NCAR | ATMOSPHERIC CHEMISTRY OBSERVATIONS & MODELING

Virtual ACOM Seminar

CI-Orbitrap: an instrument to study atmospheric reactive organic species and formation of new particles in the atmosphere

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Date: Monday, November 29th, 2021, 10:00am – 11:00am

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ABSTRACT

Over the last ten years, mass spectrometric techniques have made dramatic improvements in detecting and characterizing gas-phase oxygenated species, including radicals, of varying volatilities. In particular, chemical ionization mass spectrometry (CIMS) has become a powerful tool to characterize a wide range of different gaseous compounds. CI is a soft ionization technique where the analytes are ionized through a clustering process with the reagent product ions and undergo only minimal fragmentation. While CIMS provides very good sensitivity when coupled to TOF mass analyzers (detection limit as low as 104 molecules cm-3), with limited mass resolving power. This typically ranges from 3000 up to 14 000 for a high-performance TOF mass analyzer. The insufficient resolving power makes identification and quantification of individual organic molecules extremely challenging, especially in cases with multiple overlapping ions, yielding significant uncertainties. Indeed, "atmospheric" mass spectra acquired using the CIMS technique typically contain a large amount of information, representing a significant challenge for data analysis. Computational approaches, including ion deconvolution procedures, are required to solve this limitation to extract the maximum possible information content. In addition, as the primary method to detect highly oxygenated organic molecules (HOMs) has hitherto been based on the chemical ionization atmospheric pressure interface time-of-flight mass spectrometry (CI-APi-TOF), the main obtained information is the elemental composition. No structure and/or physicochemical properties (e.g., volatility) can be derived from such measurement.

To overcome these obstacles, one possibility is to take the advantage of the Orbitrap technology (i.e., very high mass resolving power: 140 000 at m/Q 200 Th). Hence, we coupled an Orbitrap to an extractive electrospray ionization (EESI) inlet and to a CI inlet to characterize at a molecular level the composition of the particle and gas phases, respectively. Through various experiments performed in laboratory and field campaigns, the ultra-high resolving power of the EESI or CI-Orbitrap allowed an unambiguous identification of all ions, even in cases where traditional TOF mass analyzers are unable to separate ions. In addition, the use of tandem mass spectral analyses provides novel and useful structural information that helped identify key components of atmospheric aerosol formation. In sum, these new analytical instruments can help to answer some of the questions that so far were unable to be answered due to the pre-existing instrument limitations.

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