Peregrine Ion Trap Mass Spectrometer (PITMS) PDS Data Plan and Users' Guide

Prepared by:

Barbara Cohen

Name: Barbara A. Cohen
(Printed Name) *(Signature)*
Title: PITMS Principal Investigator
Date: October 1, 2024

Orenthal J. Tucker

Name: Orenthal J. Tucker
(Printed Name) *(Signature)*
Title: PITMS PDS Lead
Date: October 1, 2024

No information in this document is subject to EAR restrictions.

Change Record

Issue	Date	Section(s) Affected	Description of Change/Change Request Reference/Remarks
A	May 31, 2024	All	First draft including raw and calibrated data products
B	September 19, 2024	All	Revised according to PDS review comments

THE CONTENT WITHIN THIS DOCUMENT INCLUDES YELLOW HIGHLIGHT TO INDICATE PENDING CONTENT.

Table of Contents

1. Overview

1.1 Purpose and scope of document

This User's Guide describes the data products in the CLPS_TO_2AB PITMS archive in sufficient detail to enable a user to read and understand the data. It also describes the Planetary Data System (PDS) archive bundle, the structure in which the data products, documentation, and supporting material are stored. This User's Guide is intended for the scientists who will analyze PITMS data, including those associated with the project and those in the general planetary science community. The PITMS data set consists of mass spectra of the gaseous molecular species in the lunar exosphere and derived species and abundance data.

1.2 Applicable and reference documents

These publications or websites describe the Planetary Data System Standards used to produce the PITMS archive. These documents are archived in the PDS system and are not found specifically in the PITMS archive. These documents are revised approximately every six months with each new release of the PDS Information Model. Current and previous versions may be found at the links below.

- Planetary Data System Standards Reference, https://pds.nasa/gov/datastandards/documents/sr/current
- PDS4 Data Dictionary, https://pds.nasa.gov/datastandards/documents/dd/current
- Planetary Data System(PDS) PDS4 Information Model Specification, https://pds.nasa.gov/datastandards/documents/im/current
- Data Providers' Handbook: Archiving Guide to the PDS4 Data Standards, https://pds.nasa.gov/datastandards/documents/dph/current

The documents below are not PDS documents but are publications or websites that offer additional mission and instrument details.

- Cohen et al. (2024a) The Peregrine Ion Trap Mass Spectrometer (PITMS) Investigation Development and Pre-Flight Planning. The Planetary Science Journal, DOI: 10.3847/PSJ/ad6e7b.
- Cohen et al. (2024b) The Peregrine Ion Trap Mass Spectrometer (PITMS) Results from a CLPS-Delivered Mass Spectrometer. The Planetary Science Journal, submitted.
- Peregrine Mission-1 on the Astrobotic web site, https://www.astrobotic.com/lunar-delivery/landers/peregrine-lander/
- Astrobotic (2024) Peregrine Mission-1 Post-Mission Report. https://www.astrobotic.com/wp-content/uploads/2024/08/PM1_Post-Mission-Report_2024-1.pdf

2. Instrument and Mission overview

The Peregrine Ion Trap Mass Spectrometer (PITMS) was a NASA project to investigate the lunar exosphere using a mass spectrometer. PITMS 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 in response to natural (*e.g.,* diurnal temperature cycle) and artificial (*e.g.,* landing event, lander activities) stimuli. The PITMS project was a partnership between NASA Goddard Space Flight Center and The Open University (OU), NASA, and the European Space Agency (ESA).

2.1 Mission overview

PITMS was manifested on the first flight of Astrobotic's Peregrine lander via the Commercial Lunar Payload Services (CLPS) program. This arrangement was the first of its kind, where NASA negotiated a firm fixed price contract to deliver NASA science payloads to the Moon. Thus, many aspects of the lander hardware, development, etc. were not available to the PITMS team and accordingly, there was no higher-level science "mission" of which PITMS was a part.

The Astrobotic team provided multiple public updates during the mission on their website (https://www.astrobotic.com/category/press/), and published a Post-Mission report (Astrobotic, 2024); the relevant details are summarized here.

The Peregrine lander with PITMS aboard launched on January 8, 2024. ULA's Vulcan rocket inserted Peregrine into the planned translunar trajectory without issue. Peregrine began receiving telemetry via the NASA Deep Space Network. The lander avionics systems, including the primary command and data handling unit, as well as the thermal, propulsion, and power controllers, all powered on and performed as expected. During initialization of the propulsion system, an anomaly occurred. During initialization of the propulsion system, an anomaly occurred when a valve between the helium pressurant and the oxidizer failed to reseal after actuation during initialization. This led to a rush of high-pressure helium that spiked the pressure in the oxidizer tank beyond its operating limit and ruptured the tank.

The failure within the propulsion system caused a rapid loss of oxidizer that both rendered the nominal propulsion nominal propulsion system incapable of accomplishing a landing on the Moon and introduced a difficult-to-characterize, dynamic thrust vector to the spacecraft. Though the critical loss of the oxidizer meant that the lander lost the ability to use its descent engine to soft land on the Moon, Astrobotic successfully used the bipropellant system to operate the Attitude Control System (ACS) thrusters nominally, maintaining the spacecraft in a stable, sun-pointing state. The loss of propellant and unplanned thrust vector caused the spacecraft to deviate from its intended trajectory and placed Peregrine on a path to intercept the Earth during its planned flyby. Astrobotic positioned the Peregrine spacecraft for a safe, controlled re-entry to

Earth over a remote area of the South Pacific which occurred on January 18 at 21:04 UTC, concluding the mission.

During the 10-day operational lifetime, NASA and Astrobotic prioritized maximizing the science and data that the lander could capture in cislunar space. Astrobotic posted regular updates on the time remaining on the spacecraft until the fuel was projected to run out, causing loss of control authority. These expectations were updated each day, because the leak was decreasing in pressure with time and the spacecraft team got better at understanding how to control the spacecraft. Nevertheless, PITMS and all the instruments operated in emergency response mode each day as if it were the last time.

PITMS operated in four sessions over the Peregrine mission, for 8.5 hrs total instrument operation time. Major successful operations included turning on, applying critical software patches, conducting a functional test with filaments and detector off, conducting a functional test with filament and detectors on, acquiring data with the dust cover closed, opening the dust cover, acquiring data with the dust cover open, and downlinking latent data.

2.2 PITMS Instrument overview

Details of the PITMS instrument design and development were reported in Cohen et al. (2024a); a brief recap is presented here for context.

The PITMS instrument consisted of an ion-trap mass spectrometer sensor coupled to a wrapper that mounted this sensor to the lander deck (Fig. 1). 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.

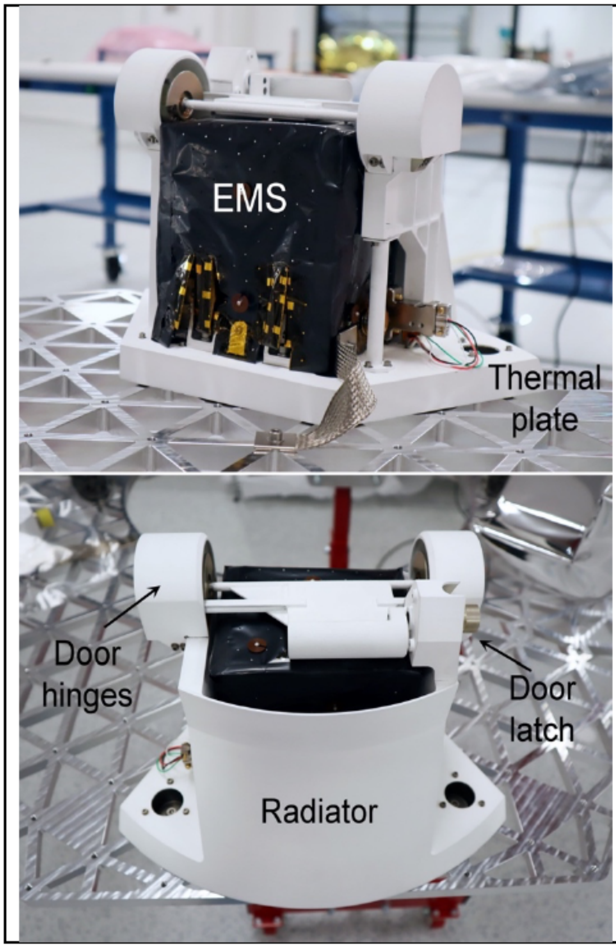

Figure 1. Views of the PITMS instrument mounted to the Peregrine deck. The EMS is shrouded in multilayer insulation (MLI) inside the white-painted wrapper.

The EMS 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, 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 ~150.

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 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. 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.

PITMS was mounted on Deck D of the Astrobotic Peregrine lander (Fig. 2). Deck D was expected to face west in a nominal landing orientation. The Peregrine lander was targeted for the Sinus Viscositatis basaltic lava plain in the northwestern part of the lunar nearside (35.25° N, 319° E). This location was chosen by NASA after PITMS delivery (and radiator angle optimization for the previous site at Lacus Mortis, 45.0° N, 27.2° E) to help optimize NASA's CLPS deliveries, as the Lunar-VISE mission will be visiting the nearby Gruithuisen Domes.

Figure 2. PITMS mounted to the Peregrine lander Deck D (left, magenta circle) in the Astrobotic cleanroom and (right) during remove-before-flight activities (with BAC for scale). The Iris rover [Potter, 2023] is mounted to the underside of deck D. The PITMS aperture opens to the +X direction of the spacecraft.

2.3 PITMS functionality

An overview of PITMS functionality is included here for reference, but the interested reader is referred to Cohen et al. (2024a) for fuller details. Ion trap mass spectrometers work by ionizing neutral gases, setting up a radio frequency (RF) voltage on a central ring electrode to trap the ions, and ramping up the RF field intensity to allow ions to escape based on their mass-to-charge ratio. The sequential ejection of ions onto a detector produces a mass spectrum. Customization of ion trap functionality can be enabled by changing voltages on components to drive the RF fields and to open and close gates for electrons and ions.

PITMS collected gaseous species in a passive mode. PITMS had a 59 mm × 43 mm rectangular array of 170 holes of diameter 3 mm at the top of its enclosure, providing an inlet aperture area of 1202 mm^2. The clear zenith view was expected to result in instrument equilibrium with the lunar exosphere external to the instrument.

During a PITMS mass spectrum acquisition, sequential manipulation for the electric fields ionizes the ambient gases in the instrument cavity, traps them, sequentially ejects them, focuses them on the detector, and counts ions as a function of the trapping field strength. The instrument scans through 2048 discrete bins for ion counts. Figure 3 illustrates the voltage profiles, raw data output, and calibrated mass spectra. 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 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 an unreal, transient spike in counts is produced by the software). Ion-molecule reactions continue to occur among species within the trapping region.

Post-settle phase. At the start of this phase, the detector gate opens [0V]. Counts climb to the background level that will be observed throughout the mass spectrum from a combination of electronics noise and ambient molecules and ions hitting the detector. 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 ions 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 (discussed in more detail in Section 6.2).

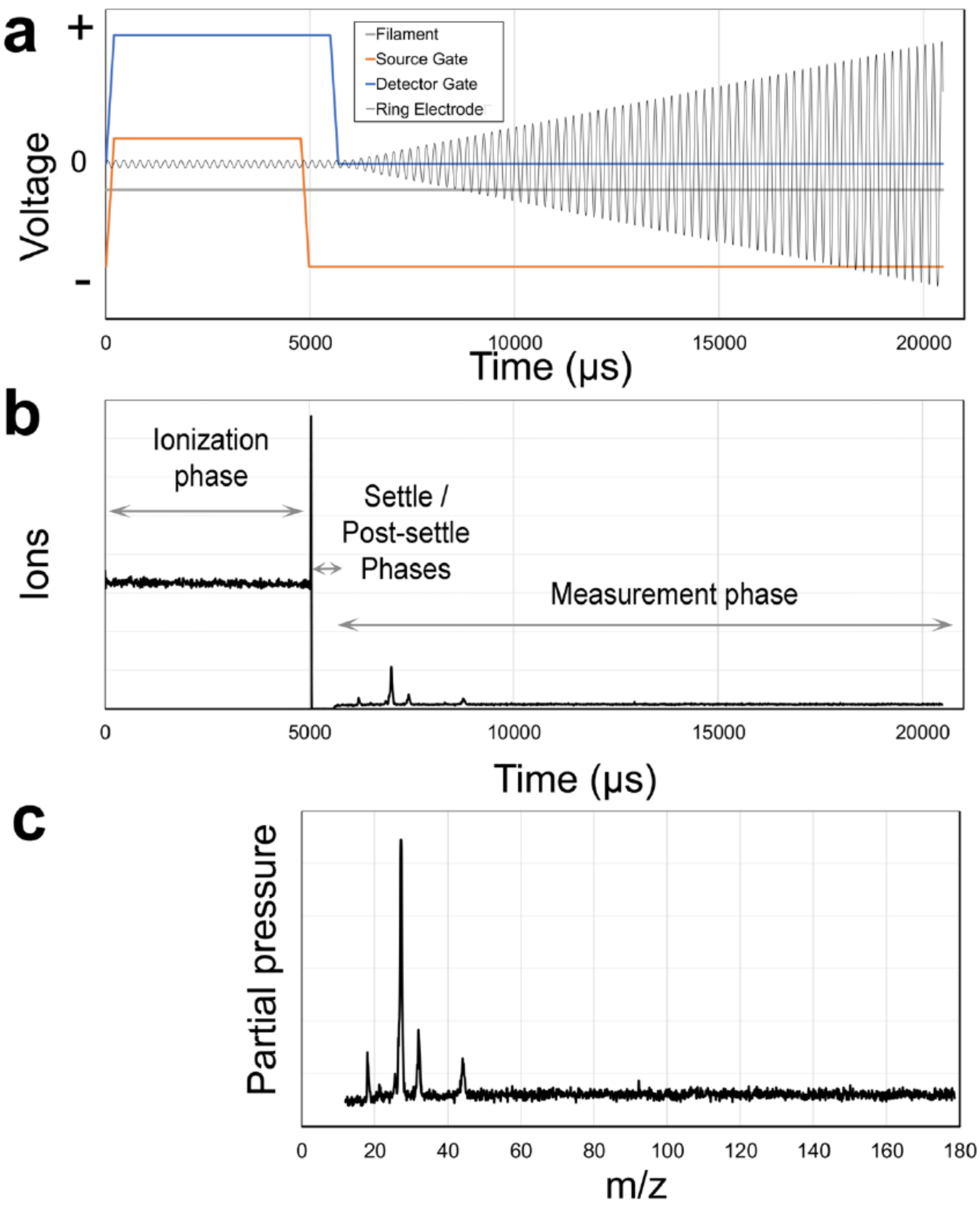

Figure 3. Illustration (non-quantitative) of a) representative voltage profiles and b) representative detector counts for the different phases of PITMS operation. The filament and detector bias are kept at constant values throughout the measurement. During the ionization phase, the source gate is open, 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.

2.4 Scan Functions and Science Sequences

Each time PITMS acquired data, it did so using a Scan Function (SF) to define the parameters applied to the sensor to acquire a mass spectrum (Table 1). These parameters determined the duration of each voltage phase and therefore feed into data parameters like mass resolution, so each data file contains the SF used to acquire the spectrum. Each SF sets the appropriate parameters and conducts the ionization, settle, and postsettle phases once, then repeats the measurement phase 1000 times and sums the measurement phase data onboard. One SF took approximately 33-45s to execute, depending on the SF used.

PITMS executed SF in groups of four, with each grouping known as a Science Sequence (SS) (Table 2). The SSs were commanded as the number of times the sequential execution of each constituent SF will be performed. Though the instrument uses SSs to operate, each spectrum is returned to the ground as a separate file with its SF, so SS is not usually reported with the data.

Table 1. PITMS Scan Function (SF) definitions. SF4 is considered a reference scan function.

Scan Function	Utility	Ionization Phase (µs)	Settle/ Post-Settle Phase (µs)	Ramp Phase* (µs)	Trapping Voltage* (m/z)	Ramp End* (m/z)	Bin duration (µs)	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 for faster scanning, lower power
SF1	Mid m/z	5000	500/500	13000	10	140	10	Shorter ramp for 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 2. 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, 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

3. PITMS Operations

Table 3 contains the as-run log for PITMS including the experiment number, Science Sequence and SFs, and the purpose/intent of each experiment. PITMS incremented its Instrument_Timeline_ID (ITL) variable each time it began a new experiment. An experiment may be thought of as a spectrum or group of spectra taken under similar circumstances for a specific science purpose. The first PITMS session assessed the instrument health and functionality by running the instrument with the filament and detectors off (ITL 11). The team planned to subsequently turn the detector and filament on to collect actual data but the spacecraft entered safe mode and cut the session short. During the first session, the team discovered that the Astrobotic-allocated onboard buffer and data rate was too low to allow PITMS data packets to be transmitted. The team worked on how to raise the data rate, along with gaining approvals to open the dust cover.

During the second session, we acquired data with the dust cover closed (ITL 12) and stored the data on the instrument. During the third session, we tested the new data downlink protocols successfully and downlinked latent data from ITL 11 and 12, but unfortunately experienced intermittent packet loss during downlink transmission that was not recovered; therefore we do not have complete spectra for ITL 11 or 12 (described further in the PDS Users Guide). In the third session, Experiments 13 and 14 were run with the PITMS dust cover still in place over the aperture, then we opened the dust cover and ran experiment 16 . Experiments 17 and 18 were run during the last session, after the dust cover had been open for about a day. Experiment 18 contains two different Science Sequences as the team did not have time to send the command to increment the ITL and run a new calibration.

Table 4 contains a list of spectra that were acquired. Each individual spectrum is referred to by the unique timestamp applied when the acquisition was initiated. The starting and ending mass numbers come from the calibrated data described in Section 6.2. The PITMS team used a set of SFs (SS2) that could be compared throughout the time PITMS was operational plus several "diagnostic" SFs that would enable the team to better understand instrument performance after the fact.

Table 3. PITMS experimental record.

Date	**Time (UTC)**	**ITL**	**Science Sequence**	**Scan Functions**	**# of cycles**	**Experiment Intent**
9-Jan-24	16:43					Turn on & software patch
9-Jan-24	18:09	11	1	1 1 1 1	1	Functional test without detector or filament on. Instrument functionality confirmed but data packets were lost during downlink[1].
9-Jan-24	19:25					Power removed (spacecraft safe mode)
12-Jan-24	08:40					Turn on & software patch
12-Jan-24	09:02	12	2	1 4 1 5	1	Functional test with filament and detector on. Instrument functionality confirmed but data packets were lost during downlink[1].
12-Jan-24	10:53	13	2	1 4 1 5	4	SS2 run 4x as a general purpose scan to compare over time
12-Jan-24	11:27					Shut down
14-Jan-24	17:28					Turn on & software patch, data downlink tests
14-Jan-24	17:59	14	2	1 4 1 5	4	SS2 run 4x as a general purpose scan to compare over time
14-Jan-24	18:28					Deploy dust cover
14-Jan-24	18:32	15				(Failed) SS2 run 4x as a general purpose scan to compare over time
14-Jan-24	19:00	16	2	1 4 1 5	4	SS2 run 4x as a general purpose scan to compare over time
14-Jan-24	19:19	17	11	4 5 11 13	4	SS11 run 4x to focus on characterize the lander environment over a wide m/z range
14-Jan-24	19:49					Science data downlink
14-Jan-24	20:44					Shut down
15-Jan-24	12:28					Turn on & software patch
15-Jan-24	12:41	18				(Failed) SS2 run 4x as a general purpose scan to compare over time
15-Jan-24	13:12	18	2	1 4 1 5	2	SS2 run 2x as a general purpose scan to compare over time
15-Jan-24	13:21	18	13	4 3 8 13	1	SS13 run 1x to get SFs with longer settle time and higher mass resolution
15-Jan-24	13:28					Shut down

[1] Each PITMS spectrum consists of six data packets; at least one and up to five data packets from each spectrum were lost during the downlink process for these experiments.

Table 4. List of PITMS spectra. Spectra from ITL 11 are not included in the raw data delivery as those packets were not downlinked. Spectra in ITL 12 have missing packets; the value for missing raw data is 65535.

Spectrum	ITL	SF	Start mass (amu)	End mass (amu)	Notes
2024-01-12T10:33:23Z	12	1	13.98	82.31	Incomplete raw data. Raw counts may exceed 11,000 counts. High-mass baseline is 8 counts below zero.
2024-01-12T10:34:00Z	12	4	51.37	134.97	Incomplete raw data. No thermal drift correction available. Noise in high-mass region is not randomly distributed.
2024-01-12T10:34:36Z	12	1	14.25	125.35	Raw counts may exceed 11,000 counts.
2024-01-12T10:35:13Z	12	5	11.62	107.55	Incomplete raw data. Raw counts may exceed 11,000 counts. Noise in high-mass region is not randomly distributed.
2024-01-12T11:12:29Z	13	1	13.84	125.87	Raw counts may exceed 11,000 counts.
2024-01-12T11:13:07Z	13	4	14.07	137.00	Raw counts may exceed 11,000 counts.
2024-01-12T11:13:43Z	13	1	13.97	125.12	Raw counts may exceed 11,000 counts.
2024-01-12T11:14:20Z	13	5	11.50	133.81	Raw counts may exceed 11,000 counts. High mass baseline is 8 counts above zero.
2024-01-12T11:14:56Z	13	1	14.15	123.56	Raw counts may exceed 11,000 counts.
2024-01-12T11:15:33Z	13	4	14.36	134.48	Raw counts may exceed 11,000 counts. High mass baseline is not symmetric around 0
2024-01-12T11:16:10Z	13	1	14.15	123.56	Raw counts may exceed 11,000 counts.
2024-01-12T11:16:47Z	13	5	11.77	131.31	Raw counts may exceed 11,000 counts.
2024-01-12T11:17:23Z	13	1	14.31	122.06	Raw counts may exceed 11,000 counts.
2024-01-12T11:18:00Z	13	4	14.53	132.84	Raw counts may exceed 11,000 counts.
2024-01-12T11:18:37Z	13	1	14.35	121.29	Raw counts may exceed 11,000 counts.
2024-01-12T11:19:15Z	13	5	11.82	130.46	Raw counts may exceed 11,000 counts.
2024-01-12T11:19:50Z	13	1	14.35	121.29	Raw counts may exceed 11,000 counts.
2024-01-12T11:20:27Z	13	4	14.56	131.98	Raw counts may exceed 11,000 counts.
2024-01-12T11:21:03Z	13	1	14.51	119.86	Raw counts may exceed 11,000 counts.
2024-01-12T11:21:40Z	13	5	12.08	128.11	Raw counts may exceed 11,000 counts.
2024-01-14T18:11:37Z	14	1	14.06	125.20	
2024-01-14T18:12:15Z	14	4	14.38	136.34	
2024-01-14T18:12:51Z	14	1	14.16	125.28	

Spectrum	ITL	SF	Start mass (amu)	End mass (amu)	Notes
2024-01-14T18:13:30Z	14	5	11.73	133.10	
2024-01-14T18:14:07Z	14	1	14.32	123.73	
2024-01-14T18:14:44Z	14	4	14.54	134.65	
2024-01-14T18:15:21Z	14	1	14.49	122.23	
2024-01-14T18:15:58Z	14	5	11.94	131.47	
2024-01-14T18:16:35Z	14	1	14.65	120.77	
2024-01-14T18:17:14Z	14	4	14.73	132.16	
2024-01-14T18:17:50Z	14	1	14.68	120.01	High mass baseline is not randomly distributed
2024-01-14T18:18:28Z	14	5	12.33	128.36	
2024-01-14T18:19:04Z	14	1	14.71	119.27	
2024-01-14T18:19:42Z	14	4	14.91	129.87	High mass baseline is not randomly distributed
2024-01-14T18:20:18Z	14	1	14.75	118.54	
2024-01-14T18:20:57Z	14	5	12.43	126.77	
2024-01-14T19:06:00Z	16	1	13.27	122.16	High mass baseline is not randomly distributed
2024-01-14T19:06:37Z	16	4	13.50	134.79	
2024-01-14T19:07:15Z	16	1	13.57	121.67	
2024-01-14T19:07:52Z	16	5	11.10	131.02	
2024-01-14T19:08:28Z	16	1	13.53	122.39	
2024-01-14T19:09:05Z	16	4	13.95	132.71	
2024-01-14T19:09:42Z	16	1	13.77	121.11	
2024-01-14T19:10:20Z	16	5	11.37	129.64	High mass baseline is not randomly distributed
2024-01-14T19:10:56Z	16	1	13.89	120.48	
2024-01-14T19:11:34Z	16	4	14.07	132.01	
2024-01-14T19:12:10Z	16	1	14.01	119.87	
2024-01-14T19:12:47Z	16	5	11.64	128.29	
2024-01-14T19:13:24Z	16	1	14.12	119.25	

Spectrum	ITL	SF	Start mass (amu)	End mass (amu)	Notes
2024-01-14T19:14:02Z	16	4	14.29	130.63	
2024-01-14T19:14:38Z	16	1	14.12	119.25	
2024-01-14T19:15:16Z	16	5	11.77	127.63	
2024-01-14T19:27:40Z	17	4	13.44	133.91	
2024-01-14T19:28:17Z	17	5	10.78	131.58	
2024-01-14T19:28:55Z	17	11	31.06	151.53	
2024-01-14T19:29:33Z	17	13	35.47	154.76	
2024-01-14T19:30:11Z	17	4	13.86	132.63	
2024-01-14T19:30:49Z	17	5	11.15	130.24	
2024-01-14T19:31:27Z	17	11	31.15	151.69	
2024-01-14T19:32:05Z	17	13	35.47	152.99	
2024-01-14T19:32:42Z	17	4	14.07	132.00	
2024-01-14T19:33:20Z	17	5	11.37	129.64	
2024-01-14T19:33:59Z	17	11	31.10	147.40	
2024-01-14T19:34:36Z	17	13	35.52	152.45	
2024-01-14T19:35:13Z	17	4	14.21	130.55	
2024-01-14T19:35:51Z	17	5	11.55	128.21	
2024-01-14T19:36:29Z	17	11	31.07	144.57	
2024-01-14T19:37:08Z	17	13	35.26	148.80	
2024-01-15T13:16:17Z	18	1	12.82	121.77	High mass baseline is not randomly distributed
2024-01-15T13:16:54Z	18	4	13.09	133.59	
2024-01-15T13:17:30Z	18	1	13.00	121.93	
2024-01-15T13:18:08Z	18	5	10.51	131.34	
2024-01-15T13:18:44Z	18	1	13.21	121.35	
2024-01-15T13:19:23Z	18	4	13.51	132.33	
2024-01-15T13:19:59Z	18	1	13.30	121.44	

Spectrum	ITL	SF	Start mass (amu)	End mass (amu)	Notes
2024-01-15T13:20:36Z	18	5	10.89	130.02	
2024-01-15T13:23:37Z	18	4	13.46	131.47	High mass baseline is not randomly distributed
2024-01-15T13:24:15Z	18	3	13.34	120.72	
2024-01-15T13:24:41Z	18	8	12.71	68.18	
2024-01-15T13:25:19Z	18	13	35.15	153.28	High mass baseline is not randomly distributed

4. Archive Organization

This section describes the organization of the PITMS archive according to the PDS4 Information Model.

4.1 The PITMS Bundle

The complete PITMS archive is organized into one bundle. The bundle's PDS Logical Identifier (LID) is "urn:nasa:pds:clps_to_2ab_pitms."

4.2 PITMS Collections

The PITMS bundle includes the collections of data products and documents shown in Table 5.

Table 5. Collections in the PITMS Bundle.

Collection Logical Identifier	**Collection Type**	**Contents**
urn:nasa:pds:clps_to_2ab_pitms:document	Document	Documentation, including this User's Guide
urn:nasa:pds:clps_to_2ab_pitms:data_raw	Data	5 .csv files; 5.xml labels
urn:nasa:pds:clps_to_2ab_pitms:data_calibrated	Data	1 .csv data file and 1 .xml label for calibration variables; 1 .csv data file and 1 .xml label file for each spectrum (80)
urn:nasa:pds:clps_to_2ab_pitms:data_derived	Data	1 .csv data file, 1 image file (.jpg), and 2 .xml label files for each SF4 spectrum

4.3 PITMS Data Organization

This PITMS data directory and subdirectory structure is given below. Within the archive root directory are subdirectories for each type of data record produced from the PITMS instrument. The PITMS data are stored in subdirectories labeled by processing level. Text in *italics* denotes unique data record numbers.

```
/clps_to_ab_pitms
     /document
          PITMS_DATA_PLAN.pdf
          PITMS_DATA_PLAN.xml
     /data_raw
          PITMS_RAW_AUX.csv
```

```
          PITMS_RAW_AUX.xml
          PITMS_RAW_CAT.csv
          PITMS_RAW_CAT.xml
          PITMS_RAW_HK.csv
          PITMS_RAW_HK.xml
          PITMS_RAW_SCI.csv
          PITMS_RAW_SCI.xml
          PITMS_RAW_DECKD.csv
          PITMS_RAW_DECKD.xml
     /data_calibrated
          PITMS_CAL_VAR.csv
          PITMS_CAL_VAR.xml
          PITMS_CAL_2024-01-14T18-19-04Z.csv
          PITMS_CAL_2024-01-14T18-19-04Z.xml
     /data_derived
          PITMS_DER_2024-01-14T18-19-04Z.csv
          PITMS_DER_2024-01-14T18-19-04Z.xml
          PITMS_DER_img_2024-01-14T18-19-04Z.jpg
          PITMS_DER_img_2024-01-14T18-19-04Z.xml
```

4.4 PITMS Product Identification and Naming

A PITMS product consists of one digital object in one file, accompanied by a PDS label file. The PDS label provides identification and other metadata for the data file. In addition to data products, the archive includes document products, which also have PDS labels. Finally, the collections and the bundle are considered products in PDS, and therefore have their own labels.

4.5 Data Products

PITMS data products in this bundle consist of raw, calibrated, and derived products. Table 6 shows a summary of the data product types.

Table 6. PITMS Product Types.

Product Name	PDS Processing Level	PDS4 bundle:collection	Product Description	PDS4 Data Type
PITMS_Data_Plan.pdf	Document	pitms:document	PITMS Data Plan, PDS Descriptions, and Users' Guide	PDF
PITMS_RAW_HK.csv	Raw	pitms:data_raw	Housekeeping data	Table_Delimited
PITMS_RAW_AUX.csv	Raw	pitms:data_raw	Auxiliary data	Table_Delimited
PITMS_RAW_SCI.csv	Raw	pitms:data_raw	Science data	Table_Delimited
PITMS_RAW_CAT.csv	Raw	pitms:data_raw	Concatenated file containing each full spectrum from the SCI file plus	Table_Delimited

			HK and AUX data relevant to each spectrum	
PITMS_RAW_DECKD	Raw	pitms:data_raw	Peregrine Deck D temperature	Table_Delimited
PITMS_CAL_VAR.csv	Calibrated	pitms:data_calibrated	Variables in the PITMS data calibration process for each spectrum	Table_Delimited
PITMS_CAL_timestamp.csv	Calibrated	pitms:data_calibrated	Calibrated mass spectra in instrument- independent units (mass to charge ratio vs ions or partial pressure)	Table_Delimited
PITMS_DER_ timestamp.csv	Derived	pitms:data_derived	Interpreted data as species and number density	Table_Delimited
PITMS_DER_img_ timestamp.csv	Derived	pitms:data_derived	Image showing spectral peak deconvolution	Image

5. Raw Data Products

PITMS raw data products are human-readable .csv files.

The PITMS instrument was thermally isolated from the lander; however, Astrobotic shared data from the thermocouple mounted on the lander Deck D, closest to PITMS. Temperature data was received by PITMS via Astrobotic's mission control interface and archived as PITMS_RAW_DECKD in the format in which it was received for the duration of the mission.

PITMS returned data as individual packets. The PITMS ground software ingested the packets and wrote four human-readable raw data files in .csv format: the HK file contains Housekeeping data, the AUX file contains auxiliary data (there is one AUX packet per science spectrum), and the SCI file contains science data (note that each spectrum is composed of six individual packets). Each file contains all the packets of that type for the entire mission duration while PITMS was turned on.

For ease of interpretation, the PITMS ground software also produced a concatenated (CAT) file to show each full science spectrum in a single row, concatenating 6 SCI packets with selected parameters from the HK and AUX files that are useful in interpreting the science spectrum. The timestamp for the CAT spectrum is the closest HK timestamp to the initiation of the spectrum acquisition.

When telemetry packets were not received on the ground, the software filled in a value of 65535 for raw counts. When the instrument did not store data values onboard but sent a full telemetry packet, it set all raw count values to zero (0). Spectra from ITL 11 are not included in the raw data delivery as none of the data packets were downlinked. Spectra in ITL 12 have both missing telemetry packets and packets with raw count values of zero.

The variables in each file are defined in the XML label for each file and in the following tables.

Table 7. Variable definitions for PITMS_RAW_HK.csv file.

Col	Variable Name	Format	Units	Range	Description
1	TIME	ASCII_Date_Time_YMD			Spacecraft clock at the time of the record
2	PITMS_PACKET_ID	ASCII_NonNegative_Integer			PITMS packet CCSDS APID
3	PACKET_COUNT	ASCII_NonNegative_Integer			The count of this packet type
4	PACKET_LENGTH	ASCII_NonNegative_Integer			The number of data bytes contained in the packet
5	TIME_IN_SECONDS	ASCII_NonNegative_Integer	s		Time that the packet was created (seconds)
6	FRACTIONS_OF_SECONDS	ASCII_NonNegative_Integer	s		Fractional Time that the packet was created (seconds_over_65535)
7	HOUSEKEEPING_PACKET_COUNT	ASCII_NonNegative_Integer			Count of Housekeeping packets
8	SOFTWARE_VERSION	ASCII_NonNegative_Integer			Software version
9	SOFTWARE_MINOR_VERSION	ASCII_NonNegative_Integer			Software minor version
10	VALID_TC_COUNTER	ASCII_NonNegative_Integer			Valid Telecommand counter
11	REJECTED_TC_COUNTER	ASCII_NonNegative_Integer			Rejected telecommand counter
12	FLASH_WRITE_ENABLE_FLAG	ASCII_String		DISABLED, ENABLED	Flash memory write enabled
13	FLASH_READ_ENABLE_FLAG	ASCII_String		DISABLED, ENABLED	Flash memory read enabled
14	MEMORY_DUMP_IN_PROGRESS_FLAG	ASCII_String		--, RUNNING	Memory dump in progress flag
15	PREPARING_MEMORY_PATCH_ FLAG	ASCII_String		--, STARTING	Preparing memory patch flag
16	CORRECT_NUMBER_PATCH_BYTES	ASCII_String		TRUE, FALSE	Correct number patch bytes received
17	PATCH_OUT_OF_SEQUENCE	ASCII_String		TRUE, FALSE	Patch data packet out of sequence
18	PATCH_TOO_LARGE	ASCII_String		TRUE, FALSE	Patch data too large
19	UART_STATUS	ASCII_String		FALSE, OK	RS422 communication Uart status
20	TIME_SIGNAL_FAILED	ASCII_String		TRUE, FALSE	Time signal failed
21	INITIALISATION_OK	ASCII_String		TRUE, FALSE	Initialisation ok
22	INVALID_PATCH_ADDRESS	ASCII_String		TRUE, FALSE	Invalid patch address
23	HV_SHUTDOWN_IN_PROGRESS	ASCII_String		TRUE, FALSE	HV shutdown in progress
24	HV_ON	ASCII_String		TRUE, FALSE	HV on
25	ACQUISITION_HAZARD_ENABLE	ASCII_String		TRUE, FALSE	Acquisition hazard enable
26	FDIR_HAZARD_ENABLE	ASCII_String		TRUE, FALSE	FDIR hazard enable
27	SOFTWARE_FLAGS_3	ASCII_NonNegative_Integer			Software flags 3
28	SOFTWARE_FLAGS_4	ASCII_NonNegative_Integer			Software flags 4
29	RECEIVED_CRC_OF_TC	ASCII_Numeric_Base16			CRC received with telecommand
30	CALCULATED_CRC_OF_TC	ASCII_Numeric_Base16			CRC calculated from received telecommand
31	STATE	ASCII_String		BOOT, SAFE, INITIALISE, STANDBY, ACQUISITION	Instrument Operational State
32	SEQUENCE	ASCII_NonNegative_Integer		0-16	Science Sequence running

33	SCIENCE_STATE_MACHINE_STATE	ASCII_String		START, DELAY_MS, DDS_FREQ_TEST_1_ST, DDS_FREQ_TEST_2, DDS_FREQ_TEST, DDS_FREQ_TST_LOOP_ST, DDS_FREQ_TESTLOOP, DDS_FREQ_TEST_END, CALC_V_PER_AMU, DDS_AMP_TEST_ST, DDS_AMP_TEST, DDS_AMP_TST_LOOP_ST, DDS_AMP_TEST_LOOP, DDS_AMP_TEST_END, RF_AMP_CAL_START, RF_AMP_SEEK_V_START1 , RF_AMP_SEEK_VOLTS_END1 , RF_AMP_SEEK_V_START2, RF_AMP_SEEK_V_END2, RF_AMP_SEEK_V_PRELOOP , RF_AMP_SEEK_V_RAMPUP, RF_AMP_SEEK_V_RAMPDOWN, RF_AMP_CALIBRATE, SCAN_SETUP, SCAN_LOOP, SCAN_WAIT_COMPLETE, SCAN_READ_RESULTS, FINISHED_SCAN, IDLE, BLOCKING_TEST_RUN, RAMP_HV_LOOP_ST, RAMP_HV_LOOP, RAMP_HV_LOOP_END, RAMP_HV_LOOP_TO_0, RAMP_HV_TO_0_LOOP_END, SHUTDOWN_HV_START, SETUP_HV_START, TWEAK_HV_START, RAMP_DET_BIAS, RAMP_FIL1DRIVE, RAMP_FIL2DRIVE, RAMP_FILBIAS, RAMP_150V, SHUTDOWN_HV_END, STARTUP_HV_END, TWEAK_HV_END, TWEAK_HV_LOOP, FINISHED_READ_RESULTS, FINISHED_SETUP	Science state machine state

Col	Variable Name	Format	Units	Range	Description
34	NUMBER_OF_HK_QUEUE_PACKETS	ASCII_NonNegative_Integer			Number of HK queue packets
35	NUMBER_OF_DROPPED_TM_PACKETS	ASCII_NonNegative_Integer			Number of dropped telemetry packets
36	LAST_RXD_S/C_TIME_S	ASCII_NonNegative_Integer	s		Last received spacecraft time (secs)
37	LAST_RXD_S/C_TIME_MS	ASCII_NonNegative_Integer	ms		Last received spacecraft time (msecs)
38	PITMS_TIME_AT_RXD_S/C_TIME_S	ASCII_NonNegative_Integer	s		PITMS internal clock time at last received spacecraft time (secs)
39	PITMS_TIME_AT_RXD_S/C_TIME_MS	ASCII_NonNegative_Integer	ms		PITMS time at Last received spacecraft time (msecs)
40	WORST_BACKGROUND_TIME	ASCII_NonNegative_Integer			Shortest time spent in background this HK period
41	RETURN_STACK_POINTER	ASCII_NonNegative_Integer			Return stack pointer
42	FLASH_WRITE_FAILURES	ASCII_NonNegative_Integer			Flash write failures
43	LAST_TC_TYPE	ASCII_String		PITMS_SENDHK, PITMS_DUMMY, PITMS_GOTO, PITMS_SAFE, PITMS_ACQUISITION, PITMS_STANDBY, PITMS_HAZARDEN, PITMS_PATCH, PITMS_DUMP, PITMS_COPYMEM, PITMS_MEMCRC, PITMS_FLASHDATA, PITMS_FLASHWREN, PITMS_CHECKASW, PITMS_LOADASW, PITMS_TRANSMITTM, PITMS_HKRATE, PITMS_ITMSHTR, PITMS_ADSORBERHTR, PITMS_SETITL, PITMS_SETADDRESS, PITMS_FDIRPARAM	Last telecommand command name
44	LAST_TC_QUALIFIER	ASCII_Numeric_Base16			Last telecommand qualifier
45	LAST_TC_ADDRESS/FUNCTION	ASCII_Numeric_Base16			Last telecommand address
46	LAST_TC_FIRST_DATA_WORD	ASCII_Numeric_Base16			Last telecommand first data word

Col	Variable Name	Format	Units	Range	Description
47	LAST_BUT_1_TC_TYPE	ASCII_String		PITMS_SENDHK, PITMS_DUMMY, PITMS_GOTO, PITMS_SAFE, PITMS_ACQUISITION, PITMS_STANDBY, PITMS_HAZARDEN, PITMS_PATCH, PITMS_DUMP, PITMS_COPYMEM, PITMS_MEMCRC, PITMS_FLASHDATA, PITMS_FLASHWREN, PITMS_CHECKASW, PITMS_LOADASW, PITMS_TRANSMITTM, PITMS_HKRATE, PITMS_ITMSHTR, PITMS_ADSORBERHTR, PITMS_SETITL, PITMS_SETADDRESS, PITMS_FDIRPARAM	Last but 1 telecommand command name
48	LAST_BUT_1_TC_TRIGGER_TIME	ASCII_NonNegative_Integer			Last but 1 TC trigger time value
49	LAST_BUT_1_TC_QUALIFIER	ASCII_Numeric_Base16			Last but 1 TC qualifier
50	LAST_BUT_1_TC_ADDRESS/FUNCTION	ASCII_Numeric_Base16			Last but 1 TC address
51	LAST_BUT_1_TC_FIRST_DATA_ WORD	ASCII_Numeric_Base16			Last but 1 TC first data word
52	SECONDS_SINCE_LAST_CALIBRATION	ASCII_NonNegative_Integer	s		Seconds since last calibration
53	ASW_IMAGE_NUMBER	ASCII_NonNegative_Integer			ASW image number
54	SOFTWARE_PATCH_ID	ASCII_NonNegative_Integer			Software patch ID
55	DATA_IN_HK_ADDRESS_POINTER	ASCII_Numeric_Base16			Data in HK address pointer
56	INSTRUMENT_TIMELINE_ID	ASCII_NonNegative_Integer			Instrument timeline identifier
57	HIGHEST_FLASH_ROM_ADDRESS_USED	ASCII_NonNegative_Integer			Highest NAND flash memory address used
58	NAND_FLASH_STATUS	ASCII_String		ENABLED, DISABLED_BY_PATCH, DISABLED_BY_INIT, DISABLED_ERASE_BLOCK1, DISABLED_ERASE_BLOCK_2, DISABLED_BY_CCSDS_PACKET, DISABLED_BY_NEXT_GOOD_BLOCK, DISABLED_BY_DEFINE	NAND flash status
59	READING_PACKETS_FROM_NAND_FLASH	ASCII_NonNegative_Integer			Reading packets from NAND flash
60	SCIENCE_PACKET_TX_COUNTER	ASCII_NonNegative_Integer			Count of Science packets transmitted

Col	Variable Name	Format	Units	Range	Description
61	AUXILLIARY_PACKET_TX_COUNTER	ASCII_NonNegative_Integer			Count of Auxiliary packets transmitted
62	HK_INTERVAL	ASCII_NonNegative_Integer			Time between housekeeping packets
63	TM_TYPES_TO_SEND	ASCII_NonNegative_Integer			Telemetry packet types to send
64	UART_DATA_RATE	ASCII_NonNegative_Integer			UART data rate
65	ASW_LOADED_IN_RAM	ASCII_NonNegative_Integer			ASW loaded in RAM
66	ION_TRAP_RF_AMPLITUDE	ASCII_Real	V	0-1000	Ion trap rf amplitude
67	ADC_1.5V_RAIL	ASCII_Real	V	1.2-1.8	ADC 1.5v rail
68	ADC_2.5V_RAIL	ASCII_Real	V	2.1-2.9	ADC 2.5v rail
69	ADC_5V_RAIL	ASCII_Real	V	4.6-5.6	ADC 5v rail
70	ADC_12V_RAIL	ASCII_Real	V	11-13	ADC 12v rail
71	ADC_-12V_RAIL	ASCII_Real	V	-11 - -13	ADC -12v rail
72	ADC_150V_RAIL	ASCII_Real	V	0-170	ADC 150v rail
73	ADC_-150V_RAIL	ASCII_Real	V	0 - -170	ADC -150v rail
74	ION_TRAP_DETECTOR_BIAS	ASCII_Real	V	0-4000	Ion trap detector bias
75	ION_TRAP_ELECTRON_FILAMENT_BIAS	ASCII_Real	V	0-120	Ion trap electron filament bias
76	ION_TRAP_ELECTRON_FILAMENT_1_DRIVE	ASCII_Real	A	0-3	Ion trap electron filament 1 drive
77	ION_TRAP_ELECTRON_FILAMENT_2_DRIVE	ASCII_Real	A	0-3	Ion trap electron filament 2 drive
78	ION_TRAP_APPROX_EMISSION_CURRENT	ASCII_Real	uA	0-150	Ion trap approximate emission current
79	ADSORBER_TEMPERATURE	ASCII_Real	DEGC	-53-700	Adsorber temperature
80	ITMS_TEMPERATURE	ASCII_Real	DEGC	-53-700	ITMS temperature
81	TRP_TEMPERATURE	ASCII_Real	DEGC	-53-63	TRP temperature
82	PROCESSOR_TEMPERATURE	ASCII_Real	DEGC	-45 - 115	Processor temperature
83	0V_REFERENCE	ASCII_Real	V	0-0.2	0V reference
84	ION_TRAP_EMISSION_CURRENT	ASCII_Real	uA		Ion trap emission current
85	LAST_PATCH_CRC	ASCII_NonNegative_Integer			CRC sent as part of the Last patch
86	CALCULATED_LAST_PATCH_CRC	ASCII_NonNegative_Integer			Calculated CRC of the last patch
87	LAST_MEMORY_CRC	ASCII_NonNegative_Integer			CRC generated by last checkmem command
88	LAST_ASW_CRC	ASCII_NonNegative_Integer			CRC generated by last checkasw command
89	LAST_TIME_SIGNAL_CRC	ASCII_NonNegative_Integer			CRC from last time message received
90	CORRUPT_FLASH_BLOCK_COUNTER	ASCII_NonNegative_Integer			Corrupt flash block counter
91	MISSING_PATCH_PACKET_INDEX	ASCII_NonNegative_Integer			Index number of Missing patch packet
92	FILAMENT_IN_USE	ASCII_NonNegative_Integer			ITMS Filament in use
93	ADSORBER_TEMPERATURE_SETPOINT	ASCII_Real			Adsorber temperature setpoint
94	ITMS_TEMPERATURE_SETPOINT	ASCII_Real			ITMS temperature setpoint

Col	Variable Name	Format	Units	Range	Description
95	FILAMENT_BIAS_SETPOINT	ASCII_Integer			Filament bias setpoint
96	DETECTOR_BIAS_SETPOINT	ASCII_Integer			Detector bias setpoint
97	ITMS_HEATER_PWM_VALUE	ASCII_Real			ITMS heater PWM value
98	ADSORBER_PWM_VALUE	ASCII_Real			Adsorber PWM value
99	150V_PWM_VALUE	ASCII_Integer			150V PWM value
100	FILAMENT_BIAS_PWM_VALUE	ASCII_Integer			Filament bias PWM value
101	FILAMENT_DRIVE_1_PWM_VALUE	ASCII_Integer			Filament drive 1 PWM value
102	FILAMENT_DRIVE_2_PWM_VALUE	ASCII_Integer			Filament drive 2 PWM value
103	DETECTOR_BIAS_PWM	ASCII_Integer			Detector bias PWM
104	PWM_VALUE_OUT_OF_RANGE	ASCII_String		TRUE, FALSE	PWM value out of range
105	ITMS_HEATER_STATUS	ASCII_String		OFF, ON	ITMS heater status
106	ADSORBER_HEATER_STATUS	ASCII_String		OFF, ON	Adsorber heater status
107	PROCESSOR_TEMPERATURE_FDIR_WARNING	ASCII_String		TRUE, FALSE	Processor temperature FDIR warning
108	ZERO_FDIR_WARNING	ASCII_String		TRUE, FALSE	Zero FDIR warning
109	DETECTOR_BIAS_FDIR_WARNING	ASCII_String		TRUE, FALSE	Detector bias FDIR warning
110	FILAMENT_BIAS_FDIR_WARNING	ASCII_String		TRUE, FALSE	Filament bias FDIR warning
111	FILAMENT_DRIVE_1_FDIR_WARNING	ASCII_String		TRUE, FALSE	Filament drive 1 FDIR warning
112	FILAMENT_DRIVE_2_FDIR_WARNING	ASCII_String		TRUE, FALSE	Filament drive 2 FDIR warning
113	EMISSION_CURRENT_FDIR_WARNING	ASCII_String		TRUE, FALSE	Emission current FDIR warning
114	ADSORBER_PRT_FDIR_WARNING	ASCII_String		TRUE, FALSE	Adsorber PRT FDIR warning
115	ITMS_PRT_FDIR_WARNING	ASCII_String		TRUE, FALSE	ITMS PRT FDIR warning
116	TRP_PRT_FDIR_WARNING	ASCII_String		TRUE, FALSE	TRP PRT FDIR warning
117	RF_FDIR_WARNING	ASCII_String		TRUE, FALSE	RF FDIR warning
118	1.5V_FDIR_WARNING	ASCII_String		TRUE, FALSE	1.5V FDIR warning
119	2.5V_FDIR_WARNING	ASCII_String		TRUE, FALSE	2.5V FDIR warning
120	5V_FDIR_WARNING	ASCII_String		TRUE, FALSE	5V FDIR warning
121	12V_FDIR_WARNING	ASCII_String		TRUE, FALSE	12V FDIR warning
122	-12V_FDIR_WARNING	ASCII_String		TRUE, FALSE	-12V FDIR warning
123	150V_FDIR_WARNING	ASCII_String		TRUE, FALSE	150V FDIR warning
124	-150V_FDIR_WARNING	ASCII_String		TRUE, FALSE	150V FDIR warning
125	PROCESSOR_TEMPERATURE_FDIR_ALARM	ASCII_String		TRUE, FALSE	Processor temperature FDIR alarm
126	ZERO_FDIR_ALARM	ASCII_String		TRUE, FALSE	Zero FDIR alarm
127	DETECTOR_BIAS_FDIR_ALARM	ASCII_String		TRUE, FALSE	Detector bias FDIR alarm
128	FILAMENT_BIAS_FDIR_ALARM	ASCII_String		TRUE, FALSE	Filament bias FDIR alarm

Col	Variable Name	Format	Units	Range	Description
129	FILAMENT_DRIVE_1_FDIR_ALARM	ASCII_String		TRUE, FALSE	Filament drive 1 FDIR alarm
130	FILAMENT_DRIVE_2_FDIR_ALARM	ASCII_String		TRUE, FALSE	Filament drive 2 FDIR alarm
131	EMISSION_CURRENT_FDIR_ALARM	ASCII_String		TRUE, FALSE	Emission current FDIR alarm
132	ADSORBER_PRT_FDIR_ALARM	ASCII_String		TRUE, FALSE	Adsorber PRT FDIR alarm
133	ITMS_PRT_FDIR_ALARM	ASCII_String		TRUE, FALSE	ITMS PRT FDIR alarm
134	TRP_PRT_FDIR_ALARM	ASCII_String		TRUE, FALSE	TRP PRT FDIR alarm
135	RF_FDIR_ALARM	ASCII_String		TRUE, FALSE	RF FDIR alarm
136	1.5V_FDIR_ALARM	ASCII_String		TRUE, FALSE	1.5V FDIR alarm
137	2.5V_FDIR_ALARM	ASCII_String		TRUE, FALSE	2.5V FDIR alarm
138	5V_FDIR_ALARM	ASCII_String		TRUE, FALSE	5V FDIR alarm
139	12V_FDIR_ALARM	ASCII_String		TRUE, FALSE	12V FDIR alarm
140	-12V_FDIR_ALARM	ASCII_String		TRUE, FALSE	-12V FDIR alarm
141	150V_FDIR_ALARM	ASCII_String		TRUE, FALSE	150V FDIR alarm
142	-150V_FDIR_ALARM	ASCII_String		TRUE, FALSE	-150VFDIR alarm

Table 8. Variable definitions for PITMS_RAW_AUX.csv file.

Col	Variable Name	Format	Units	Range	Description
1	TIME	ASCII_Date_Time_YMD			Spacecraft clock at the time of the record
2	PITMS_PACKET_ID	ASCII_Integer		0-2	PITMS packet ID calibrated value
3	PACKET_COUNT	ASCII_Integer			Packet count of this packet
4	PACKET_LENGTH	ASCII_Integer			The length of this packet
5	TIME_IN_SECONDS	ASCII_Integer	s		Time in seconds of the packet
6	FRACTIONS_OF_SECONDS	ASCII_Integer	ms		Fractions of seconds of the time in the packet
7	OPERATING_FREQUENCY	ASCII_Integer	Hz		Operating frequency
8	VOLTS_PER_AMU	ASCII_Real	V/AMU		Volts per amu
9	DAC_SCALING_GRADIENT	ASCII_Real	DN/V		DAC scaling gradient
10	DAC_SCALING_INTERCEPT	ASCII_Real	DN		DAC scaling intercept
11	START_SCALING	ASCII_Real	DN		Start scaling
12	FINAL_SCALING	ASCII_Real	DN		Final scaling
13	CALCULATED_DAC_SCALING_ GRADIENT	ASCII_Real	DN/V		Calculated DAC scaling gradient
14	CALCULATED_DAC_SCALING_INTERCEPT	ASCII_Real	DN		Calculated DAC scaling intercept
15	CALCULATED_OPERATING_FREQUENCY	ASCII_Integer	Hz		Calculated operating frequency
16	CALCULATED_VOLTS_PER_AMU	ASCII_Real	V/AMU		Calculated volts per amu
17	CALIBRATION_APPLIED	ASCII_Integer		00, 01, 02, 03	Onboard voltage ramp calibration applied (Qualifier 00: Calibrate before scan and apply the results immediately of the calibration; Qualifier 01: Calibrate before scan but do not apply the results of the calibration. ; Qualifier 02: Do not calibrate before scan and do not apply the results of the last calibration; Qualifier 03: Do not calibrate before scan but do apply the results of the last calibration.)
18	SCIENCE_SEQUENCE_NUMBER	ASCII_Integer		0-16	Science sequence number
19	SCAN_FUNCTION_NUMBER	ASCII_Integer		0-16	Scan function number

Table 9. Variable definitions for PITMS_RAW_SCI.csv file.

Col	Variable Name	Format	Units	Range	Description
1	TIME	ASCII_Date_Time_YMD_UTC			UTC converted date time of the time in the packet (SCET)
2	PITMS_PACKET_ID	ASCII_Integer			Packet ID at the beginning of the spectrum
3	PACKET_COUNT	ASCII_Integer			PITMS packet ID of this packet
4	PACKET_LENGTH	ASCII_Integer			Packet length
5	TIME_IN_SECONDS	ASCII_Integer	s		Time in seconds of the packet
6	FRACTIONS_OF_SECONDS	ASCII_Integer	ms		Fractions of seconds of the time of this packet
7	BINS_PRESENT	ASCII_String			The number of bins present
8	SCAN_FUNCTION_NUMBER	ASCII_Integer			The scan function number
9	HISTOGRAM_DATA	ASCII_Integer			Histogram data of counts in each bin

Table 10. Variable definitions for PITMS_RAW_CAT.csv file. Variables 1-27 are repeated from the AUX and HK files (Tables 7-9) but pulled together for convenience in interpretation (source file appears in the description in parentheses). The spectral data consist of six concatenated packets containing raw counts from the SCI file and appear in Variable 28 where the column number corresponds to the bin number (1-2047).

Col	Variable Name	Format	Units	Range	Description
1	TIME	ASCII_Date_Time_YMD_UTC			UTC converted date time of the time in the packet (SCET) (AUX)
2	OPERATING_FREQUENCY	ASCII_Integer	Hz		Operating frequency (AUX)
3	VOLTS_PER_AMU	ASCII_Real	V/AMU		Volts per amu (AUX)
4	DAC_SCALING_GRADIENT	ASCII_Real	DN/V		DAC scaling gradient (AUX)
5	DAC_SCALING_INTERCEPT	ASCII_Real	DN		DAC scaling intercept (AUX)
6	START_SCALING	ASCII_Real	DN		Start scaling (AUX)
7	FINAL_SCALING	ASCII_Real	DN		Final scaling (AUX)
8	CALCULATED_DAC_SCALING_GRADIENT	ASCII_Real	DN/V		Calculated DAC scaling gradient (AUX)
9	CALCULATED_DAC_SCALING_INTERCEPT	ASCII_Real	DN		Calculated DAC scaling intercept (AUX)
10	CALCULATED_OPERATING_FREQUENCY	ASCII_Integer	Hz		Calculated operating frequency (AUX)
11	CALCULATED_VOLTS_PER_AMU	ASCII_Real	V/AMU		Calculated volts per amu (AUX)
12	CALIBRATION_APPLIED	ASCII_Integer			Calibration applied (AUX)
13	SCIENCE_SEQUENCE_NUMBER	ASCII_Integer			Science sequence number (AUX)
14	SCAN_FUNCTION_NUMBER	ASCII_Integer			Scan function number (AUX)
15	REJECTED_TC_COUNTER	ASCII_NonNegative_Integer			Rejected telecommand counter (HK)
16	INSTRUMENT_TIMELINE_ID	ASCII_NonNegative_Integer			Instrument timeline identifier (HK)
17	ION_TRAP_DETECTOR_BIAS	ASCII_Real	V	0-4000	Ion trap detector bias (HK)
28	ADSORBER_TEMPERATURE	ASCII_Real	DEGC	-53-700	Adsorber temperature (HK)
19	ITMS_TEMPERATURE	ASCII_Real	DEGC	-53-700	ITMS temperature (HK)
20	TRP_TEMPERATURE	ASCII_Real	DEGC	-53- 63	TRP temperature (HK)
21	PROCESSOR_TEMPERATURE	ASCII_Real	DEGC	-45 - 115	Processor temperature (HK)
23	ION_TRAP_EMISSION_CURRENT	ASCII_Real	uA		Ion trap emission current (HK)
24	ADSORBER_TEMPERATURE_SETPOINT	ASCII_Real			Adsorber temperature setpoint (HK)
25	ITMS_TEMPERATURE_SETPOINT	ASCII_Real			ITMS temperature setpoint (HK)
26	ITMS_HEATER_STATUS	ASCII_String		OFF, ON	ITMS heater status (HK)
27	ADSORBER_HEATER_STATUS	ASCII_String		OFF, ON	Adsorber heater status (HK)
28	HISTOGRAM_DATA	ASCII_Integer			Array of 2048 bins with measured counts in each bin (SCI)

Table 11. Variable definitions for PITMS_CAL_timestamp.csv files.

Col	Variable Name	Format	Units	Range	Description
1	MASS_CALIBRATED	ASCII_Real	amu	10-160	Calibrated m/z
2	COUNTS_CORRECTED	ASCII_Real	ions	-100 to 20000	Calibrated ions per bin
3	PARTIAL_PRESSURE	ASCII_Real	mbar	0 - 100	Partial pressure (for SF4 only)

Table 12. Variable definitions for PITMS_CAL_VAR.csv file.

Col	Variable Name	Format	Units	Range	Description
1	TIME	ASCII_Date_Time_YMD_UTC			UTC converted date time of the time for the first packet in this spectrum (SCET)
2	INSTRUMENT_TIMELINE_ID	ASCII_Integer		12-18	Instrument timeline identifier (see Table 3)
3	SCAN_FUNCTION_NUMBER	ASCII_Integer		1-13	Scan function number (see Table 1)
4	ITMS_TEMPERATURE	ASCII_Real	C	25-50	ITMS temperature
5	IONIZATION_CTS	ASCII_Real	counts	3000-11000	Average value of raw counts during the ionization phase
6	IONIZATION_STDEV	ASCII_Real	counts	50-160	Standard deviation of the raw counts during the ionization phase
7	START_MASS	ASCII_Real	amu	10-52	The lowest mass measured in the spectrum
8	END_MASS	ASCII_Real	amu	45-155	The highest mass measured in the spectrum
9	1SIGMA_ERR	ASCII_Integer	counts	10-1000	The standard deviation of counts in non- peak regions of the spectrum (noise)
10	START_BIN	ASCII_Integer		600-1200	Bin corresponding to the start of the measurement phase
11	SF4_BIN_OFFSET	ASCII_Integer		-200 - 250	Bin corresponding to the start of the measurement phase, adjusted for SF
12	SF4_BIN_DIVISOR	ASCII_Integer		1-2	Factor to adjust bin width if needed
13	CALIB_SLOPE	ASCII_Real	amu	11.2-11.4	Slope of mass calibration curve from DAC values
14	CALIB_INT	ASCII_Real	amu	441-455	Intercept of mass calibration curve from DAC values
15	P1R	ASCII_Integer	amu	18, 19, 30	Known reference mass 1
16	P2R	ASCII_Integer	amu	30, 46.5	Known reference mass 2
17	P1M	ASCII_Real	amu	16-30	Measured value of reference mass 1
18	P2M	ASCII_Real	amu	29-47	Measured value of reference mass 2
19	SHIFT	ASCII_Real		-0.6 - 1.2	Spectrum shift
20	STRETCH	ASCII_Real		0.9-1.1	Spectrum stretch
21	BASELINE_A0	ASCII_Real			First baseline coefficient
22	BASELINE_A1	ASCII_Real			Second baseline coefficient
23	BASELINE_A2	ASCII_Real			Third baseline coefficient
24	BASELINE_A3	ASCII_Real			Fourth baseline coefficient
25	BASELINE_A4	ASCII_Real			Fifth baseline coefficient
26	BASELINE_A5	ASCII_Real			Sixth baseline coefficient
27	BASELINE_A6	ASCII_Real			Seventh baseline coefficient

6. Calibrated Data Products and Procedures

This section details the processing steps used to calibrate PITMS raw data to calibrated data that are in instrument-independent quantities of partial pressure per m/z (mass spectrum). The calibrated data are provided in .csv format containing the variables defined in the XML label and in Table 11. Variables needed to conduct the calibration are captured in the PITMS_CAL_VAR.csv file, defined in Table 12. For ease of reference, throughout the text:

- variables contained in PITMS_RAW data are denoted in red font
- variables in PITMS_CAL_VAR.csv are denoted in orange text
- interim variables in calculations use purple font
- variables in PITMS_CAL products appear in green text
- constants appear in **bold font**

The original concept for PITMS included an onboard calibration gas system to release known quantities of calibration gases into the ITMS to enable in situ calibration during the mission, but this system was descoped during the development process. Therefore, the PITMS calibration process uses data obtained during preflight Thermal Vacuum (TVac) testing performed on the PITMS instrument in May 2021.

The TVac calibration session targeted both quantitative and qualitative calibration. Qualitative calibration involved obtaining characteristic spectra of various gases with the different PITMS SFs and investigating other effects, such as the effect of changing the detector bias. The TVac chamber also contained background gases (e.g., air, water).

The TVac chamber contained a Residual Gas Analyzer (RGA; a mass spectrometer) and a calibrated pressure gauge. The facility provided a calibration certificate for the total pressure gauge used against the response of a gas friction manometer, traceable to the Physikalisch-Technische Bundesanstalt (PTB) national standards laboratory in Germany, with nitrogen at room temperature. This provided a scaling factor to correct the total pressure gauge output to absolute pressure value, at a range of pressures. Using the sum of partial pressure measurements of a residual air-only atmosphere by the RGA, at room temperature and over several hours, a conversion factor was derived to convert the RGA output to match the output from the total pressure gauge once this scaling factor had been applied. As calibration gases were let into the chamber, the RGA also recorded their characteristic spectra, enabling comparison with contemporaneous spectra obtained with PITMS. The total pressure recorded by the gauge was used to calculate the partial pressures of the individual test gases by the intensities recorded by the RGA.

The TVac data are proprietary data to the European Space Agency, who developed and tested the EMS, so are not included as raw data in this archive, but quantities derived from the TVac data are discussed here.

6.1 Ionization Phase

The ionization phase is when the filament and detector are on and ions are being formed but the electronic trap is not yet set up. The signal during this phase may be related to the total gas pressure in the instrument.

We computed the average value of the data in bins 100-489 for all acquired spectra. The average and standard deviation are reported in the variables IONIZATION_CTS and IONIZATION_STDEV.

6.2 Mass (x-axis) corrections

PITMS generated data by increasing the voltage on the ring electrode to eject trapped ions. The specifics of each SF determined the time (and therefore detection bin) of the mass that is ejected. The RF amplitude of the ring electrode was controlled by a DAC (Digital to Analogue) signal from the ITMS processor. The DAC signal was converted to an AC signal, amplified by the ITMS electronics and then further amplified by a tuned LC circuit to give an RF voltage on the ring electrode. Ideally the RF amplitude on the ring electrode would be proportional to the DAC voltage. However, there are two effects that result in non-linearity: a) at low DAC values, cross-over distortion of the amplifier results in a threshold below which there is no RF signal, and the RF signal then increases non-linearly; and b) the LC tuned circuit is not constant, probably due to temperature effects within the circuit at high voltages.

During calibration (preceding the first SF during an experiment), PITMS measured the tuned frequency of the LC circuit. It then scanned the DAC voltage and measured the RF signal. It determined the DAC values for m/z = 2 and m/z 135, and these values were stored as START_SCALING and FINAL_SCALING respectively. Onboard the instrument, the PITMS processor used these DAC values and assumed a linear DAC to mass calibration in the SFs. This is roughly 11.3 bins per AMU. However, as mass spectra were successively collected after the starting onboard calibration, the calibration curve can change and cause the peaks to drift.

To convert mass spectra bin numbers to mass, the PITMS team used spectra acquired during PITMS TVac testing at room temperature, with known gases added to the vacuum system, and acquired as the first spectrum after an RF calibration (to minimize the effect of drift). Because no PITMS calibration gas was included, the mass calibration further requires knowledge of the species present in the measurement to anchor the spectra. This assumption is further discussed below.

The x-axis adjustment is made in three stages:

- a ***linear adjustment*** appropriate for masses m/z 15-45 (Section 6.2.1)
- a ***thermal drift adjustment*** based on known peaks in the linear region (Section 6.2.2)
- a ***high-mass adjustment*** using a non-linear “bending” method (Section 6.2.3).

6.2.1 Linear adjustment

The linear adjustment is based on the DAC Value at m/z = 2 (START_SCALING) and the DAC Value at m/z = 135 (FINAL_SCALING) that can be found in the raw data. TVac data indicates that the mass spectrometer response is linear over the range m/z=15 to m/z = 45, so the calculated mass scale is based on a linear fit between these m/z values with constants derived from TVac calibration spectra at room temperature.

$$\text{CALIB\_INT} = (-0.3133 \times \text{START\_SCALING}) + 735.17$$

$$\text{CALIB\_SLOPE} = (-0.884\text{E-}3 \times (\text{FINAL\_SCALING} - \text{START\_SCALING})) + 13.81$$

The TVac spectra acquired immediately after a calibration used the reference scan function, SF4. This SF was designed as a reference with a starting mass of 10 amu, mass increment of 0.1 amu per bin, and start at bin 600 (See Table 1). Since the ITMS uses a linear mass calibration, the other SFs can have their bin numbers in the raw data converted to the equivalent of SF4 as follows:

$$\text{START\_BIN} = (\text{BIN} + \text{SF4\_BIN\_OFFSET}) / \text{SF4\_BIN\_DIVISOR}$$

$$\text{MASS6.2.1} = (\text{START\_BIN} - \text{CALIB\_INT}) / \text{CALIB\_SLOPE}$$

6.2.2 Thermal Drift Adjustment

The Thermal Drift adjustment fits the mass scale to two known peaks within the linear portion of the mass scale and both shifts and stretches the mass scale to force these two peaks to be in their ideal positions along the m/z scale. This correction presupposes knowledge of what species are present and what their ideal mass is. As such, it is applied carefully after preliminary knowledge from the linear mass correction. Note that this correction was not done for spectrum 2024-01-12T10:34:00Z because the data packets containing the relevant part of the spectrum were lost.

For each spectrum, we identified two peaks in the mass spectrum (P1 and P2) with ideal masses used as references (P1R and P2R) and apparent masses from the calibration in Section 6.2.1 (P1M and P2M). This step requires *a priori* knowledge of the species present in the spectrum giving rise to the peaks. For the PITMS dataset, we chose H_2O^+ (m/z=18) for P1 and NO^+ (m/z=30) for P2. The H_2O^+ comes from terrestrial atmosphere adsorbed to the instrument and lander; at the high pressures seen by PITMS, conversion of H_2O^+ ions into H_3O^+ ions is promoted, giving rise to a significant peak at m/z=19. The NO^+ arises from the Peregrine oxidizer leak, seen as a combination of NO_2^+ at m/z 46 and NO^+ at m/z 30. The team initially considered whether the P2 peak could be from either N_2^+ or CO^+ at m/z 28, but ultimately rejected these interpretations because no species that would be expected to occur along with N_2^+ or CO^+ (from, *e.g.*, terrestrial atmosphere or combustion) were present in appropriate ratios, while NO^+ and NO_2^+ (at m/z=46) from the known oxidizer leak appeared in plausible ratios. More details of these analyses and interpretations appear in Cohen et al. (2024b).

First, we calculated how much to SHIFT the mass spectrum so that P1M is locked to mass P1R. Then, we calculated STRETCH (or shrink) the mass spectrum so that the mass difference between P2M and P1M is the same as the difference between P2R and P1R. These were used to recalculate the mass.

SHIFT = P1R - P1M

STRETCH = (P2R - P1R) / (P2M - P1M)

MASS6.2.2 = (((MASS6.2.1 + SHIFT) - P1R) × STRETCH) + P1R

6.2.3 High-mass adjustment

Masses obtained by assuming a linear mass calibration curve deviate from measured masses for species with a mass > 45 amu; a second order polynomial gives a better fit to the high- mass data. TVAC data acquired when krypton and xenon were added to the vacuum system were used to derive a correction to the curve obtained after the drift correction. In effect, the high-end mass scale is bent to fit the ideal-mass krypton and xenon peaks.

A final "bending" is applied to all species with the following constants:

BENDING_A = -4.789E-4
BENDING_B = 1.011
BENDING_C = 5.305E-3

MASS_CALIBRATED = (**BENDING_A** * (MASS6.2.2)^2) + (**BENDING_B** * MASS6.2.2) + **BENDING_C**

This correction shifts the perfectly placed masses from Step 3.2 by ~0.1 m/z. However, if we were only to apply the correction to masses heavier than m/z 35, then there would be a discontinuity of 0.2 amu. This would cause problems when doing the curve fitting.

6.2.4 Precision and accuracy of the calibrated m/z scale

The precision on each MASS_CALIBRATED value is 0.01 amu. We report all values to two decimal places. MASS_CALIBRATED is accurate to ± 0.2 amu from 15 to 45 amu and ± 1 amu at masses heavier than 45 amu. However, all masses should covary systematically.

6.3 Intensity (y-axis) corrections

6.3.1 Baseline fitting and correction

We used OriginPro to fit and subtract a baseline to the data to account for background counts. Because of the way the mission unfolded, there was no "blank" data that we could use to subtract, only the instrument noise function without any gas to be measured. Therefore, we fit and subtracted a baseline for each individual spectrum.

The OriginPro baseline fit function used "anchors" at the midpoint of the noise to constrain the fit. We chose anchors at masses where species were not expected to be present in the dataset. These anchors included several points at the low and midrange masses (13-14 amu, 24-27 amu, 32-38 amu), and over the full high mass range (50+ amu). The placement of the anchors was generally the same across data files (accounting for each SF's mass range) but sometimes the team shifted the anchor points slightly (~0.1amu) to better match the midpoint of the noise. We smoothed each spectrum using an 11-point averaging window, applied the anchor points to the smoothed spectrum, and then allowed OriginPro to fit the smoothed spectrum.

Experience with the PITMS TVac data showed that a 6th order polynomial generally produced the best fit to the measurement phase data, so we adopted this method for baseline fitting to the smoothed dataset. The baseline fit to each smoothed dataset follows the following equation, where x = baseline mass and y = baseline counts. The baseline coefficients are included in the PITMS_CAL_VAR.csv table.

$$y = \text{BASELINE\_A0} + \text{BASELINE\_A1}\, x + \text{BASELINE\_A2}\, x^2 + \text{BASELINE\_A3}\, x^3 + \text{BASELINE\_A4}\, x^4 + \text{BASELINE\_A5}\, x^5 + \text{BASELINE\_A6}\, x^6$$

We subtracted the fitted baseline function from the raw (unsmoothed) data to produce COUNTS_CORRECTED. The subtraction function could allow fractional counts, which we then used for peak fitting and integration (Section 7) because these activities were part of the OriginPro workflow.

6.3.2 Baseline fit assessment and Limit of Detection

We assessed the baseline fit by examining the non-peak data variability after baseline subtraction in two mass regions: low-mass measurements (13-56 amu) and high-mass measurements (>56 amu). Non-peak counts arise from a combination of electronics noise, ambient molecules and ions hitting the detector, etc. If the non-peak counts were truly random, these counts would fit a normal distribution, and if the baseline fit the centerline of the noise, the distribution would be centered at zero.

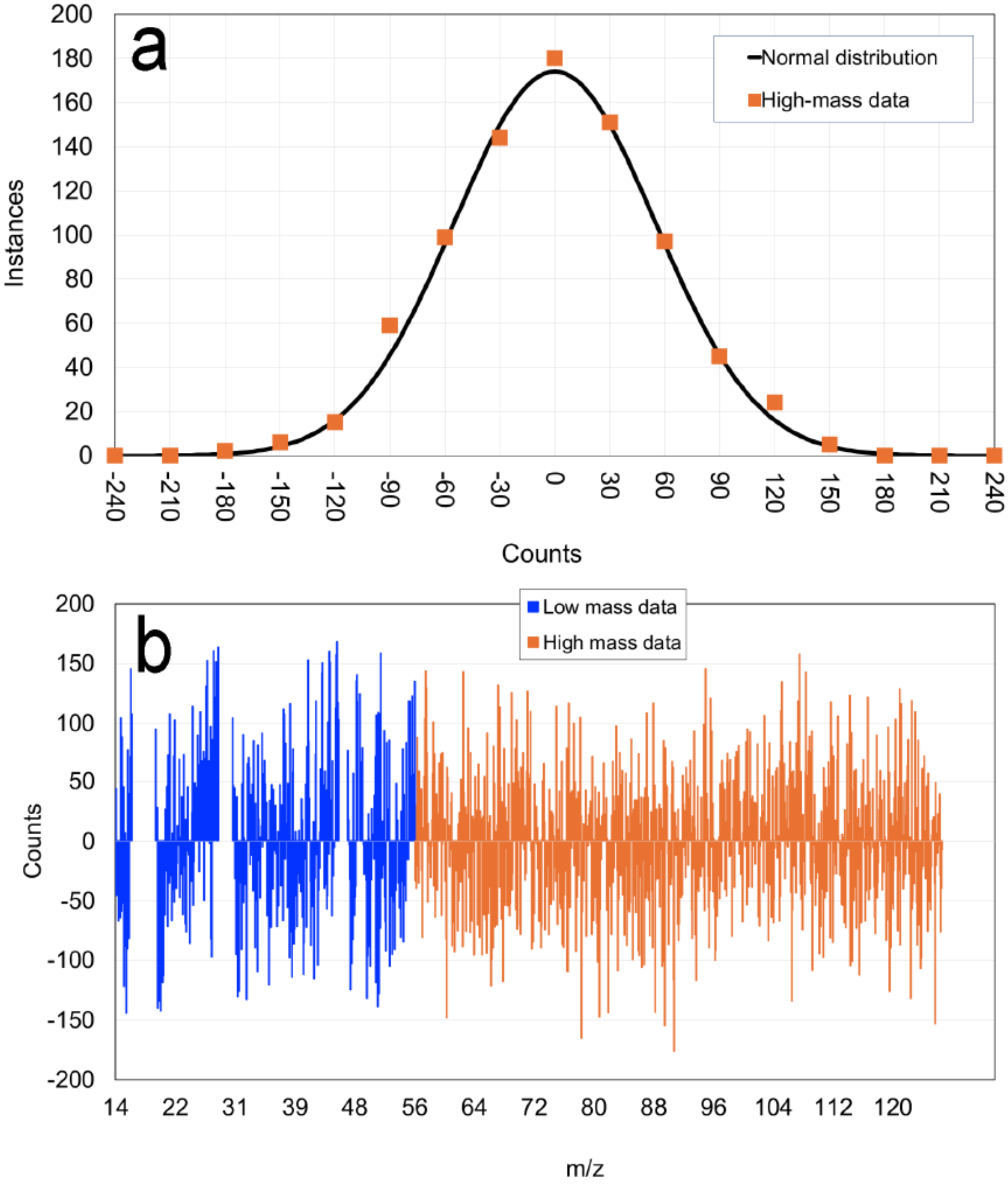

Fig. 4. Examples of baseline assessment using baseline-corrected data, excluding peak data. a) A histogram of the noise counts (orange line) follows a normal distribution model (black line), symmetrically distributed and centered at zero, indicating that the baseline was a good fit. The 1σ width of the fitted normal distribution was taken as the error in any given data point and the 3σ width of the normal distribution was taken as the Limit of Detection (LOD). b) The distribution of noise counts (positive and negative) around the zero line is not randomly distributed in this example, showing some “waviness” arising from correlated noise counts introduced by the 6th order polynomial baseline fit. Spectra displaying this property were refit to remove or at least minimize this artifact.

For each baseline-corrected spectrum, we masked mass regions with peak data and plotted a histogram of the remaining data points for the low- and high-mass regions (Fig. 4). We then fit the data using a normal distribution (Gaussian function) centered at zero. If the histogram was offset from the center at zero or asymmetrically distributed, we repeated the baseline fit procedure, offsetting the anchor points to better capture the center of the noise, until the baseline-corrected noise data were captured by a normal distribution (we defined a threshold for this distribution as within 3 counts of the zero line). We also assessed the distribution of positive and negative noise counts around the centerline to ensure that there were no systematic correlations (waviness) in the distribution. Not all spectra could be perfectly corrected; notes on the baseline fits are provided in Table 6.

The parameters of the normal distribution of the non-peak data were used to define measurement uncertainty and limit of detection (LOD). The 1σ width of the fitted normal distribution was taken as the error in any given data point (1SIGMA_ERR). The 3σ width of the normal distribution was taken as the LOD, the intensity threshold over which we can identify peaks in individual spectra.

6.3.3 Convert counts to ions

The PITMS electron multiplier worked in pulse counting mode, where one count resulted from one ion. This assumption holds true as long as ions hit the detector at discrete times and did not overcome the detector dead time. Ground experiments indicate that count limiting (from multiple ions striking the detector within the time constant of the detector) occured around 11,000 raw counts. Peaks with raw counts above 11,000 should be treated with caution as they may not accurately represent the number of ions present in the mass spectrometer. Spectra with peaks exceeding 11,000 counts are noted in Table 6.

6.3.4 Convert ions to partial pressure

The PITMS quantitative calibration (QC) defines the relationship between detected ion counts and volumetric number density of the parent molecule. The PITMS QC is based on nitrogen, chosen because N_2 is stable, does not react in the ion trap, was present in the calibration session and was expected to be present in mission data. The QC process using N_2 assumes that the RGA and PITMS were in equilibrium during TVac testing (*i.e.,* encountered the same gases, at same temperatures, same number densities), that the RGA was factory-calibrated to convert counts to pressure using the ambient chamber temperature, and that the RGA signal at m/z 28 gives a measure of partial pressure of N_2 in the TVac chamber. Applying this QC to all PITMS data further assumes that the sensitivity of PITMS to each species is the same as that of N_2.

The PITMS QC additionally assumes that the instrument conditions in the TVac chamber were similar to the instrument conditions during the flight measurements, including instrument temperature, gas molecule temperature, total pressure, and equilibrium conditions. The QC included in the PITMS calibrated data release is based on these assumptions being true, though further refinements may be possible by evaluating these assumptions. PITMS measured several instrument temperatures included in the RAW data files; ITMS_TEMPERATURE is the most representative of the instrument temperature. The Peregrine lander measured temperatures using a thermocouple attached to Deck D, where PITMS was mounted (though PITMS was thermally isolated from Deck D). Ambient gas molecule temperatures may reasonably be assumed to follow the Deck D temperature profile, provided with the PITMS_RAW data.

Eleven spectra from the TVac campaign were identified as being obtained with N_2 present while conditions were stable, reducing thermal effects and enabling time-correlating of PITMS spectra with RGA spectra. The partial pressure of N_2 in the chamber was calculated using the RGA partial pressure and the total pressure from the chamber gauge as "ground truth." We then processed the PITMS TVac chamber spectra following the procedures for mass calibration and baseline fitting. We used OriginPro to fit and integrate the N_2 peak data in the PITMS TVac spectra to assign a total number of counts to the nitrogen abundance provided by the RGA and pressure gauge.

The resulting **QC FACTOR** = 5.29 E-11 mbar / count for N_2. The **QC UNCERTAINTY** is estimated as ± 1.69E-11 mbar, derived via a product of (a) error between the recorded partial pressures during TVAC testing and the back-calculated pressure values using the QC factor, and (b) systematic errors arising from converting to absolute pressure against the gas-friction manometer.

PARTIAL_PRESSURE = COUNTS_CORRECTED × **QC FACTOR**

This PITMS QC factor is, *senso stricto*, only applicable to spectra acquired using SF4 because that was the only SF used in the TVac test campaign. Accordingly, only SF4 spectra contain a calculated PARTIAL_PRESSURE variable (spectra using other SFs have PARTIAL_PRESSURE set to -999.9). The PITMS team did not develop any further QC factors to apply to spectra acquired with different SFs. Application of our reported **QC FACTOR** to other spectra by the user may be considered with caution - for example, by assuming that the rate of change of the sample environment is low with respect to the rate of collection of data from each SF, one could cross-calibrate from SF4 to any near-contemporaneous SF. Note that this assumption is less likely to be true when the door was closed, because self-heating would cause an increase in outgassing throughout an operational session.

6.3.5 Precision and accuracy of the calibrated data

The PITMS_CAL data files report CORRECTED_COUNTS as integers after baseline subtraction, conforming to the precision of the input data as integer counts.

We define the uncertainty in any given measurement or data point by the variability in measuring the same amount of gas multiple times under identical circumstances. Because PITMS was not able to make such a measurement with calibration gases in flight, we use the noise measurement developed in Section 6.3.2 as the measurement uncertainty (1SIGMA_ERR).

The uncertainty in the calculated PARTIAL_PRESSURE for each bin comes from the uncertainty in each measurement and the uncertainty in **QC FACTOR**, calculated as:

$$= \text{PARTIAL\_PRESSURE} \times \sqrt{\left(\frac{\text{1SIGMA\_ERR}}{\text{CORRECTED\_COUNTS}}\right)^2 + \left(\frac{\textbf{QC UNCERTAINTY}}{\textbf{QC FACTOR}}\right)^2}$$

For bins with high counts, the uncertainty is around 33%; for bins where counts are near the LOD, the uncertainty can be as high as ~100%.

7. Derived Data Products and Procedures

This section will detail the interpretation of PITMS calibrated data to infer the species measured and their abundance. The derived data will be provided in .csv format containing the variables defined in the XML label and in Table X.

8. Tools

All raw data are provided as .csv files that may be opened by any spreadsheet or plotting program, such as Excel or OpenOffice. No special tools are needed to view raw data products. The PITMS team used the OriginPro software package to produce calibrated and derived data products. Descriptions of these tools are provided in the appropriate sections.

9. Appendices

9.1 Acronyms

AB	Astrobotic Technology
AOS	Acquisition of Signal
CLPS	Commercial Lunar Payload Services
EAR	Export Administration Regulations
EDR	Experiment Data Record
EMS	Exosphere Mass Spectrometer
ESA	European Space Agency
GSFC	Goddard Space Flight Center
HK	Housekeeping
HW	Hardware
ICD	Interface Control Document
ITAR	International Traffic in Arms Regulations
ITL	Instrument Timeline variable (also known as experiment number)
ITMS	Ion Trap Mass Spectrometer
LOS	Loss of Signal

MLI	Multi-Layer Insulation
MOC	Mission Operations Center
MS	Mass Spectrometer
NAIF	Navigation and Ancillary Information Facility
NASA	National Aeronautics and Space Administration
NSSDCA	National Space Science Data Coordinated Archive
Open MCT	Open Mission Control Technologies
OU	Open University
PDS	Planetary Data System
PI	Principal Investigator
PITMS	Peregrine Ion-Trap Mass Spectrometer
PL	Payload
RAL	Rutherford Appleton Laboratory Space
RD	Reference Document
RDR	Reduced Data Record
SF	Scan Function
SIS	Software Interface Specification
SPICE	Spacecraft, Planet, Instrument, Pointing C-matrix, and Event kernels (historical acronym for navigation and ancillary data)
SS	Science Sequence
SW	Software
TBC	To Be Confirmed
TBD	To Be Determined
TVac	Thermal Vacuum
URL	Uniform Resource Locator