

The Peregrine Ion Trap Mass Spectrometer (PITMS) Investigation Development and Pre-Flight Planning

Corresponding Author: Barbara A. Cohen, NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA

Barbara Cohen¹, Simeon Barber², Phillip A. Driggers¹, David Heather⁴, Chris Howe³, Pete Landsberg², Tom Morse³, Roland Trautner⁴, Feargus Abernethy², Emma-May Butroid³, Natalie M. Curran¹, Christophe Delepaut⁴, Ellis Elliott³, Javier Fernandez Salgado⁴, Joseph A. Generie¹, Philipp Hager⁴, Sophie Hall³, Fiona Hillier³, Max Hodgkins³, Sara Iacobellis⁴, Alicja Kasjanowicz³, Ewout Koekkoek⁴, Mark Leese², Karin Lundmark⁴, Jeremy Mayers³, Andrew Morse², James Mortimer², Hume L. Peabody¹, Patrick Reast³, Simon Sheridan², Richard Stamper³, Peter J. Steigner¹, Harald Stier⁴, Lauren Summers³, Orenthal J. Tucker¹, Martin Whalley³, Simon Woodward³

¹NASA Goddard Space Flight Center, 8800 Greenbelt Rd., Greenbelt, MD, 20771 USA

²School of Physical Sciences, The Open University, Walton Hall, Milton Keynes, Buckinghamshire, MK7 6AA, UK

³STFC RAL Space, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX, UK

⁴European Space Agency, P.O. Box 299, Noordwijk, South Holland, 2200AG, The Netherlands

ABSTRACT

The Peregrine Ion Trap Mass Spectrometer (PITMS) is a mass spectrometer instrument that operated during the Astrobotic Peregrine Mission-1 as part of the NASA Commercial Lunar Payload Services (CLPS) initiative. This paper describes the instrument and investigation design, development, and planning conducted by the PITMS team consisting of a successful partnership between NASA Goddard Space Flight Center (GSFC), The Open University (OU), NASA, and ESA. PITMS was designed to measure the abundance and temporal variability of volatile species in the near-surface lunar exosphere from a landed platform on the lunar surface. The PITMS instrument consisted of an ESA-provided Exospheric Mass Spectrometer (EMS; including sensor, electronics, controller, power supply boards) and a GSFC wrapper that provided structural elements, thermal control, and a deployable dust cover. PITMS was designed to operate as a passive sampler, where ambient gases would enter PITMS through an aperture, diffuse around the mass analyzer cavity, become ionized by electron impact and trapped in a radiofrequency field, then sequentially released to a detector to build a mass spectrum. PITMS was capable of measuring species with a mass-to-charge ratio (m/z) from 10 to 150 Da, with a mass resolution of approximately 0.5 amu. The PITMS science investigation was planned to be operated by GSFC with an international team of scientists. Though the mission did not achieve its lunar landing, information about the PITMS instrument and planning is provided to be able to understand and effectively use data that will be forthcoming from the investigation.

1. INTRODUCTION

The Peregrine Ion Trap Mass Spectrometer (PITMS) (formerly named PROSPECT Ion Trap Mass Spectrometer) was designed to investigate the lunar exosphere from a landed mission using a compact mass spectrometer. PITMS was intended to characterize the lunar exosphere at the lunar surface throughout the lunar day

to understand the release and movement of volatile species of interest to both science and human exploration. PITMS would have been the first landed mass spectrometer on the lunar surface since the LACE experiment, an ALSEP investigation in 1972.

The PITMS project is a partnership between NASA Goddard Space Flight Center and The Open University (OU), NASA, and the European Space Agency (ESA). The PITMS instrument consisted of an ion-trap mass spectrometer coupled to a wrapper that provides structural, thermal, and mechanical support. The mass spectrometer and electronics make up the Exospheric Mass Spectrometer (EMS), built by OU in collaboration with RAL Space under contract from ESA. The wrapper, built by NASA GSFC, provided structural elements to mate the EMS to the lander, thermal control via a baseplate and radiator, and a deployable aperture cover. The PITMS investigation was conducted by a science team consisting of members from all partner institutions.

The PITMS instrument was proposed by NASA GSFC (Principal Investigator: Barbara Cohen) and selected for development by NASA under the NASA Provided Lunar Payloads (NPLP) solicitation. PITMS was selected for flight with the Commercial Lunar Payload Services (CLPS) initiative in 2019 and manifested for flight on Astrobotic's Peregrine lunar lander mission for launch, which occurred in January 2024. The measurement results of the flight phase of the instrument will be reported elsewhere (Cohen, Barber, Gawronska, et al., 2024); this paper focuses on the design of the PITMS science investigation and operations, with details of the PITMS instrument and its pre-flight characterization provided as needed to understand its operation. A more detailed description of the design, build, test, and calibration of the EMS for PITMS will be provided in a companion paper.

PITMS, as other NPLP projects, was a very small, risk-forward instrument developed on a short timeline (<2 years) and on a small budget (\$1M US and €1.25M Euro). The EMS and wrapper hardware were designed, built, integrated, tested, and delivered in ~18 months during the COVID-19 pandemic. PITMS was designed for a very short mission duration (8 terrestrial days) and was not designed to survive lunar night.

Peregrine flew as a co-manifested payload aboard the first flight of the United Launch Alliance Vulcan Centaur vehicle. The lander targeted the Sinus Viscositatis basaltic lava plain in the north-western part of the lunar nearside (landing ellipse ~2km near 35.07° N, 41.76° W; Fig. 1). This location was chosen by NASA to help optimize NASA's CLPS deliveries, as the Lunar Vulkan Imaging and Spectroscopy Explorer (Lunar-VISE) mission will be visiting the nearby Gruithuisen Domes (Donaldson Hanna, Benavente, Bennett, et al., 2023). PITMS was mounted on Deck D of the Peregrine lander, which was expected to face west in a nominal landing orientation. PITMS operations were planned to commence soon after touchdown with the release of the dust cover and continue through the duration of the lunar day. However, the Peregrine Mission-1 did not achieve its lunar landing due to a propulsion system anomaly in the spacecraft (<https://www.astrobotic.com/final-update-for-peregrine-mission-one/>). The details of the as-flown mission and PITMS investigation will appear in a companion paper (Cohen, Barber, Gawronska, et al., 2024).

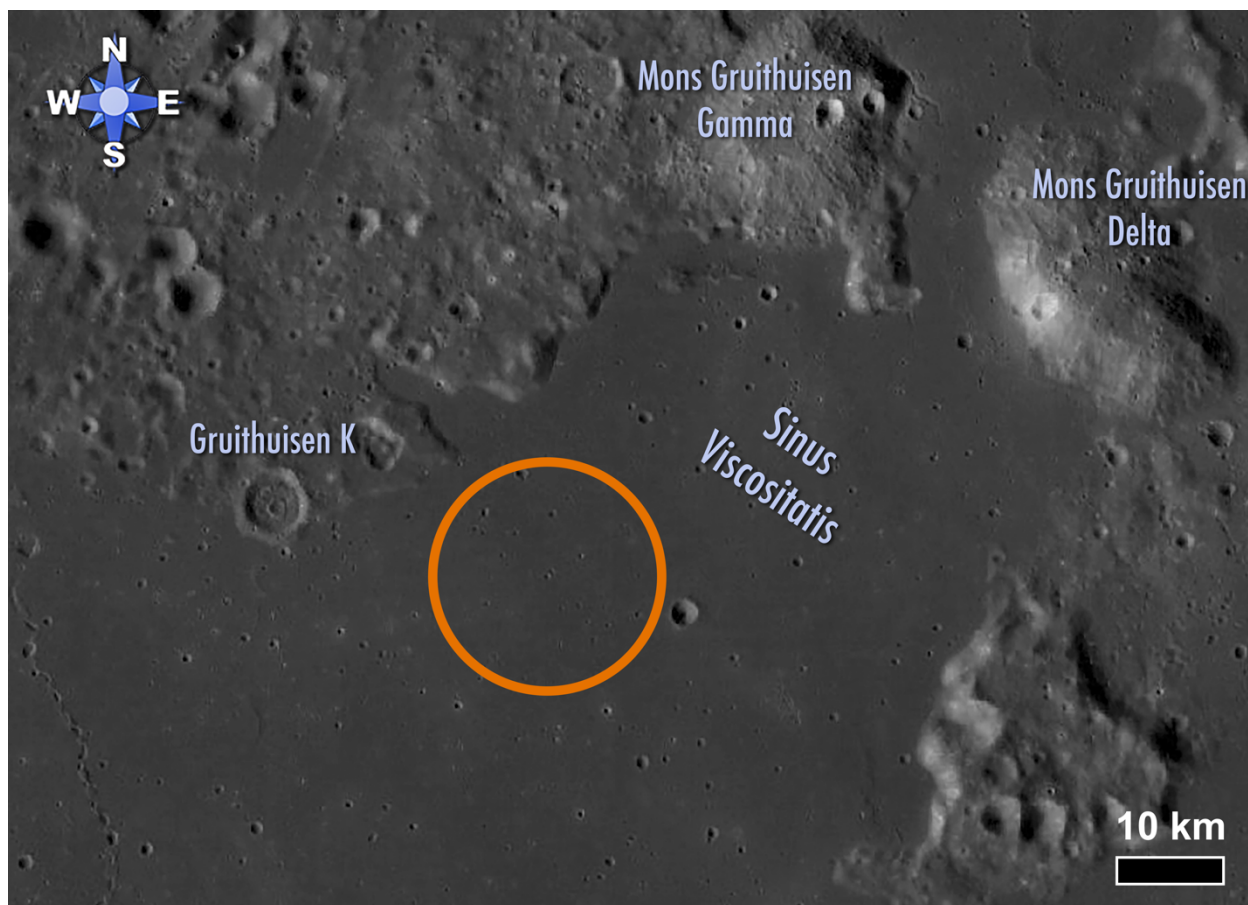


Figure 1. The Gruithuisen domes and Sinus Viscositatis as identified in the IAU Nomenclature Gazetteer (<https://planetarynames.wr.usgs.gov/Feature/16118>). The planned Peregrine Mission-1 landing region is shown in orange (centered at 35.07° N, 41.76° W); the actual landing site within this region would have been chosen during the mission.

2. PITMS SCIENCE INVESTIGATION

The science goal of PITMS was to monitor the tenuous near-surface lunar exosphere in response to natural (*e.g.*, diurnal temperature cycle) and artificial (*e.g.*, landing event, lander activities) stimuli. The PITMS investigation would characterize the lunar exosphere after descent and landing, and throughout the lunar day to understand the release and movement of volatile species. The science results would provide measurements of the exosphere to significantly improve our knowledge of the abundance and behavior of volatiles on the Moon and contribute to understanding the spatial and temporal nature of the lunar exosphere and how it responds to perturbations such as lander or thruster exhaust.

Landed mass spectrometers such as PITMS are uniquely positioned to assess the volatile components of the lunar regolith and exosphere and observe their behavior from dawn to dusk, addressing NASA science and exploration goals. The Moon has a tenuous atmosphere (exosphere) primarily made of hydrogen, helium, neon, and argon (Killen, & Ip, 1999; Stern, 1999; Benna, Mahaffy, Halekas, et al., 2015; Hurley, Cook, Retherford, et al., 2017), with smaller abundances of methane, sodium, and potassium (Colaprete, Sarantos, Wooden, et al., 2016; Hodges Jr., 2016). Because of the rate at which atoms escape from the lunar atmosphere, there must be a continuous

source of particles to maintain even a tenuous atmosphere (Stern, 1999; Benna, Hurley, Stubbs, et al., 2019). Characterizing lunar volatile reservoirs and evaluating their interrelations is a high priority for both lunar science and for exploration purposes, as water could represent a key resource for in situ resource utilization.

Multiple spacecraft have remotely observed water and hydroxyl in lunar regolith at non-polar latitudes as detected in the 2.8-micron absorption feature in the IR reflectance spectrum (Clark, 2009; Pieters, Goswami, Clark, et al., 2009; Sunshine, Farnham, Feaga, et al., 2009; Li, Lucey, Milliken, et al., 2018; Hendrix, Hurley, Farrell, et al., 2019). This surface reflectance feature may exhibit seasonal and possibly even diurnal variability. The Lunar Atmosphere and Dust Environment Explorer (LADEE) Neutral Mass Spectrometer (NMS) and Ultra-violet Spectrometer (UVS) identified the primary atmospheric constituents at the LADEE orbit (50 km), their density, and variability (Benna, Mahaffy, Halekas, et al., 2015; Colaprete, Sarantos, Wooden, et al., 2016). To date, water and OH have been reported in the exosphere only during meteor stream events by the LADEE NMS and UVS (Benna, Hurley, Stubbs, et al., 2019). A definitive observation of exospheric water and OH released from the surface during nominal times remains elusive.

The only corresponding surface measurement was made by the Lunar Atmospheric Composition Experiment (LACE) on Apollo 17. LACE was a miniature magnetic deflection mass spectrometer deployed on the surface and oriented to intercept and measure the downward flux of gases. This instrument had a mass range of 1-110 amu and an instrument sensitivity to N_2 of $5.0E-5$ amp/torr, which was sufficient to measure the concentration of gas species in the mPa range (Hoffman, 1975). Over its nine months of operation, LACE was swamped by artifacts emanating from the nearby lunar module descent stage and other abandoned equipment during the lunar daytime, but obtained firm detections of two species, argon and helium. Possible pre-sunrise detections of other species were obtained (see review in Stern, 1999), but only upper limits were determined for most of the volatile species of interest, including N_2 , CO, CO_2 , and CH_4 ; OH/ H_2O was not determined due to the high backgrounds both inside and outside the instrument (Schläppi, Altwegg, Balsiger, et al., 2010).

The science objectives of PITMS therefore included monitoring the lunar exospheric background and comparing data with other mass spectrometers and LADEE; measuring lunar regolith degassing from thermal cycling and artificial disturbances; and characterizing the dynamics of volatile evolution after their release. While the PITMS instrument was designed to have better sensitivity than LACE, the ability for any mass spectrometer to meet detailed science objectives, such as measuring the isotope signatures of water and other volatiles to infer their origin and determining the composition of trace compounds as potential contaminants for future water ice extraction, will depend on characterizing and minimizing the contribution of spacecraft outgassing by placement on the spacecraft, cleanliness of the spacecraft and the instrument, and bakeout procedures before the measurements .

Each lunar landing represents a unique active experiment, providing the opportunity for sensors to monitor evolution of the exosphere after perturbation by a relatively well-characterized source (Prem, Hurley, Goldstein, & Varghese, 2020). Small to mid-sized landers release volatiles in the form of exhaust gases after landing and blow away the upper several centimeters of dust to sand-sized grains from the lunar surface exposing the

underlying lunar soil (Metzger, Li, Immer, & Lane, 2009). The few top centimeters of the lunar surface are thought to be a highly insulating (thermally) dry regolith layer, overlying a more conductive hydrated layer (Vasavada, Paige, & Wood, 1999; Benna, Hurley, Stubbs, et al., 2019). If the dry regolith layer were thin, it is likely to be blown away, exposing the hydrated subsurface layer that will contribute to the water release. The lander exhaust gases and any released lunar water will mix in the lunar exosphere. Part of this volatile mixture would have greater velocity than the lunar escape velocity and will be lost to space. The remaining volatiles, whose origin will be a mixture between lunar water and lander exhaust, could persist in the lunar environment for 2 or more lunar days (Prem, Hurley, Goldstein, & Varghese, 2020), adsorbing and diffusing into the lunar regolith and/or migrating towards the lunar poles. PITMS will observe these phenomena to provide further constraints on modeling capabilities linking measurements to fundamental physical interactions.

Exposed lunar regolith is constantly being activated through bombardment by the solar wind and impactors, creating sites that can bind water from anthropogenic or natural sources. Laboratory observations of water bound to lunar regolith show a distribution of activation energies peaking near 0.7 eV, but with a high energy tail beyond 1 eV (Hibbitts, Grieves, Poston, et al., 2011; Farrell, Hurley, & Zimmerman, 2015; Poston, Grieves, Aleksandrov, et al., 2015). If *in situ* lunar regolith has the same properties, the water molecules would outgas from the surface over time as the surface is progressively warmed. If PITMS sensed considerable water surface outgassing near local noon (~400K), it would imply that the surfaces contain sites with very high activation energy for water trapping, with values above 1.0 eV, as one might expect for mature highland samples. In this case, the surface is a potent sorption substrate. If, however, the local regolith has little outgassing at local noon, then this may imply that *in situ* exposed surfaces have outgassed at lower temperatures, implying lower activation energy. In this case, the surface may be a far less potent sorption substrate than environmentally dormant samples used in the laboratory, affecting our models of plume-originating water retention in the actual space environment (Farrell, Prem, Tucker, et al., 2022; Lucey, Petro, Hurley, et al., 2022).

Though the other instruments aboard Peregrine did not constitute a traditional, highly-synergistic "mission," they had the potential to contribute to the PITMS investigation by providing additional context. For example, the composition of the surface is key for knowing how water is bonded (*e.g.*, loose water ice, physisorbed water ice, or water molecules formed from hydroxyls linked to MgO and TiO₂). Surface mineralogy inferred from water ice release temperatures could have been compared to data from the Near-Infrared Volatile Spectrometer System (NIRVSS) (Roush, Colaprete, Cook, et al., 2020). Neutron Spectrometer Subsystem (NSS) observations of subsurface water and its depth structure (via thermal/epithermal ratios) would have been useful in constraining the depth at which thermal penetration will be likely to release subsurface volatiles (Peplowski, Elphic, Fritzler, & Wilson, 2023). Radiation monitoring instruments M42 and LETS would have provided the solar flux throughout the mission, which could be used to understand whether the sputter rate may change throughout the mission (Stoffle, Pinsky, Kroupa, et al., 2015; Berger, Marsalek, Aeckerlein, et al., 2019; Wurz, Fatemi, Galli, et al., 2022). The Iris Rover and COLMENA micro-rovers would have disturbed the regolith at known times and locations, which may release loosely-bound molecules that could have been observed with the high time resolution afforded by PITMS.

Coordinated planning among NASA-provided, international, and commercial instruments and payloads was extremely valuable during mission planning to maximize scientific return.

3. PITMS INSTRUMENT DEVELOPMENT

3.1 Exospheric Mass Spectrometer (EMS)

ESA contracted with Open University (OU), Milton Keynes, UK to build the Exospheric Mass Spectrometer (EMS), which is the ion-trap mass spectrometer and its associated electronics. The EMS had direct heritage from the Ptolemy mass spectrometer that made the first *in situ* measurements of volatiles and organics on comet 67P Churyumov-Gerasimenko with the Rosetta lander, Philae (Wright, Barber, Morgan, et al., 2006; Andrews, Morse, Barber, et al., 2012; Morse, Mousis, Sheridan, et al., 2015). The PITMS EMS also provided an early flight pathfinder for the ongoing development of a similar instrument for the PROSPECT mission (Heather, Sefton-Nash, Trautner, et al., 2023).

The EMS (Fig. 2) consisted of an ion trap mass analyzer mounted above a set of printed circuit boards (PCBs). Gases would enter the EMS via the zenith-looking aperture and diffuse around the mass analyzer cavity. A heated tungsten wire filament emits electrons to ionize the admitted gases inside the ion trap, and the resulting positively charged ions are trapped in a radiofrequency field formed by application of suitable potentials to a set of three hyperbolic electrodes. Appropriate manipulation of the field facilitates the ejection of the ions into the electron multiplier detector in order of increasing mass-to-charge ratio (m/z). The detector output constitutes a mass spectrum with the ion species m/z as a function of the time of detection and the amplitude of the output representing the ion abundance. The PITMS EMS had a mass resolution (FWHM) of approximately 0.5 amu and could measure species to an upper limit of $m/z \approx 150$.

The EMS was developed rapidly over a period of ~16 months. Because there was no qualification or engineering unit developed, the development resulted in a single instrument known as a Proto-Flight Model, or PFM. A Ground Reference Model (GRM) replicates EMS to calibrate and optimize its performance; the GRM also served as an operations planning testbed and supported validation of command sequences.

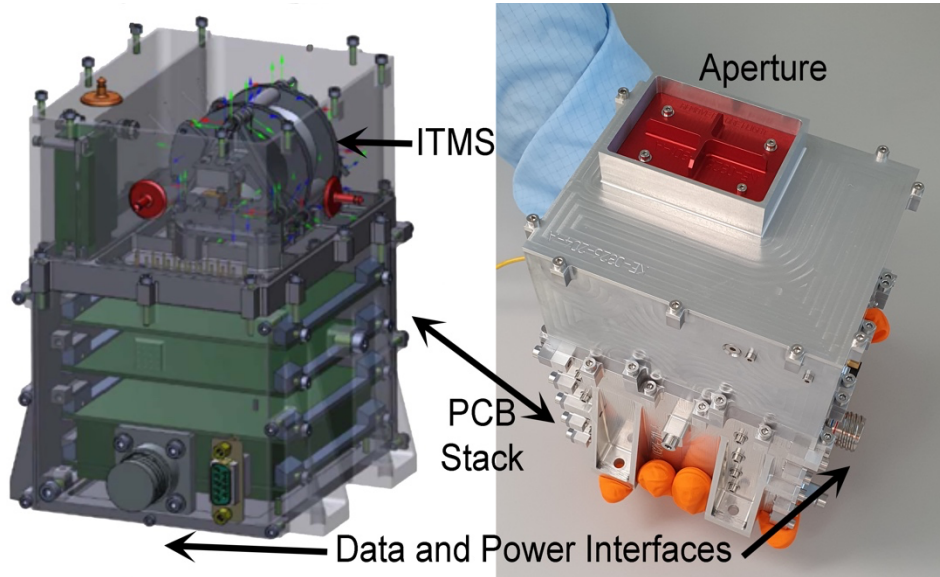


Figure 2. (left) A solid model of the EMS proto-flight model and (right) the as-built EMS proto-flight model. The ITMS is in a clean cavity that is isolated from the printed circuit boards (PCBs) stacked below it, with separate outgassing paths.

3.2 Wrapper

A GSFC-built wrapper mounted the EMS to the Peregrine lander (Fig. 3). The wrapper was made from aluminum 6061T6. Because PITMS was required to be thermally isolated from the lander deck, the wrapper also provided thermal control for PITMS via a space-facing radiator and two survival heaters with passive thermal actuation (-45 to -36.67 C). Surfaces that had an external view were painted with white Z93C55 paint; other surfaces were covered in irridite. Titanium isolators were installed at our mounting points to the lander deck. The radiator was curved outward to increase surface area and canted at an angle optimized for the original Lacus Mortis landing site, but providing adequate thermal control for the slightly warmer latitudes of Sinus Viscositatis. The wrapper also provided a deployable cover using an EBAD P-10 pin puller actuator to protect the EMS from dust and debris entering the zenith-looking aperture during spacecraft integration and testing, launch, cruise, and landing.

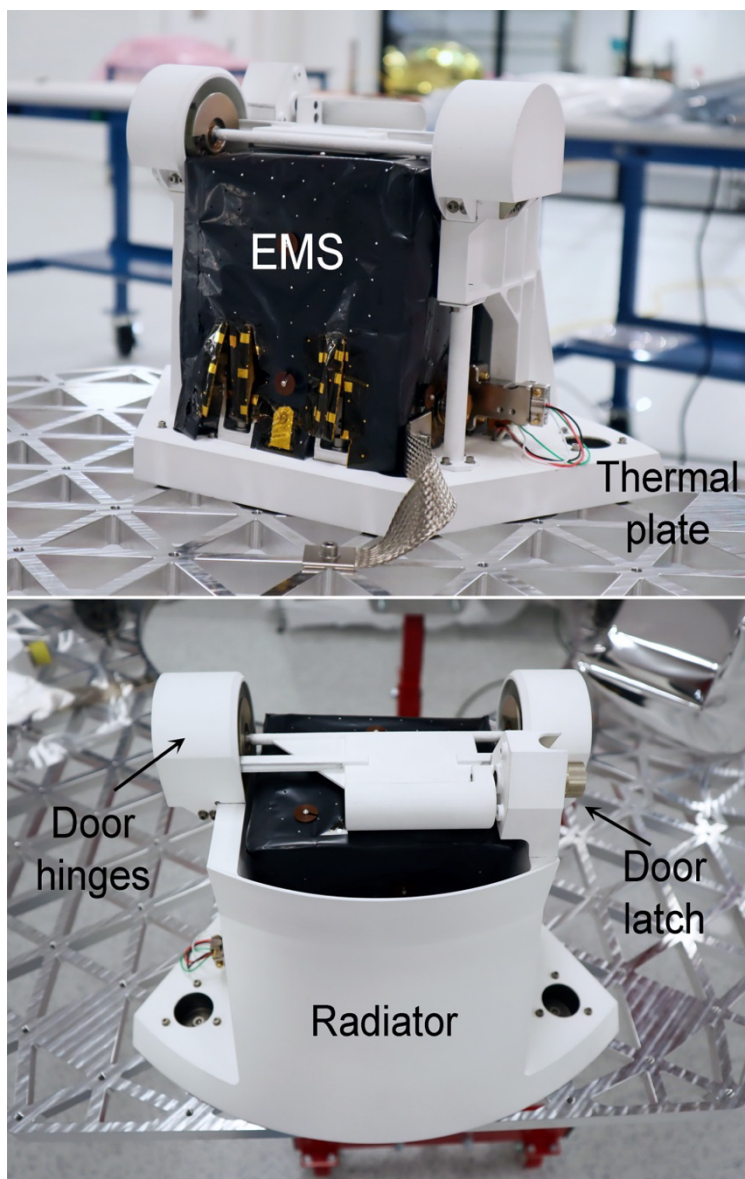


Figure 3. Views of the PITMS instrument mounted to the Peregrine deck. The EMS is shrouded in multilayer insulation (MLI) inside the white-painted Wrapper.

3.3 Project development

The PITMS instrument was classed as “Do no harm” and as such fell outside NASA NPR 7120.5 or 7120.8 governance. Under this classification, the only requirement on the instrument was not to harm the host platform, and no mishap would be declared if the payload didn't function. Because of the “do no harm” classification, extremely low cost, and compressed schedule availability, we employed a highly tailored approach to mission development. At the proposal stage, the interface requirements were those contained Astrobotic Payload Users Guide (Version 2.3), including 28V regulated power and 4 kbps downlink capacity. The instruments each needed to have their own thermal regulation both in cruise and on the surface, their own data storage and processing units, and any supporting capabilities such as operations space and IT support interfacing to Astrobotic's server.

GSFC served as the managing institution, employing the PI as the project manager, an Instrument Systems Engineer as the technical lead, a mechanical lead engineer and a thermal lead engineer. GSFC managed the Interface Control Document (ICD) to Astrobotic and was party to the EMS-Wrapper ICD held by ESA. Most technical interface requirements (Table 1) originated from the Astrobotic Interface Definition Document or the NASA contractual limits. Some PITMS-level requirements, such as thermal limits and mechanical loads, resulted in a set of derived requirements that were applied at the wrapper-to-EMS interface. For the wrapper, PDR- and CDR-equivalent tabletop reviews were held at appropriate points with experts at NASA GSFC throughout the project lifetime. For EMS, a classical but simplified and accelerated PDR-, CDR-, QR- and acceptance review cycle was implemented by ESA. Interface definition was supported by GSFC and ESA subject-matter experts and reduced-scale analyses and documentation.

Table 1. PITMS key technical specifications.

Characteristic	As-built specification
Mass (kg)	3.27
Dimensions (mm)	355 x 235 x 227
Power (W)	5.9 (standby) 9.4 (operational) 17.5 (bakeout heaters)
Mechanical loads	Notched GEVS
Thermal range (°C)	-40 to +50 (operational) -45 to +65 (survival)
Radiation tolerance	5 krad
EMC compliance	Mil std 461G
Data interface	RS422 supporting up to 115 kbits/sec (default rate < 37 kbit/s)
Electrical interface	Glenair 233 13-pin

The EMS development also followed a highly tailored approach that was new to ESA (Trautner, Barber, Leese, et al., 2021). Developing the EMS for PITMS was seen as an attractive pathfinder activity and approved for development by the ESA ministerial under a NASA-ESA MOU. Though this ensured funding for the EMS development, the EMS-wrapper interface definition and MOU signature that needed to be completed before the start of related industrial activities introduced a delay of more than a year in the originally envisaged PITMS development schedule along with schedule compression. The PITMS development team also faced the unique challenges of Brexit and COVID-SARS-19 restrictions on personnel travel and availability as well as supply-chain limitations. Despite these challenges, the PITMS instrument was delivered to GSFC in July 2021 and then delivered to Astrobotic for mechanical and electrical integration and functional testing.

4. PITMS COMPONENTS AND OPERATION

The PITMS ion-optical system comprised an electron source, an ion trap mass analyzer, and an ion detector (Fig. 4). Electrons created by thermionic emission from a heated filament are focused via the electron gate and lens assembly and pass through holes in the end-cap electrode. Interaction between electrons and neutral species in the

cavity creates ions through electron-impact ionization. With suitable radiofrequency (RF) potentials applied to the ring electrode, ions above a threshold m/z value (known as the low mass cut off, or LMCO) become "trapped" within stable orbits within the cavity. After a defined trapping period, the amplitude of the RF is increased in a linear ramp, which increases the threshold for ion orbit stability (*i.e.*, increases the LMCO). This causes ions with m/z below the LMCO to lose stability in order of increasing m/z ; crucially, the instability develops more quickly in the z direction and so exiting ions pass through holes in the detector end cap and impinge upon the detector. This sequential ejection of ions onto a detector produces a mass spectrum. Customization of the PITMS ion trap functionality was enabled by changing voltages on components to drive the RF fields and to open and close gates for electrons and ions.

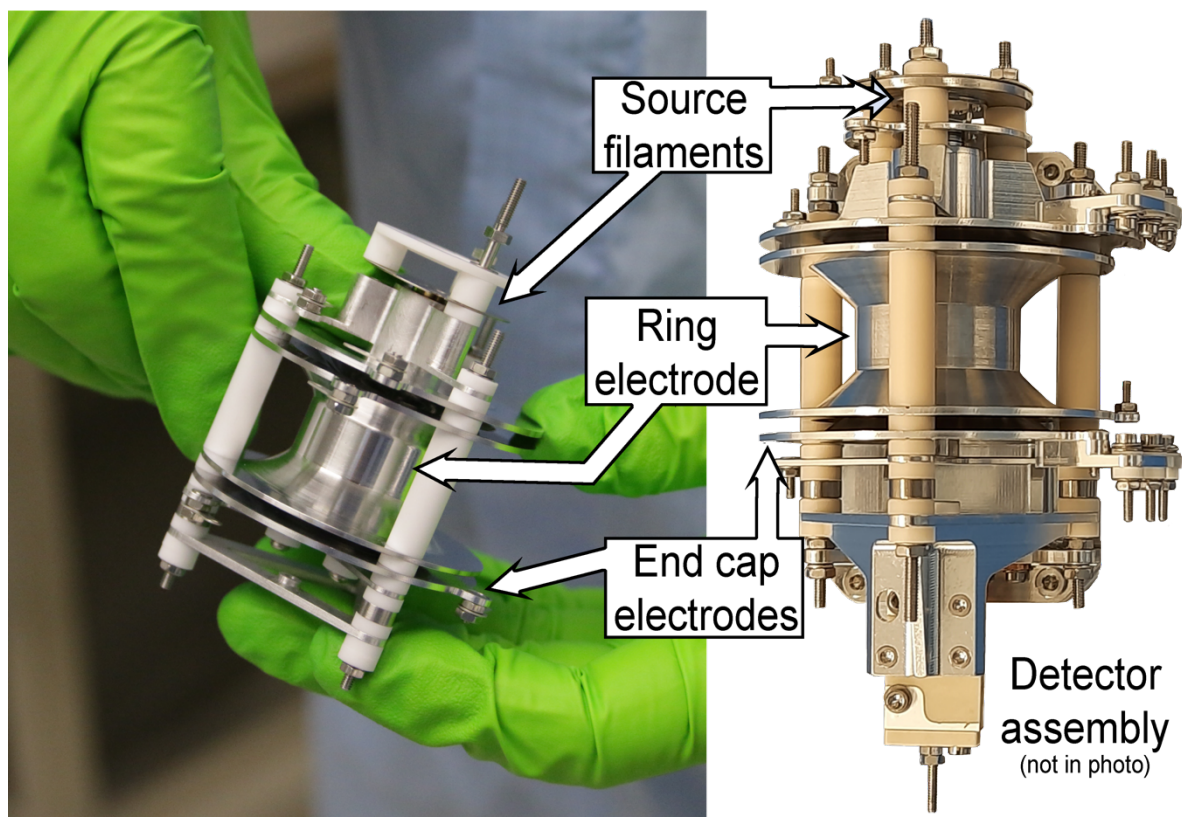


Figure 4. (left) A prototype of the PITMS ion-trap hardware and (right) schematic showing the parts of the sensor.

4.1 Ionization

The PITMS ionization source used one of two custom-built tungsten filaments; the other providing redundancy. When a suitable current is passed through the active filament, it heats to around 2000 °C and releases electrons through thermionic emission. An electron gate allows to direct electrons into or away from the central cavity. When the gate is open (held at positive potential), electrons are accelerated into the trap and collide with molecules inside the instrument, creating (almost exclusively) positive ions. The efficiency of this electron impact ionization (EI) process depends on the energy of the incident electrons and the nature of the

target species. For PITMS, the incident electron energy from the bias at the “open” electron gate minus the fixed filament bias (plus a small contribution from the RF voltage) was approximately 105 eV.

4.2 Ion Trapping

During the ion trapping phase, the RF voltage is set at a constant amplitude (albeit still cycling from positive to negative at its characteristic frequency), referred to as the "Trapping Voltage." For each species of given m/z , stable orbits exist at a given DC and RF (amplitude) voltage for an ion trap of given physical dimensions. This results in the ability to set the RF voltage that best "traps" the ions in the mass region of interest. The choice of trapping voltage is a compromise; it must be set below the lightest m/z ion of interest, but if set too low, the trapping efficiency for all ions will be low. There is no unique value of storage m/z that is optimal for all target m/z values. For this reason, the value of the storage m/z could be selected during PITMS operations according to the m/z range of interest (further discussed in Section 4.5).

4.3 Ion Ejection and Detection

To build a spectrum, PITMS employed mass-selective ejection, in which trapped ions are ejected onto a detector by increasing the amplitude of the RF field in a linear ramp. PITMS used a Channel Electron Multiplier (CEM) detector separated from the end cap electrode by a detector gate electrode. When trapped ions become destabilized by increasing RF, they escape along the z axis towards the detector. The detector is exposed to ions via the detector gate, which is closed at positive voltage and open at zero or negative voltage. The CEM operating voltage is biased such that the front funnel end is at a constant -2500 V so that ions that pass the detector gate are accelerated into the CEM. During ionization, the detector gate is positive voltage so that ions created but not stored in the trap do not reach the detector, preserving its useful lifetime. Each ion incident on the detector releases secondary electrons, which are accelerated down the channel by a positive bias. These electrons create further secondaries and this avalanche process results in a pulse of charge of up to 10^8 electrons arriving at the output end of the channel. The pulse was detected by the EMS electronics for processing.

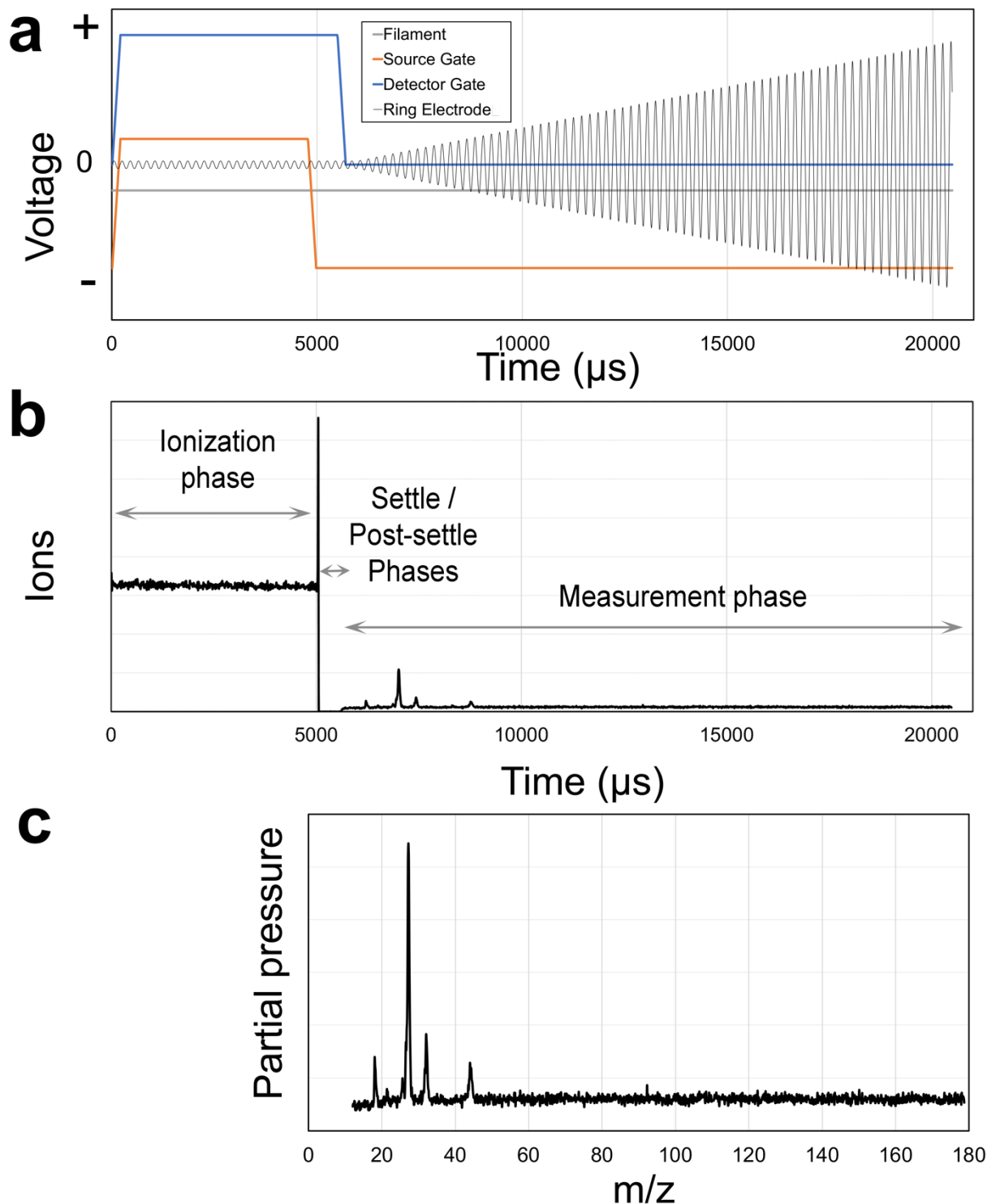


Figure 5. Illustration (non-quantitative) of a) representative voltage profiles and b) representative detector counts for the different phases of PITMS operation. The filament and detector bias are kept at constant values throughout the measurement. During the ionization phase, the source gate is open, creating ions that are trapped in the ring electrode field. The settle and post-settle phases allow the source gate to close and the detector gate to open. During the measurement phase, the amplitude of the ring electrode field is increased, sequentially ejecting ions of increasing m/z value. c) The detector counts would be calibrated to produce instrument-independent mass spectra in units of partial pressure as a function of m/z .

4.4 Generation of Mass Spectra

PITMS was intended to collect exospheric species in a passive mode. PITMS had a 59x43mm rectangular array of 170 holes of diameter 3 mm at the top of its enclosure, providing an inlet aperture area of 1202 mm². The clear zenith view was expected to result in instrument equilibrium with the lunar exosphere external to the instrument. During a mass spectrum acquisition, sequential manipulation of the electric fields would ionize the ambient gases in the instrument cavity, trap them, sequentially eject them, focus them on the detector, and count ions as a function of the trapping field magnitude. Figure 5 illustrates the voltage profiles and detector counts during operation of the ion trap throughout a scan function. The phases in this process are summarized below.

Ionization phase. The ring electrodes are set to the storage voltage, forming the ion trap. The electron gun is on and the source gate is open [+20V], accelerating electrons into the trapping region, forming ions, which are trapped. The detector gate is closed during this phase [+130V], but high counts are observed on the detector as a result of stray ions impinging upon the detector. These counts may serve as a proxy for the total pressure inside the instrument.

Settle phase. At the start of this phase, the source gate closes [-120V] and near-zero counts are observed with the source and detector gates closed (though a transient spike in counts is observed as a feature of the software). Ion-molecule reactions may occur among species within the trapping region (Cooks, & Kaiser, 1990; Barber, 1998).

Post-settle phase. At the start of this phase, the detector gate opens [0V]. Counts begin to climb to the background level that will be observed throughout the mass spectrum. This phase allows for delays in the voltage switch as the detector gate opens before the RF voltage ramp begins.

Measurement Phase. The voltage on the ring electrode is increased at a pre-determined rate to eject trapped species and create the mass spectrum. The instrument has an onboard calibration routine to determine the relationship between mass and RF field intensity to execute the correct ramp for the desired mass range.

4.5 Scan Functions and Science Sequences

The term "Scan Function" (SF) was used to describe the set of parameters applied to the instrument to acquire mass spectra. To maximize flexibility in the short surface mission under uncertain conditions, PITMS provided storage of 16 SFs on board (Table 2). Of these, 14 were conceived before launch to provide the mass spectra that were anticipated to be of interest to the science team, which allowed these to be pre-loaded into the instrument in a memory-efficient manner. A further two SF were stored in a more memory-intensive, but consequently editable, format that could be patched during the missions if updates were required. Each scan function would repeat the set parameters to sum over 1000 scans (default value, but selectable) and report the summed spectrum. 1000 summed scans would take approximately 33-45s to execute, with the exact time dependent on the scan function used.

PITMS execute SFs in groups of four, with each grouping known as a Science Sequence (SS) (Table 3). Each SS was conceived to facilitate the types of investigations desired during the mission. The command to execute a SS also contained a parameter to indicate how many times it should be executed, enabling the instrument to continue collecting data during periods without communications with ground control.

Table 2. PITMS Scan Function (SF) definitions. SF4 is considered a reference scan function.

Scan Function	Utility	Ionization Phase (μ s)	Settle/Post-Settle Phase (μ s)	Ramp Phase* (μ s)	Trapping Voltage* (m/z)	Ramp End* (m/z)	Bin duration (μ s)	Description
SF4	Reference	5000	500/500	14500	10	155	10	Used as Reference SF
SF0	Mid m/z	5000	500/500	10000	10	110	10	Shorter ramp \rightarrow faster scanning, lower power
SF1	Mid m/z	5000	500/500	13000	10	140	10	Shorter ramp \rightarrow faster scanning, lower power
SF2	Diagnostic	1000	500/500	15000	10	160	10	Reduced ionization time for lower sensitivity – in case of higher pressures
SF3	Diagnostic	5000	500/2500	13000	10	140	10	Extended post-settle time to promote ion-molecule reactions
SF5	Mid m/z	5000	500/500	14500	7	152	10	Slightly lower trapping voltage variant of reference SF
SF6	Low m/z	5000	500/500	13000	2.5	132.5	10	Significantly lower trapping voltage variant of reference SF
SF7	Low m/z	5000	500/500	13000	0.01	130.01	10	Minimum definable trapping voltage
SF8	Diagnostic	5000	500/500	4000	10	50	5	Shorter bin time samples detector output at higher cadence
SF9	Low m/z	5000	500/500	13000	0.1	130.1	10	Reduced trapping voltage for low m/z species
SF10	Low m/z	5000	500/500	13000	0.5	130.5	10	Reduced trapping voltage for low m/z species
SF11	High m/z	5000	500/500	15000	30	180	10	Increased trapping voltage for higher m/z species
SF12	High m/z	5000	500/500	12000	30	150	10	Increased trapping voltage for higher m/z species
SF13	High m/z	5000	500/500	14500	35	180	10	Increased trapping voltage for higher m/z species
SF14	Editable	5000	500/500	14500	10	155	10	Editable version of SF4
SF15	Editable	5000	500/500	14500	7	152	10	Editable version of SF5

*The duration of the Ramp Phase is defined in conjunction with the Trapping Voltage and Ramp End to achieve the desired mass-selective ejection ramp gradient (m/z per time).

Table 3. PITMS Science Sequence (SS) definitions.

Science Sequence	Scan Functions	Purpose	Description
0	4, 0, 0, 0	Mid m/z	Lowest power / fastest scanning, with SF4 for reference
1	1, 1, 1, 1	Mid m/z	Lower power / faster scanning, with SF4 for reference
2	1, 4, 1, 5	Mid m/z	Executes mid-range SFs, with SF4 for reference
3	4, 3, 4, 3	Diagnostic	Tests for ion-molecule reactions through comparison with SF4 reference
4	4, 13, 4, 13	Mid & high m/z	Highest trapping voltage, with SF4 for reference
5	4, 2, 4, 2	Diagnostic	Shorter ionization time for high pressures, with SF4 reference
6	4, 9, 10, 6	Low m/z	Executes three lower trapping voltages, with SF4 for reference
7	4, 7, 4, 7	Low m/z	Lowest trapping voltage, with SF4 for reference
8	4, 8, 9, 8	Diagnostic	Obtains high m/z resolution, compares with low trapping voltage and SF4 reference
9	4, 12, 11, 13	High m/z	Executes all 3 high trapping voltage SFs, with SF4 for reference
10	1, 9, 6, 12	Low, mid & high- m/z	Executes mid, high and two low trapping voltage SFs
11	4, 5, 11, 13	High mass	Executes mid and two high trapping voltage SFs, with SF4 reference
12	4, 7, 9, 13	Low-, mid- & high-range	Executes lowest, second lowest, and highest trapping voltages, with SF4 reference
13	4, 3, 8, 13	Diagnostic	Tests for ion-molecule reactions, obtains high m/z resolution, executes highest trapping voltage SFs, with SF4 reference
14	4, 14, 14, 14	Editable	Executes editable SF14 and SF4 for reference
15	4, 15, 15, 15	Editable	Executes editable SF15 and SF4 for reference

Reference scan function: SF4. This SF was included within multiple SS as a recurring reference throughout the mission, as well as to provide an internal standard within a SS. It used a trapping voltage corresponding to $m/z = 10$, a compromise value to enable trapping of low-mass and heavier ions. The ionization phase duration was 5000 μs , followed by settle and post-settle phases each of 500 μs . The mass-selective ejection scan ramped up to m/z 155 over a duration of 14,500 μs , selected to provide a gradient of 100 μs per Da. Throughout the SF, the detector bin width was set to 10 μs , resulting in a mass spectral sampling rate of 10 bins per Da.

Mid- m/z range scan functions: SF0, SF1, SF5. These SFs are variants of the reference SF4. SF0 employed a shorter mass-selective ejection ramp ending at m/z 110, resulting in a lower-duration and lower-power SF. SF1 was broadly similar, with an upper m/z of 140. SF5 used a lower trapping voltage of m/z 7 (compared to m/z 10 in SF4), designed to increase the trapping efficiency at lower m/z , at the cost of lower efficiency at higher m/z . In these SFs, the ramp phase duration was adjusted to maintain the mass spectral sampling rate of 10 bins per Da.

Low- m/z range scan functions: SF6, SF7, SF9, SF10. These SFs used lower trapping voltage values to maximize the efficiency of trapping low m/z ions, such as H_2^+ , He^+ and O^{2+} . In each case, the ramp end value was chosen to achieve the reference a mass spectral sampling rate of 10 bins per Da.

High- m/z range scan functions: SF11, SF12, SF13. These scan functions used higher trapping voltage values of m/z 30 (SF11, SF12) or 35 (SF13) to preferentially trap heavier ions.

Diagnostic scan functions: SF2, SF3, SF8. These SFs were designed to probe specific phenomena that may occur within the ion trap to aid interpretation of spectra from other categories. SF2 used a shorter ionization phase (1000 μs), designed to result in fewer trapped ions to investigate phenomena such as quantitative dynamic range. SF3 used an extended post-settle time to allow additional time for ion-molecule reactions to proceed, thus aiding identification of ion-molecule chemistry. SF8 used a shorter bin duration of 5 μs (compared to standard value of 10 μs); the narrower bins provide finer m/z resolution but terminating at a lower m/z value.

Editable scan functions: SF14, SF15. The hardware can execute complex scan functions, including up to 32 linear ramps of RF, each with any duration, start/end amplitudes, state of the gates and rate of binning. Each of the 32 sections also supports looping structures, allowing highly complex scan functions to be devised. To accommodate the possibility that more complex sequences might be desired, memory for two editable scan functions was available on PITMS. Since the full description of any scan function of this format would be prohibitively large, the editable scan functions SF14 and SF15 were pre-populated to the equivalent of SF4 and SF5 at PITMS power-up. Thereafter, it would be possible to customize SF14 and SF15 by uplinking software patches.

4.6 PITMS Electronics and Software

The PITMS electronics were similar to those used on the Ptolemy instrument developed by The Open University and RAL Space for the Philae lander of the ESA Rosetta mission (Wright, Barber, Morgan, et al., 2006). The architecture spanned four main circuit boards (Power Supply, Processor, High Voltage, and Mass Spectrometer Driver and Control) underneath the ion trap, as well as a smaller preamplifier board in a small pocket close to the detector. Electrical connectivity was made between the chambers via sealed (but non-hermetic) feedthroughs. This arrangement keeps most of the electronics away from the spectrometer (avoiding potential outgassing directly into the measurement volume) while still allowing proximity measurement of the sensitive detector output.

The EMS flight software provided all the logic and functionality to drive the mass spectrometer, collecting mass spectra and storing these to local memory. The flight software included two separate but loosely coupled pieces of software: the Boot Software (BSW) and the Application Software (ASW). Boot software was limited in capabilities but provided all functionality to safely drive the essential electronics and receive and respond to telecommands. The ASW was responsible for handling the main execution of operations while the instrument was in flight: responding to telecommands, transmitting telemetry packets, instigating collection of science data and driving the mass spectrometer electronics, retrieving science data and formatting them for internal storage and downlink via serial link. The ASW carried onboard warnings that alert to user in real time when parameters near a limit and fault limits that would automatically return the instrument to a safe state if limits were violated (or when commanded).

The instrument accepted commands from the spacecraft and acted on them immediately if they were valid for the operational state. The EMS design assumed that the lander would provide a time-tagged command queue, so this capability was not implemented with the instrument. However, the lander only provided pass-through communications, so the instrument was required to be commanded from the ground in real time while the lander was in communication with the ground segment.

5. PITMS CALIBRATION AND PERFORMANCE CHARACTERIZATION

The PITMS calibration campaign established two aspects of performance: calibration of the mass scale to enable assignment of spectral peaks to chemical species, and calibration of the quantitative response of the instrument to enable species quantification. The original proposal for PITMS would have included an on-board calibration gas mixture, which could be released in measured doses to produce characteristic spectral peaks enabling real-time calibration of the m/z scale and quantitative response. However, the programmatic challenges described in Section 3.3 prevented the implementation of a calibration system for the PITMS instrument. The implications of this limitation will be highlighted in the following sections.

5.1 Electron source and detector calibration

A pre-flight test campaign on the PFM led to the selection of 20 μA for the default electron source emission current. Both filaments were demonstrated to be fully functional before and after the environmental test campaign. Peak heights obtained for each filament under identical conditions were comparable within a factor 2 which is

considered acceptable, with Filament 2 providing higher counts. Therefore Filament 1 was used for most tests performed on PFM to preserve Filament 2 for flight operations.

The electron multiplier detector bias was set to -2500 V for ground testing, slightly below saturation level to reduce aging of the detector during testing (aging is broadly a function of total accumulated charge and the pressures of certain, particularly carbonaceous, gases during operation).

5.2 Mass range and linearity

A test campaign was conducted on the PFM to establish its sensitivity and linearity. The experiments were conducted in vacuum systems containing the full EMS instrument, which achieved vacuum conditions in the approximate range $1\text{E-}6$ to $1\text{E-}7$ mbar. Therefore, the results achieved must be extrapolated to lunar vacuum conditions.

A gas metering system introduced laboratory-grade pure gases (hydrogen, methane, neon, nitrogen, argon, krypton, xenon) into the UHV chamber containing the PFM. These gases were selected to provide characteristic peaks throughout the m/z range of interest. Data were acquired for varying partial pressure mixes of each gas. Multiple m/z range tests demonstrate that the EMS is capable of collecting mass spectra of individual gas species of interest distributed through the required m/z range. The EMS was shown to provide the anticipated trend of increasing counts with increasing gas partial pressure. Methane data were used to show good linearity at partial pressure $(1-3) \times 10^{-8}$ mbar, and neon data suggests that linearity is still achieved at pressures $(2-4) \times 10^{-9}$ mbar.

The test campaign did not successfully achieve the goal of detection of H_2^+ ions at $m/z = 2$. This finding was not unexpected, because of restrictions on availability of electronic components during the design and build process. Combined with the temperature-dependence of the RF generation circuitry, this means that the amplitude of the RF is poorly constrained at the low amplitudes required for trapping low m/z ions.

5.3 Sensitivity and Detection Limits

Sensitivity of the PITMS was defined as the number of counts recorded by the detector as a function of the partial pressure of the detected species within the ion trap cavity. Calibration was traced back to a calibrated Residual Gas Analyzer (RGA) employed during the Thermal Vacuum testing of the instrument. This RGA recorded the partial pressure of ions in the range m/z 1 to 200 throughout the test cycle. The resulting mass spectra typically contained the background gases nitrogen, oxygen and carbon dioxide, plus water during warmer portions of the test cycle. At specific times, test gases were introduced into the chamber to obtain further calibration cross-referenced to the ITMS spectra.

The Limit of Detection (LOD) requires consideration of not only sensitivity, but also noise. Sources of noise in PITMS include instrument sources such as dark current, feedback, or effects within the detector, along with unwanted counts from ions striking the detector but not as part of the mass-selective ejection. Typically, the noise is smaller than the signal from a real incident ion. PITMS did not specifically characterize the noise levels arising from intrinsic instrument sources, but rather employed thresholding of the detector output to limit

these effects (discarding the signals from these effects while counting the signals from the maximum number of real incident ions). The larger source of unwanted counts would be caused by ions that may reach the detector independently of the ion storage and ejection functions.

These noise sources produce a background that must be accounted for when determining true counts at a given m/z . During calibration, different gas species were measured using a range of different settings, including detector bias. These tests were typically conducted at pressures in the range of $(3-12) \times 10^{-8}$ mbar. The data showed that there was no strong correlation between detector bias or scan function and higher or lower baseline noise (and therefore LODs). Higher baseline noise strongly correlated to background pressure, because the formation and detection of untrapped ions is a pressure-dependent phenomenon. As pressure falls, this effect lessens, and a lower detection limit may potentially be achieved. Summing multiple scans in data analysis may help elevate small peaks above the background noise.

While not all species were investigated for absolute lower limits, Table 4 gives the LOD for test species at the lowest partial pressures detected during testing. Some species, notably N_2 , O_2 and Kr, were either present throughout in the chamber background or only investigated once a higher pressure had accumulated. The high number of counts above the LOD indicates that a lower pressure detection would be possible for these gases. Further details on quantitative PITMS calibration will be included when data are reported.

Table 4. Partial pressure detections, as an average of 5 successful acquisitions. Each acquisition summed 1000 individual scans, taking approximately 33-45s to execute, with the exact time dependent on the scan function used.

Species	m/z	Detector Bias (V)	Scan Function(s)	Counts above LOD	RGA pressure (mbar)
Methane	16	-2500	6	34	3.42E-09
Water	18	-2590	1,4	40	9.02E-09
Neon	20	-2590	4	22	1.27E-09
Nitrogen	28	-2590	1, 4	1205	3.35E-08
Oxygen	32	-2590	1, 4	246	7.06E-09
Argon	40	-2500	0, 4	2	5.36E-10
Krypton	84	-2590	11, 12	304	8.74E-09

5.4 Mass scale thermal stability

The electronics circuits used to generate the RF applied to the ring electrode are temperature-sensitive. The effect of changing temperature would be to change the gain of the circuit, and therefore the magnitude of the RF signal output to the ring electrode. This would have two distinct, but related, effects: a) the commanded value of the RF results in a slightly lower or higher actual RF being applied, shifting the LMCO away from the desired value and causing ions to be recorded in earlier or later bins respectively. This would affect both the storage m/z , hence the start value of the mass-selective ejection ramp, and the gradient of the ramp (bins per amu); and b) shifts in the sensitivity of the ITMS for each m/z value.

These effects could be operationally mitigated by recalibrating the RF gain before acquiring a spectrum to compensate for the thermal change of the electronics. However, the PITMS recalibration command could only be

run once at the beginning of a Science Sequence. As a commanded acquisition would proceed through the Science Sequence, the thermal drift effects would be manifested as mass peaks shifting along the apparent m/z axis. Further calibration of temperature on the RF amplitude, and therefore the m/z scale, will be achieved through data processing and testing using the Ground Reference Model.

6. PITMS MISSION OPERATIONS

Because the Peregrine mission was designed with limited duration, with surface and operational conditions that may rapidly change, the PITMS Science Team planned to participate in the surface mission in real time. The PITMS payload and science investigation was designed to operate at NASA GSFC with secure, virtual connections to Science Team Member institutions using the GSFC virtual Multi Mission Operations Center (vMMOC; Ido, 2017). Science Team operational roles included taking shifts operating the instrument, evaluating downlinked products, and/or creating science products for use and interpretation by the team.

The Peregrine mission planned for a 24-hour operations cadence, with seven hours of continuous communication and one hour loss-of-signal. As discussed in Section 4.6, the PITMS design did not allow command queuing or time-tagged command execution, so all PITMS activities needed to be real-time commanded. To protect against loss of communications and/or loss of command authority, the PITMS team developed a Default Science Plan and procedure that would have been the first commanded activity after instrument power on and checkout (once at landing and after any planned or unplanned instrument power off). In the Default Science Plan, the instrument was expected to drift out of calibration as the thermal conditions changed. Therefore, the Default Science Plan consisted of repeating a Science Sequence consisting of four scans across different trapping voltages. This would enable at least one of the science scan functions to capture optimized data throughout the course of the mission.

The PITMS team also created a Strategic Science Plan as a guide to the science sequences and calibration cadence that would be expected to provide the best science return over the anticipated mission timeline. The Strategic Science Plan was planned to be implemented during nominal operations when real-time commanding was available and to run throughout periods of planned loss of communications. When real-time communications were available, the PITMS team would also have the ability to respond to real-time changes on the lunar surface and tactically command the instrument into a mode or Science Sequence that may better capture the activity or situation, superseding the Strategic Plan activities.

6.1 Operations Roles

During the cruise and surface mission, roles would be staffed for PITMS at all times on a shift schedule to provide continuous operations. In-person shift handovers, console log with timestamped commands, and shift logs including major decisions, activities, timestamped commands, and any instrument changes that affect future operations, would be used to maintain operations continuity and documentation. The various roles developed and trained within the operations team are defined below.

Principal Investigator (PI): The PI had primary responsibility for PITMS success. The PI would be responsible for leading the team throughout operations training and the mission, working with Astrobotic and NASA to ensure that PITMS got desired data within the mission guidelines. The PI would maintain the Strategic Plan as tactical changes rippled through planning. The PI would work with the instrument developers to troubleshoot any off-nominal behavior in the instrument. The PI would support all NASA and Astrobotic meetings and report out for the PITMS team. The PI would also facilitate a daily PITMS tag-up with an overview of activities, look-ahead plan, health and safety assessment, and anomaly reporting.

PITMS Uplink Lead (PUL): The PUL would be responsible for operating the instrument safely and making tactical decisions that maximize the science return. The PUL would be responsible for understanding the science and engineering intent for near-term PITMS activities and maintaining situational awareness of mission activities. The PUL would create, deliver, and confirm instrument commands and procedures while in open communication with the Astrobotic Payload Operations Center. The PUL would also monitor the health and safety of the instrument, including trends or anomalies, and serve as the Science Team lead for their shift, working with the Science team to ensure that PITMS activities would be modified, if needed, to be consistent with the science intent (tactical commanding) and supporting the preparation and development of upcoming strategic and tactical activities.

PITMS Documentarian: The Documentarian would maintain situational awareness of PITMS and Astrobotic operations and keep a record of the major events and decisions during operations. The Documentarian also would act as a second set of eyes for the PITMS operator, verifying commands are as intended before they were uplinked. The Documentarian would keep a real-time play-by-play document available to the full team that included science observations, major decisions, instrument and mission activities, and anomalies.

PITMS Downlink Lead (PDL): The PDL would be responsible for reviewing received data products and ensuring their completeness, maintaining the data products on the vMMOC so that the full team has access to them. The PDL would also develop and create "quick-look" data products for the team to use, including generating spectra, monitoring intensity of key species, and plotting trends in instrument health parameters. Because the PDL would have insight into the data, the PDL was well-positioned to advise the team of any changes or trends that might affect planning or operations.

PITMS Science analysts: The role of the science analysts was to understand the science unfolding on the Moon and tactically respond to maximize science return. They would help prepare data products and work on science presentations and publications. All team members were to participate as analysts.

6.2 Operations Software

NASA GSFC. All science operations software was hosted at NASA GSFC. Team members would use their own institutionally managed laptops or computers. To participate in operations and data processing, each PITMS team member required both IT and Physical access to NASA and Goddard resources, which required working with NASA security and international visitor services.

The PITMS team used Slack as a persistent chat service and Box as an internal, secure archive. Team meetings were conducted virtually on Webex and Teams. At the NASA level, the project scientist used Playbook to visualize

the resources needed by each payload throughout surface operations. The NASA virtual Multi-Mission Operations Center (vMMOC; Ido, 2017) hosted PITMS operations in a virtualized Windows environment. This environment facilitated a single point of access for instrument commanding and distribution of downlinked data to the team. The PITMS project also created and employed several custom scripts using Python to develop quick-look products, archival data products, and conduct data reduction activities. These activities were packaged as executables that could be run by any team member on the vMMOC or their own machines.

RAL Space. The PITMS ground system software (Electrical Ground Support Equipment, or EGSE) was the ground support software developed for EMS/PITMS by RAL Space. It was made up of standalone Windows executables (modules) that interface with each other using Windows Pipe constructs. The Archive Distribution Engine (ADE) would read data on the RAL EGSE pipe, timestamp each data packet with receipt time, and store it in archive files. The RAL synoptic display (RatSD) module would read data from the ADE pipe and display it. Histogram plotter would connect to the ADE output pipe and display the science data as a histogram and automatically save each histogram's values in a text file. The Command tool module would allow the user to generate command strings either by typing at a prompt or selecting from several drop-down menus.

6.3 Operations timeline

PITMS was planned to be turned on at least once during lunar orbit to confirm payload post-launch survival and cleanliness before landing. PITMS planned to be turned on as soon as practical after landing, conduct a self-test, deploy the aperture cover, and then operate continuously during the surface operations phase. Continuous operations would have allowed PITMS to have a maximum chance to detect changes arising from warming of the lunar surface and lander systems, or from surface disturbance due to rover or instrument deployments. If continuous operations were not feasible, PITMS operations would have been planned with a knowledge of the scheduled lander operations. PITMS requested several data collection periods in lunar orbit, at Astrobotic's discretion.

The planned PITMS default state was ON-ACQUISITION during nominal operations to continuously collect mass spectra, buffering these and passing to the lander for downlink to Earth. Other states would be requested as needed during the surface mission, *e.g.*, bakeout operations, data downlink, software patch operations. The permissible duty cycle would have been dependent upon the mission power budget.

Launch. PITMS would be in the OFF state during launch.

Cruise & Lunar Orbit. PITMS would be in the OFF state during cruise, except for its survival heaters. PITMS would conduct a short functional test during cruise to verify that the instrument survived launch. PITMS requested to acquire science data (with the instrument dust cover closed) during lunar orbit if possible.

Descent and Landing. No PITMS operations were planned during this phase.

Surface operations. PITMS planned its power-on, checkout, and science activities soon after landing. PITMS was designed to be operated continuously throughout the surface mission. During periods without real-time commanding, data would be stored on board the instrument and passed to the lander for later downlink to Earth.

Surface siesta. During the hottest part of the day (around noon local lunar time), the lander was expected to enter a low-power state known as "siesta" to maintain thermal control. All payload services were expected to be off during the surface siesta period. PITMS would power off before this period and power on afterward.

6.4 Data Products and Archiving

PITMS data products consist of telemetry, raw data, calibrated data, and derived products. PITMS raw, calibrated, and derived data products would be delivered to and archived in NASA's Planetary Data System (PDS) Atmospheres node and mirrored on the European Space Agency's Planetary Science Archive (PSA) within 6 months of mission completion.

PITMS telemetry data would be retrieved with the PITMS ground software and locally archived. The PITMS ground software would ingest the packets and write human-readable raw data files in text format. PITMS raw data products would be archived as text files that are machine-readable and may be opened by any spreadsheet or plotting program, conforming to Findable, Accessible, Interoperable, and Readable (FAIR) standards.

The team would create calibrated mass spectra using calibration data and instrument knowledge, along with derived data products that would provide interpretations of the detected gas species and their number density in the lunar exosphere. The calibrated and derived data products would be described in the PDS documentation archived with the processed data and presented in publications.

7. SUMMARY

The Peregrine Ion-Trap Mass spectrometer was designed as a standalone instrument to investigate the gas species in the lunar exosphere on a landed mission. The instrument calibration and test campaign has been shown to perform well in ground testing and is expected to provide useful scientific measurements of gas species during the mission. The NASA-ESA partnership to develop, build, and operate PITMS worked extremely well even during a compressed schedule and the COVID-19 pandemic. Development of PITMS took place in the early stages of the NASA CLPS initiative. Its design, build, and operation presented challenges and lessons learned for this class of instrument development within development for NASA and ESA.

PITMS was only the first mass spectrometer to aim for the lunar surface in the upcoming decade. Upcoming CLPS deliveries and international missions are also planning to include mass spectrometers (*e.g.*, Benna, Malespin, Hurley, et al., 2019; Colaprete, 2021; Heather, Sefton-Nash, Trautner, et al., 2023), each of which would perform its own mission but also measure the ambient lunar exosphere. Though selected individually, the multiple mass spectrometers may be thought of as a network that will provide temporally- and spatially-resolved measurements of volatile species, including OH/H₂O, on the lunar surface, along with improved quantification of exospheric species of interest to both science and human exploration. Measuring volatile species before the exosphere is swamped by robotic and human activity could elucidate key details of lunar interior structure and composition. Multiple measurements of the lunar atmosphere and surface-lander interactions can be incredibly valuable, particularly from multiple landing sites and during different seasons. These investigations will provide measurements of the exosphere

to significantly improve our knowledge of the abundance and behavior of volatiles on the Moon, linking the lunar surface to measurements from orbit, and informing future robotic and human mission design.

ACKNOWLEDGEMENTS

PITMS was developed under the NASA Provided Lunar Payloads (NPLP) program and manifested using the Commercial Lunar Payload Services (CLPS) initiative. We thank Ryan Stephan, Paul Niles, and Chris Culbert for shepherding PITMS through the NPLP and CLPS programs to flight. We are indebted to the NASA GSFC reviewers and SMEs who helped mature the PITMS design and build. We are grateful to the GSFC Solar System Exploration Division and Goddard management, administration, and IT support and the GSFC vMMOC for ensuring the success of the international PITMS team and investigation, particularly Katrice Tanner.

The EMS team at The Open University acknowledges the support of UK Space Agency for the financial and strategic support that has underpinned the technology development over a sustained period. We gratefully acknowledge the OU's administrative, legal, technical, IT and external engagement teams for supporting the development of a space flight instrument during a pandemic which caused unprecedented operational challenges. We are also indebted to external support provided by Darren Yau and Keith Wells (DASTEC Consulting Ltd.), Jon-Jordan Cooper (Knights AMC Ltd.) and Mike Tucker.

EMS was built at STFC RAL Space by the Mechanical and Electrical Production Groups. The authors would like to thank the following individuals whose dedication and professionalism created the physical EMS instrument: Dario Alves, Mark Anderson, Terry Almond, Brett Bignell, Sarah Bonas, Luke Bushnell, Dean Cox, John Foley and Kim Morgan.

EMS was developed as a Moon Mission of Opportunity within the SciSpacE program of ESA's Human and Robotic Exploration program. The authors would like to specifically thank the following individuals, whose professionalism and excellent support enabled the successful development and flight qualification of the spectrometer within a very short time: Elena Grashchenkova, Cathal Mooney, Silvana Radu, Juliette Kaysan, Advenit Makaya, Narimane Brahimi, Robert Lindner, Leo Farhat, Gianni Corocher, Andrea Santovincenzo, Johannes Wolf, and numerous other ESA experts. We'd also like to thank Bérengère Houdou and James Carpenter for their support during the selection, approval and implementation process of the EMS activity.

REFERENCES

- Andrews, D.J., Morse, A.D., Barber, S.J., et al., 2012, *Planet Space Sci* 66: 179.
- Barber, S.J., 1998, PhD Thesis.
- Benna, M., Hurley, D.M., Stubbs, T.J., Mahaffy, P.R., & Elphic, R.C., 2019, *Nature Geosci* 12(5): 333.
- Benna, M., Mahaffy, P.R., Halekas, J.S., Elphic, R.C., & Delory, G.T., 2015, *Geophys Res Lett* 42(10): 3723.
- Benna, M., Malespin, C.A., Hurley, D.H., et al., 2019, *Lunar Planet Sci Conf* 2364.
- Berger, T., Marsalek, K., Aeckerlein, J., et al., 2019, *Review of Scientific Instruments* 90(12): 125115.
- Clark, R.N., 2009, *Science* 326(5952): 562.
- Cohen, B.A., Barber, S.J., Gawronska, A.J., et al., 2024, *The Planetary Science Journal*: in preparation.

- Colaprete, A., 2021, VIPER (Volatiles Investigating Polar Exploration Rover) Proposal Information Package (PIP).
- Colaprete, A., Sarantos, M., Wooden, D.H., et al., 2016, *Science* 351(6270): 249.
- Cooks, R.G., & Kaiser, R.E., Jr., 1990, *Accounts of Chemical Research* 23(7): 213.
- Donaldson Hanna, K.L., Benavente, J., Bennett, K., et al., 2023, *Lunar Planet Sci Conf* 2152.
- Farrell, W.M., Hurley, D.M., & Zimmerman, M.I., 2015, *Geophys Res Lett* 42(9): 3160.
- Farrell, W.M., Prem, P., Tucker, O.J., et al., 2022, *Icarus* 376: 114857.
- Heather, D.J., Sefton-Nash, E., Trautner, R., et al., 2023, *Lunar Planet Sci Conf*: 2047.
- Hendrix, A.R., Hurley, D.M., Farrell, W.M., et al., 2019, *Geophys Res Lett* 46(5): 2417.
- Hibbitts, C.A., Grieves, G.A., Poston, M.J., et al., 2011, *Icarus* 213(1): 64.
- Hodges Jr., R.R., 2016, *Geophys Res Lett* 43(13): 6742.
- Hoffman, J.H., 1975, NASA Technical Report NASA-CR-150946.
- Hurley, D.M., Cook, J.C., Retherford, K.D., et al., 2017, *Icarus* 283: 31.
- Ido, H.K., 2017, *Ground System Architectures Workshop (GSAW)* <https://ntrs.nasa.gov/citations/20170002276>.
- Killen, R.M., & Ip, W.-H., 1999, *Reviews of Geophysics* 37(3): 361.
- Li, S., Lucey, P.G., Milliken, R.E., et al., 2018, *Proceedings of the National Academy of Sciences* 115(36): 8907.
- Lucey, P.G., Petro, N., Hurley, D.M., et al., 2022, *Geochemistry* 82(3): 125858.
- Metzger, P., Li, X., Immer, C., & Lane, J., 2009, *47th AIAA Aerospace Sciences Meeting*: 10.2514/6.2009.
- Morse, A., Mousis, O., Sheridan, S., et al., 2015, *Astron Astrophys* 583(A42).
- Peplowski, P.N., Elphic, R.C., Fritzler, E.L., & Wilson, J.T., 2023, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 1049: 168063.
- Pieters, C.M., Goswami, J.N., Clark, R.N., et al., 2009, *Science* 326(5952): 568.
- Poston, M.J., Grieves, G.A., Aleksandrov, A.B., et al., 2015, *Icarus* 255: 24.
- Prem, P., Hurley, D.M., Goldstein, D.B., & Varghese, P.L., 2020, *Journal of Geophysical Research: Planets* 125(8): e2020JE006464.
- Roush, T.L., Colaprete, A., Cook, A., et al., 2020, *Lunar Planet Sci Conf* #2581.
- Schläppi, B., Altwegg, K., Balsiger, H., et al., 2010, *Journal of Geophysical Research: Space Physics* 115(A12).
- Stern, S.A., 1999, *Reviews of Geophysics* 37(4): 453.
- Stoffle, N., Pinsky, L., Kroupa, M., et al., 2015, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 782: 143.
- Sunshine, J.M., Farnham, T.L., Feaga, L.M., et al., 2009, *Science* 326(5952): 565.
- Trautner, R., Barber, S., Leese, M., et al., 2021, *International Astronautical Congress*.
- Vasavada, A.R., Paige, D.A., & Wood, S.E., 1999, *Icarus* 141: 179.
- Wright, I.P., Barber, S.J., Morgan, G.H., et al., 2006, *Space Sci Rev* 128: 363.
- Wurz, P., Fatemi, S., Galli, A., et al., 2022, *Space Sci Rev* 218(3): 10.