IUPAC Task Group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet V.A1.10 HI10

This Data sheet last evaluated: January 2008. Last change in preferred values: January 2008.

NH_3 + ice

Uptake coefficient data

Parameter	Temp./K	Reference	Technique/Comments
γ			
$3.8 \pm 1.4 \times 10^{-4}$	189.9 ± 0.5	Jin and Chu, 2007	CWFT-MS(a)

Comments

(a) The ice film (≈ 3.5 μm thick) was condensed from the vapour phase at the experimental temperature. Uptake of NH_3 (P_{NH3} = 5.3 x 10^{-7} – 2.9 x 10^{-6} mbar) was continuous, irreversible and independent of the NH_3 partial pressure. The uptake coefficients varied with ice film thickness and were corrected for pore diffusion.

Preferred values

Parameter	**Value**	**T/K**
γ	4×10^{-4}	190 - 200
Reliability		
$\Delta \log \gamma$	± 0.5	190 - 200

Comments on preferred values

Jin and Chu (2007) report continuous and irreversible uptake of NH_3 onto ice films, with the amount taken up exceeding monolayer coverage by more than a factor of 10, thus indicating possible formation of stable hydrates or solid-liquid phase change under the conditions employed. Based on an estimated diffusion coefficient on ice, Jin and Chu (2007) suggest that diffusion into their ice cannot account for the continuous uptake. This contrasts the conclusions of Hoog et al., who analysed the NH_4^+ content (by ion chromatography subsequent to melting) of ice crystals that had been exposed to NH_3 at significantly higher concentrations (≈ 6-100 × 10^{-4} mbar).
Theoretical work suggests that remaining in the gas-phase is energetically more favourable than incorporation into the bulk ice for single NH_3 at infinite dilution. An adsorption free energy of 11 kJ mol^{-1} has been calculated (Pártay et al., 2007). Spectroscopic evidence for hydrogen bonded NH_3 on ice has been obtained at 38 K, with no evidence for thermal

desorption up to ≈ 140 K. Evidence for ionisation of NH_3 to $NH_4^+$and subsequent transfer to the bulk of the ice surface was however obtained at these temperatures (Ogasawara et al., 2000) and would presumably also take place at higher temperatures.

References

Hoog, I., Mitra, S. K., Diehl, K. and Borrmann, S.: J. Atmos. Chem. 57, 73-84, 2007.
Jin, R. and Chu, L.T.: J. Phys. Chem. A, 111, 7833, 2007.
Ogasawara, H., Horimoto, N. and Kawai, M.: J. Chem. Phys. 112, 8229-8232, 2000.
Pártay, L. B., Jedlovszky, P., Hoang, P. N. M., Picaud, S. and Mezei, M.: J. Phys. Chem. C 111, 9407-9416, 2007.