G.A.S. Technical Note

Working principle of the GC-IMS technology

Ion Mobility Spectrometry (IMS) is an analytical technology to separately detect gaseous compounds in a mixture of analytes. The separation is based on the specific *drift times*, that ionized compounds need to pass a fixed distance (*drift tube*) in a defined electric field. Compared to other techniques e.g. TOF-MS, ions travel at atmospheric pressure versus a flow of inert *drift gas*. The drift time of each substance is determined by its ion's mass and geometric structure, as slowing collisions with the drift gas molecules are more frequent for sterically demanding structures. Therefore IMS can even differentiate isobaric molecules. For detection, the resulting ion current is measured by an electrometer as a function of time.

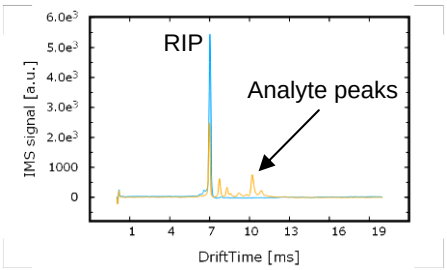

Figure 1: IMS spectra with and without analyte

Atmospheric Ionization of molecules can be obtained by several techniques. G.A.S. uses photoionization with a 10.6eV UV-lamp or soft chemical-ionization initiated by a low-radiation tritium (H3) source (below exemption limits of EURATOM). While the first directly produces positive ions, the latter generates *rectand ions* with the gas atmosphere by a cascade of reactions following the collision of a fast electron emitted from the *β*-radiator H^3[1]. The so-called Reaction Ion Peak (RIP) representing the total of all ions available is formed. In nitrogen and air, resp., the *reactand ions* can be descibed as $H^+(H_2O)_n$ and $O_2^-(H_2O)_n$. Chemical ionization of analytes by *reactant ions* then result in the formation of specific analyte ions, when the affinity of the analyte towards the reactand ion is higher when compared to water. The proton affinity of water is 691kJ/mol, so all molecules with a higher proton affinity will be ionized by proton transfer, which is typically given for all heteroatom-organic compounds. The ionization takes place at ambient pressure, so that the analyte concentration is not diluted as compared to other analytical methods where a vacuum has to be applied. Therefore IMS is extremely sensitive. The detection limits typically are in the low ppb-range for *volatile organic compounds* (VOC).

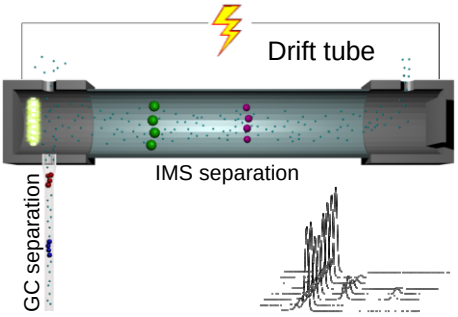

Figure 2: Sketch of the analyte flow in a GC-IMS

Figure 1 exemplarily shows the IMS spectrum without analyte (azur) and with analyte (orange). The RIP is formed as a sharp signal proving the cleanliness of the system and at a specific position that is used as internal standard. The spectrum containing analytes shows a decreased RIP, while new (analyte) peaks are correspondingly formed. The drift time is specific of an ion, therefore analyte identification is possible. The peak height and area correlate to the analyte concentration, so that a quantification is also possible.

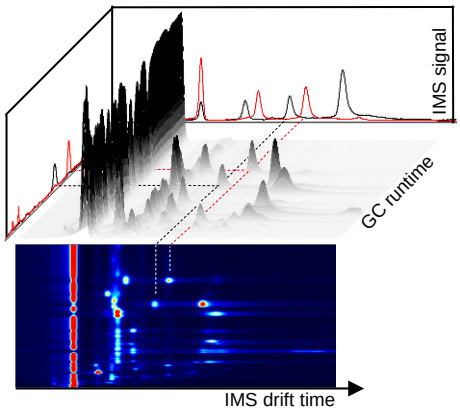

Figure 3: 3D GC-IMS measurement dataset

Complex analyte mixtures, like e.g. food flavours, often demand a second and independant separation step in order to seperately analyse the multiplicity of compounds at low concentrations. G.A.S. equips its IMS systems with gas chromatographic (GC) columns. The volatile compounds of *samples under testing* are pre-serparated in time by a GC column. The discrete compounds are consecutively fed into the IMS ionization chamber, so that analyte and/or ion interactions are prevented (*Figure 2*). Furthermore a competition of analytes on the *reactand ions* is excluded, enhancing the sensitivity of the individual compounds.

The **GC-IMS setup** enables a twofold separation of analyte mixtures and the detection by the IMS electrometer. Since the IMS measurements are extremely fast (21ms / spectrum) a continuous and high-resolution recording of analyte signals is provided. *Figure 3* sketches the GC-IMS measurment's 3D-dataset and the corresponding heatmap visualization.

[1] Eiceman, G. and Karpas, Z., Ion Mobility Spectrometry, ISBN 0-88493-2247-2

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