Method development to characterization of polar VOC-oxidations products in cloud water and aerosol with LC-MS

D. Hofmann and H. Herrmann

Institut für Troposphärenforschung e.V., Permoserstraße 15, D-04318 Leipzig, Germany
Tel.: (0341) 235 2614
Fax: (0341) 235 2325
e-mail: hofmann@tropos.de

Present knowledge about the composition of the organic part of the fine aerosol fraction is small. Organic components represent 15 - 55 % of the particle mass in anthropogenic influenced regions. Up to now only a part of 10 - 20 % of these compounds could be characterized (Rogge et al., 1993, Facchini et al., 1998). Investigations were performed mainly using GC-MS methods with and without derivatization. The application of other advanced analytical techniques like Curie-point-pyrolysis-GC-MS and capillary electrophoresis could increase the spectrum of examinable classes of substances (Neusüß et al., 2000) regarding higher molecular and ionic compounds. Secondary organic carbon (SOC) form (i) through adsorptive and/or absorptive condensation or nucleation of products of gas-phase hydrocarbon oxidation and (ii) by cloud and aerosol chemical conversions. These products should represent substances with high polarity showing thermal instability and possessing several functional groups. Latest, soft techniques like API-MS do not need derivatisation and should contribute to further characterization of the organics in aerosols. First API-MS experiments, partly in combination with liquid chromatography, were performed by Kwok et al. (1996), Aschmann et al. (1997), Hoffmann et al. (1998) and Glasius et al. (1999) for characterization of products from smog chamber experiments. The intention of this study is to use API-MS techniques for structural elucidation of organics from different field experiments. To this end, first results from chromatographical and mass spectrometric method development (optimization of detection limits and chromatographic separation regarding mass spectrometric detection, comparison of different possible MS/MS investigations as well as sample concentrations with a modified and miniaturized light phase rotary perforator) regarding the example of nitro- and dinitrophenols in (cloud) water.

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