Chlorinated Paraffins Analysis by High-Resolution Mass Spectrometry Coupled with an Atmospheric Pressure Glow Discharge Micro-Plasma Ionization

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CPs mixtures contain hundreds of thousands of homologues. The single-chain CP-materials also contain a small amount of chlorinated olefins (COs), which are their transformation product that can interfere. Monitoring CPs currently requires a chromatographic method coupled to a MS and induction of chlorine adduct formation by adding dichlorometane to a methanol: water solution.

The liquid sampling - atmospheric pressure glow discharge (LS-APGD) micro-plasma ionization source is a proven method to obtain atomic and molecular (CAM) information from a variety of analytes[1]. To further extend upon the already versatile capabilities of the LS-APGD ionization source, it was coupled to a high-resolution Orbitrap MS as a new technique for the challenging analysis of Chlorinated Paraffins (CPs) materials.

As the complexity of CP mixtures requires both high resolution (e.g. R ≈ 120'000 at m/z …)[2] and high sensitivity, we coupled the CAM-Orbitrap LTQ XL system to an external high-performance data acquisition (DAQ) system (FTMS Booster X2). The employed DAQ system enables mass spectra representation in the absorption mode Fourier transform helping to improve mass spectral resolution and dynamic range[3].

Synthetized C18-chloroparaffin material of low, medium and high chlorination degrees of different concentrations was analysed and detected for the first time as nitrate adduct in a methanol: water solution. We will present the ability to resolve CPs from the COs interferences (separated by 18 mDa) already with a resolution of 30'000 at m/z …. The DAQ proved to be able to double the resolution, provide the spectral dynamic range of 3.5 orders of magnitude, and improve the sensitivity.

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[2] Knobloch M.C. et al., *Chemosphere*, **2021**, 283, 131199
[3] Jacob R. Bills et al., J. Am. Soc. Mass Spectrom, **2021**, 32, 1224-1236