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Oligomerization as a potential mechanism for Secondary Organic Aerosol (SOA) formation in clouds

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Electrospray ionization - mass spectrometry (ESI-MS) has been used to investigate oligomer formation in dark chamber experiments designed to study the polymerization conditions of common atmospheric photooxidation products without photochemical action. Methylglyoxal has been selected as the monomer considering, it is a gas-phase product from the atmospheric oxidation of isoprene and terpenes (biogenic sources) as well as of aromatic compounds (anthropogenic sources). Aqueous-phase oligomer formation of methylglyoxal has been investigated in a simulated cloud matrix, under dark conditions in view of its short life time (1̃.6 hrs). A mechanistic pathway for the growth of oligomers via aldol condensation under cloud conditions and in the absence of UV-light and the OH radical is proposed here for the first time.

Soluble oligomers (n=1-12) formed in the course of acid-catalyzed aldol condensation have been detected and identified by positive and negative ion ESI-MS, while their relative abundance is estimated from the full-scan mass spectra. In particular, oligomer abundances and their adduct formation was considered with special emphasis on the structural elucidation of these oligomers and their corresponding adduct products. The oligomer series starts with a -hydroxy ketone via aldol condensation and oligomers are formed by multiple addition of C3H4O2 units (72 Da) to the parent -hydroxy ketone. MS2 ion trap experiments have been performed to structurally characterize the oligomers.

Oligomers could form under conditions encountered in clouds even at micromolar concentrations and thus could significantly result in secondary organic aerosol (SOA) after cloud droplet evaporation. Therefore, it is proposed that oligomer formation does not only occur during droplet evaporation when the concentrations of products increase but could as well be an in-cloud process and substantially enhance in-cloud SOA yields.