A gently ionizing electrospray ionization mass spectrometer for high mass organic and biomolecule detection.

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This project focuses on the development of a novel, gently-ionizing electrospray source for mass spectral analysis of biomolecules and other high-mass organics (100-1000+ AMU) in future spacecraft missions. By leveraging existing micro-thruster technology and adapting it for use as an electrospray mass spectrometry ionization source, intact organics may be studied by on-orbit or lander spacecraft with minimal fragmentation effects. Unlike current spacecraft mass spectrometers, this new, soft ionization technique would mimic the ideal, state-of-the-art laboratory methods used on Earth for detection of fragile biomolecules that have heretofore been impossible for spacecraft instrumentation. The source can be optimized for direct ionization of organics in solution or as a desorption secondary ion (DESI) source that ionizes surface material, either directly on the planetary object or from captured ejecta particles.

One of the key aspects of any mass spectrometer (MS) is the method of ionization. In laboratory settings, electrospray ionization (ESI) is a preferred method of ionization for high-mass, fragile biomolecules because it is comparatively gentle and thus minimizes molecular fragmentation relative to other techniques. However, ESI sources are optimized for terrestrial use and require atmospheric pressures and/or buffer gases to operate. While some attempts have been made to operate them at lower pressures [1], none have been able to operate in a space-like vacuum.

The search for biomolecules at icy ocean worlds and for prebiotic organics across the solar system is of high scientific priority, especially in light of the detection of as-of-yet unidentified high-mass organics in icy dust grains ejected from Enceladus's subsurface liquid water ocean [2]. The most recent NASA Planetary Science Decadal Survey names the Enceladus Orbilander concept as the second-highest priority new flagship mission for the upcoming decade, in part because previous studies of Enceladus by the Cassini spacecraft resulted in "fragmentation of large molecules, and ambiguity as to the precise identity of the parent organic molecules" [3]. Even in the absence of life, assessing the inventory and distribution of organic compounds is a critical step in habitability assessments and in studying the origin of terrestrial life [4], but fragmentation effects may complicate the detection and identification of such molecules. Thus, a spacecraft ESI-MS that mimics the terrestrial laboratory gold standard for gentle ionization of analytes may enable new biomolecular searches across the solar system.

By adapting ESI propulsion systems that are designed natively to work in space and have been flown on a number of cubesats [5], we have created a proof-of-concept vacuum-compatible ESI-MS system. These ionization sources use ionic liquids (liquids that do not evaporate or sublimate in vacuum pressures and that readily produce ions) that are brought to the tip of a needle at high potential relative to an extractor grid or plate. The high electric fields at the needle tip ionize the molecules and launch them at high velocity through the extractor grid. Importantly, ions produced from the ionic liquid may grab onto organic molecules that otherwise may not be readily ionized themselves, thus enabling their acceleration into a time-of-flight (TOF) MS system.

Fig. shows a preliminary comparison between mass spectra from EMI-BF_4, a common ionic liquid, and EMI-BF_4 with a suspension of cellulose. The spectra with suspended cellulose show an additional line corresponding to a glucose-EMI-BF_4 complex. These results, taken in direct ionization mode, show that the ionic liquid ESI source may be able to detect potential biomolecules. Ongoing work will confirm these initial results and study a large variety of other potential biomarker organics. Future work will convert the ESI-MS to operate in the DESI mode, wherein the source is fired at a solid to ionize surface material for TOF-MS.

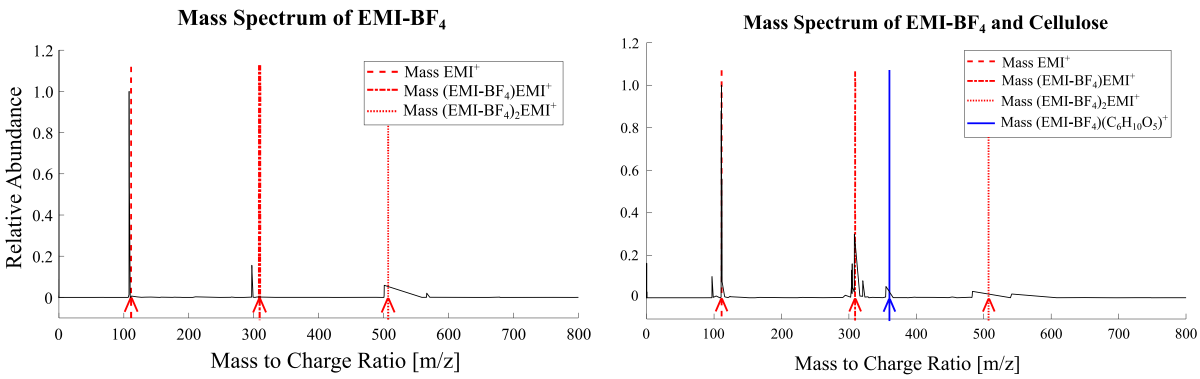

Figure 1: Left: Spectrum of EMI-BF_4. Right: Spectrum of EMI-BF_4 with a suspension of cellulose. The blue line shows a detection of a glucose-EMI-BF_4 complex. These initial results show the potential of the ESI-MS to detect possible biomolecules or other high-mass organics.

References

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