

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A2.13 MD13

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H₂O₂ + mineral oxide (dust) surfaces

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Experimental uptake coefficients: γ</i>			
1.5×10^{-3} (TiO ₂ , 15% RH)	298	Pradhan et al., 2010a	AFT-CIMS (a)
5.0×10^{-4} (TiO ₂ , 70% RH)			
$(3.33 \pm 0.26) \times 10^{-4}$ (Gobi sand, 15% RH)		Pradhan et al., 2010b	AFT-CIMS (b)
$(6.03 \pm 0.42) \times 10^{-4}$ (Gobi sand, 70% RH)			
$(6.20 \pm 0.22) \times 10^{-4}$ (Saharan dust, 15% RH)			
$(9.42 \pm 0.41) \times 10^{-4}$ (Saharan dust, 70% RH)			

Comments

- (a) H₂O₂ (initial concentration $\approx 4.1 \times 10^{12}$ molecule cm⁻³) was detected by CIMS using CF₃O⁻ (m/z = 85) as a reagent ion. A sub-micron aerosol was generated by nebulising an aqueous dispersion of TiO₂ particles followed by diffusion drying. Particle number and size distribution was analysed using a DMA, giving typically surface area of $S_a = 6 \times 10^{-3}$ cm² cm⁻³ and D_{\max} of 0.45 μ m at 40% RH. The uptake coefficient was calculated using the time- and aerosol area dependent loss rate of H₂O₂, which was first order in all cases. Uptake coefficients (γ) were measured at relative humidities of 15, 35 and 70 %.
- (b) Experimental method as in comment (a). For Gobi sand the available surface area was mainly from particles of diameter ~ 0.4 μ m, for Saharan dust ~ 0.2 μ m. The relative humidity was varied between 15 and 70 % (not all uptake coefficients obtained are listed in the table above).

Preferred Values

Parameter	Value	T/K
γ (15-70 % RH)	$6.24 \times 10^{-4} - 1.87 \times 10^{-6} \text{ RH} + 9.37 \times 10^{-8} (\text{RH})^2$	298
<i>Reliability</i>		
$\Delta \log (\gamma)$	0.5	

Comments on Preferred Values

The uptake kinetics of H₂O₂ on mineral dust material has been reported in two publications from the same group (Pradhan et al, (2010a, 2010b). Pradhan et al., found irreversible uptake of

H₂O₂ to sub micron Saharan dust, Gobi sand and TiO₂ aerosol substrates, but no gas phase products were detected. For TiO₂, an increase of γ was observed as RH decreased below $\sim 40\%$, but γ remained approximately constant above 50% RH. This was attributed to competition between water molecules and H₂O₂ for surface sites. In contrast, the uptake of H₂O₂ to both Gobi sand and Saharan dust became more efficient with increasing RH. No dependence of γ on [H₂O₂] was observed. In this case, the authors argue that the increasing uptake with RH is due to dissolution of H₂O₂ in surface adsorbed water.

Our preferred values are based on the data for Saharan dust, which is most likely to best represent atmospheric mineral aerosol. The parameters were derived by fitting a polynomial to data read from a graph and should not be extrapolated beyond the range given. The error limits are expanded to reflect this and the fact that (to date) the data are only reported in a discussion paper.

References

- Pradhan, M., Kalberer, M., Griffiths, P. T., Braban, C. F., Pope, F. D., Cox, R. A. and Lambert, R. M., *Environ. Sci. Technol.*, 44, 1360-1365, 2010a.
Pradhan, M., Kyriakou, G., Archibald, T., Papageorgiou, A. C., Kalberer, M., and Lambert, R. M.: *Atmos. Chem. Phys. Disc.* 10, 11081-11107, 2010b.

