Geophysical Research Abstracts
Vol. 13, EGU2011-11104, 2011
EGU General Assembly 2011


# Mechanistic studies on the OH-initiated oxidation of acetone in the aqueous phase

Janine Schindelka and Hartmut Herrmann
Leibniz-Institut für Troposphärenforschung, Permoserstraße 15, 04318 Leipzig, Germany (schindelka@tropos.de)

Acetone is a ubiquitous compound due to its source strength of about 95 Tg/yr and poor reactivity in the gas phase [1]. The latter allows acetone to reach the upper troposphere where it is mainly removed by photolysis reactions. Acetone degradation has an impact on the oxidizing capacity of the (upper) troposphere producing $HO_x$ and ozone. Another potential sink for acetone in the tropospheric multiphase system is the oxidation in aqueous solution. According to the low Henrys law constant of acetone it was thought that this pathway is only of minor importance. However, a recent study detected much higher concentrations in cloud water than expected [2]. An increased uptake into the aqueous phase could be of importance for the formation of SOA (secondary organic aerosol) since acetone serves as precursor for semi volatile organic compounds. Furthermore, an additional effective sink for acetone in turn influences also the $HO_x$ budget of the troposphere. Phase transfer processes as well as degradation reactions of acetone in the aqueous phase are still not completely understood and need further investigation.

Within this work the degradation mechanism of acetone in the aqueous phase was investigated by stepwise identification and quantification of the oxidation products. For the reaction with OH radicals an aqueous solution of 0.1 mM acetone and 1 mM hydrogen peroxide was irradiated with a variable number of laser pulses at $\lambda$ = 248 nm. The mean laser energy per pulse was E = 250 mJ producing a concentration of [OH] = 7.5 $\mu$M. Generated carbonyl compounds as well as acetone were analyzed by HPLCESIMS after derivatization with 2,4dinitrophenylhydrazine and purification using solid phase extraction. In addition analysis for mono- and dicarboxylic acids were done with CEUV.

Identified primary products are acetic acid, methylglyoxal and hydroxyacetone. The further oxidation of these compounds leads to the formation of pyruvic acid, oxalic acid and formic acid. The concentration profiles of acetone and its oxidation products as a function of the number of laser pulses were used to develop a reaction scheme which can be implemented in multiphase chemistry models. Furthermore, the ratio between the two primary degradation pathways was calculated and compared with other studies [3][4][5].

## 1 References

[1] Jacob, D. J., et al. (2002), Atmospheric budget of acetone, *Journal of Geophysical Research-Atmospheres*, 107

[2] van Pinxteren, D., et al. (2005), Schmucke hill cap cloud and valley stations aerosol characterisation during FEBUKO (II): Organic compounds, *Atmospheric Environment*, 39, 4305-4320

[3] Zegota, H., et al. (1986), Acetonylperoxyl Radicals, $CH_3COCH_2O_2$ - a Study on the Gamma-Radiolysis and Pulse-Radiolysis of Acetone in Oxygenated Aqueous-Solutions, *Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences*, 41, 1015-1022

[4] Stefan, M. I., and J. R. Bolton (1999), Reinvestigation of the acetone degradation mechanism in dilute aqueous solution by the UV/H2O2 process, *Environmental Science & Technology*, 33, 870-873

[5] Poulain, L., et. al. (2010), In-cloud multiphase behaviour of acetone in the troposphere: Gas uptake, Henry's law equilibrium and aqueous phase photooxidation, *Chemosphere*, 81, 312-320