Recent advances in mass spectrometry techniques to determine the composition and reactivity of atmospheric aerosols

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Atmospheric aerosol particles are important in many atmospheric processes such as light scattering, light absorption, and cloud formation. Oxidation reactions continuously change the chemical composition of aerosol particles, especially organic components, which are often a dominant fraction and lead to highly complex compound mixtures in ambient aerosols. These ageing processes are poorly understood but are known to affect for example the cloud formation potential of aerosol particles.
The use of conventional analytical techniques often limits a comprehensive characterization of organic aerosol composition and processes due to the thousands of compounds present in organic aerosol particles and the often only small amounts of sample (in the μg range) available for analysis. In addition, organic aerosol components cover a very large chemical space, e.g., with regard to polarity, solubility or functional group distribution. Most conventional analytical separation 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 two instrumental aspects, better mass resolution 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.
The use of high resolution and ultra-high resolution mass spectrometers allows identifying the elemental composition of thousands of unknown organic compounds and a detailed characterization of particle phase reaction products such as oligomers (1-3). High resolution mass spectrometers are very successfully deployed in field measurements and significantly advanced our qualitative and quantitative understanding of atmospheric aerosol composition and the effect of oxidative aging processes (4). A wide range of novel ionization techniques (e.g., direct desorption electrospray ionization (5)) allows for simplified sample preparation procedures, which potentially lead to less measurement artifacts 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.

References

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