

CubeSatTOF: Planetary Atmospheres Analyzed with a 1U High-Performance Time-Of-Flight Mass Spectrometer

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ABSTRACT

This paper presents design and performance of a miniature time-of-flight mass spectrometer of 1U size for a CubeSat platform for quantitative chemical composition analysis of thin atmospheres. The atmospheres of solar system bodies harbor key information to answer questions about its origin and evolution, night-side transport, satellite drag including seasonal variation of it, chemical sputtering of satellites, and even the feasibility of earthquake forecast system has been suggested. Highly sensitive chemical analyses with our mass spectrometer will allow to obtain insight into atmospheric processes. We designed a compact multipurpose instrument. Its application is discussed for two mission concepts, namely orbiting Earth in a terrestrial swarm configuration or descending through the atmosphere of a planetary object during a flyby. Our measurements demonstrate that the instrument has mass range of about m/z 1 – 300 and a mass resolution so that the heavy noble gases such as krypton and xenon can be quantified in situ. Thanks to its ion optical performance, the CubeSatTOF instrument serves as a baseline technology for future analysis of both the terrestrial and extraterrestrial exospheres.

INTRODUCTION

Knowledge of the chemical composition of solar system objects allows better understanding of the origin and evolution of planetary objects. Chemical composition measurements on space missions have been repeatedly performed with various instrumentation. However, mass spectrometers provide a high dynamic range of 10^{10} , a sensitivity in measurements of atomic abundances to the ppm level and below, and an identification of many molecular species. In addition, the analyses of atmosphere composition (elemental, isotopic, and molecular) improve our understanding of the atmosphere formation and evolution processes, atmospheric escape flux, and provide insight into planetary surface composition as well as habitability¹.

Mass spectrometers have been used on several planetary missions so far and visited several planets to perform in situ chemical composition of planetary atmospheres^{2,3}. The GPMS / Galileo Probe⁴ analyzing Jupiter as well as the INMS / Cassini⁵ and the GCMS / Cassini-Huygens⁶ analyzing Saturn are perhaps the best examples of earlier used mass spectrometers designed to investigate tenuous atmospheres. Present technology provides possibilities to considerably improve performance of mass spectrometers especially regarding mass, power consumption, sensitivity, and mass resolution within a small volume. The system presented here is an example of an improved instrument. There are also smaller instruments available, though they have either limited mass resolution so that an analysis of heavier species is not possible or they need to scan the

mass range resulting in a lower sensitivity due to the duty cycle of the scan⁷⁻⁹.

The instruments designed for application on space missions are typically optimized for their weight, size, and power consumption. The development time of such instruments include time for the design, the construction of prototype and flight models as well as test phases. These lead typically to high costs. For example, typical durations for the development of mass spectrometers on-board major missions have been in the order of 5 (NIM / PEP / JUICE)¹⁰ to more than 13 years (MASPEX / Europa Clipper)¹¹, not counting development phases before. In the time frame between the start of the development and the finalization of the instrument, the underlying technology, of which electronic parts are a considerable fraction, has advanced its performance considerably. Therefore, these long development times of space instrumentation in general lead to both the need of launching outdated technology to space and mass spectrometers that are costly.

To date, planetary mass spectrometers performing in situ measurements are either designed to measure at a low ambient pressure ($p \lesssim 10^{-4}$ mbar) or at a higher ambient pressure ($p \gtrsim 0.5$ bar), which can be roughly translated into altitude considering the density of the expected planetary atmosphere. For low pressure-type mass spectrometers, the mass spectrometers analyze the ambient gas directly without a dedicated or only a simple sample inlet. Thus, such instruments operate either like a residual gas analyzer if the species have

thermal velocities, i.e. in a vacuum chamber, or as a neutral and/or ion mass spectrometer with a given field-of-view to analyze species at orbital velocities (~ 8 km/s). To perform high pressure measurements, a mass spectrometer needs to be integrated into a vacuum system and the sample needs to be transferred via a sophisticated sample inlet subsystem from the surrounding atmosphere into the ion source of the mass spectrometer¹². Also, the ion optical requirements differ when analyzing thermal species or species with orbital velocities as the initial starting energies in the ion source differ by orders of magnitude. The ion optics need to project the ion source to the detector by focusing the ion beam from the ion source with several ion optical lenses. This focusing is improved by a larger system and by limiting the ions to a narrow distribution of initial starting energies. Consequently, the mass spectrometers differ considerably for both cases. This approach has led to the development of customized mass spectrometers which were applicable to mostly one specific type of missions.

In current contribution, we describe a time-of-flight mass spectrometer designed for an operation on a CubeSat platform, the CubeSatTOF. This mass spectrometer has high-performance, low cost, and a modular structure so that it can be easily applied for investigation on various solar system objects. The instrument can be used to analyze ambient gas in a potentially mobile vacuum chamber and as a neutral and ion mass spectrometer to analyze species with orbital velocities. Therefore, we designed and developed the next generation of time-of-flight mass spectrometer to fit into one standardized unit (1U) of a CubeSat platform by optimizing the ion optical system of its predecessors (NGMS / Luna-Resurs, NIM / PEP / JUICE, and RTOF / ROSINA / Rosetta).

SCIENCE CASE

The scientific rationale defining the requirements of this instrument is threefold. In the first use case, the instrument will analyze the terrestrial upper atmosphere in situ as an orbiter, whereas the other use cases consider an application in extraterrestrial atmospheres or vacuum chambers.

Earth's Upper Atmosphere

Although the Earth's upper atmosphere is key for understanding the evolution of planetary objects, not all details are understood, and sensitive composition analysis are still required. The upper atmosphere is a complex region which is poorly constrained in terms of chemical composition, drivers, their exact contribution, and their localization. The thermosphere remarks the region of the atmosphere that is above ~ 90 km. In this

region, among others, both photo-chemical reactions and subsequent ion-neutral and neutral-neutral reactions convert the irradiation energy provided by the solar EUV flux into kinetic energy of the species heating the thermosphere. In this region, the gas density is still high enough so that collisions between species dominate their trajectories. Once the number density of the species becomes low enough with increasing altitude, the mean free path of the species becomes high enough so that the species follow ballistic trajectories upon reactions or collisions. This region in the atmosphere is defined as the exosphere, and the region where the transition occurs is referred to as the exobase.

Starting from the exobase, species are modeled to follow an exponentially decreasing number density profile with increasing altitude (see also Figure 1C). The negative inverse of this exponent of this function represents the atmospheric scale height of the species, which are not well constrained given the lack of accurate in situ measurements. These scale heights depend on both the species present and the planet itself and can be derived from the total number density if the chemical composition at the according altitude, i.e. exobase, is accurately known. For the Earth, the atmosphere is assumed to be in hydrostatic equilibrium and thus the species-specific scale heights can be converted into exospheric temperatures as a first order approximation. More dedicated models exist¹³, but they lack accurate data.

Knowledge of current exospheric temperatures constrains the atmospheric escape rates and the evolution of it. Jeans escape is one of the dominant atmospheric escape mechanisms, which occurs if the kinetic energy and the direction of the species allow for an escape of the gravity field of the host planet. In this case, the current atmospheric loss rates of species depend on the scale heights. This allows for modeling of the actual terrestrial chemical composition and the atmospheric loss rates in the past¹⁴. This evolution of Earth's atmosphere serves as a baseline for comparative planetology to answer questions about the difference between Earth's, Mars', and Venus' atmosphere although, for example, Füri and Marty¹⁵ indicated the similarities of these planets at its early stage. However, the scale heights only represent an exponential approximation of the real time-dependent density profile of species, but not even these scale heights are accurately known. In fact, neither the altitude of the exobase nor the chemical composition of it is well constrained.

The altitude of the exobase (and thus the scale heights) may adapt in response to exogenous and endogenous drivers in several timescales. On Earth, potential drivers

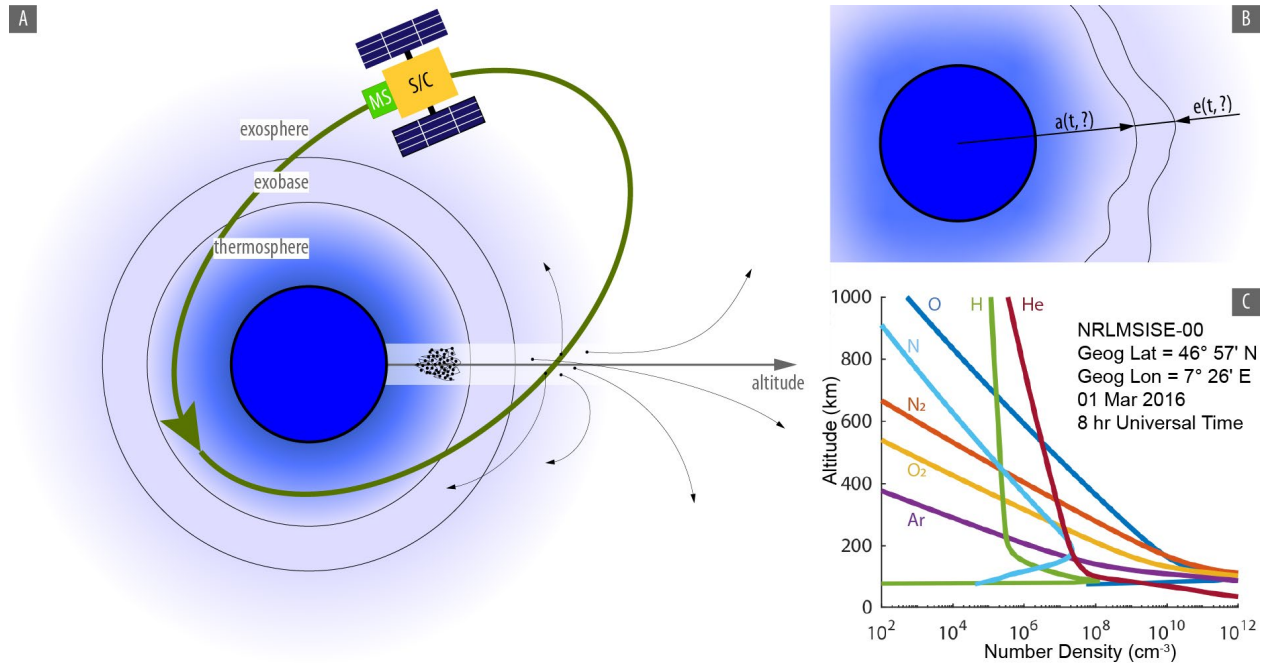


Figure 1A: Measurement situation of the CubeSatTOF instrument in an idealized atmosphere. B: The instrument will identify the actual altitude (a) of the exobase, its thickness (e), its composition, and corresponding drivers (?) over time (t). C: The exponential fit of the number densities of species represent the current knowledge, which corresponds to the idealized model illustrated in panel A.

are discussed in the literature^{16,17} and could include drivers such as the rotation of the Earth, solar wind, solar activity in general, emanation of material of the Earth¹⁸, and anthropologic drivers¹⁹. Besides a variation of the chemical composition, such drivers cause a variation of the number densities at fixed altitudes so that the range of the number densities easily exceeds one order of magnitude¹⁷. Other exemplary effects caused by these drivers are the night-side transport of the species. This diurnal variation of the exosphere has already been extensively studied on extraterrestrial planets such as, for example, Venus and Mars^{20–22}. For Earth, however, the scientific community still lacks detailed in situ measurements of such phenomena.

Table 1: Required species to be measured.

	Major species	Minor species	Traces of elements
Neutrals	H, N, O, N ₂ , CO, NO, O ₂	D, ¹⁵ N, ¹⁷ O, ¹⁸ O	Noble gases, ...
Ions	H ⁺ , He ⁺ , N ⁺ , O ⁺ , N ₂ ⁺	D ⁺ , ¹⁵ N ⁺ , ¹⁷ O ⁺ , ¹⁸ O ⁺	NO ⁺ , OH ⁺ , ...

Table 1 shows an overview of species that are likely present near the exobase. The table refers to altitudes around 1,000 and 200 km, which approximately corresponds to a total number density of 10⁶ and

10¹⁰ cm⁻³, respectively. It remains unclear, which species are present and in which concentration they can be found.

Extraterrestrial Upper Atmosphere

The satellite embarking the CubeSatTOF instrument can be deployed as a descent probe from a primary payload either during a gravity assist maneuver at Venus²³ or a dedicated flyby of a planetary object. Descent probes have been discussed for flybys of Europa²⁴ or deep space missions to, for example, Uranus and Neptune²⁵. Those two planets remain widely unexplored, which is why even the basic measurement of H₂, HD, and He are still to be done¹² in addition to the ones presented in Table 1. Note that these measurements require a different target mass resolution of about $m/\Delta m = 1000$ (FWHM, including margin) to resolve these species when compared to the others, for which a mass resolution of about $m/\Delta m = 200$ (FWHM) is sufficient. All of these planets require measurements of especially the heavier noble gases such as krypton and xenon to improve our understanding of their evolution. Noble gases are chemically inert and thus mostly not involved in planetary processes serving as a fingerprint of the evolution of the object. However, these data are not available with the desired accuracy. Especially, an isotope ratio with an accuracy of about 1 – 10 %²⁶ is desired.

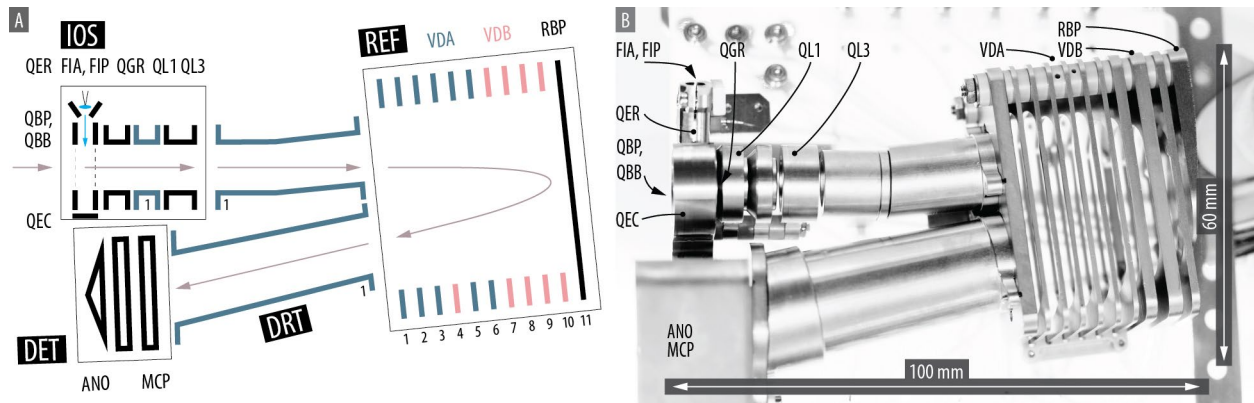


Figure 2: Layout of the ion optical system (A) and its mechanical realization (B). The color coding in REF represent the configuration in the Orbit Modes (upper electrodes) and in Thermal Gas Mode (lower electrodes). See text for the labels.

Analysis of Dense Atmospheres or Vacuum Chambers

This instrument can be used in various scientific and industrial applications. There is an increasing interest in analyzing the deep atmospheric composition of planets and moons²⁷. When comparing to measurements of the upper atmosphere, analyzing the lower part of a dense atmosphere requires to reach a certain depth as most of the heavier species (except e.g. noble gases) are condensed in clouds at certain altitudes. Such measurements provide a more surface-like atmospheric composition than exospheric measurements do. Given the entry speeds for such missions, a deceleration of the probe is required to establish a depth profile of the atmosphere. Thus, a probe could benefit from a low mass consumption of this instrument as both the mass of the instrument itself and the mass of the instrument's vacuum chamber can be reduced. The vacuum system will especially include a dedicated sample inlet to regulate the pressure inside both the ion source and the mass analyzer. In this case, the instrument analyses ambient gas with thermal velocities. As such, it can also be used in other scientific applications to monitor processes in the vacuum chamber by live measurements of the chemical composition as it has been done by others^{28,29}, but with the advantage of measuring the whole mass range at once and only consuming little space in the vacuum chamber.

INSTRUMENT

The CubeSat-type Time-Of-Flight mass spectrometer (CubeSatTOF) is a modular compact mass spectrometer designed for high-performance measurements. The time-of-flight technique has the advantage that it allows for recording of the complete mass range at once without the necessity of scanning over the masses of interest as it is the case for quadrupole mass analysers³⁰. This approach results in superior efficiency over quadrupole mass analyzers, which is beneficial for the

scientific measurements, but it becomes a necessity when orbiting a planet, where the time needed for recording a spectrum directly translates into spatial resolution. When orbiting Earth and measuring constantly, the minimum time to record one mass spectrum is designed to 100 ms, which roughly translates into 700 – 800 m spatial resolution on the ground track depending on the chosen orbit.

Concept of Operation in Low Earth Orbit

Although the application of this instrument is versatile, we focus on an application in Low Earth Orbit (LEO) in this section for exemplary reasons. Figure 1A shows the idealized spherical model of Earth (blue circle in the center), the thermosphere, the exobase, and the exosphere. An elliptical orbit of the satellite, i.e. apogee 1'000 km – perigee 200 km, implies that the mass spectrometer crosses the regions of interest at different heights so that the number density profiles as shown in Figure 1C (data from NRLMSISE-00 model¹³) can be derived from these measurements. Additionally, not shown in Figure 1, a second mass spectrometer on-board a second satellite should be placed in a sun-synchronous orbit (SSO), i.e. at 600 km altitude, to allow for measurements at constant local times. This assistive though necessary satellite allows to constrain the diurnal variation, which has a major impact on the chemical composition, with a high precision.

Table 2: Operation modes of the instrument.

	Neutral species	Ions
Thermal velocities	Thermal Gas Mode	–
Orbital velocities	Orbit Mode Neutrals	Orbit Mode Ions

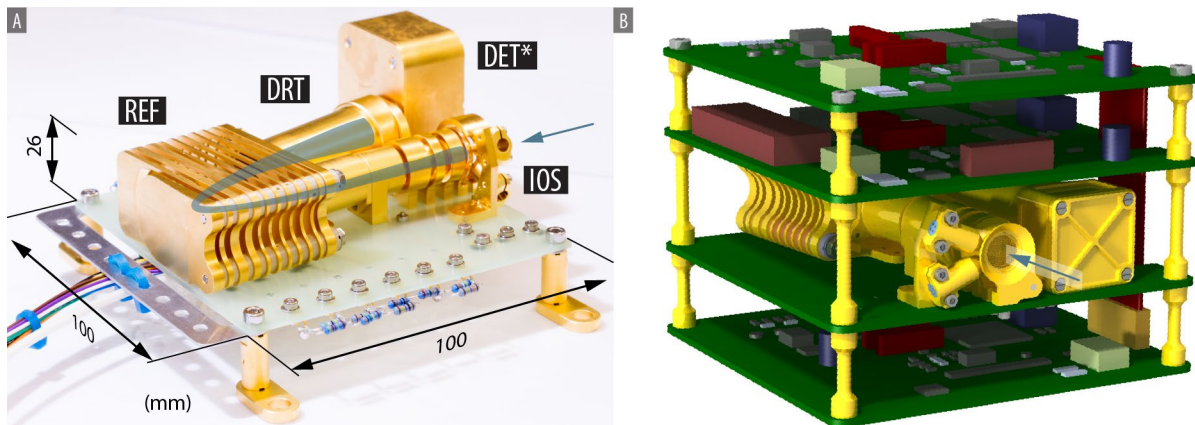


Figure 3A: Flight-like ion optical system mounted on a mockup PCB with a prototype (*) detector. See text for explanations of the labels B: Computer model of the CubeSatTOF instrument with the flight-like detector.

The instrument has three main operation modes (Table 2). It analyzes neutral species at thermal velocities (Thermal Gas Mode), neutral species with orbital velocities (Orbit Mode Neutrals), and ions with orbital velocities (Orbit Mode Ions). Ions at low energies could be analyzed but this use case is considered as unlikely because the pericenter of the orbit is well above the bulk ionosphere.

The main difference between the modes is the necessity of an active electron source for electron ionization of the incoming species in Orbit Mode Neutrals and in Thermal Gas Mode when compared to the Orbit Mode Ions. Also, the actual voltages which are applied to the sensor (voltage sets) differ slightly. This change of configuration of the voltages can easily be varied without any change on the instrument as it is implemented in the electronics. Thus, the instrument itself remains the same for different types of application as the design driving factor was the same namely to design an initial energy spread tolerant ion mirror. In fact, the ion source can accept even higher energies (velocities) to be compatible with potentially upcoming mission scenarios of flybys.

Ion Optical System

Figure 2 shows the layout of the ion optical system. In Orbit Mode Neutrals, neutral species enter the ion source (IOS), where they are ionized, from the dedicated opening (QBB) which points into flight direction (arrow). Once the gate (high voltage pulser, QBP) is active, the ions fly through an acceleration region consisting of lenses into the field-free drift tube (DRT), where the species separate along their flight trajectory. Afterwards, they enter the grid-less ion mirror³¹ so that the species reach the detector (DET) after passing another drift tube. The time difference

between triggering the gate and the signal registered at the detector results in the time spectrum, which can easily be converted into a mass spectrum during post processing as the time-of-flight of a species is proportional to the square root of the mass-per-charge ratio.

Simulations of the instrument showed that it is reasonable to constrain the field-of-view (FOV) to nominal value of $\pm 5^\circ$. This is mainly limited by the mass resolution for higher masses and can thus be extended to $\pm 20^\circ$ in a limited mass range.

Figure 3A shows the flight-like mechanical design of the ion optical system on a mockup PCB. Thanks to its direct mount on the electronic boards, which are part of the structure, both the ion optical system and the structural design in general are robust, simple, and easily manufactured leading to relatively cheap subsystems. This reduction in complexity has a particular impact in the simplification of the electronics, as most of the harness becomes obsolete (Figure 3B). Thus, the signal-to-noise ratio can be increased as the burden of electromagnetic interference is reduced thanks to the lack of cables, which otherwise serve as antennas. Also, the mass is reduced as only little shielding for electromagnetic compatibility is needed.

Modularity

The system is designed so that the ion optics is the same for various missions with similar requirements, but the operating electronics is selectable. The main electronical subunits of typical space-borne mass spectrometers are roughly the same for every instrument namely read-out electronics, a data processing unit, power supplies, and a high voltage pulser³². The design of this instrument allows replacement of various modules depending on the

requirements of the particular mission. For example, an exospheric entry probe on Jupiter's moon Ganymede has different requirements concerning a radiation tolerant design when comparing to an application in LEO with a carefully selected orbit. Although a radiation tolerant design of the electronics³² and the ion detector^{33,34} is possible, this limits the number of available parts for engineering in case of exploring the Jupiter system. However, on Ganymede, an increased power consumption might be acceptable as the mission duration is shorter. Thus, an even more sensitive read-out electronics can be implemented. The modularity of this system provides the possibility to exchange the nominally foreseen commercial off-the-shelf (COTS) parts with hi-reliability (Hi-Rel) parts if and where desired.

The design of our system allows easy exchange of subcomponents or individual components. Also overlaying subsystems can be tailored to the mission requirements. For most of the hardware components, no change in software is needed when demanding for Hi-Rel parts. Otherwise, some adaptations on the software has to be made to account for both a change of the hardware and likely to the interfaces to the spacecraft, but the vast majority of the software code remains the same and can be imported from modules using preexisting libraries. This approach paves the way for reuse of the software in a modular way, which is a considerable budgetary item.

Ion Optical Performance

The results of tests with the hardware shown in Figure 3A demonstrate the ion optical capabilities in Thermal Gas Mode. The ion detector used in the mass spectrometer represents a state-of-the-art detector, which was developed for the NIM / PEP / JUICE instrument¹⁰. The measuring currents are approximately 10^{-4} A/mbar resulting in a dynamic range of $\sim 10^6$ within 1 s. The active area of this detector is smaller than the flight detector, which results in a reduced sensitivity but not affecting the mass resolution. For the tests, we used a calibration gas mixture consisting of 99.7 % He, 0.1 % Ne, Kr, and Xe each and added it to an ambient gas pressure of $6.0 \cdot 10^{-7}$ mbar to reach a final pressure of $6.0 \cdot 10^{-6}$ mbar. Laboratory power supplies replaced the ones of the instrument, the high voltage pulser is a custom-made prototype with a rise time of 1.2 ns (20 % – 80 %, 10 kHz repetition frequency) and an Acquiris digitizer card U1084A001, 4 GHz, 20 mV/div, with a 3 dB attenuator acquired the spectrum consisting of 10,000 waveforms. The spectra were background corrected for illustration purposes³⁵, but the analysis was performed on raw data.

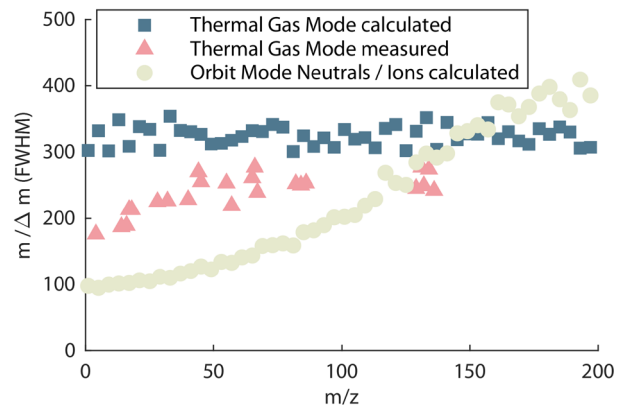


Figure 4: Calculated (blue, green) and measured (red) mass resolution of the ion optical system (FWHM).

Figure 4 shows the performance of the ion optical system. The measured mass resolution $m/\Delta m$ (FWHM) was 176 for m/z 4 and > 240 for the isotope mass peaks of xenon at masses around m/z 136 in Thermal Gas Mode. This mass resolution demonstrates the analyzer's capability to resolve the krypton and xenon isotopes sufficiently for calculation of the isotope abundances (see also Figure 5). Accounting for the laboratory setup, this is well within the expectations.

For comparison, the calculated mass resolution of the ion optical system is indicated for the Thermal Gas Mode, the Orbit Mode Neutrals, and the Orbit Mode Ions. A similar mass resolution in both orbital modes (ion, neutrals) can be achieved. In these modes, the mass resolution is observed to increase for higher masses. Also, the ion optical transmission increases when compared to the Thermal Gas Mode. The measurements presented above demonstrate that the instrument is capable of resolving masses in a range of about m/z 1 – 300 in Thermal Gas Mode. Consequently, isotope ratios of species such as xenon can be quantified.

Figure 5 shows the background corrected mass spectrum with an integration time of 1 s. The isotopes of the noble gases present in the calibration gas mixture can easily be analyzed in addition to the ambient gas in the vacuum chamber. The insert shows the pattern of the isotope ratio of xenon, demonstrating the resolving power of the instrument. The dynamic range is mainly dependent on the mission-specific read-out electronics. The ion optical performance, however, does not limit the dynamic range given the high transmission of the ion optical system.

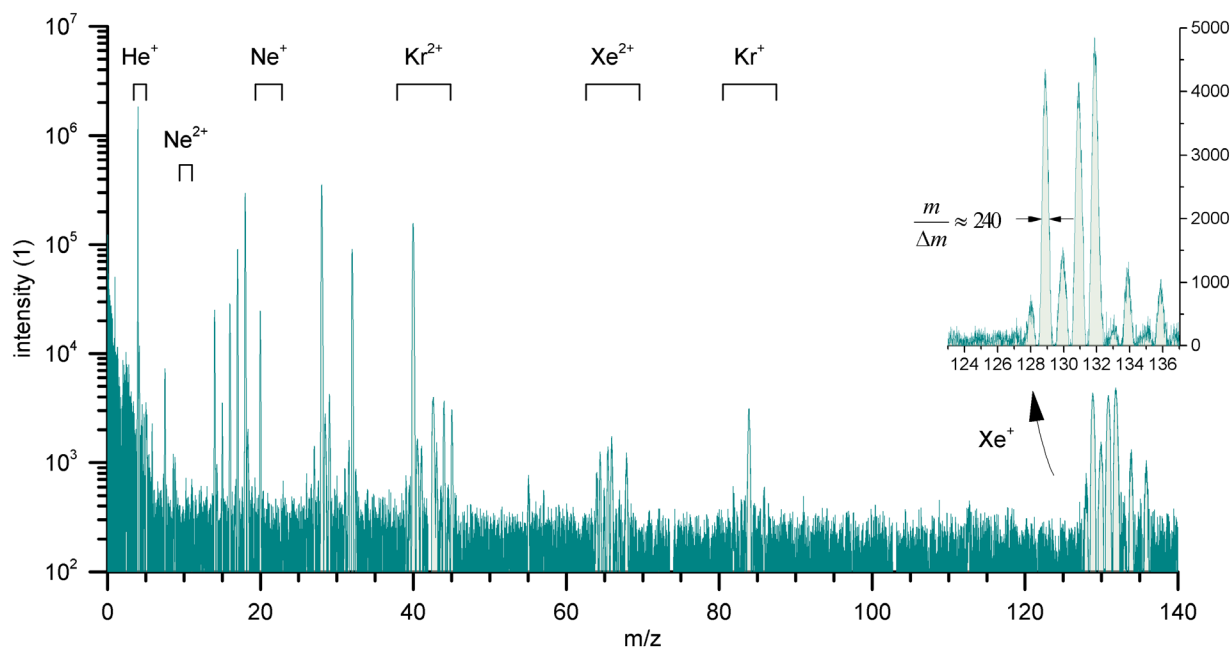


Figure 5: Mass spectrum of the CubeSatTOF ion optics in Thermal Gas Mode. The mass resolution of this instrument is enough to separate noble gases with margin.

DISCUSSION

The CubeSatTOF instrument anticipates the upcoming wave of space exploration by responding to it with the next generation of low resource consumptive though high-performance mass spectrometer. We broke down the mission requirements of likely upcoming missions that we consider as the next logic steps in planetary exploration, unified them where possible, and created a modular design of a mass spectrometer that is tailored to those missions. The design contains a mass analyzer that is tolerant to extended ranges of initial starting energies of the analytes so that multiple operation modes can be selected with the same instrument without losing relevant performance. The initial energy spread can be compensated by a simple reconfiguration of the electrodes in the software if the ion optical system is designed accordingly. Thus, this instrument provides the possibility to be considered for analysis of the exospheres of Earth, Venus, Mars, and other objects as a primary or a secondary scientific goal of a mission.

Given the possibility to deploy this instrument from a primary payload as a descent probe, the mission designers of future major space missions need to reconsider their mission designs. A satellite consisting of a service module, the CubeSatTOF instrument, and an additional payload has weight of no more than 3 kg. This satellite, which communicates with the primary spacecraft, and the corresponding communication module on the primary spacecraft add only little mass and complexity to an overall mission (e.g. Dragonfly³⁶).

Thus, such decent probes should preferably be included in all future space missions. If not considered in the main mission scenario, then the designers should at least foresee the possibility to consider such a probe for a ride sharing in case of not fully exhausting the allocated mass margin of the primary spacecraft. A major ESA mission is designed with 5 – 20 % margin concerning the mass budget³⁷ depending on the technical readiness level of the subsystems, which is comparable to NASA missions³⁸. For example, assuming that a total mass of 420 kg for a rotorcraft of the upcoming Dragonfly mission to Titan³⁶, the conservative 5 % margin equals 21 kg, which fits well within a mass requirement for such a descent probe system. As mass budgets are mostly not fully exhausted, this suggests that a selection for ridesharing is likely. The return on science of the whole mission can considerably be increased by the implementation of such an option.

With a mass range of about m/z 1 – 300 and a comparable mass resolution, the instrument has the capability to resolve the heavy noble gases such as xenon and krypton with good margin as demonstrated, which is unique for CubeSat-type instruments. Its performance is about an order of magnitude higher (about factor 6 in Thermal Gas Mode; about factor 25 in both orbital modes) than instruments with a comparable form factor^{7,9}. Thus, the instrument fulfills the requirements of likely upcoming descent probes. For example, it is likely that such a descent probe can

analyze those noble gases on Venus²³ directly without the uncertainty of modeling the results due to on-board concentrators, which have species-dependent characteristics⁸. Also, it can analyze species on-board a descent probe as a residual gas analyzer to probe the deep atmosphere of Uranus or Neptune¹² if the instrument is coupled to the according chemical pre-separators.

This instrument is ideal to analyze the chemical composition of terrestrial upper atmosphere as well. Thanks to both the high transmission of the ion optical system and the modularity of the instrument, the system can be configured with the according electronics to meet the requirements of the dynamic range, which depends on the orbit selected. Thanks to this modularity and the accelerated engineering process, latest technology can be directly implemented where desired. Such a system will allow to collect a chemical inventory of the species present in the upper atmosphere. This allows for modeling of the evolution of the atmosphere by knowing the atmospheric escape rates of the species¹⁴.

CONCLUSION

We developed a compact time-of-flight mass spectrometer that fits into 1U of a CubeSat platform, has high-performance, and allows for highly dynamic measurements of the mass range of about m/z 1 – 300 in Thermal Gas Mode and of about m/z 1 – 1000 in Orbit Mode Neutrals and in Orbit Mode Ions. Thanks to this unique mass range for this class of instruments empowered by its mass resolution, the CubeSatTOF instrument serves as a baseline technology for future analysis of exospheres as it is designed to improve our understanding of the origin and evolution of celestial objects.

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