Ground-truthing the performance of Orbitrap-iso for ice core nitrate stable isotope ratios by comparison to traditional Isotope Ratio Mass Spectrometer (IRMS) measurements

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Innovative enhancements to the bioanalytical Orbitrap mass spectrometer now allow quantification of stable isotope ratios of soluble species. The novel technique, known as Orbitrap-iso, enables deeper-than-ever isotopic analysis of ice core oxyanions, including nitrate and sulfate.

On paper, the Orbitrap-iso methodology presents a compelling alternative to the established Isotope Ratio Mass Spectrometry (IRMS) approach for quantification of isotope ratios of ice core oxyanions. Unlike IRMS, which necessitates the conversion of nitrate samples into gases (N₂, O₂) for analysis, Orbitrap-iso directly measures isotopologue ratios on intact ions in liquid solution. This streamlined process significantly simplifies sample preparation and enables additional quantification of enrichments in multiply-substituted (clumped) isotopologues in ice core oxyanions. These enrichments can offer valuable insights into the historical oxidative environment of Earth’s atmosphere.

Moreover, Orbitrap-iso boasts the capability to deliver simultaneous measurements of multiple isotopologue ratios from minuscule sample quantities, as low as nanomoles. This requirement represents a monumental reduction in sample size compared to IRMS, empowering the extraction of higher temporal resolution records from ice cores.

Despite these notable advantages of the Orbitrap-iso method, questions linger regarding its accuracy, reproducibility, and precision relative to the long-established industry standard, IRMS. In an effort to validate the quality of Orbitrap-iso isotopologue ratio measurements, our study rigorously compares the analysis of identical ice core nitrate samples using both systems, aiming to establish a ground truth for the Orbitrap-iso methodology.