Geophysical Research Abstracts, Vol. 8, 02950, 2006
SRef-ID: 1607-7962/gra/EGU06-A-02950

Temperature dependent reactions of the NO_3-radical with *para*-substituted phenols in aqueous solution

C. Weller, D. Hoffmann and H. Herrmann

Leibniz-Institut für Troposphärenforschung, Germany

(weller@tropos.de)

The NO_3-radical is one of the most important radicals in the atmosphere besides OH. In general, the atmospheric decomposition or transformation of a variety of organic compounds is initiated by radicals. These processes take place in the gas phase as well as in the liquid phase (cloud droplets, fog, rain, deliquescent particles). Substituted phenols can be directly emitted into the atmosphere or they are formed through oxidation of precursor substances. NO_3-radicals may react with substituted phenols faster in the liquid phase than in the gas phase since there is the possibility for the direct electron transfer besides the H-atom abstraction reaction mechanism [1]. Moreover, liquid phase atmospheric reactions have the potential to form toxic compounds like nitrated phenols and cresols via nitration. For the kinetic investigation of the temperature dependent reactions of NO_3-radicals with substituted phenols a laser flash photolysis-long path laser absorption (LFP – LPLA) setup has been used. NO_3-radicals were generated in a reaction cell in aqueous solution (pH = 0.5 with $HClO_4$) by nitrate-anion photolysis ([NO_3] = 0.05 M) at a wavelength of λ = 248 nm [2, 3]. Pseudo first order rate constants for the reactions of NO_3 with (1) 4-aminophenol, (2) 4-methylphenol, (3) 4-methoxyphenol, (4) 4-nitrophenol and (5) 4-hydroxybenzoic acid were measured between 278 and 318 K. From these measurements second order rate constants were derived and the activation parameters were determined. The kinetic and thermodynamic parameters have been compared with literature values and will be discussed.

[1] Herrmann, H. and Zellner, R.; In *N-Centered Radicals;* Alfassi, Z.B.; Ed., Wiley: Chichester, **1998**, 291

[2] Umschlag, T.; Zellner, R.; Herrmann, H.; *Phys. Chem. Chem. Phys.*, 4, **2002**, 2975

[3] Barzaghi, P. and Herrmann, H.; *Phys. Chem. Chem. Phys.*, 6, **2004**, 5379