Secondary organic aerosol from catechol as a model for atmospheric HULIS: Formation and processing with respect to transformation of functional groups

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A particular fraction of the Secondary Organic Aerosol (SOA) termed Humic Like Substances (HULIS) attracted attention in atmospheric aerosol science only recently, initiating a discourse about their aromaticity and other properties, such as reactivity and hygroscopicity (Grabner & Rudich, 2006). A major portion of HULIS originates from volatile organic compounds, which are formed by abiotic oxidation reactions involving mainly OH radicals and ozone. Subsequently, the particles provide surface for heterogeneous reactions with atmospheric trace gases like halogens released by sea-salt activation. For studying those possible reactions in aerosol smog chambers a HULIS model aerosol is needed, the qualities of which are known in detail. Latest research was only focused towards aerosol formation yields (Coeur-Tourneur et al., 2009). However for heterogeneous chemistry on organic aerosol particles, investigations on chemical composition and structure are a matter of particular interest.

The SOA was produced in a 700 L aerosol smog chamber, equipped with a solar simulator. SOA formation from catechol and guaiacol was investigated at simulated environmental conditions (humidity, light, and presence of oxidizers) and characterized with respect to HULIS properties by particle classifiers, Fourier Transform IR spectroscopy (by long-path absorption and attenuated total reflection), UV/VIS spectroscopy, ultrahigh-resolution mass-spectroscopy, and temperature-programmed-desorption mass-spectrometry. High-resolution imaging was obtained using Field Emission Gun Scanning Electron Microscopy (FEGSEM).

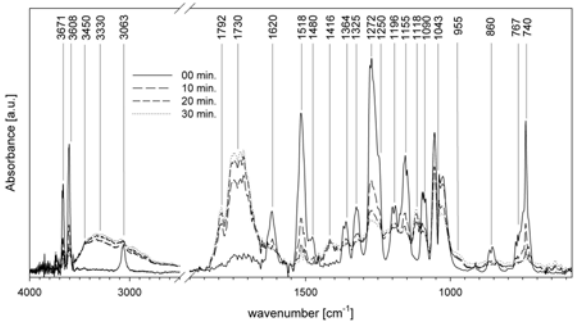

Figure 1. Long-path FTIR spectra of aerosol formation from the reaction of catechol with ozon

Those methods provide a detailed view of the physical-chemistry of the HULIS properties within the organic aerosols without analyzing every single compound the aerosol is built-on. Especially different FTIR methods allow determining the formation and degradation of different functional groups and structural elements during aerosol formation (Figure 1).

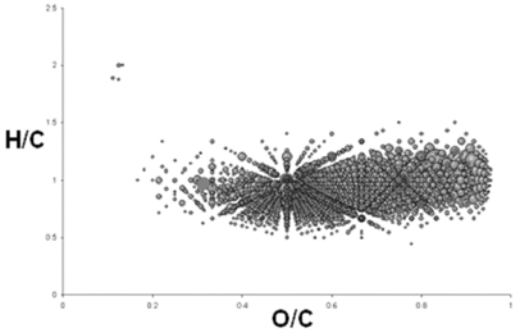

Figure 2. van Krevelen diagram of humic like SOA from catechol obtained from 12 Tesla ICR-FT/MS

Those investigations show that aromatic precursors like catechol and guaiacol are suitable models to form synthetic HULIS for laboratory-scale measurements with the same physical and chemical properties described in literature. The so formed model aerosol has similar O:C rations (Figure 2) as natural oxidized organic aerosols recently described in literature (Jimenez et al., 2009). However, sunlight and relative humidity play a major role in particle production and composition. Here, the functional groups are the anchor points for heterogeneous atmospheric chemistry, e.g. with atmospheric halogen species, which is the focus of our interest.

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