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SSHADE-BandList, the new database of spectroscopy band lists of solids

Bernard Schmitt, Manon Furrer, Damien Albert, Philippe Bollard, Maria Gorbacheva, Lydie Bonal, and Olivier Poch
CNRS / Univ. Grenoble Alpes, Institut de Planétologie et Astrophysique de Grenoble, Grenoble Cedex 9, France (bernard.schmitt@univ-grenoble-alpes.fr)

Introduction

The SSHADE database infrastructure (1) (http://www.sshade.eu) hosts the databases of about 30 experimental research groups in spectroscopy of solids from 15 countries. It currently provides to all researcher over 4000 spectra of many different types of solids (ices, minerals, carbonaceous matters, meteorites…) over a very wide range of wavelengths (mostly X-ray and VUV to sub-mm)

However, although these data are invaluable for the community, one type of information is still critically missing to easily interpret observations: the list of the characteristics of all the absorption bands of a given solid, called its 'band list'.

This type of database is well developed for gases (see e.g. the VAMDC portal (2)), and it is even frequently the only type of spectral data available. But for solids (and liquids) there is currently almost no database which provide such information (only in some restricted fields, such as Raman spectroscopy of minerals, e.g. the WURM database (3)).

This critical lack triggered us to develop such a band list database containing the characteristics of electronic, vibration and phonon bands of various solids (ices, simple organics, minerals) of astrophysical interest to help:

- identify absorption or emission bands from solids observed in various astrophysical environments or in laboratory simulations
- determine the environment of the molecule or mineral (composition, isotopes, mixing, phase, T, P, …)
- select the best spectra in SSHADE to compare with observation, or to use in models

What is a band list of a solid?

A 'band list' is a list of band parameters and vibration modes of a molecule in a simple molecular constituent (3 species maximum), or of a mineral or a ionic/covalent solid, with a well-defined phase and composition (fixed or small range). It includes the bands of all isotopes (sub-bandlists) and can be provided for different environments (T, P, …).

The SSHADE 'band list' database provides the band parameters (position, width, peak and/or

integrated intensity, and their accuracy, isotopic species involved, mode assignment, ...) of a progressively increasing number of solids and simple compounds (with different compositions) of astrophysical and planetary interest in various phases (crystallines, amorphous, ...) at different temperatures or pressures.

We are feeding this database through exhaustive compilations and critical reviews of all data published in various journals for pure ices and molecular solids and their simple compounds (solid solution, hydrates, clathrates, ...), including the own works of the SSHADE consortium partners. We will continue in a second step with band lists of minerals. However, this is a tremendous scientific work, expected to last many years… For example, the infrared spectrum of pure solid CO in its cubic α phase has been the subject of more than 35 papers scattered in 25 different journals over the period 1961-2020…

SSHADE band list database and interface

A specific data model, SSDM-BL (Solid Spectroscopy Data Model – Band List), has been first developed in order to accurately describe and link all the parameters necessary to describe both the solid constituent and the band list itself. A structured database storing all these data and metadata, has then be set up based on this data model. A data review tool (excel file), a data convertor to a XML import file, as well as a data import tool have been developed to feed the database.

Then an efficient search tool allows you to search either a band list or a specific band thanks to a combination between a 'search bar' and a set of filters on various parameters, such as band position, width and intensity, expected molecular or atomic composition, type of vibration, temperature and pressure. The search result are provided as a table with band list title or the main band parameters allowing the users to select the most relevant ones. He can then display the selected band list graphically, thanks to a simulator of 'band list spectra', with various unit and display options. The data can be exported as a table containing the main parameters of all the bands of the band list, as well as detailed metadata of the band list and all its bands. A data reference and a DOI will be associated with each band list.

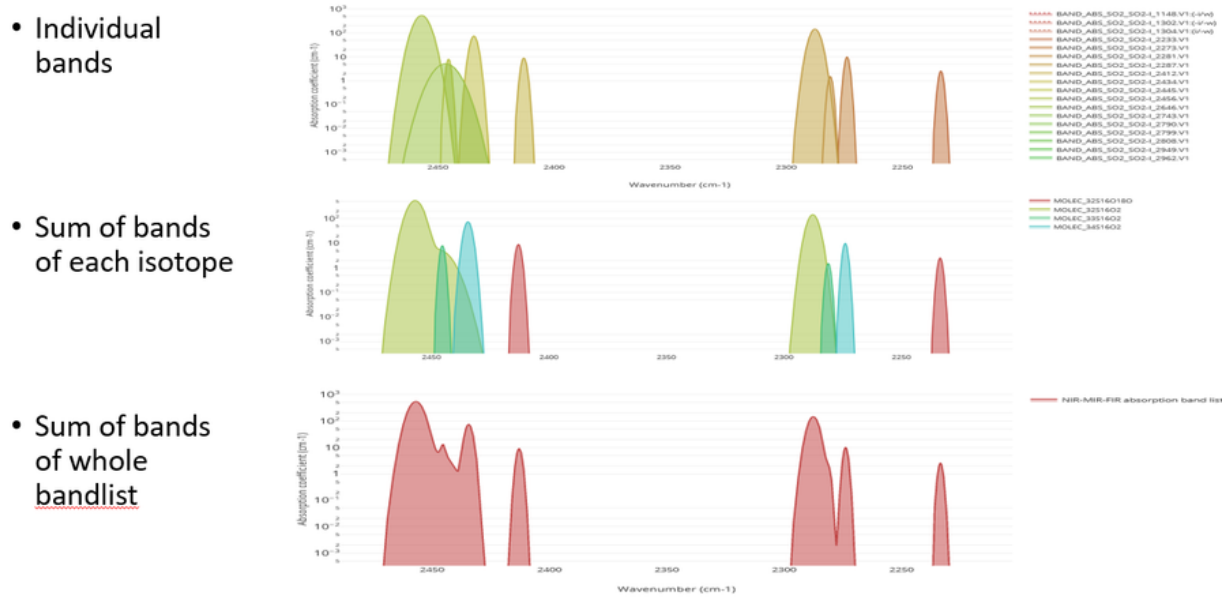

Figure 1: *the plotting tool allow to simulate the indivudual bands, the spectrum with all bands of a given isotope, as well as the full spectrum of the band list.*

SSHADE in Virtual Observatory

SSHADE-Bandlist will be later a service of the VESPA Virtual Planetary Observatory. It will be

accessible via the EPN-TAP protocol, which will allow comparison with observational data and mass processing in the VESPA environment through a series of dedicated spectroscopy plotting and analysing tools.

Conclusion

This band list database should become a key tool for astronomers and planetary scientists to identify unknown absorption bands observed in the spectra of the surface or atmosphere of many astrophysical and solar system objects. Once the best candidate solid found by the user, the tool will link to the most relevant spectral datasets present in the SSHADE databases. These data can then be used for direct comparison with observations, or to model them through radiative transfer codes.

However its feeding will strongly depend on the scientific manpower available, and on the contribution of the SSHADE partners and of the community.

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