. LossO3R + 1. LossO3 + $CH_3C(O)OO$ + HNO_3	1.4E-12*EXP(-1900./temp)	Sander et al. (2011)
G4210	TrGC	CH_3COOH + OH → 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. (2001)
G4211b	TrGC	$CH_3C(O)OO$ + HO_2 → 1. ProdO3R + 1. ProdO3 + CH_3COOH + O_3	4.3E-13*EXP(1040./temp)/(1.+ 37.*EXP(-660./temp))	Tyndall et al. (2001)
G4212	TrGCN	$CH_3C(O)OO$ + NO → 1. ProdO3R + 1. ProdO3 + CH_3O_2 + CO_2 + NO_2	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
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. LossO3R + 1. 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., 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. (2001)
G4218	TrGC	$CH_3C(O)OOH$ + OH → $CH_3C(O)OO$ + 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 → 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)*
G4300	TrGC	C_3H_8 + OH → .82 $iC_3H_7O_2$ + .18 $C_2H_5O_2$ + H_2O	1.65E-17*temp*temp*EXP(-87./temp)	Atkinson (2003)

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

#	labels	reaction	rate coefficient	reference
G4301	TrGC	$C_3H_6 + O_3 \rightarrow$ 1. LossO3R + 1. 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	$C_3H_6 + OH \rightarrow CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,8.E-27,3.5, 3.E-11,0.,0.5)	Wallington et al.
G4303	TrGCN	$C_3H_6 + NO_3 \rightarrow$ 1. LossO3R + 1. LossO3 + LC4H9NO3	4.6E-13*EXP(-1155./temp)	Wallington et al.
G4304	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	k_PrO2_HO2	Atkinson (1997)
G4305	TrGCN	$iC_3H_7O_2$ + NO $\rightarrow$ 1. ProdO3R + 1. ProdO3 + .96 CH_3COCH_3 + .96 HO_2 + .96 NO_2 + .04 $iC_3H_7ONO_2$	k_PrO2_NO	Wallington et al.
G4306	TrGC	$iC_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3$ + .8 HCHO + .8 HO_2 + .2 CH_3OH	k_PrO2_CH3O2	Kirchner and Stockwell (1996)
G4307	TrGC	iC_3H_7OOH + OH $\rightarrow$ .3 $iC_3H_7O_2$ + .7 CH_3COCH_3 + .7 OH	k_CH3OOH_OH	see note*
G4308	TrGC	$CH_3CH(O_2)CH_2OH + HO_2 \rightarrow CH_3CH(OOH)CH_2OH$	6.5E-13*EXP(650./temp)	Müller and Brasseur (1995)
G4309	TrGCN	$CH_3CH(O_2)CH_2OH$ + NO $\rightarrow$ 1. ProdO3R + 1. 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 $\rightarrow$ .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 $\rightarrow$ $CH_3COCH_2O_2 + H_2O$	1.33E-13+3.82E-11*EXP(-2000./ temp)	Sander et al. (2011)
G4312	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	8.6E-13*EXP(700./temp)	Tyndall et al. (2001)
G4313	TrGCN	$CH_3COCH_2O_2$ + NO $\rightarrow$ 1. ProdO3R + 1. ProdO3 + $CH_3C(O)OO$ + HCHO + NO_2	2.9E-12*EXP(300./temp)	Sander et al. (2011)
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow$ .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. (2001)
G4315	TrGC	$CH_3COCH_2O_2H$ + OH $\rightarrow$ .3 $CH_3COCH_2O_2$ + .7 MGLYOX + .7 OH	k_CH3OOH_OH	see note*
G4316	TrGC	CH_3COCH_2OH + OH $\rightarrow$ MGLYOX + HO_2	2.15E-12*EXP(305./temp)	Dillon et al. (2006)
G4317	TrGC	MGLYOX + OH $\rightarrow$ $CH_3C(O)OO$ + CO	8.4E-13*EXP(830./temp)	Tyndall et al. (1995)
G4320	TrGCN	$iC_3H_7ONO_2$ + OH $\rightarrow$ $CH_3COCH_3 + NO_2$	6.2E-13*EXP(-230./temp)	Wallington et al.
G4400	TrGC	C_4H_{10} + OH $\rightarrow$ $LC_4H_9O_2 + H_2O$	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)
G4401	TrGC	$LC_4H_9O_2 + CH_3O_2 \rightarrow$ .88 MEK + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	k_PrO2_CH3O2	see note*

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

#	labels	reaction	rate coefficient	reference
G4402	TrGC	$LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$	k_PrO2_HO2	see note*
G4403	TrGCN	$LC_4H_9O_2 + NO \rightarrow$ 1. ProdO3R + 1. ProdO3 + .84 NO_2 + .56 MEK + .56 HO_2 + .28 $C_2H_5O_2$ + .28 CH_3CHO + .16 LC4H9NO3	k_PrO2_NO	see note*
G4404	TrGC	$LC_4H_9OOH + OH \rightarrow$ .15 $LC_4H_9O_2$ + .85 MEK + .85 OH + .85 H_2O	k_CH3OOH_OH	see note*
G4405	TrGC	MVK + $O_3 \rightarrow$ 1. LossO3R + 1. 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 → 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 → 1. ProdO3R + 1. 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 → CH_3COCH_2OH + MGLYOX + .5 CO + .5 HCHO + HO_2	2.E-12	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH → MVKO2	3.E-11	Pöschl et al. (2000)
G4413	TrGC	MEK + OH → LMEKO2	1.3E-12*EXP(-25./temp)	Wallington et al.
G4414	TrGC	LMEKO2 + $HO_2 \rightarrow$ LMEKOOH	k_PrO2_HO2	see note*
G4415	TrGCN	LMEKO2 + NO → 1. ProdO3R + 1. ProdO3 + .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 LC4H9NO3	k_PrO2_NO	see note*
G4416	TrGC	LMEKOOH + OH → .8 BIACET + .8 OH + .2 LMEKO2	k_CH3OOH_OH	see note*
G4417	TrGCN	LC4H9NO3 + OH → MEK + NO_2 + H_2O	1.7E-12	Wallington et al.
G4418	TrGCN	MPAN + OH → CH_3COCH_2OH + NO_2	3.2E-11	Orlando et al. (2002)
G4419	TrGCN	MPAN → MVKO2 + NO_2	k_PAN_M	see note*
G4500	TrGC	$C_5H_8 + O_3 \rightarrow$ 1. LossO3R + 1. 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)

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

#	labels	reaction	rate coefficient	reference
G4501	TrGC	C_5H_8 + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGCN	C_5H_8 + NO_3 → 1. LossO3R + 1. LossO3 + ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO_2 → ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)
G4504	TrGCN	ISO2 + NO → 1. ProdO3R + 1. 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(^{3}P) → 2. LossO3Cl + 2. LossO3 + Cl + O_2	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → 2. LossO3Cl + 2. LossO3 + Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2. LossO3Cl + 2. LossO3 + 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → 1. LossO3Cl + 1. LossO3 + Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(1.72E-27*EXP(8649./temp))	Atkinson et al. (2007), Sander et al. (2011)*
G6200	StGCl	Cl + H_2 → HCl + H	tag_kG6200	Atkinson et al. (2007)
	tag: FHM	$^{FHM}H_2$ + Cl → Cl + ^{FHM}HCl + ^{FHM}H + PTLFHMH2	tag_kG6200	
	tag: FHM	$^{FHMr}H_2$ + Cl → Cl + ^{FHMr}HCl + ^{FHMr}H + PTLFHMrH2	tag_kG6200	
G6201a	StGCl	Cl + HO_2 → HCl + O_2	tag_kG6201a	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HO_2$ + Cl → Cl + ^{FHM}HCl	tag_kG6201a	
	tag: FHM	$^{FHMr}HO_2$ + Cl → Cl + ^{FHMr}HCl	tag_kG6201a	
G6201b	StGCl	Cl + HO_2 → ProdO3Cl + ProdO3 + ClO + OH	tag_kG6201b	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HO_2$ + Cl → Cl + ^{FHM}OH + PTPFHMOH	tag_kG6201b	
	tag: FHM	$^{FHMr}HO_2$ + Cl → Cl + ^{FHMr}OH + PTPFHMrOH	tag_kG6201b	
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	tag_kG6202	Atkinson et al. (2007)
	tag: FHM	$^{FHM}H_2O_2$ + Cl → Cl + ^{FHM}HCl + $^{FHM}HO_2$	tag_kG6202	
	tag: FHM	$^{FHMr}H_2O_2$ + Cl → Cl + ^{FHMr}HCl + $^{FHMr}HO_2$	tag_kG6202	
G6203	StGCl	ClO + OH → LossO3Cl + LossO3 + 0.94 Cl + 0.94 HO_2 + 0.06 HCl + 0.06 O_2	tag_kG6203	Atkinson et al. (2007)
	tag: FHM	^{FHM}OH + ClO → ClO + 0.94 $^{FHM}HO_2$ + 0.06 ^{FHM}HCl + PTLFHMOH	tag_kG6203	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}OH + ClO \rightarrow ClO + 0.94\ ^{FHMr}HO_2 + 0.06\ ^{FHMr}HCl$ + PTLFHMrOH	tag_kG6203	
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl + O_2$	tag_kG6204	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HO_2 + ClO \rightarrow ClO + {}^{FHM}HOCl$	tag_kG6204	
	tag: FHM	$^{FHMr}HO_2 + ClO \rightarrow ClO + {}^{FHMr}HOCl$	tag_kG6204	
G6205	StTrGCl	$HCl + OH \rightarrow Cl + H_2O$	tag_kG6205	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HCl + OH \rightarrow OH + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG6205	
	tag: FHM	$^{FHMr}HCl + OH \rightarrow OH + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kG6205	
	tag: FHM	$^{FHM}OH + HCl \rightarrow HCl + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG6205	
	tag: FHM	$^{FHMr}OH + HCl \rightarrow HCl + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG6205	
G6206	StGCl	$HOCl + OH \rightarrow ClO + H_2O$	tag_kG6206	Sander et al. (2011)
	tag: FHM	$^{FHM}HOCl + OH \rightarrow OH + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kG6206	
	tag: FHM	$^{FHMr}HOCl + OH \rightarrow OH + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kG6206	
	tag: FHM	$^{FHM}OH + HOCl \rightarrow HOCl + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O + PTLFHMOH	tag_kG6206	
	tag: FHM	$^{FHMr}OH + HOCl \rightarrow HOCl + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O + PTLFHMrOH	tag_kG6206	
G6300	UpStTrGClN	$ClO + NO \rightarrow NO_2 + Cl$	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGClN	$ClO + NO_2 \rightarrow ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31, 3.4,7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGClN	$ClNO_3 \rightarrow ClO + NO_2$	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGClN	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGClN	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3$	tag_kG6400	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_4 + Cl \rightarrow Cl + {}^{FHM}HCl + {}^{FHM}CH_3$ + PTLFHMCH4	tag_kG6400	
	tag: FHM	$^{FHMr}CH_4 + Cl \rightarrow Cl + {}^{FHMr}HCl + {}^{FHMr}CH_3$ + PTLFHMrCH4	tag_kG6400	
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	tag_kG6401	Atkinson et al. (2006)
	tag: FHM	$^{FHM}HCHO + Cl \rightarrow Cl + {}^{FHM}HCl + {}^{FHM}HO_2$	tag_kG6401	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}HCHO + Cl \rightarrow Cl + {}^{FHMr}HCl + {}^{FHMr}HO_2$	tag_kG6401	
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	tag_kG6402	Atkinson et al. (2006)
	tag: FHM	$^{FHM}CH_3OOH + Cl \rightarrow Cl + {}^{FHM}HCHO + {}^{FHM}HCl + {}^{FHM}OH$ + PTPFHMOH	tag_kG6402	
	tag: FHM	$^{FHMr}CH_3OOH + Cl \rightarrow Cl + {}^{FHMr}HCHO + {}^{FHMr}HCl + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG6402	
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow$ LossO3Cl + LossO3 + HO_2 + Cl + HCHO	tag_kG6403	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3O_2 + ClO \rightarrow ClO + {}^{FHM}HO_2 + {}^{FHM}HCHO$	tag_kG6403	
	tag: FHM	$^{FHMr}CH_3O_2 + ClO \rightarrow ClO + {}^{FHMr}HO_2 + {}^{FHMr}HCHO$	tag_kG6403	
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow$ 4.0 ProdLCl + LCARBON + ClO + 3 Cl	3.3E-10	Sander et al. (2011)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow$ 2 LHYDROGEN + ProdLCl + LossO3Cl + LossO3 + LCARBON + OH + Cl	tag_kG6405	
	transfer:	$CH_3Cl \rightarrow$ OH		
	tag: FHM	$O(^1D) + {}^{FHM}CH_3Cl \rightarrow O(^1D) + {}^{FHM}OH$ + PTPFHMOH	tag_kG6405	
	tag: FHM	$O(^1D) + {}^{FHMr}CH_3Cl \rightarrow O(^1D) + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG6405	
G6406	StGCl	$CH_3Cl + OH \rightarrow$ 2 LHYDROGEN + ProdLCl + LCARBON + H_2O + Cl	tag_kG6406	Sander et al. (2011)
	transfer:	$OH \rightarrow H_2O$		
	tag: FHM	$CH_3Cl + {}^{FHM}OH \rightarrow CH_3Cl + {}^{FHM}H_2O$ + PTPFHMH2O + PTLFHMOH	tag_kG6406	
	tag: FHM	$CH_3Cl + {}^{FHMr}OH \rightarrow CH_3Cl + {}^{FHMr}H_2O$ + PTPFHMrH2O + PTLFHMrOH	tag_kG6406	
	transfer:	$CH_3Cl \rightarrow$		
	tag: FHM	$OH + {}^{FHM}CH_3Cl \rightarrow OH$ + Dummy	tag_kG6406	
	tag: FHM	$OH + {}^{FHMr}CH_3Cl \rightarrow OH$ + Dummy	tag_kG6406	
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow$ 2 LHYDROGEN + 3 ProdLCl + LossO3Cl + LossO3 + 2 LCARBON + OH + 3 Cl	tag_kG6407	
	transfer:	$CH_3CCl_3 \rightarrow$ OH		
	tag: FHM	$O(^1D) + {}^{FHM}CH_3CCl_3 \rightarrow O(^1D) + {}^{FHM}OH$ + PTPFHMOH	tag_kG6407	
	tag: FHM	$O(^1D) + {}^{FHMr}CH_3CCl_3 \rightarrow O(^1D) + {}^{FHMr}OH$ + PTPFHMrOH	tag_kG6407	

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

#	labels	reaction	rate coefficient	reference
G6408	StTrGCCl	CH_3CCl_3 + OH → 2 LHYDROGEN + 3 ProdLCl + 2 LCARBON + H_2O + 3 Cl	tag_kG6408	Sander et al. (2011)
	transfer:	OH → H_2O		
	tag: FHM	CH_3CCl_3 + ^{FHM}OH → CH_3CCl_3 + $^{FHM}H_2O$ + PTPFHMH2O + PTLFHMOH	tag_kG6408	
	tag: FHM	CH_3CCl_3 + ^{FHMr}OH → CH_3CCl_3 + $^{FHMr}H_2O$ + PTPFHMrH2O + PTLFHMrOH	tag_kG6408	
	transfer:	CH_3CCl_3 →		
	tag: FHM	OH + $^{FHM}CH_3CCl_3$ → OH + Dummy	tag_kG6408	
	tag: FHM	OH + $^{FHMr}CH_3CCl_3$ → OH + Dummy	tag_kG6408	
G6409	TrGCCl	Cl + C_2H_4 → 1.6666669 PHYDROGEN + .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)
G6500	StGClF	CF_2Cl_2 + O(^{1}D) → 2.0 ProdLCl + LCARBON + 2 LFLUORINE + ClO + Cl	1.4E-10	Sander et al. (2011)
G6501	StGClF	$CFCl_3$ + O(^{1}D) → 3.0 ProdLCl + LCARBON + LFLUORINE + ClO + 2 Cl	2.3E-10	Sander et al. (2011)
G7100	StTrGBr	Br + O_3 → BrO + O_2	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	BrO + O(^{3}P) → 2. LossO3Br + 2. LossO3 + Br + O_2	1.9E-11*EXP(230./temp)	Atkinson et al. (2007)
G7102a	StTrGBr	BrO + BrO → 2. LossO3Br + 2. LossO3 + 2 Br + O_2	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	BrO + BrO → 2. LossO3Br + 2. LossO3 + Br_2 + O_2	2.9E-14*EXP(840./temp)	Atkinson et al. (2007)
G7200	StTrGBr	Br + HO_2 → HBr + O_2	tag_kG7200	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HO_2$ + Br → Br + ^{FHM}HBr	tag_kG7200	
	tag: FHM	$^{FHMr}HO_2$ + Br → Br + ^{FHMr}HBr	tag_kG7200	
G7201	StTrGBr	BrO + HO_2 → HOBr + O_2	tag_kG7201	Atkinson et al. (2007)
	tag: FHM	$^{FHM}HO_2$ + BrO → BrO + ^{FHM}HOBr	tag_kG7201	
	tag: FHM	$^{FHMr}HO_2$ + BrO → BrO + ^{FHMr}HOBr	tag_kG7201	
G7202	StTrGBr	HBr + OH → Br + H_2O	tag_kG7202	Atkinson et al. (2007)
	tag: FHM	^{FHM}HBr + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG7202	
	tag: FHM	^{FHMr}HBr + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7202	
	tag: FHM	^{FHM}OH + HBr → HBr + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7202	
	tag: FHM	^{FHMr}OH + HBr → HBr + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7202	

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

#	labels	reaction	rate coefficient	reference
G7203	StGBr	HOBr + O(^{3}P) → LossO3Br + LossO3 + OH + BrO	tag_kG7203	Atkinson et al. (2007)
	tag: FHM	^{FHM}HOBr + O(^{3}P) → O(^{3}P) + ^{FHM}OH + PTPFHMOH	tag_kG7203	
	tag: FHM	^{FHMr}HOBr + O(^{3}P) → O(^{3}P) + ^{FHMr}OH + PTPFHMrOH	tag_kG7203	
G7204	StTrGBr	Br_2 + OH → ProdO3Br + ProdO3 + HOBr + Br	tag_kG7204	Atkinson et al. (2007)
	tag: FHM	^{FHM}OH + Br_2 → Br_2 + ^{FHM}HOBr + PTLFHMOH	tag_kG7204	
	tag: FHM	^{FHMr}OH + Br_2 → Br_2 + ^{FHMr}HOBr + PTLFHMrOH	tag_kG7204	
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)*
G7303	TrGBrN	$BrNO_3$ → 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 → HBr + CO + HO_2	tag_kG7400	Atkinson et al. (2006)
	tag: FHM	^{FHM}HCHO + Br → Br + ^{FHM}HBr + ^{FHM}HO_2	tag_kG7400	
	tag: FHM	^{FHMr}HCHO + Br → Br + ^{FHMr}HBr + ^{FHMr}HO_2	tag_kG7400	
G7401	TrGBr	Br + CH_3OOH → CH_3O_2 + HBr	tag_kG7401	Kondo and Benson (1984)
	tag: FHM	^{FHM}CH_3OOH + Br → Br + ^{FHM}CH_3O_2 + ^{FHM}HBr	tag_kG7401	
	tag: FHM	^{FHMr}CH_3OOH + Br → Br + ^{FHMr}CH_3O_2 + ^{FHMr}HBr	tag_kG7401	
G7402a	TrGBr	BrO + CH_3O_2 → HOBr + HCHO	tag_kG7402a	Aranda et al. (1997)
	tag: FHM	^{FHM}CH_3O_2 + BrO → BrO + ^{FHM}HOBr + ^{FHM}HCHO	tag_kG7402a	
	tag: FHM	^{FHMr}CH_3O_2 + BrO → BrO + ^{FHMr}HOBr + ^{FHMr}HCHO	tag_kG7402a	
G7402b	TrGBr	BrO + CH_3O_2 → LossO3Br + LossO3 + Br + HCHO + HO_2	tag_kG7402b	Aranda et al. (1997)
	tag: FHM	^{FHM}CH_3O_2 + BrO → BrO + ^{FHM}HCHO + ^{FHM}HO_2	tag_kG7402b	
	tag: FHM	^{FHMr}CH_3O_2 + BrO → BrO + ^{FHMr}HCHO + ^{FHMr}HO_2	tag_kG7402b	
G7403	StTrGBr	CH_3Br + OH → 2 LHYDROGEN + ProdLBr + LCARBON + H_2O + Br	tag_kG7403	Sander et al. (2011)
	transfer:	OH → 0.5 H_2O		
	tag: FHM	CH_3Br + ^{FHM}OH → CH_3Br + 0.5 ^{FHM}H_2O + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7403	
	tag: FHM	CH_3Br + ^{FHMr}OH → CH_3Br + 0.5 ^{FHMr}H_2O + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7403	
	transfer:	CH_3Br → 0.5 H_2O		
	tag: FHM	OH + ^{FHM}CH_3Br → OH + 0.5 ^{FHM}H_2O + 0.5 PTPFHMH2O	tag_kG7403	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	OH + $^{FHMr}CH_3Br$ → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7403	
G7404	TrGBrC	Br + C_2H_4 → 1.6666669 PHYDROGEN + .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 → HBr + $CH_3C(O)OO$	1.8e-11*EXP(-460./temp)	Atkinson et al. (2006)
G7407	TrGBr	$CHBr_3$ + OH → 3 ProdSBr + LCARBON + H_2O + 3 Br	tag_kG7407	Sander et al. (2011)
	transfer:	OH → 0.5 H_2O		
	tag: FHM	$CHBr_3$ + ^{FHM}OH → $CHBr_3$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7407	
	tag: FHM	$CHBr_3$ + ^{FHMr}OH → $CHBr_3$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7407	
	transfer:	$CHBr_3$ → 0.5 H_2O		
	tag: FHM	OH + $^{FHM}CHBr_3$ → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG7407	
	tag: FHM	OH + $^{FHMr}CHBr_3$ → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7407	
G7408	TrGBr	CH_2Br_2 + OH → LHYDROGEN + 2 ProdSBr + LCARBON + H_2O + 2 Br	tag_kG7408	Sander et al. (2011)
	transfer:	OH → 0.5 H_2O		
	tag: FHM	CH_2Br_2 + ^{FHM}OH → CH_2Br_2 + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7408	
	tag: FHM	CH_2Br_2 + ^{FHMr}OH → CH_2Br_2 + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7408	
	transfer:	CH_2Br_2 → 0.5 H_2O		
	tag: FHM	OH + $^{FHM}CH_2Br_2$ → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG7408	
	tag: FHM	OH + $^{FHMr}CH_2Br_2$ → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7408	
G7600	TrGBrCl	Br + BrCl → Br_2 + Cl	3.32E-15	Manion et al. (2015)
G7601	TrGBrCl	Br + Cl_2 → BrCl + Cl	1.10E-15	Dolson and Leone (1987)
G7602	TrGBrCl	Br_2 + Cl → BrCl + Br	2.3E-10*EXP(135./temp)	Bedjanian et al. (1998)
G7603a	StTrGBrCl	BrO + ClO → 0.5 LossO3Br + 0.5 LossO3Cl + 1. LossO3 + Br + OClO	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G7603b	StTrGBrCl	BrO + ClO → 1. LossO3Br + 1. LossO3Cl + 2. LossO3 + Br + Cl + O_2	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGBrCl	BrO + ClO → 1. LossO3Br + 1. LossO3Cl + 2. LossO3 + BrCl + O_2	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G7604	TrGBrCl	BrCl + Cl → Br + Cl_2	1.45E-11	Clyne and Cruse (1972)
G7605	TrGBrCl	$CHCl_2Br$ + OH → ProdSBr + LCARBON + 2 LCHLORINE + H_2O + Br	tag_kG7605	
	transfer:	OH → 0.5 H_2O		
	tag: FHM	$CHCl_2Br$ + ^{FHM}OH → $CHCl_2Br$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7605	
	tag: FHM	$CHCl_2Br$ + ^{FHMr}OH → $CHCl_2Br$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7605	
	transfer:	$CHCl_2Br$ → 0.5 H_2O		
	tag: FHM	OH + $^{FHM}CHCl_2Br$ → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG7605	
	tag: FHM	OH + $^{FHMr}CHCl_2Br$ → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7605	
G7606	TrGBrCl	$CHClBr_2$ + OH → 2 ProdSBr + LCARBON + LCHLORINE + H_2O + 2 Br	tag_kG7606	
	tag: FHM	$^{FHM}CHClBr_2$ + OH → OH + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG7606	
	tag: FHM	$^{FHMr}CHClBr_2$ + OH → OH + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG7606	
	tag: FHM	^{FHM}OH + $CHClBr_2$ → $CHClBr_2$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG7606	
	tag: FHM	^{FHMr}OH + $CHClBr_2$ → $CHClBr_2$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG7606	
G7607	TrGBrCl	CH_2ClBr + OH → LHYDROGEN + ProdSBr + LCARBON + LCHLORINE + H_2O + Br	tag_kG7607	Sander et al. (2011)
	transfer:	OH → 0.333 H_2O		
	tag: FHM	CH_2ClBr + ^{FHM}OH → CH_2ClBr + 0.333333333333333 $^{FHM}H_2O$ + 0.3333333 PTPFHMH2O + PTLFHMOH	tag_kG7607	
	tag: FHM	CH_2ClBr + ^{FHMr}OH → CH_2ClBr + 0.333333333333333 $^{FHMr}H_2O$ + 0.3333333 PTPFHMrH2O + PTLFHMrOH	tag_kG7607	
	transfer:	$CHClBr_2$ → 0.333 H_2O		

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	OH + CH_2ClBr → OH + CH_2ClBr + 0.333333333333333 $^{FHM}H_2O$ + 0.3333333 PTPFHMH2O	(tag_kG7607)*tag_src_fFHMCHClBr2	
	tag: FHM	OH + CH_2ClBr → OH + CH_2ClBr + 0.333333333333333 $^{FHMr}H_2O$ + 0.3333333 PTPFHMrH2O	(tag_kG7607)*tag_src_fFHMrCHClBr2	
	transfer:	CH_2ClBr → 0.333 H_2O		
	tag: FHM	OH + $^{FHM}CH_2ClBr$ → OH + 0.333333333333333 $^{FHM}H_2O$ + 0.3333333 PTPFHMH2O	tag_kG7607	
	tag: FHM	OH + $^{FHMr}CH_2ClBr$ → OH + 0.333333333333333 $^{FHMr}H_2O$ + 0.3333333 PTPFHMrH2O	tag_kG7607	
G9200	StTrGS	SO_2 + OH → 2 PHYDROGEN + ProdO3S + ProdO3 + H_2SO_4 + HO_2	tag_kG9200	Sander et al. (2011)
	transfer:	OH → HO_2		
	tag: FHM	SO_2 + ^{FHM}OH → SO_2 + $^{FHM}HO_2$ + PTLFHMOH	tag_kG9200	
	tag: FHM	SO_2 + ^{FHMr}OH → SO_2 + $^{FHMr}HO_2$ + PTLFHMrOH	tag_kG9200	
	transfer:	H_2O → H_2SO_4		
	tag: FHM	OH + SO_2 → OH + SO_2 + $^{FHM}H_2SO_4$	(tag_kG9200)*tag_src_fFHMH2O	
	tag: FHM	OH + SO_2 → OH + SO_2 + $^{FHMr}H_2SO_4$	(tag_kG9200)*tag_src_fFHMrH2O	
G9400a	TrGCS	DMS + OH → ProdO3S + ProdO3 + CH_3SO_2 + HCHO + H_2O	tag_kG9400a	Atkinson et al. (2004)
	transfer:	OH → 0.5 H_2O		
	tag: FHM	DMS + ^{FHM}OH → DMS + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O + PTLFHMOH	tag_kG9400a	
	tag: FHM	DMS + ^{FHMr}OH → DMS + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O + PTLFHMrOH	tag_kG9400a	
	transfer:	DMS → 0.5 H_2O + CH_3SO_2 + HCHO + CH_3O_2		
	tag: FHM	OH + ^{FHM}DMS → OH + $^{FHM}CH_3SO_2$ + $^{FHM}HCHO$ + 0.5 $^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kG9400a	
	tag: FHM	OH + ^{FHMr}DMS → OH + $^{FHMr}CH_3SO_2$ + $^{FHMr}HCHO$ + 0.5 $^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kG9400a	
G9400b	TrGCS	DMS + OH → ProdO3S + ProdO3 + DMSO + HO_2	tag_kG9400b	Atkinson et al. (2004)
	transfer:	OH → HO_2		
	tag: FHM	DMS + ^{FHM}OH → DMS + $^{FHM}HO_2$ + PTLFHMOH	tag_kG9400b	
	tag: FHM	DMS + ^{FHMr}OH → DMS + $^{FHMr}HO_2$ + PTLFHMrOH	tag_kG9400b	
	transfer:	DMS → DMSO		
	tag: FHM	OH + ^{FHM}DMS → OH + $^{FHM}DMSO$	tag_kG9400b	

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	OH + ^{FHMr}DMS → OH + ^{FHMr}DMSO	tag_kG9400b	
G9401	TrGCNS	DMS + NO_3 → CH_3SO_2 + HNO_3 + HCHO	tag_kG9401	Atkinson et al. (2004)
	tag: FHM	^{FHM}DMS + NO_3 → NO_3 + $^{FHM}CH_3SO_2$ + $^{FHM}HNO_3$ + ^{FHM}HCHO	tag_kG9401	
	tag: FHM	^{FHMr}DMS + NO_3 → NO_3 + $^{FHMr}CH_3SO_2$ + $^{FHMr}HNO_3$ + ^{FHMr}HCHO	tag_kG9401	
G9402	TrGCS	DMSO + OH → 0.40000004 ProdO3S + 0.40000004 ProdO3 + 0.6 H_2O + 0.6 SO_2 + HCHO + 0.6 CH_3 + 0.4 HO_2 + 0.4 CH_3SO_3H	tag_kG9402	Hynes and Wine (1996)
	transfer:	DMSO → CH_3O_2 + HCHO + CH_3SO_3H + 0.5 H_2O + CH_3		
	tag: FHM	OH + ^{FHM}DMSO → OH + 0.3 $^{FHM}H_2O$ + 0.3 PTPFHMH2O + ^{FHM}HCHO + 0.6 $^{FHM}CH_3$ + 0.4 $^{FHM}CH_3SO_3H$	tag_kG9402	
	tag: FHM	OH + ^{FHMr}DMSO → OH + 0.3 $^{FHMr}H_2O$ + 0.3 PTPFHMrH2O + ^{FHMr}HCHO + 0.6 $^{FHMr}CH_3$ + 0.4 $^{FHMr}CH_3SO_3H$	tag_kG9402	
	transfer:	OH → HO_2 + 0.5 H_2O		
	tag: FHM	DMSO + ^{FHM}OH → DMSO + 0.3 $^{FHM}H_2O$ + 0.3 PTPFHMH2O + 0.4 $^{FHM}HO_2$ + PTLFHMOH	tag_kG9402	
	tag: FHM	DMSO + ^{FHMr}OH → DMSO + 0.3 $^{FHMr}H_2O$ + 0.3 PTPFHMrH2O + 0.4 $^{FHMr}HO_2$ + PTLFHMrOH	tag_kG9402	
G9403	TrGS	CH_3SO_2 → SO_2 + CH_3	tag_kG9403	Barone et al. (1995)
	tag: FHM	$^{FHM}CH_3SO_2$ → $^{FHM}CH_3$	tag_kG9403	
	tag: FHM	$^{FHMr}CH_3SO_2$ → $^{FHMr}CH_3$	tag_kG9403	
G9404	TrGS	CH_3SO_2 + O_3 → CH_3SO_3	tag_kG9404	Barone et al. (1995)
	tag: FHM	$^{FHM}CH_3SO_2$ + O_3 → O_3 + $^{FHM}CH_3SO_3$	tag_kG9404	
	tag: FHM	$^{FHMr}CH_3SO_2$ + O_3 → O_3 + $^{FHMr}CH_3SO_3$	tag_kG9404	
G9405	TrGS	CH_3SO_3 + HO_2 → CH_3SO_3H	tag_kG9405	Barone et al. (1995)
	tag: FHM	$^{FHM}CH_3SO_3$ + HO_2 → HO_2 + 0.75 $^{FHM}CH_3SO_3H$	tag_kG9405	
	tag: FHM	$^{FHMr}CH_3SO_3$ + HO_2 → HO_2 + 0.75 $^{FHMr}CH_3SO_3H$	tag_kG9405	
	tag: FHM	$^{FHM}HO_2$ + CH_3SO_3 → CH_3SO_3 + 0.25 $^{FHM}CH_3SO_3H$	tag_kG9405	
	tag: FHM	$^{FHMr}HO_2$ + CH_3SO_3 → CH_3SO_3 + 0.25 $^{FHMr}CH_3SO_3H$	tag_kG9405	
G9600	TrGCClS	DMS + Cl → ProdO3S + ProdO3 + CH_3SO_2 + HCl + HCHO	tag_kG9600	Atkinson et al. (2004)

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

#	labels	reaction	rate coefficient	reference
	tag: FHM	^{FHM}DMS + Cl → Cl + $^{FHM}CH_3SO_2$ + ^{FHM}HCl + ^{FHM}HCHO	tag_kG9600	
	tag: FHM	^{FHMr}DMS + Cl → Cl + $^{FHMr}CH_3SO_2$ + ^{FHMr}HCl + ^{FHMr}HCHO	tag_kG9600	
G9700	TrGBrCS	DMS + Br → ProdO3S + ProdO3 + CH_3SO_2 + HBr + HCHO	tag_kG9700	Jefferson et al. (1994)
	tag: FHM	^{FHM}DMS + Br → Br + $^{FHM}CH_3SO_2$ + ^{FHM}HBr + ^{FHM}HCHO	tag_kG9700	
	tag: FHM	^{FHMr}DMS + Br → Br + $^{FHMr}CH_3SO_2$ + ^{FHMr}HBr + ^{FHMr}HCHO	tag_kG9700	
G9701	TrGBrCS	DMS + BrO → DMSO + Br	tag_kG9701	Ingham et al. (1999)
	tag: FHM	^{FHM}DMS + BrO → BrO + ^{FHM}DMSO	tag_kG9701	
	tag: FHM	^{FHMr}DMS + BrO → BrO + ^{FHMr}DMSO	tag_kG9701	
G6413	StTrGClN	Cl + CH_3ONO_2 → ProdO3Cl + ProdO3 + HCl + HCHO + NO_2	tag_kG6413	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3ONO_2$ + Cl → Cl + ^{FHM}HCl + ^{FHM}HCHO	tag_kG6413	
	tag: FHM	$^{FHMr}CH_3ONO_2$ + Cl → Cl + ^{FHMr}HCl + ^{FHMr}HCHO	tag_kG6413	
G6414	StTrGClN	Cl + CH_3ONO → HCl + HCHO + NO	tag_kG6414	Sokolov et al. (1999)
	tag: FHM	$^{FHM}CH_3ONO$ + Cl → Cl + ^{FHM}HCl + ^{FHM}HCHO	tag_kG6414	
	tag: FHM	$^{FHMr}CH_3ONO$ + Cl → Cl + ^{FHMr}HCl + ^{FHMr}HCHO	tag_kG6414	
G6415	StTrGCl	Cl + CH_3O_2 → 0.5 ProdO3Cl + 0.5 ProdO3 + 0.5 ClO + 0.5 CH_3O + 0.5 HCl + 0.5 CO + 0.5 HO_2 + 0.5 OH	tag_kG6415	Sander et al. (2011)
	tag: FHM	$^{FHM}CH_3O_2$ + Cl → Cl + 0.5 $^{FHM}CH_3O$ + 0.5 ^{FHM}HCl + 0.5 $^{FHM}HO_2$ + 0.5 ^{FHM}OH + 0.5 PTPFHMOH	tag_kG6415	
	tag: FHM	$^{FHMr}CH_3O_2$ + Cl → Cl + 0.5 $^{FHMr}CH_3O$ + 0.5 ^{FHMr}HCl + 0.5 $^{FHMr}HO_2$ + 0.5 ^{FHMr}OH + 0.5 PTPFHMrOH	tag_kG6415	
G01Diag	StTrG	O_3(s) → LO_3(s)	k_O3s	Roelofs and Lelieveld (1997)

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 $k_0(T)$, $k_{\mathrm{inf}}(T)$, and k_{ratio}, `k_3rd` is defined as:

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

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

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \quad (3)$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_\mathrm{c}^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}}))^2}\right)} \quad (4)$$

A similar function, called `k_3rd_iupac` here, is used by T. J. Wallington et al. (2014) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

$$k_{\mathrm{ratio}} = \frac{k_0(T)M}{k_{\mathrm{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_\mathrm{c}) \quad (8)$$

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

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 $k^{1\mathrm{st}} = 2 \times \sqrt{k_{\mathrm{self}} \times \texttt{k\_CH3O2}} \times [\mathrm{RO_2}]$ 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 $[\mathrm{RO_2}]$ = 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.

`G3109`: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)`.

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

`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 ≈ 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.

`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).

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow$ 2. ProdO3O + 2. ProdO3 + $O(^3P)$ + $O(^3P)$	jx(ip_O2)	Sander et al. (2014)
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	jx(ip_O1D)	Sander et al. (2014)
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	jx(ip_O3P)	Sander et al. (2014)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	tag_kJ2100a	Sander et al. (2014)
	tag: FHM	$^{FHM}H_2O + h\nu \rightarrow h\nu + {}^{FHMr}H + {}^{FHMr}OH$ + PTPFHMrOH + PTLFHMH2O	tag_kJ2100a	
	tag: FHM	$^{FHMr}H_2O + h\nu \rightarrow h\nu + {}^{FHMr}H + {}^{FHMr}OH$ + PTPFHMrOH + PTLFHMrH2O	tag_kJ2100a	
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2$ OH	tag_kJ2101	Sander et al. (2014)
	tag: FHM	$^{FHM}H_2O_2 + h\nu \rightarrow h\nu + 2.0\ {}^{FHM}OH$ + 2.0 PTPFHMOH	tag_kJ2101	
	tag: FHM	$^{FHMr}H_2O_2 + h\nu \rightarrow h\nu + 2.0\ {}^{FHMr}OH$ + 2.0 PTPFHMrOH	tag_kJ2101	
J3100	UpStGJN	$N_2O + h\nu \rightarrow$ 1. ProdO3N + 1. ProdO3 + $O(^1D)$ + N_2	jx(ip_N2O)	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow$ 1. ProdO3N + 1. ProdO3 + N + $O(^3P)$	jx(ip_NO)	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO2O)	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow$ 2. LossO3N + 2. LossO3 + NO + O_2	jx(ip_NOO2)	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N2O5)	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow NO + OH$	tag_kJ3200	Sander et al. (2014)
	tag: FHM	$^{FHM}HONO + h\nu \rightarrow h\nu + {}^{FHM}OH$ + PTPFHMOH	tag_kJ3200	
	tag: FHM	$^{FHMr}HONO + h\nu \rightarrow h\nu + {}^{FHMr}OH$ + PTPFHMrOH	tag_kJ3200	
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	tag_kJ3201	Sander et al. (2014)
	tag: FHM	$^{FHM}HNO_3 + h\nu \rightarrow h\nu + {}^{FHM}OH$ + PTPFHMOH	tag_kJ3201	
	tag: FHM	$^{FHMr}HNO_3 + h\nu \rightarrow h\nu + {}^{FHMr}OH$ + PTPFHMrOH	tag_kJ3201	
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow 0.333$ ProdO3N + 0.333 ProdO3 + 0.667 NO_2 + 0.667 HO_2 + 0.333 NO_3 + 0.333 OH	tag_kJ3202	Sander et al. (2014)
	tag: FHM	$^{FHM}HNO_4 + h\nu \rightarrow h\nu + 0.667\ {}^{FHM}HO_2 + 0.333\ {}^{FHM}OH$ + 0.333 PTPFHMOH	tag_kJ3202	
	tag: FHM	$^{FHMr}HNO_4 + h\nu \rightarrow h\nu + 0.667\ {}^{FHMr}HO_2 + 0.333\ {}^{FHMr}OH$ + 0.333 PTPFHMrOH	tag_kJ3202	
J41000	StTrGJ	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	tag_kJ41000	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3OOH + h\nu \rightarrow h\nu + {}^{FHM}CH_3O + {}^{FHM}OH$ + PTPFHMOH	tag_kJ41000	
	tag: FHM	$^{FHMr}CH_3OOH + h\nu \rightarrow h\nu + {}^{FHMr}CH_3O + {}^{FHMr}OH$ + PTPFHMrOH	tag_kJ41000	

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41001a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	tag_kJ41001a	Sander et al. (2014)
	tag: FHM	$^{FHM}HCHO + h\nu \rightarrow h\nu + {}^{FHM}H_2 + PTPFHMH2$	tag_kJ41001a	
	tag: FHM	$^{FHMr}HCHO + h\nu \rightarrow h\nu + {}^{FHMr}H_2 + PTPFHMrH2$	tag_kJ41001a	
J41001b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	tag_kJ41001b	Sander et al. (2014)
	tag: FHM	$^{FHM}HCHO + h\nu \rightarrow h\nu + {}^{FHM}H + {}^{FHM}HO_2$	tag_kJ41001b	
	tag: FHM	$^{FHMr}HCHO + h\nu \rightarrow h\nu + {}^{FHMr}H + {}^{FHMr}HO_2$	tag_kJ41001b	
J41002	StGJ	$CO_2 + h\nu \rightarrow$ 1. ProdO3C + 1. ProdO3 + CO + $O(^3P)$	jx(ip_CO2)	Sander et al. (2014)
J41003	StGJ	$CH_4 + h\nu \rightarrow$ 0.0864 ProdO3C + 0.0864 ProdO3 + 0.42 CH_3 + 0.62 H + 0.7912 H_2 + 0.0864 HCHO + 0.0864 $O(^3P)$ + 0.1584 OH + 0.1584 HO_2 + 0.2112 CO_2 + 0.1824 CO + 0.024 H_2O + 0.1 LCARBON	tag_kJ41003	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_4 + h\nu \rightarrow h\nu + 0.42\ {}^{FHM}CH_3 + 0.62\ {}^{FHM}H + 0.7912\ {}^{FHM}H_2$ + 0.7912 PTPFHMH2 + 0.0864 $^{FHM}HCHO$ + 0.1584 ^{FHM}OH + 0.1584 PTPFHMOH + 0.1584 $^{FHM}HO_2$ + 0.024 $^{FHM}H_2O$ + 0.024 PTPFHMH2O + PTLFHMCH4	tag_kJ41003	
	tag: FHM	$^{FHMr}CH_4 + h\nu \rightarrow h\nu + 0.42\ {}^{FHMr}CH_3 + 0.62\ {}^{FHMr}H + 0.7912\ {}^{FHMr}H_2$ + 0.7912 PTPFHMrH2 + 0.0864 $^{FHMr}HCHO$ + 0.1584 ^{FHMr}OH + 0.1584 PTPFHMrOH + 0.1584 $^{FHMr}HO_2$ + 0.024 $^{FHMr}H_2O$ + 0.024 PTPFHMrH2O + PTLFHMrCH4	tag_kJ41003	
J41004	StTrGJN	$CH_3ONO + h\nu \rightarrow CH_3O + NO$	tag_kJ41004	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3ONO + h\nu \rightarrow h\nu + {}^{FHM}CH_3O$	tag_kJ41004	
	tag: FHM	$^{FHMr}CH_3ONO + h\nu \rightarrow h\nu + {}^{FHMr}CH_3O$	tag_kJ41004	
J41005	StTrGJN	$CH_3ONO_2 + h\nu \rightarrow$ ProdO3C + ProdO3 + CH_3O + NO_2	tag_kJ41005	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3ONO_2 + h\nu \rightarrow h\nu + {}^{FHM}CH_3O$	tag_kJ41005	
	tag: FHM	$^{FHMr}CH_3ONO_2 + h\nu \rightarrow h\nu + {}^{FHMr}CH_3O$	tag_kJ41005	
J41006	StTrGJN	$CH_3O_2NO_2 + h\nu \rightarrow$ 1.333 ProdO3C + 1.333 ProdO3 + 0.667 NO_2 + 0.667 CH_3O_2 + 0.333 NO_3 + 0.333 CH_3O	tag_kJ41006	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3O_2NO_2 + h\nu \rightarrow h\nu + 0.667\ {}^{FHM}CH_3O_2 + 0.333\ {}^{FHM}CH_3O$	tag_kJ41006	
	tag: FHM	$^{FHMr}CH_3O_2NO_2 + h\nu \rightarrow h\nu + 0.667\ {}^{FHMr}CH_3O_2 + 0.333\ {}^{FHMr}CH_3O$	tag_kJ41006	
J41008	StTrGJ	$CH_3O_2 + h\nu \rightarrow HCHO + OH$	tag_kJ41008	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3O_2 + h\nu \rightarrow h\nu + {}^{FHM}HCHO + {}^{FHM}OH$ + PTPFHMOH	tag_kJ41008	
	tag: FHM	$^{FHMr}CH_3O_2 + h\nu \rightarrow h\nu + {}^{FHMr}HCHO + {}^{FHMr}OH$ + PTPFHMrOH	tag_kJ41008	

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41009	StTrGJ	$HCOOH + h\nu \rightarrow CO + HO_2 + OH$	tag_kJ41009	Sander et al. (2014)
	tag: FHM	$^{FHM}HCOOH + h\nu \rightarrow h\nu + {}^{FHM}HO_2 + {}^{FHM}OH + PTPFHMOH$	tag_kJ41009	
	tag: FHM	$^{FHMr}HCOOH + h\nu \rightarrow h\nu + {}^{FHMr}HO_2 + {}^{FHMr}OH + PTPFHMrOH$	tag_kJ41009	
J4200	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)
J4201	TrGJC	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	Sander et al. (2014)
J4202	TrGJC	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J4203	TrGJCN	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	von Kuhlmann (2001)
J4204	TrGJCN	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	Sander et al. (2014)
J4300	TrGJC	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)
J4301	TrGJC	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	Sander et al. (2014)
J4302	TrGJC	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note*
J4303	TrGJC	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	Sander et al. (2014)
J4304	TrGJC	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HCHO + OH$	jx(ip_CH3OOH)	see note*
J4306	TrGJCN	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*jx(ip_PAN)	von Kuhlmann et al. (2003)*
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	$Cl_2O_2 + h\nu \rightarrow 2.\ LossO3Cl + 2.\ LossO3 + 2\ Cl$	jx(ip_Cl2O2)	Sander et al. (2014)
J6101	StTrGJCl	$OClO + h\nu \rightarrow 1.\ ProdO3Cl + 1.\ ProdO3 + ClO + O(^3P)$	jx(ip_OClO)	Sander et al. (2014)
J6200	StGJCl	$HCl + h\nu \rightarrow Cl + H$	tag_kJ6200	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHM}HCl + h\nu \rightarrow h\nu + {}^{FHM}H$	tag_kJ6200	
	tag: FHM	$^{FHMr}HCl + h\nu \rightarrow h\nu + {}^{FHMr}H$	tag_kJ6200	
J6201	StTrGJCl	$HOCl + h\nu \rightarrow LossO3Cl + LossO3 + OH + Cl$	tag_kJ6201	Sander et al. (2014)
	tag: FHM	$^{FHM}HOCl + h\nu \rightarrow h\nu + {}^{FHM}OH + PTPFHMOH$	tag_kJ6201	
	tag: FHM	$^{FHMr}HOCl + h\nu \rightarrow h\nu + {}^{FHMr}OH + PTPFHMrOH$	tag_kJ6201	
J6300	TrGJClN	$ClNO_2 + h\nu \rightarrow 1.\ ProdO3Cl + 1.\ ProdO3 + Cl + NO_2$	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	$CH_3Cl + h\nu \rightarrow ProdLCl + Cl + CH_3$	tag_kJ6400	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3Cl + h\nu \rightarrow h\nu + {}^{FHM}CH_3$	tag_kJ6400	
	tag: FHM	$^{FHMr}CH_3Cl + h\nu \rightarrow h\nu + {}^{FHMr}CH_3$	tag_kJ6400	
J6401	StGJCl	$CCl_4 + h\nu \rightarrow 4.0\ ProdLCl + LCARBON + 4\ Cl$	jx(ip_CCl4)	Sander et al. (2014)
J6402	StGJCCl	$CH_3CCl_3 + h\nu \rightarrow 3\ LHYDROGEN + 3\ ProdLCl + 2\ LCARBON + 3\ Cl$	tag_kJ6402	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3CCl_3 + h\nu \rightarrow h\nu$	tag_kJ6402	
	tag: FHM	$^{FHMr}CH_3CCl_3 + h\nu \rightarrow h\nu$	tag_kJ6402	
J6500	StGJClF	$CFCl_3 + h\nu \rightarrow 3.0\ ProdLCl + LCARBON + LFLUORINE + 3\ Cl$	jx(ip_CFCl3)	Sander et al. (2014)
J6501	StGJClF	$CF_2Cl_2 + h\nu \rightarrow 2.0\ ProdLCl + LCARBON + 2\ LFLUORINE + 2\ Cl$	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	$HOBr + h\nu \rightarrow LossO3Br + LossO3 + Br + OH$	tag_kJ7200	Sander et al. (2014)
	tag: FHM	$^{FHM}HOBr + h\nu \rightarrow h\nu + {}^{FHM}OH + PTPFHMOH$	tag_kJ7200	
	tag: FHM	$^{FHMr}HOBr + h\nu \rightarrow h\nu + {}^{FHMr}OH + PTPFHMrOH$	tag_kJ7200	
J7300	TrGJBrN	$BrNO_2 + h\nu \rightarrow 1.\ ProdO3Br + 1.\ ProdO3 + Br + NO_2$	jx(ip_BrNO2)	Sander et al. (2014)
J7301	StTrGJBrN	$BrNO_3 + h\nu \rightarrow 5.9604645\times10^{-}8\ ProdO3Br + 5.9604645\times10^{-}8\ ProdO3 + .85\ Br + .85\ NO_3 + .15\ BrO + .15\ NO_2$	jx(ip_BrNO3)	Sander et al. (2014)*
J7400	StGJBr	$CH_3Br + h\nu \rightarrow ProdLBr + Br + CH_3$	tag_kJ7400	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3Br + h\nu \rightarrow h\nu + {}^{FHM}CH_3$	tag_kJ7400	
	tag: FHM	$^{FHMr}CH_3Br + h\nu \rightarrow h\nu + {}^{FHMr}CH_3$	tag_kJ7400	
J7401	TrGJBr	$CH_2Br_2 + h\nu \rightarrow 2\ LHYDROGEN + 2\ ProdSBr + LCARBON + 2\ Br$	tag_kJ7401	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_2Br_2 + h\nu \rightarrow h\nu$	tag_kJ7401	
	tag: FHM	$^{FHMr}CH_2Br_2 + h\nu \rightarrow h\nu$	tag_kJ7401	

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7402	TrGJBr	$CHBr_3 + h\nu \rightarrow$ LHYDROGEN + 3 ProdSBr + LCARBON + 3 Br	tag_kJ7402	Sander et al. (2014)
	tag: FHM	$^{FHM}CHBr_3 + h\nu \rightarrow h\nu$	tag_kJ7402	
	tag: FHM	$^{FHMr}CHBr_3 + h\nu \rightarrow h\nu$	tag_kJ7402	
J7500	StGJBrF	$CF_3Br + h\nu \rightarrow$ 1.0 ProdLBr + LCARBON + 3 LFLUORINE + Br	jx(ip_CF3Br)	Sander et al. (2014)
J7600	StTrGJBrCl	$BrCl + h\nu \rightarrow Br + Cl$	jx(ip_BrCl)	Sander et al. (2014)
J7601	StGJBrClF	$CF_2ClBr + h\nu \rightarrow$ 1.0 ProdLBr + 1.0 ProdLCl + LCARBON + 2 LFLUORINE + Br + Cl	jx(ip_CF2ClBr)	Sander et al. (2014)
J7602	TrGJBrCl	$CH_2ClBr + h\nu \rightarrow$ 2 LHYDROGEN + ProdSBr + ProdSCl + LCARBON + Br + Cl	tag_kJ7602	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_2ClBr + h\nu \rightarrow h\nu$	tag_kJ7602	
	tag: FHM	$^{FHMr}CH_2ClBr + h\nu \rightarrow h\nu$	tag_kJ7602	
J7603	TrGJBrCl	$CHCl_2Br + h\nu \rightarrow$ LHYDROGEN + ProdSBr + 2 ProdSCl + LCARBON + Br + 2 Cl	tag_kJ7603	Sander et al. (2014)
	tag: FHM	$^{FHM}CHCl_2Br + h\nu \rightarrow h\nu$	tag_kJ7603	
	tag: FHM	$^{FHMr}CHCl_2Br + h\nu \rightarrow h\nu$	tag_kJ7603	
J7604	TrGJBrCl	$CHClBr_2 + h\nu \rightarrow$ LHYDROGEN + 2 ProdSBr + ProdSCl + LCARBON + 2 Br + Cl	tag_kJ7604	Sander et al. (2014)
	tag: FHM	$^{FHM}CHClBr_2 + h\nu \rightarrow h\nu$	tag_kJ7604	
	tag: FHM	$^{FHMr}CHClBr_2 + h\nu \rightarrow h\nu$	tag_kJ7604	
J8401a	StTrGJI	$CH_3I + h\nu \rightarrow CH_3$	tag_kJ8401a	Sander et al. (2014)
	tag: FHM	$^{FHM}CH_3I + h\nu \rightarrow h\nu + {}^{FHM}CH_3$	tag_kJ8401a	
	tag: FHM	$^{FHMr}CH_3I + h\nu \rightarrow h\nu + {}^{FHMr}CH_3$	tag_kJ8401a	

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) → jx(ip_COH2)
J(12) → jx(ip_CHOH)
J(15) → jx(ip_HOCH2CHO)
J(18) → jx(ip_MACR)
J(22) → jx(ip_ACETOL)
J(23)+J(24) → jx(ip_MVK)
J(31)+J(32)+J(33) → jx(ip_GLYOX)
J(34) → jx(ip_MGLYOX)
J(41) → jx(ip_CH3OOH)
J(53) → J($iC_3H_7ONO_2$)
J(54) → J($iC_3H_7ONO_2$)
J(55) → J($iC_3H_7ONO_2$)
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 Sander et al. (2011) for $\lambda > 300$nm and used here for the entire spectrum.

Table 3: Henry's law coefficients

substance	$\frac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\frac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^{5}$	6338.	Lind and Kok (1994)
H_2O	BIG	0.	see note
NH_3	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
N_2O_5	BIG	0.	see note
HONO	4.9×10^{1}	4780.	Schwartz and White (1981)
HNO_3	$2.45\times10^{6}/1.5\times10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3OH	2.20×10^{2}	5200.	Snider and Dawson (1985)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CH_3COOH	4.1×10^{3}	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
$C_2H_5O_2$	6.	5600.	see note
CH_3CHO	1.29×10^{1}	5890.	Sander et al. (2006)
CH_3COCH_3	28.1	5050.	Sander et al. (2006)
MGLYOX	3.70×10^{3}	7500.	Betterton and Hoffmann (1988)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.6×10^{2}	5862.	Huthwelker et al. (1995)
$ClNO_3$	BIG	0.	see note
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	1.3×10^{3}	5862.	Blatchley et al. (1992)*

Table 3: Henry's law coefficients (... continued)

substance	$\frac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\frac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	reference
$BrNO_3$	BIG	0.	see note
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
CH_3SO_3H	BIG	0.	see note
DMS	5.4×10^{-1}	3500.	Staudinger and Roberts (2001)
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*
LMEKOOH	$1.\times10^{3}$	0.	???
CH_3COCH_2OH	4.7×10^{2}	0.	???

General notes

The value "BIG" corresponds to virtually infinite solubility which is represented in the model using a very large but arbitrary number.

The temperature dependence of the Henry constants is:

$$K_{\mathrm{H}} = K_{\mathrm{H}}^{\ominus} \times \exp\left(\frac{-\Delta_{\mathrm{soln}}H}{R}\left(\frac{1}{T} - \frac{1}{T^{\ominus}}\right)\right)$$

where $\Delta_{\mathrm{soln}}H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314$ J/(mol K).

Specific notes

NO_2: The temperature dependence is from Chameides (1984).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

$C_2H_5O_2$: Assumed to be the same as $K_{\mathrm{H}}(CH_3O_2)$.

HBr: Calculated using the acidity constant from Lax (1969).

HOBr: Twice the value of HOCl, according to Blatchley et al. (1992). Same temperature dependence as for HOCl assumed.

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO_2	0.5	(default)	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
H_2O	0.0	(default)	see note
NH_3	0.06	(default)	DeMore et al. (1997)*
NO	5.0×10^{-5}	(default)	Saastad et al. (1993)*
NO_2	0.0015	(default)	Ponche et al. (1993)*
NO_3	0.04	(default)	Rudich et al. (1996)*
N_2O_5	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO_3	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO_4	(default)	(default)	DeMore et al. (1997)*
CH_3OH	(default)	(default)	see note
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
CO_2	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH_3COOH	2.0×10^{-2}	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
$C_2H_5O_2$	(default)	(default)	see note
CH_3CHO	3.0×10^{-2}	(default)	see note
CH_3COCH_3	3.72×10^{-3}	6395.	Davidovits et al. (1995)
MGLYOX	(default)	(default)	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
$ClNO_3$	0.108	(default)	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	(default)	Deiber et al. (2004)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
BrCl	0.038	6546.	see note
SO_2	0.11	(default)	DeMore et al. (1997)
H_2SO_4	0.65	(default)	Pöschl et al. (1998)*
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)
LMEKOOH	(default)	(default)	???
CH_3COCH_2OH	(default)	(default)	???

General notes

If no data are available, the following default values are used:
$\alpha^{\ominus} = 0.1$
$-\Delta_{\mathrm{obs}}H/R = 0$ K

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\begin{aligned} \frac{\alpha}{1-\alpha} &= \exp\left(\frac{-\Delta_{\mathrm{obs}}G}{RT}\right) \\ &= \exp\left(\frac{-\Delta_{\mathrm{obs}}H}{RT} + \frac{\Delta_{\mathrm{obs}}S}{R}\right) \end{aligned}$$

where $\Delta_{\mathrm{obs}}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\mathrm{obs}}H$ and $\Delta_{\mathrm{obs}}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R} \times \frac{1}{T} + \frac{-\Delta_{\mathrm{obs}}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right) \Big/ \mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R}$$

Specific notes

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NH_3: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

N_2O_5: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

CO_2: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

$C_2H_5O_2$: Estimate.

CH_3CHO: Using the same estimate as in the CAPRAM 2.4 model (`http://projects.tropos.de/capram/capram_24.html`).

HCl: Temperature dependence derived from published data at 2 different temperatures

HOCl: Assumed to be the same as α(HOBr).

$ClNO_3$: Value measured at 274.5 K.

HBr: Temperature dependence derived from published data at 2 different temperatures

HOBr: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

$BrNO_3$: Value measured at 273 K.

BrCl: Assumed to be the same as $\alpha(Cl_2)$.

H_2SO_4: Value measured at 303 K.

Table 5: 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 the file `messy_mecca_aero.f90` using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry's law constants in subroutine `mecca_aero_henry`.

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 $5{\times}10^2$ 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 $5{\times}10^2$. The ratio $5{\times}10^2/3{\times}10^5$ 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 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow$ LossO3N + LossO3 + 2 HNO_3	tag_kHET200	see general notes*
	tag: FHM	$^{FHM}H_2O + N_2O_5 \rightarrow N_2O_5 + 2.0\ ^{FHM}HNO_3$ + PTLFHMH2O	tag_kHET200	
	tag: FHM	$^{FHMr}H_2O + N_2O_5 \rightarrow N_2O_5 + 2.0\ ^{FHMr}HNO_3$ + PTLFHMrH2O	tag_kHET200	
HET201	TrHetN	$N_2O_5 \rightarrow$ 3. LossO3N + 3. LossO3 + 2 NO_3^-(aq) + 2 H^+(aq)	khet_Tr(iht_N2O5)	see general notes*
HET410	StHetCl	$HOCl + HCl \rightarrow$ LossO3Cl + LossO3 + $Cl_2 + H_2O$	tag_kHET410	see general notes*
	tag: FHM	$^{FHM}HOCl + HCl \rightarrow HCl + 0.5\ ^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kHET410	
	tag: FHM	$^{FHMr}HOCl + HCl \rightarrow HCl + 0.5\ ^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kHET410	
	tag: FHM	$^{FHM}HCl + HOCl \rightarrow HOCl + 0.5\ ^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kHET410	
	tag: FHM	$^{FHMr}HCl + HOCl \rightarrow HOCl + 0.5\ ^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kHET410	
HET420	StHetClN	$ClNO_3 + HCl \rightarrow$ LossO3Cl + LossO3 + $Cl_2 + HNO_3$	tag_kHET420	see general notes*
	tag: FHM	$^{FHM}HCl + ClNO_3 \rightarrow ClNO_3 + {}^{FHM}HNO_3$	tag_kHET420	
	tag: FHM	$^{FHMr}HCl + ClNO_3 \rightarrow ClNO_3 + {}^{FHMr}HNO_3$	tag_kHET420	
HET421	StHetClN	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	tag_kHET421	see general notes*
	tag: FHM	$^{FHM}H_2O + ClNO_3 \rightarrow ClNO_3 + {}^{FHM}HOCl + {}^{FHM}HNO_3$ + PTLFHMH2O	tag_kHET421	
	tag: FHM	$^{FHMr}H_2O + ClNO_3 \rightarrow ClNO_3 + {}^{FHMr}HOCl + {}^{FHMr}HNO_3$ + PTLFHMrH2O	tag_kHET421	
HET422	StHetClN	$N_2O_5 + HCl \rightarrow$ LossO3Cl + LossO3N + 2 LossO3 + $ClNO_2$ + HNO_3	tag_kHET422	see general notes*
	tag: FHM	$^{FHM}HCl + N_2O_5 \rightarrow N_2O_5 + {}^{FHM}HNO_3$	tag_kHET422	
	tag: FHM	$^{FHMr}HCl + N_2O_5 \rightarrow N_2O_5 + {}^{FHMr}HNO_3$	tag_kHET422	
HET510	StHetBr	$HOBr + HBr \rightarrow$ LossO3Br + LossO3 + $Br_2 + H_2O$	tag_kHET510	see general notes*
	tag: FHM	$^{FHM}HOBr + HBr \rightarrow HBr + 0.5\ ^{FHM}H_2O$ + 0.5 PTPFHMH2O	tag_kHET510	
	tag: FHM	$^{FHMr}HOBr + HBr \rightarrow HBr + 0.5\ ^{FHMr}H_2O$ + 0.5 PTPFHMrH2O	tag_kHET510	

Table 6: Heterogeneous reactions (... continued)

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHM}HBr + HOBr \rightarrow HOBr + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kHET510	
	tag: FHM	$^{FHMr}HBr + HOBr \rightarrow HOBr + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kHET510	
HET520	StHetBrN	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	tag_kHET520	see general notes*
	tag: FHM	$^{FHM}H_2O + BrNO_3 \rightarrow BrNO_3 + {}^{FHM}HOBr + {}^{FHM}HNO_3$ + PTLFHMH2O	tag_kHET520	
	tag: FHM	$^{FHMr}H_2O + BrNO_3 \rightarrow BrNO_3 + {}^{FHMr}HOBr + {}^{FHMr}HNO_3$ + PTLFHMrH2O	tag_kHET520	
HET540	StHetBrClN	$ClNO_3 + HBr \rightarrow 0.5$ LossO3Br + 0.5 LossO3Cl + LossO3 + BrCl + HNO_3	tag_kHET540	see general notes*
	tag: FHM	$^{FHM}HBr + ClNO_3 \rightarrow ClNO_3 + {}^{FHM}HNO_3$	tag_kHET540	
	tag: FHM	$^{FHMr}HBr + ClNO_3 \rightarrow ClNO_3 + {}^{FHMr}HNO_3$	tag_kHET540	
HET541	StHetBrClN	$BrNO_3 + HCl \rightarrow 0.5$ LossO3Br + 0.5 LossO3Cl + LossO3 + BrCl + HNO_3	tag_kHET541	see general notes*
	tag: FHM	$^{FHM}HCl + BrNO_3 \rightarrow BrNO_3 + {}^{FHM}HNO_3$	tag_kHET541	
	tag: FHM	$^{FHMr}HCl + BrNO_3 \rightarrow BrNO_3 + {}^{FHMr}HNO_3$	tag_kHET541	
HET542	StHetBrCl	$HOCl + HBr \rightarrow 0.5$ LossO3Br + 0.5 LossO3Cl + LossO3 + BrCl + H_2O	tag_kHET542	see general notes*
	tag: FHM	$^{FHM}HOCl + HBr \rightarrow HBr + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kHET542	
	tag: FHM	$^{FHMr}HOCl + HBr \rightarrow HBr + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kHET542	
	tag: FHM	$^{FHM}HBr + HOCl \rightarrow HOCl + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kHET542	
	tag: FHM	$^{FHMr}HBr + HOCl \rightarrow HOCl + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kHET542	
HET543	StHetBrCl	$HOBr + HCl \rightarrow 0.5$ LossO3Br + 0.5 LossO3Cl + LossO3 + BrCl + H_2O	tag_kHET543	see general notes*
	tag: FHM	$^{FHM}HOBr + HCl \rightarrow HCl + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kHET543	
	tag: FHM	$^{FHMr}HOBr + HCl \rightarrow HCl + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	tag_kHET543	
	tag: FHM	$^{FHM}HCl + HOBr \rightarrow HOBr + 0.5\ ^{FHM}H_2O + 0.5$ PTPFHMH2O	tag_kHET543	

Table 6: Heterogeneous reactions (... continued)

#	labels	reaction	rate coefficient	reference
	tag: FHM	$^{FHMr}HCl + HOBr \rightarrow HOBr + 0.5\ ^{FHMr}H_2O + 0.5$ PTPFHMrH2O	`tag_kHET543`	

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 7: Acid-base and other equilibria

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

Specific notes

Table 8: Aqueous phase reactions

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

Specific notes

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