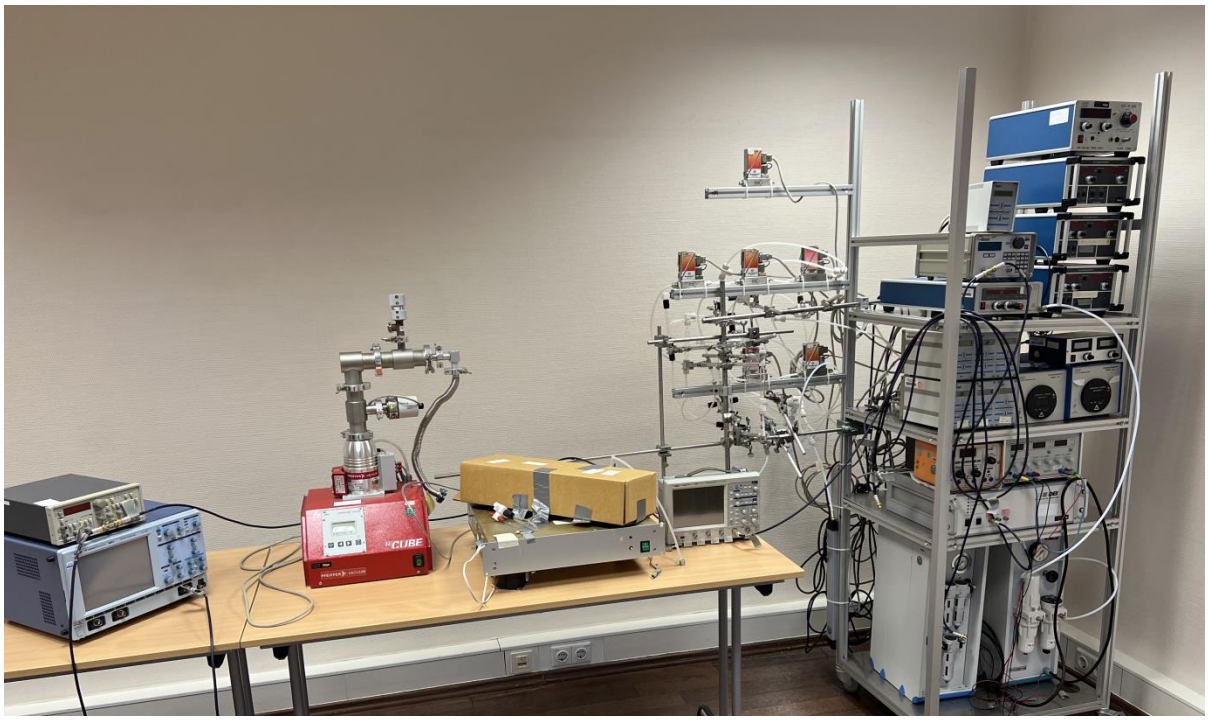
Pulsed Ion Mobility Spectrometry

Ion Mobility Spectrometry (IMS) is an analytic technology that helps to identify unknown substances, typically in the gas phase. It also supports identifying the molecular structure of substances if combined with other techniques such as mass spectrometry or optical spectroscopy.

IMS requires the ionization of the substance, which can be achieved with different techniques. We use a pulsed electron gun which allows obtaining further information about the sample by e.g. delaying ionization and detection. A gas chromatograph (GC) can be added to increase the precision of the experiments. Typical problems are resolving power too low, or response not specific enough (multiple peaks in the spectrum etc.) that we try to solve with our set up.



Apart from the experimental side, we are also working on the theoretic side by investigating how the calculation of mobilities with help of theoretic principles can be enhanced (i.e. the calculated results are close enough to the experimental results). These theoretic calculations require knowing the molecular geometry, which is then bombarded with air (nitrogen) particles in order to calculate via collision theory the collision cross section and thus the ion mobility. The molecular geometry is typically obtained in quantum-chemical structure optimization calculations, which do not necessarily represent the experimental structures; problems are temperature, internal energy, etc. We work on analyzing how different approaches can lead to better start structures by e.g. employing quantum-chemical trajectory calculations and other techniques. While larger molecules are leading to relatively good results, we are working on smaller structures with a more environmental background such as VOCs and other hazardous substances.

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