



Formation and characterization of dimeric compounds in Secondary Organic Aerosol

M. Beck and T. Hoffmann

Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University, Mainz, Germany (beck003@uni-mainz.de)

Secondary organic aerosols (SOA) are important for air quality and the global climate. The influence of aerosols depends mainly on its chemical composition. Therefore a clearer understanding of formation mechanism, growth, sources and also quantity of SOA is necessary. Today many details concerning these aspects are unknown.

SOA is formed by volatile organic compounds (VOCs) oxidized by ozone, OH- and NO₃-radicals in the atmosphere. The products of these oxidations have different kinds of functional groups (e.g. acid- and aldehyde-groups). Thus the volatility of the compounds decreases and nucleation or condensation on existing particles occurs. As monoterpenes are an important part of VOCs, the atmospheric oxidation is of high interest in aerosol research. ^[1]

Besides oxidation products with monomeric structure, such as pinic acid for example, dimers were found in SOA. The formation of these is discussed intensively. Various reactions in gas- and/or particle phase are possible. The dimers of α -pinene are of high interest due to the quantity of this terpene in the atmosphere. A lot of research hereby is focused on the compounds with the molecular mass 358 and 368. For the former very different formation pathways and chemical structures are suggested in the literature. Also the possibility of using them as marker substances for various atmospheric conditions is discussed. ^[2,3]

Ozonolysis of α -pinene and other monoterpenes in an atmospheric simulation chamber is used to get more information about the formation process. Various changes in the reaction conditions were applied, e.g. adding of OH-scavengers. The ozonolyses were monitored by an on-line APCI-IT/MSⁿ system. Thus time resolved changes of the aerosol composition could be observed. To avoid misleading results, e.g. through isomers or adduct formation in the ion source, the aerosol was sampled on filters after the reaction in the chamber had reached an equilibrium state. Mostly a methanol-water-solution was used for extraction of the filters. Also some experiments with the extracts were made, e.g. changing the pH of the solution. RP-HPLC-ESI-IT/MSⁿ was used for analysis.

References:

- [1] J.H. Kroll, J.H. Seinfeld, *Atmos. Environ.* **2008**, 42 (16), 3593-3624
- [2] L. Müller, M.C. Reinnig, H. Hayen, T. Hoffmann, *Rapid Commun. Mass Spectrom.* **2009**; 23, 971-979
- [3] F. Yasmeeen, R. Vermeylen, R. Szmigielski, Y. Iinuma, O. Böge, H. Herrmann, W. Maenhaut, M. Claeys, *Atmos. Chem. Phys. Discuss.*, **2010**, 10, 10865-10888