SSHADE Users Newsletter – July 2024 –

Raman band list of carbonates

Dear SSHADE users,

Today, we would like to present the **Raman band lists for carbonates** available in the SSHADE database. These band lists provide robust spectral information that is invaluable for a wide range of research applications, from geological studies on Earth to planetary exploration.

Composed of carbonate ions $(CO_3)^{2-}$, these minerals are prevalent in various geological formations on Earth and other planetary bodies, such as Mars, asteroids.... They are important indicators of past water presence and climatic conditions, making them essential for understanding planetary evolution and environmental history.

We started a dedicated effort to provide an extensive set of band list data of carbonates by compiling (almost-)all publications on the Raman and infrared spectra of these carbonates and reanalyzing some e-published spectra (RRUFF, ...) as well as a series of new measurements we performed at ENS-Lyon and ISTerre labs. Currently, **SSHADE offers 33 Raman band lists for carbonates**, covering a diverse array of composition. These band lists provide comprehensive spectral data, including band parameters such as position, width, intensity, and vibration modes. In addition to the "endmembers" minerals we are also developing specific band lists for the solid solution, such as for ferroan dolomite or ferroan magnesite (Fe > 0.05).

◀ **Jul** Bandlist 🏚 Constituent **Bandlist** preview list Raman bandlist of natural Ferroan Magnesite Raman bandlist of natural Ferroan Magnesite Sub-Bandlist Phonon modes 100 Band 205.0 cm⁻¹: v_T (E_a) of (CO₃)²⁻ in Ferroan Magnesite 10^{-1} Band 317.0 cm⁻¹: v_L (E_a) of (CO₃)²⁻ in Ferroan Magnesite Relative intensity Sub-Bandlist Fundamental vibration modes 10-2 Sub-Bandlist ¹²C¹⁶O₃²⁻ in Fe-Magnesite Band 735.5 cm⁻¹: v₄ (E_q) of (CO₃)²⁻ in Ferroan Magnesite 10-3 Band 874.0 cm⁻¹: v₂ (A_q) of (CO₃)²⁻ in Ferroan Magnesite 500 1000 1250 1500 1750 2000 250 750 Band 1093.0 cm⁻¹: v₁ (A_{1q}) of (CO₃)²⁻ in Ferroan Magnesite Wavenumber (cm⁻¹) Title Band 1451.0 cm⁻¹: v₃ (E_a) of (CO₃)²⁻ in Ferroan Magnesite Raman bandlist of natural Ferroan Magnesite Constituent Sub-Bandlist Combination vibration and overtone modes Ferroan Magnesite (crystalline) Sub-Bandlist ¹²C¹⁶O₃²⁻ in Fe-Magnesite Spectral range(s) 150 - 1800 cm⁻ Band 1752.0 cm⁻¹: 2v₂ (A_{1g}) of (CO₃)²⁻ in Ferroan Magnesite Number of bands

Examples of applications include the <u>Raman bandlist of natural Ferroan Magnesite</u>, relevant for Martian geology:

Another example that may interest specialists in primitive bodies of our solar system concern the return to Earth of grains from the Hayabusa 2 mission. Their analysis has highlighted the presence of 3 types of carbonates on Ryugu (calcite, dolomite, ferroan-magnesite (breunnerite)), which are evidence of varying degrees of aqueous alteration. You can also find in SSHADE the <u>Raman bandlist of natural Dolomite</u>



To explore these resources, simply navigate through the band list search tool on SSHADE. Its filters allow you to search by specific carbonate minerals or spectral parameters. **If you know one, two or three band positions of your sample** with some good accuracy (better than a few cm⁻¹) **you can unambiguously identify your carbonate mineral** within those already in the database. Once more data on band lists is available, this tool should prove much more effective and accurate in identifying carbonates than conventional methods of correlating the baseline-corrected spectrum with spectra in the database (as in RRUFF and many Raman spectra analysis softwares).

SSHA	Solid Spectroscopy Hosting Architecture of Databases and Expertise				
Q	Write your keywords here or leave it empty to get all the data				
	Search spectra	Lttl Search band lists	Ltd Search bands	Search publications	

You can then visualize the bandlist spectrum (or one of its linked measured spectrum, if available), analyze band characteristics in detail and export the data.

Whether you are studying planetary geology, conducting environmental research, or exploring the origins of life, the Raman band lists for carbonates on SSHADE offer essential resources to advance your research. Visit SSHADE now to explore these band lists and discover how they can enhance your studies. In the coming months a new series of carbonate band lists will be added to make this tool even more efficient.

Have fun with SSHADE data and stay tuned for future data and user tools.

The SSHADE Team

All previous user newsletters are stored in the dedicated 'News' page of the SSHADE Wiki

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