The Chemical Mechanism of MECCA

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Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.2E-11*EXP(70./temp)`	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2003)
G1002	StG	$O_3 + O(^1D) \rightarrow 2\ O_2$	`1.2E-10`	Sander et al. (2003)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2\ O_2$	`8.E-12*EXP(-2060./temp)`	Sander et al. (2003)
G01Diag	DiagG	$O_3(s) \rightarrow LO_3(s)$	`k_O3s`	Roelofs and Lelieveld (1997)*
G2100	StTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,5.7E-32,1.6,7.5E-11,0.,0.6)`	Sander et al. (2003)
G2101	StG	$H + O_3 \rightarrow OH$	`1.4E-10*EXP(-470./temp)`	Sander et al. (2003)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	`1.1E-10`	Sander et al. (2003)
G2103	StG	$OH + O(^3P) \rightarrow H$	`2.2E-11*EXP(120./temp)`	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	`5.5E-12*EXP(-2000./temp)`	Sander et al. (2003)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH$	`3.E-11*EXP(200./temp)`	Sander et al. (2003)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	`1.E-14*EXP(-490./temp)`	Sander et al. (2003)
G2108a	StG	$HO_2 + H \rightarrow 2\ OH$	`0.69*8.1E-11`	Sander et al. (2003)*
G2108b	StG	$HO_2 + H \rightarrow H_2$	`0.29*8.1E-11`	Sander et al. (2003)*
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	`0.02*8.1E-11`	Sander et al. (2003)*
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	`4.8E-11*EXP(250./temp)`	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`2.2E-10`	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`2.9E-12*EXP(-160./temp)`	Sander et al. (2003)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	`1.5E-11*EXP(-3600./temp)`	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`1.8E-11*EXP(110./temp)`	Sander et al. (2003)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2\ NO$	`6.7E-11`	Sander et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.9E-11	Sander et al. (2003)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2003)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Sander et al. (2003)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.6E-12*EXP(180./temp)	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2003)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./temp)	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(3.E-27*EXP(10990./temp))	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.E-31,2.6,3.6E-11,0.1, 0.6)	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,2.E-30,3.,2.5E-11,0., 0.6)	Sander et al. (2003)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2003)
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./temp))	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2003)
G4100	StG	$CH_4 + O(^1D) \rightarrow .75\ CH_3O_2 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	1.5E-10	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*log(temp)-987./temp)	Atkinson (2003)*
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	7.3E-12*EXP(-620./temp)	Sander et al. (2003)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	4.1E-13*EXP(750./temp)/(1.+1./ 497.7*EXP(1160./temp))	Sander et al. (2003)*
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	4.1E-13*EXP(750./temp)/(1.+ 497.7*EXP(-1160./temp))	Sander et al. (2003)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2003)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
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. (2003)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH$	9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2003)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2003)*

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

#	labels	reaction	rate coefficient	reference
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*log(temp)+636./temp)`	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2003)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	`1.57E-13 + cair*3.54E-33`	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	`4.E-13`	Sander et al. (2003)
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	$C_2H_4 + O_3 \rightarrow HCHO + .22\ HO_2 + .12\ OH + .23\ CO + .54\ HCOOH + .1\ H_2$	`1.2E-14*EXP(-2630./temp)`	Sander et al. (2003)*
G4202	TrGC	$C_2H_4 + OH \rightarrow .6666667\ CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,1.E-28,0.8,8.8E-12,0.,0.6)`	Sander et al. (2003)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	`7.5E-13*EXP(700./temp)`	Sander et al. (2003)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	`2.6E-12*EXP(365./temp)`	Sander et al. (2003)
G4205	TrGNC	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	`2.3E-12`	Atkinson et al. (1999)
G4206	TrGC	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	`1.6E-13*EXP(195./temp)`	see note
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	`k_CH3OOH_OH`	see note
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	`5.6E-12*EXP(270./temp)`	Sander et al. (2003)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2003)
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2$	`4.E-13*EXP(200./temp)`	Sander et al. (2003)
G4211a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	`4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))`	Tyndall et al. (2001)
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	`4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))`	Tyndall et al. (2001)
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	`8.1E-12*EXP(270./temp)`	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow PAN$	`k_PA_NO2`	Tyndall et al. (2001)
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2$	`4.E-12`	Canosa-Mas et al. (1996)
G4215a	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	`0.9*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO + CO_2$	`0.1*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	`4.9E-12*EXP(211./temp)`	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	`2.5E-12*EXP(500./temp)`	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	`k_CH3OOH_OH`	see note
G4219	TrGNC	$NACA + OH \rightarrow NO_2 + HCHO + CO$	`5.6E-12*EXP(270./temp)`	see note
G4220	TrGNC	$PAN + OH \rightarrow HCHO + NO_2$	`2.E-14`	see note
G4221	TrGNC	$PAN \rightarrow CH_3C(O)OO + NO_2$	`k_PAN_M`	Sander et al. (2003)*
G4300	TrGC	$C_3H_8 + OH \rightarrow .82\ C_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	`1.65E-17*temp*temp*EXP(-87./temp)`	Atkinson (2003)

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

#	labels	reaction	rate coefficient	reference
G4301	TrGC	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ CH_3COCHO + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	`6.5E-15*EXP(-1900./temp)`	Sander et al. (2003)*
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)`	Atkinson et al. (1999)
G4303	TrGNC	$C_3H_6 + NO_3 \rightarrow ONIT$	`4.6E-13*EXP(-1155./temp)`	Atkinson et al. (1999)
G4304	TrGC	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	`k_PrO2_HO2`	Atkinson (1997)*
G4305	TrGNC	$C_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	`k_PrO2_NO`	Atkinson et al. (1999)*
G4306	TrGC	$C_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	`k_PrO2_CH3O2`	Kirchner and Stockwell (1996)
G4307	TrGC	$C_3H_7OOH + OH \rightarrow .3\ C_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	`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	TrGNC	$CH_3CH(O_2)CH_2OH + NO \rightarrow .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ ONIT$	`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. (2003)
G4312	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001)
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	`2.9E-12*EXP(300./temp)`	Sander et al. (2003)
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ CH_3COCHO + .5\ CH_3OH + .3\ CH_3C(O)OO + .8\ HCHO + .3\ HO_2 + .2\ CH_3COCH_2OH$	`7.5E-13*EXP(500./temp)`	Tyndall et al. (2001)
G4315	TrGC	$CH_3COCH_2O_2H + OH \rightarrow .3\ CH_3COCH_2O_2 + .7\ CH_3COCHO + .7\ OH$	`k_CH3OOH_OH`	see note
G4316	TrGC	$CH_3COCH_2OH + OH \rightarrow CH_3COCHO + HO_2$	`3.E-12`	Atkinson et al. (1999)
G4317	TrGC	$CH_3COCHO + OH \rightarrow CH_3C(O)OO + CO$	`8.4E-13*EXP(830./temp)`	Tyndall et al. (1995)
G4318	TrGNC	$MPAN + OH \rightarrow CH_3COCH_2OH + NO_2$	`3.2E-11`	Orlando et al. (2002)
G4319	TrGNC	$MPAN \rightarrow MVKO2 + NO_2$	`k_PAN_M`	see note
G4320	TrGNC	$C_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	`6.2E-13*EXP(-230./temp)`	Atkinson et al. (1999)
G4400	TrGC	$C_4H_{10} + OH \rightarrow C_4H_9O_2 + H_2O$	`1.81E-17*temp*temp*EXP(114./temp)`	Atkinson (2003)
G4401	TrGC	$C_4H_9O_2 + CH_3O_2 \rightarrow .88\ CH_3COC_2H_5 + .68\ HCHO + 1.23\ HO_2 + .12\ CH_3CHO + .12\ C_2H_5O_2 + .18\ CH_3OH$	`k_PrO2_CH3O2`	see note
G4402	TrGC	$C_4H_9O_2 + HO_2 \rightarrow C_4H_9OOH$	`k_PrO2_HO2`	see note

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

#	labels	reaction	rate coefficient	reference
G4403	TrGNC	$C_4H_9O_2$ + NO → .84 NO_2 + .56 $CH_3COC_2H_5$ + .56 HO_2 + .28 $C_2H_5O_2$ + .84 CH_3CHO + .16 ONIT	k_PrO2_NO	see note
G4404	TrGC	C_4H_9OOH + OH → .15 $C_4H_9O_2$ + .85 $CH_3COC_2H_5$ + .85 OH + .85 H_2O	k_CH3OOH_OH	see note
G4405	TrGC	MVK + O_3 → .45 HCOOH + .9 CH_3COCHO + .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 → MVKOOH	1.82E-13*EXP(1300./temp)	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO → NO_2 + .25 $CH_3C(O)OO$ + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 CH_3COCHO	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO_2 → 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 → .5 CH_3COCHO + .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 + CH_3COCHO + .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	$CH_3COC_2H_5$ + OH → MEKO2	1.3E-12*EXP(-25./temp)	Atkinson et al. (1999)
G4414	TrGC	MEKO2 + HO_2 → MEKOOH	k_PrO2_HO2	see note
G4415	TrGNC	MEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 ONIT	k_PrO2_NO	see note
G4416	TrGC	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	k_CH3OOH_OH	see note
G4417	TrGNC	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	ISOP + O_3 → .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	ISOP + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO_3 → 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	TrGNC	ISO2 + NO → .88 NO_2 + .88 MVK + .88 HCHO + .88 HO_2 + .12 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)*

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#	labels	reaction	rate coefficient	reference
G4505	TrGC	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .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	TrGNC	ISON + OH → CH_3COCH_2OH + NACA	1.3E-11	Pöschl et al. (2000)
G6100	StTrGCl	Cl + O_3 → ClO	2.3E-11*EXP(-200./temp)	Sander et al. (2003)
G6101	StGCl	ClO + O(^{3}P) → Cl	3.E-11*EXP(70./temp)	Sander et al. (2003)
G6102	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Atkinson et al. (2005)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(1.27E-27*EXP(8744./temp))	Sander et al. (2003)*
G6200	StGCl	Cl + H_2 → HCl + H	3.7E-11*EXP(-2300./temp)	Sander et al. (2003)
G6201a	StGCl	Cl + HO_2 → HCl	1.8E-11*EXP(170./temp)	Sander et al. (2003)
G6201b	StGCl	Cl + HO_2 → ClO + OH	4.1E-11*EXP(-450./temp)	Sander et al. (2003)
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	1.1E-11*EXP(-980./temp)	Sander et al. (2003)
G6203a	StGCl	ClO + OH → Cl + HO_2	7.4E-12*EXP(270./temp)	Sander et al. (2003)
G6203b	StGCl	ClO + OH → HCl	6.E-13*EXP(230./temp)	Sander et al. (2003)
G6204	StTrGCl	ClO + HO_2 → HOCl	2.7E-12*EXP(220./temp)	Sander et al. (2003)
G6205	StTrGCl	HCl + OH → Cl + H_2O	2.6E-12*EXP(-350./temp)	Sander et al. (2003)
G6206	StGCl	HOCl+ OH → ClO + H_2O	3.E-12*EXP(-500./temp)	Sander et al. (2003)
G6300	StTrGNCl	ClO + NO → NO_2 + Cl	6.4E-12*EXP(290./temp)	Sander et al. (2003)
G6301	StTrGNCl	ClO + NO_2 → $ClNO_3$	k_3rd(temp,cair,1.8E-31,3.4,1.5E-11, 1.9,0.6)	Sander et al. (2003)
G6303	StGNCl	$ClNO_3$ + O(^{3}P) → ClO + NO_3	2.9E-12*EXP(-800./temp)	Sander et al. (2003)
G6304	StTrGNCl	$ClNO_3$ + Cl → Cl_2 + NO_3	6.5E-12*EXP(135./temp)	Sander et al. (2003)
G6400	StTrGCl	Cl + CH_4 → HCl + CH_3O_2	9.6E-12*EXP(-1360./temp)	Sander et al. (2003)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO_2	8.1E-11*EXP(-30./temp)	Sander et al. (2003)
G6402	StTrGCl	Cl + CH_3OOH → CH_3O_2 + HCl	5.7E-11	Sander et al. (2003)
G6403	StTrGCl	ClO + CH_3O_2 → HO_2 + Cl + HCHO	3.3E-12*EXP(-115./temp)	Sander et al. (2003)
G6404	StGCl	CCl_4 + O(^{1}D) → ClO + 3 Cl	3.3E-10	Sander et al. (2003)
G6405	StGCl	CH_3Cl + O(^{1}D) → OH + Cl	1.65E-10	Sander et al. (2003)*
G6406	StGCl	CH_3Cl + OH → H_2O + Cl	2.4E-12*EXP(-1250./temp)	Sander et al. (2003)
G6407	StGCCl	CH_3CCl_3 + O(^{1}D) → OH + 3 Cl	3.E-10	Sander et al. (2003)*
G6408	StTrGCCl	CH_3CCl_3 + OH → H_2O + 3 Cl	1.6E-12*EXP(-1520./temp)	Sander et al. (2003)
G6500	StGFCl	CF_2Cl_2 + O(^{1}D) → ClO + Cl	1.4E-10	Sander et al. (2003)
G6501	StGFCl	$CFCl_3$ + O(^{1}D) → ClO + 2 Cl	2.3E-10	Sander et al. (2003)
G7100	StTrGBr	Br + O_3 → BrO	1.7E-11*EXP(-800./temp)	Sander et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G7101	StGBr	$BrO + O(^3P) \rightarrow Br + O_2$	`1.9E-11*EXP(230./temp)`	Sander et al. (2003)
G7102a	StTrGBr	$BrO + BrO \rightarrow Br + Br$	`2.4E-12*EXP(40./temp)`	Sander et al. (2003)
G7102b	StTrGBr	$BrO + BrO \rightarrow Br_2$	`2.8E-14*EXP(869./temp)`	Sander et al. (2003)
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr$	`1.5E-11*EXP(-600./temp)`	Sander et al. (2003)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr$	`3.4E-12*EXP(540./temp)`	Sander et al. (2003)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	`1.1E-11`	Sander et al. (2003)
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	`1.2E-10*EXP(-430./temp)`	Sander et al. (2003)
G7301	StTrGNBr	$BrO + NO \rightarrow Br + NO_2$	`8.8E-12*EXP(260./temp)`	Sander et al. (2003)
G7302	StTrGNBr	$BrO + NO_2 \rightarrow BrNO_3$	`k_BrO_NO2`	Sander et al. (2003)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	`1.7E-11*EXP(-800./temp)`	Sander et al. (2003)
G7403	StTrGBr	$CH_3Br + OH \rightarrow H_2O + Br$	`2.35E-12*EXP(-1300./temp)`	Sander et al. (2003)
G7603a	StTrGClBr	$BrO + ClO \rightarrow Br + OClO$	`9.5E-13*EXP(550./temp)`	Sander et al. (2003)
G7603b	StTrGClBr	$BrO + ClO \rightarrow Br + Cl$	`2.3E-12*EXP(260./temp)`	Sander et al. (2003)
G7603c	StTrGClBr	$BrO + ClO \rightarrow BrCl$	`4.1E-13*EXP(290./temp)`	Sander et al. (2003)
G9200	TrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	`k_3rd(temp,cair,3.E-31,3.3,1.5E-12,0.,0.6)`	Sander et al. (2003)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2003)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`	Atkinson et al. (2003)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2003)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	`1.9E13*EXP(-8661./temp)`	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	`3.E-13`	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	`5.E-11`	Barone et al. (1995)

*Notes:

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

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

G1002: path leading to 2 $O(^3P)$ + O_2 neglected

G01Diag: `k_O3s = (1.7E-12 * EXP(-940./temp)) * C(KPP_OH) + (1.E-14 * EXP(-490./temp)) * C(KPP_HO2) + J_O1D * 2.2E-10 * C(KPP_H2O) / ( 3.2E-11 * EXP(70./temp) * C(KPP_O2) + 1.8E-11 * EXP(110./temp) * C(KPP_N2) + 2.2E-10 * C(KPP_H2O) )`

G2108: branching ratio from Hack et al., see note B5 of Sander et al. (2003)

G2110: The rate coefficient is: `k_HO2_HO2 = (1.5E-12 * EXP(19./temp)+1.7E-33 * EXP(1000./temp) * cair) * (1.+1.4E-21 * EXP(2200./temp) * C(KPP_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984)

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.

G3203: The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./(6.5E-34 * EXP(1335./temp) * cair) + 1./(2.7E-17 * EXP(2199./temp)) )`

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

G4103: product distribution is from Elrod et al. (2001)

G4107: The rate coefficient is: `k_CH3OOH_OH = 3.8E-12 * EXP(200./temp)`

G4109: same temperature dependence assumed as for CH_3CHO+NO_3

G4201: product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))

G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH_3OO and C_2H_5OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: same value as for G4107: CH_3OOH+OH assumed

G4213: The rate coefficient is: `k_PA_NO2 = k_3rd(temp,cair,8.5E-29,6.5,1.1E-11,1.,0.6)`.

G4216: `1.0E-11` from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)

G4218: same value as for G4107: CH_3OOH+OH assumed

G4219: according to Pöschl et al. (2000), the same value as for CH_3CHO+OH can be assumed

G4220: 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001)

G4221: The rate coefficient is: `k_PAN_M = k_PA_NO2/9.E-29 * EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G4301: product distribution is for terminal olefin carbons from Zaveri and Peters (1999)

G4304: The rate coefficient is: `k_PrO2_HO2 = 1.9E-13 * EXP(1300./temp)`. Value for generic RO_2 + HO_2 reaction from Atkinson (1997) is used.

G4305: The rate coefficient is: `k_PrO2_NO = 2.7E-12 * EXP(360./temp)`

G4306: The rate coefficient is: `k_PrO2_CH3O2 = 9.46E-14 * EXP(431./temp)`. The product distribution is from von Kuhlmann (2001).

G4307: same value as for G4107: CH_3OOH+OH assumed

G4309: products are from von Kuhlmann (2001)

G4315: same value as for G4107: CH_3OOH+OH assumed

G4319: same value as for PAN assumed

G4401: same value as for propyl group assumed (`k_PrO2_CH3O2`)

G4402: same value as for propyl group assumed (`k_PrO2_HO2`)

G4403: same value as for propyl group assumed (`k_PrO2_NO`)

G4404: same value as for G4107: CH_3OOH+OH assumed

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

G4414: same value as for propyl group assumed (`k_PrO2_HO2`)

G4415: same value as for propyl group assumed (`k_PrO2_NO`)

G4416: same value as for G4107: CH_3OOH+OH assumed

G4417: value for $C_4H_9ONO_2$ used here

G4503: same temperature dependence assumed as for other RO_2+HO_2 reactions

G4504: Yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).

G6102: The rate coefficient is: `k_ClO_ClO = k_3rd_iupac(temp,cair,2.E-32,4.,1.E-11,0.,0.45)`.

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.

G6405: average of reactions with CH_3Br and CH_3F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

G6407: extrapolated from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

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

G8101: This value was assumed by Jimenez et al. (2003).

G9400a: Abstraction path. The assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

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

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

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

G9400b: Addition path. The rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(KPP_O2) / (1.+5.0E-30*EXP(6280./temp)*C(KPP_O2))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	J_O2	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	J_O1D	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	J_O3P	see note
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	J_H2O	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	J_H2O2	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	J_N2O	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	J_NO2	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	J_NO	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	J_NO2O	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	J_NOO2	see note
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	J_N2O5	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	J_HONO	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	J_HNO3	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	J_HNO4	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	J_CH3OOH	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	J_COH2	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	J_CHOH	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	J_CO2	see note
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	J_CH3OOH	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	J_CH3CHO	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	J_PAA	see note
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*J_CHOH	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	J_PAN	see note
J4300	TrGCJ	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	J_CH3OOH	see note
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	J_CH3COCH3	see note
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*J_CHOH	see note
J4303	TrGCJ	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	J_CH3COCHO	see note
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	J_CH3OOH	see note
J4305	TrGNCJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	J_PAN	see note
J4306	TrGNCJ	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*J_PAN	see note
J4400	TrGCJ	$C_4H_9OOH + h\nu \rightarrow OH + .67\ CH_3COC_2H_5 + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	J_CH3OOH	see note
J4401	TrGCJ	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	0.019*J_COH2+.015*J_CH3COCHO	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4402	TrGCJ	MVKOOH + hν → OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	J_CH3OOH	see note
J4403	TrGCJ	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*J_CHOH	see note
J4404	TrGCJ	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	J_CH3OOH	see note
J4405	TrGCJ	MeCOCO + hν → 2 $CH_3C(O)OO$	2.15*J_CH3COCHO	see note
J4406	TrGNCJ	ONIT + hν → NO_2 + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	3.7*J_PAN	see note
J4500	TrGCJ	ISOOH + hν → MVK + HCHO + HO_2 + OH	J_CH3OOH	see note
J4501	TrGNCJ	ISON + hν → MVK + HCHO + NO_2 + HO_2	3.7*J_PAN	see note
J6000	StTrGClJ	Cl_2 + hν → Cl + Cl	J_Cl2	see note
J6100	StTrGClJ	Cl_2O_2 + hν → 2 Cl	1.4*J_Cl2O2	see note
J6101	StTrGClJ	OClO + hν → ClO + O(^{3}P)	J_OClO	see note
J6200	StGClJ	HCl + hν → Cl + H	J_HCl	see note
J6201	StTrGClJ	HOCl + hν → OH + Cl	J_HOCl	see note
J6301	StTrGNClJ	$ClNO_3$ + hν → Cl + NO_3	J_ClNO3	see note
J6400	StGClJ	CH_3Cl + hν → Cl + CH_3O_2	J_CH3Cl	see note
J6401	StGClJ	CCl_4 + hν → 4 Cl	J_CCl4	see note
J6402	StGCClJ	CH_3CCl_3 + hν → 3 Cl	J_CH3CCl3	see note
J6500	StGFClJ	$CFCl_3$ + hν → 3 Cl	J_CFCl3	see note
J6501	StGFClJ	CF_2Cl_2 + hν → 2 Cl	J_CF2Cl2	see note
J7000	StTrGBrJ	Br_2 + hν → Br + Br	J_Br2	see note
J7200	StTrGBrJ	HOBr + hν → Br + OH	J_HOBr	see note
J7301	StTrGNBrJ	$BrNO_3$ + hν → Br + NO_3	J_BrNO3	see note
J7400	StGBrJ	CH_3Br + hν → Br + CH_3O_2	J_CH3Br	see note
J7500	StGFBrJ	CF_3Br + hν → Br	J_CF3Br	see note
J7600	StTrGClBrJ	BrCl + hν → Br + Cl	J_BrCl	see note
J7601	StGFBrJ	CF_2ClBr + hν → Br + Cl	J_CF2ClBr	see note

*Notes: J-values are calculated with an external module and then supplied to the MECCA chemistry

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the Cl_2O_2 formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed Cl_2O_2/ClO ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the Cl_2O_2 formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

Table 3: PSC reactions

#	labels	reaction	rate coefficient	reference
PSC200	StPscN	$N_2O_5 + H_2O \rightarrow HNO_3 + HNO_3$	`khet_N2O5_H2O`	see note
PSC410	StPscCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_HOCl_HCl`	see note
PSC420	StPscNCl	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_ClNO3_HCl`	see note
PSC421	StPscNCl	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_ClNO3_H2O`	see note
PSC510	StPscBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_HOBr_HBr`	see note
PSC520	StPscNBr	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_BrNO3_H2O`	see note
PSC540	StPscNClBr	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_ClNO3_HBr`	see note
PSC541	StPscNClBr	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_BrNO3_HCl`	see note
PSC542	StPscClBr	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_HOCl_HBr`	see note
PSC543	StPscClBr	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_HOBr_HCl`	see note

*Notes: PSC reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see `http://www.messy-interface.org` for details)

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