Optimization of the LAb-CosmOrbitrap experiment negative ion mode

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Abstract

Mass spectrometry is a reliable instrumentation for the characterization of atomic and molecular compounds in the planetary environments. The growing interest for astrobiological questions is driving us to develop instruments with better determination capabilities than those that previously flew.
A new generation of space mass analyzer based on OrbitrapTM technology (Makarov, 2000) with a high mass resolving power allowing to deeply constrain the composition of samples, is developed by a consortium of 6 laboratories and is called CosmOrbitrap. Previous studies performed with a Laser-CosmOrbitrap prototype have shown convincing performances in the positive ion mode (Selliez *et al.*, 2019, Arevalo *et al.*, 2018).

Detection of negative ion has relevant interest for small bodies and icy worlds exploration. Here we present first results of the laboratory prototype in this mode.

The laboratory prototype used for this work is composed of a commercial laser ablation/desorption system (pulsed Nd-YAG laser at 266 nm) coupled with the CosmOrbitrap, thereafter called LAb-CosmOrbitrap. A vacuum chamber maintained at 10-8 mbar was designed to host a sample holder and the Orbitrap cell is located in a second vacuum chamber maintained at 10-9 mbar. An ion optics composed of 6 lenses focuses the ion beam into the Orbitrap cell. Variable output energy of laser beam can be operated thanks to a polarizing prism. Under development CosmOrbitrap subsystems (currently at Technology Readiness Level between 4 and 5) have been set in the negative ion mode.

The first step of the study is the optimization of the voltage applied to the 6 electrodes composing the ion optics to enhance the transmission between the sample holder and the Orbitrap cell. The samples used are reference materials such as pure tin and pure gold, analyzed during distinct experiments. Metal samples are pressed onto an indium stub located at the surface of the sample holder. The LAb-CosmOrbitrap prototype enables detection of these inorganic compounds with a high mass resolution (m/m $>$ 100000, Full Width Half Maximum (FWHM)) and a low mass measurement error ($<$ 10 ppm) during a single laser shot experiment. A part of the work also aims to achieve accurate relative isotopic abundances.

Previous studies in positive ion mode have shown the capabilities of the LAb-CosmOrbitrap

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prototype to detect organic molecules such as pure adenine with ultra-high mass resolution. The second part of the study aims to prove similar capabilities in negative ion mode. We present here the results on organic molecules samples. Two preparation of pure adenine has been made: pressed onto an indium stub and dried on aluminum surface of the sample holder. The prototype allow us detection with a mass resolution and accuracy similar to the reference samples. Furthermore, the fragmentation pattern of adenine in negative ion mode shows similarities with the one obtained in positive ion mode.

These results are part of a study of the capabilities of the LAb-CosmOrbitrap prototype to detect and identify organics molecules with an astrobiological interest mixed in salts analog to Europa's surface.

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