

Tables S1-S4: Aqueous chemistry and gas-phase halogen chemistry

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The tables listed here give the reactions used to represent aqueous and halogen chemistry in the model described by *Sillman et al.* [2007] (Reactive mercury in the troposphere: Model formation and results for Florida, the northeastern U.S. and the Atlantic Ocean, *J. Geophys. Res.*, 10.1029/2006JD008227, 2007).

Reactions for atmospheric mercury are not included here. They are described separately (Tables S5-S8).

The mechanism for gas-phase photochemistry (other than mercury or halogens) is described in Appendix A of *Ito et al.* [2007].

The reactions and rates included here are taken from compilations by *Jacob et al.* [1986], *Pandis and Seinfeld* [1989], *Lelieveld et al.* [1990], *Liu et al.* [1997], *Sander and Crutzen* [1996] and *Sander et al.* [2003]. These studies are cited as references for the individual rates. Readers are referred there for the primary sources.

This file includes the following tables:

- Table S1: Henry's law coefficients
- Table S2: Aqueous equilibrium coefficients.
- Table S3: Aqueous reactions.
- Table S4: Gas-phase reactions involving halogens.

Table S1
Henry's Law coefficients

Values here represent the physical Henry constants (K_H) and do not take into account enhanced solubilities due to dissociation equilibria.

Abbreviations and units:

K_{H298} =Henry's law coefficient at 298 K, expressed in $M \text{ atm}^{-1}$.

ΔH = enthalpy of solution, expressed as $\Delta H/R$ (where R represents the gas constant) in units $^{\circ}K$.

The temperature dependence is represented by $K_H = K_{H298} \exp[-\Delta H/R(1/T - 1/298)]$ for temperature T in $^{\circ}K$.

Species	K_{H298}	$\Delta H/R$	Reference
CO ₂	3.4E-02	2420.	<i>Pandis, 1989</i>
H ₂ O ₂	7.73E+04	-7310.	<i>JPL, 2003</i>
OH	2.5E+01	-5280.	<i>Jacob, 1986</i>
HO ₂	2.0E+03	-6640.	<i>Jacob, 1986</i>
O ₃	1.03E-02	-2830.	<i>JPL, 2003</i>
NO ₂	1.0E-02	-2500.	<i>Pandis, 1989</i>
NO	1.9E-03	-1480.	<i>Pandis, 1989</i>
HNO ₃	2.1E+05	0.	<i>Lelieveld, 1991,</i> <i>Sander, 1996</i>
HONO	5.1E-04	1260.	<i>Pandis, 1989</i>
NH ₃	7.5E+01	-3400.	<i>Pandis, 1989</i>
PAN	2.9E+00	-5910.	<i>Pandis, 1989</i>
CH ₃ CO ₃	1.0E+02	0.	<i>Pandis, 1989</i>
CH ₃ C(O)OOH	4.73E+02	-6170.	<i>Pandis, 1989</i>
CH ₃ O ₂	6.0E+00	-5600.	<i>Pandis, 1989</i>
CH ₃ OOH (MP)	2.27E+02	-5610.	<i>Pandis, 1989</i>
HCHO	6.3E+03	-6460.	<i>Pandis, 1989</i>
CH ₃ CHO	1.14E+01	-6460.	<i>Hermann, 2000</i>

CH ₃ OH	2.2E+02	-4900.	<i>Pandis, 1989</i>
CH ₃ COOH (Acetic acid)	5.5E+03	-5740.	<i>Hermann, 2000</i>
H ₂ SO ₄ ¹	1.0E+08	0.	See note 1
HCl	1.1E+00	2023.	<i>Sander, 1996</i>
Cl ₂	9.2E-02	0.	<i>Sander, 1996</i>
HOCl	4.8E+02	1633.	<i>Sander, 1996</i>
HBr	7.2E-01	6077.	<i>Sander, 1996</i>
HOBr	4.8E+01	0.	<i>Sander, 1996</i>

1. H₂SO₄ and other species that form soluble aerosols are represented by a gas-phase pseudo-species with a very high Henry constant, which insures rapid incorporation into the aqueous phase. This is used in model calculations that do not include explicit treatment of aerosols.

Table S2
Aqueous equilibrium coefficients

K_{aq} represents the equilibrium constant for reactions with the form $C \rightleftharpoons A+B$, with format $K_{aq} = [A][B]/[C]$, in M.

Abbreviations and units:

K_{aq298} =equilibrium constant at 298 K, in M.

ΔH = reaction enthalpy, expressed as $\Delta H/R$ (where R represents the gas constant) in units $^{\circ}K$.

The temperature dependence is represented by $K_{aq} = K_{aq298} \exp[-\Delta H/R(1/T - 1/298)]$ for temperature T in $^{\circ}K$.

Reaction	K_{aq298}	$\Delta H/R$	Reference
$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.46E-07	1000.	<i>Pandis, 1989</i>
$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$	4.68E-11	1760.	<i>Pandis, 1989</i>
$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.23E-02	1960.	<i>Pandis, 1989</i>
$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.61E-08	-1500.	<i>Sander, 1996</i>
$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E+03		<i>Pandis, 1989</i>
$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.02E-02	-2720.	<i>Pandis, 1989</i>
$H_2O_2 \rightleftharpoons H^+ + HO_2^-$	2.2E-12	3730.	<i>Pandis, 1989</i>
$HO_2 \rightleftharpoons H^+ + O_2^-$	1.6E-05	0.	<i>Sander, 1996</i>
$HNO_3 \rightleftharpoons H^+ + NO_3^-$	1.54E+01	-8700.	<i>Pandis, 1989</i>
$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-04	1260.	<i>Pandis, 1989</i>
$NH_3 \rightleftharpoons OH^- + NH_4^+$	1.7E-05	-4325.	<i>Pandis, 1989</i>
$HCHO + H_2O \rightleftharpoons H_2C(OH)_2$	1.82E+03 ¹	-4020.	<i>Pandis, 1989,</i> <i>Sander, 2004</i>
$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.78E-04	20.	<i>Pandis, 1989</i>
$HOCH_2SO_3^-$ (HMS-) \rightleftharpoons $H^+ + OCH_2SO_3^{2-}$	2.0E-12		<i>Jacob et al., 1986</i>

$\text{CH}_3\text{C}(\text{O})\text{OOH} \leftrightarrow \text{H}^+ + \text{CH}_3\text{C}(\text{O})\text{OO}^-$	1.78E-04	0.	assumed equal to HCOOH
$\text{CH}_3\text{COOH} \leftrightarrow \text{H}^+ + \text{CH}_3\text{COO}^-$	1.75E-05	0.	<i>Hermann, 2000</i>
$\text{HCl} \leftrightarrow \text{H}^+ + \text{Cl}^-$	1.74E+06	-6900.	<i>Sander, 1996</i>
$\text{Cl} \leftrightarrow \text{H}^+ + \text{ClOH}^-$	6.19E-08	0.	<i>Pandis, 1989,</i> <i>Sander, 1996. see note 1</i>
$\text{HOCl} \leftrightarrow \text{H}^+ + \text{OCl}^-$	3.2E-08	0.	<i>Sander, 1996</i>
$\text{HBr} \leftrightarrow \text{H}^+ + \text{Br}^-$	1.0E+09	0.	<i>Sander, 1996</i>
$\text{HOBr} \leftrightarrow \text{H}^+ + \text{OBr}^-$	2.100E-09	0.	<i>Sander, 1996</i>
$\text{Cl}_2 \leftrightarrow \text{Cl} + \text{Cl}^-$	5.26E-06		<i>Sander, 1996</i>
$\text{Br}_2 \leftrightarrow \text{Br} + \text{Br}^-$	9.1E-06		<i>Sander, 1996</i>

Notes:

1. This equilibrium coefficient is derived from the rates reported by *Pandis and Seinfeld* [1989] and *Sander and Crutzen* [1996] for the reactions $\text{Cl} \rightarrow \text{H}^+ + \text{ClOH}^-$ and $\text{H}^+ + \text{ClOH}^- \rightarrow \text{Cl}$.

Table S3
Aqueous reactions

k_{298} : rate constant at 298 K, in $M s^{-1}$ (for reactions involving two species) or s^{-1} for reactants involving a single species.

E_a : activation energy, expressed as E_a/R (where R represents the gas constant) in units $^{\circ}K$.

The temperature dependence is represented by $k_T = k_{298} \exp[-E_a/R(1/T - 1/298)]$ for temperature T in $^{\circ}K$.

Reaction	k_{298}	E_a/R	References
$OH + HO_2 \rightarrow$	7.0E+09	1500.	<i>Pandis, 1989</i>
$OH + O_2^- \rightarrow OH^-$	1.0E+10	1500	<i>Pandis, 1989</i>
$OH + H_2O_2 \rightarrow HO_2$	2.7E+07	1700.	<i>Pandis, 1989</i>
$HO_2 + HO_2 \rightarrow H_2O_2$	8.6E+05	2365.	<i>Pandis, 1989</i>
$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E+08	1500.	<i>Pandis, 1989</i>
$O_2^- + O_2^- \rightarrow H_2O_2 + 2OH^-$	3.0E-01	0.	<i>Pandis, 1989</i>
$HO_2 + H_2O_2 \rightarrow OH$	5.0E-01		<i>Pandis, 1989</i>
$O_2 + H_2O_2 \rightarrow OH$	1.3E-01		<i>Pandis, 1989</i>
$OH + O_3 \rightarrow HO_2$	2.0E+09		<i>Pandis, 1989</i>
$HO_2 + O_3 \rightarrow OH$	1.0E+04		<i>Pandis, 1989</i>
$O_2^- + O_3 \rightarrow OH + OH^-$	1.5E+09	1500.	<i>Pandis, 1989</i>
$OH^- + O_3 \rightarrow HO_2 + O_2^-$	7.0E+01		<i>Pandis, 1989</i>
$HO_2^- + O_3 \rightarrow OH + O_2^-$	2.8E+06	0.	<i>Pandis, 1989</i>
$HCO_3 + OH \rightarrow CO_3^-$	1.5E+07	1910.	<i>Pandis, 1989</i>
$HCO_3 + O_2^- \rightarrow CO_3^- + HO_2^-$	1.5E+06	0.	<i>Pandis, 1989</i>
$CO_3^- + O_2^- \rightarrow HCO_3 + OH^-$	4.0E+08	1500.	<i>Pandis, 1989</i>
$CO_3^- + H_2O_2 \rightarrow HCO_3 + HO_2$	8.0E+05	2820.	<i>Pandis, 1989</i>
$HCO_3 + OH \rightarrow CO_3^-$	1.4E-12	900	<i>Pandis, 1989</i>
$Cl^- + HOCl + H^+ \rightarrow Cl_2$	1.8E+04	6900.	<i>Sander, 1996¹</i>

$\text{Cl}_2 \rightarrow \text{Cl}^- + \text{HOCl}$	1.1E+01	0.	<i>Sander, 1996</i>
$\text{Cl}_2^- + \text{HO}_2 \rightarrow 2\text{Cl}^- + \text{H}^+$	4.5E+09	0.	<i>Sander, 1996</i>
$\text{Cl}_2^- + \text{O}_2^- \rightarrow 2\text{Cl}^-$	1.0E+09	0.	<i>Sander, 1996</i>
$\text{Cl}_2^- + \text{H}_2\text{O}_2 \rightarrow 2\text{Cl}^- + \text{HO}_2 + \text{H}^+$	1.4E+05	3370.	<i>Pandis, 1989</i>
$\text{Cl}_2^- + \text{OH}^- \rightarrow 2\text{Cl}^- + \text{OH}$	7.3E+06	2160.	<i>Pandis, 1989</i>
$\text{Cl} + \text{HO}_2 \rightarrow \text{Cl}^- + \text{H}^+$	3.1E+09	1500.	<i>Pandis, 1989</i>
$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{Cl}^- + \text{HO}_2 + \text{H}^+$	4.5E+07	0.	<i>Pandis, 1989</i>
$\text{Cl}^- + \text{OH}^- \rightarrow \text{ClOH}^-$	4.3E+09	1500.	<i>Pandis, 1989,</i> <i>Sander, 1996</i>
$\text{ClOH}^- \rightarrow \text{Cl}^- + \text{OH}$	6.1E+09	0.	<i>Pandis, 1989,</i> <i>Sander, 1996</i>
$\text{SO}_4^- + \text{Cl}^- \rightarrow \text{SO}_4^{=} + \text{Cl}$	2.0E+08	1500.	<i>Pandis, 1989</i>
$\text{NO}_3 + \text{Cl}^- \rightarrow \text{NO}_3^- + \text{Cl}$	1.0E+8	1500.	<i>Pandis, 1989</i>
$\text{Br}_2^- + \text{HO}_2 \rightarrow 2\text{Br}^- + \text{H}^+$	4.4E+09	0.	<i>Sander, 1996, 2004</i>
$\text{Br}_2^- + \text{O}_2^- \rightarrow 2\text{Br}^-$	1.7E+08	0.	<i>Sander, 1996</i>
$\text{Br}_2^- + \text{H}_2\text{O}_2 \rightarrow 2\text{Br}^- + \text{HO}_2 + \text{H}^+$	1.0E+05	0.	<i>Sander, 2004</i>
$\text{Br}_2^- + \text{OH}^- \rightarrow 2\text{Br}^- + \text{OH}$	1.1E+10	0.	<i>Sander, 2004</i>
$\text{HOBr} + \text{HO}_2 \rightarrow \text{Br}^-$	1.0E+09	0.	<i>Sander, 2004</i>
$\text{HOBr} + \text{O}_2^- \rightarrow \text{Br}^-$	3.5E+09	0.	<i>Sander, 2004</i>
$\text{SO}_4 + \text{Br}^- \rightarrow \text{SO}_4^- + \text{Br}$	3.5E+09	0.	<i>Sander, 1996</i>
$\text{NO}_3 + \text{Br}^- \rightarrow \text{NO}_3^- + \text{Br}$	4.0E+09	1500.	<i>Sander, 1996, 2004</i>
$\text{NO} + \text{NO}_2 \rightarrow 2\text{NO}_2^- + \text{H}^+$	2.0E+8	1500.	<i>Pandis, 1989</i>
$\text{NO}_2 + \text{NO}_2 \rightarrow \text{NO}_2^- + \text{NO}_3^- + 2\text{H}^+$	1.0E+8	1500.	<i>Pandis, 1989</i>
$\text{NO} + \text{OH}^- \rightarrow \text{NO}_2^- + \text{H}^+$	2.0E+10	1500.	<i>Pandis, 1989</i>
$\text{NO}_2 + \text{OH}^- \rightarrow \text{NO}_3^- + \text{H}^+$	1.3E+09	1500.	<i>Pandis, 1989</i>
$\text{HONO} + \text{OH}^- \rightarrow \text{NO}_2$	1.0E+09	1500.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{OH}^- \rightarrow \text{NO}_2 + \text{OH}^-$	1.0E+10	1500.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{O}_3 \rightarrow \text{NO}_3^-$	5.0E+05	6950.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_3^-$	1.2E+09	1500.	<i>Pandis, 1989</i>

$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_3^- + \text{H}^+$	1.2E+09	1500.	<i>Jacob, 1986</i>
$\text{NO}_3 + \text{O}_2^- \rightarrow \text{NO}_3^-$	1.0E+09	1500.	<i>Jacob, 1986</i>
$\text{NO}_3 + \text{H}_2\text{O}_2 \rightarrow \text{NO}_3^- + \text{HO}_2 + \text{H}^+$	1.0E+06	2800.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{CO}_3^- \rightarrow \text{NO}_2 + \text{CO}_3^{-2}$	4.0E+05	0.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{Cl}_2^- \rightarrow \text{NO}_2 + 2\text{Cl}^-$	2.5E+08	1500.	<i>Pandis, 1989</i>
$\text{NO}_2^- + \text{Br}_2^- \rightarrow \text{NO}_2 + 2\text{Br}^-$	1.7E+07	0.	<i>Sander, 2004</i>
$\text{H}_2\text{C}(\text{OH})_2 + \text{OH}^- \rightarrow \text{HCOOH} + \text{HO}_2$	2.0E+09	1500.	<i>Pandis, 1989</i>
$\text{HCOOH} + \text{OH}^- \rightarrow \text{CO}_2 + \text{HO}_2$	1.6E+08	1500.	<i>Pandis, 1989</i>
$\text{HCOO}^- + \text{OH}^- \rightarrow \text{CO}_2 + \text{HO}_2 + \text{OH}^-$	2.5E+09	1500.	<i>Pandis, 1989</i>
$\text{HCOOH} + \text{NO}_3^- \rightarrow$ $\text{NO}_3^- + \text{CO}_2 + \text{HO}_2 + \text{H}^+$	2.1E+05	3200.	<i>Pandis, 1989</i>
$\text{HCOO}^- + \text{NO}_3^- \rightarrow \text{NO}_3^- + \text{CO}_2 + \text{HO}_2$	6.0E+07	1500.	<i>Jacob, 1986</i>
$\text{HCOOH} + \text{O}_3 \rightarrow \text{CO}_2 + \text{HO}_2 + \text{OH}^-$	5.0E+00	0.	<i>Pandis, 1989</i>
$\text{HCOO}^- + \text{O}_3 \rightarrow \text{CO}_2 + \text{O}_2^- + \text{OH}^-$	1.0E+02	0.	<i>Pandis, 1989</i>
$\text{HCOO}^- + \text{CO}_3^- \rightarrow$ $\text{HCO}_3^- + \text{CO}_2 + \text{HO}_2 + \text{OH}^-$	1.1E+05	3400.	<i>Pandis, 1989</i>
$\text{HCOOH} + \text{Cl}_2^- \rightarrow$ $\text{CO}_2 + \text{HO}_2 + 2\text{Cl}^- + \text{H}^+$	6.7E+03	4300.	<i>Pandis, 1989</i>
$\text{HCOO}^- + \text{Cl}_2^- \rightarrow \text{CO}_2 + \text{HO}_2 + 2\text{Cl}^-$	1.9E+06	2600.	<i>Pandis, 1989</i>
$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH}$	4.3E+05	3000.	<i>Jacob, 1986</i>
$\text{CH}_3\text{O}_2 + \text{O}_2^- \rightarrow \text{CH}_3\text{OOH} + \text{OH}^-$	5.0E+07	1600.	<i>Jacob, 1986</i>
$\text{CH}_3\text{OOH} + \text{OH}^- \rightarrow \text{CH}_3\text{O}_2$	2.7E+07	1700.	<i>Jacob, 1986</i>
$\text{CH}_3\text{OOH} + \text{OH}^- \rightarrow \text{HCHO} + \text{OH}^-$	1.9E+07	1800.	<i>Jacob, 1986</i>
$\text{CH}_3\text{OH} + \text{OH}^- \rightarrow \text{HCHO} + \text{HO}_2$	4.5E+06	1500.	<i>Pandis, 1989</i>
$\text{CH}_3\text{OH} + \text{CO}_3^-$ $\rightarrow \text{HCHO} + \text{HO}_2 + \text{HCO}_3^-$	2.6E+03	4500.	<i>Pandis, 1989</i>
$\text{CH}_3\text{OH} + \text{Cl}_2^-$ $\rightarrow \text{HCHO} + \text{HO}_2 + 2\text{Cl}^- + \text{H}^+$	3.5E+03	4400.	<i>Pandis, 1989</i>
$\text{CH}_3\text{OH} + \text{NO}_3^-$ $\rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	1.0E+06	2800	<i>Pandis, 1989</i>

$\text{CH}_3\text{CO}_3 + \text{O}_2^- \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}^-$	1.0E+09	0.	
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CHO} \rightarrow$ $2\text{CH}_3\text{COOH} + 2\text{H}^+$	1.5E-02	0.	
$\text{SO}_2 + \text{O}_3 \rightarrow \text{H}_2\text{SO}_4$	2.4E+04	0.	<i>Pandis, 1989</i>
$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{HSO}_4^-$	3.7E+05	5530.	<i>Pandis, 1989</i>
$\text{SO}_3^{-2} + \text{O}_3 \rightarrow \text{SO}_4^{-2}$	1.5E+09	5280.	<i>Pandis, 1989</i>
$\text{SO}_2 + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{SO}_4$	1.3E+06	4430.	<i>Pandis, 1989</i>
$\text{HSO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{HSO}_4^-$	5.2E+06	3650.	<i>Sander, 2004</i>
$\text{HSO}_3^- + \text{OH}^- \rightarrow \text{SO}_5^-$	4.2E+09	1500.	<i>Pandis, 1989</i>
$\text{SO}_3^{-2} + \text{OH}^- \rightarrow \text{SO}_5^- + \text{OH}^-$	4.6E+09	1500.	<i>Pandis, 1989</i>
$\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{SO}_5^- + \text{HSO}_5^-$	3.0E+05	3100.	<i>Pandis, 1989</i>
$\text{SO}_5^- + \text{SO}_3^{-2} \rightarrow \text{SO}_4^{-2} + \text{SO}_4^-$	1.3E+07	2000.	<i>Jacob, 1986 (1.0E07)</i>
$\text{SO}_5^- + \text{O}_2^- \rightarrow \text{HSO}_5^- + \text{OH}^-$	1.0E+08	1500.	<i>Jacob, 1986</i>
$\text{SO}_5^- + \text{HCOOH} \rightarrow$ $\text{HSO}_5^- + \text{CO}_2 + \text{HO}_2$	2.0E+02	5300.	<i>Jacob, 1986</i>
$\text{SO}_5^- + \text{HCOO}^- \rightarrow$ $\text{HSO}_5^- + \text{CO}_2 + \text{O}_2^-$	1.4E+04	4000.	<i>Jacob, 1986</i>
$\text{SO}_5^- + \text{SO}_5^- \rightarrow 2\text{SO}_4^-$	2.0E+08	1500.	<i>Jacob, 1986</i>
$\text{HSO}_5^- + \text{OH}^- \rightarrow \text{SO}_5^-$	1.7E+07	1900.	<i>Jacob, 1986</i>
$\text{HSO}_5^- + \text{SO}_4^- \rightarrow \text{SO}_5^- + \text{SO}_4^{-2} + \text{H}^+$	1.0E+05	0.	<i>Jacob, 1986</i>
$\text{HSO}_5^- + \text{NO}_2^- \rightarrow \text{HSO}_4^- + \text{NO}_3^-$	3.1E-01	6650.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{HSO}_3^- \rightarrow \text{SO}_5^- + \text{SO}_4^{-2} + \text{H}^+$	1.3E+09	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{SO}_3^{-2} \rightarrow \text{SO}_5^- + \text{SO}_4^{-2}$	5.3E+08	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{HO}_2 \rightarrow \text{SO}_4^{-2} + \text{H}^+$	5.0E+09	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{O}_2^- \rightarrow \text{SO}_4^{-2}$	5.0E+09	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{OH}^- \rightarrow \text{SO}_4^{-2} + \text{OH}^-$	8.0E+07	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{H}_2\text{O}_2^- \rightarrow \text{SO}_4^{-2} + \text{HO}_2 + \text{H}^+$	1.2E+07	2000.	<i>Pandis, 1989</i>
$\text{SO}_4^- + \text{NO}_2^- \rightarrow \text{SO}_4^{-2} + \text{NO}_2$	8.8E+08	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{HCO}_3^- \rightarrow \text{SO}_4^{-2} + \text{CO}_3^- + \text{H}^+$	9.1E+06	2100.	<i>Pandis, 1989</i>

$\text{SO}_4^- + \text{HCOO}^- \rightarrow$ $\text{SO}_4^{-2} + \text{CO}_2 + \text{HO}_2$	1.7E+08	1500.	<i>Jacob, 1986</i>
$\text{SO}_4^- + \text{HCOOH} \rightarrow$ $\text{SO}_4^{-2} + \text{CO}_2 + \text{HO}_2 + \text{H}^+$	1.4E+06	2700.	<i>Jacob, 1986</i>
$\text{SO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{OH}$	1.0E+06	0.	<i>Pandis, 1989</i>
$\text{SO}_4^- + \text{CH}_3\text{OH} \rightarrow$ $\text{SO}_4^{-2} + \text{HCHO} + \text{HO}_2 + \text{H}^+$	2.5E+07	1800.	<i>Pandis, 1989</i>
$\text{SO}_4^- + \text{Cl}_2^- \rightarrow \text{SO}_4^{-2} + 2\text{Cl}^- + \text{H}^+$	3.4E+08	1500.	<i>Pandis, 1989</i>
$\text{SO}_3^- + \text{Cl}_2^- \rightarrow \text{SO}_5^- + 2\text{Cl}^-$	1.6E+08	1500.	<i>Pandis, 1989</i>
$\text{H}_2\text{O}_2(\text{aq}) + \text{h}\nu \rightarrow 2 \text{OH}(\text{aq})$	same as gas-phase $\text{H}_2\text{O}_2 + \text{h}\nu \rightarrow 2\text{OH}$		<i>Sander, 1996</i>
$\text{O}_3(\text{aq}) + \text{h}\nu \rightarrow \text{H}_2\text{O}_2(\text{aq})$	same as gas-phase $\text{O}_3 + \text{h}\nu \rightarrow \text{O}(^1\text{D})$		<i>Pandis, 1989,</i> <i>Sander, 1996</i>
$\text{HONO}(\text{aq}) + \text{h}\nu \rightarrow \text{NO} + \text{OH}$	same as gas-phase $\text{HONO} + \text{h}\nu \rightarrow$ $\text{NO} + \text{OH}$		<i>Pandis, 1989</i>
$\text{HNO}_2^- + \text{h}\nu \rightarrow \text{NO} + \text{OH}$	same as gas-phase $\text{HONO} + \text{h}\nu \rightarrow$ $\text{NO} + \text{OH}$		<i>Pandis, 1989</i>
$\text{NO}_3^- + \text{h}\nu \rightarrow \text{NO}_2 + \text{OH} + \text{OH}^-$	same as gas-phase $\text{HNO}_3 + \text{h}\nu$		<i>Pandis, 1989</i>
$\text{NO}_3 + \text{h}\nu \rightarrow \text{NO}$	same as gas-phase $\text{NO}_3 + \text{h}\nu \rightarrow \text{NO}$		<i>Pandis, 1989</i>

CH ₃ OOH+ hv→ HCHO+OH+HO ₂	5.0E-04*j _{NO2}		<i>Pandis, 1989</i>
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1. *Sander and Crutzen* [1996] give this reaction as a H⁺+Cl⁻+HOCl. We have converted this into an equivalent reaction for HCl+HOCl, with a rate equal to k_s*K_e, where k_s is the rate from *Sander and Crutzen* [1996] and K_e is the equilibrium constant for HCl↔H⁺+Cl⁻.

Table S4
Gas-phase reactions: Halogens

k_0 =rate constant at 0 K, in molec. cm⁻³ s⁻¹ (for reactions involving two species) or s⁻¹ (for reactants involving a single species).

E_a = activation energy, expressed as $-E_a/R$ (where R represents the gas constant) in units °K.

The temperature dependence is represented by $k_T = k_0 \exp[-E_a/R(1/T)]$ for temperature T in °K.

Reaction	k_0	E_a/R	References
Cl ₂ + OH→ HOCl	1.4E-12	900.	JPL, 2003
HCl+ OH→ Cl	2.6E-12	350.	JPL, 2003
HOCl+ OH→ ClO	3.0E-12	500.	JPL, 2003
Cl+ HO ₂ → HCl	1.8E-11	-170.	JPL, 2003
Cl+ HO ₂ → OH+ClO	4.1E-11	450.	JPL, 2003
ClO+ HO ₂ → HOCl	2.7E-12	-220.	JPL, 2003
ClO+ NO→ Cl+NO ₂	6.4E-12	-290.	JPL, 2003
ClO+ OH→ Cl+HO ₂	7.4E-12	-270.	JPL, 2003
ClO+ OH→ HCl	6.0E-13	-230.	JPL, 2003
Cl+ H ₂ O ₂ → HCl+HO ₂	1.1E-11	980.	JPL, 2003
Cl+ NO ₃ → ClO+NO ₂	2.4E-11	0.	JPL, 2003
Cl+ H ₂ → HCl+HO ₂	3.7E-11	2300.	JPL, 2003
Cl+ CH ₄ → HCl+CH ₃ O ₂	9.6E-12	1360.	JPL, 2003
Cl+ O ₃ → ClO	2.3E-11	200.	JPL, 2003
Br ₂ + OH→ HOBr+Br	4.2E-11		JPL, 2003.
HBr + OH→ Br	1.1E-11	0.	JPL, 2003
HOBr + OH→ BrO	3.0E-12	500.	assumed equal to HOCl+OH→ ClO

$\text{Br} + \text{HO}_2 \rightarrow \text{HBr}$	1.5E-11	600.	<i>JPL, 2003</i>
$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr}$	3.4E-12	-540.	rate from <i>JPL, 2003</i> , products from <i>Sander, 1996</i>
$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	8.8E-12	-260.	<i>JPL, 2003</i>
$\text{Br} + \text{NO}_3 \rightarrow \text{Br}_2 + \text{NO}_2$	1.6E-11	0.	<i>JPL, 2003</i>
$\text{Br} + \text{HCHO} \rightarrow$ $\text{HBr} + \text{HO}_2 + \text{CO}$	1.7E-11	800.	<i>JPL, 2003</i>
$\text{Br} + \text{O}_3 \rightarrow \text{BrO}$	1.7E-11	800.	<i>JPL, 2003</i>
$\text{Br} + \text{HO}_2 \rightarrow \text{HBr}$	1.5E-11	600.	<i>JPL, 2003</i>
$\text{Cl}_2 + \text{h}\nu \rightarrow 2 \text{Cl}$	$0.267 * j_{\text{NO}_2}$		<i>Sander, 1996</i>
$\text{Br}_2 + \text{h}\nu \rightarrow 2 \text{Br}$	$4.444 * j_{\text{NO}_2}$		<i>Sander, 1996</i>

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