P6 - NMR AEROSOLOMICS AS A TOOL TO DISTINGUISH VARIOUS TYPES OF AEROSOL SAMPLES

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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.[1,2] 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 is represented by polar, water-soluble organic compounds (WSOC).[1] NMR spectroscopy was for the purpose of aerosol chemistry "discovered" only recently[3] as it is rather insensitive method. Nevertheless, NMR has undergone rapid development and sensitivity gain of late.

Aerosolomics provides complex evaluation of aerosol composition and compound concentration.[4] It is exploiting metabolomic approach, which is applied to aerosol samples. 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. 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. 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. Up to now, 50 new compounds attributed to aerosol have been added to the database; the largest gap was found in aromatic carboxylic acids (12), compounds with sulphur (11) and amines (8). Additionally, about 30 new organic compounds (mainly hydroxyl carboxylic acids) were found in aerosol samples. These compounds were present in the original ChenomX library and have not been found in aerosol samples yet.

In the recent study, the summer and winter aerosol samples were analyzed using NMR aerosolomics approach. The samples were collected in Prague-Suchdol during summer 2008 and winter 2009 in two different particle size fractions – PM2.5 and PM10. Around 50 compounds were identified in each aerosol spectrum owing to the comprehensive library. The profile of 86 identified compounds, which were identified in the samples altogether, served as an input data for statistical analysis. Multivariate statistical analysis clearly discriminates the two groups studied. Furthermore, it is possible to determine the most significant compounds.

References

1. P. Saxena, L.M. Hildemann, *J. Atmos. Chem.* **1996**, 24(1), 57-109..
2. J. Schwarz, J. Karban, E. Chalupnickova, V. Havranek, J. Smolik, V. Zdimal, *Atmos. Res.* **2016**, 176, 108-120.
3. S. Decesari, M.C. Facchini, S. Fuzzi, E. Tagliavini, *J. Geophys. Res., [Atmos.]* **2000**, 105, 1481–1489.
4. J. Ruiz-Jimenez et al., *Aerosol Science 109*, Finnish Center of Excellency (FCoE) in physics, chemistry, biology and meteorology of atmospheric composition and climate change, Kuopio, Finland, 17-19 May, 2010.
5. ChenomX Inc., ChenomX NMR Suite 8.0, Alberta, Canada **2016**, http://www.chenomx.com/

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