Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A5.16 HNDT16

N_2O_5 + HBr (NAT) → products

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
γ			
5×10^{-3}	200	Hanson and Ravishankara, 1992	CWFT-CIMS (a)

Comments

(a) Ice surfaces (2-10 μm thick) were made by vapour deposition and doped with HNO_3 (the amount of HNO_3 was not given). The geometric surface area was used to calculate the uptake coefficient. Experiments were conducted with 5×10^{9} – 10^{11} molecule cm^{-3} HBr and 10^{11} – 10^{12} molecule cm^{-3} N_2O_5. Values of the uptake coefficient varied between a high value of $\approx 4 \times 10^{-2}$ and a low value of 5×10^{-3}, the latter being obtained at the lower HBr concentrations.

Preferred Values

Parameter	Value	T/K
γ_{ER}	2×10^{-2}	
θ_{HBr}	4.14×10^{-10} [HBr]$^{0.88}$	
Reliability		
$\Delta \log\gamma$	0.5	200

Comments on Preferred Values

There is a single study (Hanson and Ravishankara, 1992) of the reaction of N_2O_5 and HBr on a NAT-like (or HNO_3 doped) surface. The uptake coefficient was found to be enhanced compared to N_2O_5 uptake to pure NAT ($\gamma \leq 1 \times 10^{-3}$), indicative of surface reaction with possible products BrONO and HNO_3 (not observed). In order to parameterise the uptake coefficient, γ, we have assumed an Eley-Rideal type mechanism with the surface coverage of HBr the same as that for pure ice.

$\gamma = \gamma_{gs}\ \theta_{HBr}$, with [HBr] in molecule cm^{-3}.

The parameterisation above yields a value of γnet = 5×10^{-3} at concentrations of HBr close to 10^{10} molecule cm^{-3}, increasing to $\gamma = 4 \times 10^{-2}$ at HBr close to 10^{11} molecule cm^{-3}, which are consistent with the experimental observations.

References

Hanson, D. R. and Ravishankara, A. R.: J. Phys. Chem. 96, 9441-9446, 1992.