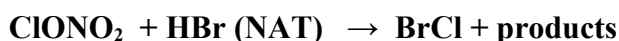


IUPAC Task Group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet V.A5.14 HNNT14

Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hard copy without explicit written permission.

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: January 2009; last change in preferred values: January 2009.



Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
γ			
> 0.3	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 either HBr ($5 \times 10^9 - 10^{11}$ molecule cm^{-3}) or ClONO_2 ($10^{10} - 10^{11}$ molecule cm^{-3}) in excess to give the same value of γ . BrCl was observed as primary gas-phase product, but not quantified. When HBr was in excess, some BrCl was converted to Br_2 . Note that the same value of γ (and the same product) was also obtained for pure ice.

Preferred Values

Parameter	Value	T/K
$\gamma_{\text{gs}}(\text{ClONO}_2)$	0.56	180 – 200 K
θ_{HBr}	$4.14 \times 10^{-10} [\text{HBr}]^{0.88}$	188 K
<i>Reliability</i>		
$\Delta \log \gamma$	0.3	200 K

Comments on Preferred Values

The single study (Hanson and Ravishankara, 1992) of the reaction of ClONO_2 and HBr on a NAT-like (or HNO_3 doped) surface shows that the reaction proceeds very efficiently and that BrCl escapes to the gas-phase at low HBr concentrations. There is no difference in the uptake coefficient if pure ice or NAT-like surfaces are used and we adopt the same parameterisation for γ_{net} as for pure ice, which relies on a parameterisation for the HBr surface coverage (see datasheet on HBr + ice).

$$\gamma_{\text{net}} = \gamma_{\text{ER}}(\text{ClONO}_2) \theta_{\text{HBr}} \text{ with } [\text{HBr}] \text{ in molecule cm}^{-3}.$$

Note that the parameterisation, which is only valid for $\theta_{\text{HBr}} \leq 1$ and assumes that the maximum coverage is 1×10^{15} molecule cm^{-2} , generates uptake coefficients that are in close to or greater than 0.3 for $[\text{HBr}] \geq 10^{10}$ molecule cm^{-3} , as observed by Hanson and Ravishankara, 1992.

References

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

