### UPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HET\_Org09

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HO2 + saturated functionalized organics  products

Experimental data

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | substrate | RH / % | Temp./K | p(HO2) / mbar | Reference | Technique/ Comments |
|  |  |  |  |  |  |  |
| *Uptake coefficients*: *γ* |  |  |  |  |  |  |
| < 0.01 | levoglucosan | 20 | 296 ± 2 | 4×10-9 | Taketani et al., 2010 | AFT-LIF (a) |
| 0.01± 0.01 | polystyrene latex | 22 | 296 ± 2 | 4×10-9 |  |  |
| 0.02± 0.01 |  | 58 |  |  |  |  |
| 0.03± 0.01 |  | 92 |  |  |  |  |
| 0.07± 0.02 | succinic acid | 28 | 296 ± 2 | 4×10-9 | Taketani et al., 2013 | AFT-LIF (b) |
| 0.07± 0.03 | glutaric acid | 28 |  |  |  |  |
| 0.02± 0.01 | adipic acid | 28 |  |  |  |  |
| 0.06± 0.01 | adipic acid | 68 |  |  |  |  |
| 0.06± 0.03 | pimelic acid | 28 |  |  |  |  |
| < 0.004 | stearic acid | 32-75 | 293±2 | 4×10-8 | Lakey et al., 2015 | AFT-LIF (c) |

Comments

(a) Uptake of HO2 to levoglucosan particles (mean surface area weighted diameter of around 100 nm, aerosol surface area up to a few 10-4 cm2 cm-3). Only data at RH<30% are listed in the table. Water content not defined. HO2 was generated by the photolysis of H2O in air and detected as OH (by LIF) following conversion in reaction with NO.

(b) Setup and conditions as in (a); uptake to dicarboxylic acid particles (mean surface area weighted diameter of 110-200 nm, aerosol surface area up to a few 10-4 cm2 cm-3) was measured at RH values of 28 and 68 %; except for adipic acid, which was likely effloresced at both RHs, only values at 28% are listed in the table to represent the pure carboxylic acid in its effloresced amorphous or crystalline form.

(c) Uptake of HO2 to stearic acid particles generated by homogeneous nucleation (peak surface area weighted diameter of 84 nm, aerosol surface area up to 10-4 cm2 cm-3) at RH between 30 and 80 %. HO2 was generated by the photolysis of H2O in N2 or air and detected as OH (by LIF) following conversion in reaction with NO.

Preferred Values

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | **T/K** |
| *γ* | < 0.004 | 290 – 300 |

Comments on Preferred Values

Uptake coefficients of HO2 to aerosol particles containing saturated organic compounds including acids, alcohol and carbonyl functionalities are much lower than those to deliquesced aqueous particles containing dissolved organic components.

The discrepancy between the Taketani et al. (2010, 2013) and the Lakey et al. (2015) studies is also found for other substrates and may be related to differing residence times, surface to volume ratio and differences in the configuration of the FAGE system for the detection of OH following conversion of HO2 in an excess of NO.

In view of the consistency between the Lakey et al. (2015) data on aqueous substrates (see datasheet on aqueous organic substrates) with the bulk aqueous phase kinetics of HO2, we prefer the upper limit provided by Lakey et al. (2015) for stearic acid as a proxy for unsaturated organic compounds.

Taketani et al. (2010) discuss the option of uptake being driven by uptake of hydrated HO2, HO2-H2O (Aloisio et al., 2000), to explain the dependence of the uptake coefficient on RH on solid polystyrene latex particles.

# References

Lakey, P. S. J., George, I. J., Whalley, L. K., Baeza-Romero, M. T., and Heard, D. E.: Environ. Sci. Technol., 49, 4878-4885, 2015.

Taketani, F. and Kanaya, Y.: J. Phys. Chem. Lett., 1, 1701-1704, 2010.

Taketani, F., Kanaya, Y., and Akimoto, H.: Int. J. Chem. Kinet., 45, 560-565, 2013.