IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.33 HI33

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

HOI (Ice) → Products

Experimental Data

Parameter	Temp./K	Reference	Technique/Comments
Experimental uptake coefficients: γ, γ_0			
$\gamma = 3.2 \times 10^{-2}$	180	Allanic and Rossi, 1999	Knudsen-MS (a)
$\gamma = 4.9 \times 10^{-2}$	190		
$\gamma = 5.7 \times 10^{-2}$	200		
$\gamma_0 > 10^{-2}$	243	Holmes et al., 2001	CWFT-MS (b)

Comments

(a) HOI (at concentrations of ~10^{10} molecule cm^{-3}) was formed in the reaction of $O(^3P)$ with C_2H_5I. The ice film was formed by vapour deposition. The uptake did not saturate (time independent) under these conditions and displayed a negative temperature dependence. It was found to be independent of HOI concentration (varied over a factor of four). The values of γ listed are averages from 3-5 datasets. Individual values scatter by a factor of up to two for unchanged conditions. The only gas-phase product detected was I_2 with no recoverable HOI after the evaporation of the 20 μm thick ice film.

(b) HOI (at concentrations <10^{10} molecule cm^{-3}) was formed in the reaction of $O(^3P)$ with C_3H_7I. The ice film was formed by freezing liquid water at 258 K. The uptake coefficient decreased with exposure time and HOI was observed to desorb from the ice film after exposure stopped, indicating a (partially) reversible process. Diffusion limitation prevented precise measurement of the initial uptake coefficient.

Preferred Values

none

Comments on Preferred Values

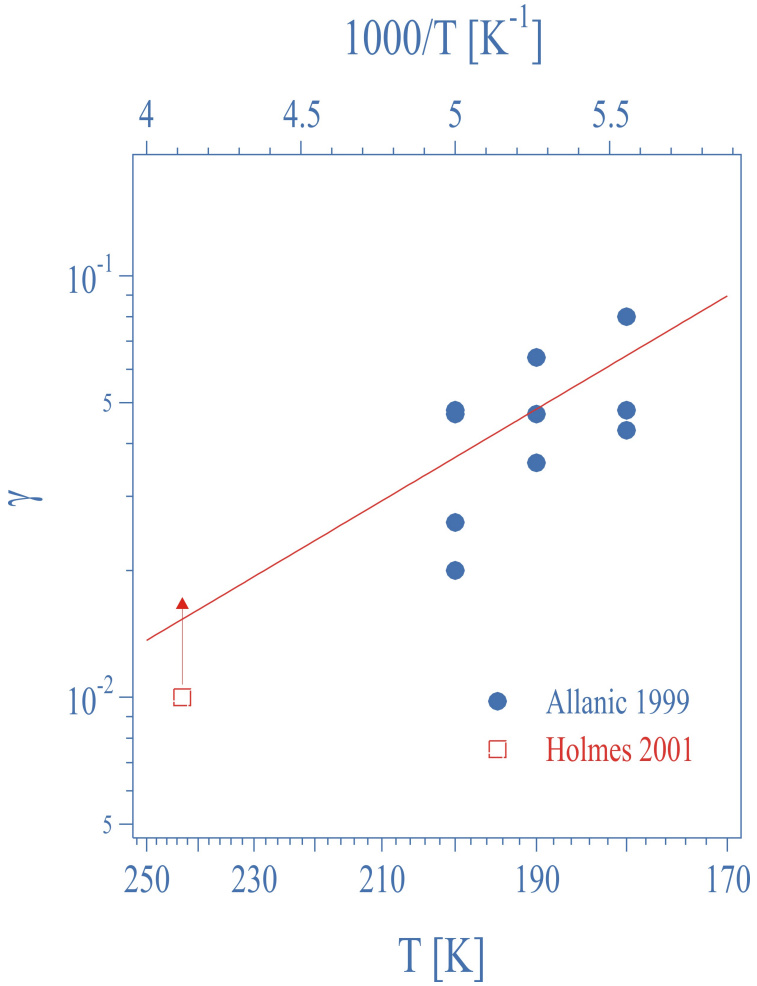
The results of Allanic and Rossi (1999) and Holmes et al (2001) were obtained in different temperature ranges and concur that the uptake coefficient is large. A parameterisation, $\gamma = 5 \times 10^{-5} \exp(1000/T)$ generates uptake coefficients that are consistent with both datasets. At the lower temperatures covered by Allanic and Rossi (1999), the uptake is observed to be irreversible, whereas Holmes et al. (2001) observe partially reversible adsorption at 243 K.

From the experimental datasets it is not obvious how HOI reacts with the ice surface. Both studies observed I_2 as product and Holmes et al (2001) suggest that this may arises from self-reaction of HOI (or reaction of HOI with $IONO_2$ impurity) on the ice surface. It is possible that on a pure ice surface, HOI will adsorb reversibly unless high concentrations and low temperatures result in formation of a thermodynamically stable phase (e.g. formation of hydrates). For this reason we make no recommendation for uptake to pure ice, whilst noting that HOI reacts readily on ice surfaces containing reactive species (Allanic and Rossi, 1999; Holmes et al., 2001).

References

Allanic, A. and Rossi, M.J.: J. Geophys. Res. 104, 18689-18696, 1999.

Holmes, N. S., Adams, J. W., and Crowley, J. N.: Phys. Chem. Chem. Phys, 3, 1679-1786, 2001.



Experimental uptake coefficients for HOI interaction with ice.