

UPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HET_Org09

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This datasheet last evaluated: June 2017; last change in preferred values: June 2017

HO₂ + saturated functionalized organics → products

Experimental data

substrate	RH / %	Temp./K	p(HO ₂) / mbar	Reference	Technique/ Comments	
<i>Uptake coefficients: γ</i>						
< 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.