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Analysis of the unresolved organic fraction in aerosols with ultrahigh resolution 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 research. Earth's energy balance by scattering and absorption of radiation. 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 describe the main chemical characteristics of complexe oligomeric organic fraction extracted from different aerosols collected in urban, indoor and rural area in Germany, Hungary and Canada. Hundreds of organic compounds (hydrocarbons, carboxylic acids, etc.) have been determined in atmospheric aerosol particles, mostly by selective analysis of filter or impactor samples with gas or liquid chromatography, capillary electrophoresis, UV/VIS and mass spectrometry. Generally, however, no more than 10-40% of the OPM content estimated from OC measurements have been identified on a molecular level. Several studies using a wide range of spectroscopic, chromatographic and hyphenated bioanalytical techniques indicate that macromolecular components such as biopolymers from soil

or atmospheric transformation of biogenic and anthropogenic precursors, and highly oxygenated hydrocarbon derivatives account for significant fractions of the unknown substances. They have a largely unexplored potential for adverse health effects, and can be efficiently modified by heterogeneous reactions in the atmosphere or during the sampling process, which can lead to significant analytical artefacts. 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 (FT-MS) is an ultrahigh resolution MS system that allow new approach in the analysis of complex mixtures. The mass resolution ($<$ 200 ppb) allow to assign the element composition (C, H, O, N, SĚ) 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 author in the non targeted environmental metabolomic approach in the molecular level characterization of natural organic matter (NOM) from terrestrial, marine and aquatic environments.

Novel aspects: Data and data evaluations/visualizations from the analysis of unknown polar organic fractions from aerosols as measured with NMR and Chip ESI-FT/MS.