S3.2 Phase transfer

Table S10 Henry's Law constants

	Species	$K_H(298\,\mathrm{K})$ / M atm^{-1}	$\Delta H/R$ / K	**Reference/comment**
H1 $^{\otimes}$	Cl_2	9.15×10^{-2}	-2490	Wilhelm et al. (1977)
H2 $^{\oplus}$	Cl	0.2		Mozurkewich (1995)
H3 $^{\ominus}$	ClO	660	-5862	estimated ($K_{H,\,\mathrm{H3}} \approx K_{H,\,\mathrm{H6}}$), correction of Halogen Module 1.0
H4 $^{\oplus}$	ClO_2	1.0	3300	Lide et al. (1995)
H5 $^{\otimes}$	HCl	1.1	-2020	Marsh and McElroy (1985)
H6 $^{\ominus}$	HOCl	660	-5862	Huthwelker et al. (1995), correction of Halogen Module 1.0
H7	ClNO	5.0×10^{-2}		upper limit, Scheer et al. (1997)
H8 $^{\otimes}$	$ClNO_2$	4.6×10^{-2}		upper limit, Frenzel et al. (1998)
H9	$ClNO_3$	2.1×10^{5}	-8700	estimated same as nitric acid
H10	CH_2ClCO_3	669	-5893	estimated same as acetylperoxyl radical
H11	$CH_2ClCOOH$	5.5×10^{3}	-5890	estimated same as acetic acid
H12	$CH_3COCClO$	1.4	-7541	estimated same as methylglyoxal
H13	$COCl_2$	7.0×10^{-2}		Law et al. (2007)
H14	CHOCl	3.0×10^{3}	-7216	estimated same as formaldehyde
H15 $^{\otimes}$	Br_2	0.76	-4100	Law et al. (2007)
H16 $^{\oplus}$	Br	1.2		Mozurkewich (1995)
H17 $^{\oplus}$	BrO	93	-5862	estimated ($K_{H,\,\mathrm{H17}} \approx K_{H,\,\mathrm{H19}}$)
H18 $^{\ominus}$	HBr	1.3	-10239	Brimblecombe and Clegg (1989)
H19 $^{\ominus}$	HOBr	93	-5862	von Glasow et al. (2002a), temperature dependency estimated same as H6
H20 $^{\otimes}$	$BrNO_2$	0.3		Frenzel et al. (1998)
H21	$BrNO_3$	2.1×10^{5}	-8700	estimated same as nitric acid
H22 $^{\oslash}$	BrCl	0.94	-5600	Bartlett and Margerum (1999)
H23	CH_2BrCO_3	669	-5893	estimated same as acetylperoxyl radical
H24	$CH_2BrCOOH$	5.5×10^{3}	-5890	estimated same as acetic acid

Table S10 (continued) Henry's Law constants

	Species	K_H**(298 K) / M atm**$^{-1}$	$\Delta H/R$ **/ K**	**Reference/comment**
H25	$CH_3COCBrO$	1.4	-7541	estimated same as methylglyoxal
H26	$COBr_2$	7.0×10^{-2}		estimated ($K_{H,\ H26} \approx K_{H,\ H13}$)
H27	CHOBr	3.0×10^3	-7216	estimated same as formaldehyde
H28	I_2	3.0	-4431	Palmer et al. (1985)
H29	I	8.0×10^{-2}		Mozurkewich (1986)
H30	IO	450	-5862	von Glasow et al. (2002a), estimated ($K_{H,\ H30} \approx K_{H,\ H6}$)
H31	OIO	2.1×10^5	-8700	estimated same as nitric acid
H32	I_2O_2	2.1×10^5	-8700	estimated same as nitric acid
H33	HI	2.5	-9800	Brimblecombe and Clegg (1989)
H34	HOI	450	-5862	von Glasow et al. (2002a), estimated ($K_{H,\ H34} \approx K_{H,\ H6}$)
H35	HIO_3	2.1×10^5	-8700	estimated same as nitric acid
H36	INO_2	2.1×10^5	-8700	estimated same as nitric acid
H37	INO_3	2.1×10^5	-8700	estimated same as nitric acid
H38	ICl	110	-5600	von Glasow et al. (2002a), temperature dependency estimated same as bromine chloride
H39	IBr	24	-5600	von Glasow et al. (2002a), temperature dependency estimated same as bromine chloride
H40	CH_2ICO_3	669	-5893	estimated same as acetylperoxyl radical
H41	CH_2ICOOH	5.5×10^3	-5890	estimated same as acetic acid
H42	COI_2	7.0×10^{-2}		estimated ($K_{H,\ H42} \approx K_{H,\ H13}$)
H43	CHOI	3.0×10^3	-7216	estimated same as formaldehyde

$^{\otimes}$already implemented in CAPRAM; $^{\oplus}$already implemented in the Halogen Module 1.0; $^{\ominus}$update of the Halogen Module 1.0

Table S11 Mass accommodation coefficients and gas phase diffusion coefficients

	Species	α	**Reference**	$D_g{}^a$	**Reference**	**Comment**
H1 $^{\otimes}$	Cl_2	0.08		1.28	Schwartz (1986)	α estimated

Table S11 (continued) Mass accommodation coefficients and gas phase diffusion coefficients

	Species	α	Reference	D_g [a]	Reference	Comment
H2 ⊖	Cl	0.05		1.82	Fuller (1986)	α estimated same as OH, [b]
H3 ⊖	ClO	0.064		1.55	Fuller (1986)	α estimated, [b]
H4 ⊖	ClO_2	0.05		1.39	Fuller (1986)	α estimated same as OH, [b]
H5 ⊘	HCl	0.1026	Schweitzer et al. (2000)	1.89	Marsh and McElroy (1985)	
H6 ⊖	HOCl	0.5	Abbatt and Waschewsky (1998)	1.51	Fuller (1986)	α estimated same as H19 , [b]
H7	ClNO	0.01		1.39	Fuller (1986)	α estimated same as H8 , [c]
H8 ⊘	$ClNO_2$	0.01	Schweitzer et al. (1998)	1.27	Fuller (1986)	[b]
H9	$ClNO_3$	0.1	Schweitzer et al. (1998)	1.18	Fuller (1986)	[c]
H10	CH_2ClCO_3	0.019		0.94	Fuller (1986)	α estimated same as acetylperoxyl radical, [c]
H11	$CH_2ClCOOH$	0.0322		0.97	Fuller (1986)	α estimated same as acetic acid, [c]
H12	$CH_3COCClO$	0.03		0.88	Fuller (1986)	α estimated same as methylglyoxal, [c]
H13	$COCl_2$	0.02		1.02	Fuller (1986)	α estimated same as formaldehyde, [c]
H14	CHOCl	0.02		1.23	Fuller (1986)	α estimated same as formaldehyde, [c]
H15 ⊗	Br_2	0.08		1.00	Schwartz (1986)	α estimated
H16 ⊖	Br	0.05		1.29	Fuller (1986)	α estimated same as OH, [b, d]
H17 ⊖	BrO	0.06	Sander and Crutzen (1996)	1.19	Fuller (1986)	[b, d]
H18 ⊖	HBr	0.0481	Schweitzer et al. (2000)	1.26	Fuller (1986)	[b, d]
H19 ⊖	HOBr	0.5	Abbatt and Waschewsky (1998)	1.16	Fuller (1986)	[b, d]
H20 ⊘	$BrNO_2$	0.01	Schweitzer et al. (1998)	1.06	Fuller (1986)	[b, d]
H21	$BrNO_3$	0.8	Hanson et al. (1996)	1.01	Fuller (1986)	[b, d]
H22 ⊘	BrCl	0.33	(Katrib et al.)	1.05	Fuller (1986)	[b, d]
H23	CH_2BrCO_3	0.019		0.84	Fuller (1986)	α estimated same as acetylperoxyl radical, [c, d]
H24	$CH_2BrCOOH$	0.0322		0.84	Fuller (1986)	α estimated same as acetic acid, [c]
H25	$CH_3COCBrO$	0.03		0.79	Fuller (1986)	α estimated same as methylglyoxal, [c, d]
H26	$COBr_2$	0.02		0.81	Fuller (1986)	α estimated same as formaldehyde, [c, d]
H27	CHOBr	0.02		1.02	Fuller (1986)	α estimated same as formaldehyde, [c, d]
H28	I_2	0.0126	Pechtl et al. (2005)	0.86	Fuller (1986)	α estimated, [c, e]

Table S11 **(continued)** Mass accommodation coefficients and gas phase diffusion coefficients

	Species	α	Reference	$D_g{}^a$	Reference	Comment
H29	I	0.05		1.16	Fuller (1986)	α estimated same as OH, $^{c,\,f}$
H30	IO	0.558	Pechtl et al. (2005)	1.10	Fuller (1986)	α estimated, $^{c,\,f}$
H31	OIO	1.00	Pechtl et al. (2005)	1.04	Fuller (1986)	α estimated, $^{c,\,f}$
H32	I_2O_2	0.123	Pechtl et al. (2005)	0.80	Fuller (1986)	α estimated, $^{c,\,f}$
H33	HI	0.057	Schweitzer et al. (2000)	1.14	Fuller (1986)	α estimated, $^{c,\,f}$
H34	HOI	0.5	Pechtl et al. (2005)	1.08	Fuller (1986)	α estimated, $^{c,\,f}$
H35	HIO_3	0.0126	Pechtl et al. (2005)	0.98	Fuller (1986)	α estimated, $^{c,\,f}$
H36	INO_2	0.123	Pechtl et al. (2005)	0.99	Fuller (1986)	α estimated, $^{c,\,f}$
H37	INO_3	0.123	Pechtl et al. (2005)	0.96	Fuller (1986)	α estimated, $^{c,\,f}$
H38	ICl	0.0126	Pechtl et al. (2005)	0.98	Fuller (1986)	α estimated, $^{c,\,f}$
H39	IBr	0.0126	Pechtl et al. (2005)	0.88	Fuller (1986)	α estimated, $^{c,\,f}$
H40	CH_2ICO_3	0.019		0.80	Fuller (1986)	α estimated same as acetylperoxyl radical, $^{c,\,f}$
H41	CH_2ICOOH	0.0322		0.82	Fuller (1986)	α estimated same as acetic acid, ^{c}
H42	COI_2	0.02		0.76	Fuller (1986)	α estimated same as formaldehyde, $^{b,\,d}$
H43	CHOI	0.02		0.96	Fuller (1986)	α estimated same as formaldehyde, $^{b,\,d}$

$^{\otimes}$already implemented in CAPRAM; $^{\oslash}$update of CAPRAM; $^{\oplus}$already implemented in the Halogen Module 1.0; $^{\ominus}$update of the Halogen Module 1.0
^{a}in 10^5 m^2 s^{-1} at 288 K; ^{b}correction of D_g in the Halogen Module 1.0; $^c D_g$ calculated with the FSG method (Fuller, 1986); $^d v_{Br}$ estimated with 34.8; $^e v_{I_2}$ estimated with 77.3; $^f v_I$ estimated with 40

S3.3 Gas phase chemistry

Table S12 Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G1 $^{\ominus}$	$Cl + O_3 \rightarrow ClO + O_2$	1.21×10^{-11}	250		*Atk07*
G2	$Cl + H_2 \xrightarrow{O_2} HCl + HO_2$	1.68×10^{-14}	2310		*Atk07*
G3	$Cl + HO_2 \rightarrow HCl + O_2$	3.40×10^{-11}			*Atk07*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G4	$Cl + HO_2 \rightarrow ClO + OH$	9.30×10^{-12}	570		*Atk07*
G5	$Cl + H_2O_2 \rightarrow HCl + HO_2$	4.10×10^{-13}	980		*Atk07*
G6	$Cl_2 + OH \rightarrow HOCl + Cl$	6.42×10^{-14}	1200		*Atk07*
P_g1 ⊖	$Cl_2 \xrightarrow{h\nu} 2\,Cl$	*(2.99×10^{-3})*		$\Phi = 1.0^{Cal/Pit66}$; see Tab. S14	*Dem97*
G7 ⊖	$ClO + O_3 \rightarrow ClO_2 + O_2$	1.13×10^{-17}	3600	upper limit	*Atk07*
G8	$ClO + O_3 \rightarrow OClO + O_2$	1.48×10^{-18}	4000	upper limit	*Atk07*
G9	$ClO + OH \rightarrow$ $0.94\,HO_2 + 0.94\,Cl + 0.06\,HCl + 0.06\,O_2$	2.00×10^{-11}	-300		*Atk07*
G10 ⊖	$ClO + HO_2 \rightarrow HOCl + O_2$	6.89×10^{-12}	-340		*Atk07*
G11	$ClO + ClO \rightarrow Cl_2 + O_2$	4.82×10^{-15}	1590		*Atk07*
G12	$ClO + ClO \rightarrow Cl + ClO_2$	8.06×10^{-15}	2450		*Atk07*
G13	$ClO + ClO \rightarrow Cl + OClO$	3.53×10^{-15}	1370		*Atk07*
G14	$ClO + ClO \xrightarrow{M} Cl_2O_2$	1.52×10^{-15}		TYP: TROE; see Tab. S13	*San06*
P_g2	$ClO \xrightarrow{h\nu} Cl + O$	*(2.64×10^{-4})*		$\Phi = 1.0^i$; see Tab. S14	*San06*
G15	$Cl + O_2 \xrightarrow{M} ClO_2$	5.17×10^{-14}		TYP: TROE; see Tab. S13	*San06*
G16 ⊖	$ClO_2 \xrightarrow{M} Cl + O_2$	6.23×10^{-13}	1820		*Atk07*
G17	$Cl + ClO_2 \rightarrow 0.95\,Cl_2 + 0.95\,O_2 + 0.1\,ClO$	2.42×10^{-10}			*San06*
G18	$Cl_2O_2 \xrightarrow{M} 2\,ClO$	2.87×10^{-3}		TYP: TROEXP; see Tab. S13	*Atk07*
G19	$Cl_2O_2 + O_3 \rightarrow ClO + ClO_2 + O_2$	1.00×10^{-19}		upper limit	*Atk07*
G20	$Cl_2O_2 + Cl \rightarrow Cl_2 + ClO_2$	9.45×10^{-11}	-65		*Atk07*
P_g4	$Cl_2O_2 \xrightarrow{h\nu} Cl + ClO_2$	*(1.83×10^{-3})*		$\Phi = 1.0^i$; see Tab. S14	*San03*
G21	$OClO + OH \rightarrow HOCl + O_2$	1.05×10^{-11}	-600		*Atk07*
G22	$Cl + OClO \rightarrow 2\,ClO$	5.66×10^{-11}	-170		*Atk07*
G23	$ClO + OClO \xrightarrow{M} Cl_2O_3$	1.08×10^{-19}		TYP: TROE; see Tab. S13	*Atk07*
P_g3	$OClO \xrightarrow{h\nu} ClO + O$	*(0.10)*		$\Phi = 1.0^i$; see Tab. S14	*San06*
G24	$Cl_2O_3 \xrightarrow{M} ClO + OClO$	6.17×10^{-2}		TYP: TROEXP; see Tab. S13	*Atk07*

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} (j_{max})[a]	E_A/R[b]	Comment	Reference
P_g5	$Cl_2O_3 \xrightarrow{h\nu} ClO + OClO$	*(9.80×10^{-4})*		$\Phi = 1.0^i$; further products omitted; see Tab. S14	*Atk07*
G25 ⊖	$HCl + OH \rightarrow Cl + H_2O$	7.86×10^{-13}	230		*Atk07*
G26	$HOCl + OH \rightarrow ClO + H_2O$	5.60×10^{-13}	500	E_A/R estimated	*San06*
G27	$HOCl + Cl \rightarrow$ $0.76\,HCl + 0.76\,ClO + 0.24\,Cl_2 + 0.24\,OH$	1.62×10^{-12}	130	branching ratios from Vogt and Schindler (1993)	*San06*
P_g6 ⊖	$HOCl \xrightarrow{h\nu} Cl + OH$	*(3.63×10^{-4})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G28	$ClO + NO \rightarrow Cl + NO_2$	1.67×10^{-11}	-295		*Atk07*
G29	$OClO + NO \rightarrow ClO + NO_2$	3.56×10^{-13}	-350		*Atk07*
G30	$Cl + NO_3 \rightarrow ClO + NO_2$	2.40×10^{-11}			*Atk07*
G31	$ClO + NO_3 \rightarrow 0.68\,ClO_2 + 0.32\,OClO + NO_2$	4.61×10^{-13}			*Kuk94*
G32	$Cl + NO \xrightarrow{M} ClNO$	1.92×10^{-12}		TYP: SPEC2; see Tab. S13	*San06*
G33	$Cl + ClNO \rightarrow Cl_2 + NO$	8.11×10^{-11}	-100		*San06*
P_g7	$ClNO \xrightarrow{h\nu} Cl + NO$	*(5.48×10^{-4})*		see Tab. S14	*Atk07*
G34	$Cl + NO_2 \xrightarrow{M} ClNO_2$	5.80×10^{-14}		TYP: TROE; see Tab. S13	*San06*
G35	$ClNO_2 + OH \rightarrow HOCl + NO_2$	3.62×10^{-14}	1250		*Atk07*
P_g8 ⊖	$ClNO_2 \xrightarrow{h\nu} Cl + NO_2$	*(4.81×10^{-4})*		see Tab. S14	*Atk07*
G36	$ClO + NO_2 \xrightarrow{M} ClNO_3$	1.85×10^{-19}		TYP: TROEF; see Tab. S13	*Atk07*
G37	$ClNO_3 \xrightarrow{M} ClO + NO_2$	1.47×10^{-3}	11438	TYP: SPEC4	*And/Fah90*
G38	$ClNO_3 + OH \rightarrow$ $0.5\,ClO + 0.5\,HNO_3 + 0.5\,HOCl + 0.5\,NO_3$	3.97×10^{-13}	330	branching ratios from Pechtl et al. (2005)	*Atk07*
G39	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	1.01×10^{-11}	-145		*Atk07*
P_g9	$ClNO_3 \xrightarrow{h\nu} Cl + NO_3$	*(5.16×10^{-5})*		$\Phi = 0.6 - 1.0$; see Tab. S14	*Dem97*
P_g10	$ClNO_3 \xrightarrow{h\nu} ClO + NO_2$	*(1.09×10^{-5})*		$\Phi = 0.4 - 0.0$; see Tab. S14	*Dem97*
G40 ⊖	$Cl + CH_4 \xrightarrow{O_2} HCl + MO_2$	1.03×10^{-13}	1240	*g, A*	*Atk06*
G41	$Cl + OP1 \rightarrow HCl + MO_2$	5.70×10^{-11}		*A, B*	*San06*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} (j_{max})[a]	E_A/R[b]	Comment	Reference
G42	Cl + MO_2 → 0.5 HCHO + 0.5 ClO + 0.5 HO_2 − 0.5 O_2 + 0.5 HCl + 0.5 ORA1	1.60×10^{-10}		branching ratios as in Pechtl et al. (2005) with revised products for H-abstraction, [A, C]	*San06*
G43	ClO + MO_2 $\xrightarrow{O_2}$ ClO_2 + HCHO + HO_2	1.63×10^{-12}	238	further products omitted, [h, A]	*Atk08*
G44	Cl + ETH $\xrightarrow{O_2}$ HCl + ETHP	5.93×10^{-11}	100	[g, D, E]	*Atk06*
G45	Cl + HC3 $\xrightarrow{O_2}$ HCl + HC3P	1.47×10^{-10}	-13	estimated, [F, G]	
G46	Cl + HC5 $\xrightarrow{O_2}$ HCl + HC5P	2.14×10^{-10}		estimated, [H, I]	
G47	Cl + HC8 $\xrightarrow{O_2}$ HCl + HC8P	4.38×10^{-10}		estimated, [J, K]	
G48	Cl + TOL $\xrightarrow{O_2}$ HCl + TOLP	5.15×10^{-11}		estimated, [L, M]	
G49	Cl + HCHO $\xrightarrow{O_2}$ HCl + CO + HO_2	7.23×10^{-11}	34	[h]	*Atk06*
G50	ClO + HCHO $\xrightarrow{O_2}$ HOCl + CO + HO_2	8.70×10^{-16}	2100	upper limit	*San06*
G51	Cl + CH_3CHO $\xrightarrow{O_2}$ HCl + ACO_3	8.00×10^{-11}		[N]	*Atk06*
G52	Cl + ALD $\xrightarrow{O_2}$ HCl + ACO_3	8.00×10^{-11}		estimated ($k_{G52} \approx k_{G51}$), [N, O]	
G53	Cl + CH_3COCH_3 $\xrightarrow{O_2}$ HCl + KETP	2.08×10^{-11}	815		*Atk06*
G54	Cl + KET $\xrightarrow{O_2}$ HCl + KETP	2.08×10^{-11}	815	estimated ($k_{G54} \approx k_{G53}$), [P, Q]	
G55	Cl + $CH_3COCH_2CH_3$ $\xrightarrow{O_2}$ HCl + KETP	3.60×10^{-11}		[Q]	*Atk06*
G56	Cl + HKET $\xrightarrow{O_2}$ HCl + HO_2 + MGLY	5.70×10^{-11}		[R, S]	*Orl99*
G57	Cl + MGLY $\xrightarrow{O_2}$ HCl + ACO_3	4.80×10^{-11}		[N, S]	*Gre90*
G58	Cl + GLY $\xrightarrow{O_2}$ HCl + 2 CO + HO_2	3.80×10^{-11}		[T]	*Nik85*
G59	Cl + CHOCH2OH $\xrightarrow{O_2}$ HCl + ACO_3	7.00×10^{-11}		[N]	*Nik87*
G60	Cl + ETI $\xrightarrow{O_2, M}$ 0.26 CHOCl + 0.21 Cl + 0.53 HCl + 0.21 GLY + 1.32 CO + 0.79 HO_2	4.60×10^{-11}		TYP: TROE; see Tab. S13; [d, ,T U]	*Atk06*
G61	Cl + ETE $\xrightarrow{O_2, M}$ $CH_2ClCH_2O_2$	8.46×10^{-11}		TYP: TROE; see Tab. S13; [g, V]	*Atk06*
G62	$CH_2ClCH_2O_2$ + MO_2 → 0.2 CH_2ClCH_2OH + 0.8 HCHO + 0.2 CH_2ClCHO + 0.2 CH_3OH + 0.4 O_2 + 0.6 CH_2ClCH_2O + 0.6 HO_2	2.00×10^{-12}		estimated (RO_2 = MO_2), [A]	*MCM*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G63	$CH_2ClCH_2O_2 + CH_2ClCH_2O_2 \rightarrow 1.28\,CH_2ClCH_2O + 0.36\,CH_2ClCH_2OH + 0.36\,CH_2ClCHO + O_2$	3.29×10^{-12}	-1300	branching ratio at 298 K	*Atk08*
G64	$CH_2ClCH_2O_2 + NO \rightarrow CH_2ClCH_2O + NO_2$	9.70×10^{-12}			*Atk08*
G65	$CH_2ClCH_2OH + OH \xrightarrow{O_2} CH_2ClCHO + H_2O + HO_2$	4.60×10^{-12}			*MCM*
G66	$CH_2ClCH_2O + O_2 \rightarrow CH_2ClCHO + HO_2$	9.48×10^{-15}	550		*MCM*
G67	$CH_2ClCHO + OH \xrightarrow{O_2} CH_2ClCO_3 + H_2O$	3.10×10^{-12}		[g]	*Atk08*
P_g13	$CH_2ClCHO \xrightarrow{h\nu, 2\,O_2} CH_2ClO_2 + CO + HO_2$	*(3.26×10^{-5})*		see Tab. S14	*MCM*
G68	$CH_2ClCO_3 + HO_2 \rightarrow 0.71\,CH_2ClCO_3H + 0.71\,O_2 + 0.29\,CH_2ClCOOH + 0.29\,O_3$	1.41×10^{-11}	-1040		*MCM*
G69	$CH_2ClCO_3 + MO_2 \rightarrow 0.3\,CH_2ClCOOH + HCHO + 0.7\,CH_2ClO_2 + 0.7\,CO_2 + 0.7\,HO_2 - 0.4\,O_2$	1.00×10^{-11}		estimated ($RO_2 = MO_2$), [A]	*MCM*
G70	$CH_2ClCO_3 + NO \xrightarrow{O_2} CH_2ClO_2 + CO_2 + NO_2$	2.00×10^{-11}	-270		*MCM*
G71	$CH_2ClCO_3 + NO_2 \xrightarrow{M} CH_2ClC(O)OONO_2$	1.11×10^{-11}		TYP: TROEF; see Tab. S13	*MCM*
G72	$CH_2ClC(O)OONO_2 \xrightarrow{M} CH_2ClCO_3 + NO_2$	3.48×10^{-4}		TYP: TROEXP; see Tab. S13	*MCM*
G73	$CH_2ClC(O)OONO_2 + OH \rightarrow O_2CHClC(O)OONO_2 + H_2O$	6.26×10^{-13}		[e]	*MCM*
G74	$O_2CHClC(O)OONO_2 + NO \rightarrow CHOCl + CO + O_2 + 2\,NO_2$	1.36×10^{-11}	-360	estimated	
G75	$CH_2ClCO_3H + OH \rightarrow CH_2ClCO_3 + H_2O$	4.29×10^{-12}			*MCM*
P_g14	$CH_2ClCO_3H \xrightarrow{h\nu, O_2} CH_2ClO_2 + CO_2 + OH$	*(5.79×10^{-6})*		see Tab. S14	*MCM*
G76	$CH_2ClCOOH + OH \xrightarrow{O_2} CH_2ClO_2 + CO_2 + H_2O$	3.59×10^{-12}	-190		*MCM*
G77	$Cl + C_3H_6 \xrightarrow{O_2, M} CH_3CHO_2CH_2Cl$	2.52×10^{-10}		TYP: TROE; see Tab. S13	*Atk06*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G78	$CH_3CHO_2CH_2Cl + MO_2 \rightarrow 0.2\,CH_3CHOHCH_2Cl + 0.8\,HCHO + 0.2\,CH_3COCH_2Cl + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_3CHOCH_2Cl + 0.6\,HO_2$	4.00×10^{-14}		estimated ($RO_2 = MO_2$), [c, A]	*MCM*
G79	$CH_3CHO_2CH_2Cl + NO \rightarrow CH_3CHOCH_2Cl + NO_2$	9.04×10^{-12}	-360	further products omitted, [c]	*Atk06*
G80	$CH_3CHOHCH_2Cl + OH \xrightarrow{O_2} CH_3COCH_2Cl + H_2O + HO_2$	5.09×10^{-12}	-200	products as in MCM, [c]	*Atk06*
G81	$CH_3CHOCH_2Cl + O_2 \rightarrow CH_3COCH_2Cl + HO_2$	6.93×10^{-15}	230	[c]	*Atk06*
G82	$CH_3COCH_2Cl + OH \xrightarrow{O_2} CH_3COCHClO_2 + H_2O$	1.05×10^{-13}	1320	[c, g]	*Atk06*
P_g11	$CH_3COCH_2Cl \xrightarrow{h\nu} 0.7\,COCl + 0.7\,ACO3 + 0.3\,CH_2ClCO_3 + 0.3\,MO2 - 1.3\,O_2$	*(3.83×10^{-3})*		$\Phi = 1.0^i$; see Tab. S14	*San06*
G83	$CH_3COCHClO_2 + MO_2 \rightarrow 0.2\,CH_3COCHClOH + 0.8\,HCHO + 0.2\,CH_3COCClO + 0.2\,CH_3OH - 0.2\,O_2 + 0.6\,ACO_3 + 0.6\,CHOCl + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [c, A, N]	*MCM*
G84	$CH_3COCHClO_2 + NO \xrightarrow{O_2} ACO_3 + CHOCl + NO_2$	8.00×10^{-12}		[c, N]	*Atk06*
G85	$CH_3COCHClOH + OH \xrightarrow{O_2} CH_3COCClO + H_2O + HO_2$	3.00×10^{-12}		[c]	*MCM*
P_g12	$CH_3COCClO \xrightarrow{h\nu, O_2} COCl + ACO3$	*(2.78×10^{-5})*		estimated same as methylglyoxal; see Tab. S14	*MCM*
G86	$C_2Cl_4 + OH \xrightarrow{O_2} CCl_2OHCCl_2O_2$	1.60×10^{-13}	920	[g]	*Atk08*
G87	$CCl_2OHCCl_2O_2 + MO_2 \rightarrow 0.3\,CCl_2OHCCl_2OH + HCHO + 1.4\,COCl_2 + 1.4\,HO_2 - 0.4\,O_2$	9.20×10^{-14}		estimated ($RO_2 = MO_2$), [d, A]	*MCM*
G88	$CCl_2OHCCl_2O_2 + NO \xrightarrow{O_2} 2\,COCl_2 + HO_2 + NO_2$	1.87×10^{-11}	-360		*MCM*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G89	$CCl_2OHCCl_2OH + OH \xrightarrow{O_2} 2\,COCl_2 + H_2O + HO_2$	7.18×10^{-14}		^{d}	*MCM*
G90	$C_2HCl_3 + OH \xrightarrow{O_2} 0.5\,CHClOHCCl_2O_2 + 0.5\,CCl_2OHCHClO_2$	2.0×10^{-12}	-565	branching ratios as in MCM, ^{g}	*Atk*08
G91	$CHClOHCCl_2O_2 + MO_2 \rightarrow 0.3\,CCl_2OHCHClOH + HCHO + 0.7\,COCl_2 + 0.7\,CHOCl + 1.4\,HO_2 - 0.4\,O_2$	9.20×10^{-14}		estimated ($RO_2 = MO_2$), $^{d,\,A}$	*MCM*
G92	$CHClOHCCl_2O_2 + NO \xrightarrow{O_2} COCl_2 + CHOCl + NO_2 + HO_2$	1.87×10^{-11}	-360	^{d}	*MCM*
G93	$CCl_2OHCHClO_2 + MO_2 \rightarrow 0.2\,CCl_2OHCHClOH + 0.8\,HCHO + 0.2\,CCl_2OHCClO + 0.2\,CH_3OH - 0.2\,O_2 + 0.6\,COCl_2 + 0.6\,CHOCl + 1.2\,HO_2$	8.80×10^{-13}		estimated ($RO_2 = MO_2$), $^{d,\,A}$	*MCM*
G94	$CCl_2OHCHClO_2 + NO \xrightarrow{O_2} COCl_2 + CHOCl + NO_2 + HO_2$	1.87×10^{-11}	-360	^{d}	*MCM*
G95	$CCl_2OHCHClOH + OH \xrightarrow{O_2} CCl_2OHCClO + H_2O + HO_2$	2.85×10^{-13}			*MCM*
G96	$CCl_2OHCClO + OH \rightarrow COCl_2 + CO + Cl + H_2O$	3.59×10^{-14}			*MCM*
P_g15	$CCl_2OHCClO \xrightarrow{h\nu,O_2} COCl_2 + CO + Cl + HO_2$	*(1.99×10^{-5})*		see Tab. S14	*MCM*
G97	$CH_3CCl_3 + OH \xrightarrow{O_2} CCl_3CH_2O_2 + H_2O$	9.56×10^{-15}	1440	^{g}	*Atk*08
G98	$CH_3CCl_3 + Cl \xrightarrow{O_2} CCl_3CH_2O_2 + HCl$	6.89×10^{-15}	1790	^{g}	*Atk*08
G99	$CCl_3CH_2O_2 + MO_2 \rightarrow 0.2\,CCl_3CH_2OH + 0.8\,HCHO + 0.2\,CCl_3CHO + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CCl_3CH_2O + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$); ^{A}	*MCM*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G100	$CCl_3CH_2O_2 + NO \rightarrow CCl_3CH_2O + NO_2$	1.36×10^{-11}	-360		*MCM*
G101	$CCl_3CH_2O + O_2 \rightarrow CCl_3CHO + HO_2$	9.48×10^{-15}	550		*MCM*
G102	$CCl_3CH_2OH + OH \xrightarrow{O_2} CCl_3CHO + H_2O + HO_2$	2.56×10^{-12}			*MCM*
G103	$CCl_3CHO + OH \xrightarrow{O_2} CCl_3CO_3 + H_2O$	8.04×10^{-13}	240		*Atk08*
P_g16	$CCl_3CHO \xrightarrow{h\nu, 3/2\,O_2} Cl + COCl_2 + CO + HO_2$	*(1.06×10^{-4})*		$\Phi = 1.0$; see Tab. S14	*Atk08*
G104	$CCl_3CO_3 + MO_2 \xrightarrow{O_2} CCl_3O_2 + CO_2 + HCHO + HO_2 + O_2$	1.00×10^{-11}		estimated ($RO_2 = MO_2$); [A]	*MCM*
G105	$CCl_3CO_3 + NO \xrightarrow{O_2} CCl_3O_2 + CO_2 + NO_2$	2.00×10^{-11}	-270	[g]	*MCM*
G106	$CCl_3CO_3 + NO_2 \xrightarrow{M} CCl_3C(O)OONO_2$	1.11×10^{-11}		TYP: TROEF; see Tab. S13	*MCM*
G107	$CCl_3C(O)OONO_2 \xrightarrow{M} CCl_3CO_3 + NO_2$	3.48×10^{-4}		TYP: TROEXP; see Tab. S13	*MCM*
G108	$CHCl_3 + OH \xrightarrow{O_2} CCl_3O_2 + H_2O$	1.04×10^{-13}	850	[g]	*Atk08*
G109	$CHCl_3 + Cl \xrightarrow{O_2} CCl_3O_2 + HCl$	1.10×10^{-13}	920	[g]	*Atk08*
G110	$CCl_3O_2 + HO_2 \rightarrow COCl_2 + HOCl + O_2$	5.09×10^{-12}	-710		*Atk08*
G111	$CCl_3O_2 + MO_2 \rightarrow 0.3\,CCl_3OH + HCHO + 0.3\,O_2 + 0.7\,CCl_3O + 0.7\,HO_2$	6.60×10^{-12}		branching ratios from MCM, [A]	*IUPAC*
G112	$CCl_3O_2 + CCl_3O_2 \rightarrow 2\,CCl_3O + O_2$	3.95×10^{-12}	-740		*Atk08*
G113	$CCl_3O_2 + NO \rightarrow COCl_2 + Cl + NO_2$	1.81×10^{-11}	-270		*San06*
G114	$CCl_3O_2 + NO_2 \xrightarrow{M} CCl_3OONO_2$	1.41×10^{-12}		TYP: TROEF; see Tab. S13	*Atk08*
G115	$CCl_3OONO_2 \xrightarrow{M} CCl_3O_2 + NO_2$	0.26		TYP: TROEXP; see Tab. S13	*Atk08*
G116	$CCl_3OH + OH \rightarrow CCl_3O + H_2O$	3.60×10^{-14}			*MCM*
G117	$CCl_3O \xrightarrow{M} COCl_2 + Cl$	7.91×10^{6}	4600	TYP: SPEC4	*Atk08*
G118	$CH_2Cl_2 + OH \xrightarrow{O_2} CHCl_2O_2 + H_2O$	1.00×10^{-13}	860	[g]	*Atk08*
G119	$CH_2Cl_2 + Cl \xrightarrow{O_2} CHCl_2O_2 + HCl$	3.40×10^{-13}	850	[g]	*Atk08*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G120	$CHCl_2O_2 + HO_2 \rightarrow 0.3\,CHOCl + 0.3\,HOCl + 0.7\,COCl_2 + 0.7\,H_2O + O_2$	5.87×10^{-12}	-700		*Atk08*
G121	$CHCl_2O_2 + MO_2 \rightarrow 0.2\,COCl_2 + 0.2\,CH_3OH + 0.2\,CHCl_2OH + 0.8\,HCHO + 0.4\,O_2 + 0.6\,HO_2 + 0.6\,CHOCl + 0.6\,Cl$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [d, A]	*MCM*
G122	$CHCl_2O_2 + CHCl_2O_2 \rightarrow 2\,CHOCl + 2\,Cl + O_2$	7.00×10^{-12}			*Atk08*
G123	$CHCl_2O_2 + NO \rightarrow CHOCl + Cl + NO_2$	1.87×10^{-11}	-360	[d]	*MCM*
G124	$CHCl_2OH + OH \xrightarrow{O_2} COCl_2 + H_2O + HO_2$	9.34×10^{-13}			*MCM*
G125	$COCl_2 + OH \rightarrow COCl + HOCl$	5.00×10^{-15}		upper limit	*Atk08*
G126	$CH_3Cl + OH \xrightarrow{O_2} CH_2ClO_2 + H_2O$	3.62×10^{-14}	1210		*Atk08*
G127	$CH_3Cl + Cl \xrightarrow{O_2} CH_2ClO_2 + HCl$	4.85×10^{-13}	1150		*Atk08*
G128	$CH_2ClO_2 + HO_2 \rightarrow 0.3\,CH_2ClO_2H + 0.7\,CHOCl + 0.7\,H_2O + O_2$	5.01×10^{-12}	-820		*Atk08*
G129	$CH_2ClO_2 + MO_2 \rightarrow 0.2\,CH_2ClOH + 0.8\,HCHO + 0.2\,CHOCl + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_2ClO + 0.6\,HO_2$	2.50×10^{-12}		branching ratios from corresponding RO_2 reaction in MCM, [A]	*IUPAC*
G130	$CH_2ClO_2 + CH_2ClO_2 \rightarrow 2\,CH_2ClO + O_2$	3.52×10^{-12}	-870		*Atk08*
G131	$CH_2ClO_2 + NO \rightarrow CH_2ClO + NO_2$	1.92×10^{-11}	-300		*San06*
G132	$CH_2ClO_2H + OH \rightarrow CH_2ClO_2 + H_2O$	3.59×10^{-12}	-190		*MCM*
G133	$CH_2ClO_2H + OH \rightarrow CHOCl + OH + H_2O$	4.14×10^{-12}			*MCM*
P_g17	$CH_2ClO_2H \xrightarrow{h\nu} CH_2ClO + OH$	*(5.79×10^{-6})*		see Tab. S14	*MCM*
G134	$CH_2ClOH + OH \xrightarrow{O_2} CHOCl + H_2O + HO_2$	1.08×10^{-12}			*MCM*
G135	$CH_2ClO + O_2 \rightarrow CHOCl + HO_2$	9.48×10^{-15}	550		*MCM*
G136	$CHOCl + OH \rightarrow COCl + H_2O$	5.00×10^{-13}		upper limit	*Atk08*
G137	$CHOCl + Cl \rightarrow HCl + COCl$	7.48×10^{-13}	710		*Atk08*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
P_g18	$CHOCl \xrightarrow{h\nu, O_2} Cl + CO + HO_2$	*(2.71×10^{-7})*		$\Phi = 1.0^{Fan/Liu01}$; see Tab. S14	*Atk08*
G138	$COCl \xrightarrow{M} CO + Cl$	4.98×10^{5}	2960	TYP: SPEC4	*Atk07*
G139	$CO + Cl \xrightarrow{M} COCl$	3.33×10^{-14}		TYP: SPEC2; see Tab. S13	*Atk07*
G140 ⊕	$Br + O_3 \rightarrow BrO + O_2$	1.16×10^{-12}	800	better reference	*Atk07*
G141 ⊖	$Br + HO_2 \rightarrow HBr + O_2$	1.70×10^{-12}	450		*Atk07*
G142	$Br + H_2O_2 \rightarrow HBr + HO_2$	4.25×10^{-16}	3000		*San06*
G143	$Br_2 + OH \rightarrow HOBr + Br$	4.48×10^{-11}	-240		*Atk07*
P_g19 ⊖	$Br_2 \xrightarrow{h\nu} 2\,Br$	*(3.86×10^{-2})*		$\Phi = 1.0^{Fan/Liu01}$; see Tab. S14	*See/Bri64*
G144 ⊖	$BrO + O_3 \rightarrow 0.9\,Br + 0.1\,OBrO + 1.9\,O_2$	2.17×10^{-17}	3200	products from Atkinson et al. (2007); upper limit	*San06*
G145	$BrO + OH \rightarrow Br + HO_2$	4.16×10^{-11}	-250		*Atk07*
G146 ⊖	$BrO + HO_2 \rightarrow HOBr + O_2$	2.41×10^{-11}	-500	further products omitted	*Atk07*
G147	$BrO + BrO \rightarrow 1.7\,Br + 0.15\,Br_2 + O_2$	3.24×10^{-12}	-210		*Atk07*
P_g20	$BrO \xrightarrow{h\nu} Br + O(^3P)$	*(4.86×10^{-2})*		$\Phi = 1.0$; see Tab. S14	*San03*
P_g21	$OBrO \xrightarrow{h\nu} BrO + O(^3P)$	*(0.56)*		$\Phi = 1.0^{Fle05,\,i}$; see Tab. S14	*San06*
P_g22 ⊖	$HOBr \xrightarrow{h\nu} Br + OH$	*(2.80×10^{-3})*		$\Phi = 1.0$; see Tab. S14	*San03*
G148 ⊖	$HBr + OH \rightarrow Br + H_2O$	1.13×10^{-11}	-155		*Atk07*
G149	$Br + NO_2 \xrightarrow{M} BrNO_2$	1.43×10^{-12}		TYP: TROEF; see Tab. S13	*Atk07*
P_g23 ⊖	$BrNO_2 \xrightarrow{h\nu} Br + NO_2$	*(5.87×10^{-3})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G150	$Br + NO_3 \rightarrow BrO + NO_2$	1.60×10^{-11}			*Atk07*
G151	$BrO + NO \rightarrow Br + NO_2$	2.08×10^{-11}	-260		*Atk07*
G152	$BrO + NO_2 \xrightarrow{M} BrNO_3$	1.87×10^{-12}		TYP: TROEF; see Tab. S13	*Atk07*
G153	$BrNO_3 \rightarrow BrO + NO_2$	2.75×10^{-5}	12360		*Orl/Tyn96*
G154	$BrNO_3 + Br \rightarrow Br_2 + NO_3$	4.9×10^{-11}			*Orl/Tyn96*
P_g24	$BrNO_3 \xrightarrow{h\nu} Br + NO_3$	*(1.26×10^{-3})*		$\Phi = 0.71$; see Tab. S14	*San03*
P_g25	$BrNO_3 \xrightarrow{h\nu} BrO + NO_2$	*(5.13×10^{-4})*		$\Phi = 0.29$; see Tab. S14	*San03*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G155	$HBr + NO_3 \rightarrow Br + HNO_3$	1.0×10^{-16}		upper limit	*Atk07*
G156	$Br + Cl_2O_2 \rightarrow BrCl + ClO_2$	3.34×10^{-12}	170		*Atk07*
G157	$Br + OClO \rightarrow BrO + ClO$	3.44×10^{-13}	1300		*Atk07*
G158	$BrO + ClO \rightarrow Br + OClO$	6.77×10^{-12}	-430		*Atk07*
G159	$BrO + ClO \rightarrow Br + ClO_2$	6.07×10^{-12}	-220		*Atk07*
G160	$BrO + ClO \rightarrow BrCl + O_2$	1.03×10^{-12}	-170		*Atk07*
G161	$Br_2 + Cl \rightarrow BrCl + Br$	3.62×10^{-10}	-135		*Bed98*
G162	$BrCl + Br \rightarrow Br_2 + Cl$	3.32×10^{-15}			*Bau81*
G163	$Br + Cl_2 \rightarrow BrCl + Cl$	1.10×10^{-15}			*Dol/Leo87*
G164	$BrCl + Cl \rightarrow Br + Cl_2$	1.45×10^{-11}			*Cly/Cru72*
P_g26 ⊖	$BrCl \xrightarrow{h\nu} Br + Cl$	*(1.32×10^{-2})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G165	$Br + OP1 \rightarrow HBr + MO_2$	1.18×10^{-14}	1610	*A, B*	*Kon/Ben84*
G166	$BrO + MO_2 \rightarrow 0.25\,BrO_2 + 0.25\,HCHO + 0.25\,HO_2 - 0.25\,O_2 + 0.75\,HOBr + 0.75\,ORA1$	6.01×10^{-12}	-800	*A, C*	*IUPAC*
G167 ⊕	$Br + HCHO \xrightarrow{O_2} HBr + CO + HO_2$	1.16×10^{-12}	800	better reference	*San06*
G168	$BrO + HCHO \xrightarrow{O_2} HOBr + CO + HO_2$	1.50×10^{-14}			*Han99*
G169	$Br + CH_3CHO \xrightarrow{O_2} HBr + ACO_3$	3.84×10^{-12}	460	*N*	*Atk06*
G170	$Br + ALD \xrightarrow{O_2} HBr + ACO_3$	3.84×10^{-12}	460	estimated ($k_{G170} \approx k_{G169}$), *N, O*	*Atk06*
G171	$Br + ETI \xrightarrow{O_2, M} 0.17\,CHOBr + 0.09\,Br + 0.74\,HBr + 0.09\,GLY + 1.65\,CO + 0.91\,HO_2$	2.78×10^{-14}	-440	*d, ,T U*	*Atk06*
G172	$Br + ETE \xrightarrow{M, O_2} CH_2BrCH_2O_2$	2.25×10^{-13}	-277	fitted to Arrhenius expression, *g, U*	*Atk06*
G173	$CH_2BrCH_2O_2 + MO_2 \rightarrow 0.2\,CH_2BrCH_2OH + 0.8\,HCHO + 0.2\,CH_2BrCHO + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_2BrCH_2O + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), *e A*	*MCM*
G174	$CH_2BrCH_2O_2 + CH_2BrCH_2O_2 \rightarrow 1.14\,CH_2BrCH_2O + 0.43\,CH_2BrCH_2OH + 0.43\,CH_2BrCHO + O_2$	3.98×10^{-12}	-1250		*Atk08*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G175	$CH_2BrCH_2O_2 + NO \rightarrow CH_2BrCH_2O + NO_2$	9.70×10^{-12}		*e*	*Atk*08
G176	$CH_2BrCH_2OH + OH \xrightarrow{O_2} CH_2BrCHO + H_2O + HO_2$	4.60×10^{-12}		*e*	*MCM*
G177	$CH_2BrCH_2O + O_2 \rightarrow CH_2BrCHO + HO_2$	9.48×10^{-15}	550	*e*	*MCM*
G178	$CH_2BrCHO + OH \xrightarrow{O_2} CH_2BrCO_3 + H_2O$	3.10×10^{-12}		*e, g*	*Atk*08
P_g29	$CH_2BrCHO \xrightarrow{h\nu, 2\,O_2} CH_2BrO_2 + CO + HO_2$	*(3.26×10^{-5})*		estimated same as P_g13, see Tab. S14	*MCM*
G179	$CH_2BrCO_3 + HO_2 \rightarrow 0.71\,CH_2BrCO_3H + 0.71\,O_2 + 0.29\,CH_2BrCOOH + 0.29\,O_3$	1.41×10^{-11}	-1040	*e*	*MCM*
G180	$CH_2BrCO_3 + MO_2 \xrightarrow{O_2} 0.3\,CH_2BrCOOH + HCHO + 0.7\,CH_2BrO_2 + 0.7\,CO_2 + 0.7\,HO_2 - 0.4\,O_2$	1.00×10^{-11}		estimated ($RO_2 = MO_2$), *e A*	*MCM*
G181	$CH_2BrCO_3 + NO \xrightarrow{O_2} CH_2BrO_2 + CO_2 + NO_2$	2.00×10^{-11}	-270	*e*	*MCM*
G182	$CH_2BrCO_3 + NO_2 \xrightarrow{M} CH_2BrC(O)OONO_2$	1.11×10^{-11}		TYP: TROEF; see Tab. S13, *e*	*MCM*
G183	$CH_2BrC(O)OONO_2 \xrightarrow{M} CH_2BrCO_3 + NO_2$	3.48×10^{-4}		TYP: TROEXP; see Tab. S13, *e*	*MCM*
G184	$CH_2BrC(O)OONO_2 + OH \rightarrow O_2CHBrC(O)OONO_2 + H_2O$	6.26×10^{-13}		*e*	*MCM*
G185	$O_2CHBrC(O)OONO_2 + NO\,C(O)OONO_2 + NO\,CHOBr + CO + O_2 + 2\,NO_2$	1.36×10^{-11}	-360	estimated	
G186	$CH_2BrCO_3H + OH \rightarrow CH_2BrCO_3 + H_2O$	4.29×10^{-12}		*e*	*MCM*
P_g30	$CH_2BrCO_3H \xrightarrow{h\nu, O_2} CH_2BrO_2 + CO_2 + OH$	*(5.79×10^{-6})*		estimated same as P_g14, see Tab. S14	*MCM*
G187	$CH_2BrCOOH + OH \xrightarrow{O_2} CH_2BrO_2 + CO_2 + H_2O$	3.59×10^{-12}	-190	*e*	*MCM*
G188	$Br + C_3H_6 \xrightarrow{M, O_2} CH_3CHO_2CH_2Br$	3.60×10^{-12}		*g*	*Atk*06

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G189	$CH_3CHO_2CH_2Br + MO_2 \rightarrow 0.2\,CH_3CHOHCH_2Br + 0.8\,HCHO + 0.2\,CH_3COCH_2Br + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_3CHOCH_2Br + 0.6\,HO_2$	4.00×10^{-14}		estimated ($RO_2 = MO_2$), [c, A]	*MCM*
G190	$CH_3CHO_2CH_2Br + NO \rightarrow CH_3CHOCH_2Br + NO_2$	9.04×10^{-12}	-360	further products omitted, [c]	*Atk06*
G191	$CH_3CHOHCH_2Br + OH \xrightarrow{O_2} CH_3COCH_2Br + H_2O + HO_2$	5.09×10^{-12}	-200	further products omitted, [c]	*Atk06*
G192	$CH_3CHOCH_2Br + O_2 \rightarrow CH_3COCH_2Br + HO_2$	6.93×10^{-15}	230	[c]	*Atk06*
G193	$CH_3COCH_2Br + OH \xrightarrow{O_2} CH_3COCHBrO_2 + H_2O$	1.05×10^{-13}	1320	[c, g]	*Atk06*
P_g27	$CH_3COCH_2Br \xrightarrow{h\nu} 0.7\,COBr + 0.7\,ACO3 + 0.3\,CH_2BrCO_3 + 0.3\,MO2 - 1.3\,O_2$	(5.87×10^{-3})		$\Phi = 1.0^i$; see Tab. S14	*San06*
G194	$CH_3COCHBrO_2 + MO_2 \rightarrow 0.2\,CH_3COCHBrOH + 0.8\,HCHO + 0.2\,CH_3COCBrO + 0.2\,CH_3OH - 0.2\,O_2 + 0.6\,ACO_3 + 0.6\,CHOBr + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [c, A, N]	*MCM*
G195	$CH_3COCHBrO_2 + NO \xrightarrow{O_2} ACO_3 + CHOBr + NO_2$	8.00×10^{-12}		[c, N]	*Atk06*
G196	$CH_3COCHBrOH + OH \xrightarrow{O_2} CH_3COCBrO + H_2O + HO_2$	3.00×10^{-12}		[c]	*MCM*
P_g28	$CH_3COCBrO \xrightarrow{h\nu,O_2} COBr + ACO3$	(2.78×10^{-5})		estimated same as methylglyoxal; see Tab. S14	*MCM*
G197	$CHBr_3 + OH \xrightarrow{O_2} CBr_3O_2 + H_2O$	1.80×10^{-13}	600		*San06*
G198	$CHBr_3 + Cl \xrightarrow{O_2} CBr_3O_2 + HCl$	2.80×10^{-13}	850		*San06*
P_g31	$CHBr_3 \xrightarrow{h\nu,O_2} Br + CHBr_2O_2$	(1.77×10^{-6})		$\Phi = 1.0^i$; see Tab. S14	*Dem97*
G199	$CBr_3O_2 + HO_2 \rightarrow COBr_2 + HOBr + O_2$	5.09×10^{-12}	-710	[e]	*Atk08*

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} (j_{max})[a]	E_A/R[b]	Comment	Reference
G200	$CBr_3O_2 + MO_2 \rightarrow 0.3\,CBr_3OH + 0.3\,O_2 + HCHO + 0.7\,CBr_3O + 0.7\,HO_2$	6.60×10^{-12}		branching ratios from MCM, [e, A]	*MCM*
G201	$CBr_3O_2 + CBr_3O_2 \rightarrow 2\,CBr_3O + O_2$	3.95×10^{-12}	-740	[e]	*Atk08*
G202	$CBr_3O_2 + NO \rightarrow COBr_2 + Br + NO_2$	1.81×10^{-11}	-270	[e]	*San06*
G203	$CBr_3O_2 + NO_2 \xrightarrow{M} CBr_3OONO_2$	1.41×10^{-12}		TYP: TROEF; see Tab. S13; [e]	*Atk08*
G204	$CBr_3OONO_2 \xrightarrow{M} CBr_3O_2 + NO_2$	0.26		TYP: TROEXP; see Tab. S13; [e]	*Atk08*
G205	$CBr_3OH + OH \rightarrow CBr_3O + H_2O$	3.60×10^{-14}		[e]	*MCM*
G206	$CBr_3O \rightarrow COBr_2 + Br$	7.91×10^{6}	4600	[e]	*Atk08*
G207	$CH_2Br_2 + OH \xrightarrow{O_2} CHBr_2O_2 + H_2O$	1.11×10^{-13}	775		*Atk08*
G208	$CH_2Br_2 + Cl \xrightarrow{O_2} CHBr_2O_2 + HCl$	4.30×10^{-13}	800		*San06*
P_g32	$CH_2Br_2 \xrightarrow{h\nu, O_2} Br + CH_2BrO_2$	*(8.22×10^{-10})*		$\Phi = 1.0$[i]; see Tab. S14	*Atk08*
G209	$CHBr_2O_2 + HO_2 \rightarrow 0.3\,CHOBr + 0.3\,HOBr + 0.7\,COBr_2 + 0.7\,H_2O + O_2$	5.87×10^{-12}	-700	[e]	*Atk08*
G210	$CHBr_2O_2 + MO_2 \rightarrow 0.2\,CHBr_2OH + 0.8\,HCHO + 0.2\,COBr_2 + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CHOBr + 0.6\,Br + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [d, e, A]	*MCM*
G211	$CHBr_2O_2 + CHBr_2O_2 \rightarrow 2\,CHOBr + 2\,Br + O_2$	7.00×10^{-12}		[e]	*Atk08*
G212	$CHBr_2O_2 + NO \rightarrow CHOBr + Br + NO_2$	1.70×10^{-11}			*Atk08*
G213	$CHBr_2OH + OH \xrightarrow{O_2} COBr_2 + H_2O + HO_2$	9.34×10^{-13}		[e]	*MCM*
G214	$COBr_2 + OH \rightarrow COBr + HOBr$	5.00×10^{-15}		upper limit, [e]	*Atk08*
P_g33	$COBr_2 \xrightarrow{h\nu} 2\,Br + CO$	*(3.32×10^{-6})*		$\Phi = 1.0$[i]; products estimated the same as in the phosgene reaction in MCM; see Tab. S14	*San06*
G215	$CH_3Br + OH \xrightarrow{O_2} CH_2BrO_2 + H_2O$	2.88×10^{-14}	1215		*Atk08*
G216	$CH_3Br + Cl \xrightarrow{O_2} CH_2BrO_2 + HCl$	4.42×10^{-13}	1030		*San06*

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G217	$CH_2BrO_2 + HO_2 \rightarrow$ $0.85\,CH_2BrO_2H + 0.15\,CHOBr + 0.15\,H_2O + O_2$	6.70×10^{-12}			*Atk08*
G218	$CH_2BrO_2 + MO_2 \rightarrow$ $0.2\,CH_2BrOH + 0.8\,HCHO + 0.2\,CHOBr +$ $0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_2BrO + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [A]	*MCM*
G219	$CH_2BrO_2 + CH_2BrO_2 \rightarrow 2\,CH_2BrO + O_2$	1.05×10^{-12}		products from Atkinson et al. (2008b)	*Vil/Les95*
G220	$CH_2BrO_2 + NO \rightarrow CH_2BrO + NO_2$	1.10×10^{-11}			*Atk08*
G221	$CH_2BrO_2H + OH \rightarrow CH_2BrO_2 + H_2O$	3.59×10^{-12}	-190		*MCM*
G222	$CH_2BrO_2H + OH \rightarrow CHOBr + OH + H_2O$	5.79×10^{-12}			*MCM*
P_g34	$CH_2BrO_2H \xrightarrow{h\nu} CH_2BrO + OH$	*5.79×10^{-6}*		see Tab. S14	*MCM*
G223	$CH_2BrOH + OH \xrightarrow{O_2} CHOBr + H_2O + HO_2$	1.06×10^{-12}			*MCM*
G224	$CH_2BrO + O_2 \rightarrow CHOBr + HO_2$	9.48×10^{-15}	550		*MCM*
G225	$CHOBr + OH \rightarrow Br + CO + H_2O$	1.16×10^{-12}			*MCM*
G226	$CHOBr + Cl \rightarrow COBr + HCl$	7.48×10^{-13}	710	[e]	*Atk08*
P_g35	$CHOBr \xrightarrow{h\nu, O_2} Br + CO + HO_2$	*(1.77×10^{-5})*		$\Phi = 1.0$[i]; see Tab. S14	*San06*
G227	$COBr \xrightarrow{M} CO + Br$	4.98×10^{5}	2960	TYP: SPEC4, [e]	*Atk07*
G228	$CO + Br \xrightarrow{M} COBr$	3.33×10^{-14}		TYP: SPEC2; see Tab. S13, [e]	*Atk07*
G229	$I + I \rightarrow I_2$	2.99×10^{-11}			*Hip73*
G230	$I + O_3 \rightarrow IO + O_2$	1.30×10^{-12}	830		*Atk07*
G231	$I_2 + OH \rightarrow I + HOI$	2.10×10^{-10}			*Atk07*
P_g36	$I_2 \xrightarrow{h\nu} 2\,I$	*(0.18)*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G232	$I + HO_2 \rightarrow HI + O_2$	3.87×10^{-13}	1090		*Atk07*
G233	$IO + HO_2 \rightarrow HOI + O_2$	8.57×10^{-11}	-540		*Atk07*
G234	$IO + IO \rightarrow 0.38\,OIO + 0.485\,I_2O_2 + 0.6\,I +$ $0.135\,O_2 + 0.025\,I_2$	8.03×10^{-11}	-500	branching ratios from Sander and Kerkweg (2005)	*San06*
P_g37	$IO \xrightarrow{h\nu} I + O(^3P)$	*(2.07×10^{-3})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G235	$OIO + OH \rightarrow 0.5\,HIO_3 + 0.5\,HOI + 0.5\,O_2$	2.00×10^{-10}		assumed	*Gla02a*

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G236	$OIO + OIO \rightarrow I_2O_2 + O_2$	5.00×10^{-11}		assumed	*Gla02b*
P_g38	$OIO \xrightarrow{h\nu} I + O_2$	*(3.37×10^{-2})*		$\Phi = 0.15$; upper limit; see Tab. S14	*San06*
P_g39	$OIO \xrightarrow{h\nu} IO + O(^3P)$	*(1.57×10^{-3})*		$\Phi = 0.007$; upper limit; see Tab. S14	*San06*
G237	$I_2O_2 \rightarrow 2\,IO$	20.0		assumed	*Jim03*
P_g40	$I_2O_2 \xrightarrow{h\nu} 2\,I + O_2$	*(1.83×10^{-3})*		$\Phi = 1.0^i$; see Tab. S14	*San03*
G238	$HI + OH \rightarrow I + H_2O$	7.00×10^{-11}	-440		*Atk07*
P_g41	$HI \xrightarrow{h\nu, O_2} I + HO_2$	*(1.58×10^{-4})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
P_g42	$HOI \xrightarrow{h\nu, O_2} I + OH$	*(1.16×10^{-2})*		$\Phi = 1.0$; see Tab. S14	*Atk07*
G239	$I + NO \xrightarrow{M} INO$	9.38×10^{-14}		TYP: TROE; see Tab. S13	*Atk07*
P_g43	$INO \xrightarrow{h\nu} I + NO$	*(3.84×10^{-3})*		$\Phi = 1.0^i$; see Tab. S14	*San06*
G240	$I + NO_2 \xrightarrow{M} INO_2$	1.10×10^{-70}		TYP: TROEF; see Tab. S13	*Atk07*
P_g44	$INO_2 \xrightarrow{h\nu} I + NO_2$	*(3.89×10^{-3})*		$\Phi = 1.0^i$; see Tab. S14	*San06*
G241	$I + NO_3 \rightarrow IO + NO_2$	4.50×10^{-10}			*Cha92*
G242	$I_2 + NO_3 \rightarrow I + INO_3$	1.50×10^{-12}			*Atk07*
G243	$IO + NO \rightarrow I + NO_2$	1.96×10^{-11}	-300		*Atk07*
G244	$IO + NO_2 \xrightarrow{M} INO_3$	4.13×10^{-12}		TYP: TROEF; see Tab. S13	*Atk07*
P_g45	$INO_3 \xrightarrow{h\nu} I + NO_3$	*(5.17×10^{-2})*		$\Phi = 0.85$ (estimated same as $BrNO_3$ in Sander et al. (2006)), see Tab. S14	*San06*
P_g46	$INO_3 \xrightarrow{h\nu} IO + NO_2$	*(9.11×10^{-3})*		$\Phi = 0.15$ (estimated same as $BrNO_3$ in Sander et al. (2006)), see Tab. S14	*San06*
G245	$OIO + NO \rightarrow IO + NO_2$	6.78×10^{-12}	-542		*Atk07*
G246	$HI + NO_3 \rightarrow I + HNO_3$	2.80×10^{-15}	1830		*Atk07*
G247	$INO + INO \rightarrow I_2 + 2\,NO$	1.28×10^{-14}	2620		*Atk07*
G248	$INO_2 + INO_2 \rightarrow I_2 + 2\,NO_2$	1.73×10^{-15}	1670		*Atk07*
G249	$INO_2 \xrightarrow{M} I + NO_2$	2.4		estimated; TYP: SPEC2	*Gla02a*
G250	$INO_3 \xrightarrow{M} IO + NO_2$	2.92×10^{-3}	12060	TYP: SPEC4	*Atk07*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G251	$I_2 + Cl \rightarrow I + ICl$	2.10×10^{-10}			*Bed96*
G252	$I_2 + Br \rightarrow I + IBr$	1.20×10^{-10}			*Bed97*
G253	$I + BrO \rightarrow IO + Br$	1.20×10^{-11}			*San06*
G254	$IO + ClO \rightarrow$ $0.8\,I + 0.55\,OClO + 0.25\,Cl + 0.2\,ICl + 0.45\,O_2$	1.20×10^{-11}	-280		*Atk07*
G255	$IO + BrO \rightarrow 0.8\,OIO + Br + 0.2\,I + 0.2\,O_2$	8.31×10^{-11}	-510		*Atk07*
P_g47	$ICl \xrightarrow{h\nu} I + CL$	*(2.77×10^{-2})*		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state	*Atk07*
P_g48	$IBr \xrightarrow{h\nu} I + Br$	*(8.21×10^{-2})*		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state	*Atk07*
G256	$C_3H_7I + OH \xrightarrow{O_2} CH_3CIO_2CH_3 + H_2O$	1.60×10^{-12}		further products omitted, [g]	*Cot03*
P_g49	$C_3H_7I \xrightarrow{h\nu,O_2} I + CH_3CHO_2CH_3$	*(3.00×10^{-5})*		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state	*San06*
G257	$CH_3CIO_2CH_3 + MO_2 \xrightarrow{O_2}$ $CH_3CIOCH_3 + HCHO + HO_2 + O_2$	2.40×10^{-14}		estimated ($RO_2 = MO_2$), [c, A]	*MCM*
G258	$CH_3CIO_2CH_3 + CH_3CIO_2CH_3 \rightarrow$ $2\,CH_3CIOCH_3 + O_2$	5.57×10^{-16}	2200	[c]	*Atk06*
G259	$CH_3CIO_2CH_3 + NO \rightarrow CH_3CIOCH_3 + NO_2$	9.04×10^{-12}	-360	[c]	*Atk06*
G260	$CH_3CIOCH_3 \rightarrow CH_3COCH_3 + I$	10		estimated	
G261	$C_2H_5I + OH \xrightarrow{O_2}$ $0.13\,CH_3CHIO_2 + 0.87\,CH_2ICH_2O_2 + H_2O$	3.69×10^{-13}	800	products as in MCM, [e]	*San06*
P_g50	$C_2H_5I \xrightarrow{h\nu,O_2} I + CH_3CH_2O_2$	*(1.08×10^{-5})*		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state	*San06*
G262	$CH_2ICH_2O_2 + MO_2 \xrightarrow{O_2}$ $0.2\,CH_2ICH_2OH + 0.8\,HCHO + 0.2\,CH_2ICHO +$ $0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_2ICH_2O + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), [e, A]	*MCM*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G263	$CH_2ICH_2O_2 + CH_2ICH_2O_2 \rightarrow 1.14\,CH_2ICH_2O + 0.43\,CH_2ICH_2OH + 0.43\,CH_2ICHO + O_2$	3.98×10^{-12}	-1250	[f]	*Atk08*
G264	$CH_2ICH_2O_2 + NO \rightarrow CH_2ICH_2O + NO_2$	9.70×10^{-12}		[e]	*Atk08*
G265	$CH_2ICH_2OH + OH \xrightarrow{O_2} CH_2ICHO + H_2O + HO_2$	4.60×10^{-12}		[e]	*MCM*
G266	$CH_2ICH_2O + O_2 \rightarrow CH_2ICHO + HO_2$	9.48×10^{-15}	550	[e]	*MCM*
G267	$CH_2ICHO + OH \xrightarrow{O_2} CH_2ICO_3 + H_2O$	3.10×10^{-12}		[e, g]	*Atk08*
P_g51	$CH_2ICHO \xrightarrow{h\nu, 2\,O_2} CH_2IO_2 + CO + HO_2$	*(3.26×10^{-5})*		estimated same as P_g13, see Tab. S14	*MCM*
G268	$CH_2ICO_3 + HO_2 \rightarrow 0.71\,CH_2ICO_3H + 0.71\,O_2 + 0.29\,CH_2ICOOH + 0.29\,O_3$	1.41×10^{-11}	-1040	[e]	*MCM*
G269	$CH_2ICO_3 + MO_2 \xrightarrow{2\,O_2} 0.3\,CH_2ICOOH + HCHO - 0.4\,O_2 + 0.7\,CH_2IO_2 + 0.7\,CO_2 + 0.7\,HO_2$	1.00×10^{-11}		estimated ($RO_2 = MO_2$), [e, A]	*MCM*
G270	$CH_2ICO_3 + NO \xrightarrow{O_2} CH_2IO_2 + CO_2 + NO_2$	2.00×10^{-11}	-270	[e]	*MCM*
G271	$CH_2ICO_3 + NO_2 \xrightarrow{M} CH_2IC(O)OONO_2$	1.11×10^{-11}		TYP: TROEF; see Tab. S13, [e]	*MCM*
G272	$CH_2IC(O)OONO_2 \xrightarrow{M} CH_2ICO_3 + NO_2$	3.48×10^{-4}		TYP: TROEXP; see Tab. S13, [e]	*MCM*
G273	$CH_2IC(O)OONO_2 + OH \rightarrow O_2CHIC(O)OONO_2 + H_2O$	6.26×10^{-13}		[e]	*MCM*
G274	$O_2CHIC(O)OONO_2 + NO \rightarrow CHOI + CO + O_2 + 2\,NO_2$	1.36×10^{-11}	-360	estimated	
G275	$CH_2ICO_3H + OH \rightarrow CH_2ICO_3 + H_2O$	4.29×10^{-12}		[e]	*MCM*
P_g52	$CH_2ICO_3H \xrightarrow{h\nu, O_2} CH_2IO_2 + CO_2 + OH$	*(5.79×10^{-6})*		estimated (wie P_g14), see Tab. S14	*MCM*
G276	$CH_2ICOOH + OH \xrightarrow{O_2} CH_2IO_2 + CO_2 + H_2O$	3.59×10^{-12}	-190	[e]	*MCM*
G277	$CH_3CHIO_2 + MO_2 \rightarrow 0.2\,CH_3CHIOH + 0.8\,HCHO + 0.2\,CH_3CIO + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_3CHO + 0.6\,I + 0.6\,HO_2$	8.80×10^{-13}		estimated ($RO_2 = MO_2$), [d, e, A]	*MCM*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G278	$CH_3CHIO_2 + NO \rightarrow CH_3CHO + I + NO_2$	1.87×10^{-11}	-360	$^{d, e}$	*MCM*
G279	$CH_3CHIOH + OH \xrightarrow{O_2} CH_3CIO + H_2O + HO_2$	2.77×10^{-12}		^{e}	*MCM*
G280	$CH_3CIO + OH \xrightarrow{O_2} CIOCH_2O_2 + H_2O$	3.88×10^{-14}		^{e}	*MCM*
G281	$CIOCH_2O_2 + MO_2 \rightarrow I + CO + 2\,HCHO + HO_2$	2.00×10^{-12}		$^{d, e, A}$	*MCM*
G282	$CIOCH_2O_2 + NO \rightarrow I + CO + HCHO + NO_2$	1.36×10^{-11}	-360	$^{d, e}$	*MCM*
G283	$CH_2I_2 + OH \xrightarrow{O_2} CHI_2O_2 + H_2O$	2.75×10^{-14}	929	estimated	
G284	$CH_2I_2 + Cl \xrightarrow{O_2} CHI_2O_2 + HCl$	4.70×10^{-13}	1135	estimated	
P_g53	$CH_2I_2 \xrightarrow{h\nu, O_2} I + CH_2IO_2$	(1.13×10^{-2})		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state	*San06*
G285	$CHI_2O_2 + HO_2 \rightarrow 0.3\,CHOI + 0.3\,HOI + 0.7\,COI_2 + 0.7\,H_2O + O_2$	5.87×10^{-12}	-700	^{e}	*Atk08*
G286	$CHI_2O_2 + MO_2 \rightarrow 0.2\,CHI_2OH + 0.8\,HCHO + 0.2\,COI_2 + 0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CHOI + 0.6\,I + 0.6\,HO_2$	2.00×10^{-12}		estimated ($RO_2 = MO_2$), $^{e, A}$	*MCM*
G287	$CHI_2O_2 + CHI_2O_2 \rightarrow 2\,CHOI + 2\,I + O_2$	7.00×10^{-12}		^{e}	*Atk08*
G288	$CHI_2O_2 + NO \rightarrow CHOI + I + NO_2$	1.70×10^{-11}		^{h}	*Atk08*
G289	$CHI_2OH + OH \xrightarrow{O_2} COI_2 + H_2O + HO_2$	9.34×10^{-13}		^{e}	*MCM*
G290	$COI_2 + OH \rightarrow COI + HOI$	5.00×10^{-15}		upper limit, ^{e}	*Atk08*
G291	$CH_3I + OH \xrightarrow{O_2} CH_2IO_2 + H_2O$	1.00×10^{-13}	1120		*Atk08*
G292	$CH_3I + Cl \xrightarrow{O_2} CH_2IO_2 + HCl$	1.01×10^{-12}	1000		*San06*
P_g54	$CH_3I \xrightarrow{h\nu, O_2} I + MO_2$	(9.55×10^{-6})		$\Phi = 1.0$; see Tab. S14; exited atoms are treated like atoms in ground state, ^{A}	*San06*

Table S12 (continued) Gas phase reactions

	Reaction	k_{298} $(j_{max})^a$	E_A/R^b	Comment	Reference
G293	$CH_2IO_2 + HO_2 \rightarrow$ $0.85\,CH_2IO_2H + 0.15\,CHOI + 0.15\,H_2O + O_2$	6.70×10^{-12}		^{f}	*Atk08*
G294	$CH_2IO_2 + MO_2 \rightarrow$ $0.2\,CH_2IOH + 0.8\,HCHO + 0.2\,CHOI +$ $0.2\,CH_3OH + 0.4\,O_2 + 0.6\,CH_2IO + 0.6\,HO_2$	2.00×10^{-12}		$^{e,\,A}$	*MCM*
G295	$CH_2IO_2 + CH_2IO_2 \rightarrow 2\,CH_2IO + O_2$	1.05×10^{-12}		^{f}	*Vil/Les95*, *Atk08*
G296	$CH_2IO_2 + NO \rightarrow CH_2IO + NO_2$	1.10×10^{-11}		^{f}	*Atk08*
G297	$CH_2IO_2H + OH \rightarrow CH_2IO_2 + H_2O$	3.59×10^{-12}	-190	^{e}	*MCM*
G298	$CH_2IO_2H + OH \rightarrow CHOI + OH + H_2O$	5.79×10^{-12}		^{f}	*MCM*
P_g55	$CH_2IO_2H \xrightarrow{h\nu} CH_2IO + OH$	*(5.79×10^{-6})*		estimated same as P_g17, see Tab. S14	*MCM*
G299	$CH_2IOH + OH \xrightarrow{O_2} CHOI + H_2O + HO_2$	1.06×10^{-12}		^{f}	*MCM*
G300	$CH_2IO + O_2 \rightarrow CHOI + HO_2$	9.48×10^{-15}	550	^{e}	*MCM*
G301	$CHOI + OH \rightarrow I + CO + H_2O$	1.16×10^{-12}		^{f}	*MCM*
G302	$CHOI + Cl \rightarrow COI + HCl$	7.48×10^{-13}	710	^{e}	*Atk08*
P_g56	$CHOI \xrightarrow{h\nu,O_2} I + CO + HO_2$	*(2.71×10^{-7})*		estimated same as P_g18, see Tab. S14	*Atk08*
G303	$COI \xrightarrow{M} CO + I$	4.98×10^{5}	2960	TYP: SPEC4, ^{e}	*Atk07*
G304	$CO + I \xrightarrow{M} COI$	3.33×10^{-14}		TYP: SPEC2; see Tab. S13, ^{e}	*Atk07*
P_g57	$CH_2ICl \xrightarrow{h\nu,O_2} I + CH_2ClO_2$	*(2.04×10^{-4})*		$\Phi = 1.0$ (estimated); see Tab. S14	*Atk08*

Table S12 **(continued)** Gas phase reactions

	Reaction	k_{298} (j_{max})[a]	E_A/R[b]	Comment	Reference
P_g58	$CH_2IBr \xrightarrow{h\nu, O_2} I + CH_2BrO_2$	*(6.87 × 10⁻⁴)*		Φ = 1.0; see Tab. S14	[Atk08]

[⊕]already implemented in the Halogen Module 1.0; [⊖]update of the Halogen Module 1.0

[a]in cm^3 $molecules^{-1}$ s^{-1} (*slanted* values in parentheses represent j_{max} in s^{-1} for photolysis reactions); [b]in K; [c]estimated X = H (X = Cl, Br, I); [d]reactions combined; [e]estimated X = Cl (X = Br, I); [f]estimated I = Br; [g]immediate reaction with oxygen; [h]immediate hydrogen abstraction; [i]estimated

[A]MO_2 = methyl peroxyl radical; [B]OP1 = methyl hydrogen peroxide; [C]ORA1 = formic acid; [D]ETH = ethane; [E]ETHP = peroxyl radical formed from ETH; [F]HC3 = alkanes, alcohols, esters, and alkynes with OH rate constant (298 K, 1 atm) less than 3.4×10^{-12} cm^3 $molecules^{-1}$ s^{-1}; [G]HC3P = peroxyl radical formed from HC3; [H]HC5 = alkanes, alcohols, esters, and alkynes with OH rate constant (298 K, 1 atm) between 3.4×10^{-12} cm^3 $molecules^{-1}$ s^{-1} and 6.8×10^{-12} cm^3 $molecules^{-1}$ s^{-1}; [I]HC5P = peroxyl radical formed from HC5; [J]HC8 = alkanes, alcohols, esters, and alkynes with OH rate constant (298 K, 1 atm) greater than 6.8×10^{-12} cm^3 $molecules^{-1}$ s^{-1}; [K]HC8P = peroxyl radical formed from HC8; [L]TOL = Toluene and less reactive aromatics; [M]TOLP = peroxyl radical formed from TOL; [N]ACO_3 = acetylperoxyl and higher saturated acylperoxyl radicals; [O]ALD = higher aldehydes; [P]KET = ketones; [Q]KETP = peroxyl radical formed from KET; [R]HKET = hydroxy ketone; [S]MGLY = methylglyoxal; [T]GLY = glyoxal; [U]ETI = acetylene; [V]ETE = ethylene

[Atk07]Atkinson et al. (2007); [Dem97]DeMore et al. (1997); [Cal/Pit66]Calvert and Pitts (1966); [San06]Sander et al. (2006); [San03]Sander et al. (2003); [Kuk94]Kukui et al. (1994); [And/Fah90] Mallard et al. (1998) mit Werten von Anderson and Fahey (1990); [Atk06]Atkinson et al. (2006); [Atk08]Atkinson et al. (2008b); [Orl99]Orlando et al. (1999); [Gre90]Green et al. (1990); [Nik85]Niki et al. (1985); [Nik87]Niki et al. (1987); [MCM]Pilling et al. (2008); [IUPAC]Atkinson et al. (2008a); [See/Bri64]Seery and Britton (1964); [Fan/Liu01]Fang and Liu (2001); [Fle05]Fleischmann et al. (2005); [Orl/Tyn96]Orlando and Tyndall (1996); [Bed98]Bedjanian et al. (1998); [Bau81]Baulch et al. (1981); [Dol/Leo87]Dolson and Leone (1987); [Cly/Cru72]Clyne and Cruse (1972); [Kon/Ben84]Kondo and Benson (1984); [Han99]Hansen et al. (1999); [Vil/Les95]Villenave and Lesclaux (1995); [Hip73]Hippler et al. (1973); [Gla02a]von Glasow et al. (2002a) (ESM); [Jim03]Jimenez et al. (2003); [Gla02b]von Glasow et al. (2002a); [Cha92]Chambers et al. (1992); [Bed96]Bedjanian et al. (1996) [Bed97]Bedjanian et al. (1997)

Table S13 Parameters for pressure dependent reactions

	Reaction	TYPE	k_0[a]	k_∞[a]	F_C[b]
G14	$ClO + ClO \xrightarrow{M} Cl_2O_2$	TROE	$1.6 \times 10^{-32}(T/300)^{-4.5}$	$2.0 \times 10^{-12}(T/300)^{-2.4}$	
G15	$Cl + O_2 \xrightarrow{M} ClO_2$	TROE	$2.2 \times 10^{-33}(T/300)^{-3.1}$	1.8×10^{-10}	
G18	$Cl_2O_2 \xrightarrow{M} 2\,ClO$	TROEXP	$3.7 \times 10^{-7}e^{-7690/T}$	$7.9 \times 10^{15}e^{-8820/T}$	0,45
G23	$ClO + OClO \xrightarrow{M} Cl_2O_3$	TROE	$6.2 \times 10^{-32}(T/300)^{-4.7}$	2.4×10^{-11}	
G24	$Cl_2O_3 \xrightarrow{M} ClO + OClO$	TROEXP	$1.4 \times 10^{-10}e^{-3810/T}$	$2.5 \times 10^{12}e^{-4940/T}$	
G32	$Cl + NO \xrightarrow{M} ClNO$	SPEC2	$7.6 \times 10^{-32}(T/300)^{-1,8}$		
G34	$Cl + NO_2 \xrightarrow{M} ClNO_2$	TROE	$1.8 \times 10^{-31}(T/300)^{-2}$	$1.0 \times 10^{-10}(T/300)^{-1}$	

Table S13 (continued) Parameters for pressure dependent reactions

	Reaction	TYPE	k_0 [a]	k_∞ [a]	F_C [b]
G36	$ClO + NO_2 \xrightarrow{M} ClNO_3$	TROEF	$1.6 \times 10^{-31}(T/300)^{-3.4}$	7.0×10^{-11}	0.4
G60	$Cl + ETI^{c} \xrightarrow{O_2, M}$ $0.26\,CHOCl + 0.21\,Cl + 0.53\,HCl +$ $0.21\,GLY^{d} + 1.32\,CO + 0.79\,HO_2$	TROE	$6.10 \times 10^{-30}(T/300)^{-3.0}$	2.0×10^{-10}	
G61	$Cl + ETE^{e} \xrightarrow{O_2, M} CH_2ClCH_2OO$	TROEF	$1.85 \times 10^{-29}(T/300)^{-3.3}$	6.0×10^{-10}	0.4
G71	$CH_2ClCO_3 + NO_2 \xrightarrow{M}$ $CH_2ClC(O)OONO_2$	TROEF	$2.7 \times 10^{-28}(T/300)^{-7.1}$	$1.2 \times 10^{-11}(T/300)^{-0.9}$	0.3
G72	$CH_2ClC(O)OONO_2 \xrightarrow{M}$ $CH_2ClCO_3 + NO_2$	TROEXP	$4.9 \times 10^{-3}e^{-12100/T}$	$5.4 \times 10^{16}e^{-13830/T}$	0.3
G77	$Cl + C_3H_6 \xrightarrow{O_2, M} CH_3CHOOCH_2Cl$	TROE	4.0×10^{-28}	2.8×10^{-10}	
G106	$CCl_3CO_3 + NO_2 \xrightarrow{M} CCl_3C(O)OONO_2$	TROEF	$2.7 \times 10^{-28}(T/300)^{-7.1}$	$1.2 \times 10^{-11}(T/300)^{-0.9}$	0.3
G107	$CCl_3C(O)OONO_2 \xrightarrow{M} CCl_3CO_3 + NO_2$	TROEXP	$4.9 \times 10^{-3}e^{-12100/T}$	$5.4 \times 10^{16}e^{-13830/T}$	0.3
G114	$CCl_3OO + NO_2 \xrightarrow{M} CCl_3OONO_2$	TROEF	$9.2 \times 10^{-29}(T/300)^{-6.0}$	$1.5 \times 10^{-12}(T/300)^{-0.7}$	0.32
G115	$CCl_3OONO_2 \xrightarrow{M} CCl_3OO + NO_2$	TROEXP	$4.3 \times 10^{-3}e^{-10235/T}$	$4.8 \times 10^{16}e^{-11820/T}$	0.32
G139	$CO + Cl \xrightarrow{M} COCl$	SPEC2	$1.3 \times 10^{-33}(T/300)^{-3.8}$		
G149	$Br + NO_2 \xrightarrow{M} BrNO_2$	TROEF	$4.2 \times 10^{-31}T/300)^{-2.4}$	2.7×10^{-11}	0.55
G152	$BrO + NO_2 \xrightarrow{M} BrNO_3$	TROEF	$4.7 \times 10^{-31}(T/300)^{-3.1}$	1.8×10^{-11}	0.4
G182	$CH_2BrCO_3 + NO_2 \xrightarrow{M}$ $CH_2BrC(O)OONO_2$	TROEF	$2.7 \times 10^{-28}(T/300)^{-7.1}$	$1.2 \times 10^{-11}(T/300)^{-0.9}$	0.3
G183	$CH_2BrC(O)OONO_2 \xrightarrow{M}$ $CH_2BrCO_3 + NO_2$	TROEXP	$4.9 \times 10^{-3}e^{-12100/T}$	$5.4 \times 10^{16}e^{-13830/T}$	0.3
G203	$CBr_3OO + NO_2 \xrightarrow{M} CBr_3OONO_2$	TROEF	$9.2 \times 10^{-29}(T/300)^{-6.0}$	$1.5 \times 10^{-12}(T/300)^{-0.7}$	0.32
G204	$CBr_3OONO_2 \xrightarrow{M} CBr_3OO + NO_2$	TROEXP	$4.3 \times 10^{-3}e^{-10235/T}$	$4.8 \times 10^{16}e^{-11820/T}$	0.32
G228	$CO + Br \xrightarrow{M} COBr$	SPEC2	$1.3 \times 10^{-33}(T/300)^{-3.8}$		
G239	$I + NO \xrightarrow{M} INO$	TROE	$1.8 \times 10^{-32}(T/300)^{-1.0}$	1.7×10^{-11}	
G240	$I + NO_2 \xrightarrow{M} INO_2$	TROEF	$3.0 \times 10^{-31}(T/300)^{-1.0}$	6.6×10^{-11}	0.63

Table S13 (continued) Parameters for pressure dependent reactions

	Reaction	TYPE	k_0[a]	k_∞[a]	F_C[b]
G244	$IO + NO_2 \xrightarrow{M} INO_3$	TROEF	$7.7 \times 10^{-31}(T/300)^{-5.0}$	1.6×10^{-11}	0.4
G271	$CH_2ICO_3 + NO_2 \xrightarrow{M} CH_2IC(O)OONO_2$	TROEF	$2.7 \times 10^{-28}(T/300)^{-7.1}$	$1.2 \times 10^{-11}(T/300)^{-0.9}$	0.3
G272	$CH_2IC(O)OONO_2 \xrightarrow{M} CH_2ICO_3 + NO_2$	TROEXP	$4.9 \times 10^{-3}e^{-12100/T}$	$5.4 \times 10^{16}e^{-13830/T}$	0.3
G304	$CO + I \xrightarrow{M} COI$	SPEC2	$1.3 \times 10^{-33}(T/300)^{-3.8}$		

Rate constants calculated with TROE formula: $k(T) = \frac{k_0[M]}{1+\frac{k_0[M]}{k_\infty}} \cdot F_C^{(1+\lg(k_0[M]/k_\infty))^{-2}}$

[a]in $\frac{cm^{3n}}{molecules^n\ s}$, n = order of reaction; [b]if other than $F_C = 0.6$; [c]ETI = acetylene; [d]GLY = glyoxal; [e]ETE = ethylene

S3.4 Photolysis reactions

Table S14 Parameters for gas phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_g1 $\ominus$	$Cl_2 \xrightarrow{h\nu} 2\,Cl$	3.827×10^{-3}	0.543	0.244	DeMore et al. (1997) with quantum yields from Calvert and Pitts (1966)
P_g2	$ClO \xrightarrow{h\nu} Cl + O(^3P)$	4.755×10^{-4}	1.258	0.588	Sander et al. (2006)[a]
P_g3	$OClO \xrightarrow{h\nu} ClO + O(^3P)$	0.133	0.416	0.244	Sander et al. (2006)[a]
P_g4	$Cl_2O_2 \xrightarrow{h\nu} Cl + ClO_2$	2.294×10^{-3}	0.745	0.223	Sander et al. (2003)[a]
P_g5	$Cl_2O_3 \xrightarrow{h\nu} ClO + OClO$	1.558×10^{-3}	1.324	0.462	further products omitted, Atkinson et al. (2007)[a]
P_g6 $\ominus$	$HOCl \xrightarrow{h\nu} Cl + OH$	4.615×10^{-4}	0.656	0.240	Atkinson et al. (2007)
P_g7	$ClNO \xrightarrow{h\nu} Cl + NO$	4.755×10^{-3}	0.408	0.217	Atkinson et al. (2007)
P_g8 $\ominus$	$ClNO_2 \xrightarrow{h\nu} Cl + NO_2$	6.219×10^{-4}	0.774	0.255	Atkinson et al. (2007)
P_g9	$ClNO_3 \xrightarrow{h\nu} Cl + NO_3$	6.420×10^{-5}	0.648	0.217	DeMore et al. (1997)

Table S14 (continued) Parameters for gas phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_g10	$ClNO_3 \xrightarrow{h\nu} ClO + NO_2$	1.393×10^{-5}	1.052	0.243	DeMore et al. (1997)
P_g11	$CH_3COCH_2Cl \xrightarrow{h\nu} 0.7\,COCl + 0.7\,ACO_3 + 0.3\,CH_2ClCO_3 + 0.3\,MO_2 - 1.3\,O_2$	1.675×10^{-4}	1.003	0.296	Sander et al. (2006)[a, c, d]
P_g12	$CH_3COCClO \xrightarrow{h\nu,O_2} COCl + ACO_3$	1.853×10^{-4}	0.583	0.225	estimated same as methylglyoxal[c]
P_g13	$CH_2ClCHO \xrightarrow{h\nu,2\,O_2} CH_2ClO_2 + CO + HO_2$	4.642×10^{-5}	0.762	0.353	Pilling et al. (2008)
P_g14	$CH_2ClCO_3H \xrightarrow{h\nu,O_2} CH_2ClO_2 + CO_2 + OH$	7.649×10^{-6}	0.682	0.279	Pilling et al. (2008)
P_g15	$CCl_2OHCClO \xrightarrow{h\nu,O_2} COCl_2 + CO + Cl + HO_2$	2.792×10^{-5}	0.805	0.338	Pilling et al. (2008)
P_g16	$CCl_3CHO \xrightarrow{h\nu,3/2\,O_2} Cl + COCl_2 + CO + HO_2$	1.442×10^{-4}	1.027	0.302	Atkinson et al. (2008b)
P_g17	$CH_2ClO_2H \xrightarrow{h\nu} CH_2ClO + OH$	7.649×10^{-6}	0.682	0.279	Pilling et al. (2008)
P_g18	$CHOCl \xrightarrow{h\nu,O_2} Cl + CO + HO_2$	3.905×10^{-7}	1.936	0.362	Atkinson et al. (2008b) with quantum yields from Fang and Liu (2001)
P_g19 ⊖	$Br_2 \xrightarrow{h\nu} 2\,Br$	4.773×10^{-2}	0.193	0.213	Seery and Britton (1964) with quantum yields from Fang and Liu (2001)
P_g20	$BrO \xrightarrow{h\nu} Br + O(^3P)$	6.368×10^{-2}	0.605	0.269	Sander et al. (2003)
P_g21	$OBrO \xrightarrow{h\nu} BrO + O(^3P)$	0.688	0.144	0.198	Sander et al. (2006) with quantum yields from Fleischmann et al. (2005)
P_g22 ⊖	$HOBr \xrightarrow{h\nu} Br + OH$	3.464×10^{-3}	0.441	0.214	Sander et al. (2003)
P_g23 ⊖	$BrNO_2 \xrightarrow{h\nu} Br + NO_2$	7.443×10^{-3}	0.355	0.236	Atkinson et al. (2007)
P_g24	$BrNO_3 \xrightarrow{h\nu} Br + NO_3$	1.558×10^{-3}	0.490	0.216	Sander et al. (2003)
P_g25	$BrNO_3 \xrightarrow{h\nu} BrO + NO_2$	6.363×10^{-4}	0.492	0.215	Sander et al. (2003)
P_g26 ⊖	$BrCl \xrightarrow{h\nu} Br + Cl$	1.650×10^{-2}	0.297	0.224	Atkinson et al. (2007)
P_g27	$CH_3COCH_2Br \xrightarrow{h\nu} 0.7\,COBr + 0.7\,ACO_3 + 0.3\,CH_2BrCO_3 + 0.3\,MO_2 - 1.3\,O_2$	3.523×10^{-4}	0.885	0.283	Sander et al. (2006)[a, c, d]
P_g28	$CH_3COCBrO \xrightarrow{h\nu,O_2} COBr + ACO_3$	1.853×10^{-4}	0.583	0.225	estimated same as methylglyoxal[c]

Table S14 (continued) Parameters for gas phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_g29	$CH_2BrCHO \xrightarrow{h\nu, 2\,O_2} CH_2BrO_2 + CO + HO_2$	4.642×10^{-5}	0.762	0.353	estimated same as P_g13, Pilling et al. (2008)
P_g30	$CH_2BrCO_3H \xrightarrow{h\nu, O_2} CH_2BrO_2 + CO_2 + OH$	7.649×10^{-6}	0.682	0.279	estimated same as P_g14, Pilling et al. (2008)
P_g31	$CHBr_3 \xrightarrow{h\nu, O_2} Br + CHBr_2O_2$	2.228×10^{-6}	1.471	0.230	DeMore et al. (1997)
P_g32	$CH_2Br_2 \xrightarrow{h\nu, O_2} Br + CH_2BrO_2$	5.600×10^{-9}	2.763	1.922	Atkinson et al. (2008b)
P_g33	$COBr_2 \xrightarrow{h\nu} 2\,Br + CO$	4.377×10^{-6}	1.360	0.273	Sander et al. (2006) products estimated same as phosgene from Pilling et al. (2008)
P_g34	$CH_2BrO_2H \xrightarrow{h\nu} CH_2BrO + OH$	7.649×10^{-6}	0.682	0.279	Pilling et al. (2008)
P_g35	$CHOBr \xrightarrow{h\nu, O_2} Br + CO + HO_2$	2.547×10^{-5}	1.393	0.361	Sander et al. (2006)
P_g36	$I_2 \xrightarrow{h\nu} 2\,I$	0.217	0.125	0.185	Atkinson et al. (2007)
P_g37	$IO \xrightarrow{h\nu} I + O(^3P)$	2.640×10^{-3}	0.240	0.240	Atkinson et al. (2007)
P_g38	$OIO \xrightarrow{h\nu} I + O_2$	4.054×10^{-2}	0.119	0.185	Sander et al. (2006)
P_g39	$OIO \xrightarrow{h\nu} IO + O(^3P)$	1.894×10^{-3}	0.119	0.185	Sander et al. (2006)
P_g40	$I_2O_2 \xrightarrow{h\nu} 2\,I + O_2$	2.294×10^{-3}	0.745	0.223	estimated same as P_g4, products from von Glasow et al. (2002a)
P_g41	$HI \xrightarrow{h\nu, O_2} I + HO_2$	2.104×10^{-4}	1.123	0.281	Atkinson et al. (2007)
P_g42	$HOI \xrightarrow{h\nu, O_2} I + OH$	1.469×10^{-2}	0.342	0.236	Atkinson et al. (2007)
P_g43	$INO \xrightarrow{h\nu} I + NO$	4.849×10^{-3}	0.284	0.232	Sander et al. (2006)
P_g44	$INO_2 \xrightarrow{h\nu} I + NO_2$	5.036×10^{-3}	0.568	0.256	Sander et al. (2006)
P_g45	$INO_3 \xrightarrow{h\nu} I + NO_3$	6.599×10^{-2}	0.528	0.244	Sander et al. (2006)
P_g46	$INO_3 \xrightarrow{h\nu} IO + NO_2$	1.165×10^{-2}	0.528	0.244	Sander et al. (2006)
P_g47	$ICl \xrightarrow{h\nu} I + CL$	3.403×10^{-2}	0.179	0.207	Atkinson et al. (2007)[b]
P_g48	$IBr \xrightarrow{h\nu} I + Br$	0.1	0.149	0.197	Atkinson et al. (2007)[b]
P_g49	$C_3H_7I \xrightarrow{h\nu, O_2} I + HC3P$	3.731×10^{-5}	1.292	0.217	Sander et al. (2006)[b, e]

Table S14 (continued) Parameters for gas phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_g50	$C_2H_5I \xrightarrow{h\nu, O_2} I + ETHP$	1.386×10^{-5}	1.324	0.224	Sander et al. (2006)[b, f]
P_g51	$CH_2ICHO \xrightarrow{h\nu, 2\,O_2} CH_2IO_2 + CO + HO_2$	4.642×10^{-5}	0.762	0.353	estimated same as P_g13, Pilling et al. (2008)
P_g52	$CH_2ICO_3H \xrightarrow{h\nu, O_2} CH_2IO_2 + CO_2 + OH$	7.649×10^{-6}	0.682	0.279	estimated same as P_g14, Pilling et al. (2008)
P_g53	$CH_2I_2 \xrightarrow{h\nu, O_2} I + CH_2IO_2$	1.496×10^{-2}	0.801	0.265	Sander et al. (2006)[b]
P_g54	$CH_3I \xrightarrow{h\nu, O_2} I + MO_2$	1.206×10^{-5}	1.254	0.231	Sander et al. (2006)[b, d]
P_g55	$CH_2IO_2H \xrightarrow{h\nu} CH_2IO + OH$	7.649×10^{-6}	0.682	0.279	estimated same as P_g17, Pilling et al. (2008)
P_g56	$CHOI \xrightarrow{h\nu, O_2} I + CO + HO_2$	2.547×10^{-5}	1.393	0.361	estimated same as P_g35
P_g57	$CH_2ICl \xrightarrow{h\nu, O_2} I + CH_2ClO_2$	2.038×10^{-4}	1.057	0.238	Atkinson et al. (2008b)
P_g58	$CH_2IBr \xrightarrow{h\nu, O_2} I + CH_2BrO_2$	8.824×10^{-4}	0.976	0.250	Atkinson et al. (2008b)

Photolysis reactions are parameterised with $j = l \times \cos^m \chi \times \exp\{-n \times \sec \chi\}$.
[a]quantum yield estimated with $\Phi = 1$, [b]exited atoms are treated like atoms in ground state, [c]MO_2 = methyl peroxyl radical, [d]ACO_3 = acetyl peroxyl radical, [e]HC3P = peroxyl radical formed from alkanes, alcohols, esters, and alkynes with OH rate constant (298 K, 1 atm) less than 3.4×10^{-12} cm^3 molecules^{-1} s^{-1}, [f] ETHP = ethyl peroxyl radical

Table S15 Parameters for aqueous phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_a1	$Cl_2 \xrightarrow{h\nu} 2\,Cl$	2.548×10^{-5}	0.612	0.298	Zimmerman and Strong (1957) with quantum yields from Grossweiner and Matheson (1955)
P_a2	$HOCl \xrightarrow{h\nu} Cl + OH$	2.517×10^{-5}	0.892	0.289	Zimmerman and Strong (1957)[a]
P_a3	$ClO^- \xrightarrow{h\nu, H_2O} Cl + OH^- + OH$	4.205×10^{-4}	0.870	0.284	Anbar and Dostrovsky (1954) with quantum yields from Herrmann (2007)

Table S15 (continued) Parameters for aqueous phase photolysis reactions

	Reaction	l/s^{-1}	m	n	Reference/comment
P_a4	$Cl_3^- \xrightarrow{h\nu} Cl_2 + Cl^-$	5.140×10^{-4}	0.843	0.103	Zimmerman and Strong (1957)[a]
P_a5	$Br_2 \xrightarrow{h\nu} 2\,Br$	4.501×10^{-4}	0.154	0.262	Buckles and Mills (1953)[b] with quantum yields from Grossweiner and Matheson (1955)
P_a6	$HOBr \xrightarrow{h\nu} Br + OH$	1.396×10^{-4}	0.584	0.289	Anbar and Dostrovsky (1954)[a]
P_a7	$BrO^- \xrightarrow{h\nu,\ H_2O} Br + OH^- + OH$	7.510×10^{-4}	0.548	0.300	Anbar and Dostrovsky (1954)[a]
P_a8	$BrCl \xrightarrow{h\nu} Br + Cl$	6.121×10^{-3}	0.456	0.298	Pungor et al. (1959)[a]
P_a9	$I_2 \xrightarrow{h\nu} 2\,I$	1.816×10^{-5}	0.088	0.243	Buckles and Mills (1953)[b] with quantum yields from Grossweiner and Matheson (1955)
P_a10	$ICl \xrightarrow{h\nu} I + Cl$	3.909×10^{-3}	0.130	0.239	Buckles and Mills (1953)[a, b]
P_a11	$IBr \xrightarrow{h\nu} I + Br$	7.940×10^{-3}	0.108	0.250	Buckles and Mills (1954)[a, b]

Photolysis reactions are parameterised with $j = l \times \cos^m \chi \times \exp\{-n \times \sec \chi\}$.
[a]quantum yield estimated with $\Phi = 0.1$; [b]estimated with measurement of the extinction coefficient ϵ in the solvent carbon tetrachloride (CCl_4)

S3.5 Aqueous phase chemistry

Table S16 Aqueous phase irreversible reactions

	Reaction	k_{298}[a]	E_A/R[b]	Comment	Reference
A1	$Cl + Cl \rightarrow Cl_2$	8.75×10^{7}			*Wu80*
A2	$Cl_2^- + Cl \rightarrow Cl_2 + Cl^-$	2.1×10^{9}			*Yu/Bak03*
A3 ⊘	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2\,Cl^-$	1.8×10^{9}			*Jac99*
A4	$Cl^- + O_3 \rightarrow ClO^- + O_2$	3.0×10^{-3}			*Hoi85*
A5	$Cl + H_2O_2 \rightarrow H^+ + Cl^- + HO_2$	2.0×10^{9}			*Yu/Bak03*
A6 ⊗	$Cl_2^- + H_2O_2 \rightarrow 2\,Cl^- + H^+ + HO_2$	5×10^{4}	3340		*Jac99*
A7 ⊘	$Cl_2^- + H_2O \rightarrow H^+ + Cl^- + ClOH^-$	23.4		revised products from Yu and Barker (2003)	*Jac96/Bux98*
A8 ⊗	$Cl_2^- + HO_2 \rightarrow 2\,Cl^- + H^+ + O_2$	1.3×10^{10}			*Jac96*
A9 ⊗	$Cl_2^- + O_2^- \rightarrow 2\,Cl^- + O_2$	6.0×10^{9}			*Jac96*
A10	$Cl_2^- + OH \rightarrow HOCl + Cl^-$	1.0×10^{9}			*Wag86*
A11 ⊗	$Cl_2^- + OH^- \rightarrow 2\,Cl^- + OH$	4.0×10^{6}			*Jac96*
A12	$Cl_3^- + HO_2 \rightarrow Cl_2^- + H^+ + Cl^- + O_2$	1.0×10^{9}			*Bje81*
A13	$Cl_3^- + O_2^- \rightarrow Cl_2^- + Cl^- + O_2$	3.8×10^{9}		estimated	*Mat/Ana06*
P_a4	$Cl_3^- \xrightarrow{h\nu} Cl_2 + Cl^-$	*(4.64×10^{-4})*		$\Phi = 0.1$[c]; see Tab. S15	*Zim/Str57*
A14 ⊕	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+ + O_2$	1.0×10^{9}			*Bje81*
A15 ⊕	$Cl_2 + O_2^- \rightarrow Cl_2^- + O_2$	1.0×10^{9}		estimated ($k_{A15} \approx k_{A14}$)	*Her03*
P_a1	$Cl_2 \xrightarrow{h\nu} 2\,Cl$	*(1.89×10^{-5})*		$\Phi = 0.01$[Gro/Mat55]; see Tab. S15	*Zim/Str57*
A16	$HOCl + H_2O_2 \rightarrow H^+ + Cl^- + H_2O + O_2$	1.1×10^{4}			*Con47*
A17	$ClO^- + H_2O_2 \rightarrow Cl^- + H_2O + O_2$	1.7×10^{5}			*Con47*
A18 ⊕	$HOCl + HO_2 \rightarrow Cl + H_2O + O_2$	7.5×10^{6}		estimated ($k_{A18} \approx k_{A19}$)	*Her03*
A19 ⊕	$HOCl + O_2^- \rightarrow Cl + OH^- + O_2$	7.5×10^{6}			*Lon/Bie80*
A20	$ClO^- + O_2^- \xrightarrow{H_2O} Cl + 2\,OH^- + O_2$	2.0×10^{8}		estimated	*Mat/Ana06*
A21 ⊕	$HOCl + OH \rightarrow ClO + H_2O$	2.0×10^{9}		estimated ($k_{A21} \approx k_{A105}$)	*Her03*
A22	$ClO^- + OH \rightarrow ClO + OH^-$	8.8×10^{9}			*Bux/Sub72*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	k_{298}[a]	E_A/R[b]	Comment	Reference
P_a2	$HOCl \xrightarrow{h\nu} Cl + OH$	*(1.89×10^{-5})*		$\Phi = 0.1^c$; see Tab. S15	*Anb/Dos54*
P_a3	$ClO^- \xrightarrow{h\nu} Cl + OH^- + OH$	*(3.17×10^{-4})*		$\Phi = 4.8155 \cdot \exp\{-0.0113\lambda\}$, fit to measurements of Herrmann (2007); see Tab. S15	*Zim/Str57*
A23 ⊗	$Cl_2^- + HSO_3^- \rightarrow 2\,Cl^- + H^+ + SO_3^-$	1.7×10^8	400		*Jacua96*
A24 ⊗	$Cl_2^- + SO_3^{2-} \rightarrow 2\,Cl^- + SO_3^-$	6.2×10^7			*Jacua96*
A25	$HOCl + SO_3^{2-} \rightarrow Cl^- + HSO_4^-$	7.6×10^8			*Fog89*
A26 ⊕	$HOCl + HSO_3^- \rightarrow Cl^- + H^+ + HSO_4^-$	7.6×10^8		estimated ($k_{A26} \approx k_{A25}$)	*Her03*
A27	$Cl^- + HSO_5^- \rightarrow HOCl + SO_4^{2-}$	1.8×10^{-3}	7352		*For60*
A28 ⊗	$Cl_2^- + CH_2OHSO_3^- \rightarrow 2\,Cl^- + CH_2OHSO_3$	5.0×10^5			*Bar97*
A29 ⊗	$Cl_2^- + NO_2^- \rightarrow 2\,Cl^- + NO_2$	6.0×10^7			*Jac96*
A30 ⊗	$Cl^- + NO_2^+ \rightarrow ClNO_2$	1.0×10^{10}			*Geo99*
A31 ⊗	$Cl_2^- + Fe^{2+} \rightarrow 2\,Cl^- + Fe^{3+}$	1.0×10^7	3030		*Tho/Lau73*
A32 ⊗	$Cl_2^- + Fe^{2+} \rightarrow FeCl^{2+} + Cl^-$	4.0×10^6	3490		*Tho/Lau73*
A33 ⊗	$Cl^- + FeO^{2+} \xrightarrow{H_2O} Fe^{3+} + ClOH^- + OH^-$	100			*Jacs98*
A34 ⊗	$Cl_2^- + Mn^{2+} \rightarrow MnCl_2^+$	2.0×10^7	4090		*Lau/Tho73*
A35 ⊗	$MnCl_2^+ \rightarrow Cl_2^- + Mn^{2+}$	3.0×10^5			*Lau/Tho73*
A36 ⊗	$MnCl_2^+ \rightarrow 2\,Cl^- + Mn^{3+}$	2.1×10^5			*Lau/Tho73*
A37 ⊗	$Cl_2^- + Cu^+ \rightarrow 2\,Cl^- + Cu^{2+}$	1.0×10^8		estimated ($k_{A37} \approx 10 \cdot k_{A31}$)	
A38	$Cl + CO_3^{2-} \rightarrow Cl^- + CO_3^-$	5.0×10^8			*Mer/Son95*
A39	$Cl + HCO_3^- \rightarrow Cl^- + H^+ + CO_3^-$	2.2×10^8			*Mer/Son95*
A40 ⊗	$Cl_2^- + CO_3^{2-} \rightarrow 2\,Cl^- + CO_3^-$	2.7×10^6		estimated	
A41 ⊗	$Cl_2^- + HCO_3^- \rightarrow 2\,Cl^- + H^+ + CO_3^-$	2.7×10^6		estimated	
A42 ⊗	$Cl_2^- + CH_3OOH \rightarrow H^+ + 2\,Cl^- + CH_3OO$	5.0×10^4	3340	estimated ($k_{A42} \approx k_{A6}$)	
A43	$Cl + CH_3OH \rightarrow H^+ + Cl^- + CH_2OH$	1.0×10^9	4089		*Wic03*
A44 ⊘	$Cl_2^- + CH_3OH \rightarrow H^+ + 2\,Cl^- + CH_2OH$	5.1×10^4	5533		*Jac99*
A45	$Cl + C_2H_5OH \rightarrow H^+ + Cl^- + CH_3CHOH$	1.6×10^9			*Par06*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	$k_{298}{}^{a}$	E_A/R^{b}	Comment	Reference
A46 $\otimes$	$Cl_2^- + C_2H_5OH \rightarrow 2\,Cl^- + H^+ + CH_3CHOH$	1.2×10^5		better reference	*Jac99*
A47	$Cl + C_3H_7OH \rightarrow H^+ + Cl^- + C_2H_5CHOH$	2.2×10^9	2285		*Wic03*
A48	$Cl_2^- + C_3H_7OH \rightarrow 2\,Cl^- + H^+ + C_2H_5CHOH$	1.0×10^5			*Jac99*
A49	$Cl + CH_3CHOHCH_3 \rightarrow$ $H^+ + Cl^- + CH_3COHCH_3$	3.2×10^9	2766		*Wic03*
A50	$Cl_2^- + CH_3CHOHCH_3 \rightarrow$ $2\,Cl^- + H^+ + CH_3COHCH_3$	1.9×10^5			*Jac99*
A51	$Cl + CH_2(OH)_2 \rightarrow H^+ + Cl^- + CH(OH)_2$	1.4×10^9	3127	hydration calculated from K with ~1	*Wic03*
A52 $\otimes$	$Cl_2^- + CH_2(OH)_2 \rightarrow 2\,Cl^- + H^+ + CH(OH)_2$	3.6×10^4	4330		*Jac99*
A53	$Cl + CH_3CHO \rightarrow H^+ + Cl^- + CH_3CO$	6.0×10^8	1928	hydration calculated from K with 1:1	*Par06*
A54	$Cl + CH_3CH(OH)_2 \rightarrow$ $H^+ + Cl^- + CH_3C(OH)_2$	6.0×10^8	1928		*Par06*
A55 $\otimes$	$Cl_2^- + CH_3CHO \rightarrow 2\,Cl^- + H^+ + CH_3CO$	4.0×10^4			*Jac96*
A56 $\otimes$	$Cl_2^- + CH_3CH(OH)_2 \rightarrow$ $H^+ + 2\,Cl^- + CH_3C(OH)_2$	4.0×10^4			*Jac96*
A57	$Cl + C_2H_5CHO \rightarrow H^+ + Cl^- + C_2H_5CO$	7.5×10^8	1566	hydration calculated from K with 1:1	*Par06*
A58	$Cl + C_2H_5CH(OH)_2 \rightarrow$ $H^+ + Cl^- + C_2H_5C(OH)_2$	7.5×10^8	1566		*Par06*
A59	$Cl + C_3H_7CHO \rightarrow H^+ + Cl^- + C_3H_7CO$	2.2×10^9	1686	hydration calculated from K with 2:1 (unhydrated/hydrated)	*Par06*
A60	$Cl + C_3H_7CH(OH)_2 \rightarrow$ $H^+ + Cl^- + C_3H_7C(OH)_2$	1.1×10^9	1686		*Par06*
A61	$Cl + CH_3COCH_3 \rightarrow H^+ + Cl^- + CH_3COCH_2$	7.8×10^7			*Wic03*
A62	$Cl_2^- + CH_3COCH_3 \rightarrow$ $2\,Cl^- + H^+ + CH_3COCH_2$	1.4×10^3			*Jac99*
A63	$Cl + HCOOH \rightarrow H^+ + Cl^- + COOH$	2.8×10^9	2405		*Wic03*
A64	$Cl + HCOO^- \rightarrow Cl^- + COOH$	4.2×10^9	1924		*Bux00*
A65 $\otimes$	$Cl_2^- + HCOOH \rightarrow 2\,Cl^- + H^+ + COOH$	8.0×10^4	4450		*Jac99*
A66 $\otimes$	$Cl_2^- + HCOO^- \rightarrow 2\,Cl^- + COOH$	1.3×10^6			*Jac99*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	$k_{298}{}^a$	E_A/R^b	Comment	Reference
A67	$Cl + CH_3COOH \rightarrow H^+ + Cl^- + CH_2COOH$	1.0×10^8	4930		*Wic03*
A68	$Cl + CH_3COO^- \rightarrow Cl^- + CH_3 + CO_2$	3.7×10^9	1684		*Bux00*
A69 ⊗	$Cl_2^- + CH_3COOH \rightarrow$ $2\,Cl^- + H^+ + CH_2COOH$	1.5×10^3	4930		*Jac99*
A70 ⊗	$Cl_2^- + CH_3COO^- \rightarrow 2\,Cl^- + CH_3 + CO_2$	2.6×10^5	4800		*Jac99*
A71	$Cl + C_2H_5COOH \rightarrow$ $H^+ + Cl^- + CH_3CHCOOH$	1.2×10^9	5292		*Wic03*
A72	$Cl + C_2H_5COO^- \rightarrow Cl^- + CH_3CHCOO^-$	1.2×10^9	5292	estimated ($k_{A72} \approx k_{A71}$)	
A73 ⊗	$Cl_2^- + HC_2O_4^- \rightarrow 2\,Cl^- + H^+ + C_2O_4^-$	1.3×10^6		estimated (ETR)	
A74 ⊗	$Cl_2^- + C_2O_4^{2-} \rightarrow 2\,Cl^- + C_2O_4^-$	4.0×10^6		estimated (ETR)	
A75 ⊗	$Cl_2^- + CH(OH)_2CH(OH)_2 \rightarrow$ $2\,Cl^- + H^+ + C(OH)_2CH(OH)_2$	4.0×10^4			
A76 ⊗	$Cl_2^- + CH(OH)_2C(O)OH \rightarrow$ $2\,Cl^- + H^+ + C(OH)_2C(O)OH$	4.0×10^4		estimated ($k_{A76} \approx k_{A75}$)	
A77	$CH_2ClC(OH)_2O_2 \rightarrow CH_2ClCOOH + HO_2$	1.0×10^3		estimated (Cl = H)	
A78	$CH_2ClC(OH)_2O_2 \rightarrow$ $CH_2ClCOO^- + 2\,H^+ + O_2^-$	1.0×10^5		estimated (Cl = H)	
A79	$CH_3COCClO + H_2O \rightarrow$ $CH_3COCOOH + H^+ + Cl^-$	350		estimated same as acetyl chloride	*Pra01*
A80	$CHOCl \rightarrow CO + H^+ + Cl^-$	1.0×10^4			*Pra01*
A81	$CHOCl + OH^- \rightarrow HCOO^- + H^+ + Cl^-$	2.5×10^4			*Pra01*
A82	$COCl_2 + H_2O \rightarrow ClCOOH + H^+ + Cl^-$	10			*Pra01*
A83	$COCl_2 + OH^- \rightarrow ClCOOH + Cl^-$	2.8×10^4			*Pra01*
A84	$ClCOOH \rightarrow CO_2 + H^+ + Cl^-$	1.0×10^5		lower limit	*Pra01*
A85	$Br + Br \rightarrow Br_2$	1.0×10^9		estimated	*Kla/Wol85*
A86 ⊗	$Br_2^- + Br_2^- \rightarrow Br_2 + 2\,Br^-$	1.7×10^9			*Ree99*
A87	$Br^- + O_3 \rightarrow BrO^- + O_2$	210	4450		*Haa/Hoi83*
A88	$Br + HO_2 \rightarrow H^+ + Br^- + O_2$	1.6×10^8			*Wag/Str87*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	$k_{298}{}^{a}$	E_A/R^b	Comment	Reference
A89	$Br + H_2O_2 \rightarrow H^+ + Br^- + HO_2$	4.0×10^9			*Sut65*
A90 ⊕	$Br_2 + HO_2 \rightarrow H^+ + Br_2^- + O_2$	1.1×10^8			*Sut/Dow72*
A91 ⊕	$Br_2 + O_2^- \rightarrow Br_2^- + O_2$	5.6×10^9			*Sut/Dow72*
A92	$Br_2 + H_2O_2 \rightarrow 2\,H^+ + 2\,Br^- + O_2$	1.3×10^3			*Wag/Str87*
A93	$Br_2^- + OH \rightarrow Br^- + HOBr$	1.0×10^9			*Wag/Str87*
A94 ⊗	$Br_2^- + OH^- \rightarrow 2\,Br^- + OH$	1.1×10^4			*Jac96*
A95 ⊘	$Br_2^- + HO_2 \rightarrow 2\,Br^- + H^+ + O_2$	4.4×10^9			*Mat03*
A96	$Br_2^- + HO_2 \xrightarrow{H^+} Br_2 + H_2O_2$	4.4×10^9			*Mat03*
A97 ⊗	$Br_2^- + O_2^- \rightarrow 2\,Br^- + O_2$	1.7×10^8			*Wag/Str87*
A98 ⊗	$Br_2^- + H_2O_2 \rightarrow 2\,Br^- + H^+ + HO_2$	1.0×10^5			*Ree97*
P_a5	$Br_2 \xrightarrow{h\nu} 2\,Br$	*(3.46×10^{-4})*		$\Phi = 0.01^{Gro/Mat55}$; ϵ estimated with measurement in CCl_4; see Tab. S15	*Buc/Mil53*
A99	$Br_3^- + HO_2 \rightarrow Br_2^- + H^+ + Br^- + O_2$	1.0×10^7			*Sut/Dow72*
A100	$Br_3^- + O_2^- \rightarrow Br_2^- + Br^- + O_2$	3.8×10^9			*Sut/Dow72*
A101 ⊕	$BrO + BrO \xrightarrow{H_2O} BrO_2^- + BrO^- + 2\,H^+$	2.8×10^9			*Kla/Wol85*
A102 ⊕	$BrO_2^- + BrO \rightarrow BrO_2 + BrO^-$	4.0×10^8			*Ami/Tre70*
A103 ⊕	$Br_2^- + BrO_2^- \rightarrow 2\,Br^- + BrO_2$	8.0×10^7			*Bux/Dai68*
A104 ⊕	$BrO_2^- + OH \rightarrow BrO_2 + OH^-$	1.8×10^9			*Bux/Dai68*
A105 ⊕	$HOBr + OH \rightarrow BrO + H_2O$	2.0×10^9			*Kla/Wol85*
A106	$BrO^- + OH \rightarrow BrO + OH^-$	4.5×10^9			*Bux/Dai68*
A107 ⊕	$HOBr + HO_2 \rightarrow Br + H_2O + O_2$	1.0×10^9		estimated	*Sut/Dow72*
A108 ⊕	$HOBr + O_2^- \rightarrow Br + OH^- + O_2$	3.5×10^9			*Schw/Bie86*
A109	$BrO^- + O_2^- \xrightarrow{H_2O} Br + 2\,OH^- + O_2$	2.0×10^8		upper limit	*Schw/Bie86*
A110	$HOBr + H_2O_2 \rightarrow H^+ + Br^- + H_2O + O_2$	3.5×10^6			*You50*
A111	$BrO^- + H_2O_2 \rightarrow Br^- + H_2O + O_2$	2.0×10^5		estimated	*Mat/Ana06*
P_a6	$HOBr \xrightarrow{h\nu} Br + OH$	*(1.05×10^{-4})*		$\Phi = 0.1^c$; see Tab. S15	*Anb/Dos54*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	k_{298} [a]	E_A/R [b]	Comment	Reference
P_a7	$BrO^- \xrightarrow{h\nu} Br + OH^- + OH$	*(5.56×10^{-4})*		$\Phi = 0.1^c$; see Tab. S15	*Anb/Dos54*
A112 ⊗	$Br_2^- + HSO_3^- \rightarrow 2\,Br^- + H^+ + SO_3^-$	5.0×10^7	780		*Jac96*
A113 ⊗	$Br_2^- + SO_3^{2-} \rightarrow 2\,Br^- + SO_3^-$	3.3×10^7	650		*Jac96*
A114 ⊗	$Br^- + SO_4^- \rightarrow Br + SO_4^{2-}$	2.1×10^9			*Her97*
A115	$HOBr + SO_3^{2-} \rightarrow Br^- + HSO_4^-$	5.0×10^9			*Tro/Mar91*
A116 ⊕	$HOBr + HSO_3^- \rightarrow H^+ + Br^- + HSO_4^-$	5.0×10^9		estimated ($k_{A116} \approx k_{A115}$)	*Fog89*
A117	$Br^- + HSO_5^- \rightarrow HOBr + SO_4^{2-}$	1.0	5338		*For60*
A118 ⊗	$Br_2^- + CH_2OHSO_3^- \rightarrow 2\,Br^- + CH_2OHSO_3$	5.0×10^4		estimated ($k_{A118} \approx 0.1 \cdot k_{A28}$)	
A119 ⊗	$Br^- + NO_3 \rightarrow Br + NO_3^-$	3.8×10^9			*Zel96*
A120 ⊗	$Br_2^- + NO_2^- \rightarrow 2\,Br^- + NO_2$	1.2×10^7	1720		*Jac96*
A121 ⊗	$Br^- + NO_2^+ \rightarrow BrNO_2$	1.0×10^{10}			*Geo99*
A122 ⊗	$Br^- + BrNO_2 \rightarrow Br_2 + NO_2^-$	2.55×10^4			*Geo99*
A123 ⊗	$Br_2^- + Fe^{2+} \rightarrow 2\,Br^- + Fe^{3+}$	3.6×10^6	3330		*Tho/Lau73*
A124 ⊗	$MnBr_2^+ \rightarrow 2\,Br^- + Mn^{3+}$	2.2×10^5			*Tho/Lau73*
A125 ⊗	$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	6.3×10^6	4330		*Tho/Lau73*
A126 ⊗	$MnBr_2^+ \rightarrow Br_2^- + Mn^{2+}$	3.0×10^5			*Tho/Lau73*
A127 ⊗	$Br_2^- + Cu^+ \rightarrow 2\,Br^- + Cu^{2+}$	3.6×10^6		estimated ($k_{A127} \approx k_{A123}$)	
A128	$Br + HCO_3^- \rightarrow H^+ + Br^- + CO_3^-$	1.0×10^6		estimated	*Mat/Ana06*
A129	$Br_2^- + CO_3^{2-} \rightarrow 2\,Br^- + CO_3^-$	1.1×10^5			*Hui91*
A130 ⊗	$Br_2^- + HCO_3^- \rightarrow 2\,Br^- + H^+ + CO_3^-$	1.1×10^5		estimated	
A131	$Br_2^- + Cl_2^- \rightarrow Br_2 + 2\,Cl^-$	4.0×10^9		estimated	*Mat/Ana06*
A132 ⊕	$Br^- + HOCl \xrightarrow{H^+} BrCl + H_2O$	1.3×10^6			*Kum/Mar87*
A133	$Br^- + ClO^- \xrightarrow{H^+} BrCl + OH^-$	3.65×10^{10}			*Kum/Mar87*
A134 ⊗	$Br^- + ClNO_2 \rightarrow BrCl + NO_2^-$	5.0×10^6			*Geo99*
A135 ⊗	$BrNO_2 + Cl^- \rightarrow BrCl + NO_2^-$	10			*Geo99*
P_a8	$BrCl \xrightarrow{h\nu} Br + Cl$	*(4.54×10^{-3})*		$\Phi = 0.1^c$; see Tab. S15	*Pun59*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	k_{298} [a]	E_A/R [b]	Comment	Reference
A136 $^{\otimes}$	$Br_2^- + CH_3OOH \rightarrow 2\,Br^- + H^+ + CH_3OO$	1.0×10^5		estimated ($k_{A136} \approx k_{A98}$)	
A137	$Br + CH_3OH \rightarrow H^+ + Br^- + CH_2OH$	4.1×10^4	3368		*Par*06
A138 $^{\otimes}$	$Br_2^- + CH_3OH \rightarrow 2\,Br^- + H^+ + CH_2OH$	1.0×10^3			*Ree*97
A139	$Br + C_2H_5OH \rightarrow H^+ + Br^- + CH_3CHOH$	8.2×10^5	2285		*Par*06
A140 $^{\otimes}$	$Br_2^- + C_2H_5OH \rightarrow 2\,Br^- + H^+ + CH_3CHOH$	3.8×10^3			*Ree*99
A141	$Br + C_3H_7OH \rightarrow H^+ + Br^- + C_2H_5CHOH$	3.8×10^5	1564		*Par*06
A142	$Br + CH_3CHOHCH_3 \rightarrow H^+ + Br^- + CH_3COHCH_3$	1.8×10^6	3127		*Par*06
A143	$Br + CH_2(OH)_2 \rightarrow H^+ + Br^- + CH(OH)_2$	3.0×10^5	3608	hydration calculated from K with ~1	*Par*06
A144 $^{\otimes}$	$Br_2^- + CH_2(OH)_2 \rightarrow 2\,Br^- + H^+ + CH(OH)_2$	3.0×10^3		estimated	
A145	$Br + CH_3CHO \rightarrow H^+ + Br^- + CH_3CO$	1.75×10^7	1804	hydration calculated from K with 1:1	*Par*06
A146	$Br + CH_3CH(OH_2) \rightarrow H^+ + Br^- + CH_3C(OH_2)$	1.75×10^7	1804		*Par*06
A147 $^{\otimes}$	$Br_2^- + CH_3CHO \rightarrow 2\,Br^- + H^+ + CH_3CO$	2.15×10^5	2526		*Par*06
A148 $^{\otimes}$	$Br_2^- + CH_3CH(OH)_2 \rightarrow 2\,Br^- + H^+ + CH_3C(OH)_2$	2.15×10^5	2526		*Par*06
A149	$Br + C_2H_5CHO \rightarrow H^+ + Br^- + C_2H_5CO$	2.85×10^7	842	hydration calculated from K with 1:1	*Par*06
A150	$Br + C_2H_5CH(OH_2) \rightarrow H^+ + Br^- + C_2H_5C(OH_2)$	2.85×10^7	842		*Par*06
A151	$Br_2^- + C_2H_5CHO \rightarrow 2\,Br^- + H^+ + C_2H_5CO$	4.95×10^5	3614		*Par*06
A152	$Br_2^- + C_2H_5CH(OH_2) \rightarrow 2\,Br^- + H^+ + C_2H_5C(OH_2)$	4.95×10^5	3614		*Par*06
A153	$Br + C_3H_7CHO \rightarrow H^+ + Br^- + C_3H_7CO$	6.67×10^7	1203	hydration calculated from K with 2:1	*Par*06
A154	$Br + C_3H_7CH(OH_2) \rightarrow H^+ + Br^- + C_3H_7C(OH_2)$	3.33×10^7	1203	(unhydrated/hydrated)	*Par*06
A155	$Br_2^- + C_3H_7CHO \rightarrow 2\,Br^- + H^+ + C_3H_7CO$	2.6×10^5	2289		*Par*06
A156	$Br_2^- + C_3H_7CH(OH_2) \rightarrow 2\,Br^- + H^+ + C_3H_7C(OH_2)$	1.3×10^5	2289		*Par*06

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	k_{298}[a]	E_A/R[b]	Comment	Reference
A157	$Br + HCOOH \rightarrow H^+ + Br^- + COOH$	7.7×10^5	2288		*Par06*
A158	$Br + HCOO^- \rightarrow Br^- + COOH$	4.6×10^8			*Mer/Lin94*
A159 ⊗	$Br_2^- + HCOOH \rightarrow 2\,Br^- + H^+ + COOH$	4.0×10^3			*Ree99*
A160 ⊗	$Br_2^- + HCOO^- \rightarrow 2\,Br^- + COOH$	4.9×10^3			*Jac96*
A161 ⊗	$Br_2^- + CH_3COOH \rightarrow 2\,Br^- + H^+ + CH_2COOH$	10			*Ree99*
A162 ⊗	$Br_2^- + CH_3COO^- \rightarrow 2\,Br^- + CH_3 + CO_2$	100			*Jac96*
A163 ⊗	$Br_2^- + HC_2O_4^- \rightarrow 2\,Br^- + H^+ + C_2O_4^-$	3.7×10^3		estimated (ETR)	
A164 ⊗	$Br_2^- + C_2O_4^{2-} \rightarrow 2\,Br^- + C_2O_4^-$	1.1×10^4		estimated (ETR)	
A165 ⊗	$Br_2^- + CH(OH)_2CH(OH)_2 \rightarrow 2\,Br^- + H^+ + C(OH)_2CH(OH)_2$	500		estimated (H-abstraction)	
A166 ⊗	$Br_2^- + CH(OH)_2COOH \rightarrow 2\,Br^- + H^+ + C(OH)_2COOH$	500		estimated ($k_{A166} \approx k_{A165}$)	
A167	$CH_2BrC(OH)_2O_2 \rightarrow CH_2BrCOOH + HO_2$	1.0×10^3		estimated (Br = H)	
A168	$CH_2BrC(OH)_2O_2 \rightarrow CH_2BrCOO^- + 2\,H^+ + O_2^-$	1.0×10^5		estimated (Br = H)	
A169	$CH_3COCBrO + H_2O \rightarrow H^+ + Br^- + CH_3COCOOH$	350		estimated same as acetyl chloride	*Pra01*
A170	$CHOBr \rightarrow CO + H^+ + Br^-$	1.0×10^4		estimated ($k_{A170} \approx k_{A80}$)	*Pra01*
A171	$CHOBr + OH^- \rightarrow HCOO^- + H^+ + Br^-$	2.5×10^4		estimated ($k_{A171} \approx k_{A81}$)	*Pra01*
A172	$COBr_2 + H_2O \rightarrow BrCOOH + H^+ + Br^-$	10		estimated ($k_{A172} \approx k_{A82}$)	*Pra01*
A173	$COBr_2 + OH^- \rightarrow BrCOOH + Br^-$	2.8×10^4		estimated ($k_{A173} \approx k_{A83}$)	*Pra01*
A174	$BrCOOH \rightarrow CO_2 + H^+ + Br^-$	1.0×10^5		lower limit; estimated ($k_{A174} \approx k_{A84}$)	*Pra01*
A175	$I + I \rightarrow I_2$	1.1×10^{10}			*Bux07*
A176	$I + I_2^- \rightarrow I_3^-$	6.5×10^9			*Bux07*
A177	$I_2^- + I_2^- \rightarrow I_3^- + I^-$	2.5×10^9			*Bux07*
A178	$I^- + O_3 \xrightarrow{H^+} HOI + O_2$	2.17×10^9	8790		*Mag97*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	$k_{298}{}^{a}$	E_A/R^b	Comment	Reference
A179	$I_2 + HO_2 \rightarrow I_2^- + H^+ + O_2$	6.0×10^9		estimated ($k_{A179} \approx k_{A180}$)	*Bux07*
A180	$I_2 + O_2^- \rightarrow I_2^- + O_2$	6.0×10^9			*Bux07*
P_a9	$I_2 \xrightarrow{h\nu} 2\,I$	*(1.42×10^{-5})*		$\Phi = 0.01^{Gro/Mat55}$; ϵ estimated with measurement in CCl_4; see Tab. S15	*Buc/Mil53*
A181	$I_3^- + HO_2 \rightarrow I_2^- + H^+ + I^- + O_2$	2.5×10^8		estimated ($k_{A181} \approx k_{A182}$)	*Bux07*
A182	$I_3^- + O_2^- \rightarrow I_2^- + I^- + O_2$	2.5×10^8			*Bux07*
A183	$HIO_2 + H_2O_2 \rightarrow H^+ + IO_3^- + H_2O$	60			*Fur87*
A184	$IO_2^- + H_2O_2 \rightarrow IO_3^- + H_2O$	60		estimated same as A183	
A185	$IO + IO \xrightarrow{H_2O} HOI + HIO_2$	1.5×10^9			*Bux86*
A186	$I_2 + HSO_3^- \xrightarrow{H_2O} 2\,H^+ + 2\,I^- + HSO_4^-$	1.0×10^6			*Ols/Eps91*
A187	$HOI + SO_3^{2-} \rightarrow I^- + HSO_4^-$	5.0×10^9		estimated ($k_{A187} \approx k_{A115}$)	*Pec07*
A188	$HOI + HSO_3^- \rightarrow H^+ + I^- + HSO_4^-$	5.0×10^9		estimated ($k_{A188} \approx k_{A187}$)	*Pec07*
A189	$I^- + ICl \rightarrow I_2 + Cl^-$	1.1×10^9			*Mar86*
A190	$I^- + HOCl \xrightarrow{H^+} ICl + H_2O$	3.5×10^{11}		changed into reaction of third order at pH≅3.5 according to von Glasow et al. (2002a)	*Nag88*
A191	$I^- + HOBr \rightarrow IBr + OH^-$	5.0×10^9			*Tro/Mar91*
P_a10	$ICl \xrightarrow{h\nu} I + Cl$	*(3.08×10^{-3})*		$\Phi = 0.1^c$; ϵ estimated with measurement in CCl_4; see Tab. S15	*Buc/Mil53*
P_a11	$IBr \xrightarrow{h\nu} I + Br$	*(6.18×10^{-3})*		$\Phi = 0.1^c$; ϵ estimated with measurement in CCl_4; see Tab. S15	*Buc/Mil54*
A192	$HOI + Cl_2 \xrightarrow{H_2O} HIO_2 + 2\,H^+ + 2\,Cl^-$	1.0×10^6			*Len96*
A193	$HOI + HOCl \rightarrow HIO_2 + H^+ + Cl^-$	5.0×10^5			*Cit/Eps88*
A194	$HOI + HOBr \rightarrow HIO_2 + H^+ + Br^-$	1.0×10^6			*Chi/Sim96*
A195	$HIO_2 + HOCl \rightarrow IO_3^- + Cl^- + 2\,H^+$	1.5×10^3			*Len96*
A196	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5×10^3		estimated same as A195	
A197	$HIO_2 + HOBr \rightarrow IO_3^- + Br^- + 2\,H^+$	1.0×10^6			*Chi/Sim96*

Table S16 (continued) Aqueous phase irreversible reactions

	Reaction	$k_{298}{}^{a}$	E_A/R^{b}	Comment	Reference
A198	$IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$	1.0×10^{6}		estimated same as A197	
A199	$CH_2IC(OH)_2O_2 \rightarrow CH_2ICOOH + HO_2$	1.0×10^{3}		estimated (I = H)	
A200	$CH_2IC(OH)_2O_2 \rightarrow CH_2ICOO^- + 2\,H^+ + O_2^-$	1.0×10^{5}		estimated (Cl = H)	
A201	$CHOI \rightarrow CO + H^+ + I^-$	1.0×10^{4}		estimated ($k_{A201} \approx k_{A80}$)	*Pra01*
A202	$CHOI + OH^- \rightarrow HCOO^- + H^+ + I^-$	2.5×10^{4}		estimated ($k_{A202} \approx k_{A81}$)	*Pra01*
A203	$COI_2 + H_2O \rightarrow ICOOH + H^+ + I^-$	10		estimated ($k_{A203} \approx k_{A82}$)	*Pra01*
A204	$COI_2 + OH^- \rightarrow ICOOH + I^-$	2.8×10^{4}		estimated ($k_{A204} \approx k_{A83}$)	*Pra01*
A205	$ICOOH \rightarrow CO_2 + H^+ + I^-$	1.0×10^{5}		lower limit; estimated ($k_{A205} \approx k_{A84}$)	*Pra01*

$^{\otimes}$already implemented in CAPRAM; $^{\oslash}$update of CAPRAM; $^{\oplus}$already implemented in the Halogen Module 1.0
^{a}in $M^{-1}\,s^{-1}$; ^{b}in K; ^{c}estimation according to Herrmann (2007)
[Wu80]Wu et al. (1980); [Yu/Bak03]Yu and Barker (2003); [Jac99]Jacobi et al. (1999); [Hoi85]Hoigné et al. (1985); [Jac96]Jabobi (1996); [Bux98]Buxton et al. (1998); [Wag86]Wagner et al. (1986); [Bje81]Bjergbakke et al. (1981); [Mat/Ana06]Matthew and Anastasio (2006); [Zim/Str57]Zimmerman and Strong (1957); [Her03]Herrmann (2003); [Gro/Mat55]Grossweiner and Matheson (1955); [Con47]Connick (1947); [Lon/Bie80]Long and Bielsky (1980); [Bux/Sub72]Buxton and Subhani (1972); [Anb/Dos54]Anbar and Dostrovsky (1954); [Jacua96]Jacobi et al. (1996); [Fog89]Fogelman et al. (1989); [For60]Fortnum et al. (1960); [Bar97]Barlow et al. (1997); [Zel96]Zellner et al. (1996); [Geo99]George, C. (pers. comm., 1999); [Tho/Lau73]Thornton and Laurence (1973); [Jacs98]Jacobsen et al. (1998); [Lau/Tho73]Laurence and Thornton (1973); [Mer/Son95]Mertens and von Sonntag (1995); [Pra01]Prager et al. (2001); [Wic03]Wicktor et al. (2003); [Par06]Parajuli (2006); [Bux00]Buxton et al. (2000); [Kla/Wol85]Kläning and Wolff (1985); [Ree99]Reese et al. (1999); [Haa/Hoi83]Haag and Hoigné (1983); [Wag/Str87]Wagner and Strehlow (1987); [Sut65]Sutton et al. (1965); [Sut/DOW72]Sutton and Downes (1972); [Mat03]Matthew et al. (2003); [Ree97]Reese (1997); [Buc/Mil53]Buckles and Mills (1953); [Ami/Tre70]Amichai and Treinin (1970); [Bux/Dai68]Buxton and Dainton (1968); [Schw/Bie86]Schwarz and Bielski (1986); [You50]Young (1950); [Her97]Herrmann et al. (1997); [Tro/Mar91]Troy and Margerum (1991); [Gla02]von Glasow et al. (2002a); [Pun59]Pungor et al. (1959); [Hui91]Huie et al. (1991); [Kum/Mar87]Kumar and Margerum (1987); [Mer/Lin94]Merényi and Lind (1994); [Bux07]Buxton and Mulazzani (2007); [Mag97]Magi et al. (1997); [Fur87]Furrow (1987); [Bux86]Buxton et al. (1986); [Chi/Sim96]Chinake and Simoyi (1996); [Schm00]Schmitz (2000); [Ols/Eps91]Olsen and Epstein (1991); [Pec07]Pechtl et al. (2007); [Mar86]Margerum et al. (1986); [Nag88]Nagy et al. (1988); [Buc/Mil54]Buckles and Mills (1954); [Len96]Lengyel et al. (1996); [Cit/Eps88]Citri and Epstein (1988)

Table S17 Aqueous phase equilibria

	Reaction	K^a	$k_{f,298}{}^b$	E_A/R^c	Reference	$k_{b,298}{}^b$	E_A/R^c	Reference	Comm.
E1 $\otimes$	$Cl + Cl^- \rightleftharpoons Cl_2^-$	1.4×10^5	8.5×10^9		*Bux98*	6.0×10^4		*Bux98*	
E2	$Cl_2 + Cl^- \rightleftharpoons Cl_3^-$	0.18	2.0×10^4		*Ers04*	1.1×10^5		*Ers04*	
E3 $\oslash$ d	$Cl_2 + H_2O \rightleftharpoons$ $H^+ + Cl^- + HOCl$	$1.9 \times 10^{-5}e^{-4500/T}$	0.4	8000	*Wan/Mar94*	2.1×10^4	3500	*Wan/Mar94*	*e*
E4 $\otimes$	$HCl \rightleftharpoons H^+ + Cl^-$	1.72×10^6	5.0×10^{11}	-6890	*Mar/Elr85*	2.9×10^5		*Gra/Wes81*	*f*
E5 $\oplus$	$HOCl \rightleftharpoons H^+ + ClO^-$	3.0×10^{-8}	1.5×10^3		*Atk96*	5.0×10^{10}			*g, h*
E6 $\otimes$	$Cl^- + OH \rightleftharpoons ClOH^-$	0.7	4.3×10^9		*Jay73*	6.1×10^9		*Jay73*	
E7	$Cl + OH^- \rightleftharpoons ClOH^-$	7.83×10^8	1.8×10^{10}		*Kla/Wol85*	23		*Kla/Wol85*	
E8 $\otimes$	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	5.1×10^6	2.1×10^{10}		*Jay73*	4.1×10^3		*Jacs97*	
E9 $\otimes$	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	2.2×10^{-4}	1.0×10^4		*Gri87*	4.5×10^7		*Gri87*	
E10 $\otimes$	$Cl^- + SO_4^- \rightleftharpoons Cl + SO_4^{2-}$	1.2	2.52×10^8		*Bux99a*	2.1×10^8		*Bux99a*	
E11 $\otimes$	$Cl^- + NO_3 \rightleftharpoons Cl + NO_3^-$	3.4	3.4×10^8	4300	*Bux99b*	1.0×10^8		*Bux99b*	
E12 $\otimes$	$Cl^- + Fe^{3+} \rightleftharpoons FeCl^{2+}$	1.39	3.0×10^3		*Mar/Sil64*	2.16×10^3			
E13	$CH_2ClCO_3 + H_2O \rightleftharpoons$ $CH_2ClC(OH)_2O_2$	367	1.1×10^7			3.0×10^4			*i*
E14	$CH_2ClCOOH \rightleftharpoons$ $CH_2ClCOO^- + H^+$	1.75×10^{-5}	8.75×10^5	-46		5.0×10^{10}			*i*
E15 $\otimes$	$Br + Br^- \rightleftharpoons Br_2^-$	6.32×10^5	1.2×10^{10}		*Mer/Lin94*	1.9×10^4		*Mer/Lin94*	
E16	$Br_2 + Br^- \rightleftharpoons Br_3^-$	17.5	9.6×10^8		*Ers04*	5.5×10^7		*Ers04*	
E17 $\otimes$ $\oplus$	$Br_2 + H_2O \rightleftharpoons$ $H^+ + Br^- + HOBr$	1.06×10^{-10}	1.7	7500	*Bec96*	1.6×10^{10}		*Bec96*	*d*
E18 $\oplus$	$HBr \rightleftharpoons H^+ + Br^-$	1.0×10^9	5.0×10^{11}		*Atk96*	5.0×10^2			*j, k, l*
E19 $\oplus$	$HOBr \rightleftharpoons H^+ + BrO^-$	2.0×10^{-9}	100		*Atk96*	5.0×10^{10}			*g, h*
E20 $\otimes$	$Br^- + OH \rightleftharpoons BrOH^-$	333	1.1×10^{10}		*Zeh/Rab72*	3.3×10^7		*Zeh/Rab72*	
E21 d $\otimes$	$Br + OH^- \rightleftharpoons BrOH^-$	3.1×10^3	1.3×10^{10}		*Kla/Wol85*	4.2×10^6		*Zeh/Rab72*	
E22 $\otimes$	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	1.8×10^{12}	4.4×10^{10}		*Zeh/Rab72*	2.45×10^{-2}		*Kla/Wol85*	
E23 $\otimes$	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	70	1.9×10^8		*Zeh/Rab72*	2.7×10^6		*Vio81*	

Table S17 (continued) Aqueous phase equilibria

	Reaction	K^a	$k_{f,298}{}^a$	E_A/R^b	Reference	$k_{b,298}{}^a$	E_A/R^b	Reference	Comm.
E24 $\oplus$	$HOBr + HOBr \rightleftharpoons H^+ + Br^- + HBrO_2$	6.7×10^{-12}	2.0×10^{-5}		*Fie86*, *Fie/For86*	3.0×10^{6}		*Fie/For86*	
E25 $\oplus$	$HBrO_2 \rightleftharpoons H^+ + BrO_2^-$	1.3×10^{-5}	6.3×10^{5}		*Fie86*	5.0×10^{10}			*g, h*
E26 $\oplus$	$HOBr + HBrO_2 \rightleftharpoons 2\,H^+ + Br^- + BrO_3^-$	1.7	3.2		*Fie86*, *Fie/For86*	2.0		*Fie/For86*	
E27 $\oplus$	$HBrO_2 + HBrO_2 \rightleftharpoons HOBr + H^+ + BrO_3^-$	3.0×10^{11}	3.0×10^{3}		*Fie86*, *Fie/For86*	1.0×10^{-8}		*Fie/For86*	
E28 $\oplus$	$Br_2O_4 + H_2O \rightleftharpoons H^+ + BrO_3^- + HBrO_2$	52.6	2.2×10^{3}		*Fie86*, *Fie/For86*	42		*Fie/For86*	
E29 $\oplus$	$Br_2O_4 \rightleftharpoons 2\,BrO_2$	5.3×10^{-5}	7.4×10^{4}		*Fie86*, *Fie/For86*	1.4×10^{9}		*Fie/For86*	
E30	$Br^- + CO_3^- \rightleftharpoons Br + CO_3^{2-}$	0.05	1.0×10^{5}		*Mat/Ana06*	2.0×10^{6}		*Mat/Ana06*	*h, l*
E31 $\oplus$	$BrCl \overset{H_2O}{\rightleftharpoons} HOBr + H^+ + Cl^-$	1.8×10^{-5}	1.0×10^{5}		*Wan94*	5.6×10^{9}			*k*
E32	$BrCl^- \rightleftharpoons Br^- + Cl$	1.6×10^{-7}	1.9×10^{3}		*Don02*	1.2×10^{10}		*Don02*	
E33	$BrCl^- \rightleftharpoons Br + Cl^-$	6.1×10^{-4}	6.1×10^{4}		*Don02*	1.0×10^{8}		*Don02*	
E34	$BrCl^- + Br^- \rightleftharpoons Br_2^- + Cl^-$	1.86×10^{3}	8.0×10^{9}		*Ers04*	4.3×10^{6}		*Ers04*	
E35	$BrCl^- + Cl^- \rightleftharpoons Cl_2^- + Br^-$	2.75×10^{-8}	110		*Ers04*	4.0×10^{9}		*Ers04*	
E36 $\oplus$	$Br_2Cl^- \rightleftharpoons BrCl + Br^-$	5.6×10^{-5}	4.3×10^{5}		*Wan94*	7.7×10^{9}			*j, m*
E37 $\ominus$	$Br_2Cl^- \rightleftharpoons Br_2 + Cl^-$	0.76	3.8×10^{4}		*Wan94*	5.0×10^{4}		*Mat/Ana06*	*h, l*
E38 $\ominus$	$BrCl_2^- \rightleftharpoons BrCl + Cl^-$	0.17	1.7×10^{5}		*Ers04*	1.0×10^{6}		*Ers04*	
E39 $\ominus$	$BrCl_2^- \rightleftharpoons Br^- + Cl_2$	1.5×10^{-6}	9.0×10^{3}		*Ers04*	6.0×10^{9}		*Ers04*	
E40	$Br^- + ClOH^- \rightleftharpoons BrCl^- + OH^-$	333.3	1.0×10^{9}		*Mat/Ana06*	3.0×10^{6}		*Mat/Ana06*	*l, m*
E41	$BrOH^- + Cl^- \rightleftharpoons BrCl^- + OH^-$	9.5	1.9×10^{8}		*Mat/Ana06*	2.0×10^{7}		*Mat/Ana06*	*h, l*
E42	$CH_2BrCO_3 + H_2O \rightleftharpoons CH_2BrC(OH)_2O_2$	367	1.1×10^{7}			3.0×10^{4}			*i*
E43	$CH_2BrCOOH \rightleftharpoons CH_2BrCOO^- + H^+$	1.75×10^{-5}	8.75×10^{5}	-46		5.0×10^{10}			*i*
E44	$I + I^- \rightleftharpoons I_2^-$	1.36×10^{5}	9.1×10^{9}		*Bux07*	6.7×10^{4}		*Bux07*	

Table S17 (continued) Aqueous phase equilibria

	Reaction	K^a	$k_{f,298}{}^a$	E_A/R^b	Reference	$k_{b,298}{}^a$	E_A/R^b	Reference	Comm.
E45	$I_2 + I^- \rightleftharpoons I_3^-$	713	6.2×10^9		*Bux07*	8.7×10^6		*Bux07*	
E46	$HI \rightleftharpoons H^+ + I^-$	3.2×10^9	5.0×10^{11}		*Schw00*	156			*j, k, l*
E47	$HOI \rightleftharpoons H^+ + IO^-$	3.16×10^{-11}	1.58		*Lid95*	5.0×10^{10}			*g, h*
E48	$HOI + H^+ + I^- \overset{H_2O}{\rightleftharpoons} I_2$	1.47×10^{12}	4.4×10^{12}		*Eig/Kus62*	3.0		*Eig/Kus62*	*j, m*
E49	$HOI + HOI \rightleftharpoons HIO_2 + H^+ + I^-$	1.25×10^{-9}	25		*Schm04*	2.0×10^{10}		*Edb87*	*j, m*
E50	$HOI + HOI \rightleftharpoons IO_2^- + 2\,H^+ + I^-$	1.25×10^{-9}	25		*Schm04*	2.0×10^{10}			*h, j, m*
E51	$HIO_2 \rightleftharpoons H^+ + IO_2^-$	2.51×10^{-2}	1.26×10^9			5.0×10^{10}			*g, h*
E52	$HIO_3 \rightleftharpoons H^+ + IO_3^-$	0.17	8.5×10^9		*Lid95*	5.0×10^{10}			*g, h*
E53	$HIO_2 + HOI \rightleftharpoons$ $IO_3^- + I^- + 2\,H^+$	0.2	2.4×10^2		*Fur87*	1.2×10^3		*Schm00*	
E54	$IO_2^- + HOI \rightleftharpoons IO_3^- + I^- + H^+$	0.2	2.4×10^2			1.2×10^3		*Schm00*	*l*
E55	$IO_2^- + I_2 \overset{H_2O}{\rightleftharpoons} IO_3^- + 2\,I^- + 2\,H^+$	1.3×10^{-13}	5.5×10^{-5}			4.2×10^8		*Schm00*	*l, m*
E56	$IBr + I^- \rightleftharpoons I_2 + Br^-$	4.2×10^5	2.0×10^9		*Far93*	4.74×10^3		*Far93*	*m*
E57	$HOI + H^+ + Cl^- \overset{H_2O}{\rightleftharpoons} ICl$	1.2×10^4	2.9×10^{10}		*Wan89*	2.4×10^6		*Wan89*	*j, m*
E58	$HOI + H^+ + Br^- \overset{H_2O}{\rightleftharpoons} IBr$	5.1×10^6	4.1×10^{12}		*Far93*	8.0×10^5		*Far93*	*j, m*
E59	$ICl + Cl^- \rightleftharpoons ICl_2^-$	77	4.24×10^9			5.5×10^7			*g, h*
E60	$IBr + Br^- \rightleftharpoons IBr_2^-$	290	4.93×10^6			1.7×10^5			*g, h*
E61	$ICl + Br^- \rightleftharpoons IClBr^-$	1.8×10^4	7.7×10^9			4.3×10^5			*h, l, n*
E62	$IBr + Cl^- \rightleftharpoons IClBr^-$	1.3	5.0×10^4			3.8×10^4			*h, l, n*

Table S17 (continued) Aqueous phase equilibria

	Reaction	K^a	$k_{f,298}{}^a$	E_A/R^b	Reference	$k_{b,298}{}^a$	E_A/R^b	Reference	Comm.
E63	$CH_2ICO_3 + H_2O \rightleftharpoons CH_2IC(OH)_2O_2$	367	1.1×10^7			3.0×10^4			^{i}
E64	$CH_2ICOOH \rightleftharpoons CH_2ICOO^- + H^+$	1.75×10^{-5}	8.75×10^5	-46		5.0×10^{10}			^{i}

$^{\otimes}$already implemented in CAPRAM; $^{\oslash}$update of CAPRAM; $^{\oplus}$already implemented in the Halogen Module 1.0; $^{\ominus}$update of the Halogen Module 1.0 (when subscripts are present in remarks: superscripts concern only forward reaction and subscript concern only backward reaction)
^{a}in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; ^{b}in $M^{-1}\ s^{-1}$; ^{c}in K; ^{d}now implemented as equilibrium in CAPRAM; ^{e}correction of CAPRAM value; $^f k_f$ = speed of hydrogen bond breaking in water; $^g k_f$ calculated based on K; $^h k_b$ estimated; ^{i}estimated X = H (X = Cl, Br, I) ^{j}diffusion controlled; $^k k_b$ calulated based on K; $^l k_f$ estimated; ^{m}upper limit; $^n K$ estimated
[Bux98]Buxton et al. (1998); [Ers04]Ershov (2004); [Wan/Mar94]Wang and Margerum (1994); [Mar/Elr85]Marsh and McElroy (1985); [Gra/Wes81]Graedel and Weschler (1981); [Atk96]ATKINS, 1996; [Jay73]Jayson et al. (1973); [Kla/Wol85]Kläning and Wolff (1985); [Jacs97]Jacobsen et al. (1997); [Gri87]Grigor'ev et al. (1987); [Bux99a]Buxton et al. (1999a); [Bux99b]Buxton et al. (1999b); [Mar/Sil64]Martell and Sillen (1964); [Mer/Lin94]Merényi and Lind (1994); [Bec96]Beckwith et al. (1996); [Zeh/Rab72]Zehavi and Rabani (1972); [Vio81]Fornier de Violet (1981); [Fie86]FIELD, 1986; [Fie/For86]Field and Försterling (1986); [Mat/Ana06]Matthew and Anastasio (2006); [Wan94]Wang et al. (1994); [Don02]Donati (2002); [Bux07]Buxton and Mulazzani (2007); [Eig/Kus62]Eigen and Kustin (1962); [Schw00]Schweitzer et al. (2000); [Lid95]Lide et al. (1995); [Schm04]Schmitz (2004); [Edb87]Edblom et al. (1987); [Schm00]Schmitz (2000); [Far93]Faria et al. (1993); [Wan89]Wang et al. (1989); [Tro91]Troy et al. (1991); [Tro/Mar91]Troy and Margerum (1991)

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