

Real-time measurements of organic pollutants in atmospheric aerosols



General Introduction

Understanding the composition of fine particulate matter in the atmosphere, particularly the role of organic trace substances, is crucial for tracking environmental pollution and its impact on human health and Earth's climate. Organic molecules originate from both anthropogenic activities and natural sources. Through generous funding from the REACT-EU program, we have acquired a high-resolution mass spectrometer (Orbitrap Exploris 120, Thermo Fisher Scientific). This instrument enables in-situ and real-time measurements of aerosol composition, with a specific focus on analyzing particle-bound organic pollutants in urban and rural areas. Emphasizing the detection and characterization of emissions from individual sources such as biomass burning, agricultural activities and chemical transformation reactions, this poster presents our initial findings.

Working principle of an Orbitrap-MS

The orbitrap mass spectrometer (MS) operates by introducing a liquid or gaseous sample into the ion source, where the molecules are ionized, giving them a positive or negative charge. After ionization, the molecules enter the vacuum within the orbitrap system, where they are accelerated and pass through a series of lenses. During this process, neutral (non-charged) molecules are filtered out. Subsequently, the ions enter the quadrupole, from which either all or only selected ions can exit into the C-trap and the following Ion Routing Multipole (IRM). Here, ions can either undergo fragmentation or exit the IRM and re-enter the C-trap, where they are focused before being injected into the Orbitrap. The stable trajectory of ions in the Orbitrap is determined by their mass-to-charge (m/z) ratio and the electromagnetic fields generated by the electrodes, with the frequency of these orbits being characteristic for individual molecules or molecule fragments.

Area of application

The Orbitrap system was acquired with two main areas of application. The first application is for real-time measurements in a laboratory setting, where we generate secondary organic aerosols (SOA) under controlled conditions using simplified oxidative systems (Fig. 2b). Secondly, it facilitates field studies by allowing the measurement of ambient aerosols with a very high mass and temporal resolution. An additional explicit advantage of the Orbitrap Exploris 120 is its compact design, making it ideal for installation in space-constrained areas such as measurement containers (Fig. 2a). In the future we will deploy the instrument near Frankfurt airport and at the Taunus Observatory.

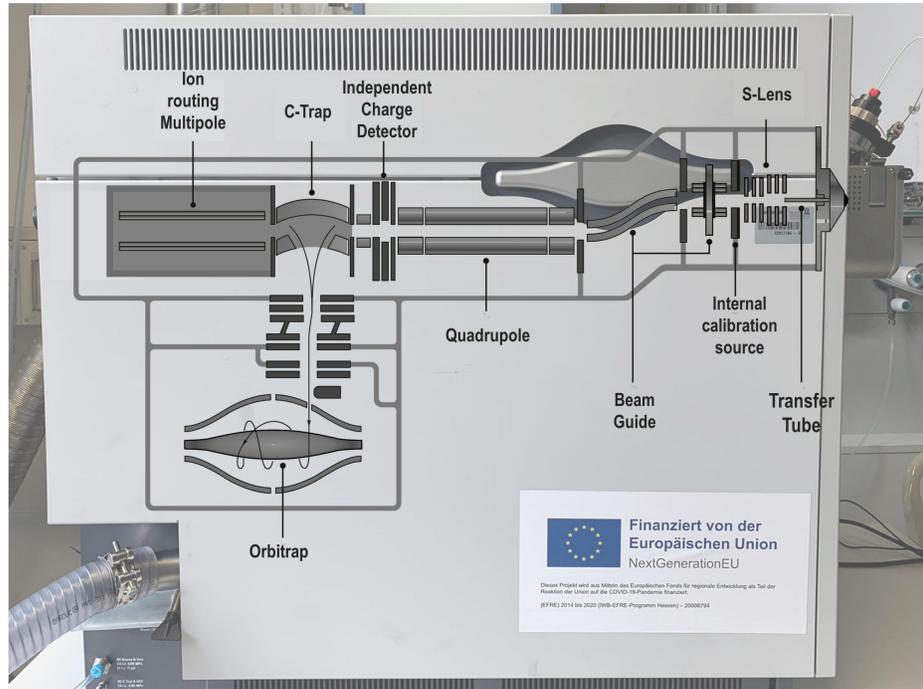


Fig. 1: Orbitrap Exploris 120 system with a sketch depicting its internal components



Fig. 2: a) Orbitrap-MS system inside the ALFA measurement container; b) Orbitrap-MS setup for laboratory experiments



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