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NMR AEROSOLOMICS: A CONVENIENT ROUTE TO ORGANIC AEROSOL ANALYSIS

Štěpán HORNÍK, Jaroslav SCHWARZ, Jan SÝKORA

Institute of Chemical Process Fundamentals of the CAS, Prague, Czech Republic,
hornik@icpf.cas.cz

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INTRODUCTION

Atmospheric aerosols are a small but very important part of the Earth's atmosphere. The proportion of inorganic and organic compounds in aerosol particles seems to be equal on average (Saxena, 1996; Schwarz, 2016). While the inorganic composition of aerosols is well explored, knowledge about the organic part is still very limited. It is well known that the major part of organic aerosol compounds (Saxena, 1996) is represented by polar, water-soluble organic compounds (WSOC). So far GC-MS is the most frequently used method for WSOC analysis. GC-MS is a very sensitive technique; furthermore, it exploits huge spectra libraries accumulated over decades. Therefore, its role in the determination of aerosol composition is indisputable. Primarily owing to GC-MS, about 150 organic compounds have been identified in aerosol particles. NMR spectroscopy for the purpose of aerosol chemistry was "discovered" only recently (Decesari, 2000) as it is rather insensitive method. Nevertheless, NMR has undergone rapid development and sensitivity gain of late. Moreover, it is fully quantitative method and no sample derivatization is needed. So far, the use of NMR spectroscopy has been limited to so called Functional group analysis (Chalbot, 2014). In this analysis the whole NMR spectrum is divided into parts and subsequently integrated according to functional groups.

EXPERIMENTAL SETUP

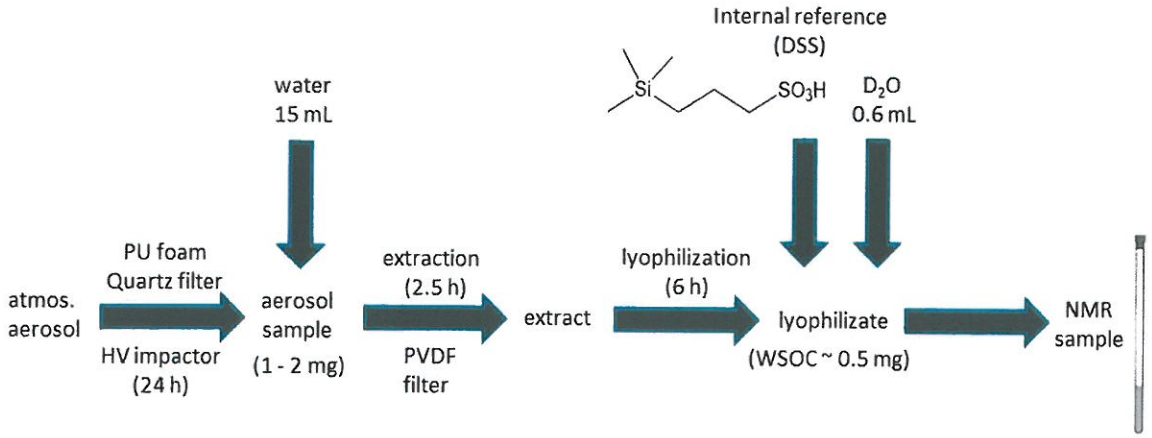

Fig. 1: Scheme of a NMR sample preparation

The optimized procedure for an aerosol sample preparation starts with aerosol filter extraction into deionized water. The extract is lyophilized and the lyophilizate is dissolved in proper amount of deuterated water containing internal standard and the sample is transferred into NMR tube. The ^{1}H NMR spectrum is usually obtained in the overnight measurement.

Aerosol samples usually come from a high-volume cascade impactor, that collects appropriate amount of aerosol matter for NMR analysis within reasonable time period (24 - 48 hours). The samples from high-volume cascade impactor are divided according to their particle size. Aerosol source samples (from diesel combustion engines and from biomass burning) come from various institutions.

RESULTS AND CONCLUSIONS

Here we propose to employ the metabolomic approach for the complex evaluation of aerosol composition. In NMR aerosolomics the assignment of dominant signals is based on precise chemical shift of the compound which enables identification of organic compounds in given aerosol sample and the original aerosol source. For this purpose, a comprehensive library of high—res ^{1}H NMR spectra of organic compounds that are known to be present in aerosol particles is essential. Originally, NMR aerosolomics was exploiting the original metabolomic library. The database of the ChenomX NMR Suite program[5] contains about 70 compounds that have also been found in aerosol samples according to the literature. We were able to identify more than 30 compounds in every analyzed sample. Up to now, 50 new compounds attributed to aerosol have been added to the database; the largest gap was in aromatic carboxylic acids (12), compounds containing sulphur (11) and amines (8). Subsequently, the score of identified compounds in real spectra jumped to over 50. Additionally, about 30 new organic compounds (mainly hydroxy carboxylic acids) were found in aerosol samples. These compounds were present in the original ChenomX library and had not been found in aerosol samples so far. The obtained results clearly show that NMR metabolomics is very powerful methods and can be implemented also in the analysis of organic compounds contained in aerosols.

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