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The PANGAEA mineralogical database

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ABSTRACT

Future human missions to the surface of the Moon and Mars will involve scientific exploration requiring new support tools to enable rapid and high quality science decision-making. Here, we describe the PANGAEA (Planetary ANalogue Geological and Astrobiological Exercise for Astronauts) Mineralogical Database developed by ESA (European Space Agency): a catalog of petrographic and spectroscopic information on all currently known minerals identified on the Moon, Mars, and associated with meteorites. The catalog also includes minerals found in the analog field sites used for ESA's geology and astrobiology training course PANGAEA, to broaden the database coverage. The Mineralogical Database is composed of the Summary Catalog of Planetary Analog Minerals and of the Spectral Archive and is freely available in the public repository of ESA PANGAEA. The Summary Catalog provides essential descriptive information for each mineral, including name (based on the International Mineralogical Association recommendation), chemical formula, mineral group, surface abundance on planetary bodies, geological signifi-

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cance in the context of planetary exploration, number of collected VNIR and Raman spectra, likelihood of detection using different spectral methods, and bibliographic references evidencing their detection in extraterrestrial or terrestrial analog environments. The Spectral Archive provides a standard library for planetary in-situ human and robotic exploration covering Visual-Near-Infrared reflective (VNIR) and Raman spectroscopy (Raman). To populate this library, we collected VNIR and Raman spectra for mineral entries in the Summary Catalog from open-access archives and analyzed them to select the ones with the best spectral features. We also supplemented this collection with our own bespoke measurements. Additionally, we compiled the chemical compositions for all the minerals based on their empirical formula, to allow identification using the measured abundances provided by LIBS and XRF analytical instruments. When integrated into an operational support system like ESA's Electronic Fieldbook (EFB) system, the Mineralogical Database can be used as a real-time and autonomous decision support tool for sampling operations on the Moon, Mars and during astronaut geological field training. It provides both robust spectral libraries to support mineral identification from instrument outputs, and relevant contextualized information on detected minerals.

Specifications Table

Subject	Earth and Planetary Sciences
Specific subject area	Space and Planetary Science
Type of data	Two main data types: 1. Summary Catalog of Planetary Analog Minerals – combined spreadsheet tables 2. Spectral Archive - An archive of representative Raman and VNIR spectra for each mineral, averaged over as many valid mineral instances from different spectral archives. It is produced solely from minerals which have more than three different Raman or VNIR measurements available from different sources. For each spectral method and mineral, the compiled data were processed to produce weighted mean homogenized spectra.
How data was acquired	The Summary Catalog was compiled from bibliographic research, and includes several spreadsheets: • Database – mineral classification, occurrence (cited), mineral abundance and description on extraterrestrial bodies and in ESA PANGAEA analog training sites. • Chemical abundances – calculated from each mineral's empirical formula on www.webmineral.com , or using the Python software *Molmass* in some cases. To determine the percentage of each element, the molecular weight from the empirical formula was divided by the sums of the atomic weights of each element. • Physical properties – mineral hardness, relative density and crystal system based on literature and mineralogical portals like https://www.mindat.org/ and http://www.webmineral.com/ The spectroscopic libraries for planetary and terrestrial analog minerals are compiled from: *Open-access archive* • Visual-NIR-SWIR spectral libraries: RELAB spectral archive of NASA Reflectance Experiment Laboratory; United States Geological Survey (USGS); and ECOSTRESS (formely ASTER), and others (see additional information below).

(*continued on next page*)

	• Raman spectral libraries: RRUFF database of Raman spectra [2], SOLSA Open Database of Raman Spectra [3] and others (see additional information below). *Ours and our collaborators' spectroscopic measurements from various VNIR/SWIR reflective and Raman spectrometers:* • VNIR/SWIR spectrometer "TerraSpec HALO" by ASD/Malvern-Panalytical; • Raman spectrometers: "XploRA" by HORIBA Scientific; "Inspector 300 ″ by SciAps, "BRAVO" by Bruker
Data format	Mixed (Raw + Processing) Analyzed Filtered
Parameters for data collection	The Summary Catalog aims to record all currently known extraterrestrial, and terrestrial planetary analog minerals confirmed to be present with one or more analytical methods. This can be from in-situ measurements, remote sensing, or laboratory studies on return samples. Whilst the International Mineralogical Association (IMA) has approved almost all of the mineral species listed in the database, we did include several that have not yet been approved due to their relevance to planetary geology. For the Spectra Archive, only the high-quality data is included. Data considered outliers by our analysis were rejected.
Description of data collection	The Summary Catalog was created from a literature review. This involved analyzing over 600 articles describing the identification of minerals from rock samples of the Moon, Mars, meteorites, and PANGAEA planetary analog sites: Nördlinger Ries impact crater (Germany), Lanzarote (Spain), Bletterbach (Italy) and Lofoten (Norway). The Raman and VNIR/SWIR spectra were collected by searching spectroscopic archives matching mineral names and their known synonyms.
Data source location	Moon, Mars, meteorites, terrestrial analog sites: Nördlinger Ries impact crater (Germany), Lanzarote (Spain), Bletterbach (Italy) and Lofoten (Norway).
Data accessibility	On Mendeley Data the version of the database associated to this article: Direct URL: https://data.mendeley.com/datasets/6dfkgnh9bp/1 DOI: doi:10.17632/6dfkgnh9bp.1 The present version of the dataset is also available at the ESA ATD repository. Future updates of the database will be available in this repository. Repository name: ESA PANGAEA Mineralogical Database Direct URL to data: https://atd.eac.esa.int/sites/PANGAEAMinDB

Value of the data

- The PANGAEA Mineralogical Database aims to enhance the recognition of planetary minerals through creating a custom structured database containing analytical information on all known minerals present on the Moon, Mars and other planetary bodies. Combined together, the mineral catalog, cross-validated multi-spectral archives, and multivariate classification software (not included in this data archive) will enable fast, reliable recognition of rocks and minerals in-situ, something that is crucial for decision support in future human and robotic planetary surface exploration missions.
- The Summary Catalog section of the Mineralogical Database has been integrated into the PANGAEA Electronic FieldBook (EFB) and used successfully for geological training during the PANGAEA astronaut training course [8,9]. In the future, it could be used for human planetary exploration missions, as well as for in-situ identification of minerals during the terrestrial fieldwork. The Mineralogical Database could also contribute to the design of future planetary exploration missions and In Situ Resources utilization (ISRU) activities, by providing a robust database for the evaluation of suitable spectroscopic instruments [5].
- The compiled archive of Raman and VNIR averaged spectra were cross-matched to select the most representative examples for inclusion in the spectroscopic library.
- The calculated mineral chemical composition provides additional complementary information, allowing for better mineral identification when combining VNIR/Raman spectra with the measured abundances provided by LIBS and XRF analytical instruments.

1. Data description

The PANGAEA Mineralogical Database (MDB) aims to enhance the recognition of planetary minerals, offering a custom structured database containing information on all known minerals present on the Moon, Mars and other planetary bodies. This database can act as an input source for novel data analysis methods, such as Machine Learning, to enable in-situ spectroscopic identification of these minerals. To this end, the MDB has already been successfully tested by ESA during the PANGAEA field campaigns with mineral recognition software to examine and develop its potential as a real-time decision support tool for future human and robotic planetary surface exploration missions. It also acts as a planetary mineral information repository, allowing mineral detections to be enhanced with additional relevant information for decision support purposes.

The MDB can be viewed as two distinct products: a catalog of petrographic information (Summary Catalog), and an analytical library (Spectral Archive). The catalog consists of petrographic information on all currently known minerals identified on Moon, Mars, and associated with meteorites. The catalog is envisioned to provide essential analytical in-field information for each mineral to assist in rapid identification and understanding of significance in real time geological exploration. Each mineral entry includes: name (based on IMA recommendation), chemical formula, mineral group, surface abundance on planetary bodies, geological significance in the context of planetary exploration, number of collected VNIR and Raman spectra, likelihood of detection using different spectral methods, and bibliographic references evidencing their detection in extraterrestrial or terrestrial analog environments. In addition, supplementary characteristics for each mineral that may help with its identification are also included, such as chemical abundances calculated from the known empirical chemical formula, and basic physical properties (hardness, specific gravity, crystal system). The database was compiled through systematic literature research, followed by the careful cross-validation ("out-of-sample" testing) of all characteristic mineral information (including flagging of doubtful or erroneous data).

The second major contribution provided by the PANGAEA Mineralogical Database is the Spectral Archive, a customized library of analytical data from all known planetary terrestrial analog minerals and mineraloids. This covers vibrational spectra obtained from two analytical methods: reflective Visual-to-Near- & Shortwave-Infrared (VNIR), and Raman spectroscopy. In addition, the database provides information about elemental compositions for each mineral, allowing it to be used for additional recognition through atomic spectroscopy like Laser-Induced-Breakdown Spectroscopy (LIBS), and X-Rays Fluorescence (XRF), even when those spectra are not provided in our library.

The PANGAEA MDB is envisioned as part of the PANGAEA EFB [15]. The EFB is a deployable system that supports field mission operations, enabling scientific documentation of traverses and sampling, and interaction between mission support and field teams through the exchange of contextual data. The EFB can interface with handheld instrumentation intended for planetary exploration, and use them to feed the instrument agnostic Machine Learning algorithms and Mineralogical Database with mineral signatures, allowing the documentation and categorization of samples to be completed within one integrated information system. When combining this set of capabilities, the EFB with the Mineralogical Database will enable fast and reliable *in-situ* recognition of rocks and minerals, and has potential to become a crucial decision support tool for future human and robotic planetary surface exploration missions.

Although targeted for use in space exploration, the PANGAEA Mineralogical Database could be used for several terrestrial applications. Its structured database of mineral information connected with spectral libraries allows for fast mineral characterization. This has uses for field geology and petrographic research, or even the mining industry.

The Summary Catalog of the Mineralogical Database is presented as an Excel workbook file comprising four spreadsheets: ‘Database’, ‘Chemical Abundances’, ‘Properties’, ‘Census & Legend’. The latter one represents the statistics related to the analysis of minerals and the number of

VNIR and Raman spectra. The first spreadsheet, titled ‘Database’, provides summary information about the minerals as specified in the ‘Database’ content table below.

‘Database’ content table

Name	Name and commonly used synonyms of the mineral separated by “/”. Most of the names are approved by the International Mineralogical Association (IMA), except for a few that do not commonly occur on Earth, or are awaiting publication. In some cases, different varieties of the same IMA mineral (i.e. ranges of mineral solutions) have been included since they can be systematically distinguished by different spectra. The synonyms include some obsolete mineral names [11], allowing for matches from past analytical data and information.[1]
Formula	Chemical Formula of Mineral
Group	Mineral Groups are adopted from Nickel-Strunz chemical-structural classification
Subgroup 1	Version 10, (last accessed June 2020)
Subgroup 2	http://www.webmineral.com/help/StrunzClass.shtml
Structural Groupname [a]	Fleischer’s Groupname: structural group for minerals by Fleischer’s Glossary [4] as reported by the IMA https://rruff.info/ima/
# Raman spectra [b]	Total number of Raman spectra in our archive
Raman detectability	The average classification accuracy – based on our Machine Learning code and the best spectra where there are more than 3 measurements available [6].
# VNIR spectra [b]	Total number of VNIR spectra in our archive
VNIR detectability	The average classification accuracy – based on our ML code and the best spectra where there are more than 3 measurements available
Mars [c]	The presence or absence of the mineral on Mars
Mars Occurrence [d]	Qualitative estimate of the mineral’s occurrence on Mars based on literature review
Moon [c]	The presence or absence of the mineral on the Moon
Moon Occurrence [d]	Qualitative estimate of the mineral’s occurrence on the Moon based on literature review
Meteorites [c]	The presence or absence of the mineral on meteorites
PANGAEA analogs [e]	Presence of the mineral in the PANGAEA campaign’s analog environments [7]: Lanzarote, Ries, Lofoten and Bletterbach
Earth Occurrence [f]	Qualitative estimate of the mineral’s occurrence on the terrestrial analogs based on literature review
General description	Short description of the mineral and its general geological significance
Moon Description [g]	Description related to the mineral’s geological significance on the Moon
Mars description [g]	Description related to the mineral’s geological significance on Mars
Meteorites description [g]	Description related to the mineral’s geological significance in Meteorites
Moon References	Bibliographic reference(s) indicating the mineral’s presence on the Moon
Mars references	Bibliographic reference(s) indicating the mineral’s presence on Mars
Meteorites references	Bibliographic reference(s) indicating the mineral’s presence in Meteorites
Bletterbach references	Bibliographic reference(s) indicating the mineral’s presence in Bletterbach
Lofoten references	Bibliographic reference(s) indicating the mineral’s presence in Lofoten
Lanzarote references	Bibliographic reference(s) indicating the mineral’s presence in Lanzarote
Ries references	Bibliographic reference(s) indicating the mineral’s presence in Ries

[1] For example, the currently approved “Chabazite-Ca” name has been changed from “Chabazite” [10], thus it is listed as its synonym. However, other members of the Chabazite series (such as “Chabazite-Na”) do not include the “Chabazite” as their synonym.

Notes to Database content table:

(a) IMA-approved minerals, and relevant non IMA-approved minerals with a high potential to be found on the extraterrestrial bodies.
(b) A spectra collection (Raman and VNIR) from online open access libraries and our own measurements.
(c) Based on the published data from scientific papers and the data from the rovers and satellites.
(d) Qualitative estimate of the mineral’s abundance on an extraterrestrial body surface based on the published data. Some of the minerals have been marked as ‘‘likely to be found’’ as they are either present in lunar meteorites and therefore could be found on the surface

of the Moon, or they are believed to form on certain extraterrestrial bodies on the base of the result of laboratory experiments on Earth (with references for each case).
(e) Based on literature research, see <u>*Section 3.1*</u>. Minerals on Lanzarote which were marked as a ''rare'' are likely to be more abundant on the other Canary Islands.
(f) Qualitative estimate of the mineral's abundance in terrestrial analog sites based on the published data.
(g) Based only on published data from scientific papers.

The two spreadsheets following the 'Database' spreadsheet contain additional analytical information. The 'Chemical Abundances' sheet contains the calculated molecular mass (in %) of chemical elements in each mineral's empirical formula. The 'Properties' sheet contains information on mineral hardness, relative density and the crystal system.

We consider this combined set of information to be essential for performing mineral identification in the field. Chemical abundances, when combined with analytical instruments such as XRF or LIBS, can confirm mineral composition. This can be combined with information on the mineral crystal system from Raman or VNIR/SWIR spectra, enhancing the accuracy of mineral classification. Raman and VNIR spectroscopy are particularly important analytical tools because of their complementarity in identifications of minerals to X-ray diffraction [10, 12]. They can highlight differences in crystallography where spatial variation in chemical composition is on a scale, or has a morphology, that precludes the use of X-ray diffraction.

2. Experimental design, materials and methods

2.1. The PANGAEA mineralogical database – bibliographic analysis

To populate the Summary Catalog portion of the Mineralogical Database, we conducted a systematic literature search using combinations of three keywords on four databases/search engines: the SAO/NASA ADS, JSTOR, ScienceDirect, and Ingentaconnect. All searches were conducted across the full-text of each paper, and combined the following keywords: 'Petrography' or 'Mineralogy', and specific keyword related to the celestial body/locality: 'Moon', 'Lunar', 'Mars', 'Meteorite', 'Nördlinger Ries impact crater', 'Lanzarote', 'Lofoten' and 'Bletterbach'. In addition, we searched for the list of confirmed minerals from the above localities using www.mindat.org. The physical properties of each mineral, such as hardness, relative density and the crystal systems, were reported based on the data from www.mindat.org and www.webmineral.com. The chemical abundances for each mineral were generated using bespoke python code, with each mineral's empirical formula as its input. The obtained parameters were compared with the values from http://www.webmineral.com to check reliability.

2.2. Raman and VNIR spectroscopic libraries

2.2.1. Online open access archives

The Mineralogical Database contains a collection of Raman and VNIR spectra for each mineral entry in the Summary Catalog, where they were possible to acquire. To achieve this, our library is composed of spectra acquired from online libraries, and from our own measurements conducted at European Astronaut Center (see Section 2.2.2). In both cases, only high quality spectra (defined as those with clearly identified spectral features or those validated through our own learning validation methodology through machine learning [6]) were selected, and measurements containing mineral mixtures were omitted in favor of those taken from pure samples (crystals or powders).

We searched several open access online archives for VNIR and Raman spectra for all the mineral entries in the Summary Catalog:

- VNIR-SWIR
  - NASA Reflectance Experiment Laboratory (RELAB) spectral database issued on December 31st 2019 at Brown University (5690 spectra — 88% of our VNIR spectra library): http://www.planetary.brown.edu/relab
  - United States Geological Survey (USGS) Spectral Library Version 7 [13] (1084 spectra) https://archive.usgs.gov/archive/sites/speclab.cr.usgs.gov/spectral-lib.html
  - ECOSTRESS (formerly ASTER) VNIR-SWIR spectral library version 1.0 [1] (724 spectra) that includes data from other spectral libraries, including spectral archives of Johns Hopkins University and Jet Propulsion Laboratory https://speclib.jpl.nasa.gov
  - CSIRO Mineral Spectral Libraries (64 VNIR spectra) https://mineralspectrallibraries.csiro.au/Home/SpectralLibraryDetails/4
  - Stony Brook University, Vibrational Spectroscopy Laboratory (a few VNIR spectra) http://aram.ess.sunysb.edu/tglotch/nir.html
- Raman
  - RRUFF database of Raman spectra http://rruff.info version from 2020 to 01–28. We have only used “excellent”- and “fair”- qualified spectra of the minerals confirmed with X-ray diffraction and/or Electron microprobe analysis (5408 spectra for 350 minerals — 88% of our Raman spectra library)
  - SOLSA Open Database of Raman Spectra used for the SOLSA H2020 project last updated on 2019–10–15 (284 spectra of 71 minerals) https://solsa.crystallography.net/rod/index.php
  - ‘Handbook of Raman Spectra for Geology’ is an archive of Laboratoire de Géologie de Lyon (34 spectra); http://www.geologie-lyon.fr/Raman/
  - The mineral Raman spectra of Parma University (66 spectra of 42 minerals); http://www.fis.unipr.it/phevix/ramandb.php
  - Romanian Database of Raman Spectroscopy http://rdrs.uaic.ro/ (60 spectra of 45 minerals)

2.2.2. ESA and collaborators spectroscopic measurements

The majority of existing spectral databases contain metadata attached to each mineral spectra. This includes information such as measurement parameters and sample details. However, often the information is incomplete and the quality of the spectra varies significantly. To address this shortcoming in our database, we have cross matched various spectra and selected the best in terms of sample purity and spectral features qualities. Initially, we aimed to collect at least three different samples per mineral species. However, it was often impossible to find enough high quality spectra for each of the required minerals. Therefore, we attempted to fill in the missing data by conducting our own measurements. Our spectra were acquired at two PANGAEA astronaut-training locations (Ries Crater, Germany, and Lanzarote, Spain), and from minerals kindly provided by partner museums and mineralogical collections, including:

- Mineralogical Museum Bonn (43 mineral species).
- GeoMuseum Cologne (43 minerals)
- Mineralogical State Collection in Munich (95 minerals)
- Ries Crater Museum (22 minerals)
- Lanzarote PANGAEA sites (26 minerals)

In addition, we were generously provided with the additional spectroscopic measurements:

- MSC-RD - Mineralogical State Collection Raman Database [14], so far this database is not yet completed and not online. However, data can be obtained on demand. The MSC-RD consists of data from terrestrial minerals, as well as from meteorites originating from Mars, the Moon and other unknown origins. Measurements were made with green (532 nm), red (638 nm) and IR (785 nm) lasers. Laser power was varied from 1 µW to 40 mW.

The following VNIR/SWIR reflective and Raman spectrometers were used for our measurements:

- VNIR/SWIR spectrometer: TerraSpec HALO by ASD/Malvern-Panalytical
- Raman spectrometers: XploRA by HORIBA Scientific; Inspector 300 by SciAps, BRAVO by Bruker

At the time of writing, we have collected 443 VNIR/SWIR spectra from 109 minerals and 695 Raman spectra from 153 minerals.

2.3. Spectra processing and creating the average spectra

Individual Raman and VNIR spectral compilations for each mineral were processed to produce mean homogenized spectra. Before this process began, the baseline (continuum) of the unprocessed (raw) Raman spectra were automatically fitted and subtracted. This was not carried out for the VNIR/SWIR spectra. Following this, all spectra were subject to:

- Interpolation to the same linear spectral resolution and range (1 cm^{-1}, 85..1800 cm^{-1} for Raman; 1 nm, 350..2500 nm for VNIR/SWIR)
- "Min-max" normalization of the spectral intensities to the range from 0 to 1.
- Missing values were masked out before weight-averaging of the spectra
- Spurious (outlying) spectra were removed if their cosine distance from the average spectrum was higher than 0.5. Outlier removal was performed to ensure that the final averaged spectra was not skewed by extremely divergent spectra originating from random instrument artifacts or sample misclassification.

Fig. 1 shows an example of Raman and VNIR spectra for Dolomite, with the average spectra created following our masked weight-average procedure. The average spectra and the standard deviations are saved as delimited text files that use a comma to separate values ("CSV"). Each filename is written as "'Mineral name'-ave_'total number of averaged spectra'".

The first two lines of these CSV files include headers (denoted with "#") that provide information on the mineral name. The codes and numbers after the name are related to the amount and archive sources of individual spectra used to generate the averaged spectra: 'ESA' refers to the number of our measurements, while USGS, ECOSPEC, RELAB, RRUFF, etc. correspond to the spectral numbers from corresponding archives.

Below are examples of the calculated average VNIR and Raman spectra for mineral Dolomite:

<u>Folder:</u> Mean_VNIR/

File: Dolomite-ave_104.txt

 # Dolomite(104):ESA=1,USGS=7,ECOSTRESS=12,RELAB=84
 # Wavelength [nm], Reflectance(mean), STDs
350.0, 0.162094, 0.220057
...

<u>Folder:</u> Mean_Raman

<u>File:</u> Dolomite-ave_77.txt

 # Dolomite(77):ESA=8,RRUFF=69
 # Wavenumber [cm-1], Raman scattering(mean), STDs
85.0, 0.006337, 0.002590
...

Overall, our spectroscopic archive contains 213 average VNIR- and 215 average Raman-spectra.

The current census of planetary analog minerals and archived VNIR and Raman spectra is presented in Fig. 2.

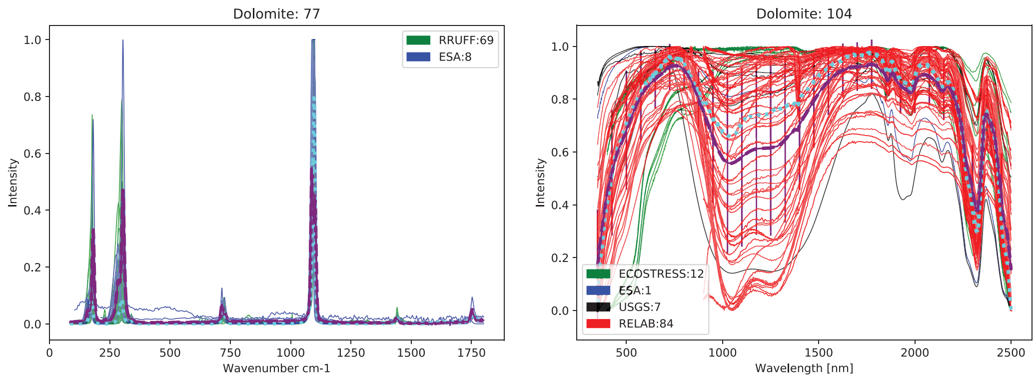

Fig. 1. A comparison of all Raman and VNIR spectra collected for Dolomite, including calculated masked weighted-averages (dashed purple), masked median (dotted cyan) spectra, and some standard deviations from the average spectra.

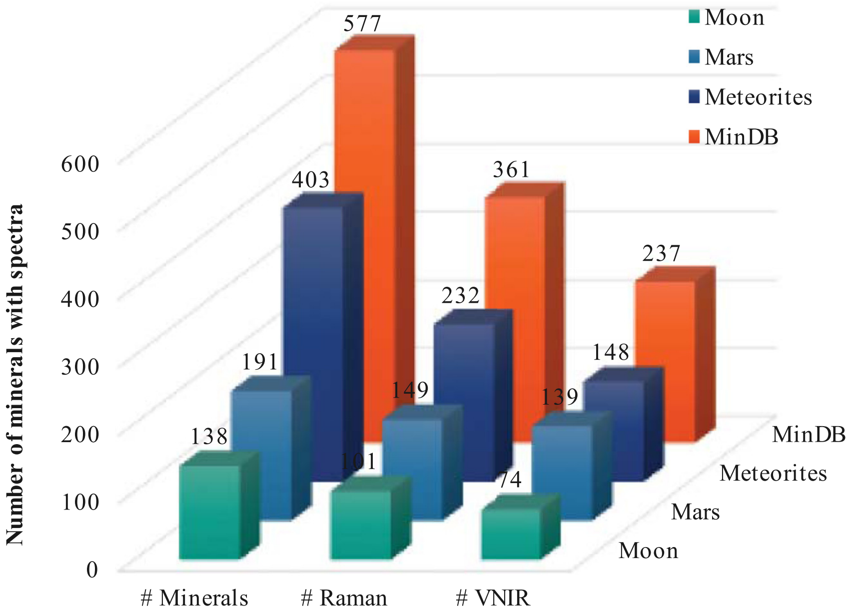

Fig. 2. The current census of the minerals with archived molecular spectra.

Declaration of Competing Interest

The authors declare that there are no known competing financial interests or personal relatiosnhips that have or could be perceived to have influenced the work reported in this article.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2020.105985.

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