
The new VUV-Vis-IR Bandlist database of ices and minerals in the SSHADE European database infrastructure

Bernard Schmitt^{*1}, Damien Albert², Manon Furrer¹, Philippe Bollard², Lucia Mandon³, Maria Gorbacheva⁴, Apolline Leclef⁵, Lydie Bonal⁵, Olivier Poch⁵, and Pierre Beck⁵

¹Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) – Centre National d'études Spatiales [Toulouse], observatoire des sciences de l'univers de Grenoble, i, Centre National d'études Spatiales [Toulouse] – France

²Observatoire des Sciences de l'Université de Grenoble – Institut National des Sciences de l'Univers : UAR832 / UMS832, Université Savoie Mont Blanc, Centre National de la Recherche Scientifique : UAR832 / UMS832, Institut National de Recherche pour l'Agriculture, l'Alimentation et l'Environnement : UMS1484, Université Grenoble Alpes, Météo-France – France

³Laboratoire d'études spatiales et d'instrumentation en astrophysique – Institut National des Sciences de l'Univers : UMR8109, Observatoire de Paris, Sorbonne Université, Centre National de la Recherche Scientifique : UMR8109, Université Paris Cité : UMR₈₁₀₉ – *France*

⁴Flex-Studia – non – France

⁵Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) – Centre National de la Recherche Scientifique : UMR5274, Institut national des sciences de l'Université : UMS832, Université Grenoble Alpes, Centre national d'études spatiales - CNES (FRANCE), Institut national des sciences de l'Université : UMS832 – France

Résumé

The SSHADE database infrastructure (www.sshade.eu) hosts more than 5000 spectra from about 30 experimental research groups in spectroscopy of solids from 15 countries. In particular it provides a large number of transmission, reflection and Raman spectra (and their products: absorption coefficients, optical constants...) of ices, minerals/rocks, organic materials, meteorites, ... in various phases (amorphous and crystalline) over a very wide range of wavelengths (mostly from VUV to sub-mm). Although these data are invaluable for the community, one type of information is still critically missing to help interpret laboratory, field or astronomical spectra: the list of the characteristics (band position, width, peak and integrated intensities, transition attribution, ...) of all the absorption bands of a given molecular solid or mineral, called its 'band list', complemented with a number of other metadata. There is currently almost no database which provides such information.

This triggered us to develop (within the Europlanet-2024 RI program) such a band list database containing the VUV-Vis-IR and Raman characteristics of electronic, vibration and phonon bands of various fundamental solids (molecular solids and minerals) to help:

- identify absorption or emission bands from laboratory, field or astronomical spectra.
- determine the composition and phase of the molecular solid or mineral

^{*}Intervenant

- select spectral data in SSHADE to compare with observation, or to use in models.

Two new interfaces in SSHADE ("search bandlists" & "search bands") allow to search solids within a given spectral range or with the position from one to three bands, complemented by other spectral constraints, as well as constraints on its chemical composition and environment (T, P).

We will present this band list database and its interfaces, opened a few months ago. We started to fill the database with VUV-Vis-IR and Raman data of fundamental minerals and inorganic and organic ices, after a dedicated and extensive review of the literature, sometimes complemented with detailed analyses of relevant high-quality spectra stored in SSHADE.