IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation
Data Sheet HI1; V.A1.1

The citation for this datasheet is: Crowley, J. N., Ammann, M., Cox, R. A., Hynes, R. G., Jenkin, M. E., Mellouki, A., Rossi, M. J., Troe, J., and Wallington, T. J., Atmos. Chem. Phys., 10, 9059-9223, 2010; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.
This datasheet last evaluated: June 2014; last change in preferred values: June 2009

$O(^3P)$ + ice → products

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
Uptake coefficients: γ			
$\gamma_0 = 7 \times 10^{-6}$ for $[O_2] = 0$	112-151	Murray and Plane, 2003	CWFT-RF (a)
$\gamma = 7 \times 10^{-6} + 2.6 \times 10^{-24} \exp(1372 \pm 72/T)$ for $[O_2]$ up to 1×10^{15} cm^{-3}	112-151		

Comments

(a) Cubic ice formed by vapour deposition at 90 K and annealed to 160 K. Uptake experiments performed using a fast flow reactor equipped with resonance fluorescence detection of O atoms at 130 nm. The BET surface area was used in the calculation of the uptake coefficients. A pulsed version of the O uptake experiment in the same flow tube was also performed and a chromatographic analysis of the pulse shape showed that O atoms were relatively strongly bound to some ice sites.

Preferred Values

Parameter	Value	T/K
γ	$7 \times 10^{-6} + 2.6 \times 10^{-24} \exp(1370/T)\ [O_2]$	110-150
Reliability		
$\Delta \log(\gamma)$	±0.3	110-150
$\Delta(E/R)$ /K	±200	110-150

Comments on Preferred Values

Kinetic modelling indicated two mechanisms for O uptake: one that was independent of temperature and $[O_2]$ between 112-151 K, and one that was dependent on $[O_2]$ and had a negative temperature dependence. The preferred values are those reported in the single study of Murray and Plane (2003), with expanded errors. An Eley-Rideal mechanism was suggested as the mechanism by which adsorbed O atoms are removed from the ice surface by collisions with gas-phase O atoms or O_2 to form O_2 or O_3, respectively. Quantum chemical calculations showed that O atoms bind to either a single dangling hydrogen on a perfectly crystalline ice surface or to two dangling hydrogens in a disordered ice structure.

References

Murray, B.J. and Plane J.M.C.: Phys. Chem. Chem. Phys. 5, 4129, 2003.