

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.23 HI23

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1-C₄H₉OH + ice

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Partitioning coefficients: K_{inc}</i>			
$K_{inc} = 358$	221	Sokolov and Abbatt, 2002	CWFT-MS (a)
$K_{inc} = 101$	228		
$K_{inc} = 42.7$	233		
$K_{inc} = 7.4 \times 10^{-16} \exp(9000/T)$	221-233		

Comments

- (a) Ice film made by freezing distilled water. Uptake was found to be reversible and equilibrium surface coverages were calculated using the geometric ice surface area. Equilibrium uptake of C₄H₉OH to ice at various temperatures was analysed using the Langmuir isotherm. The values for K_{inc} at individual temperatures given in the Table uses the reported values of K_{LangP} (221 K) = 4.6×10^4 , K_{LangP} (228 K) = 1.34×10^4 , K_{LangP} (233 K) = 5.2×10^3 (units of Torr⁻¹) and N_{max} (221 K) = 3.4×10^{14} , N_{max} (228 K) = 3.2×10^{14} and N_{max} (233 K) = 3.4×10^{14} (units of molecule cm⁻²). No errors were reported. The temperature dependent expression of K_{inc} was derived by fitting to these three data points.

Preferred Values

$$K_{inc} = 7.4 \times 10^{-16} \exp(9000/T) \text{ cm over the range 210 K to 250 K.}$$

$$N_{max} = 3.3 \times 10^{14} \text{ molecules cm}^{-2}, \text{ independent of temperature.}$$

Reliability

$$\Delta(E/R) = \pm 1000 \text{ K.}$$

$$\Delta \log N_{max} = 0.15$$

Comments on Preferred Values

There is only one study of the reversible uptake of C₄H₉OH to pure ice surfaces. The value of N_{max} derived from Langmuir analyses is consistent with other straight chain alcohols (Sokolov and Abbatt, 2002). The uncertainty on the preferred value of K_{inc} is increased to reflect that this is the sole study to date.

References

Sokolov, O. and Abbatt, J. P. D.: J. Phys. Chem. 106, 775-782, 2002.