Characterization of Organic Aerosol Composition with Ultra-High Resolution Mass Spectrometry Techniques

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Atmospheric particles play an important role in the climate system and are linked to human health effects in polluted air. A significant fraction of the atmospheric particle mass is composed of organic compounds but the chemical composition of this organic material, their sources and atmospheric chemical and physical processing such as oxidation and aerosol-cloud interactions are poorly understood.

The lack of understanding of organic aerosol properties and processes are partly due to the highly complex mixtures present in organic aerosols with thousands of organic compounds being observed. In addition, organic aerosol components cover a very large chemical space, e.g., with regard to polarity, solubility or functional group distribution and often only small amounts of sample (in the µg range) are available for analysis. Most conventional analytical techniques are selective to a rather narrow section of this large chemical space and thus for conventional analytical techniques a majority of the compounds present in organic aerosol is not accessible due to these fundamental limitations. Mass spectrometry is the only analytical technique that combines sufficient sensitivity and separation power to characterize the complex compound mixtures in organic aerosols.

Developments of high mass resolution mass spectrometers and novel ionization techniques, contributed to an advanced understanding of atmospheric aerosol composition in recent years and examples of both aspects will be discussed here. Especially ultra-high resolution mass spectrometers allow identifying the elemental composition of thousands of unknown organic compounds and a detailed characterization of particle phase reaction products such as oligomers (Nizkorodov et al., 2011; Kourtchev 2014). A wide range of novel ionization techniques (e.g., nano-electrospray or direct desorption electrospray ionization (Roach 2010; Fuller 2012) allows for simplified sample preparation procedures, which potentially lead to less measurement artefacts and higher sample throughput. New ionization techniques such as online extractive electrospray ionization also allow following in detail kinetics of particle phase reactions with high time resolution, which is not possible with conventional techniques (Gallimore 2013).

References

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