The citation for this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.

This data sheet last evaluated: March 2010; last change to preferred values: March 2010.

CH_3CHO + ice

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
γ, γ_0			
$\gamma_0 > 0.1$	120-145	Hudson et al., 2002	Knudsen (a)
$\gamma_0 > 0.04$	150		
$\gamma_0 > 0.01$	155		
$\gamma_0 > 5\text{x}10^{-3}$	160		
K_{linC} (cm)			
$3.8 \times 10^{-10} \exp(4174/T)$	140-170	Hudson et al., 2002	Knudsen (c)
2.08 ± 0.19	203	Petitjean et al., 2009	CWFT-MS (b)
0.95 ± 0.09	213		
0.46 ± 0.04	223		

Comments

(a) Vapour deposited ice film of geometric area ≈ 5 cm^2. γ_0 values taken from a Figure. The geometric surface area of the vapour deposited ice film was used to calculate the uptake coefficient, γ_0, which is a lower limit as, especially at the higher temperatures, adsorption and desorption were not separated in time.

(b) Ice film (40-100 μm thick) made from freezing liquid water at 263 K. Adsorption isotherms were measured with CH_3CHO concentrations between 5.7×10^{11} and 8.35×10^{14} molecule cm^{-3}. The data analysed using full Langmuir isotherms and the linear dependence of surface coverage on concentration to derive the partition coefficients listed in the table.

(c) Equilibrium uptake of ≈ 4×10^{-7} mbar acetaldehyde (≈ 10^{10} molecule cm^{-3}) to ice at various temperatures was analysed using the Langmuir isotherm. The expression for K_{linC} uses the reported value of ΔS_{ads} (via Trouton's rule) = -87.9 $Jmol^{-1}$ K^{-1} and ΔH_{ads} = -34.7 $kJmol^{-1}$ and is derived from K_{LangP} (atm^{-1}) = $\exp\{-(T^* 87.9 - 34700) / 8.314^*T\}$ using $N_{max} = 4 \times 10^{14}$ molecules cm^{-2}.

Preferred Values

Parameter	Value	T/K
K_{linC} / cm	$7.0 \times 10^{-8} \exp(3500/T)$	203-223
N_{max} / molecule cm^{-2}	1.3×10^{14}	
Reliability		
$\Delta(E/R)$	± 300	203-223
$\Delta \log N_{max}$	0.15	

Comments on Preferred Values

Petitjean et al. (2009) found the uptake of CH_3CHO to ice surfaces to be completely reversible. They report partition coefficients and also derive an adsorption enthalpy of –16 (± 3) kJ mol^{-1} by an unconstrained Van't Hoff-type analysis of data at 203, 213 and 223 K only. In a second approach the analysis was constrained with adsorption entropy of –87.3 to derive an adsorption enthalpy of –42 kJ mol^{-1}. The preferred values for K_{linC} above were obtained by fitting to the data of Petitjean et al. (2009) obtained in the linear coverage regime between 203 and 223 K. The adsorption enthalpy is ~ -29 kJ mol^{-1}. Hudson et al. (2002) found that the interaction of CH_3CHO with ice was too weak to detect close to atmospherically relevant temperatures. Extrapolation of their data to the temperatures covered by Petitjean et al. (2009) results in discrepancies of a factor of 5-10. The value of N_{max} given was that obtained by Petitjean et al. (2009).
Petitjean also found the uptake of CH_3CHO to ice surfaces that contained HNO_3 was enhanced by 1-2 orders of magnitude at their temperatures, presumable due to dissolution in super-cooled HNO_3 / H_2O mixtures. In contrast, Hudson et al. (2002) observed no uptake of CH_3CHO on super-cooled HNO_3 / H_2O surfaces at 200 K.

References

Hudson, P. K., Zondlo, M. A. and Tolbert, M. A.: J. Phys. Chem. A 106, 2882-2888, 2002.
Petitjean, M., Mirabel, Ph. and Le Calvé, S.: J. Phys. Chem. A 113, 5091-5098, 2009.