**Table 1a: Henry's Law Constants of halogen containing compounds**

| | Species | $K_{H\,298}$, M $atm^{-1}$ | $\Delta H / R$, K | Reference |
|---|---|---|---|---|
| 1 | BrO | 48 | | $K_{H\,1}=K_{H\,4}$ |
| 2 | ClO | 926 | | $K_{H\,2}=K_{H\,5}$ |
| 3 | HBr | 0.72 | 6077 | Sander and Crutzen, 1996 |
| 4 | HOBr | 48 | | Sander and Crutzen, 1996 |
| 5 | HOCl | 926 | | Huthwelker, 1995 |
| 6 | BrCl | 0.94 | | Sander and Crutzen, 1996 |
| 7 | Br | 1.2 | | Mozurkewich, 1986 |
| 8 | Cl | 0.2 | | Mozurkewich, 1986 |
| 9 | $ClO_2$ | 1.0 | 3300 | Lide and Frederikse, 1995 |

**Table 1a: Photolysis processes of halogen containing compounds in the gas phase**

| | Species | $\alpha$ | Literatur | $D_g$ [$10^5$ $m^2$ $s^{-1}$] | Literatur |
|---|---|---|---|---|---|
| 1 | BrO | 0.06 | Sander and Crutzen, 1996 | 1.31 | Fuller, 1986 [a)] |
| 2 | ClO | 0.064 | $\alpha_{H2} = \alpha_{H3}$ | 1.45 | Fuller, 1986 [a)] |
| 3 | HBr | 0.01 | abgeschätzt | 1.41 | Fuller, 1986 [a)] |
| 4 | HOBr | 0.06 | Vogt *et al.*, 1996 | 1.27 | Fuller, 1986 [a)] |
| 5 | HOCl | 0.064 | Vogt *et al.*, 1996 | 1.41 | Fuller, 1986 [a)] |
| 6 | BrCl | 0.01 | Sander and Crutzen, 1996 | 1.12 | Fuller, 1986 [a)] |
| 7 | Br | 0.05 | estimated equal as OH | 1.46 | Fuller, 1986 [a)] |
| 8 | Cl | 0.05 | estimated equal as OH | 1.71 | Fuller, 1986 [a)] |
| 9 | $ClO_2$ | 0.05 | estimated equal as OH | 1.29 | Fuller, 1986 [a)] |

[a)] method by Fuller,1986 (T=288,15 K, p=1013,15 hPa)

**Table 2a: Photolysis processes of halogen containing compounds in the gas phase**

| Nr. | Reaction | $j_{max}$ [$s^{-1}$] | Reference |
|---|---|---|---|
| 1 | $Br_2 + h\nu \rightarrow Br + Br$ | $3.93 \cdot 10^{-2}$ | Röth, 1992 |
| 2 | $HOBr + h\nu \rightarrow Br + OH$ | $9.37 \cdot 10^{-4}$ | ″ |
| 3 | $Cl_2 + h\nu \rightarrow Cl + Cl$ | $2.69 \cdot 10^{-3}$ | ″ |
| 4 | $HOCl + h\nu \rightarrow Cl + OH$ | $2.63 \cdot 10^{-4}$ | ″ |
| 5 | $BrCl + h\nu \rightarrow Br + Cl$ | $1.24 \cdot 10^{-2}$ | ″ |
| 6 | $BrNO_2 + h\nu \rightarrow Br + NO_2$ | $3.99 \cdot 10^{-4}$ | ″ |
| 7 | $ClNO_2 + h\nu \rightarrow Cl + NO_2$ | $3.99 \cdot 10^{-4}$ | ″ |

**Table 2b: Reactions of halogen containing compounds in the gas phase**

| | Reaktion | $k_{298}$, $M^{-n}\ s^{-1}$ | $E_a$ / R, K | Reference |
|---|---|---|---|---|
| HG1 | $Br + O_3 \rightarrow BrO + O_2$ | $1.16 \cdot 10^{-12}$ | 800 | DeMore *et al.,* 1997 |
| HG2 | $BrO + HO_2 \rightarrow HOBr + O_2$ | $1.43 \cdot 10^{-11}$ | -520 | Elrod *et al.,* 1996 |
| HG3 | $BrO + O_3 \rightarrow Br + 2\ O_2$ | $5.0 \cdot 10^{-17}$ | | Atkinson *et al.*, 1997 |
| HG4 | $Cl + O_3 \rightarrow ClO + O_2$ | $1.21 \cdot 10^{-11}$ | 260 | DeMore *et al.,* 1997 |
| HG5 | $ClO + HO_2 \rightarrow HOCl + O_2$ | $5.5 \cdot 10^{-12}$ | -700 | DeMore *et al.,* 1997 |
| HG6 | $ClO + O_3 \rightarrow ClO2 + O_2$ | $1.4 \cdot 10^{-17}$ | | DeMore *et al.,* 1997 |
| HG7 | $ClO_2 \xrightarrow{[M]} Cl + O_2$ | $6.2 \cdot 10^{-13}$ | 1820 | Atkinson *et al.*, 1997 |
| HG8 | $CH_4 + Cl \rightarrow HCl + CH_3$ | $1.1 \cdot 10^{-13}$ | 1400 | DeMore *et al.,* 1997 |
| HG9 | $Br + HO_2 \rightarrow HBr + O_2$ | $2.0 \cdot 10^{-12}$ | 600 | DeMore *et al.,* 1997 |
| HG10 | $Br + C_2H_4\ (+\ 2\ O_2) \rightarrow HBr + CH_3O_2 + CO_2$ | $2.5 \cdot 10^{-14}$ | | Sander and Crutzen,1996 |
| HG11 | $Br + OLT \rightarrow HBr + CH_3O_2$ | $2.5 \cdot 10^{-14}$ | | " |
| HG12 | $Br + HCHO \rightarrow HBr + CO + HO_2$ | $1.16 \cdot 10^{-11}$ | 800 | DeMore *et al.,* 1997 |
| HG13 | $HCl + OH \rightarrow Cl$ | $8.0 \cdot 10^{-13}$ | 350 | DeMore *et al.,* 1997 |
| HG14 | $HBr + OH \rightarrow Br$ | $1.0 \cdot 10^{-11}$ | | DeMore *et al.,* 1997 |

OLT: terminale alkenes

**Table 3: Reactions of halogen containing compounds in aqueous solution**

| | Reaction | $k_{298}$. $M^{-n}\ s^{-1}$ | Reference |
|---|---|---|---|
| R1 | $HO_2 + HOCl \rightarrow H_2O + O_2 + Cl$ | $7.5 \cdot 10^6$ | $k_{R2} = k_{R1}$ |
| R2 | $HO_2 + Cl_2 \rightarrow Cl_2^- + O_2 + H^+$ | $1.0 \cdot 10^9$ | Bjergbakke *et al.*, 1981 |
| R3 | $O_2^- + HOCl \rightarrow OH^- + O_2 + Cl$ | $7.5 \cdot 10^6$ | Long and Bielski, 1980 |
| R4 | $O_2^- + Cl_2 \rightarrow Cl_2^- + O_2$ | $1.0 \cdot 10^9$ | $k_{R4} = k_{R2}$ |
| R5 | $HOCl + OH \rightarrow H_2O + ClO$ | $2.0 \cdot 10^9$ | $k_{R5} = k_{R12}$ |
| R6 | $HOCl + HSO_3^- \rightarrow HSO_4^- + H^+ + Cl^-$ | $7.6 \cdot 10^8$ | $k_{HSO3-}=k_{SO32-}$ (Fogelman *et al.*, 1989) |
| R7 | $HOCl + Br^- \rightarrow BrCl + OH^-$ | $1.6 \cdot 10^3$ | Kumar, 1987 |
| R8 | $HO_2 + HOBr \rightarrow H_2O + O_2 + Br$ | $1.0 \cdot 10^9$ | estimated (Sutton and Downes, 1972) |
| R9 | $HO_2 + Br_2 \rightarrow Br_2^- + O_2 + H^+$ | $1.1 \cdot 10^8$ | Sutton and Downes, 1972 |
| R10 | $O_2^- + HOBr \rightarrow OH^- + O_2 + Br$ | $3.5 \cdot 10^9$ | Schwarz and Bielski, 1986 |
| R11 | $O_2^- + Br_2 \rightarrow Br_2^- + O_2$ | $5.6 \cdot 10^9$ | Sutton and Downes, 1972 |
| R12 | $HOBr + OH \rightarrow H_2O + BrO$ | $2.0 \cdot 10^9$ | Kläning and Wolff, 1985 |
| R13 | $HOBr + HSO_3^- \rightarrow HSO_4^- + H^+ + Br^-$ | $5.0 \cdot 10^9$ | $k_{HSO3-}=k_{SO32-}$ (Fogelman *et al.*, 1989) |
| R14 | $BrO + BrO \rightarrow BrO_2^- + OBr^- + 2\ H^+$ | $2.8 \cdot 10^9$ | Klaning and Wolff, 1985 |
| R15 | $BrO_2^- + BrO \rightarrow OBr^- + BrO_2$ | $4.0 \cdot 10^8$ | Amichai and Treinin, 1970 |
| R16 | $Br_2^- + BrO_2^- \rightarrow 2\ Br^- + BrO_2$ | $8 \cdot 10^7$ | Buxton and Dainton, 1968 |
| R17 | $BrO_2^- + OH \rightarrow BrO_2 + OH^-$ | $1.8 \cdot 10^9$ | Buxton and Dainton, 1968 |
| R19 | $H^+ + Cl^- + HOCl \rightarrow Cl_2 + H_2O$ | $2.1 \cdot 10^4$ | Wang and Margerum, 1994 |
| R20 | $H^+ + Br^- + HOBr \rightarrow Br_2 + H_2O$ | $1.6 \cdot 10^{10}$ | Eigen and Kustin, 1962 |

**Table 4: Aqueous Phase equilibria**

| | Equilibrium | K, M | Reference | $k_{(hin)\ 298}/s^{-1}$<br>$k_{(rück)\ 298}/M^{-n}\ s^{-1}$ | Reference |
|---|---|---|---|---|---|
| E1 | $HOBr \rightleftharpoons H^+ + BrO^-$ | $2.0\cdot10^{-9}$ | Atkins, 1990 | $1.0\cdot10^{2}$ | calculated based on K |
| | | | | $5.0\cdot10^{10}$ | estimated |
| E2 | $HOCl \rightleftharpoons H^+ + ClO^-$ | $3.0\cdot10^{-8}$ | Atkins, 1996 | $1.5\cdot10^{3}$ | calculated based on K |
| | | | | $5.0\cdot10^{10}$ | estimated |
| E3 | $BrCl\ (+H_2O) \rightleftharpoons HOBr + Cl^- + H^+$ | $1.8\cdot10^{-5}$ | Wang *et al,*, 1994 | $1.0\cdot10^{5}$ | Wang *et al,*, 1994 |
| | | | | $5.6\cdot10^{9}$ | calculated based on K |
| E4 | $Br_2Cl^- \rightleftharpoons BrCl + Br^-$ | $5.6\cdot10^{-5}$ | Wang *et al,*, 1994 | $4.3\cdot10^{5}$ | calculated based on K |
| | | | | $7.7\cdot10^{9}$ | estimated equal as E4 |
| E5 | $BrCl_2^- \rightleftharpoons BrCl + Cl^-$ | $1.6\cdot10^{-1}$ | Wang *et al,*, 1994 | $1.3\cdot10^{9}$ | calculated based on K |
| | | | | $7.7\cdot10^{9}$ | estimated equal as E4 |
| E6 | $Br_2Cl^- \rightleftharpoons Br_2 + Cl^-$ | $7.7\cdot10^{-1}$ | Wang *et al,*, 1994 | $5.9\cdot10^{9}$ | calculated based on K |
| | | | | $7.7\cdot10^{9}$ | estimated equal as E4 |
| E7 | $BrCl_2^- \rightleftharpoons Cl_2 + Br^-$ | $7.7\cdot10^{-1}$ | estimated equal as E6 | $5.9\cdot10^{9}$ | calculated based on K |
| | | | | $7.7\cdot10^{9}$ | Wang *et al,*, 1994 |
| E8 | $HBr \rightleftharpoons H^+ + Br^-$ | $1.0\cdot10^{9}$ | Atkins, 1990 | $5.0\cdot10^{11}$ | estimated (limitation by diffusion) |
| | | | | $5.0\cdot10^{2}$ | calculated based on K |
| E9 | $HBrO_2 \rightleftharpoons H^+ + BrO_2^-$ | $1.3\cdot10^{-5}$ | Field, 1986 | $6.3\cdot10^{5}$ | calculated based on K |
| | | | | $5.0\cdot10^{10}$ | abgeschätzt |
| E10 | $2\ HOBr \rightleftharpoons H^+ + Br^- + HBrO_2$ | $6.7\cdot10^{-12}$ | Field, 1986 | $2.0\cdot10^{-5}$ | Field and Försterling, 1986 |
| | | | | $3.0\cdot10^{6}$ | Field and Försterling, 1986 |
| E11 | $HOBr+HBrO_2 \rightleftharpoons 2\ H^+ + Br^- + BrO_3^-$ | 1.7 | Field, 1986 | 3.2 | Field and Försterling, 1986 |
| | | | | 2.0 | Field and Försterling, 1986 |
| E12 | $2\ HBrO_2 \rightleftharpoons H^+ + BrO_3^- + HOBr$ | $3.0\cdot10^{11}$ | Field, 1986 | $3.0\cdot10^{3}$ | Field and Försterling, 1986 |
| | | | | $1.0\cdot10^{-8}$ | Field and Försterling, 1986 |
| E13 | $Br_2O_4+H_2O \rightleftharpoons H^+ + BrO_3^- + HBrO_2$ | 52.6 | Field, 1986 | $2.2\cdot10^{3}$ | Field and Försterling, 1986 |
| | | | | 42 | Field and Försterling, 1986 |
| E14 | $Br_2O_4 \rightleftharpoons 2\ BrO_2$ | $5.3\cdot10^{-5}$ | Field, 1986 | $7.4\cdot10^{4}$ | Field and Försterling, 1986 |
| | | | | $1.4\cdot10^{9}$ | Field and Försterling, 1986 |

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