IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.16 HI16

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HCHO + ice

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
Surface partitioning coefficients: K_{linC} $K_{linC} = 0.7 \pm 0.3$	198-223	Winkler et al., 2002	CWFT-MS (a)

Comments

(a) Ice surface formed by freezing water. The geometric surface area was used to calculate the coverage. The formaldehyde uptake data showed neither a dependence on temperature nor an approach to saturation, thus precluding an analysis using Langmuir isotherms. K_{linC} (cm^{-2}/cm^{-3}) was determined from a linear relationship between N (surface coverage in molecule cm^{-2} of ice) and [HCHO] (units of molecule cm^{-3}) at low coverage where $N < 1 \times 10^{13}$ molecule cm^{-2}.

Preferred Values

Parameter	Value	T/K
K_{linC} / cm	0.7	198 - 233
N_{max} / molecules cm^{-2}	2.7×10^{14}	
Reliability		
$\Delta \log K_{linC}$	0.5	198 - 233
$\Delta \log N_{max}$	0.2	198 - 233

Comments on Preferred Values

The sole experimental study of the formaldehyde- ice interaction by Winkler et al. (2002) shows that the adsorption of formaldehyde to ice is completely reversible, and that the interaction is quite weak. This could be confirmed in a theoretical study (Hantal et al. 2007), which found a much lower heat of adsorption for formaldehyde (≈ -30 kJ mol^{-1}) compared to methanol although in both cases the thermodynamic driving force was the formation of hydrogen-bonds.

References

Hantal, G., Jedlovzky, P., Hoang, P. N. M., and Picaud, S.: J. Phys. Chem. C 111, 14170, 2007.
Winkler, A.K., Holmes, N.S. and Crowley, J.N.: Phys. Chem. Chem. Phys. 4, 5270 2002.