Direct Measurement of Neutral Gas during Hypervelocity Planetary Flybys

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Abstract—**Planetary flybys at hypervelocity provide the opportunity for sensitive, in situ chemical composition analysis performed with mass spectrometers to identify both simple and complex species in search of the origin and evolution of life in the Solar System. Current mass spectrometric instrumentation handles the fast flow of neutral gas (and ions) streaming into the instrument with an open or closed ion source system. In an open source system, the particles enter the ion source directly without contact with any element, are ionized there, and then are deflected into the mass analyzer section by electrostatic means. The advantage of an open source is that there is no particle alteration by surface interactions, but the electrostatic deflection limits the upper velocity of incoming particles to about 5 km/s. In a closed source system, the particles enter an antechamber through a small hole first. Many collisions with the chamber wall thermalize them before they enter the actual ion source as thermalized gas. The advantages of a closed source system include the large velocity range and the increased sensitivity resulting from the ram pressure enhancement. Its disadvantage is that the particles may fragment, or chemically alter as they hit the wall leading to complicated fractionation patterns in the recorded mass spectrum. Thus, the larger the molecules are the more difficult, or even impossible, inferring the original molecule becomes. Here we present a novel ion optical system for a mass spectrometer that directly measures the atmospheric species at orbital velocities with an open source system, but without ion deflection into the mass analyzer section to overcome the disadvantages of both techniques and unite their advantages. Furthermore, the mass analyzer features a selectivity for the velocity of the analyzed gas allowing for the first time for sensitive mass spectrometric analysis of the atmospheric gas, while reliably knowing the influence of the background gas resulting from spacecraft outgassing. As a first realization, we built an ion optical system for 1U of a CubeSat (CubeSatTOF). Our results demonstrate that the sample acquisition system preserves the chemical nature of molecules even when relative encounter velocities of up to 20 km/s are required. Its mass range is about *m/z* 1 to 300, thanks to its mass resolution exceeding 300 (FWHM), designed for an application of analyzing Earth's exosphere. In addition, we designed a larger system (OpenTOF) with a mass range of about *m/z* 1 to 1,000 and a mass resolution of up to 1,000 (FWHM) for flybys of Enceladus, Io, Europa, Ganymede, Venus, and others, capable of analysis of complex (bio) molecules.**

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1. INTRODUCTION

The sensitive analysis of complex (bio) molecules in planetary atmospheres has challenged engineers and scientist over decades, but it is key to understand the origin and evolution of the Solar System. Upper atmospheres are the gateways to the chemical composition of celestial objects [1]. The present chemical composition is the result of the fractionation processes taking place over their evolution. The differentiation of an atmosphere during its evolution is a major reason why life exists on Earth. Mainly because of the limited sensitivity and mass range of the instruments performing the measurement in the early 1970s and 1980s ([2], [3] and references, [4]), molecules only up to argon (*m/z* 40) were detected. The ion neutral mass spectrometer (INMS) [5], [6] on board the Cassini Orbiter detected the presence of complex mixtures of species forming Enceladus' and Titan's organic atmosphere [7]–[12]. Heavier molecules were claimed to be identified in Titan's atmosphere, up to *m/z* 100 for neutral species, up to *m/z* 350 for positive ions, and up to *m/z* 10,000 for negative ions [10], [13]. Since then, (deep) space exploration with mass spectrometers has prospered as shown by the numerous proposed and selected concepts of both flyby and descent probes [1], [14]–[43].

Deep space exploration of upper atmospheres enables simple in situ analysis of celestial objects with broad chemical coverage and outstanding detail. Current major missions on the launch pad visiting the Jovian system are NASA's Europa Clipper and ESA's Jupiter icy moon explorer (JUICE) mission. Both spacecraft fly by the icy moons at hyperbolic velocities. For JUICE, relative encounter velocities are limited to about 4 – 5 km/s, which drives the design of both the mission and the mass spectrometer. Similarly, Europa Clipper flyby speeds are below 7 km/s. This velocity is mostly the result of the optimization of various parameters, especially including orbital parameters, observation conditions during flybys, the actual measurement time spent in the location of interest, and the capabilities of the mass spectrometer to manage the incoming gas stream at the given hypervelocity. As of yet, two current methods of the mass spectrometers' ion source exist to handle the fast flow of neutral gas (and ions) streaming into the instrument namely the closed and the open source system [44] (see also Figure 1B, which is adapted from [44]). In an open source system [4], [45], the particles enter the ion source directly without contact with any element, are ionized there, and then are deflected into the mass analyzer section by electrostatic means. The advantage of an open source is that there is no particle alteration by surface interactions, but the design has a limited upper velocity of about 4 – 5 km/s [6], [16], [46], which results from the electrostatic deflection. In a closed source system [45], the particles enter an antechamber through a small (pin-) hole first, where they are thermalized by many collisions with the chamber wall of the antechamber, before they proceed to the actual ion source as thermalized gas. The advantages of a closed source system are the large velocity range, the large field-of-view (almost 2π), and the good sensitivity resulting from the ram pressure enhancement. Its disadvantage is that the particles hit the wall several times where they may fragment, or chemically alter [47].

Recording meaningful data is key when exploring new worlds asking for measurements that ensure an unambiguous identification of the analyzed molecules. Recently, there has been an increasing interest to explore remote objects, where complex molecules are expected to be present [47]–[49]. For example, Europa is known to harbor complex species in its tenuous exosphere, as plumes likely transport ocean material into the exosphere [50]. Additionally, Io is thought to hold complex molecules in its upper atmosphere [49]. Its active volcanos eject complex compounds into the atmosphere providing a possible range for heavy molecules, for example, cyclic octaatomic sulfur (S_8) would be a possible heavy sulfur compound, and others. Current concepts for an in situ analysis of Io's exosphere during a flyby require a relative encounter velocity of about 15 km/s [51] implying closed ion source systems. Due to the fractionation occurring in the antechamber of presently available instrumentation, inferring the parent molecule in such a mass spectrum is already challenging for light species, but almost impossible for complex molecules in a total mass range of about *m/z* 1 to 1,000.

Furthermore, a spacecraft constantly outgases even after years in space [52], [53]. The species form a local exosphere around the spacecraft with mean velocities corresponding to thermal energies relative to the spacecraft. This local cloud interferes with the measurements of the object of interest as most of current instrumentation cannot distinguish between the origins of those molecules. Although complex requirements for both cleanliness campaigns and choice of materials during the development phases attempt to mitigate this issue to a certain extent, complex post-processing of the recorded spectra is required. The ambient gas is monitored over years in space, their time dependence, and species are identified and an adequate background subtraction of them is performed. Complications occur once the spacecraft interacts with the exosphere of the visiting object. It cannot be ruled out that the mass spectrometer measures species originating from the spacecraft itself due to: A) Sputtering or desorption of low-volatile species on spacecraft surfaces caused by the incoming gas stream hitting the surface of the spacecraft forming a local cloud of thermal gas (with respect to the spacecraft velocity). B) Classical outgassing because of an increased heat production due to modified illumination conditions, aerobraking, or consumers that are switched on for scientific measurements, or their preparation.

Our goal was to design an instrument that overcomes current velocity limitations of deflection systems used in current open source designs and the alteration of molecules in antechambers to allow for a reliable post analysis of its recorded data by design to enable the unambiguous analysis of complex species in tenuous upper atmospheres for relative encounter velocities of about 1 to 20 km/s. We analyzed available both missions and mission concepts [1], [14]–[43], adapted our ion optical system to fulfill the presented requirements, and tested the system in the laboratory to proof the concept of the instrument in an adequate environment.

2. THE ION OPTICAL DESIGN

Here we present a novel ion optical system that directly measures the atmospheric species at hypervelocity with an open source system, but without ion deflection into the mass analyzer section. Following the open and closed source terminology, we refer to this technique as direct open source. Direct Open Source Mass Spectrometry (DOeS-MS) builds

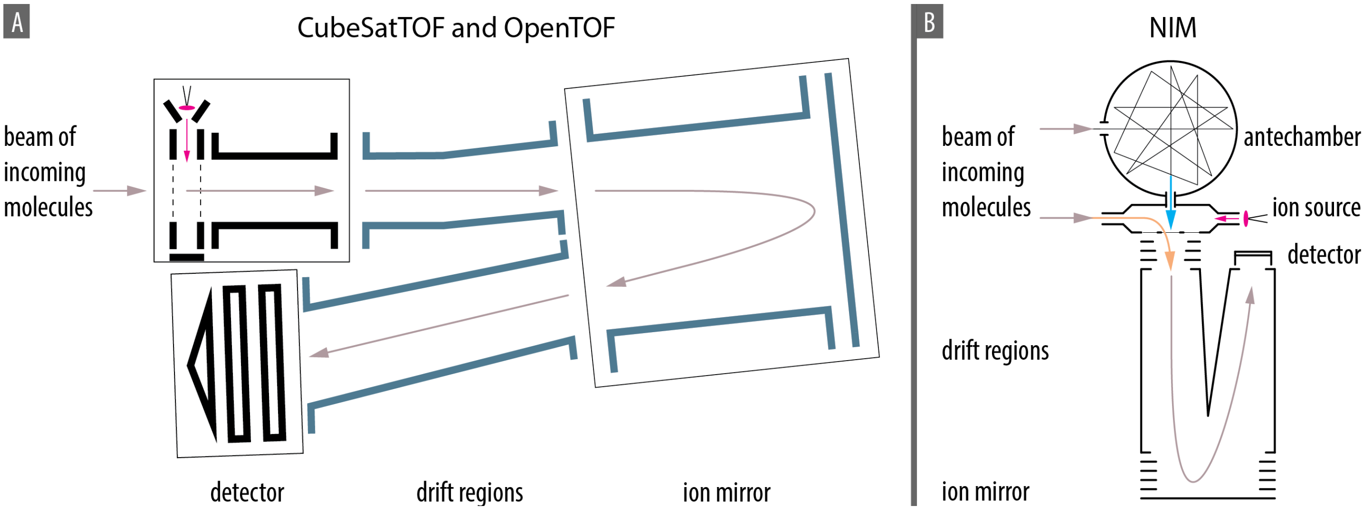

Figure 1. Schematics of the ion optical system (A). The total length of the instruments is about 100 mm or 300 mm to fit the CubeSat standards. The NIM instrument (B) either deflects the species (orange) or thermalizes them before insertion into the mass analyzer (blue). Electron ionization is indicated (magenta).

on conventional elements of a time-of-flight (TOF) mass spectrometry namely the ion source for ionization of the incoming species [16], [54]–[56], a gate for the common start signal, a field-free drift tube for separation of them, an ion mirror to compensate for variations in initial energies [57], another field-free tube, and a detector for registration [16], [58] that provides the stop signals of each species (Figure 1A). The incoming gas stream enters the ion source directly (contact-free), where the species are ionized with an orthogonal electron beam to form positive ions via electron ionization. Positive ions originating the exosphere can also be analyzed by switching the filament off. In principle, an analysis of negative ions is possible, but not pursued in the first version of it. At a cadence of 10 to about 40 kHz, the ion source is extracted by a high voltage pulser opening the gate. One of the main differences to instruments from which it draws heritage [16], [56] is the polarity of the gate. This high voltage pulser is considered as a push electrode rather than a pull electrode for the positively charged ions. The read-out electronics records a full mass spectrum simultaneously at one instance of a measurement and accumulates the data to save a full spectrum every 100 ms to about 10 s translating into < 1 km spatial resolution when in low earth orbit (LEO).

We designed the ion optical system to be tolerant towards an energy spectrum of the incoming species. The voltages applied to the electrostatic electrodes of the ion optical system are referred to as a voltage set, which can be commanded by the user. A careful selection of the voltages allows the user to analyze species from thermal energies, i.e., velocities < 1 km/s, to orbital encounter velocities of up to about 20 km/s. Thus, the system has several basic operation modes, also referred to as configurations, for example, the *thermal* mode, *orbital laboratory (1 to 4 km/s)* mode, *orbital 10 km/s* mode, *orbital 20 km/s* mode, and others [59].

The presented concepts allow for scaling of the ion optical system. Our detailed analysis of the indicated mission concepts led to the conclusion that there is a need for two versions of the DOeS-MS to reflect two trends namely I) as sensitive and reliable as possible chemical composition analysis of complex (bio) molecules and II) miniaturization of space instrumentation. Especially the first requirement asks to be prepared for unknown, heavier species that may become visible in mass spectra, thanks to the enhanced sensitivity of the instrument. Table 1 provides an overview of the instruments' current best estimates (CBE) specifications.

The 10 cm Instrument – CubeSatTOF

We designed, manufactured, and tested a version of a DOeS-MS that fits into 1 U (1 liter) of a CubeSat, the CubeSatTOF instrument, to proof both the concept of DOeS-MS and its scaling capabilities. This instrument is designed to analyze both known and unknown species in a moderate mass range of about *m/z* 1 to 200, with basically unit mass resolution (including considerable margin) of *m/Δm* of up to 400 full width at half maximum (FWHM). This approach allows for analysis of both simple and complex species including noble gases and complex organic compounds.

The ion optical system itself is directly mounted on top of a printed circuit board (PCB) for both better noise suppression and simplification of the harness. Another difference to its predecessors, the neutral gas mass spectrometer (NGMS) on board Luna-Resurs and neutral and ion mass spectrometer (NIM) as part of the particle environment package (PEP) on board JUICE [16], [56], is its increased active detector area. The NIM detector was demonstrated to provide a high sensitivity, i.e., 10^{-4} A/mbar, and short pulse widths (<500 ps) [16], [58]. Connecting it to according read-out electronics, a dynamic range of about 10^6 within 1 s is possible even for earlier systems [60], [61].

Application in LEO foresees the extensive use of commercial off-the-shelf (COTS) components. In some cases, military (MIL) grade components or even space grade components are considered, where their application considerably improves the overall probability of failure free operation and components are easily available. Shielding of the electronics is realized by enclosing the CubeSat with a shield of about 0.5 mm Ta, where necessary. An application in a harsh radiation environment can easily be adapted, as discussed for the OpenTOF instrument.

Table 1. Comparison of the designed instruments.

Feature	CubeSatTOF	OpenTOF
Characteristic size	10 cm	30 cm
Ion source type	DOeS-MS	DOeS-MS
Mass range *m/z*	1 – 200	1 – 1,000
Velocity range	thermal or 1 – 20 km/s	thermal or 1 – 20 km/s
Mass resolution *m/Δm*	up to 400	up to 1,000
Volume	1 U (< 1 l)	3 U (< 3 l)
Mass	<1 kg	3.5 kg
Extra mass for shielding	Mass includes shielding for LEO	3.8 kg for Europa flyby
Sensitivity	10^{-4} A/mbar	10^{-4} A/mbar
Dynamic range	~10^6 in 1 s	~10^6 in 1 s
Typical (extended) measurement cadence and integration time	40 kHz, 1 s (60 kHz, 0.1 s)	10 kHz, 1 s (20 kHz, 0.1 s)
Spatial resolution at: **7.8 km/s, 18 km/s**	780 m 1.8 km	780 m 1.8 km
Parts grade	mostly COTS	Hi-Rel
Typical application	LEO, descent probe for flybys (Venus)	On board instrument for deep space exploration

The 30 cm Instrument – OpenTOF

Whereas the CubeSatTOF instrument has a limited mass range, the 30 cm instrument, the OpenTOF instrument, has an extended mass range of about *m/z* 1 to 1,000. As a possible application, considering the search for bio-molecules in plumes of icy moons (e.g., Europa, Enceladus, Triton, and others), the masses of typically expected biomolecules necessitate a large mass range: amino acids of about mass 110, poly-peptides (small chains of amino acids), polycyclic aromatic hydrocarbons (PAHs) around mass 300, and lipids at mass 400, and more. OpenTOF allows for measurements of at least moderately long compounds, if present at reasonable abundance. In addition, sulfur compounds, like S_8 at mass 256, can easily be analyzed. To achieve the desired sensitivity, we aimed for a high ion-optical transmission close to 100 % in the ion optical system. The detector and read-out electronics will be comparable to current state-of-the-art instruments [16], [56]. These instruments used a 10-bit analogue to digital converter (ADC) with a single impedance-matched anode. Thanks to technological advancements, including recently updated high-reliability (Hi-Rel) components such as the high-speed ADC (12-bit, about 9.5 effective number of bits ENOB), an even better dynamic range can be expected.

Given its application beyond Earth, radiation is a design driver. In addition to a global shielding of the electronics as stated above, the detector requires considerable attention in such a case [62], [63]. For application near Europa, for example, the backplane of the ion mirror serves as shielding as implemented in the NIM instrument. The materials of the electrodes can be adapted to provide an according high atomic number (high-Z) material. Current best estimates foresee a shielding mass of about 3.8 kg for a Europa flyby and about 4.3 kg for visiting Io when assuming JUICE mission design parameters.

3. MATERIALS AND METHODS

This study reports on the tests of the CubeSatTOF instrument mainly in orbital velocity mode to proof the concept of DOeS-MS measurements and define the specifications of the OpenTOF instrument. The ion optical system is simulated with SIMON. This commercial software allows for both assessing a large parameter space and drawing seeds for laboratory-use voltage sets, which are then optimized once the instrument is operational [56].

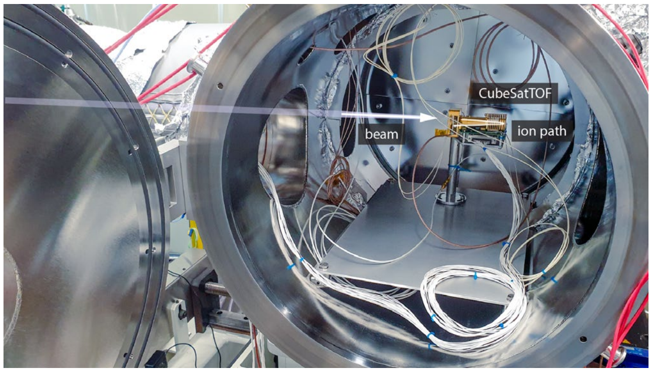

Figure 2. The CubeSatTOF instrument (10 cm) before exposure to a beam of neutral species in CASYMIR.

The CubeSatTOF instrument is exposed to a beam consisting of neutral gas. This beam simulates the encountering exosphere that the instrument experiences either during a flyby or when in orbit. The velocity (and pressure) parameter space covered by the instrument challenges the beam facilities. Fausch et al. [59] reported on measurements in thermal gas mode proofing the concept of residual gas analysis. Although test facilities providing gas velocities of > 4.5 km/s exists [64], this supersonic cation and anion source (SATANS) facilities was not available because of maintenance. Thus, the instrument was tested inside the calibration system for the mass spectrometer instrument

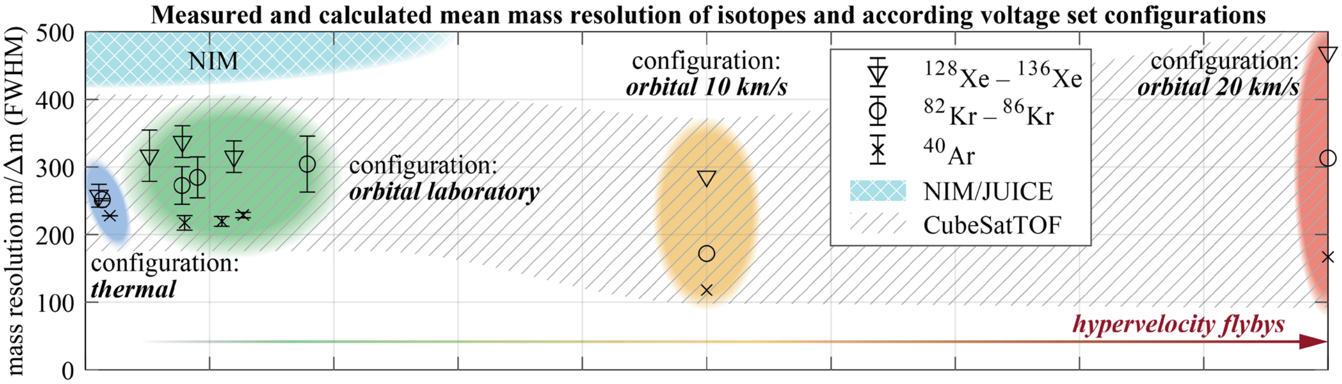

Figure 3. Demonstrated performance of the CubeSatTOF instrument. Error bars indicate the laboratory measurements. Whilst the sensitivity of NIM and CubeSatTOF are similar given the transmission of the ion optical systems, the CubeSatTOF instrument expands the design parameter space of future flyby missions.

ROSINA (CASYMIR) beam facilities [65]. The CASYMIR test facilities was developed along with the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) instrument suite flown on board ROSETTA. Its vacuum system provides vacuum at a few 10^{-10} mbar. Given the COTS components, we achieved an ambient gas pressure of about $1.2 \cdot 10^{-9}$ mbar. CASYMIR provides a supersonic molecular beam consisting of thermally distributed neutral gas, as a heated nozzle causes supersonic jet expansion of gas (mixtures) to reach maximum velocities of about 4.5 km/s for the lightest species, H_2. Although the gas can be almost arbitrarily mixed in the gas-mixing unit, the velocity of the beam considerably decreases when adding heavier compounds due to the increased mean molecular mass of the gas. The resulting beam has mean velocities of about 1 to 4 km/s depending on the gas mixture, i.e., [H_2]:[Ar], [H_2]:[Kr], and [H_2]:[Xe] in ratios of about 40:1 to 40:8 by volume. For most measurements, a pressure of about 5 to $6 \cdot 10^{-9}$ mbar was measured to be present in the chamber when the beam was applied. The voltage set of the ion optical system is adapted for these slow relative encounter velocities present in CASYMIR. We simulated the ion optical system covering available velocity range to derive a voltage set (configuration), referred to as *orbital laboratory*, which we then applied to the ion optical system in the vacuum chamber to validate our simulation. For a comparison, the results of the simulation are presented for the nominal 10 km/s use case and the 20 km/s use case until SATANS becomes available.

The beam is guided to the instrument chamber into the ion source so that the complete volume of the ion source is illuminated at 0° entry angle (Figure 2). Calculations showed that the acceptance half-angle of this type of ion source is well within 10° to 15° [66], but variations should be kept to a minimum, preferably within 5° to maximize its scientific performance.

Defining the final electronics of the CubeSatTOF is a goal of this test campaign. As a first step, we mounted a small NIM prototype detector to the ion optical system, until the larger detector is available. Because the form factor does not match well with the CubeSatTOF design, the active detection area of the microchannel plates is smaller than necessary. A reasonable signal was found, but the detector is prone to ringing given its prototype stage. It cannot be excluded that the ringing of this prototype corrupts the accuracy of the isotope ratios. Hence, sensitivity and isotope analysis would be affected. Thus, their assessment is performed in a qualitative manner as of yet until a flight-like detector is available, although the simulations promise no mass fractionation to be present at all (now and) once detector is available, thanks to the transmission of 1 of the ion optical system. Given this transmission, the sensitivity is determined by the detector and read-out electronics. As an almost similar technology that is realized for NIM will be used for the novel instruments, the sensitivity is considered to be very similar as well.

We designed a PCB with COTS components supporting the ion optical system and providing basic functions. This sensor board PCB was operated with laboratory electronics; power supplies for low voltages, high voltages, and the filament, a high voltage pulse generator (10 kHz cadence; Behlke Power Electronics LLC, USA), and a digitizer card (U1084A001, 4 GHz, 5 mV/div; Acqiris SA, Switzerland) with a 3 dB attenuator to acquire spectra. To compensate for the small active detector area, each spectrum consists of 300,000 waveforms, i.e., a histogram of 5 minutes, despite the nominal cadence shown in Table 1.

The present laboratory electronics allowed for a post analysis of the data with software [67]. The software calculates the mass resolution R to be $R = m / \Delta m$, where m is the mass of interest and Δm the full width at half maximum of its peak. The average of the isotopes' mass resolution of a given species for each velocity results in the mean mass resolutions per species, with errors resulting from both the standard deviation and from the software (integration errors). Also, the overall average and error per species is calculated. Those analyses asked for enhanced baseline corrections (wavelet thresholding) to remove the signals induced by the external high voltage pulser from the data. Despite the peak shape can be preserved with a careful selection of the de-noising process, a flatter baseline will be established once the high voltage pulser is integrated on the sensor board PCB allowing for better analog noise reduction [56]. In contrast, the mass spectra shown here are the result of a simple, linear background subtraction.

4. RESULTS

The tests demonstrate that the performance of the instrument in its target velocity range behaves as simulated and proofs the concept of the direct open source. The performance measurements of the ion optical system are summarized in Figure 3. It shows the applicable relative encounter velocity range of the CubeSatTOF instrument. An instrument not moving with respect to the gas defines the lower set of the velocity range, i.e., thermal velocities, when in *thermal* configuration (measurements of the same ion optical system from [59]), as experienced in a laboratory environment and in exospheres translating to temperatures of about 270 K – 1100 K for usage in LEO [68]. This configuration is useful either for testing in the laboratory without beam facilities during commissioning phase or for measuring the background of the spacecraft. The tests at velocities in the range of 1 to 4 km/s with the configuration *orbital laboratory* demonstrated its applicability for hypervelocity flybys. The good agreement of the simulation and measurement show that the predicted applicable velocity range is reliable. The measured mass resolution is even exceeding the basic requirement of achieving unitary mass resolution with margin. Thus, the isotopes of krypton and xenon are easily resolved and the isotope pattern matches the nominal terrestrial distributions (Figure 4).

Its high mass resolution has several benefits. It provides a margin during operation, for example, for inclined beams, and likely allows for an extension of the nominal mass range by about 10 to 50 % for slower relative encounter velocities. For higher velocities, despite adapting the voltage set for each relative encounter velocity, this margin shrinks until the mass range needs to be constrained as the transmission becomes smaller than 1. Our simulations show an upper limit of about 20 km/s for which a reasonable voltage set was found at a transmission of 1. Figure 5, left panel, shows the transmission of encountering species in the mass range between *m/z* 1 and 300 for the configuration (voltage set) that is optimized for a relative encounter velocity of 10 km/s. The region in which the species' transmission equals 1 defines the nominal case in terms of mass range of this set. Thus, the nominal mass range in this configuration is *m/z* 1 to 200. Extending the mass range would be possible while accepting either a decreased mass resolution, a lower transmission, or both. However, especially the high transmission is key as it guarantees that the CubeSatTOF and the OpenTOF instrument to be mass analyzers free of mass fractionation, translating to a high accuracy concerning isotope ratio, and ensuring a high sensitivity of the systems.

The energy tolerant ion optical system provides a selectivity between the thermal species and species encountering at higher velocities for higher masses by design (Figure 5, right panel). In orbital mode, the mass resolution increases with the mass per charge ratio *m/z*, which allows for resolving especially higher masses. Additionally, it is a function of the initial energy of the species, i.e., velocity, in the ion source. Whereas the mass resolution of species at thermal energies remains constant over the complete mass range, the mass resolution increases for higher velocity species, and at higher masses, they are better resolved the heavier they are. Although this effect starts at *m/z* 1, it becomes significant for higher masses. Thus, the mass spectra recorded in flight will consist of two superimposed mass spectra: One part containing information of the background of the spacecraft, at lower mass resolution, and another part containing information of species originating the exosphere, at higher mass resolution.

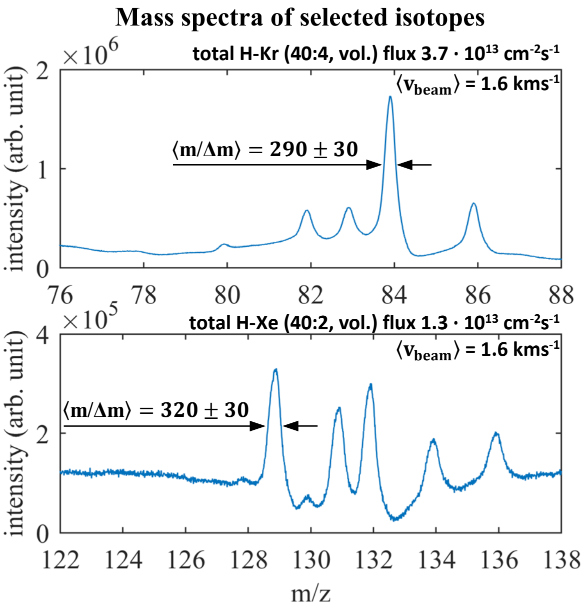

Figure 4. The CubeSatTOF instrument resolves isotopes of heavy species (Kr top panel, Xe bottom panel) when encountering at hypervelocity. For reference, the total flux at 550 km altitude, Earth, is about 2·10^{13} cm^{-2}s^{-1}.

5. DISCUSSION

Direct measurements of neutral (and ionized) gas provides the possibility to reliably detect, measure, and analyze complex (bio) molecules and biomarkers at hypervelocity, thanks to the direct open source providing versatile ion optical systems. The CubeSatTOF instrument has a much larger mass range compared to Atmosphere Explorer [4] and Dynamics Explorer [2]. Those instruments measured species to be present in Earth's exosphere in a mass range *m/z* of about 1 to 50. Heavier species might not have be observed given the sensitivity of the mass spectrometers designed in the 1980s. Recent instrumentation [19], [36] is designed to repeat those measurements within a similar mass range constrained by their limited mass resolution, which is

Simulated performance of the ion optical system optimized for a relative encounter velocity of 10 km/s

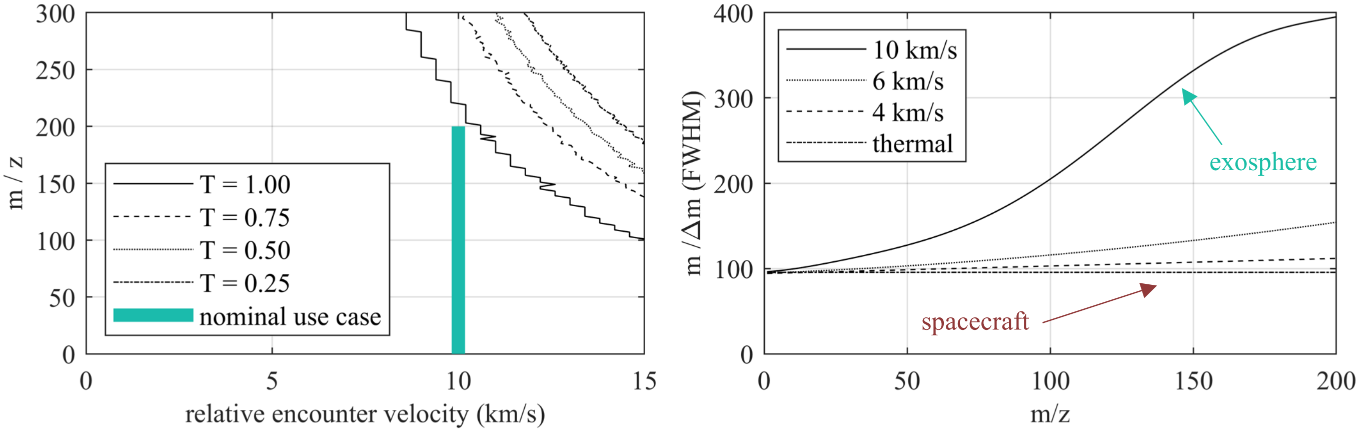

Figure 5. The transmission of 1 defines the nominal mass range of the CubeSatTOF instrument (left panel) for the 10 km/s configuration. Species in this mass range are clearly resolved including margin (right panel). The origin of species, i.e., exosphere (green) and spacecraft (red), can be determined thanks to a selectivity emanated from the velocity dependent mass resolution.

outperformed by the CubeSatTOF's mass resolution by at least a factor of 10 or even more (>30) for higher masses. The technological advancement that the CubeSatTOF provides together with its sensitivity enables the analysis of chemical species that remain undetected and a much higher cadence of recorded mass spectra.

Exploring exospheres leads to an understanding of both the formation and the transport mechanisms of heavier species. Earth serves as a baseline for habitable worlds. On Earth, atmospheric disturbances may transport those species into higher altitudes, for example, via atmospheric waves. In addition, the constant ultraviolet exposure causes constant chemical reactions forming countless new species, some of which are heavy. A prominent example is O_3. The fragile nature of this molecule requires the instrument to measure them directly as it is rapidly destroyed once it interacts with a chamber wall. Also, N_xO_y molecules are known to be present. Although it is well known that heavy species fall to lower latitudes, i.e., below the exobase where a mixing with other species occurs, some species must be present at higher altitudes. A static measurement of these species above the exobase already provides valuable data for comparative planetology. In addition, measuring the temporal and spatial behavior of those species over time will provide a better understanding of Earth's current atmosphere and its evolution [20]. Thanks to its suitable mass range, the presented instrumentation provides a baseline for such studies.

Beyond Earth, heavier species are expected to be present given either their atmospheric structure, i.e., Venus and Io, or thanks to plumes. For example, noble gases on Venus were shown to be assessable during a flyby [30]. CubeSatTOF could easily accomplish such tasks while measuring the bulk atmospheric composition simultaneously. Although it could be applied to ocean worlds as well, an application of OpenTOF with its even larger mass range is recommended. As plumes transport species from the ocean into the exosphere, the compounds expected to be present in the exosphere are even heavier than species in Venus' exosphere. Thanks to the direct open source measurement technique, both instruments can measure those heavier molecules.

Mission scenarios addressing the analysis of complex molecules have been limited by current instrumentation. Up to now, the maximal relative encounter velocity of current mass spectrometers have been a major constraint for design of their flight trajectories. Analysis of complex molecules is preferably done in open source mode. Due to the poorly understood chemical mechanisms, i.e., hypervelocity induced bond dissociation, ideal relative encounter velocities between 3 and 6 km/s were recommended for measuring bare amino and fatty acids to prevent from fractionation [47]. For higher velocities, the use of an antechamber leaves a room for interpretation of the results given the chemical alteration caused by the interaction with the walls. Both instruments presented in this study overcome this limitation and provide direct measurements at hypervelocity of up to about 20 km/s enabling mission concepts to analyze complex species during flybys reliably.

The ion optical system of the instrument has to point into ram-facing (flight) direction to measure, which may conflict pointing requirements of other scientific instruments. Cameras, for example, are often considered as a high priority payload of an orbiting mission given their possibility to identify possible landing sites for follow-up missions. Therefore, the spacecraft has to point into a nadir direction (center of the body of interest). Given the non-circular orbit during the flybys, the spacecraft actively slews to maintain the nadir pointing. Thus, the ion optical system requires a rotation mechanism to maintain the desired ram pointing of about ± 5° ram facing. Such mechanisms were successfully designed for other instruments, i.e., colour and stereo surface imaging system (CASSIS) on board ExoMars [69], and easily adaptable. Such a 1-axis rotation mechanism allows for a most independent mission design, especially for the OpenTOF instrument.

Mass spectrometers analyze the surrounding ambient gas. This gas may originate either from incoming species of the exosphere or from the actual outgassing of the spacecraft. Despite several attempts to account for the background of the outgassing spacecraft [52], [53], a systematic bias will always remain. As the DOeS technique provides an initial energy dependent mass resolution of especially for heavier species, scientists may infer the origin of species during post analysis by decomposing the superimposed mass spectra.

The shielding of the instruments' electronics protects them from fatal penetrating particle radiation. The NIM mass spectrometer on board JUICE was the first instrument to design a complete radiation shielding [16], [62], [63] and other instruments, such as the mass spectrometer for planetary exploration (MASPEX) on board Europa Clipper, followed this approach [17]. Shielding mainly concerns electronics, which is shielded against total dose. Typically, 2 mm aluminum is employed for modest radiation environments. In addition, spot shielding of sensitive electronics components is done with 0.5 mm thick tantalum sheets directly on the device. In contrast, the detector of the instrument will be shielded against instantaneous flux to minimize the background arising from penetrating radiation. High atomic number material encapsulates the NIM detector to maintain the sensitivity as it prevents from unwanted random background events occurring at the microchannel plates.

The designed ion optical system draws heritage from NIM. By now, the detector for the CubeSatTOF instrument will be designed for an application in LEO, which has a moderate radiation environment, but the current design already implements the possibility to severely increase the shielding of the components to allow for an application beyond LEO. For the main electronics, moving them to their consumer, i.e., mount the ion optical system directly on top of the PCB, has considerable advantages. Experience from the NIM instrument for JUICE showed that selecting appropriate high voltage connectors is challenging, especially due to the material constrains given the harsh radiation environment. Removing those connectors increases the reliability of the instrument while decreasing the footprint and therefore eases the mass budget in a first place, thanks to reduced mass for shielding. Shielding the larger volume, as the ion optical system is now part of the electronics, consumes the saved mass keeping the total system at the approximately same mass. However, the instrument benefits from a considerable simplification, thanks to the omitted connectors, thus, increasing the probability of failure free operation.

6. CONCLUSION

We designed two mass spectrometers, the CubeSatTOF and the OpenTOF instrument, for measurement of neutral gas during hypervelocity flybys. In this study, we demonstrated that our novel direct open source technique is capable of analyzing the fast flow of incoming molecules approaching at hypervelocity in a high mass range, thanks to an outstanding mass resolution. Mass spectrometers equipped with a direct open source represent the novel generation of instruments for analysis of complex (bio) molecules during hypervelocity flybys enabling the reliable detection of molecules in upper atmospheres while analyzing their bulk composition envisioning previously unrealistic mission scenarios.

LIST OF ABBREVIATIONS, ACRONYMS AND SYMBOLS

ADC	Analogue to Digital Converter
CaSSIS	Colour and Stereo Surface Imaging System
CASYMIR	Calibration System for the Mass Spectrometer Instrument Rosina
CBE	Current Best Estimate
COTS	Commercial Off-The-Shelf
CubeSatTOF	CubeSat Time-Of-Flight mass spectrometer
DOeS-MS	Direct Open Source Mass Spectrometry
ENOB	Effective Number Of Bits
ESA	European Space Agency
FWHM	Full Width at Half Maximum
high-Z	High atomic number (material)
Hi-Rel	High-Reliability (component)
INMS	Ion and Neutral Mass Spectrometer
JUICE	JUpiter ICy moon Explorer
LEO	Low Earth Orbit
m	Mass
m/z	Mass per charge ratio
m/Δm	Mass resolution
Δm	Peak width of the mass of interest, measured as FWHM
MASPEX	The MAss Spectrometer for Planetary EXploration
MIL	Military grade (component)
NASA	National Aeronautics and Space Administration
NGMS	Neutral Gas Mass Spectrometer
NIM	Neutral and Ion Mass spectrometer
OpenTOF	Open Time-Of-Flight Mass Spectrometer
PAH	Polycyclic Aromatic Hydrocarbons
PCB	Printed Circuit Board

PEP	Particle Environment Package
R	Mass resolution
ROSINA	Rosetta Orbiter Spectrometer for Ion and Neutral Analysis
SATANS	Supersonic cATion and ANion Source (calibration facilities)
SIMION	Commercial software for simulation of trajectories of charged particles
TOF	Time-Of-Flight
U	Unit (measure for the volume of a CubeSat)

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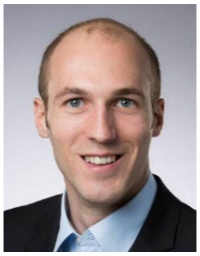
BIOGRAPHY



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