

# SSHADE Users Newsletter - September 2023

Dear SSHADE users,

As the 'new' [band list database](#) and its search / visualization / export interfaces are now online since almost 2 years and we recently passed the 50-bandlist threshold, with over 1150 absorption and Raman bands described, it's time to introduce it in some more details.

In addition, we will continue to give you tips to make your use of SSHADE easier. In this newsletter, we will show you how to **search for publications** in the SSHADE database.

## General info

On the shaded-side of the **software development for the coming months**:

- Improvement of the efficiency of the 'search bar' tool with automatic search on synonyms and words equivalent to your input.
- A series of tool to allow you to directly compare your own data to with SSHADE data
- A few additional improvements on the band list interfaces.

## Focus on the band list database

The [band list database](#), which initially went online on 1<sup>st</sup> October 2021, contains a collection of "band lists" drawn up on the basis of exhaustive compilations and critical review of all relevant data published in various journals (up to 40 articles per band list!) as well as additional analyses of spectra available in the SSHADE database or in other databases.

A 'band list' is a list of band parameters (position, width, intensity, ...) and vibration modes of:

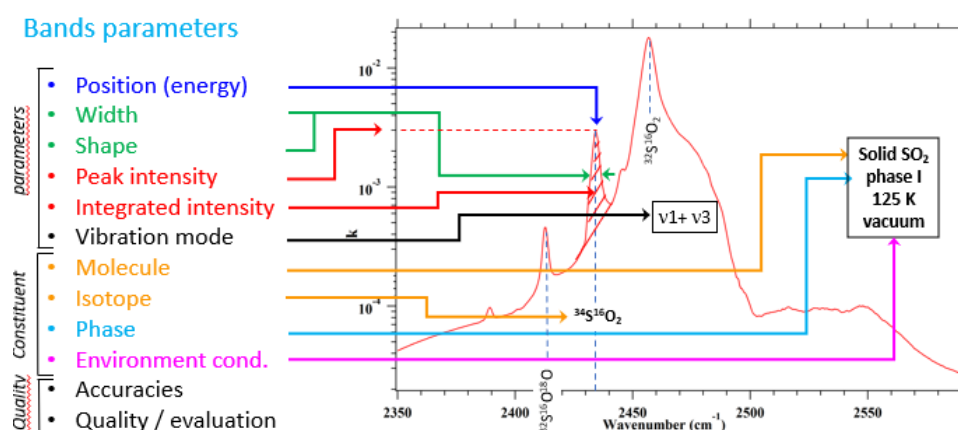
- a **molecule** in a simple solid molecular **constituent** (2-3 species maxi)
- or a **mineral** or a **ionic/covalent solid**

with well-defined **phase** and **composition** (unique or small range)

- ✓ includes bands of all isotopes (sub-band lists)
- ✓ can be provided for different environment conditions (T, P)
- ✓ cover the VUV, UV, Vis, Near-IR, Mid-IR and Far-IR ranges

Several band lists can cover several composition ranges (e.g., for solid solution series)

For example: Siderite (pure), Mg-Siderite, Fe-Magnesite, Magnesite (pure)



There are currently 54 band lists available in 2 categories: **absorption** or **Raman**

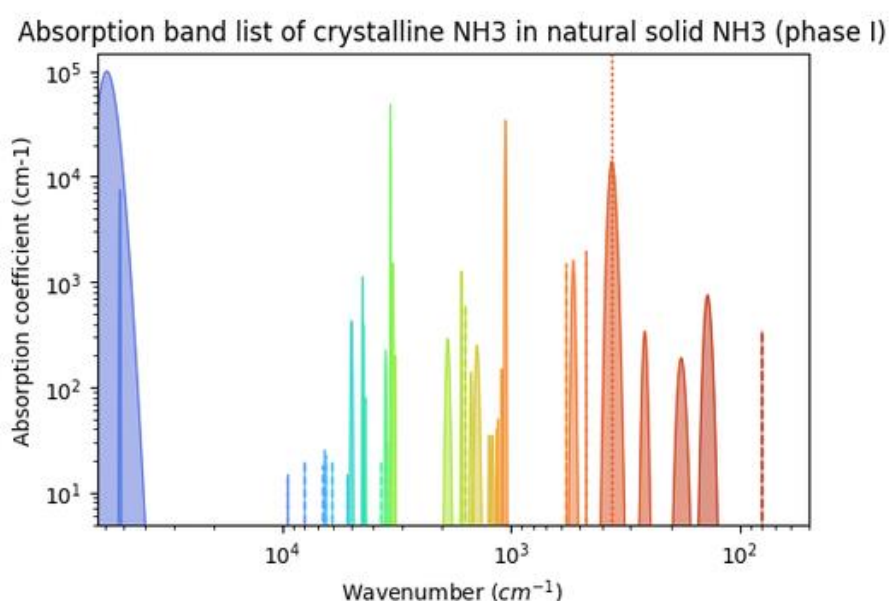
They describe the spectral bands of:

- ✓ simple ices, organics and nitriles in various amorphous and crystalline phases
- ✓ minerals (mostly carbonates yet)

Dedicated **search and visualization** interfaces have been developed for this band list database. You certainly saw the 2 additional search buttons on the front page.

In particular, the search interface, in addition to solid composition filters, allows you to **find which compound may absorb at one (or more) specific wavelength** (+/- some uncertainty), which should be very useful to identify unknown absorption or emission bands.

A special feature of the plotting tool allows you to display a band list simulated as a spectrum with several options to plot the bands separately, added as a spectrum, or grouped by isotope.



If you want more details you can look at our [EPSC-2021 poster](#) or even read the [final report of delivery of this database](#) (23p.) available in the [SSHADÉ Wiki](#).

This database, which is currently being developed as part of the Europlanet-2024 (H-2020) programme, aims to add to its content on a regular basis, but it's going to be a long-term task...

Do not hesitate to explore all the existing data in this new database, and to provide us feedback (which additional data you would like?, ...) through the [SSHADÉ contact e-mail](#) !

### [How to search for publications:](#)

With the creation of the new band list database, many major publications on VUV, infrared and Raman spectroscopy of ices and minerals have been included (and linked) in the SSHADÉ database, in addition to the publications linked to the spectra provided by each partner database. This gives us the opportunity to focus on the search for publication in this newsletter.

Currently, SSHADÉ contains **more than 550 references concerning the spectroscopy of solids** of interest for astrophysical objects, geophysics and several fields of physico-chemistry, optics...By clicking on "Search publications" on the welcome page, you can discover interesting new articles.



## Solid Spectroscopy Hosting Architecture of Databases and Expertise

You can use either the search-bar or various filters such as journal or author name, keywords, or words in the abstract. In particular specific keywords (molecule, mineral and meteorite names, spectral range...) have been extracted from each paper to provide a much more efficient and specialized search in spectroscopy of solids.

For example, searching '2023' will provide you with the last papers published in our field and recently added in the database.

The screenshot shows the SSHADE search interface. At the top, there is a search bar with the text "Write your keywords here or leave it empty to get all the data...". Below the search bar are four buttons: "Search spectra", "Search band lists", "Search bands", and "Search publications".

The search results page shows a search for "2023". The results are displayed in a table with the following columns: "First author", "Year", and "Title". There are 8 publications listed.

First author	Year	Title
Quirico E.	2023	Compositional heterogeneity of insoluble organic matter extracted from asteroid Ryugu samples
Urashima Shu-hei	2023	Non-destructive estimation of the cation composition of natural carbonates by micro-Raman spectroscopy
El Mohammad Sabah	2023	Elucidation of Metal-Sugar Complexes: When Tungstate Combines with d-Mannose
Bonal L.	2023	The thermal history of Ryugu based on Raman characterization of Hayabusa2 samples
Eschrig J.	2023	The hydration history of unequilibrated ordinary chondrites
Sultana R.	2023	Reflection, emission, and polarization properties of surfaces made of hyperfine grains, and implications for the nature of primitive small bodies
Bott N.	2023	Effects of Temperature on Visible and Infrared Spectra of Mercury Minerals Analogues.
Prestgard T.	2023	The parent bodies of CR chondrites and their secondary history

For each published article, you can find a direct link to the journal page for downloading the paper.

Do not hesitate to use this search tool and you may discover new interesting papers in the field of spectroscopy!

Have fun with SSHADE data!

The SSHADE Team

All previous user newsletters are stored in the dedicated ['News' page](#) of the [SSHADE Wiki](#)

*You are receiving this SSHADE User Newsletter because you are a registered user of SSHADE ([www.sshade.eu](http://www.sshade.eu)). If you do not wish to receive them, please send an e-mail to our contact address ([contact@sshade.eu](mailto:contact@sshade.eu)) with the subject 'unsubscribe User Newsletter'.*