

IUPAC Task Group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet V.A1.55 HI55

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Data sheet last evaluated: January 2009; last change in preferred values: January 2009.

CIOOCl + ice → products

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Uptake coefficients: γ</i>			
$5.1 \pm 3.9 \times 10^{-4}$	226	De Haan and Birks, 1997	CWFT-MS (a)

Comments

- (a) Flow tube reactor using electron-impact MS. ClOOCl was generated in the self reaction of ClO at low temperatures and detected as Cl₂O₂⁺. The ice film (300 – 900 μ m) was made by “brushing” water onto the cold flow tube surface and the geometric surface area was used to calculate the uptake coefficient. The value of γ presented is an average value from several experiments (results varied between < 3 to 11×10^{-4}), though it is not clear that these were all conducted at the same temperature and ClOOCl partial pressure (which was reported to have been varied between 10^{11} and 10^{13} molecule cm⁻³ for a variety of substrates including pure ice).

Preferred Values

Parameter	Value	T/K
γ	$\gamma = 5 \times 10^{-4}$	226 K
<i>Reliability</i>		
$\Delta \log (\gamma)$	0.7	

Comments on Preferred Values

The study De Haan and Birks (1997) reports an uptake coefficient that is close to the detection limit of the apparatus. The uptake appears to be irreversible, and He Haan and Birks (1997) suggest that a hydrolysis reaction forming H₂OCl⁺ and ClOO⁻ ions may take place. Mckeachie et al (2004) report insignificant interaction of ClOOCl to an ice surface at 213 K, but do not report an uptake coefficient. Considering that there is only one study reporting an uptake coefficient, the use of large concentrations of ClOOCl, the possible reaction of impurity reactants and the unusual mode of making the ice film, the uncertainty is considerable.

References

De Haan, D. O. and Birks, J. W.: J. Phys. Chem. 101, 8026-8034, 1997.

McKeachie, J. R., Appel, M. F., Kirchner, U., Schindler, R. N. and Benter, T.: J. Phys. Chem. B 108, 16786-16797, 2004.