



Identification of water-soluble polar organics in air and vehicular emitted particulate matter using ultrahigh resolution mass spectrometry and Capillary electrophoresis - mass spectrometry.

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The effects of aerosols on human health, atmospheric chemistry, and climate are among the central topics in current environmental health research. Detailed and accurate measurements of the chemical composition of air particulate matter (PM) represent a challenging analytical task. Minute sample amounts are usually composed of several main constituents and hundreds of minor and trace constituents. Moreover, the composition of individual particles can be fairly uniform or very different (internally or externally mixed aerosols), depending on their origin and atmospheric aging processes (coagulation, condensation / evaporation, chemical reaction). The aim of the presentation was the characterization of the organic matter (OM) fraction of environmental aerosols which is not accessible by GC-methods, either because of their high molecular weight, their polarity or due to thermal instability. We also describe the main chemical characteristics of complex oligomeric organic fraction extracted from different aerosols collected in urban and rural area in Germany and Canada.

Mass spectrometry (MS) became an essential tool used by many prominent leaders of the biological research community and the importance of MS to the future of biological research is now clearly evident as in the fields of Proteomics and Metabolomics. Especially Fourier Transform Ion Cyclotron Mass Spectrometry (ICR-FT/MS) is an ultrahigh resolution MS that allows new approach in the analysis of complex mixtures. The mass resolution (< 200 ppb) allowed assigning the elemental composition (C, H, O, N, S...) to each of the obtained mass peaks and thus already a description of the mixture in terms of molecular composition. This possibility is used by the authors together with a high resolution separation method of charged compounds: capillary electrophoresis.

A CE-ESI-MS method using an ammonium acetate based background electrolyte (pH 4.7) was developed for the determination of isomeric benzoic acids in atmospheric aerosols and vehicular emission. UltraTrol LN was employed as the pre-coated polymer to suppress the EOF (0.3×10^{-9} m²V⁻¹s⁻¹) and achieve a baseline separation of studied acids. Good repeatability for migration time (RSD $< 1\%$, N=10) was obtained without coating regeneration. The high pre-coating stability allowed coupling of CE to MS without ion suppression in MS. In scanning mode and using field-amplified sample injection with electrokinetic injection (-5 kV for 60 s), LODs (S/N =3) ranged from 2.5 to 6 μ g/L for standard target analytes prepared in deionized water. In the presence of 100 mg/L of sulphate (added to simulate a sample matrix), LODs ranged from 8 to 90 μ g/L. Several aromatic acids were identified in atmospheric and diesel-engine emitted particulate matter. In off-line combination with the electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI-FT-ICR-MS), this method provided accurate molecular mass determination of unknowns containing various functionalised carboxylic and sulfonic acids, and allowed their formula to be proposed.