

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

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### H<sub>2</sub>O<sub>2</sub> + mineral oxide (dust) surfaces

#### Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Experimental uptake coefficients: <math>\gamma</math></i>			
$1.5 \times 10^{-3}$ (TiO <sub>2</sub> , 15% RH)	298	Pradhan et al., 2010a	AFT-CIMS (a)
$5.0 \times 10^{-4}$ (TiO <sub>2</sub> , 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) H<sub>2</sub>O<sub>2</sub> (initial concentration  $\approx 4.1 \times 10^{12}$  molecule cm<sup>-3</sup>) was detected by CIMS using CF<sub>3</sub>O<sup>-</sup> (m/z = 85) as a reagent ion. A sub-micron aerosol was generated by nebulising an aqueous dispersion of TiO<sub>2</sub> particles followed by diffusion drying. Particle number and size distribution was analysed using a DMA, giving typically surface area of  $S_a = 6 \times 10^{-3}$  cm<sup>2</sup> cm<sup>-3</sup> and  $D_{\max}$  of 0.45  $\mu$ m at 40% RH. The uptake coefficient was calculated using the time- and aerosol area dependent loss rate of H<sub>2</sub>O<sub>2</sub>, which was first order in all cases. Uptake coefficients ( $\gamma$ ) 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  $\sim 0.4$   $\mu$ m, for Saharan dust  $\sim 0.2$   $\mu$ 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
$\gamma$ (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 H<sub>2</sub>O<sub>2</sub> 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

H<sub>2</sub>O<sub>2</sub> to sub micron Saharan dust, Gobi sand and TiO<sub>2</sub> aerosol substrates, but no gas phase products were detected. For TiO<sub>2</sub>, an increase of  $\gamma$  was observed as RH decreased below  $\sim 40\%$ , but  $\gamma$  remained approximately constant above 50% RH. This was attributed to competition between water molecules and H<sub>2</sub>O<sub>2</sub> for surface sites. In contrast, the uptake of H<sub>2</sub>O<sub>2</sub> to both Gobi sand and Saharan dust became more efficient with increasing RH. No dependence of  $\gamma$  on [H<sub>2</sub>O<sub>2</sub>] was observed. In this case, the authors argue that the increasing uptake with RH is due to dissolution of H<sub>2</sub>O<sub>2</sub> 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.

