This data sheet evaluated: 15$^{th}$ January 2009; last change in preferred values: 15$^{th}$ January 2009.

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## $ICl + Cl^-/Br^- \rightarrow IBr + Cl^-$
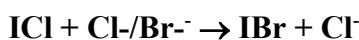
### Experimental data

| Parameter | [X]/ M | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|---|
| *Uptake coefficients:* $\gamma, \gamma_{ss}, \gamma_0$ | | | | |
| $\gamma = 2.6 \times 10^{-3}$ | 2 (Cl-) | 274 | Braban et al, 2007 | WWFT-EIMS (a) |
| $\gamma = 2.5 \times 10^{-3}$ | 2 (Br-) | | | |
| $\gamma = 3 \times 10^{-3}$ | pure water | | | |
| | 2 (Br-) | | | |
| $\gamma = (0.6 - 1.6) \times 10^{-3}$ | 15 - 209 Torr | 278 | | |
| $\alpha = 0.01 - 1.0$ | aq.NaBr aerosol | | | |
| | | | | AFT-CIMS(b) |
| $\gamma = 0.018 \pm 0.004$ | | 274 | | |
| $\gamma = (0.1 - 1) \times 10^{-3}$ | Sea salt aerosol (5-87% RH) | 274 | | |

### Comments

(a) The uptake of ICl ($4–70 \times 10^{10}$ molecules cm$^{-3}$) to aqueous surfaces was studied in the wetted-wall flow tube with MS detection at m/z = 144. Several combinations of dissolved concentrations of Cl$^-$ and Br$^-$ in solutions of different pH were used. Experiments were conducted at 274 and 293 K and at a range of flow tube pressures between 13 and 20 Torr, , and at 278K in a different system (see Holmes, et al., 2001) over the pressure range 15 – 209 Torr. The uptake coefficient values were independent of composition or pH of the solution, but increased with deceasing pressure in the flow tube. Uptake is thus gas phase diffusion limited in all cases. Gas phase diffusion coefficients for ICl of $D^{ICl}_{H2O} = 57 \pm 6$ cm$^2$ s$^{-1}$ Torr$^{-1}$, and $D^{ICl}_{He} = 289 \pm 19$ cm$^2$ s$^{-1}$ Torr$^{-1}$ at 278 K, were obtained from the pressure dependence of $\gamma$. Uptake of ICl into Br$^-$ solutions produced IBr which was partially released to the gas phase.

(b) Atmospheric pressure aerosol flow tube with ICl ($\approx 10^{13}$ molecule cm$^{-3}$) measured by CIMS, together with products Br$_2$ or IBr. Aerosols were generated from salt solutions in a constant output atomiser (TSI 3076), dried, and then equilibrated at controlled humidity by addition of 'wet' carrier gas before entry into the flow tube. The size distribution was measured with a differential mobility analyser (DMA). The area weighted radius and surface area of the aerosol in the flow tube was 100 -1000nm, and $(1 - 80) \times 10^{-3}$ cm$^2$/cm$^3$ respectively. Uptake coefficients were determined from the first order rate constants for ICl decay, corrected for wall loss, which were linearly dependent on surface area. Diffusion limitation was negligible for the size range used. Uptake of ICl onto NaBr aerosol (pH<8) led to IBr release with a yield of 0.6±0.3. Lower uptake on sea salt attributed to depletion of Br-. The uptake coefficient on NaBr aerosol was independent of RH in the range 10-70% (and hence on [Br$^-$]) and was independent of particle size. This indicates an accommodation controlled uptake process.

# Preferred Values

| Parameter | Value | T/K |
|---|---|---|
| $\alpha_b$ | 0.016 | 298 |
| $k^{II}$ (M$^{-1}$ s$^{-1}$) (Br) | $\gg 10^3$ | 298 |

*Reliability*

| | | |
|---|---|---|
| $\Delta \log (\alpha)$ | $\pm 0.3$ | 298 |

## Comments on Preferred Values

The recommended value of $\alpha$ is based on the uptake coefficient into NaBr aerosol; the reaction of ICl with Br- is fast and it is likely that reactive uptake of ICl into salt droplets is accommodation limited under atmospheric conditions. The dihalogen product IBr will partition rapidly to the gas phase. The uptake coefficient at lower [Br-] is given in terms of the resistance model :

$$\gamma = \left\{ \frac{1}{\alpha_b} + \frac{c}{4HRT\,(D_l k^I)^{0.5}} \right\}^{-1} \quad \text{where } k^I (\text{s}^{-1}) = k^{II} \times [\text{Br}^-]_{aq} \text{ (M)}$$

At 298 K: $\alpha_b = 0.016$ and the value of $k^{II} = 5.0 \times 10^4$ and can be used with $H = 110$ M atm$^{-1}$ and $D_l = 5.0 \times 10^{-6}$ cm$^2$s$^{-1}$

## References

Braban, C. F.; Adams, J.W.; Rodriguez, D.; Cox, R.A., Crowley, J.N. and Schuser, G.: Phys. Chem. Chem. Phys., **9**, 3136, 2007.
Holmes, N. S., Adams, J. W. and Crowley, J. N., Phys. Chem. Chem. Phys., **3**, 1679, 2001.