



Molecular characterization of nitrogen and sulfur containing compounds in night-time SOA

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The oxidation of volatile organic compounds (VOCs) leads to the formation of low volatile organic compounds that can form secondary organic aerosol (SOA). Studies in the past showed that laboratory generated and ambient SOA are made of polar molecules with O/C ratios generally greater than 0.5. More recent studies have shown that SOA compounds can contain heteroatoms mainly sulfur and nitrogen atoms. Offline chemical analysis with high-resolution mass spectrometers and fragmentation experiments has shown that sulphur containing compounds are mainly organosulfates and nitrogen containing species are aromatic heterocyclic compounds such as imidazole and nitrated aromatic compounds such as nitrophenols. In addition to these, SOA compounds containing both sulfur and nitrogen have been reported from the analysis of ambient organic aerosol, rainwater, fog and cloud samples. Based on the mass spectrometric evidence these compounds are attributed to nitrooxy-organosulfates originating from isoprene and monoterpenes. Although these compounds are ubiquitously detected in the ambient samples, reports about their detection in laboratory generated SOA are scarce and their formation mechanisms are not well understood. In the present study, we investigated the formation of sulfur and nitrogen containing SOA species in the oxidation of biogenic VOCs. Photooxidation and night-time oxidation experiments were performed in a smog chamber to produce SOA samples. The laboratory generated SOA samples were analysed with UPLC-IMS-TOFMS (Ultra Performance Liquid Chromatography coupled to Ion Mobility Spectrometry and Time of Flight Mass Spectrometry). The presence of highly acidic sulphate seed particles (pH0) did not promote the formation of compounds with chemical formula of C₁₀H₁₇NO₇S- and m/z value of 294.0653, indicating that the formation mechanisms of these compounds unlikely involve the ring opening reactions of epoxides and subsequent sulfation reactions. On the other hand, their formation was significantly enhanced when the night-time oxidation was performed in the presence of both neutral seed particle and gas-phase SO₂, suggesting that the presence of gas-phase SO₂ is a key for their formation.