Spaceflight Laser Desorption Orbitrap Mass Spectrometry

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Abstract

Laser Desorption Mass Spectrometry (LDMS) is an analytical technique commonly applied for measuring the chemical composition of solid materials. Advantages of LDMS include: spatially resolved measurements, enabling 2D chemical mapping; analysis of inorganic and organic compounds, providing context for detected biomarkers; and rapid experimental cadence, maximizing duty cycle. LDMS instrumentation has been developed for harsh environments, such as the surface of Mars (via the Mars Organic Molecule Analyzer – MOMA (*1*)), Titan (via the Dragonfly Mass Spectrometer – DraMS (*2*)), and the Moon (via the laser-based mass spectrometry – LIMS (*3*)). These systems, however, rely on linear ion traps or time-of-flight mass analyzers that can struggle to resolve spectral interferences. In comparison, next-generation LDMS instruments that leverage ultrahigh resolution analyzers, like the Orbitrap™, have the capacity to resolve spectral interferences (e.g. CO_2 and ^{44}Ca, or ^{54}Cr and ^{54}Fe) expanding access to a wider range of elemental, isotopic, and molecular measurements.

The Characterization of Ocean Residues and Life Signatures (CORALS) (*4*) and Characterizing Regolith And Trace Economic Resources (CRATER) (*5*) instruments are two LDMS instruments centered around an Orbitrap mass analyzer and designed for exploration of ocean worlds and the lunar surface respectively. Both investigations require approximately 10 kg of mass and less than 60 W of peak power facilitating accommodation on a wide range of spacecraft. Initial testing of these instruments (and earlier proof-of-concept prototypes) were focused on the detection of organic compounds at abundances higher than those expected in most planetary materials (e.g., wt.% levels of amino acids (*6*)) and measurements of trace element abundances in synthetic materials with unnatural major element compositions (e.g., rare earth elements in NIST SRM610 (*7*). More recently, performance testing of CORALS/CRATER has extended to isotopic ratios with permil level precision, quantification of elemental abundances in geologic materials to within 10% of true values, chemical mapping of meteorites, quantification of modal abundances of mineralogy via chemical mapping, training of machine learning models to classify mineralogy, and distinguishing biotic and abiotic sources. Here, I will review the most recent results collected from these protoflight and relevant commercial analog systems and discuss applications beyond planetary science.

References

1. F. Goesmann *et al.*, *Astrobiology*. **17**, 655–685 (2017).
2. A. Grubisic *et al.*, *Int. J. Mass Spectrom.* **470**, 116707 (2021).
3. P. Wurz *et al.*, *2023 IEEE Aerosp. Conf.*, 1–10 (2023).
4. L. Willhite *et al.*, *2021 IEEE Aerosp. Conf. 50100*, 1–13 (2021).
5. S. Ray *et al.*, *Rapid Commun. Mass Spectrom.* **38**, e9657 (2024).
6. R. Arevalo Jr *et al.*, *Rapid Commun. Mass Spectrom.* **32**, 1875–1886 (2018).
7. R. Arevalo *et al.*, *Nat. Astron.* **7**, 359–365 (2023).

Biography - Madeline Raith

I am a PhD candidate at the University of Maryland, College Park studying Geology. My primary research topics are developing spaceflight laser based mass spectrometry to conduct quantification of elemental abundances in geologic material, understanding why minerals affect organic detectability via laser desorption mass spectrometry (LDMS), and characterizing native organic distributions in Mars analog samples.

Keywords

Laser Desorption, Orbitrap, Geochemistry, Astrobiology