

IUPAC Task Group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet VI.A1.12 HET_H2OL_12

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Experimental data

Parameter	Temp./K	Reference	Technique/Comments
<i>Accommodation coefficients: α_b</i>			
0.16	263	Schweitzer et al., 2000	DT-MS (a)
6.8×10^{-2}	281		
0.26 ± 0.02	273	Li et al., 2002	DT-MS (b)
0.14 ± 0.02	283		

Comments

- (a) 80-150 μm diameter droplets with a gas-liquid interaction time of 0-20 ms. The HBr concentrations were in the range $10^{12} - 10^{14}$ molecule cm^{-3} , with most experiments performed at 10^{13} molecule cm^{-3} . Rate of uptake was time-independent as well as independent on pH in the range 7-14. Diffusion-corrected uptake coefficient is interpreted as a bulk accommodation coefficient α_b having a significant negative temperature dependence.
- (b) Droplet train experiment with ethylene glycol/water mixtures. Droplet size was in the range 70 to 300 μm , 2.6-25 mbar of (mostly) He in flow tube with trace gas species concentrations in the range 2×10^{13} to 3×10^{14} molecule cm^{-3} . The value of α_b was found to be independent of the interaction time in the range 2.5 to 17 ms, and temperature. α_b varied continuously with increasing mole fraction of H_2O from a high (pure glycol) to a low (pure H_2O) value which has been successfully modelled using surface tension data for glycol/ H_2O solutions of variable composition.

Preferred Values

Parameter	Value	T/K
α_b	2.3×10^{-2}	298
α_b	$1.3 \times 10^{-8} \exp(4290/T)$	263-281

Reliability

$\Delta \log(\alpha_b)$	± 0.3	298
$\Delta(E/R)$	$\pm 600 \text{ K}$	263-281

Comments on Preferred Values

Although both Schweitzer et al. (2000) and Li et al. (2002) present bulk accommodation coefficients with a strong negative temperature dependence, there is disagreement of a factor of between 3 and 5 in the absolute values of α_b . We have taken the data of Schweitzer et al. (2000) as the basis of our recommended values owing in part to the larger number of data taken within a larger temperature range.

References

Li, Y.Q.; Zhang, H.Z.; Davidovits, P.; Jayne, J.T.; Kolb, C.E. and Worsnop, D.R.: J. Phys. Chem. A, 106, 1220-1227, 2002.

Schweitzer, F., Mirabel, Ph. and George, C.: J. Phys. Chem. A, 104, 72-76, 2000.