

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A1.3 HI3

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This data sheet last evaluated: December 2007; last change in preferred values: December 2007.

OH + ice

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Experimental uptake coefficients: γ</i>			
$\gamma_0 = 0.1$	205-230	Cooper and Abbatt, 1996	CWFT-RF (a)
$\gamma_{ss} = 0.03 \pm 0.02$			

Comments

- (a) OH radicals generated by the reactions $F + H_2O \rightarrow HF + OH$ and $H + NO_2 \rightarrow OH + NO$. The total flow tube pressure was generally 1 Torr (1.33 mbar) with a total flow velocity of 1500-2200 $cm\ s^{-1}$.

Preferred Values

Parameter	Value	T/K
γ_{ss}	0.03	200 - 230
<i>Reliability</i>		
$\Delta \log(\gamma)$	± 0.5	200 - 230

Comments on Preferred Values

Cooper and Abbatt (1996) observed that OH radicals were irreversibly adsorbed on the ice surface. Initial uptake coefficients were large (~ 0.1) on fresh ice surfaces, but after 20 mins of OH uptake, surfaces became deactivated and uptake coefficients were reduced to a steady-state value of ~ 0.03 . The irreversible loss of OH may then be due to reaction of OH with an activated S-OH site formed from reaction of OH with a surface site, S. Cooper and Abbatt (1996) argue that this mechanism is consistent with the observed first-order loss of OH from the gas-phase if the rate limiting step is transfer of OH from the gas-phase to the activated surface (i.e. to an S-OH site). The uptake coefficient could be significantly increased (to ~ 0.2) by adsorbing HNO_3 to the surface (whilst remaining in the ice stability regime of the ice- HNO_3 phase diagram), or by melting the surface by adding a sufficient partial pressure of HCl. It should be stressed that the preferred value is representative of uptake to a clean ice surface and that in an atmospheric, chemically complex environment, the uptake coefficient could be larger (if the surface is contaminated with e.g. reactive organics) or smaller if S-OH is deactivated by trace gases other than OH.

References

Cooper, P.L. and Abbatt, J.P.D.: J. Phys. Chem. 100, 2249-2254, 1996.