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CHENOMX BASED NMR METHOD FOR ORGANIC AEROSOL ANALYSIS

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A novel NMR approach to the analysis of organic aerosol composition was tested. The method is focused on the water soluble organic compounds (WSOC) analysis, which is the least examined group of organic aerosols. So far, the use of NMR technique was limited to so called Functional Group Analysis, where measured ¹H NMR spectra of the WSOC are divided into parts and the entire area is integrated without or with very little identification of individual compounds [1]. Recently, the employment of 2D NMR techniques (COSY, HSQC) was published, however the analysis is rather challenging [2].

The proposed NMR technique exploits the NMR metabolomic approach, in which the ¹H NMR spectra of individual compounds are fitted into the complex ¹H NMR spectra. The assignment is based on precise chemical shift of dominant signals of given compound. The library spectrum is subsequently subtracted from the aerosol sample spectrum. For this purpose software ChenomX 8.0 is employed. The key to the detail analysis lies in an extensive database. ChenomX database is primarily intended for metabolite analysis, however ca. 60 compounds can be found also in WSOC fraction. Additionally, the software allows database extension and new compounds can be added.

The suitability of ChenomX was performed on both real atmospheric aerosols and model samples of coal combustion and up to 30 compounds were found in analyzed samples. Most abundant substances were mono- and dicarboxylic acids (formic, acetic, succinic acid) and their derivatives (lactic acid), followed by carbohydrates, anhydro saccharides and sugar alcohols (levoglucosan, fructose, D-threitol) and amines (methylamine, dimethylamine). The real aerosol sample was analyzed also on four different NMR spectrometers (500, 600, 700, 800 MHz) in to order to

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enhance the resolution and find less abundant substances. The frequencies of the spectrometers were chosen according to the ChemomX database. In the 800 MHz spectrum ca. 50 compounds were identified.

References:

1. Chalbot, M. C. G.; Brown, J.; Chitranshi, P.; Gamboa da Costa, G.; Pollock, E. D.; Kavouras, I. G. Functional characterization of the water-soluble organic carbon of size-fractionated aerosol in the southern Mississippi Valley. *Atmos. Chem. Phys.* **2014**, *14*, 6075–6088.
2. Chalbot, M. C. G.; Gamboa da Costa, G.; Kavouras, I. G. NMR Analysis of the Water-Soluble Fraction of Airborne Pollen Particles. *Appl. Magn. Reson.* **2013**, *44*, 1347–1358.