

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet VI.A2.15 HET_SALTS_15

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This datasheet evaluated: 15th January 2009; last change in preferred values: 15th January 2009.

I₂ + Cl⁻/Br⁻ → products

Experimental data

Parameter	[X]/ M	Temp./K	Reference	Technique/ Comments
<i>Uptake coefficients: $\gamma, \gamma_{ss}, \gamma_0$</i>				
$\gamma = (2.0 \pm 0.3) \times 10^{-3}$	2 (Cl ⁻) 0.003 (Br ⁻) pure water	274	Braban et al, 2007	WWFT-EIMS (a)
$\gamma_0 = (1.8 \pm 0.2) \times 10^{-3}$		274		

Comments

- (a) The uptake of I₂ ($(0.2-1) \times 10^{12}$ molecules cm⁻³) to aqueous surfaces was studied in the wetted-wall flow tube with MS detection at $m/z = 144$. Uptake was measured on pure water and with dissolved concentrations of Cl⁻ (2M) and Br⁻ (0.003M) to mimic sea water. Uptake was rapid and was gas phase diffusion limited in both cases, but on pure water the uptake coefficient reduced with increasing exposure length, indicating surface saturation. No gas phase products were observed.

Preferred Values

Parameter	Value	T/K
α_b	>0.01	298
<i>Reliability</i> $\Delta \log(\alpha)$	± 0.3	298

Comments on Preferred Values

The uptake of I₂ into aqueous halide is the same as into pure water, and is solubility limited, with no detectable reaction products in the gas phase. The recommended accommodation coefficient is based on an analogy with ICl uptake on the same surfaces. The time dependent uptake coefficient is given by:

$$\gamma = \left\{ \frac{1}{\alpha} + \frac{c\sqrt{\pi}}{8HRT} \sqrt{\frac{t}{D_1}} \right\}^{-1}$$

with $\alpha_b = 0.016$, $H = 24 \text{ M atm}^{-1}$ and $D_1 = 5.0 \times 10^{-6} \text{ cm}^2\text{s}^{-1}$ at 298 K.

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.