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Organic acid analysis in aerosol particles and cloud water using capillary electrophoresis – mass spectrometry

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Carboxylic acids are an important fraction of the organic aerosol. As stable products in atmospheric oxidation processes their determination allows insights into chemical reaction pathways. They are also discussed to have an influence on the hygroscopicity of aerosol particles, thereby changing their ability to act as cloud condensation nuclei.

The aim of this study was to develop and optimise a method which allows the determination of aliphatic and aromatic organic acids in aqueous extracts of atmospheric particulate matter and cloud water samples.

A capillary electrophoresis (CE) System (Agilent), coupled via an electrospray ionization (ESI) to an ion trap mass spectrometer (IT-MS) (esquire 3000+, Bruker) or a time-of-flight mass spectrometer (μ TOF-MS, Bruker) was used as instrumentation.

Based on earlier work in our group (Iinuma and Herrmann, 2003), a 20 mM Ammoniumacetate electrolyte with pH 9.1 was used for separation which exhibited a good resolution of different carboxylic acids. The optimization of different parameters influencing the efficiency of the electrospray (thereby the sensitivity of the system) was done by means of chemometric methods.

Clean-up and enrichment of the aqueous samples is done by a solid phase extraction step and subsequent blowdown of the desorption solvent (methanol). Different solid phase materials have been tested. OASIS HLB (Waters) was found to give the highest recovery for the target analytes. The process of peak identification in real sample extracts was significantly facilitated by the possibility of exact mass determination

of the μ TOF-MS. A wide range of mono- and dicarboxylic acids could be identified by comparison of mass spectra and migration times with authentic standard solutions. The identified compounds include many carboxylic acids with one ore more additional functional groups.

Figures of merit for the new analytical method will be presented and the application to real samples is shown.

References

Iinuma, Y., and H. Herrmann, J. Chrom. A, 1018 (1), 105-115, 2003.