DEVELOPMENT OF A RAMAN SPECTRAL DATABASE FOR LUNAR SCIENCE: A LITTLE SALSA ON YOUR DATA. S. Manigand[1], N. Turenne[1], S. Sidhu[1], S. Connell[1], S. M. Potin[1], D. Applin[1] and E. A. Cloutis[1]. [1]Centre for Terrestrial and Planetary Exploration (C-TAPE), University of Winnipeg, 515 Portage Avenue, Winnipeg, Manitoba, Canada.

Introduction: Raman spectroscopy is gaining interest of the community to investigate in situ geological samples in a non-destructive and remote way [e.g., 1]. Upcoming insights from the SuperCam instrument on board NASA Perseverance [2] has motivated the planning of Raman-equipped multiple remote exploration mission on Mars, with the 2022 ESA-Roscosmos Rosalind Franklin rover [3], and back on the Moon, such as the CNSA Chang'e-7 2024 lunar south pole lander and rover mission [4].

In this context, we present the development of a new Raman spectral database of lunar-relevant samples: The Spectral Analyses of Lunar Soils and Analogues Database (SALSA database). This database will support future lunar missions hosting a Raman instrument by storing and sharing the data to the scientific community, and providing a set of analytic tools to facilitate Raman spectral analysis.

Architecture and Database Features: The SALSA database is associated with the LunaR spectrometer project, conducted under the CSA's Lunar Exploration Accelerator Program (LEAP [5], currently in phase 0). LunaR is a Raman spectrometer that will be on board a future lunar rover. The spectra will be added to the database and freely accessible via a public website interface. The interface will be made the most ergonomically possible way to facilitate access to the users. Both the data and the website will be hosted by the University of Winnipeg's C-TAPE data centre (http://www.uwinnipeg.ca/c-tape).

The SALSA database is built as a normalized, relational database, based on Structured Query Language (SQL). Figure 1 shows the architecture diagram of the database. Information on the samples, the spectrum metadata, the laboratory, and the related publications are stored in different tables, linked together through elaborated SQL queries. The spectra themselves are stored in individual tables that are pointed by a single element from the spectrum meta-data table. The intrinsic limit for the number of objects that an SQL database can define offers the possibility to host a large number of spectra (>10.000.000 spectra).

In addition to the data, a set of spectral analysis tools will be freely available, as Python scripts. These tools can be used to: (1) read the exported spectra from SALSA, (2) remove sharp fluorescence or spurious peaks, (3) fit and subtract the continuum background, and (4) detect and fit Raman peaks.

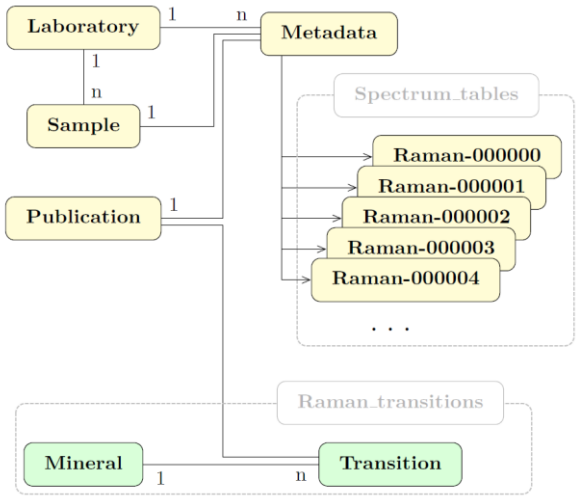

Figure 1: Architecture diagram of the SALSA database. The yellow and green boxes correspond to the tables in the initial and augmented versions of the database, respectively. Associations between tables are represented by the black lines with the modality '1' or 'n' on each side. Arrows correspond to 'one-to-one' associations.

Spectra Collection: The SALSA database focuses on Raman spectra relevant to lunar science and exploration, including new and existing laboratory Raman measurements of lunar samples, analogues, and end member minerals. The data that will be included in the database should be corrected from any instrumental bias, however, they will, in general, include the continuum background. The choice of the continuum background subtracting method is left to the user. The user-friendly website interface will allow users to upload their data on their own and update/correct the data and headers of their contributions.

We started a laboratory measurement campaign of mono-modal geological sample of lunar analogues. Currently, the data collection counts more than 200 spectra taken from more than 60 different samples, including mineral types such as ortho-/clino-pyroxenes, olivines, silicates, feldspars, ilmenites and other oxides. This first campaign will consist of ~450 spectra of ~150 samples, including a few lunar samples returned from Apollo missions, and will be a basis that the community can contribute to with time.

Augmented version: We have planned to expand the spectra database to a Raman transitions list similar, in some aspects, to the rotational transitions databases such as the widely used Cologne Database for Molecular Spectroscopy (CDMS, [6, 7]). This additional table will be linked to the spectra where the Raman signature has been found and the associated publication. Multiple assignations of the same Raman transition will allow us and the community to extract statistical information, such as the peak position distribution or the correlation between peak parameters, about the spectroscopic signature depending on the physical condition (temperature, pressure, etc.) of the sample or the mixing composition. The submission of new transitions entries will be systematically reviewed in order to ensure the consistency of the tables.

An initial batch of Raman transitions will be gathered, in relation to the minerals that compose the initial batch of Raman spectra. This collection will include both fitted transitions resulting from experimental measurements [e.g., 8, 9] and theoretical Raman studies [e.g., 11-14].

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References: [1] Hipkin V.J. et al. (2017) LEAG 2017; abstract #5054. [2] Wiens et al. (2012) Space Science Reviews, 170, 167-227. [3] Rull et al. (2017) Astrobiology, 17, 627-654. [4] Zou et al. (2020) LPSC, 51, 1755. [5] https://asc-csa.gc.ca/eng/funding-programs/programs/leap/about.asp. [6] Muller, H. S. P. et al. (2001) A&A, 370, L49-L52. [7] Muller, H. S. P. et al. (2005) J. Mol. Struct., 742, 1-3, 215-227. [8] Ling, Z. C. et al. (2011) Icarus, 211, 101-113. [9] Wang, A. et al. (2004) American Mineralogist, 89, 665-680. [11] Griffith, W. P. (1969) J. Chem. Soc. (A), 1372-1377. [12] Griffith, W. P. (1970) J. Chem. Soc. (A), 286-291. [13] Tuinstra, F. & Koenig, J. L. (1970) J. Chem. Phys., 53, 1126. [14] Chopelas, A. (1991) American Mineralogist, 76, 1101-1109.