

Pole surfaces planétaires – 17 Mai 2023

SSHADE: Database Infrastructure of Solid Spectroscopy



<https://www.sshade.eu>

Bernard Schmitt

Damien Albert, Etienne Dode, (Manon Furrer, Philippe Bolland), Lydie Bonal,
Zelia Dionnet, Lucia Mandon and the SSHADE Consortium Partners



The SSHADE database infrastructure

for Astrophysics, Planetary sciences and Geosciences

- ✓ Promote the creation of databases of laboratory & field **spectra of solids** in the **electromagnetic spectrum**
- ✓ Develop tools & interface to provide on-line the experimental data
 - ✓ Develop tools to analyze and use the data
- set of spectral databases from a Consortium of research groups
 - a common **bandlist database**



...

SSHADE European Consortium of Data Providers

Data from **20 solid spectroscopy experimental groups** in **11 countries**

20 active databases + 2 starting + 5 coming

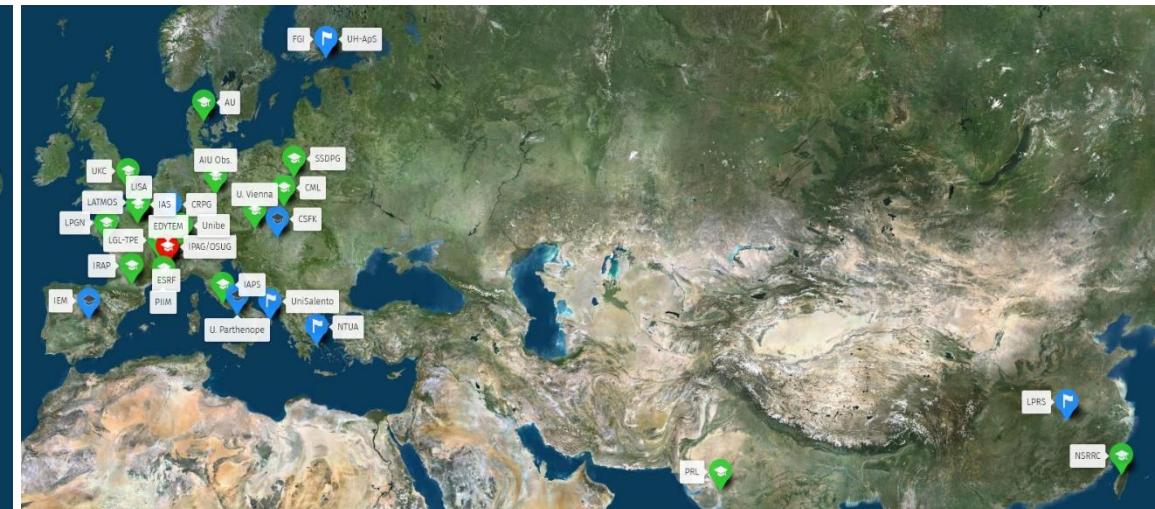
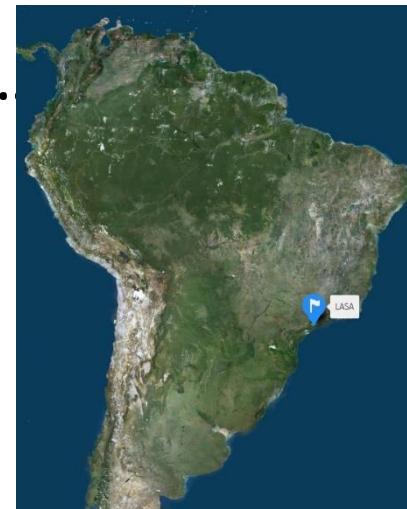
Each with particular expertise on:

- some wavelength ranges
- type of materials
- physico-chemical conditions
- specific techniques
- type of data and products, ..

> 6000 spectra in > 400 experiments

SSHADE : www.sshade.eu

SSHADE Wiki : wiki.sshade.eu



SSHADE-F : French Consortium of Data Providers

11 + 1 solid spectroscopy experimental groups (~30 people)

Planetary surfaces : 6+1 groups, Small objects : 5 groups, Aerosols : 1 group, Astro : 3 groups

- **SSHADE (OSUG, Grenoble)** **SNO5 / INSU**

(Bernard Schmitt, Philippe Bolland, Manon Furrer, Damien Albert, Lydie Bonal)

8 OSUs (OSUG, OSUPS, OMP, OSUNA, OVSQ, EFLUVE, Obs. Lyon... + OTELo)

- **IPAG / Planéto**, Grenoble (Bernard Schmitt, Lydie Bonal, Olivier Poch)

• **IRAP / PEPS**, Toulouse (Patrick Pinet, Yves Daydou)

• **IRAP / MICMAC**, Toulouse (Karine Demyk , Yves Daydou)

• **IAS**, Univ. Paris-Sud (Rosario Brunetto, Donia Baklouti, Zelia Dionnet)

• **LPG**, Univ. Nantes (Marion Massé, Manuel Giraud)

• **ESRF / FAME line**, Grenoble (Denis Testemale, Isabelle Kieffer)

• **PIIM**, Univ. Aix-Marseille (Patrice Theulé)

• **LISA**, Univ. Paris-Est (Nicolas Fray)

• **LATMOS / IMPEC**, IPSL (Nathalie Carrasco, Thomas Gautier)

• **LGL / ENS-Lyon** (Bruno Reynard, Gilles Montagnac, Razvan Caracas)

• **CRPG**, Nancy (Jessica Flahaut, Gen Ito)

Futur : **GEOPS**, Univ. Paris-Sud (François Andrieu, Frederic Schmidt)



Main aim of *SSHADE*

- Provide to the planetary, astrophysics and geophysics communities
 - Spectral and spectro-photometric data
 - on all types of solid materials (but also liquid)
 - from synthetic, terrestrial or extraterrestrial samples
 - Bandlist data
 - on fundamental minerals and simple molecular solids
 - with well documented information !!
 - on the spectra, samples, experiments ... + publications
 - with a data reference and a DOI per experiment
 - easy to cite & provides direct access to the data used

→ For the analysis, modeling and interpretation of spectroscopic observations

of planetary surfaces, small bodies, cosmomaterials, aerosols & grains, + inter- & circumstellar grains, exoplanets...

Development of *SSHADE*

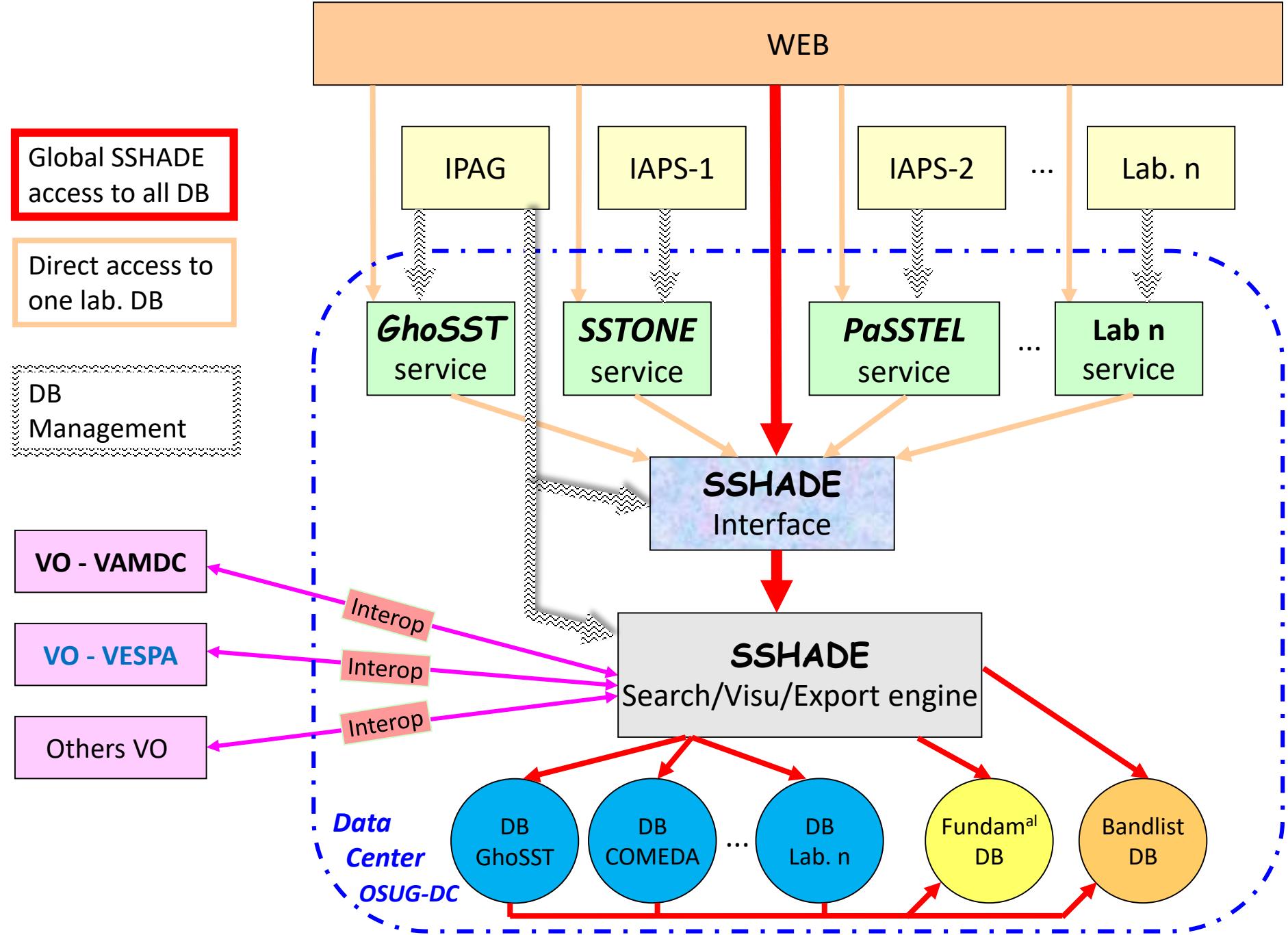
- **A common data model for Solid Spectroscopy (SSDM) describing:**

- Solid samples
 - on all types of solid materials
- Spectral data (instruments, experiments, spectra)
 - on all types of spectroscopic techniques

- **Database, interface and tools to:**

- Search, visualize, export spectral + bandlist data → for users
- To compare and analyze data (in preparation) → for users
- Prepare, import and manage
 - spectral data
 - fundamental data
 - bandlist data→ for data providers
- Manage databases en access right → for SSHADE team
- Manage databases en access right → for SSHADE bandlist
- Manage databases en access right → for SSHADE managers

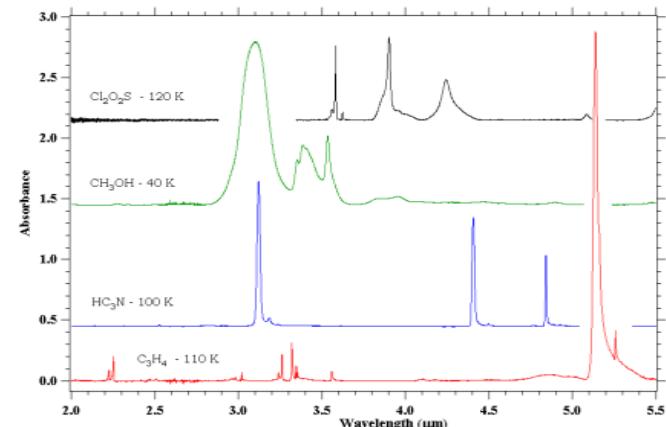
- **Tool to automatically create and validate a DOI per experiment**



Which types of materials and samples in *SSHADE-spectra* ?

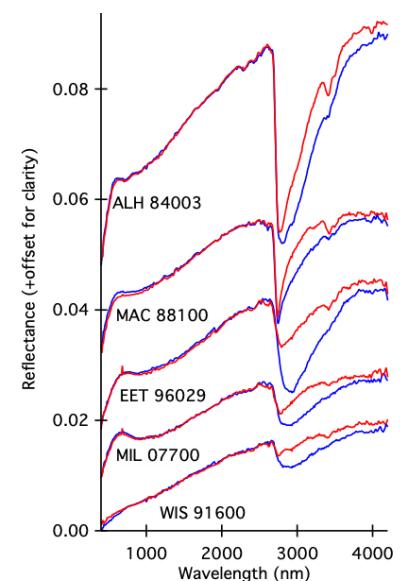
- **Materials**

- **Ices** (low/high T-P, mixtures, ...), molecular solids, snow...
- **Minerals**, rocks
- **Organic solids**, polymers, **Carbonaceous materials**, ...
- **Inorganic solids**, Metals, ...
- also some **liquids**



- **Samples**

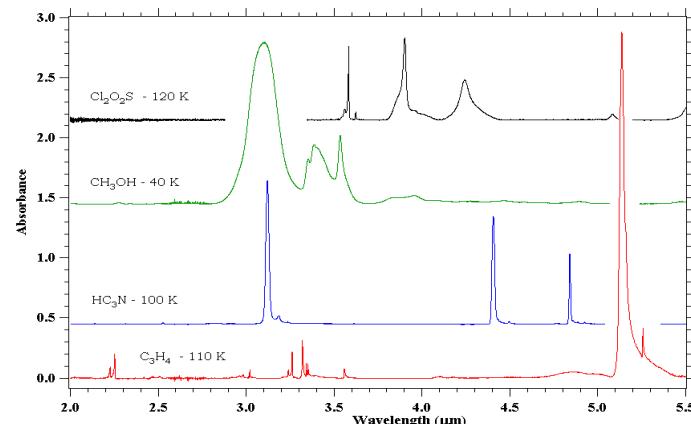
- **Synthesized** in the laboratory
- **Natural terrestrial analogues** collected or measured in the field
- **Cosmomaterials collected on Earth**: (micro-)meteorites, *IDPs*, ...
- **Extra-terrestrial samples** collected on planetary bodies: lunar soils...



Which types of spectra in SSHADE ?

- **Spectral ranges:**

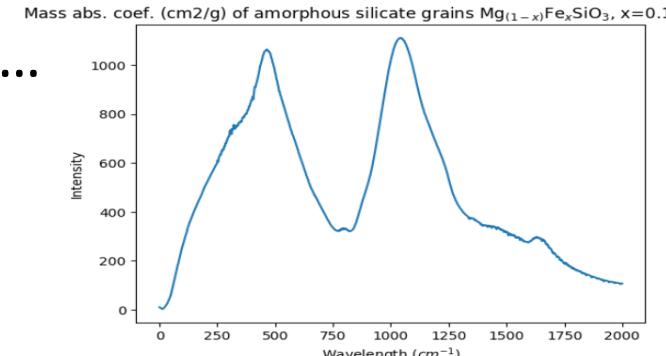
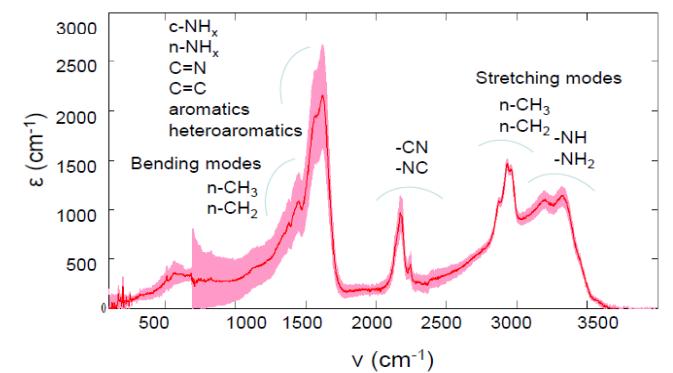
- Designed from γ -rays to radio wavelengths
- Now mostly **from VUV to sub-mm (0.2 μ m - 1mm), plus X-rays.**



- **Types of data:** (from level 1 to 5)

➤ **Spectra**

- **Transmission** spectra, absorption coefficients,
- **Optical constants** ...
- **Reflectance** spectra of surfaces, spectro-photometric functions, ...
- **Raman** spectra & micro-spectroscopy, *Fluorescence*, ...
- **XANES** spectra



Types of data for Terrestrial and Planetary surfaces

• Laboratory data:

- **Optical constants of ices** => radiative transfer
- **Reflectance** spectra of mineral, salts, organic & icy surfaces
 - Effect of grain size
 - Effect of temperature (90 – 500 K)
 - Effect of adsorption of H₂O
 - Effect of high pressure
- **Spectro-photometric functions** of mineral and icy surfaces
- **Raman** spectra & micro-spectroscopy of minerals
- **Surface processes:** differential sublimation of ices, space weathering, ...
- ...

• Planetary data:

- **Reflectance** spectra of Moon soils, ...
- **Reflectance, Raman** spectra of Meteorites, IDPs, ...

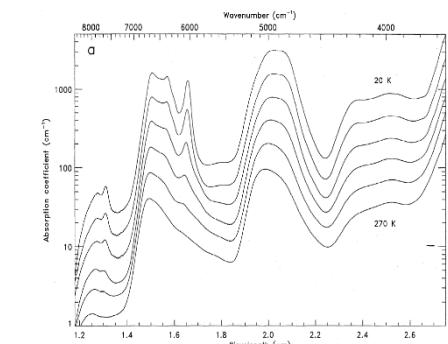
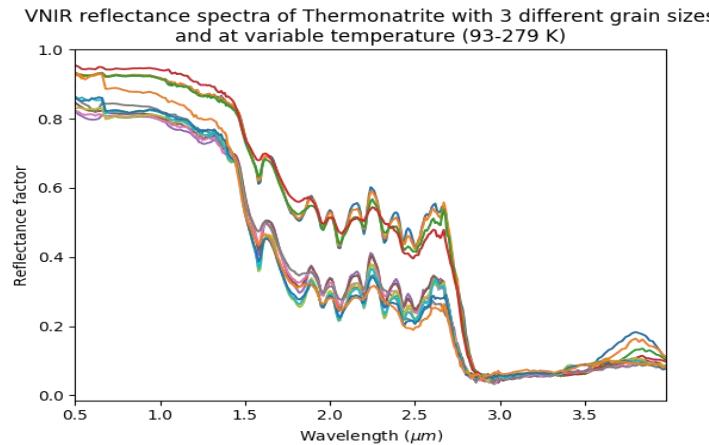


Figure 2. Illustration of the temperature dependence of our H₂O ice absorption coefficients. (a)

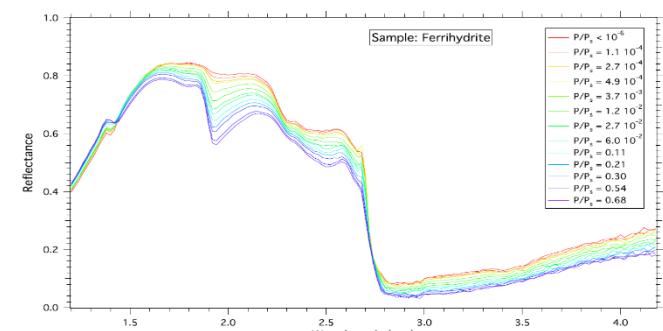


Fig. 11. Reflectance spectra of the ferrihydrite sample measured under different values of water vapor relative pressure.

SSHADE Spectral data

Types of mineral spectral data

> 3000 spectra on different minerals and rocks :

- Vis-NIR reflectance, BRDF
- MIR reflectance and transmission
- MIR specular reflection
- Optical constants
- Raman
- XANES

In various physical conditions : texture, grain size, temperature, phases, with adsorbed gases, ...

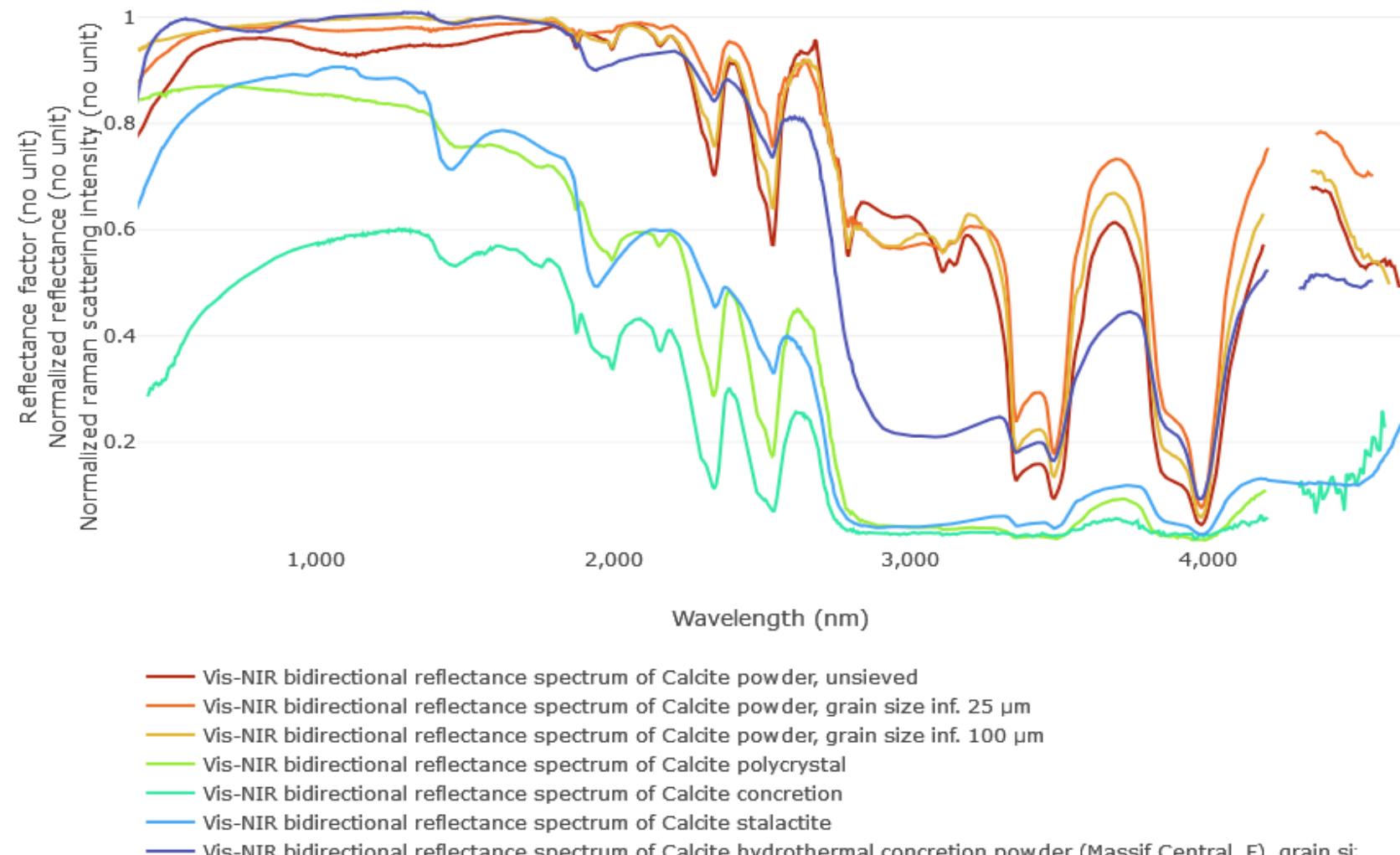
Mineral spectral data

Vis-NIR spectra: Texture



Calcites

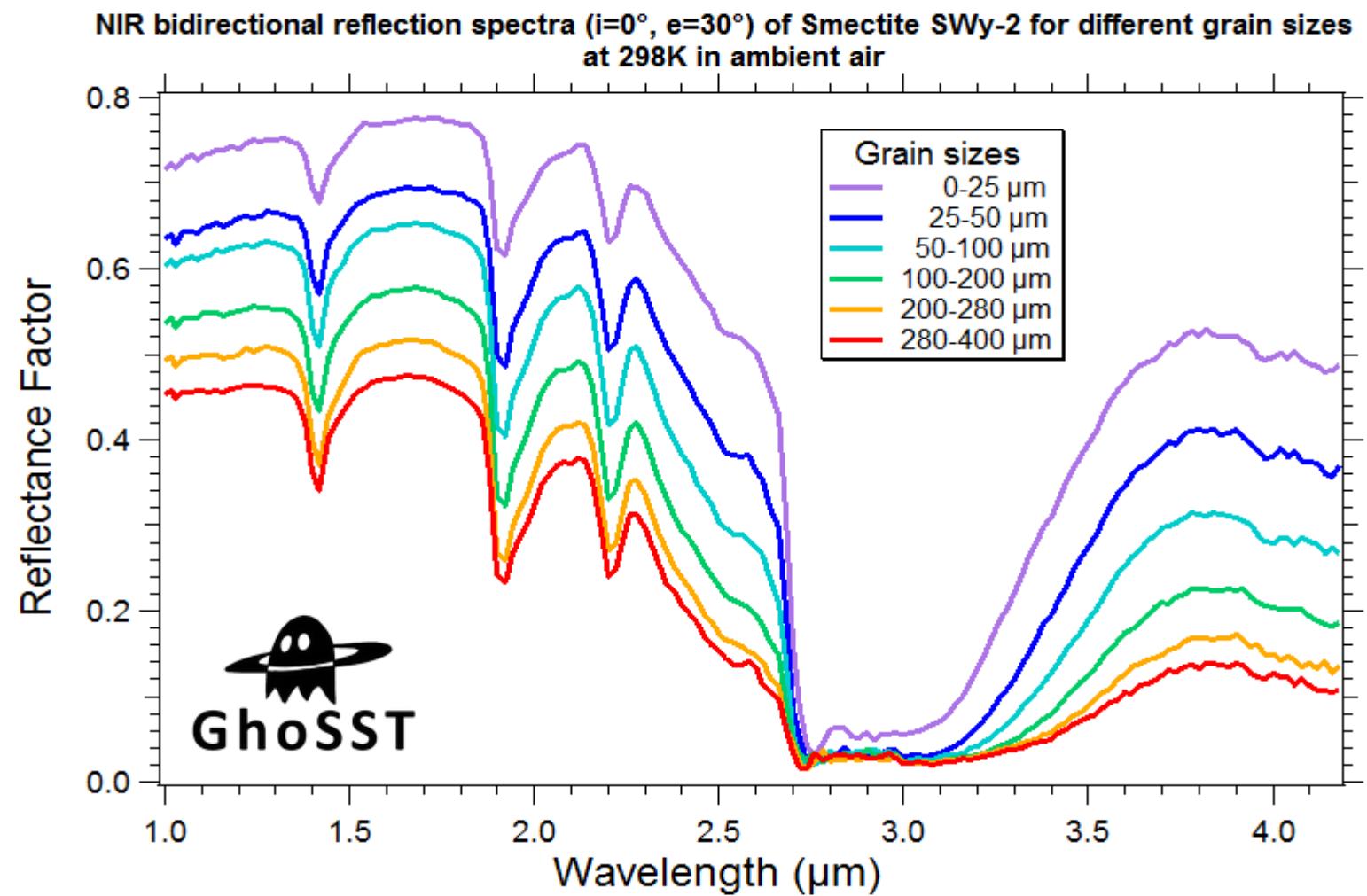
- Powders (ϕ)
- Rocks
- Concretions
- Polycrystal



Mineral spectral data

Vis-NIR spectra:
Grain size effect
25 to 400 μm

Na-Montmorillonite



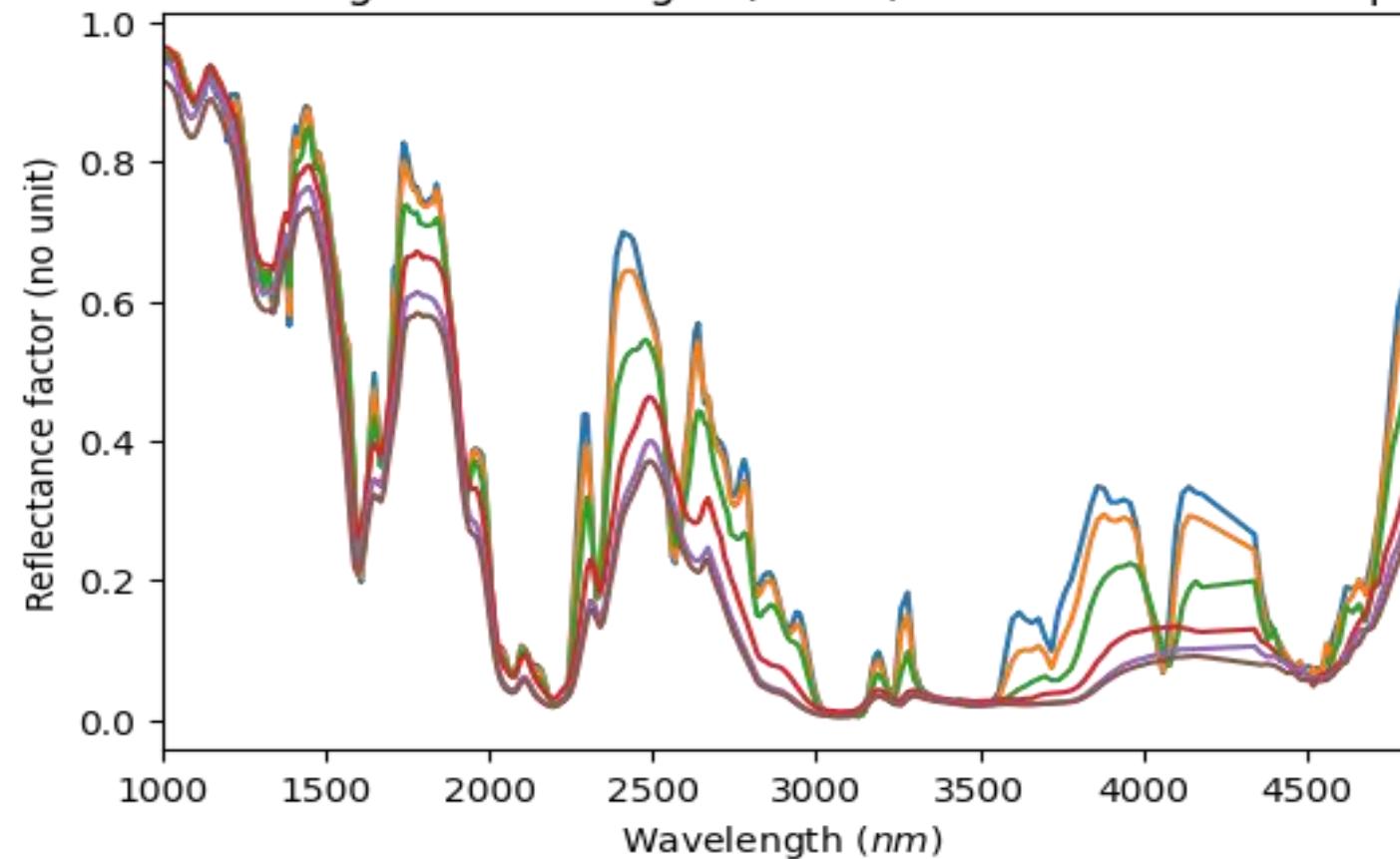
Mineral spectral data

Vis-NIR spectra:
Low temperature
(90 - 290 K)



Salammoniac &
Ammonium chloride
(phase IV)

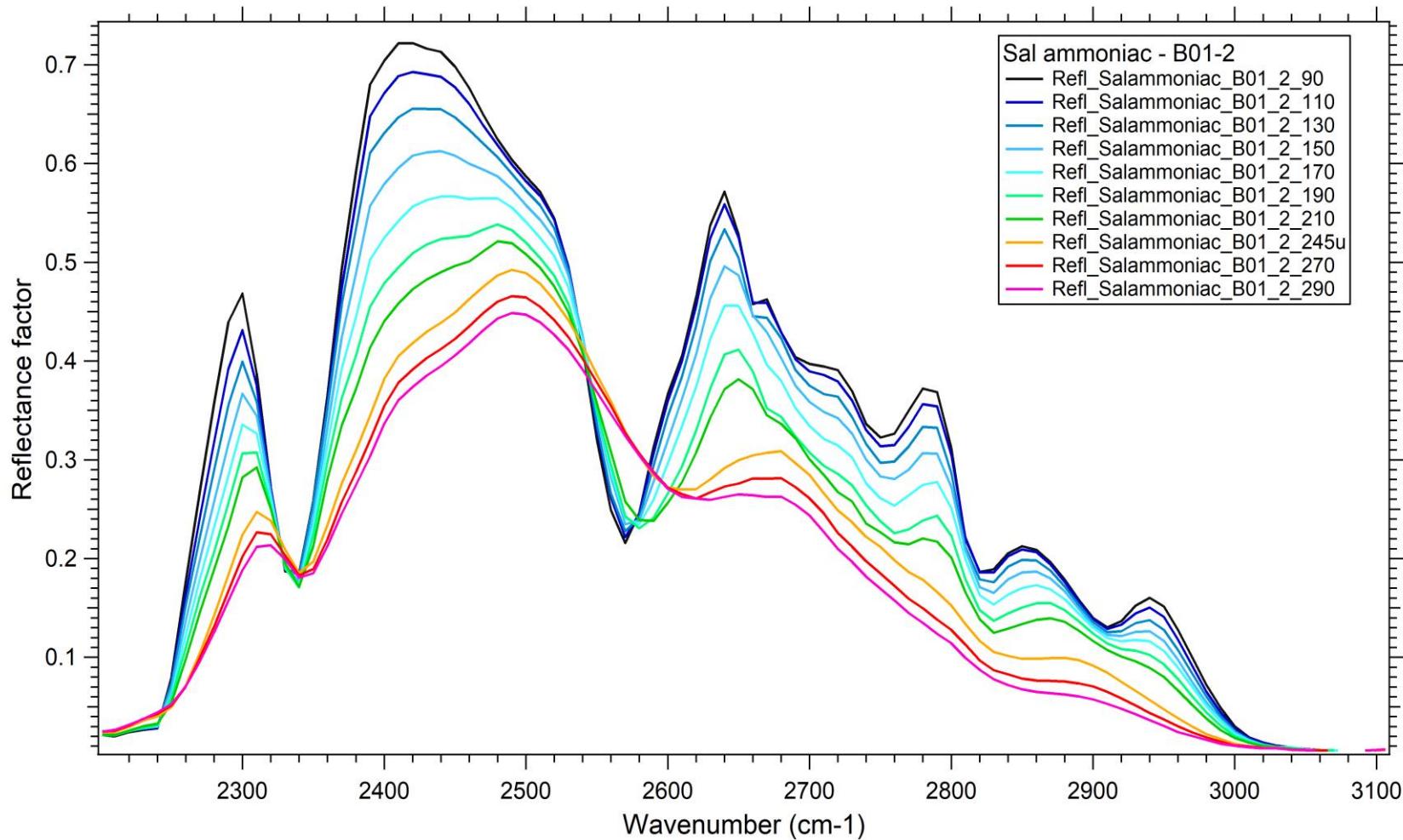
Near-infrared reflectance spectra at low temperature (300-90K) of Salammoniac and delta-Ammonium chloride (phase IV) [NH₄Cl] powders with three grain size ranges (32-80, 80-125 and 125-150μm)



Mineral spectral data

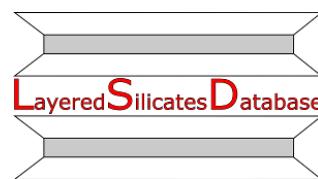
Vis-NIR spectra:
Low temperature
Phase transition
(90 - 290 K)

Salammoniac \leftrightarrow
Ammonium chloride
(phase IV)



Mineral spectral data

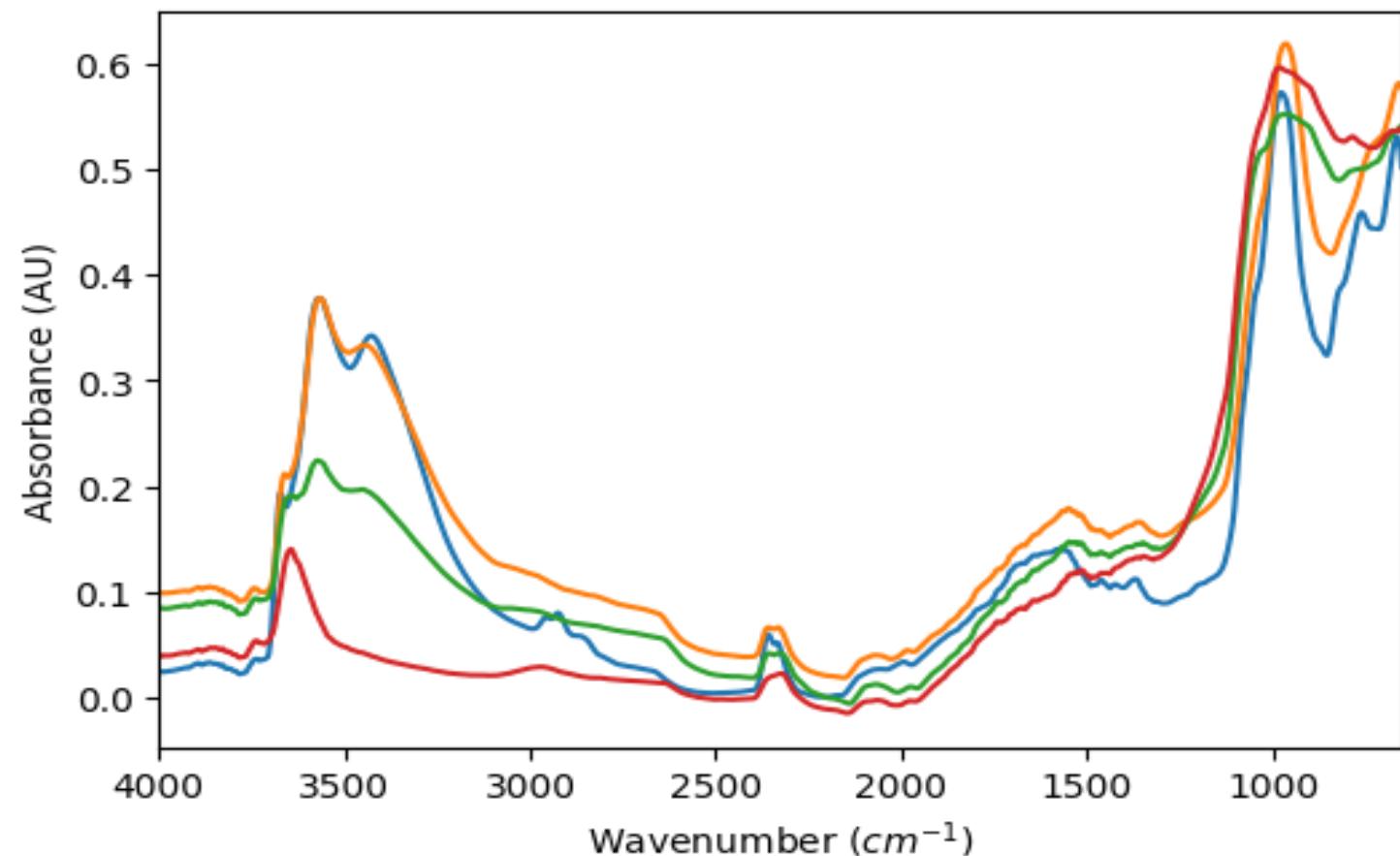
Mid-IR spectra:
High temperature
(25 – 860 °C)



Clinochlore

- at 25°C
- at 550°C
- at 700°C
- at 860°C

Mid-infrared diffuse reflectance experiment with chlorite (clinochlore) heated in-situ from 25 to 860°C

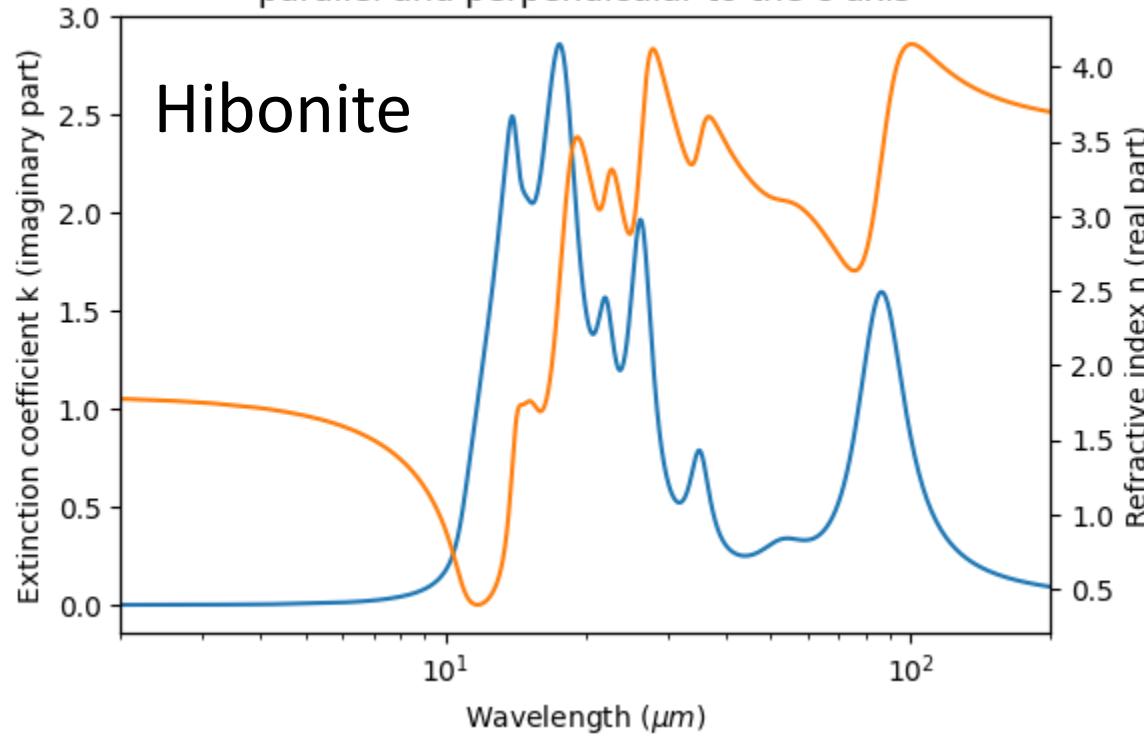


Mineral spectral data

Mid-IR spectra: Optical constants (oriented crystals)



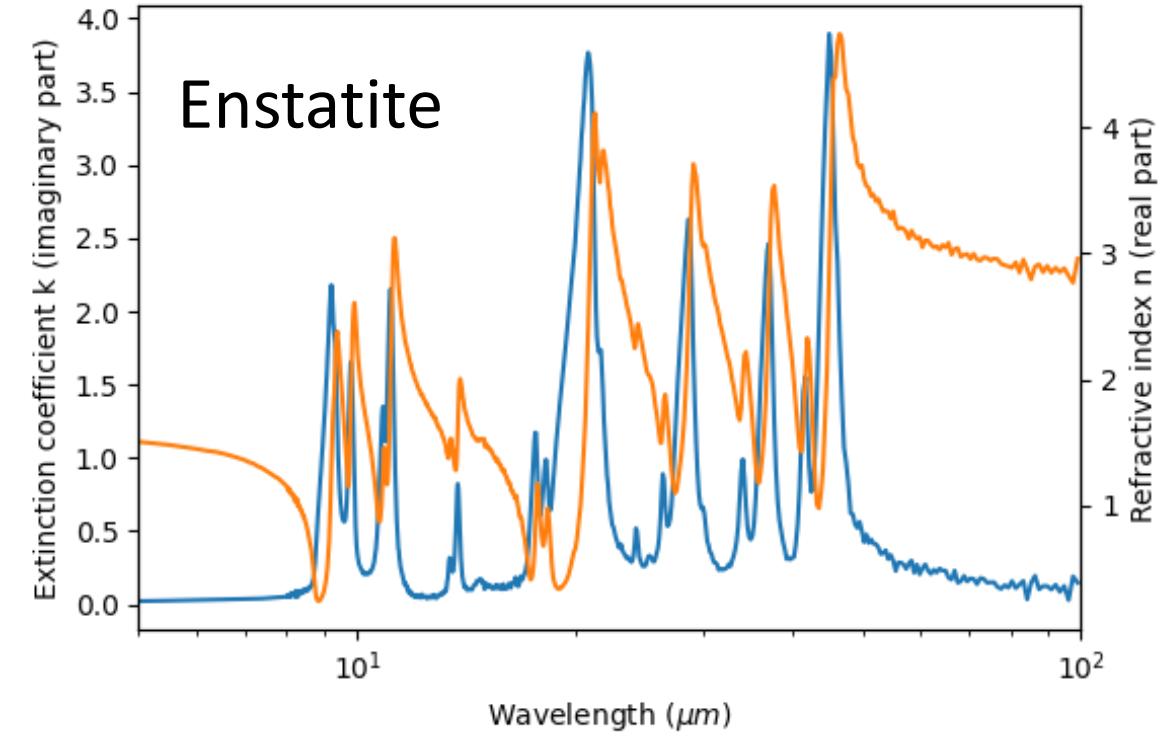
Optical constants in the MIR and FIR for oriented hibonite crystals parallel and perpendicular to the c-axis



Mutschke et al. (2002)

[10.26302/SSHADE/EXPERIMENT_SB_20200430_001](https://doi.org/10.26302/SSHADE/EXPERIMENT_SB_20200430_001)

Optical constants in the MIR and FIR for an oriented enstatite crystal parallel to the three crystallographic axes



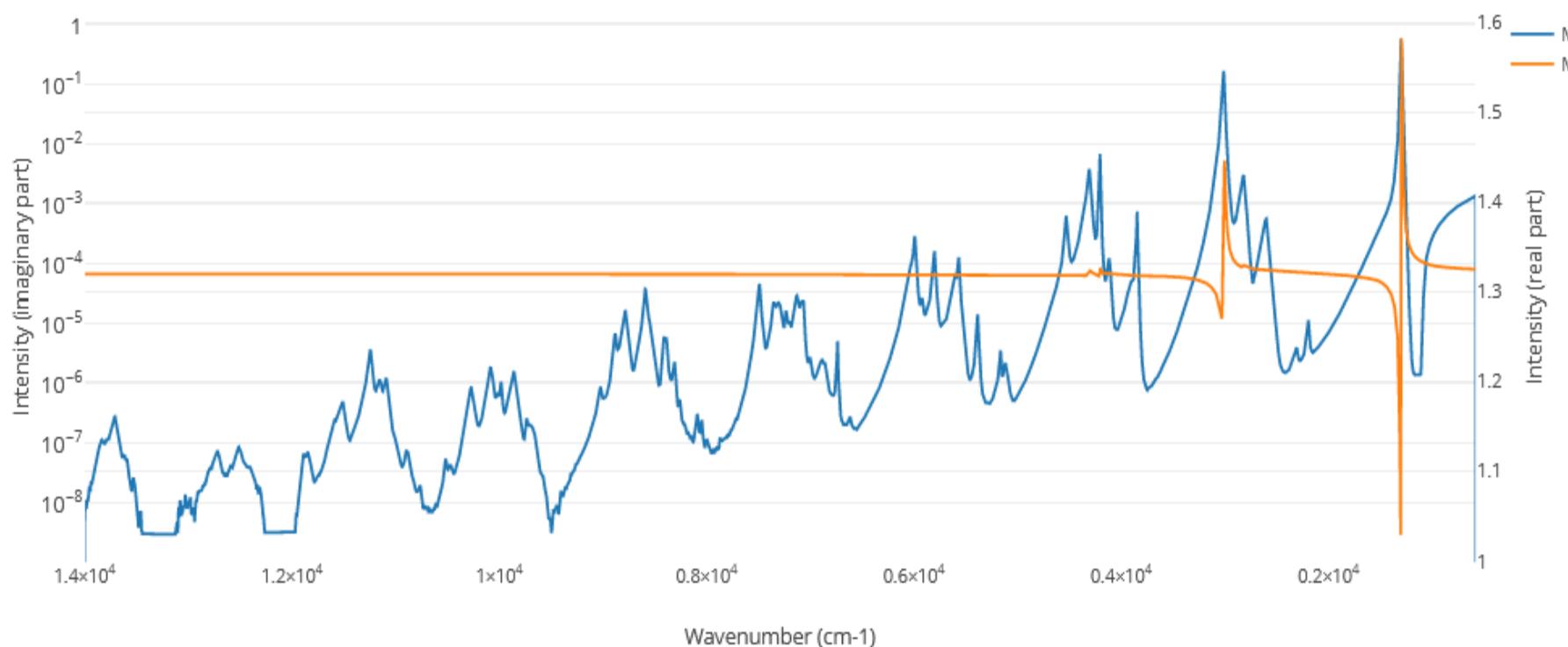
Jäger et al. (1997)

[10.26302/SSHADE/EXPERIMENT_SB_20200117_002](https://doi.org/10.26302/SSHADE/EXPERIMENT_SB_20200117_002)

Spectra of Ices

- **NIR-MIR-FIR Transmission spectra and Optical constants**

- ✓ N₂
- ✓ CO
- ✓ CH₄
- ✓ C₂H₆ ...
- ✓ CH₃OH
- ✓ H₂O
- ✓ Tholins ...



Title

Vis-NIR-MIR optical constants spectrum of crystalline CH₄-I at 39K

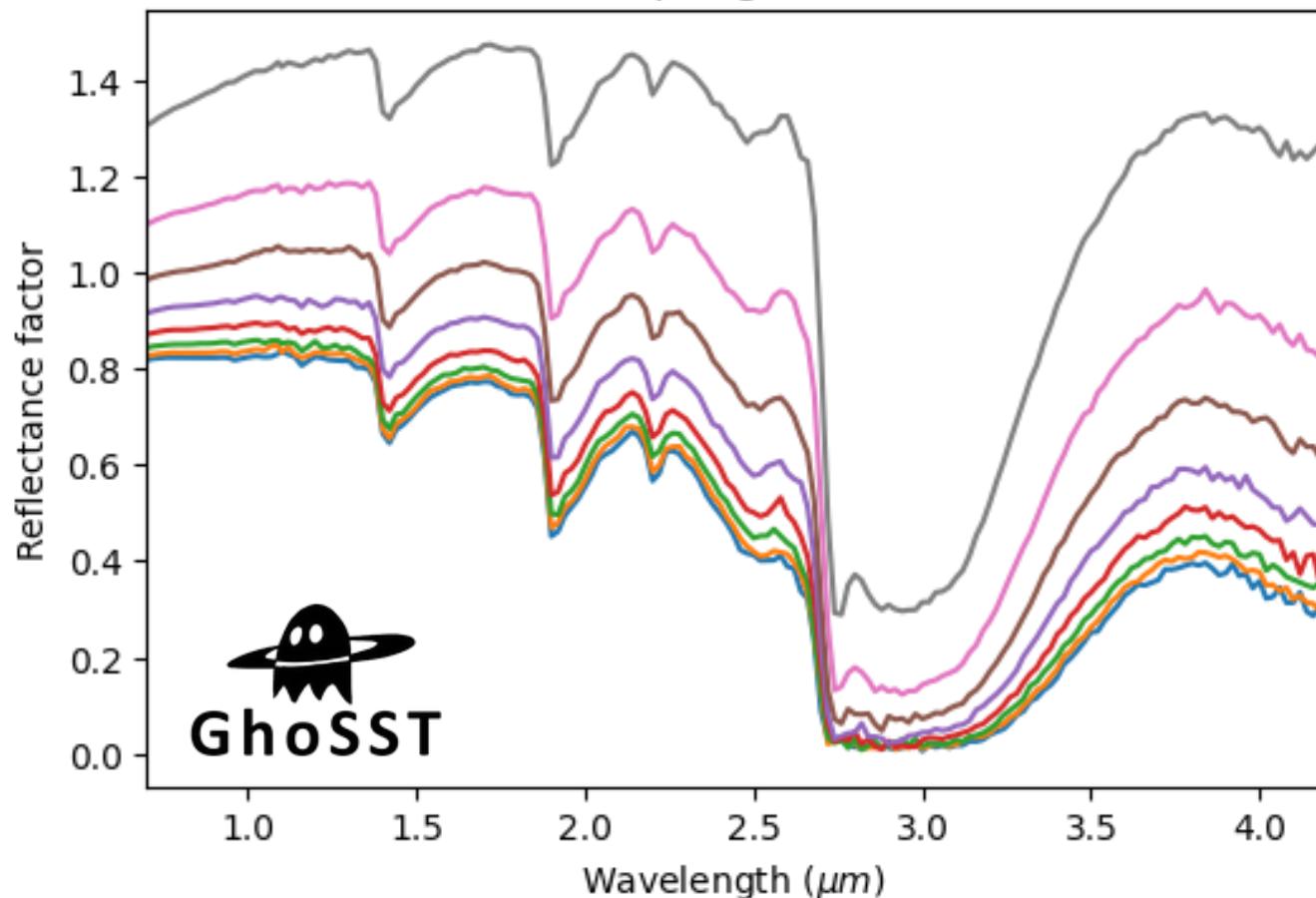
Mineral spectral data

Vis-NIR spectra: BRDF

Ca-Montmorillonite
2 μm – 263K

- i=70.0°, e=0.0°, az=180.0°, ph=70.0°
- i=70.0°, e=10.0°, az=180.0°, ph=80.0°
- i=70.0°, e=20.0°, az=180.0°, ph=90.0°
- i=70.0°, e=30.0°, az=180.0°, ph=100.0°
- i=70.0°, e=40.0°, az=180.0°, ph=110.0°
- i=70.0°, e=50.0°, az=180.0°, ph=120.0°
- i=70.0°, e=60.0°, az=180.0°, ph=130.0°
- i=70.0°, e=70.0°, az=180.0°, ph=140.0°

NIR bidirectional reflection spectra ($i=0-70^\circ/e=0-70^\circ/az=180^\circ$) of Smectite STx-1 2 μm grains at 263K, Patm



Mineral spectral data

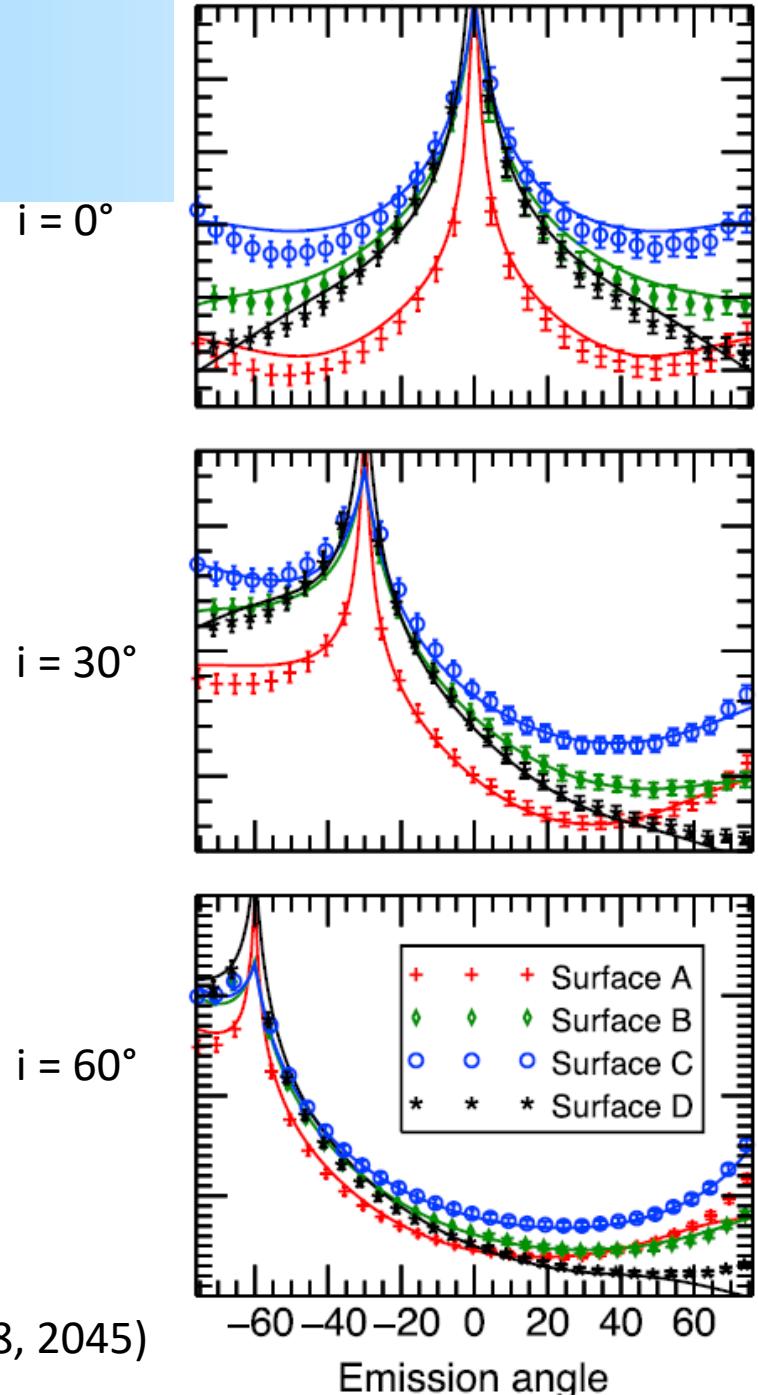
Vis-NIR photometry of surfaces: BRDF

Sols:

- Martan simulant JSC Mars-1
- 4 types of surface textures

Measurements:

- BRDF @ 650 nm (FWHM = 70nm)
- Incidence $i = 0, 30, 60^\circ$
- Emergence e : from -70° à $+70^\circ$

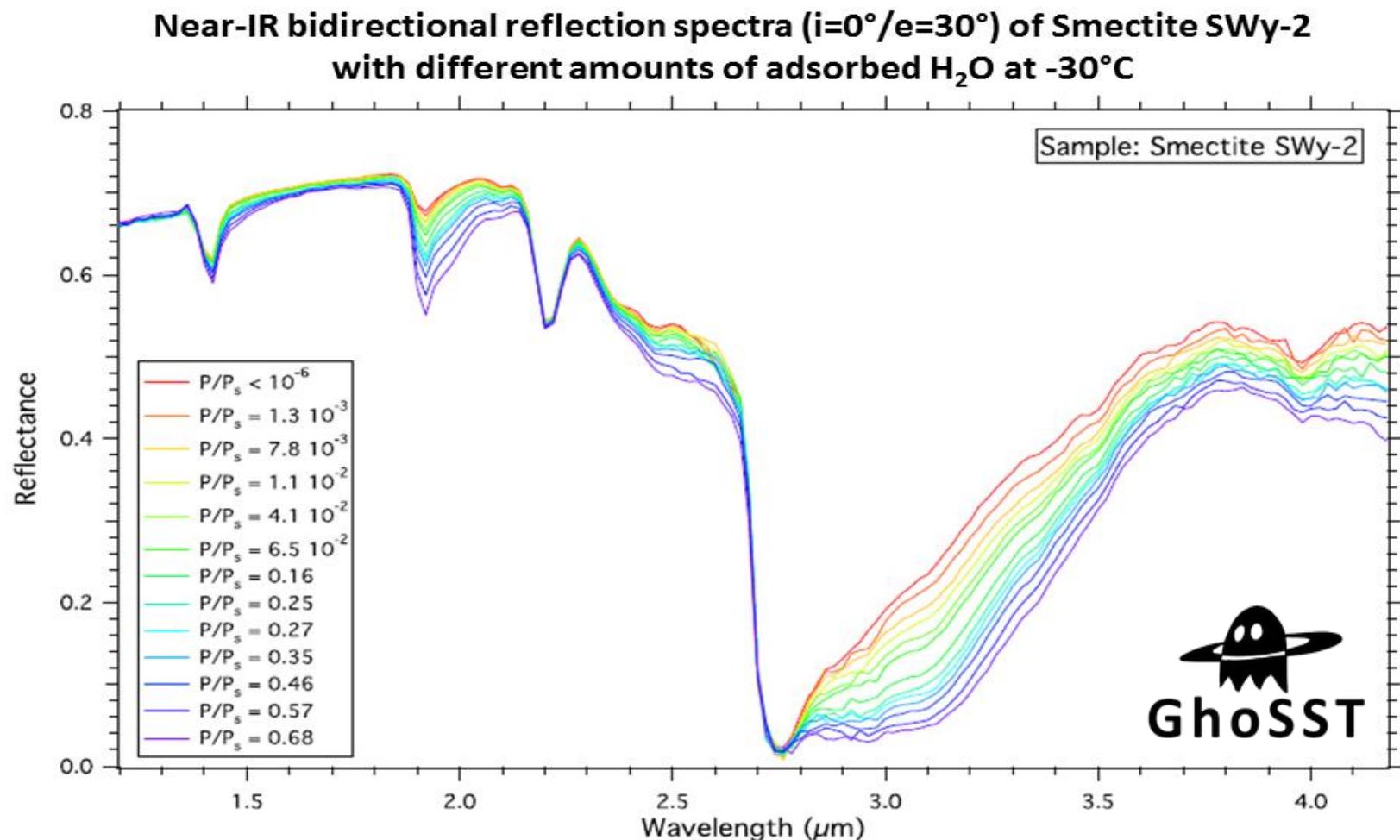


(Pommerol et al. 2013, JGRE, 118, 2045)

Mineral spectral data

Vis-NIR spectra: Adsorption of H₂O (243 K)

Na-Montmorillonite
25-50 µm

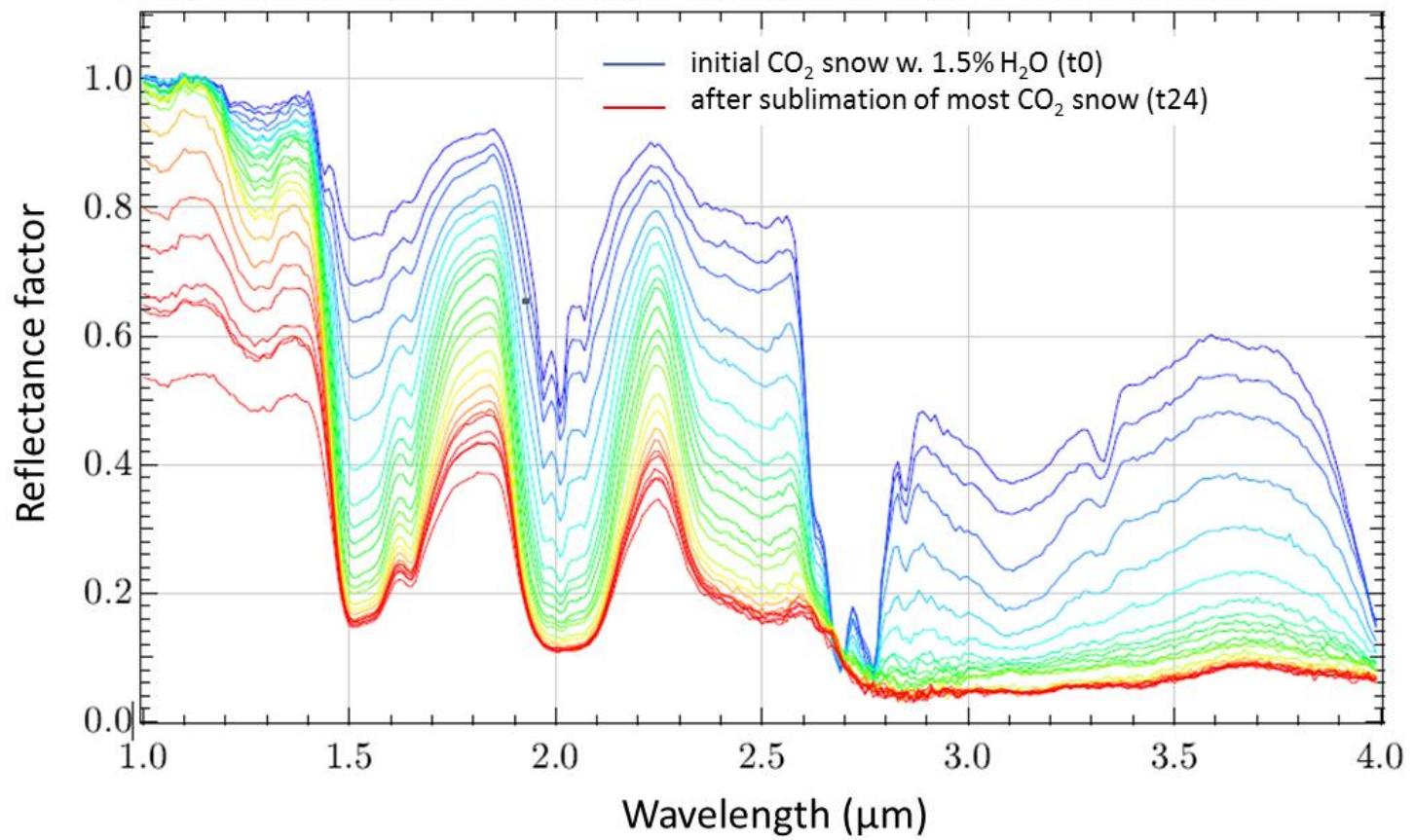


Spectra of Ices

- **NIR reflectance**

Sublimation kinetics
CO₂-H₂O mixtures

NIR reflectance spectra of a mixture of CO₂ snow and H₂O ice (1.5%), deposited over a layer of volcanic tuff, and submitted to slow sublimation under illumination



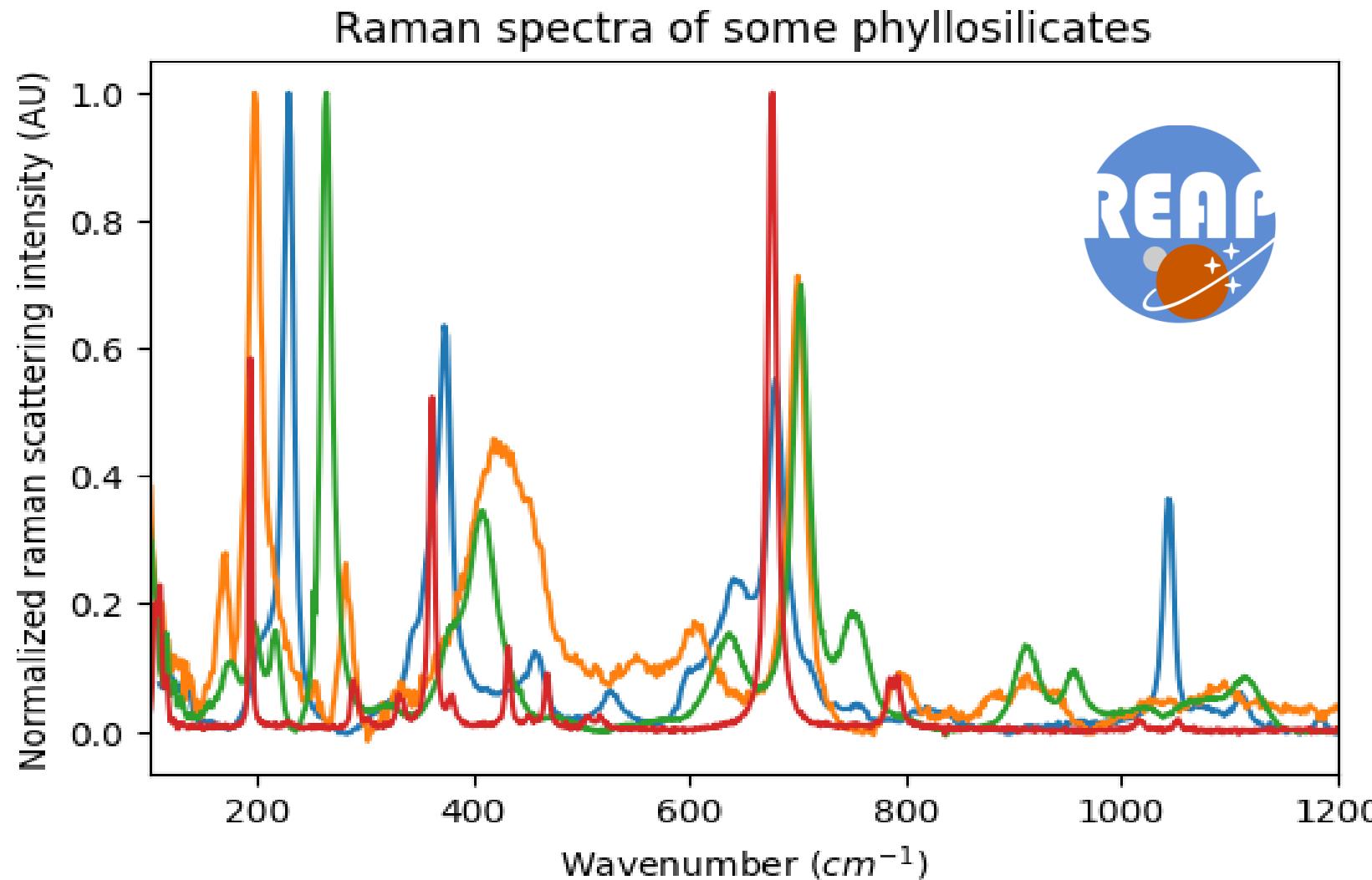
Mineral spectral data

Raman spectra

Phyllosilicates

- Antigorite
- Montmorillonite
- Muscovite
- Talc

Normalized Raman spectrum of $(Mg, Fe^{2+})_3Si_2O_5(OH)_4$ antigorite acquired with a 532 nm laser
Normalized Raman spectrum of $(Na,Ca)_{0.3}(Al,Mg)_2Si_4O_{10}(OH)_2 \cdot n(H_2O)$ Na-montmorillonite SWy-2 acquired with a 532 nm laser
Normalized Raman spectrum of $KAl_2(AlSi_3O_{10})(OH,F)_2$ muscovite acquired with a 514 nm laser
Normalized Raman spectrum of $Mg_3Si_4O_{10}(OH)_2$ talc acquired with a 514 nm laser

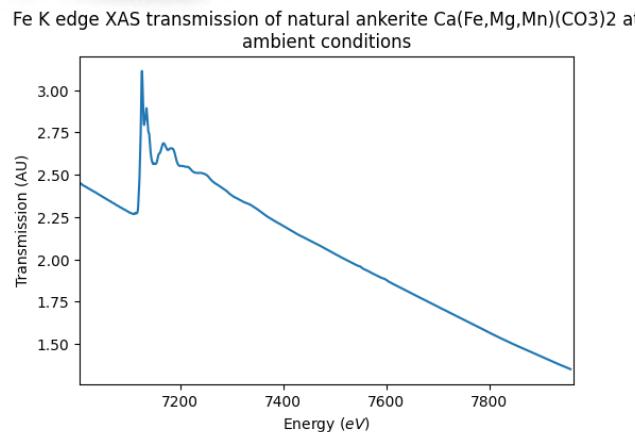


Mineral spectral data

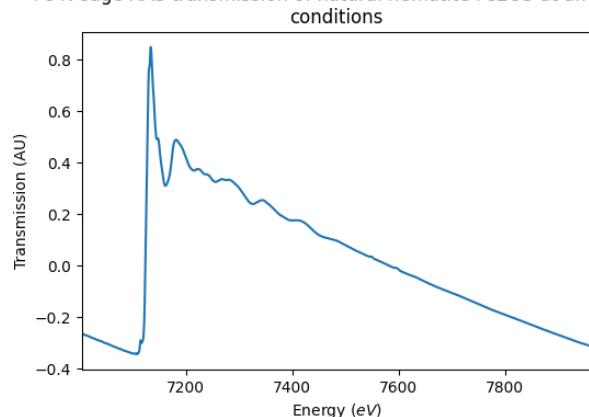
XAS fluorescence spectra



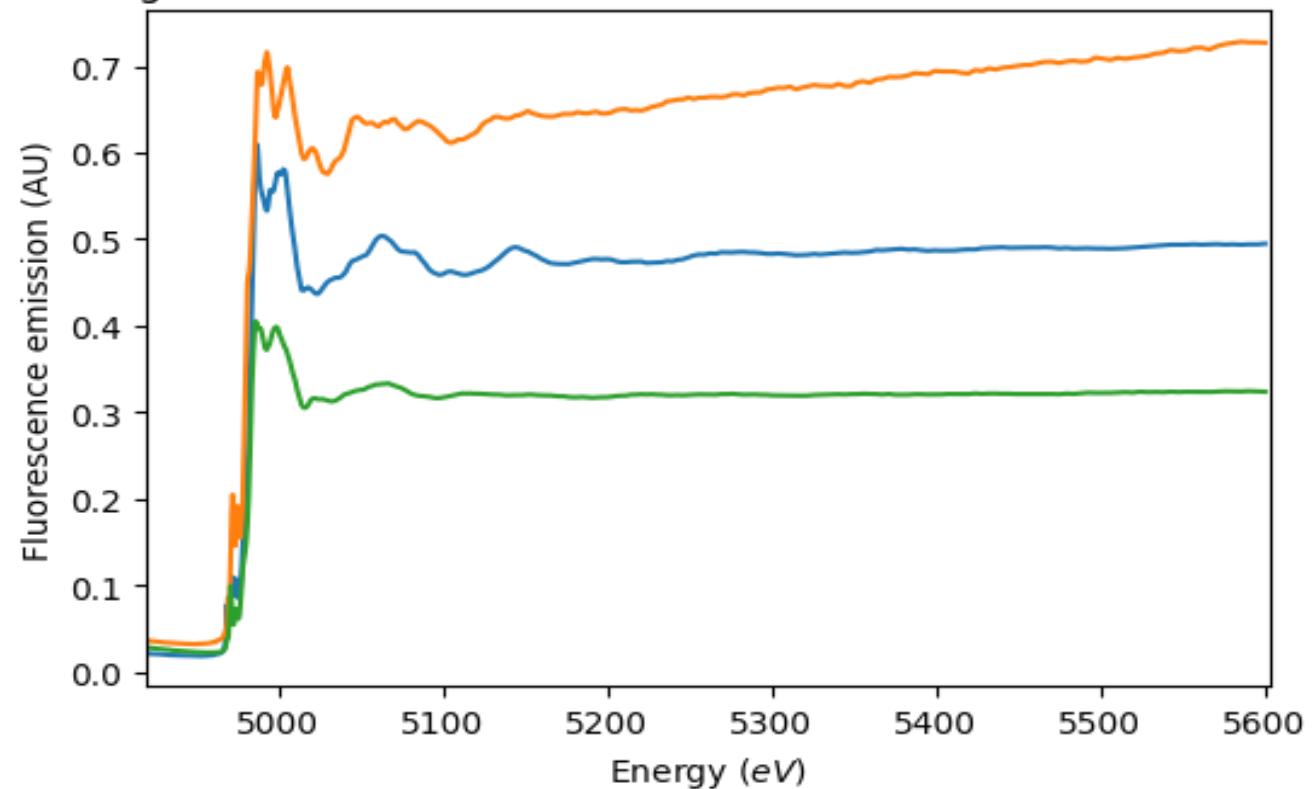
Ankerite
(Fe K edge)



Hematite
(Fe K edge)



Ti K edge XAS fluorescence of Titanium references ambient conditions



- Ti K edge XAS fluorescence of Anatase ambient conditions
- Ti K edge XAS fluorescence of Rutile ambient conditions
- Ti K edge XAS fluorescence of TiOSO₄ ambient conditions

Spectra of Meteorites

- **~1000 spectra on ~300 different meteorites:**
CM, CO, CV, CI, CR, UOC, CV, OC, EL, HED,
mesosiderites, martian, lunar, ...

- Vis-NIR reflectance: ~500 spectra
- MIR transmission ~320 spectra
- Raman : ~50 spectra
- XANES: ~120 spectra

- 11 spectra on 11 different Antarctic micro-meteorites
- 3 spectra on 3 different IDPs

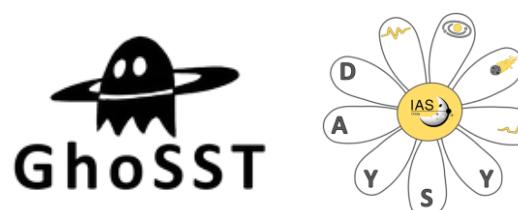
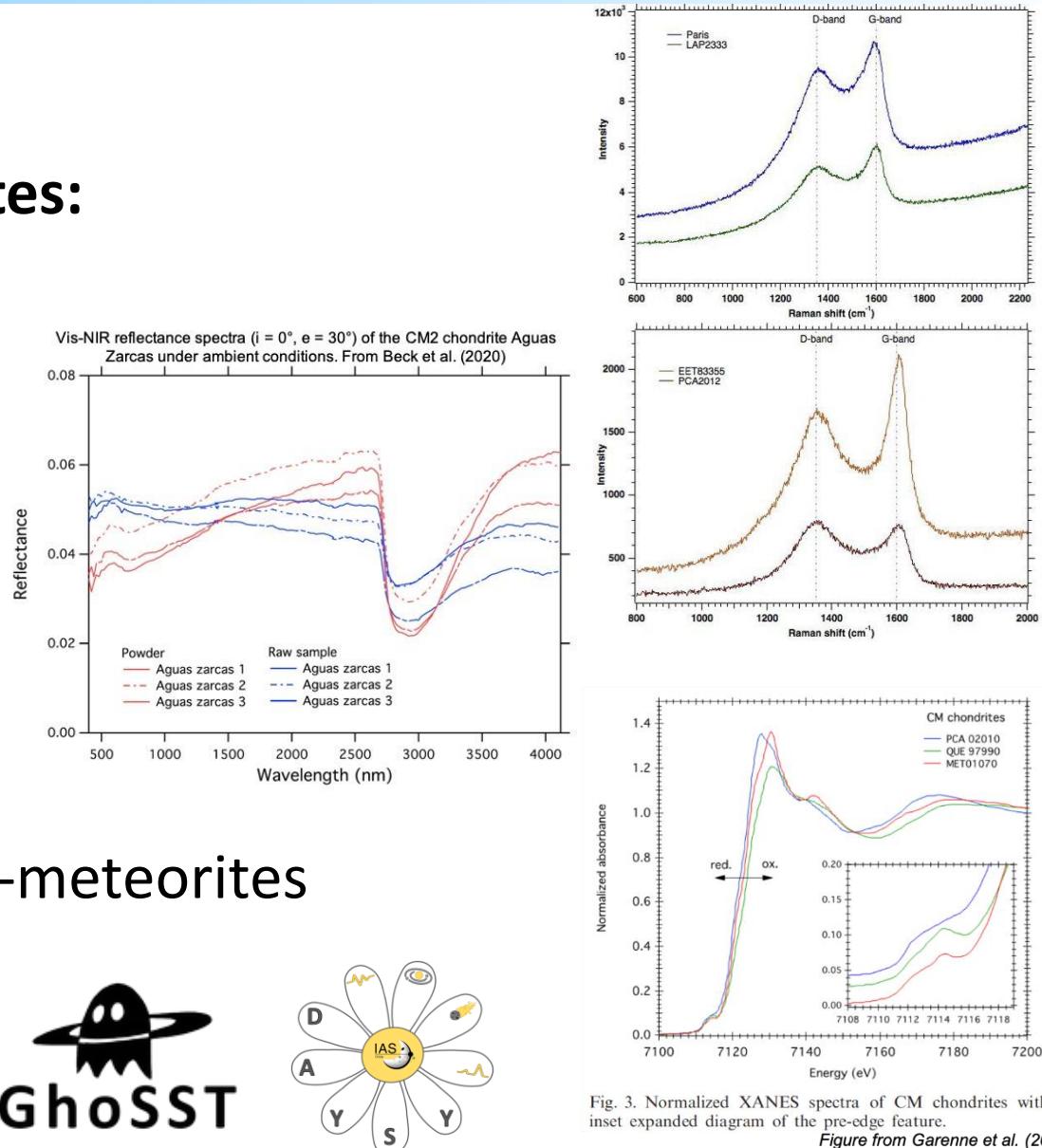


Fig. 3. Normalized XANES spectra of CM chondrites with inset expanded diagram of the pre-edge feature.

Figure from Garenne et al. (2019)

Mineral spectral data

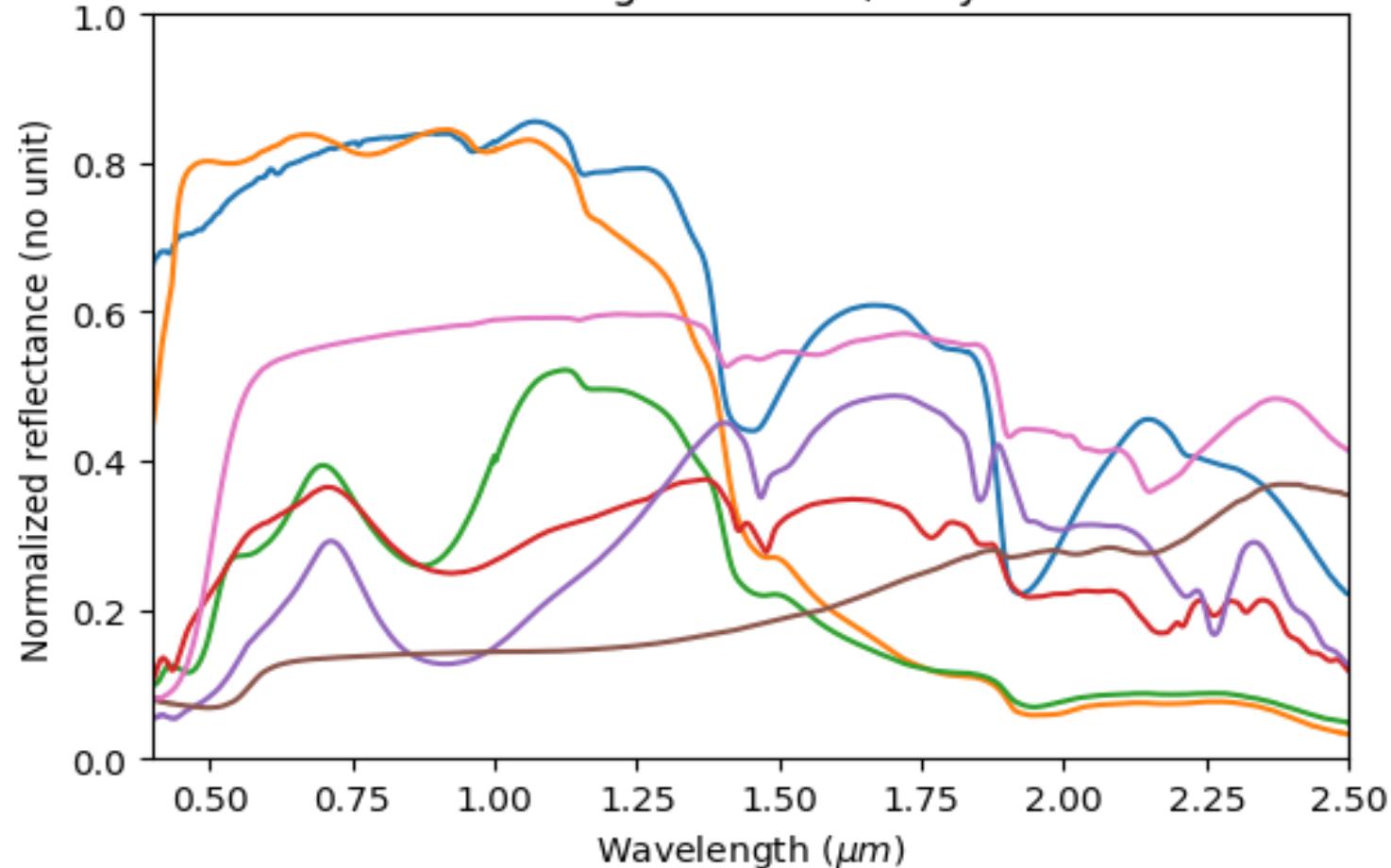
Vis-NIR spectra: Field measurements



Solfatara crater

- Visible and near infrared reflectance spectrum of amorphous silica from crater wall(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of sulfate deposits (alunogen, alum-K, Goldichite) from within a fumarolic vent(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of sulfate deposits (alunogen, alum-K) from within a fumarolic vent(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of sulfate-rich coatings (alunite) from an altered crater wall(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of sulfate-rich coatings (jarosite) from an altered crater wall(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of As and Hb -bearing sublimes from a 160°C fumarolic vent(Solfatara Crater, Italy)
- Visible and near infrared reflectance spectrum of As and Hb -bearing sublimes from a 160°C fumarolic vent(Solfatara Crater, Italy)

Visible near infrared spectra of rocks from the Solfatara crater,
Phlegrean fields, Italy

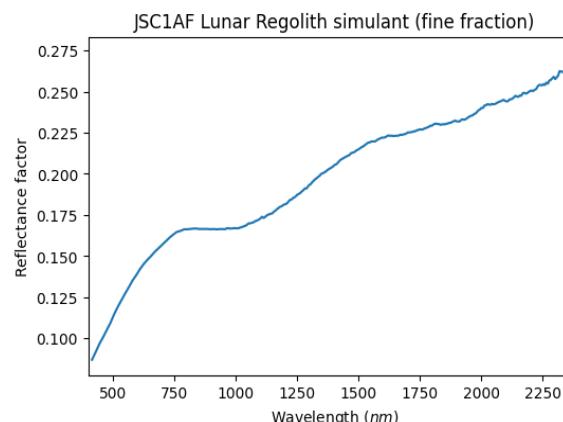
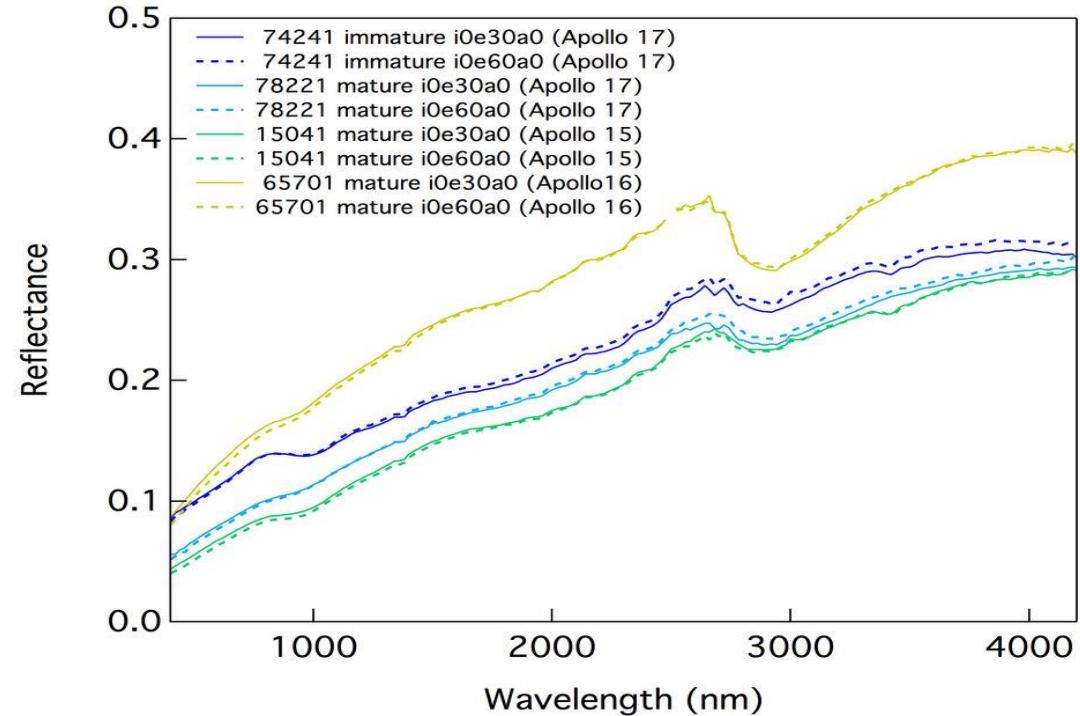


Flahaut et al. (2015) [10.26302/SSHADE/EXPERIMENT_JF_20220531_001](https://doi.org/10.26302/SSHADE/EXPERIMENT_JF_20220531_001)

Spectra of Lunar soils and simulants

- Spectra of collected lunar soils

- ✓ Apollo missions
 - ✓ Simulants: JSC-1AF, ...
-
- ✓ Vis-NIR, MIR



Simulant JSC-1AF

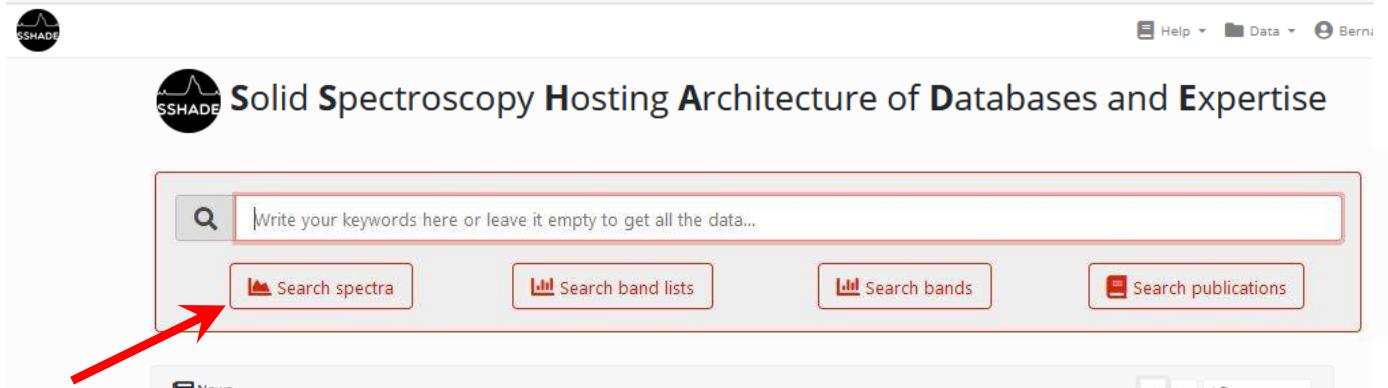


SSHADE Web Interface for Spectra

SSHADE Web interface

www.sshade.eu

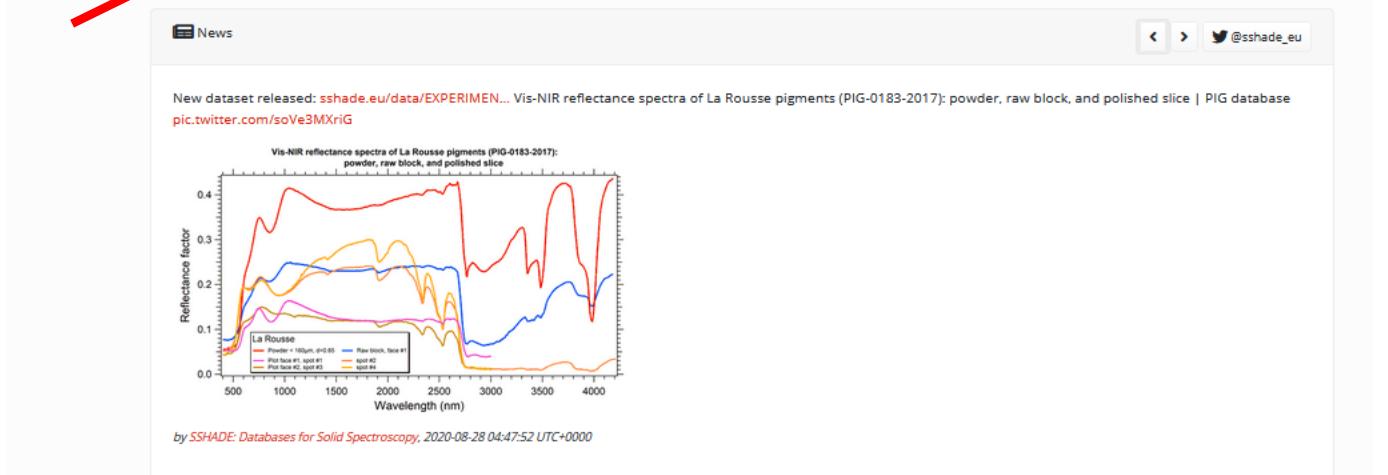
Search bar →



News and new data →

Already available:

- over 6000 spectra
- 41 bandlists (1050 bands)
- ~ 520 publications



SSHADE Web interface

Search

- Spectra
- Publications

Provide 2 complementary tools:

- ✓ “Google-style” toolbar
 - any relevant word
- ✓ Specialized filters

Spectra

- by experiment,
- by instrument parameters,
- by environment,
- by extra-terrestrial object,
- by sample,
- by composition
- by publication.

Publications

- by reference,
- by content
- by published spectrum

Spectra search

smectite NIR reflectance

Search

Filters

By experiment

By instrument parameters

By environment

By extraterrestrial object

By sample

Sample

Sample name: Water ice

Layer type: in

Texture: in

Materials

Name:

Family: snow-ice matter

Origin:

Reference code:

SSHADE Web interface

Search results

Spectra fitting the search criteria are displayed either as:

- Spectrum (one spectrum of the experiment fits your keywords)
- Experiment (several spectra of an experiment fit your keywords)

Tools:

- Unfold experiment
→ View spectra
- Quick view
→ preview popup
- Download
→ customize format
→ direct or basket

The screenshot shows the SSHADE Web interface with a search bar containing 'co2 optical'. The search results table has three rows of data. Red arrows point to several UI elements: one arrow points to the 'Native' unit selection in the top right; another arrow points to the '3 spectra' dropdown in the second row; a third arrow points to the download icons in the second row; and two more arrows point to the download icons in the last two rows.

Spectra number	Title	Spectral range(s)	Temperature	Type	Date created	Actions
3 spectra	Near-IR optical constants spectrum of crystalline CO ₂ ice at 179 K completed with 28K data	1850 - 8500 cm ⁻¹	179.0 K	optical constants	2017-11-17	
28 spectra	MIR-FIR optical constants spectrum of crystalline CO ₂ ice at 15 K	54 - 630 cm ⁻¹ 630 - 4800 cm ⁻¹	15.0 K	optical constants	2017-11-17	
5 spectra	UV-Vis optical indices of 3 oxygenated Tholins films			optical constants	2018-12-13	
	NIR Optical constants spectrum of H ₂ O Ih crystal and H ₂ O liquid from 20 to 293 K			optical constants	2017-07-04	
	NIR Optical constants spectrum of alpha-CO crystal at 21 K	4000 - 4500 cm ⁻¹ 6150 - 6450 cm ⁻¹	21.0 K	optical constants	2017-11-17	
	MIR optical constants spectrum of crystalline C ₂ H ₆ at 15K	670 - 3660 cm ⁻¹	15.0 K	optical constants	2017-11-17	
	NIR optical constant spectra of CH ₄ in solid solution in alpha and beta-N ₂ phases at 5 different temperatures (35K - 43K)			optical constants	2018-02-07	

SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ Experiment structure and parameters
 - Spectral, spatial, angular, polarization
 - Instrument used
- ✓ Spectrum and parameters



SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ Experiment structure and parameters
 - Spectral, spatial, angular, polarization
 - Instrument used
- ✓ Spectrum and parameters
- ✓ Sample structure and composition
 - composition (abundance, ...), texture,
 - physical parameters (T,P, atm...)
 - processes (irradiation)
 - 'object' (meteorite, micrometeorite, idp)

The screenshot shows the SSHADE Web interface with a sample details page. A red arrow points to the 'Sample' tab in the top navigation bar. The main content area displays detailed information about a sample named 'QUE97990 meteorite pellet Tamb'. The left sidebar lists various sample components and their properties, such as 'Material KBr matrix', 'Constituent KBr', and 'Constituent adsorbed water on KBr (Beck14)'. The right sidebar contains sections for 'Sample', 'Physical characteristics', 'Comments', 'Sample environment: Temperature', 'Sample environment: Fluid', and 'Documentation and publication'. Each section includes specific parameters like thickness (0.8 ± 0.01 mm), diameter (13.0 mm), mass (0.301 ± 0.0015 g), temperature (22.0 ± 2.0 °C), fluid pressure (0.001 mbar), and comments related to storage conditions.

SAMPLE description: Layer(s) / Material(s) / Constituent(s)

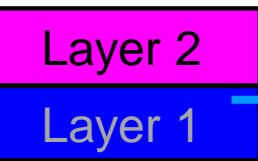
SAMPLE

LAYERS

→ superposition



n

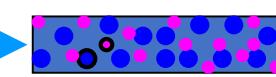


Layer 2

Layer 1

MATERIALS

→ grains mixing



n

CONSTITUENTS

→ phases arrangement



polycrystal, coating, adsorption...

	Experiment and spectra	Sample
Sample	QUE97990 meteorite pellet Tamb	
Layer	QUE97990 meteorite pellet	
Material	KBr matrix	
Constituent	KBr	
	Constituent adsorbed water on KBr (Beck14)	
Material	bulk QUE97990 powder	
Constituent	matrix QUE97990 IPAG	
Constituent	chondrules QUE97990 IPAG	
Constituent	CAIs QUE97990 IPAG	
Constituent	adsorbed water on QUE97990 bulk	

Fonctions & Bonds



n

ATOMS

(isotopes)

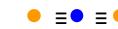


n

MOLECULES

(isotopes, isomers...)

n



ATOMS

(isotopes)

n

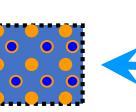
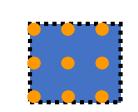
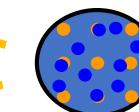
MOLECULES

(isotopes, isomers...)

n

Fundamental PHASES

(solids, minerals, liquids)



liquid, ice, mineral, polymer, clathrate, ...

Basic constituent

1

SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ Experiment structure and parameters
 - Spectral, spatial, angular, polarization
 - Instrument used
- ✓ Spectrum and parameters
- ✓ Sample structure and composition
 - composition (abundance, ...), texture,
 - physical parameters (T,P, atm...)
 - processes (irradiation)
 - 'object' (meteorite, micrometeorite, idp)
- ✓ Many linked info !
 - Publications
 - Documentation, Web sites, ...
 - Minerals, molecules / chemical bonds / atoms

To the limit of the knowledge of the data provider

The screenshot shows the SSHADE Web interface. At the top, there's a navigation bar with a logo, a 'Spectrum' dropdown, a search bar containing 'Write your keywords here', and a magnifying glass icon. To the right of the search bar are 'Help' and 'Log in / Register' links.

The main area displays a list of experiments and spectra. One experiment is highlighted in red:
Experiment MIR transmission spectra at Tamb, 150°C and 300°C of bulk CM chondrites in KBr pellets

Below this, several sub-experiments are listed:

- Sub-Experiment MIR Transmission spectra of bulk Boriskino CM chondrite at ambient temperature, T = 150°C and T = 300°C
- Spectrum MIR transmission spectrum bulk Boriskino meteorite in KBr pellet at ambient temperature
- Spectrum MIR transmission spectrum bulk Boriskino meteorite in KBr pellet at T = 150°C
- Spectrum MIR transmission spectrum bulk Boriskino meteorite in KBr pellet at T = 300°C
- Sub-Experiment MIR Transmission spectra of bulk LEW85311 CM chondrite at ambient temperature, T = 150°C and T = 300°C
- Sub-Experiment MIR Transmission spectra of bulk QUE97990 CM chondrite at ambient temperature, T = 150°C and T = 300°C
- Sub-Experiment MIR Transmission spectra of bulk Murchison CM chondrite at ambient temperature, T = 150°C and T = 300°C
- Sub-Experiment MIR Transmission spectra of bulk MCY05230 CM chondrite at ambient temperature, T = 150°C and T = 300°C
- Sub-Experiment MIR Transmission spectra of bulk LON94101 CM chondrite at ambient temperature, T = 150°C and T = 300°C

A large modal window titled 'Related data' is open on the right side, listing various instrument details and techniques:

- Instrument technique**
 - Name: Brucker Vertex 70v
- Instrument description**
 - Type: FTIR spectrometer
 - Name: Brucker Vertex 70v - transmission Mid-IR
 - Technique: transmission
- Technique description**
 - Technique type: macroscopic
 - Source: Globar-IR
 - Source wavelength: MIR-FIR
 - Source power: 30 W
 - Spectral analyzer(s): KBr/Ge Beamsplitter
 - Detector(s): DTGS-KBr
- Laboratories**
- Documentation and links**
- Spatial parameters**
- History**

SSHADE Web interface

Export

Can export:

- Spectra (+ customize export formats: •••)
- Experiment

At different level of the interface

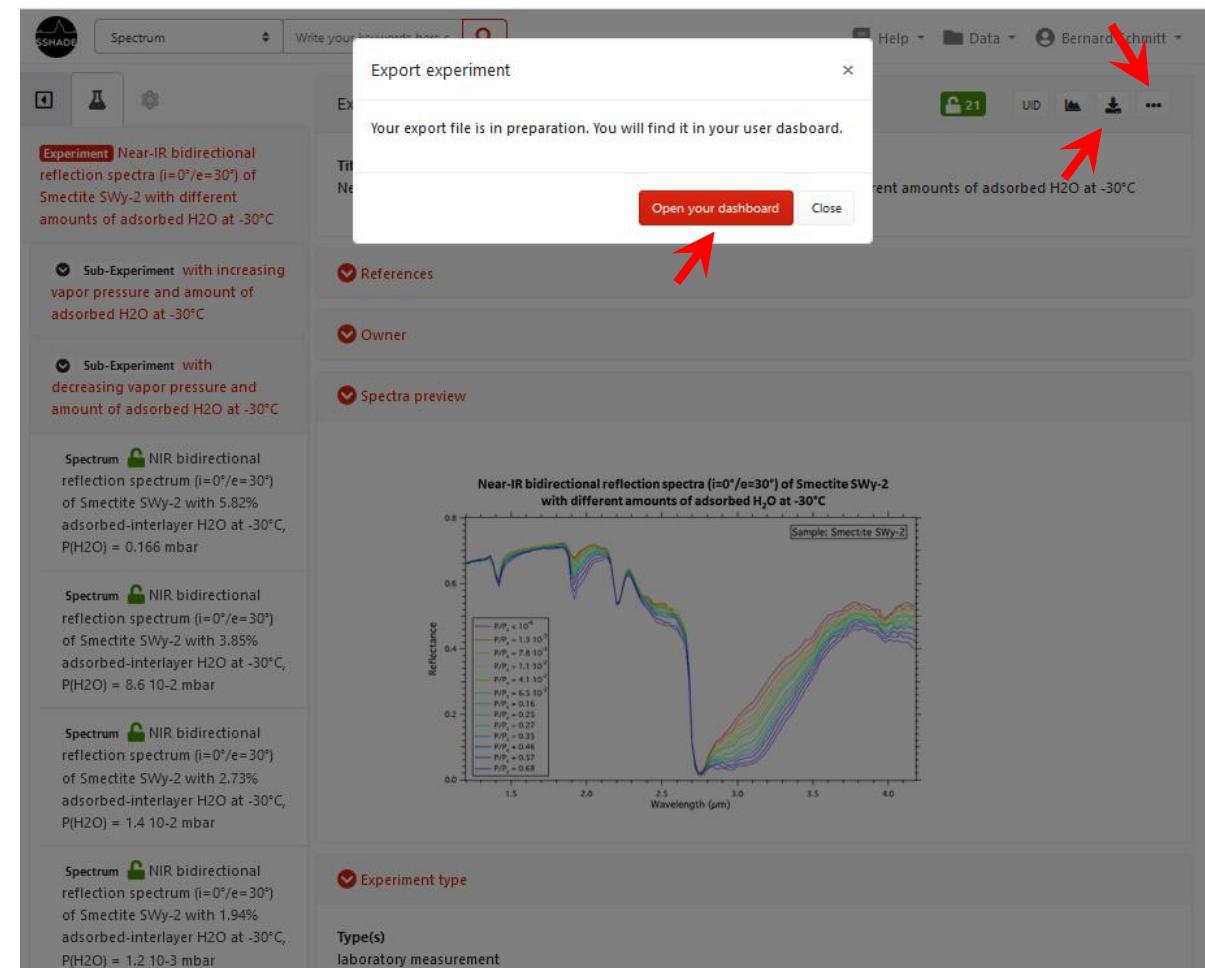
- Search results
- Detail pages of experiment and spectra

Delivered in a zip file that contains:

- all spectral data
- their experiment and sample metadata
- a ‘description’ file w. info on spectrum structure & units
- a ‘citation file’ w. references of the data (paper(s), DOI)

by asynchronous data extraction:

- stored in dashboard



How to become a SSHADE partner ?

SSHADE : partners / data providers

Who can be a SSHADE partner ?

Any group producing experimental data on solid spectroscopy who want to make them available to the community

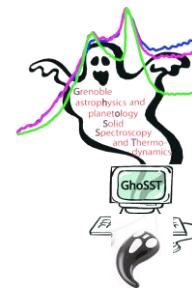
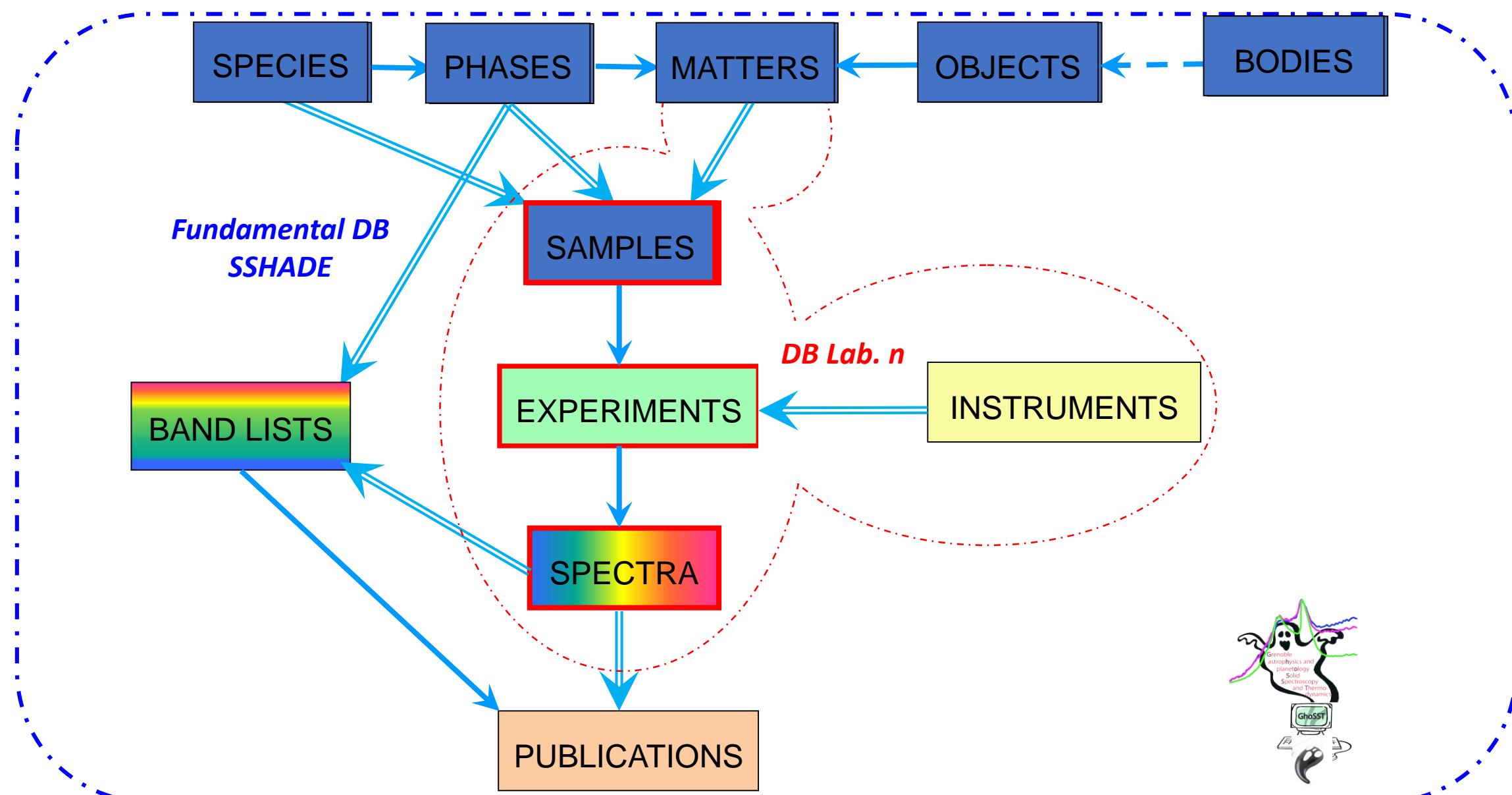
They will:

- ➔ get their own database
- ➔ be scientifically responsible of their content and quality
- ➔ get a ~2.5 days training (+ SSHADE-party) to:
 - ✓ Understand the SSHADE infrastructure and the SSDM data model
 - ✓ Learn to prepare XML import files (sample, experiment, spectra + associated files)
 - ✓ Validate, import and correct data
- ➔ get access to all preparation tools and fundamental data (atoms, molecules, minerals, solid phases...)
- ➔ get on-line technical / scientific support from the SSHADE team
- ➔ get a 'data reference' + DOI for each 'experiment' (= data set) + a reference + DOI for their database

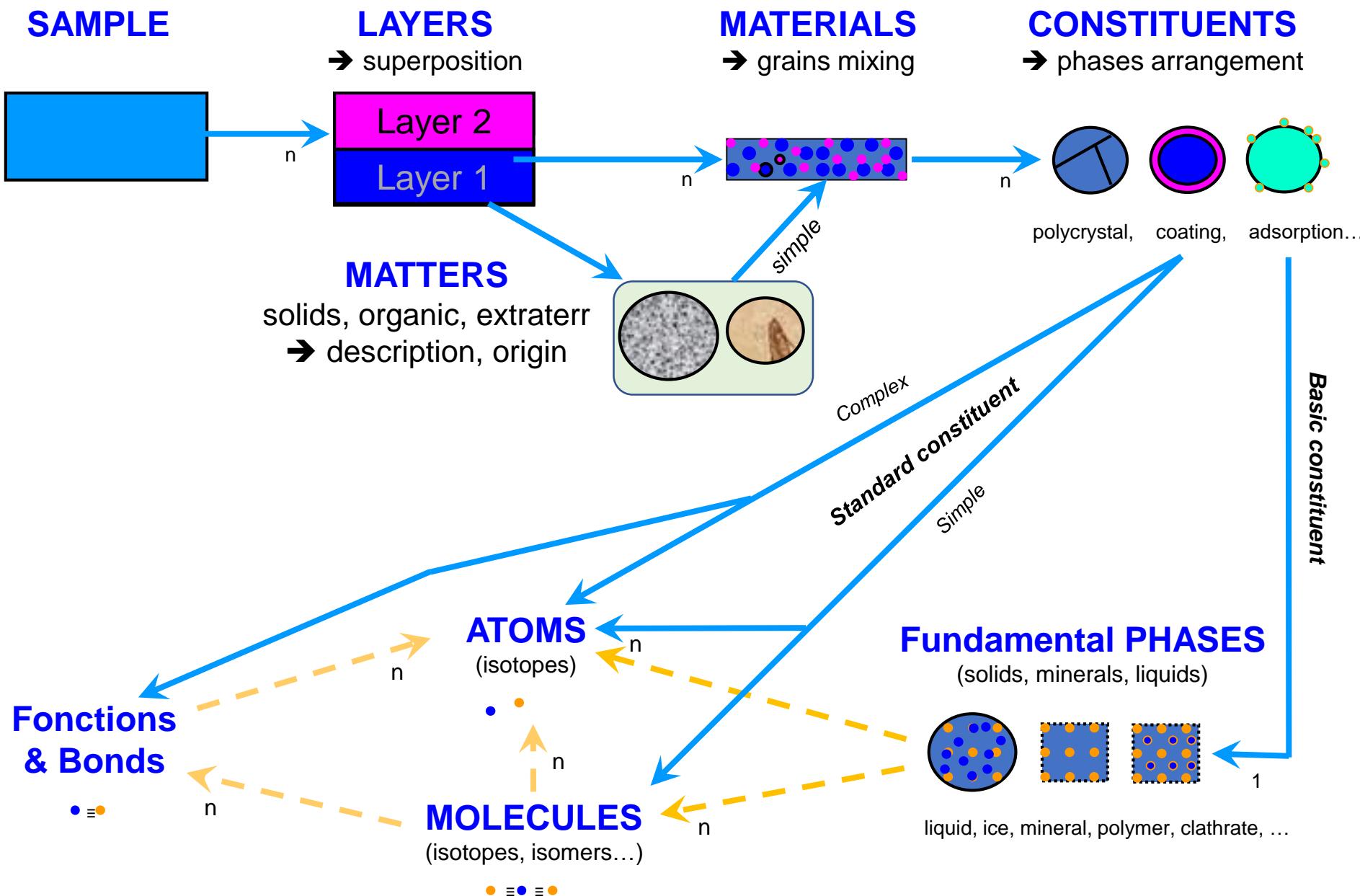
But they need

- ✓ To be motivated
- ✓ Can spend some time on data preparation (Astronomers/CNAP can count time on their service)

SSHADE: new SSDM structure



SAMPLE description: Layer(s) / Material(s) / Constituent(s)



SSHADE : partners / data providers side

Who can be a SSHADE partner ?

Any group producing experimental data on solid spectroscopy who want to make them available to the community

They will:

- ➔ get their own database
- ➔ be scientifically responsible of their content and quality
- ➔ get a ~2.5 days training (+ SSHADE-party) to:
 - ✓ Understand the SSHADE infrastructure and the SSDM data model
 - ✓ Learn to prepare XML import files (sample, experiment, spectra + associated files)
 - ✓ Validate import & correct data
- ➔ get access to all preparation tools and fundamental data (atoms, molecules, minerals, solid phases...)
- ➔ get on-line technical / scientific support from the SSHADE team
- ➔ get a 'data reference' + DOI for each 'experiment' (= data set) + a reference + DOI for their database

But they need

- ✓ To be motivated
- ✓ Can spend some time on data preparation (Astronomers/CNAP can count time on their service)

XML Templates: Data preparation

Empty '*Laboratory*' template

```
<?xml version="1.0" encoding="UTF-8"?>
<!>
<!-- Data type : Laboratory
-->
<import type="laboratory" ssdm_version="0.9.0"
        xmlns="http://ssshade.eu/schema/import"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="http://ssshade.eu/schema/import http://ssshade.eu/schema/import-0.9.xsd">

<laboratory><!-- multiple -->
    <import_mode>first import</import_mode> <!-- **ABS MANDATORY** Mode of import of the 'laboratory'</import_mode>
    <!-- **ABS MANDATORY to CREATE** Unique identifier code given to the laboratory</uid>LAB_</uid> <!-- **ABS MANDATORY at least one** -->
    <!-- **ABS MANDATORY at least one** -->
    <!-- **ABS MANDATORY** LINK to the existing manager_databases</manager_databases>
    <!-- **ABS MANDATORY** database_uid</database_uid><!-- multiple --> <!-- **ABS MANDATORY** LINK to the existing manager_databases</manager_databases>

<!-- LABORATORY DESCRIPTION -->
    <acronym></acronym> <!-- **ABS MANDATORY** Acronym of the laboratory -->
    <name><![CDATA[]]></name> <!-- **ABS MANDATORY** Full name of the laboratory -->
    <description><![CDATA[]]></description> <!-- General description of the scientific/technical organizations -->
    <!-- **MANDATORY at least one** -->
        <organization><!-- multiple -->
            <acronym></acronym> <!-- **MANDATORY** Acronym of the parent organization to which belongs the laboratory</acronym>
            <name><![CDATA[]]></name> <!-- **MANDATORY** Name of the parent organization to which belongs the laboratory</name>
        </organization>
    </organizations>
    <addresses> <!-- **ABS MANDATORY at least one** -->
        <address><!-- multiple -->
            <label></label> <!-- Label of the address (postal/geographic) or name of the geographic location</label>
            <street><![CDATA[]]></street> <!-- **MANDATORY** Street address, building number/name</street>
            <postal_code></postal_code> <!-- **MANDATORY** Postal code of the laboratory -->
            <city></city> <!-- **MANDATORY** City/locality of the laboratory -->
            <region><![CDATA[]]></region> <!-- Region, state, province, or county of the laboratory</region>
            <country_code></country_code> <!-- **ABS MANDATORY** 2-digit country code of the laboratory</country_code>
        </address>
    </addresses>

<!-- LABORATORY HISTORY -->
    <date_begin></date_begin> <!-- Beginning date of the laboratory. [Format: 'YYYY-MM-DD'] Ex: 2000-01-01</date_begin>
    <date_end></date_end> <!-- **COMPULSORY when lab stop activity** Ending date of the laboratory</date_end>

<!-- LABORATORY WEB SITES -->
    <links> <!-- **MANDATORY at least one** Link(s) to current web page(s) of the laboratory and services</links>
        <link><!-- multiple -->
            <name><![CDATA[]]></name> <!-- **MANDATORY** Name of the web page(s) -->
            <url><![CDATA[]]></url> <!-- **MANDATORY** URL address (avoid non-perennial commercial links)</url>
        </link>
    </links>
    <comments><![CDATA[]]></comments> <!-- Additional information on the laboratory (Tel, ...)</comments>
</laboratory>
</import>
```

Filled '*Laboratory*' template

```
<?xml version="1.0" encoding="UTF-8"?>
<!>
<!-- Data type : Laboratory
-->
<import type="laboratory" ssdm_version="0.9.0"
        xmlns="http://ssshade.eu/schema/import"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="http://ssshade.eu/schema/import http://ssshade.eu/schema/import-0.9.xsd">

<laboratory><!-- multiple -->
    <import_mode>correction</import_mode> <!-- **ABS MANDATORY** Mode of import of the 'laboratory'</import_mode>
    <!-- **ABS MANDATORY to CREATE** Unique identifier code given to the laboratory</uid>LAB_IAS</uid> <!-- **ABS MANDATORY at least one** -->
    <!-- **ABS MANDATORY at least one** -->
    <!-- **ABS MANDATORY** database_uid</database_uid><!-- multiple --> <!-- **ABS MANDATORY** LINK to the existing manager_databases</manager_databases>

<!-- LABORATORY DESCRIPTION -->
    <acronym>IAS</acronym> <!-- **ABS MANDATORY** Acronym of the laboratory -->
    <name>Institut d'Astrophysique Spatiale</name> <!-- **ABS MANDATORY** Full name of the laboratory -->
    <description>Astrophysics laboratory with an important implication in space instrumentation</description>
    <organizations> <!-- **MANDATORY at least one** -->
        <organization><!-- multiple -->
            <acronym>UPSUD</acronym> <!-- **MANDATORY** Acronym of the parent organization to which belongs the laboratory</acronym>
            <name>Université Paris-Sud</name> <!-- **MANDATORY** Name of the parent organization</name>
        </organization>
    </organizations>
    <addresses> <!-- **ABS MANDATORY at least one** -->
        <address><!-- multiple -->
            <label>bât 121</label> <!-- Label of the address (postal/geographic) or name of the geographic location</label>
            <street>Campus d'Orsay</street> <!-- **MANDATORY** Street address, building number/name</street>
            <postal_code>91405</postal_code> <!-- **MANDATORY** Postal code of the laboratory -->
            <city>Orsay</city> <!-- **MANDATORY** City/locality of the laboratory -->
            <region><![CDATA[file-de-France]]></region> <!-- Region, state, province, or county of the laboratory</region>
            <country_code>FR</country_code> <!-- **ABS MANDATORY** 2-digit country code of the laboratory</country_code>
        </address>
    </addresses>

<!-- LABORATORY HISTORY -->
    <date_begin>2000-01-01</date_begin> <!-- Beginning date of the laboratory. [Format: 'YYYY-MM-DD'] Ex: 2000-01-01</date_begin>
    <date_end>2010-01-01</date_end> <!-- **COMPULSORY when lab stop activity** Ending date of the laboratory</date_end>

<!-- LABORATORY WEB SITES -->
    <links> <!-- **MANDATORY at least one** Link(s) to current web page(s) of the laboratory and services</links>
        <link><!-- multiple -->
            <name>IAS website</name></link> <!-- **MANDATORY** Name of the web page(s) -->
            <url><![CDATA[http://www.ias.u-psud.fr]]></url> <!-- **MANDATORY** URL address -->
        </link>
    </links>
    <comments><![CDATA[]]></comments> <!-- Additional information on the laboratory (Tel, ...)</comments>
</laboratory>
</import>
```

The data provider « search » tool

- Allow to search data by data type
 - Number of search options and filters
 - Shows ALL data in the database
 - Gives ALL information on data

Provider Molecules search

H₂O

Search

Molecules

UID	UID	Type	Formula	Name	IUPAC name	Isotope mixture
MOLEC_1H216O	MOLEC_1H216O	molecule	¹ H ₂ ¹⁶ O	Water	(1H2,16O)Water	pure isotope
MOLEC_1H217O	MOLEC_1H217O	molecule	¹ H ₂ ¹⁷ O	Water	(1H2,17O)Water	pure isotope
MOLEC_D2O	MOLEC_D2O	molecule	D ₂ O	Heavy water	(2H ₂)Water	partly substituted
MOLEC_1H218O	MOLEC_1H218O	molecule	¹ H ₂ ¹⁸ O	Water	(1H2,18O)Water	pure isotope
MOLEC_H2O	MOLEC_H2O	molecule	H ₂ O	Water, Oxidane		terrestrial abundance
MOLEC_1HD16O	MOLEC_1HD16O	molecule	¹ H ² D ¹⁶ O	Water	(1H1,2H1,16O)Water	pure isotope
MOLEC_HDO	MOLEC_HDO	molecule	HDO	Water	(2H1)Water	partly substituted

Spectrum Write your keywords here ..

Molecule

Type molecule

Name Water

IUPAC name Water, Oxidane

Secondary names Hydrogen oxide, Dihydrogen oxide, H₂O

InChI 1S/H₂O/h1H₂

InChI key XLYOFNOQVPJJNP-UHFFFAOYSA-N

CAS number 7732-18-5

Comments natural H₂O

Structure and atomic composition

Formula H₂O

Chemical formula H₂O

Stoichiometric formula O H₂

Structural formula [OH₂]

Charge 0

Unpaired electrons 0

Atoms

SSHADE : partners / data providers side

Who can be a SSHADE partner ?

Any group producing experimental data on solid spectroscopy who want to make them available to the community

They will:

- ➔ get their own database
- ➔ be scientifically responsible of their content and quality
- ➔ get a ~2.5 days training (+ SSHADE-party) to:
 - ✓ Understand the SSHADE infrastructure and the SSDM data model
 - ✓ Learn to prepare XML import files (sample, experiment, spectra + associated files)
 - ✓ Validate, import & correct data
- ➔ get access to all preparation tools and fundamental data (atoms, molecules, minerals, solid phases...)
- ➔ get on-line technical / scientific support from the SSHADE team
- ➔ get a 'data reference' + DOI for each 'experiment' (= data set) + a reference + DOI for their database

But they need

- ✓ to be motivated
- ✓ to spend some time on data preparation (Astronomers/CNAP can count time on their service)

SSHADE Band lists

Band lists: Aims

- To provide a data base containing the **list of electronic, vibration and phonon bands (absorption and Raman) of various solids** (Ices, Simple organics, Minerals)
 - To help **identify absorption or emission bands from solids** observed on objects
 - To help **determine the environment of the molecule or mineral** (composition, isotopes, mixing, phase, T, P, ...)
 - To help **select the best spectra to compare with observation, or to use in models**
- ➔ Provide tools to **Import / Search / Visualize / Export** Band lists & Bands

Band list of solids: band parameters

Bands parameters

- Position (energy)
- Width
- Shape
- Peak intensity
- Integrated intensity

• Vibration mode

• Molecule

• Constituent

• Isotope

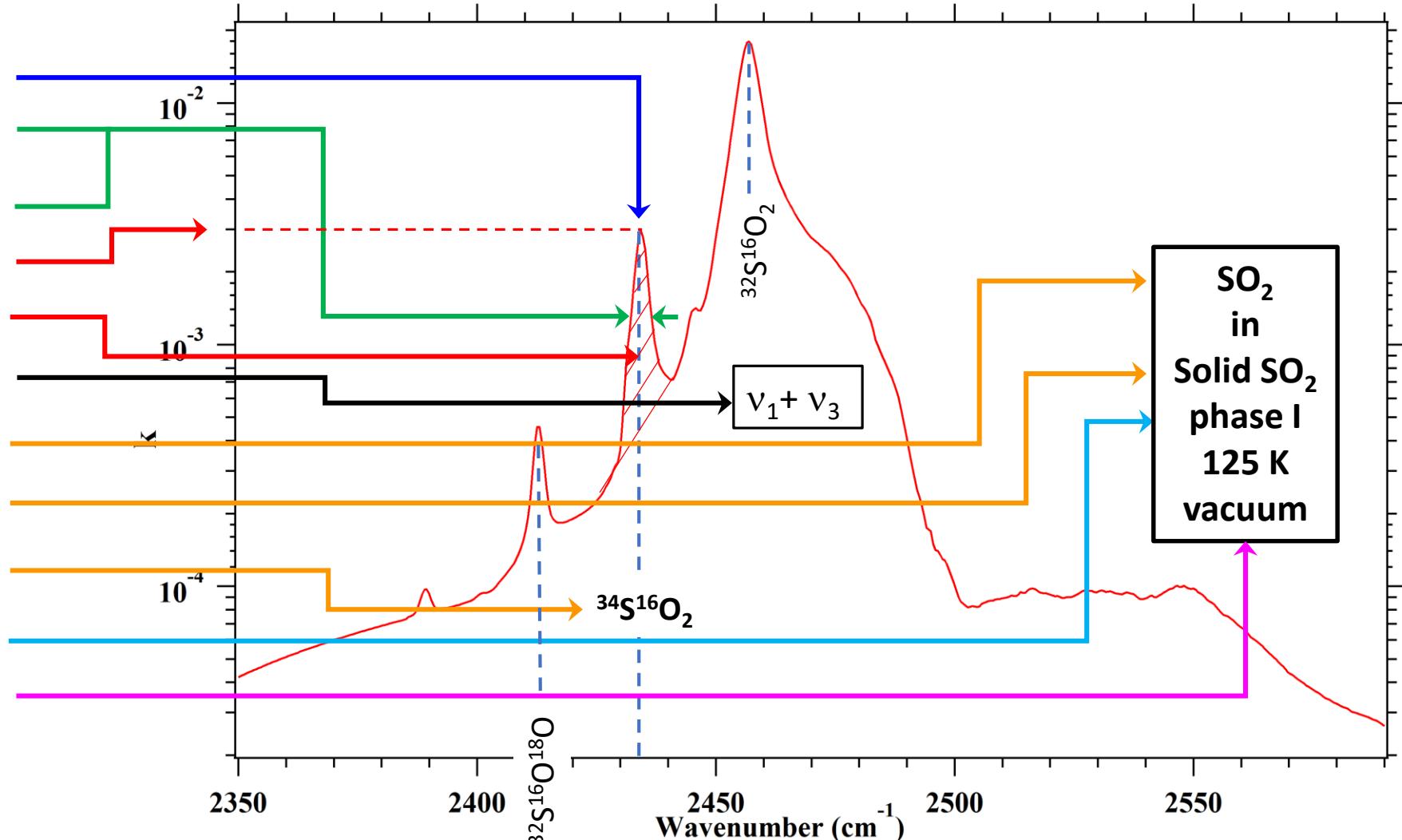
• Phase

• Environment cond.

• Accuracies

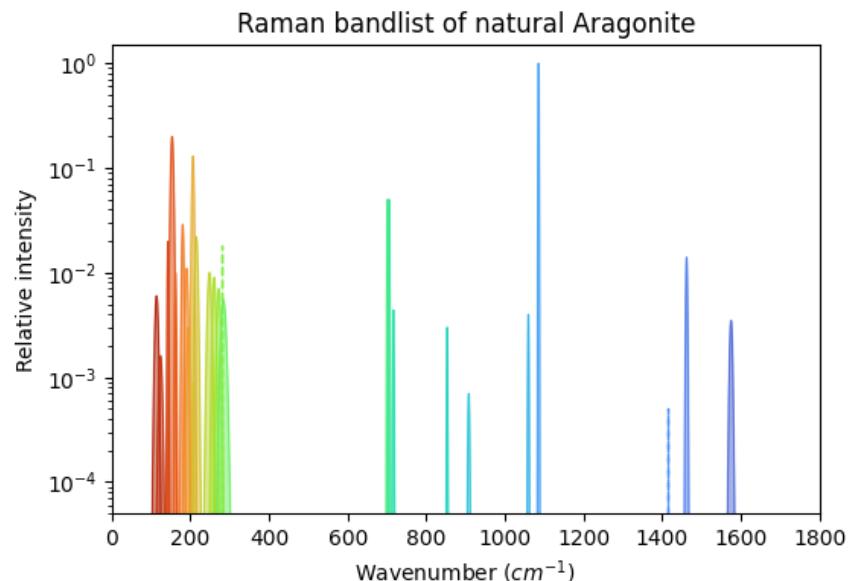
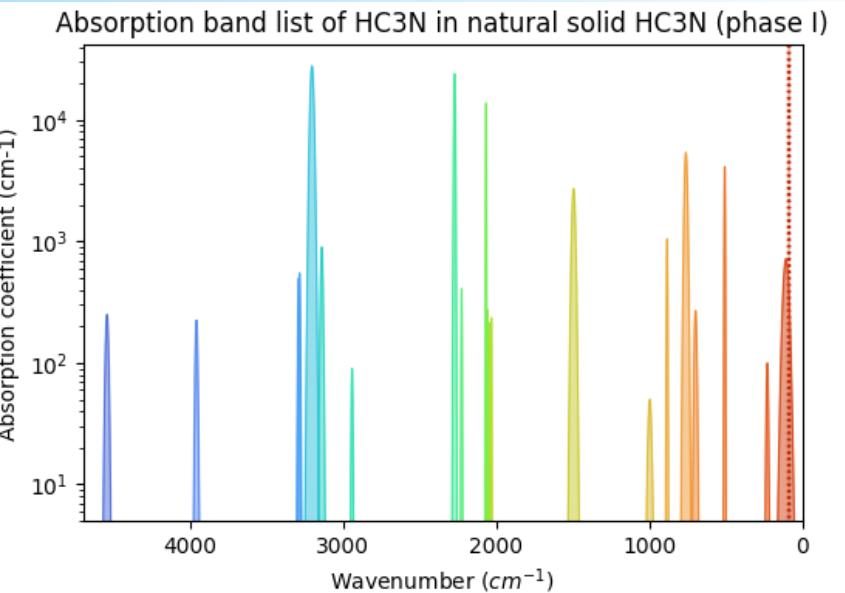
• Quality / evaluation

Spectral range : from VUV to Far-IR



Which types of bandlists in SSHADE ?

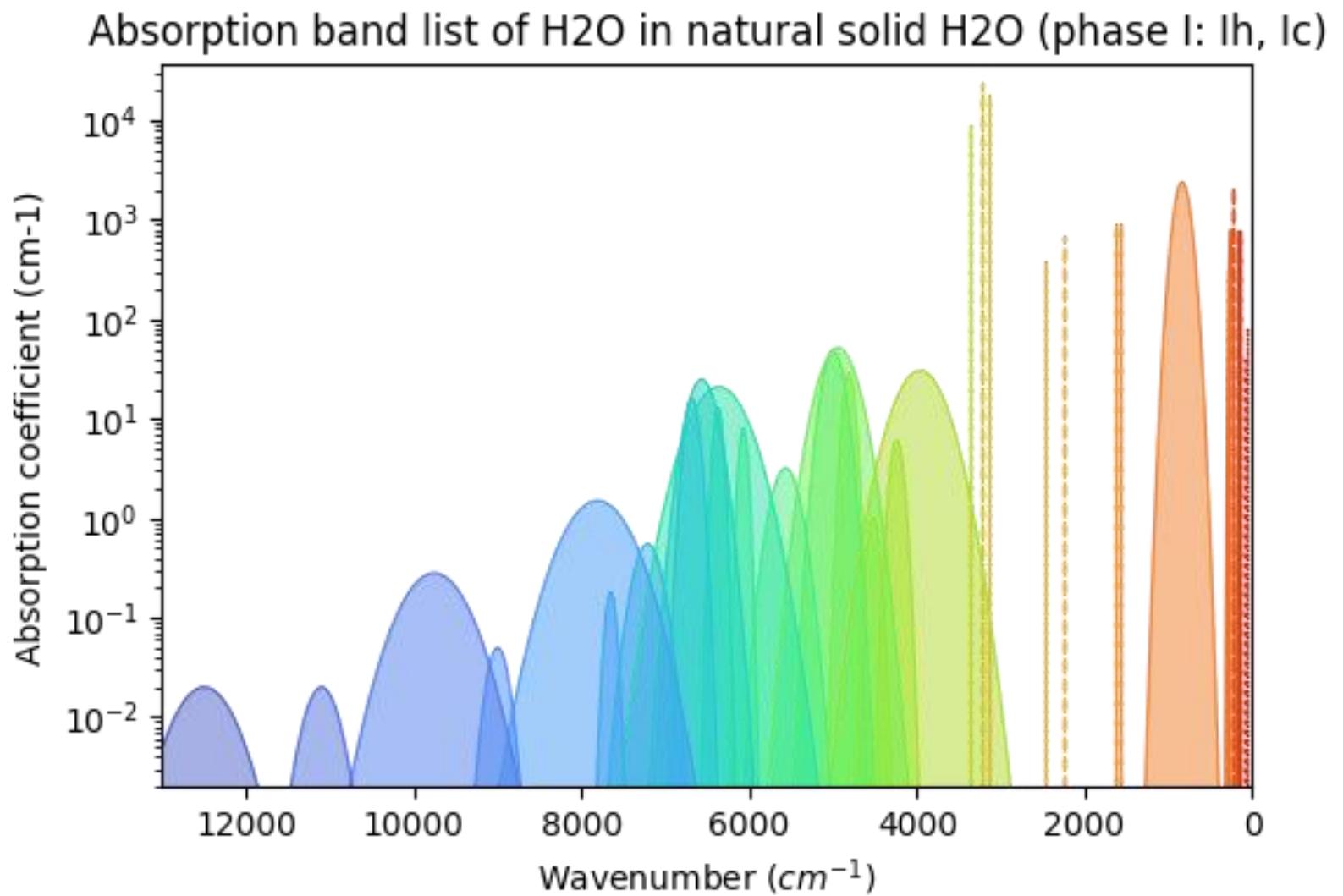
- Materials
 - Minerals
 - Ices (low/high T-P, simple compounds, ...)
 - Organic & Inorganic solids (simple)
- Spectral ranges:
 - from VUV to far-IR (0.2μm – 500μm)
- Types of data:
 - Bands
 - Absorption spectra (absorption coefficients)
 - Raman spectra



Bandlist of Ices

Absorption

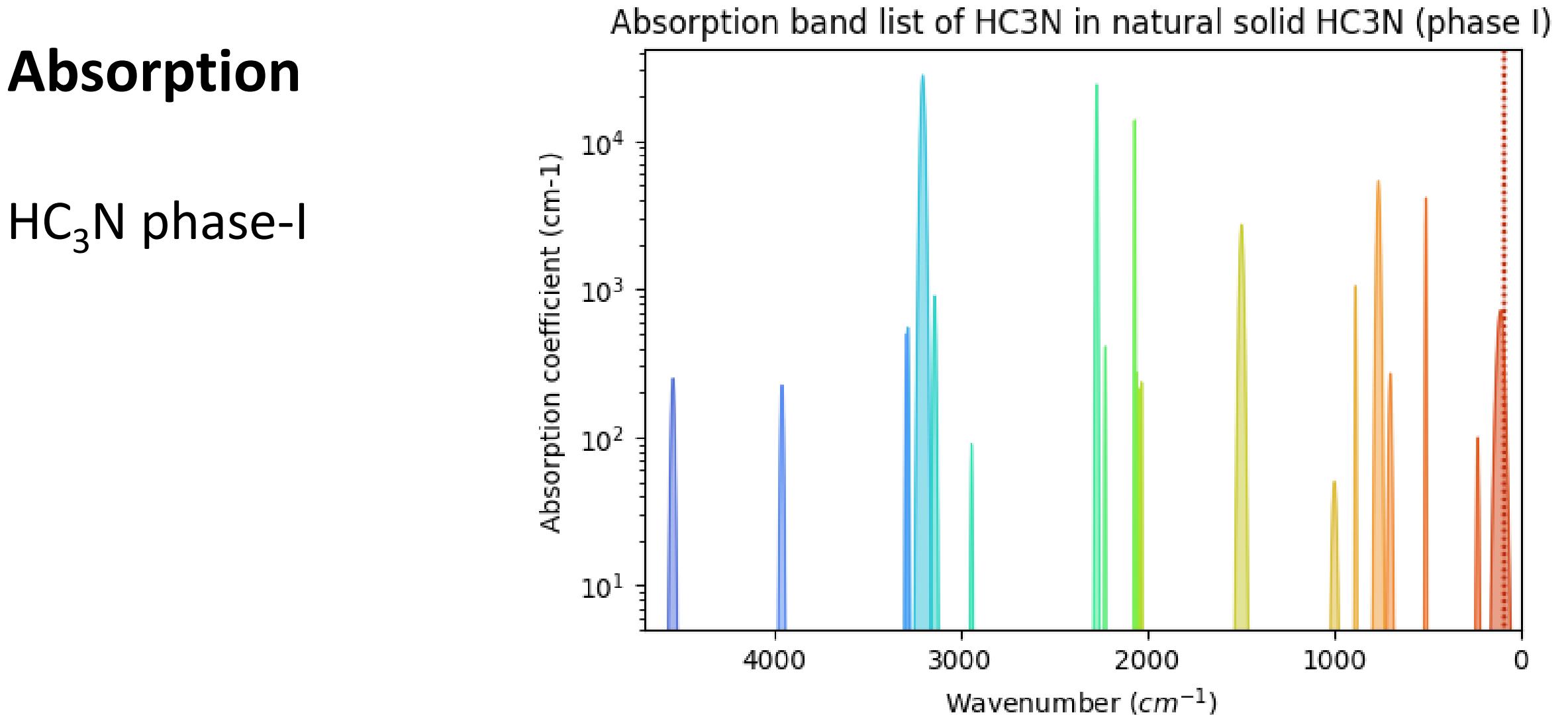
H₂O ice Ih



Bandlist of Nitriles

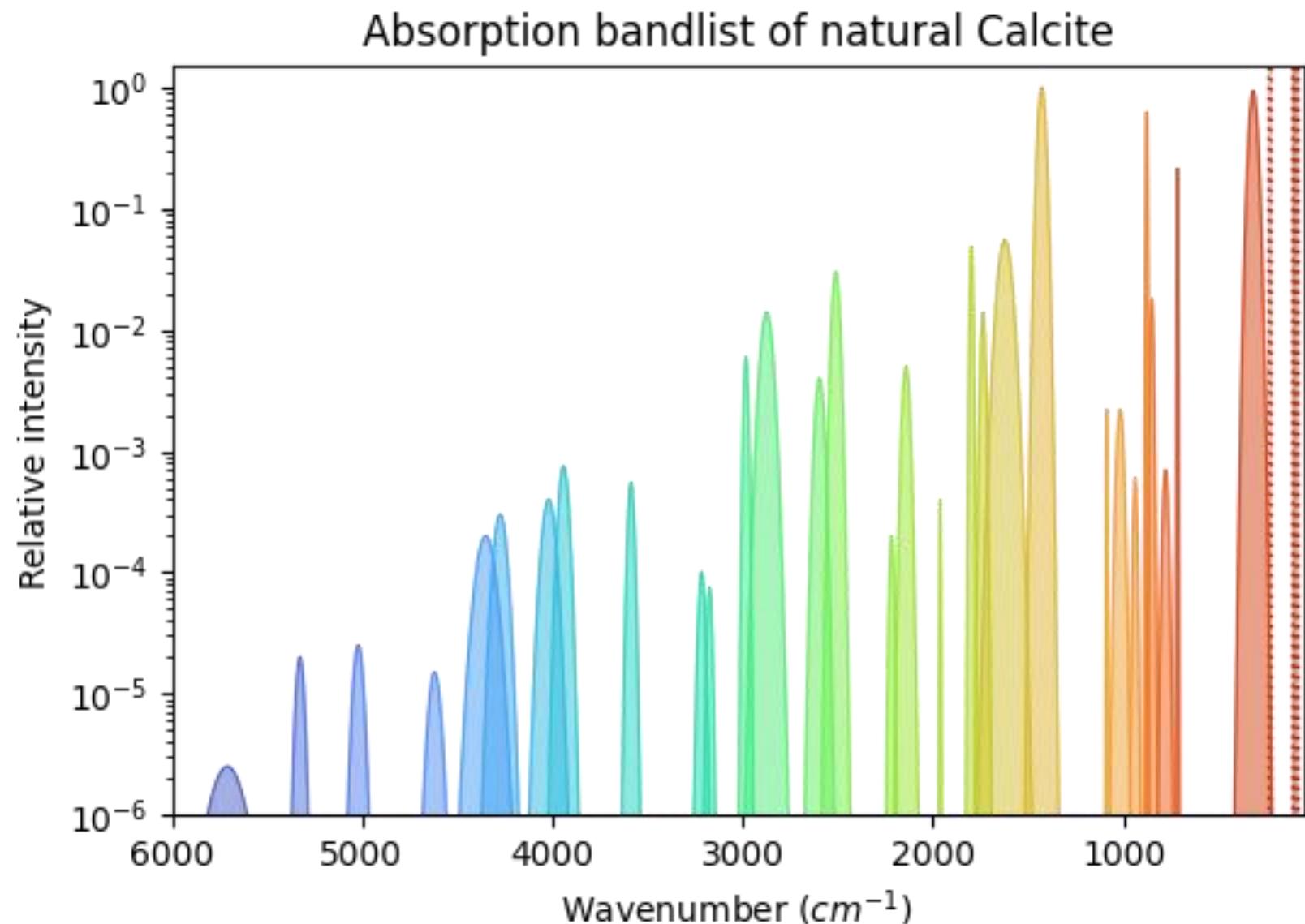
Absorption

HC_3N phase-I



Bandlist of Minerals

Absorption
Calcite

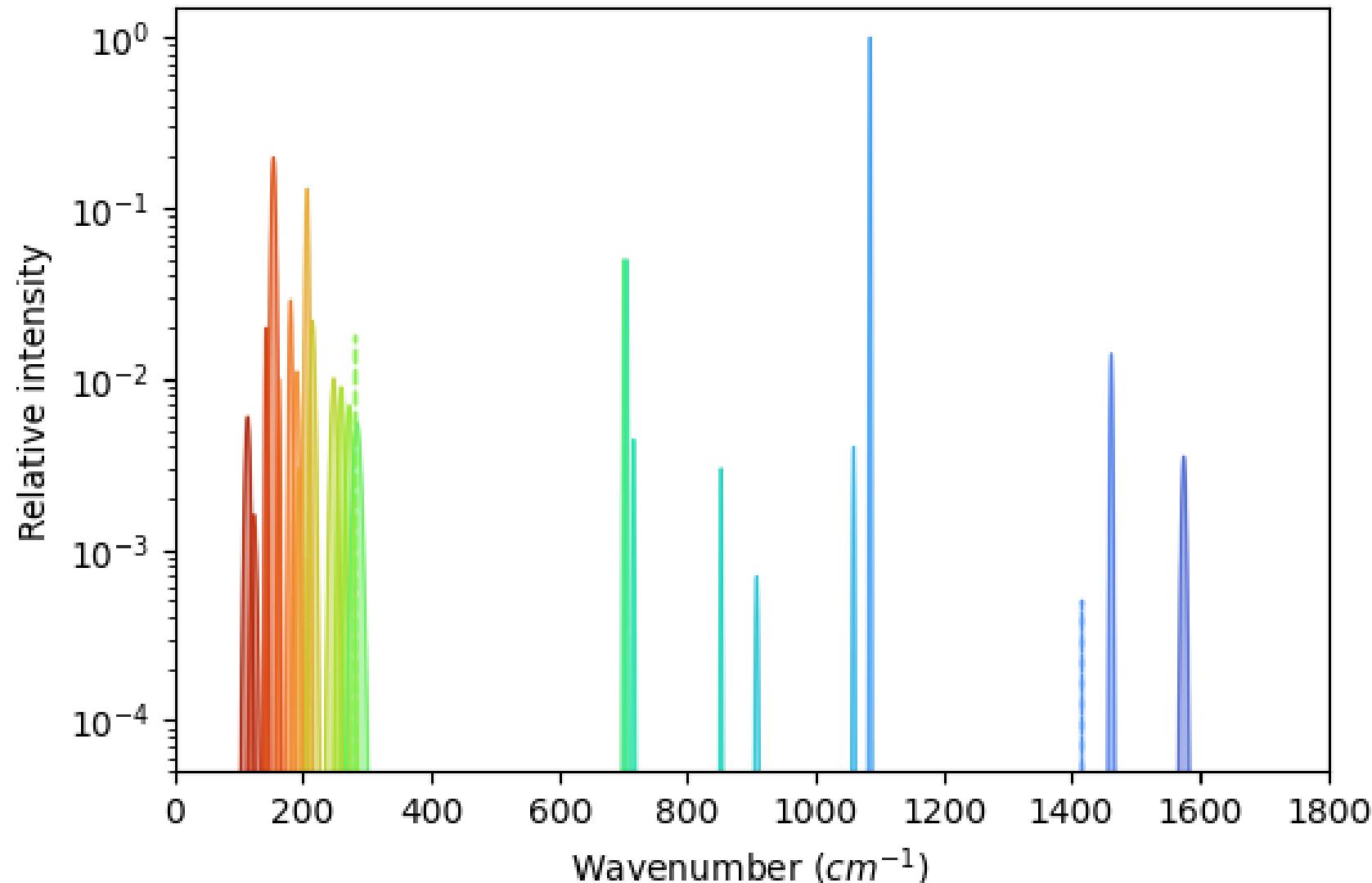


Bandlist of Minerals

Raman

Aragonite

Raman bandlist of natural Aragonite



SSHADE interface for Band lists

SSHADE Web interface

www.sshade.eu

Search bar ➔

News and new data ➔

Already available:

- over 5500 spectra
- 28 bandlists (850 bands)
- ~ 500 publications

The screenshot shows the SSHADE Web interface. At the top, there is a search bar with the placeholder "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" (which has two red arrows pointing to it), and "Search publications". The main content area features a news article titled "New dataset released: [sshade.eu/data/EXPERIMENT...](#) Vis-NIR reflectance spectra of La Rousse pigments (PIG-0183-2017): powder, raw block, and polished slice | PIG database". It includes a plot of Reflectance factor vs. Wavelength (nm) for La Rousse pigments in three states: Powder, Raw block, and Polished slice. The plot shows characteristic absorption features in the visible and infrared regions. Below the plot, the text "by SSHADE: Databases for Solid Spectroscopy, 2020-08-28 04:47:52 UTC+0000" is displayed. At the bottom of the page, there is an "About SSHADE" section with a detailed description of the project and logos for various partners: euroPLANET, CNRS/INSU, cnes, UNIVERSITÉ Grenoble Alpes, IPAG, and OSUG.

SSHADE Web interface

Search

- **Bandlist**
- **Bands**
- **Publications**

Provide 2 complementary tools:

- ✓ “Google-style” toolbar
 - any relevant word
- ✓ Specialized filters

Bandlist

- by bandlist,
- by molecule,
- By constituent
- by environment,

Band

- by bandlist,
- by molecule,
- By constituent
- by environment,

Publications

Band lists search

HC3N

Filters

By Bandlist

Type	in	absorption	
Spectral range type	in	NIR, MIR, FIR	
Spectral range min	>=	1.5	
Spectral range max	<=	40	
Category	in	micron	
fundamental vibration, overtone vibration, combination vibration			

By Molecule (for molecular solids and liquids)

Name	contains all words		
Formula	is	HC3N	
InChI + key	is		

For isotopes, put atomic mass between [] before the atom - ex: [32]S[16]O[18]O, [13]C2HD...

Options

By Constituent

Name	contains all words		
Liquid compound type	in	Nothing selected	
Solid (synthetic) compound type	in	organic molecular solid	
Mineral compound type	in	Nothing selected	
CAS number	is		

By Environment

Temperature	>=	50	K	
Temperature	<=	200	K	

Band lists & Bands: search interfaces

- **Search tool**

Band list:

Type and spectral range

Molecule, bond, chem. function
(molecular solid/liquid)

Constituent
(ice, mineral, organic...)

Environment
(T, P)

Band lists search

Write your keywords here or leave it empty to get all the data... in user S1b

Filters

By Bandlist

Type	in	Raman scattering
Spectral range type	in	NIR, MIR, FIR
Spectral range min	>=	1 micron
Spectral range max	<=	200 micron
Category	in	fundamental vibration

By Molecule (for molecular solids and liquids)

Name	contains all words	
Formula	is	
InChI + key	is	

Options

With bond	is	
With chemical function	is	

By Constituent

Name	contains all words	
Liquid compound type	in	Nothing selected
Solid (synthetic) compound type	in	Nothing selected
Mineral compound type	in	carbonate, sulfate
CAS number	is	

By Environment

Temperature	>=	250 C
Temperature	<=	350 C
Pressure	>=	bar
Pressure	<=	bar

Band:

Wavelength, intensity, width...

Molecule, bond
(molecular solid/liquid)

Constituent
(ice, mineral, organic...)

Bands search

Write your keywords here or leave it empty to get all the data... in user S1b

Filters

By Band

Type	in	absorption
Band position min	>=	2400 cm ⁻¹
Band position max	<=	2460 cm ⁻¹

Options

By Molecule

Name	contains all words	
Formula	is	SO2
InChI + key	is	

Options

By Constituent

Name	contains all words	
Liquid compound type	in	Nothing selected
Solid (synthetic) compound type	in	inorganic molecular solid
Mineral compound type	in	Nothing selected
CAS number	is	

Results 5 bands

SSHADE Web interface

Bandlist search results

Bandlists fitting the search criteria are displayed:

Info provided:

- Band number
- molecule and constituent

Tools:

- Order by title or info
- Quick view
→ preview popup
- Download
→ customize format
→ direct or basket

Title	Bands number	Molecule/Atom	Constituent	
Absorption band list of C2N2 in natural solid C2N2 (phase I)	33	C ₂ N ₂	natural C ₂ N ₂ - phase I	
Absorption band list of CH3CN in natural solid CH3CN (phase beta)	66	CH ₃ CN	natural CH ₃ CN - phase beta	
Absorption band list of CH3CN in pnatural solid CH3CN (phase alpha)	34	CH ₃ CN	natural CH ₃ CN - phase alpha	
Absorption band list of CH3OH in natural solid CH3OH (amorphous phase)	33	CH ₃ OH	natural CH ₃ OH - amorphous	
Absorption band list of CH3OH in natural solid CH3OH (phase alpha)	48	CH ₃ OH	natural CH ₃ OH - phase alpha	

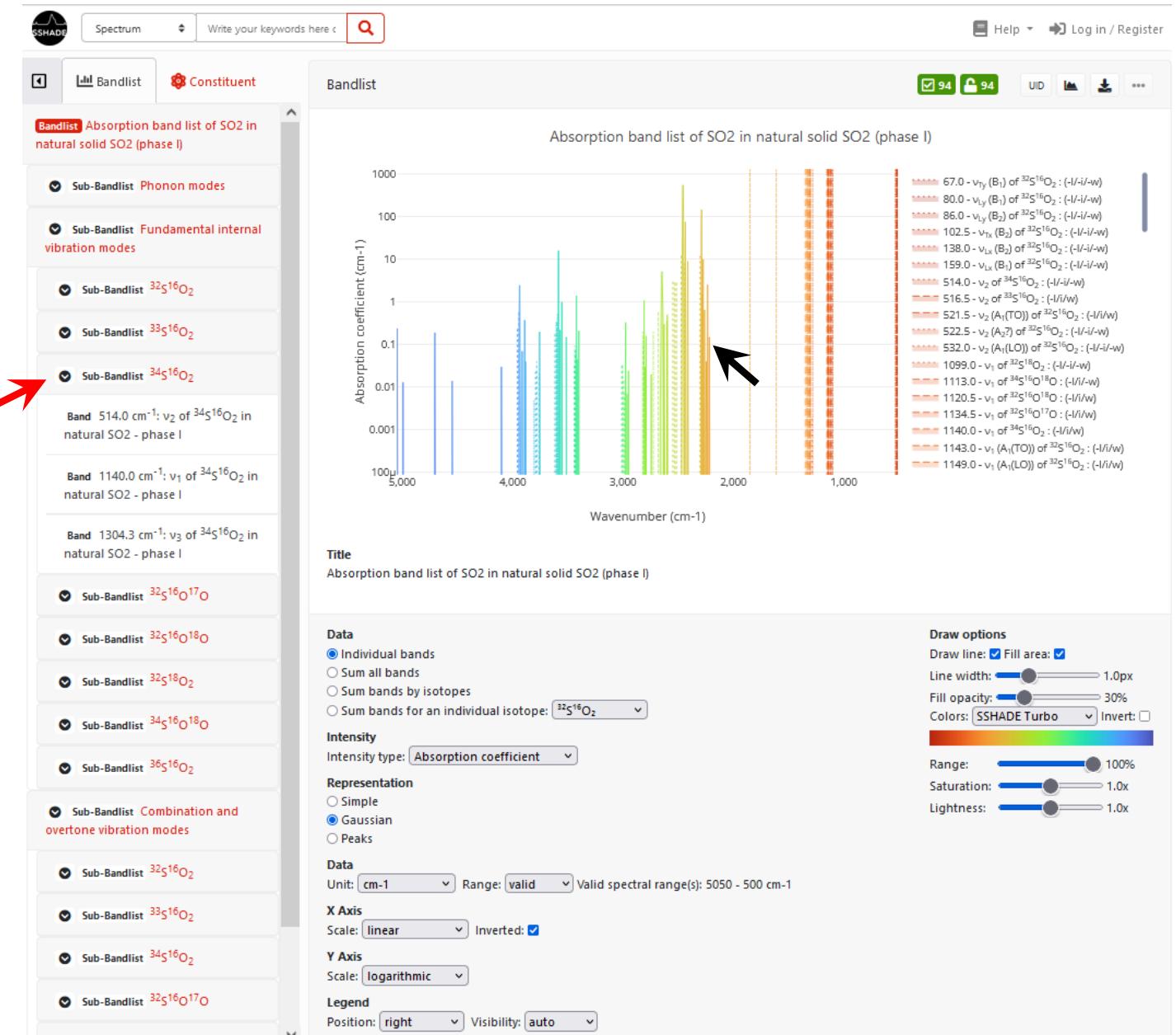
SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ **Bandlist structure and parameters**
 - Ordered by transition type and isotopes
 - Molecule, constituent
 - Spectral range, band number...

- ✓ **Bands and parameters**



SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ Bandlist structure and parameters
 - Ordered by transition type and isotopes
 - Molecule, constituent
 - Spectral range, band number...
- ✓ Bands and parameters
- ✓ Constituent structure and composition
 - Composition (abundance, ...)
 - Isotopes
 - Chemical bonds and functions
 - Crystallography
 - Optical and Physical properties

The screenshot shows the SSHADE Web interface with the following details:

- Spectrum**: A small plot area.
- Write your keywords here**: A search bar.
- Bandlist**: A button.
- Constituent**: A button.
- Constituent natural SO₂ - phase I**: The selected constituent.
- Molecule/Atom SO₂ (Sulfur dioxide)**: The molecule name with a red arrow pointing to it.
- Isotope ³²S¹⁶O₂**
- Isotope ³²S¹⁶O¹⁷O**
- Isotope ³²S¹⁶O¹⁸O**
- Isotope ³³S¹⁶O₂**
- Isotope ³³S¹⁶O¹⁷O**
- Isotope ³³S¹⁶O¹⁸O**
- Isotope ³⁴S¹⁶O₂**
- Isotope ³⁴S¹⁶O¹⁷O**
- Isotope ³⁴S¹⁶O¹⁸O**
- Isotope ³⁶S¹⁶O₂**
- Name**: natural SO₂ - phase I
- Type**: checked
- Family**: molecular solid
- Class**: polar molecular solid
- Compound type**: inorganic molecular solid
- Chemical composition**: checked
- Formula**: SO₂
- Chemical formula**: SO₂
- Elemental formula**: SO₂
- Isotope mixture type**: terrestrial abundance
- Species**: checked

Formula	Name	Family	Number min-max	Mole fraction	Isotope mole fraction	State	Relevance
SO ₂	Sulfur dioxide	molecule	1	1.0	1	pure	main

- Chemical functions and bonds**: checked
- Chemical bonds**

Bond	Number	Relevance
=S=O	2	main
- Classification**: checked
- Phase**: checked

Band lists : list of the bands

- Main band parameters + assignment + molecule, isotope, constituent + T, P

Spectrum  Write your keywords here 

Help  Data  Bernard Schmitt

 Bandlist 

Bandlist VUV-NIR-MIR-FIR absorption band list of CO in pure solid alpha-CO

 Sub-Bandlist Electronic transitions $d^3\Delta \leftarrow X^1\Sigma^+$ system

 Sub-Bandlist Electronic transitions $A^1\Pi \leftarrow X^1\Sigma^+$ system

 Sub-Bandlist Electronic transitions $a^3\Pi_r \leftarrow X^1\Sigma^+$ system

 Sub-Bandlist Vibration modes

 Sub-Bandlist Phonon modes

Bands

Show 25 entries Search:

	Position (cm ⁻¹)	Width (cm ⁻¹)	Relative intensity	Strength	Transition mode	Isotope	Bond	Mode type	Degeneracy
	51870 ± 25	512 ± 10	0.33		$a^3\Pi_r \leftarrow X^1\Sigma^+(2, 0)$	¹² C ¹⁶ O	¹² C ⁻ ≡ ¹⁶ O ⁺	intervalence charge transfer stretching	double site
	50150 ± 25	504 ± 10	0.5		$a^3\Pi_r \leftarrow X^1\Sigma^+(1, 0)$	¹² C ¹⁶ O	¹² C ⁻ ≡ ¹⁶ O ⁺	intervalence charge transfer stretching	double site
	48400 ± 25	563 ± 10	1		$a^3\Pi_r \leftarrow X^1\Sigma^+(0, 0)$	¹² C ¹⁶ O		intervalence charge transfer	double site
	6390 ± 1	43 ± 2	5.5e-07	vw	$3\nu_1 + \nu_{L,T}$	¹² C ¹⁶ O	¹² C ⁻ ≡ ¹⁶ O ⁺	stretching other	
	6337.8 ± 0.8	3.7 ± 0.2	3.1e-05	vw	$3\nu_1$	¹² C ¹⁶ O	¹² C ⁻ ≡ ¹⁶ O ⁺	stretching	
	6258 ± 0.5	3.7 ± 0.2	1.2e-08	vw	$3\nu_1$	¹² C ¹⁷ O	¹² C ⁻ ≡ ¹⁷ O ⁺	stretching	
	6199 ± 0.6	3.6 ± 0.2	3e-07	vw	$3\nu_1$	¹³ C ¹⁶ O	¹³ C ⁻ ≡ ¹⁶ O ⁺	stretching	
	6188.4 ± 0.5	3.7 ± 0.3	6.5e-08	vw	$3\nu_1$	¹² C ¹⁸ O	¹² C ⁻ ≡ ¹⁸ O ⁺	stretching	

Crystalline α -CO

Band list & bands: organisation of the bands

- Constituent

- Phonon modes

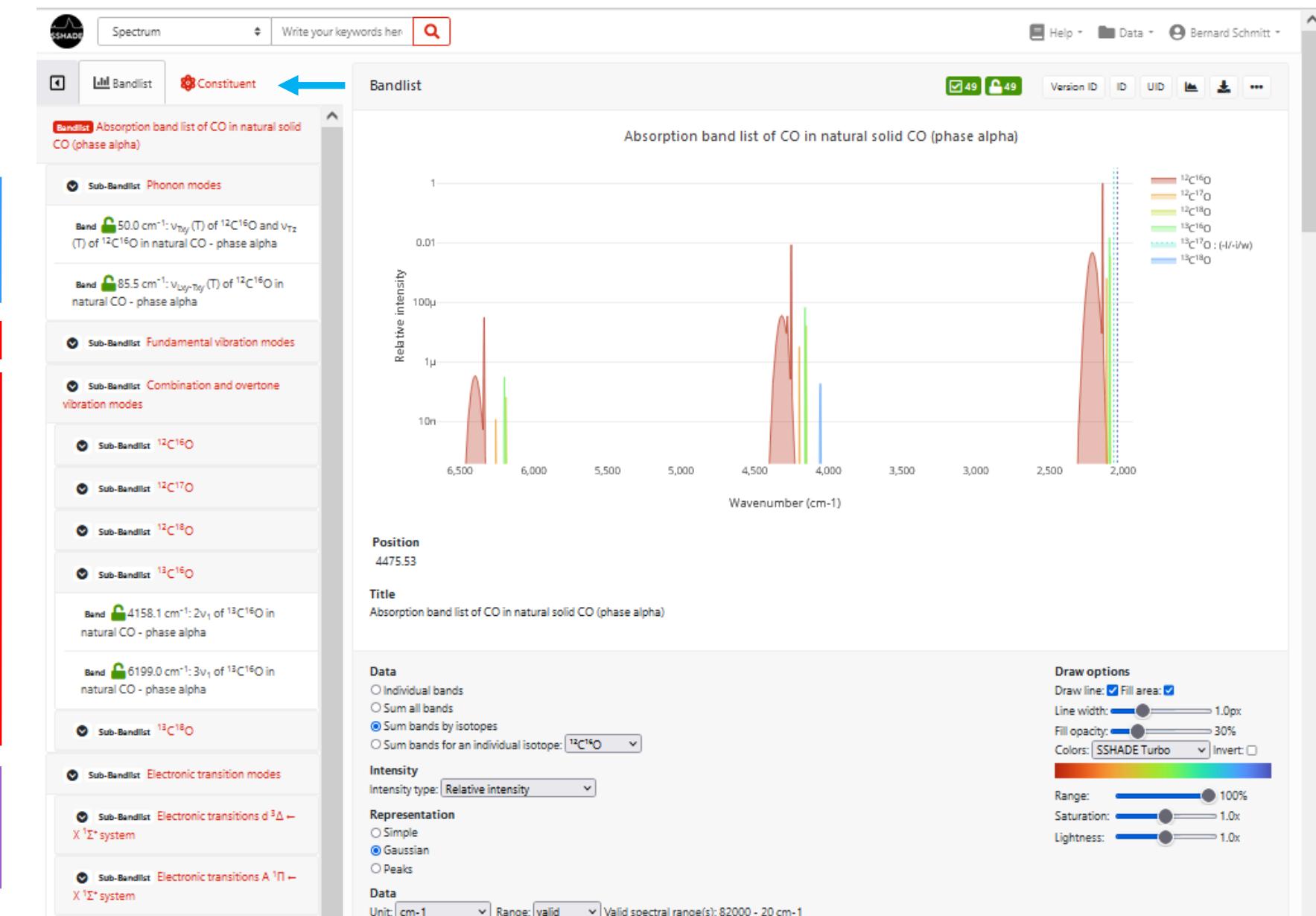
- Fundamental vibration modes

- By isotope

- Combination vibration modes

- By isotope

- Electronic bands



Band list & bands: display tools

Data

- Individual bands
- Individual isotope
- Sum of bands per isotope
- Sum of bands of whole bandlist

Intensity

- Absorption coefficient
- Relative intensity

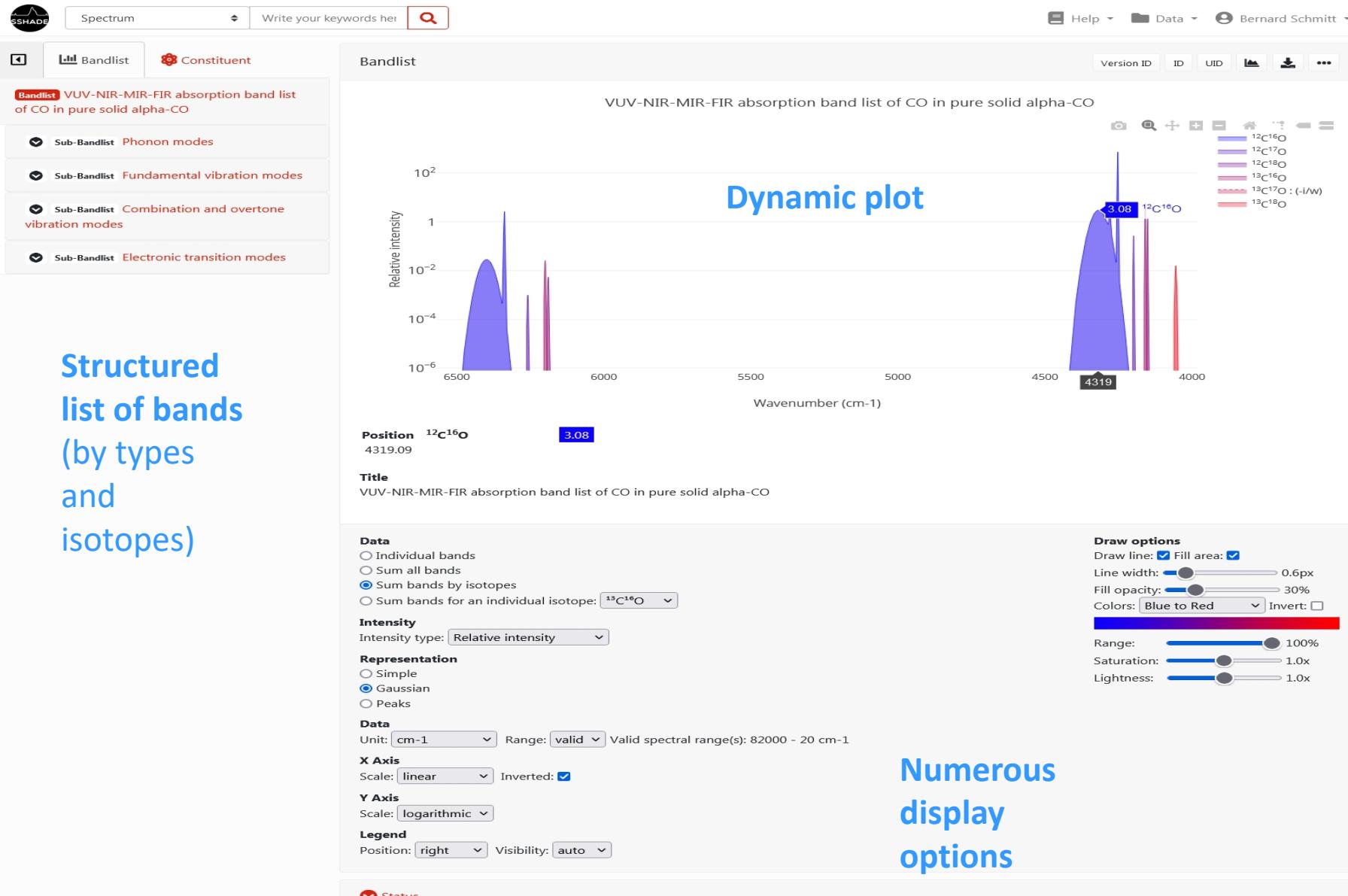
Representation

- Line (position + intensity)
- Triangle (position + width + intensity)
- Gaussian

✓ Manage missing data on width and/or intensity

Band list & bands: dynamic display tool

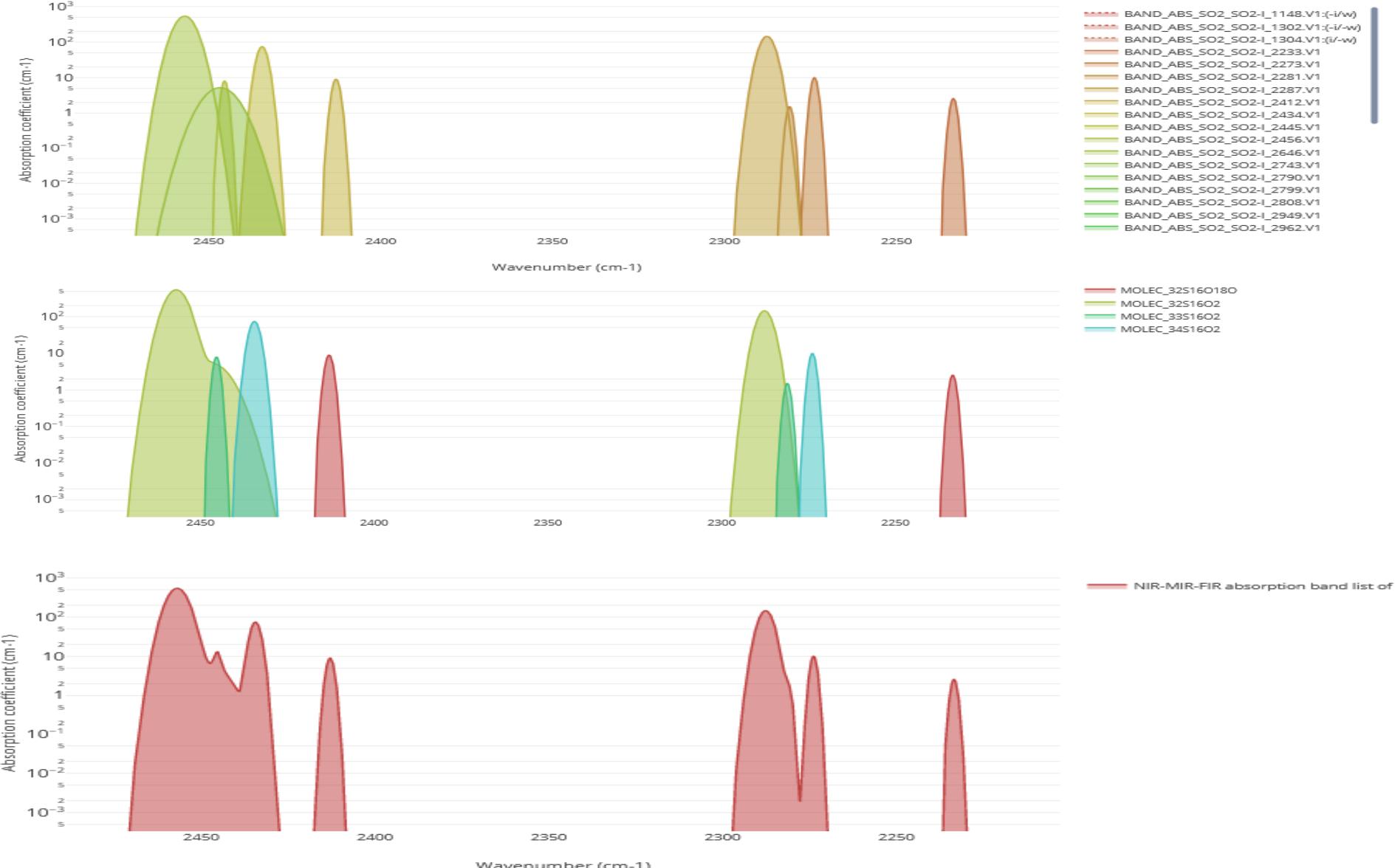
- Display tool



Band list & bands: display tools

Band list plot options

- Individual bands
- Sum of bands of each isotope
- Sum of bands of whole bandlist



SSHADE Web interface

Visualize

Provide very complete information on:

- ✓ Bandlist structure and parameters
 - Ordered by transition type and isotopes
 - Molecule, constituent
 - Spectral range, band number...
- ✓ Bands and parameters
- ✓ Constituent structure and composition
 - Composition (abundance, ...)
 - Isotopes
 - Chemical bonds and functions
 - Crystallography
 - Optical and Physical properties
- ✓ Many linked info !
 - Publications
 - Web sites, ...
 - Minerals, molecules / chemical bonds / atoms

The screenshot shows the SSHADE Web interface with a focus on a specific molecule's properties. The main navigation bar includes 'Spectrum', 'Write your keywords here', and a search icon. Below this, there are tabs for 'Bandlist' (selected) and 'Constituent'. The 'Bandlist' tab shows 'Absorption band list of HC₃N in natural solid HC₃N (phase I)'. Sub-tabs include 'Sub-Bandlist Phonon modes', 'Sub-Bandlist Fundamental vibration modes', and 'Sub-Bandlist Combination and overtone vibration modes'. A large 'Related data' panel is open, containing sections for 'Molecule', 'Name' (Cyanoacetylene), 'Name and identifiers', 'Structure and atomic composition' (with a 3D ball-and-stick model of the molecule), 'Formula' (HC₃N), 'Chemical formula' (HC₃N), 'Structural formula' ([H]-C≡C≡N), 'Charge' (0), and 'Unpaired electrons' (0). Other sections like 'Atoms', 'Stereoisomers', 'Isotopic composition', 'Nuclear spin isomers', 'Properties', 'Fundamental vibration modes', 'Chemical functions and bonds', and 'Links' are also listed. The bottom right corner of the interface has a note: 'ion 1. SSHADE (OSUG Data Center). Dataset/Band list'.

SSHADE Web interface

Export

- Band (+ customize export formats: •••)
- Band list

At different level of the interface

- Search results

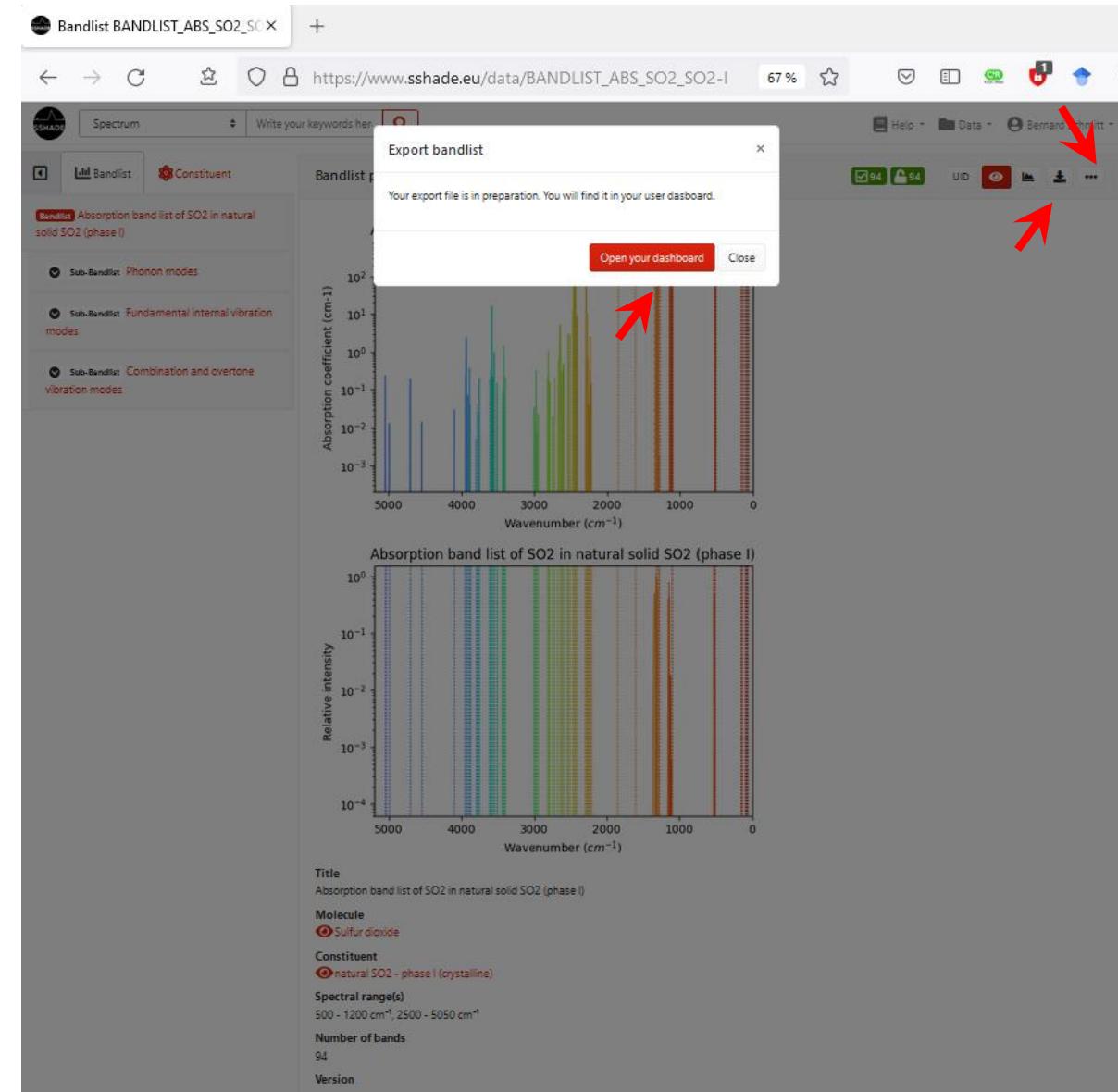
Detail pages of bandlist and bands

by asynchronous data extraction:

- stored in dashboard

Delivered in a zip file that contains:

- Band list preview
- Constituent composition
- Details on bandlist
- **Details on all bands:** parameters & mode assignments, environment ...
- **ASCII table w. main parameters of all bands**
- Description file
- Publication citation list



SSHADE-Bandlist content

- ✓ **Critical compilation** of all publications on a given fundamental phase
- ✓ + analysis of SSHADE-Spectra data + others

Prototype:

Online: 1st October 2021

with 20 band lists
~420 bands

Currently

41 band lists
~1050 bands

2024

> 75 band lists
> 1500 bands

Absorption

- Ices: H₂O(Ih), CO(α), CO₂(I), N₂(α, β), NH₃(I), CH₃OH(α, am) [+ H₂O₂, CO₂ in various matrices ...]
- Hydrocarbons : CH₄(I), C₂H₂ (am, meta, II), C₄H₂(I, am) [+ C₂H₄, C₂H₆, C₆H₆ ...]
- Nitriles: HCN(II), HC₃N(I), C₂N₂(I), CH₃CN (α, β)
- SO₂(I), SO (in Ar), S₂O (in Ar, in SO₂) [+ SO₃, S₂, S₃ ...]
- Minerals: calcite, hematite [+ carbonates, silicates,...]

Raman

- Minerals: Aragonite, Calcite, Dolomite, Magnesite, Rhodochrosite, Siderite [+ salts ...]
- Ices: CH₄(I), CO(α), CO₂(I), N₂(α, β), S₂O (in Ar, in SO₂)
- Organics: HCN(II), C₂N₂(I), CHCH₃CN (α)

Bibliography search

Database of solid spectroscopy papers

- Over 500 publications

- Paper from SSHADE data
 - Experiments
 - Band lists
 - + many others

- Specialized keywords

- Many ways to search
 - Reference
 - Content
 - Codes
 - SSHADE experiment

The screenshot shows the SSHADE database search interface. At the top, there is a navigation bar with a logo, a dropdown menu labeled "Spectrum", a search bar with placeholder text "Write your keywords here", and a magnifying glass icon. To the right of the search bar are links for "Help", "Data", and a user account for "Bernard Schmitt". Below the navigation bar is a section titled "Publications search" with a placeholder text "Write your keywords here or leave it empty to get all the data...". To the right of this is a dropdown menu "in user S1b" and a red "Search" button. Underneath the search bar is a red "Filters" button and a "Reset all filters" link. The main area contains several filter sections: "Publication" (Document type: "in" dropdown set to "review article"), "Reference" (Author family name: "contains all words" dropdown set to "Fatelli", "Only first author" checkbox), "Year" (dropdown set to "2020"), "Title" (dropdown set to "contains all words"), "Content" (Abstract, Content, Keyword dropdowns, and a "Nothing selected" message for Content), "Codes" (DOI, Identifier type, Identifier code dropdowns, and a "Nothing selected" message for Identifier type), and "Publications of an experiment" (Experiment title, Spectrum title, Experiment DOI dropdowns). The "Keyword" field contains the value "Salammonia" and is highlighted with a red border.

SSHADE @ VESPA VO

SSHADE Virtual Observatory (VO) access for VESPA

- Provide VO search on a limited number of main metadata
 - *species name/formula, compound type, object name, spectral type, T, P, grain size...*
 - Allow to retrieve metadata and data for displaying in VO and associated tools/services
 - Provide a link to the data in SSHADE (spectra in VOTable)
- For spectra: public since **summer 2019**
- For bandlist: **to be developed in 2023-2024**

The screenshot shows the VESPA VO interface. At the top, there's a banner with the VESPA logo and the text "Virtual European Solar and Planetary Access". Below the banner, there are tabs for "Form", "Query", "EPN-TAP Services" (which is selected), and "Custom Service". On the left, there's a sidebar titled "Plotting tools" with icons for TOPCAT, Aladin, SPLAT, CASSIS, and 3DView. Another sidebar titled "Example queries" shows a query for "Saturn in March 2012". A "Help" section is also present.

The main content area has a green header box titled "SSHADE - SSHADE spectra library". It contains text about SSHADE's purpose, data ranges, and links to its website and wiki. Below this, there's a table with columns for "granule_uid", "dataproduct_type", "target_name", and "time_min (d)". The table lists several entries, all of which are "SPECTRUM_YD_20190911_xxx" files, categorized as "cube", and timestamped at "2010-02-16T00:00:00".

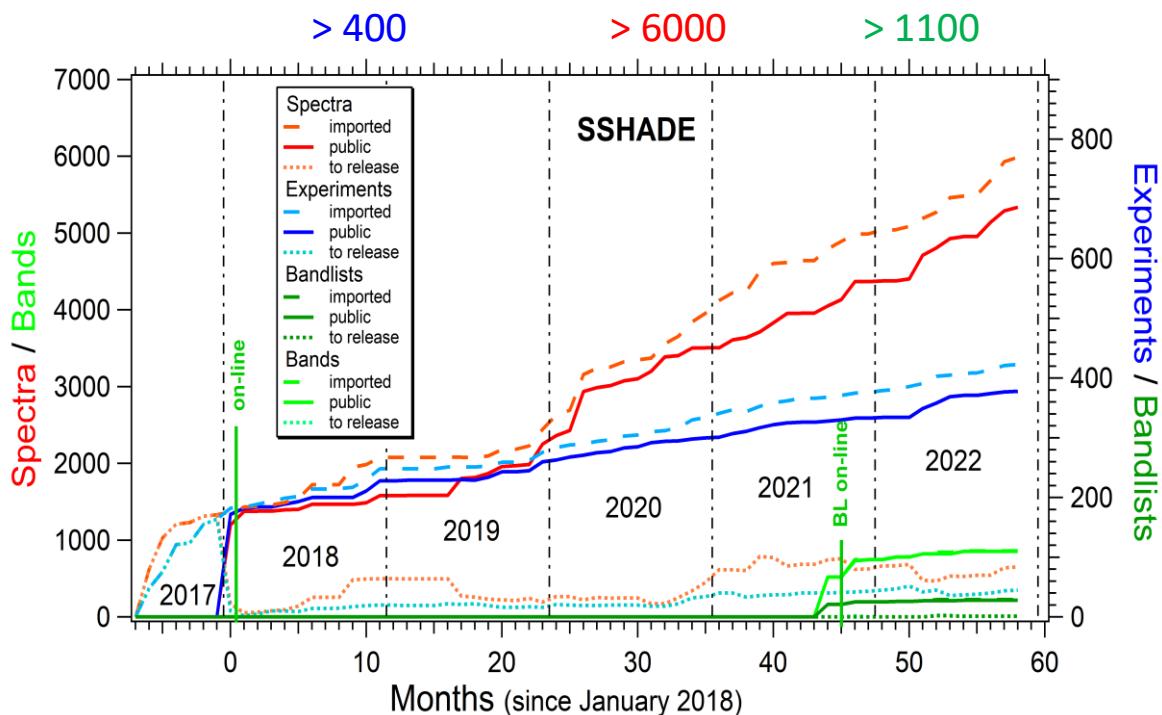
granule_uid	dataproduct_type	target_name	time_min (d)
SPECTRUM_YD_20190911_060	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_050	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_040	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_030	cube		2010-02-16T00:00:00

The users of SSHADE

Increase of content and of use

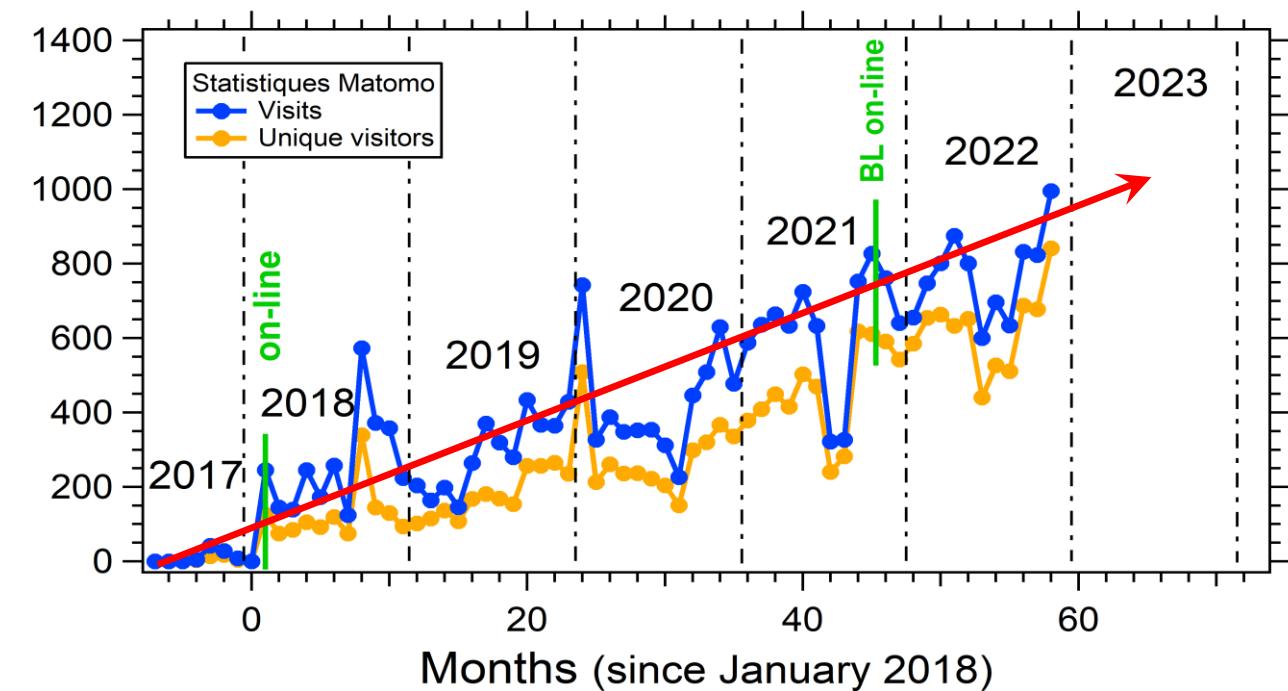
- Today : 500 researchers registered
- SSHADE data content

Experiments & Spectra & Bands



SSHADE users (Stats Matomo)

23% France, 23% Europe, 28% USA+Canada, 23% Asia



Current & near-future SSHADE developments

- **Samples collected by space missions**

- ✓ Information on collected samples and body + geolocalisation
- ✓ Moon (Apollo, Luna, Chang'e), 81P/Wild (Stardust), Itokawa & Ryugu (Hayabusa1 & 2),
- ✓ + Bennu (OSIRIS REx), Phobos (MMX)...

- **Multi-spectra and user data comparison**

- ✓ Simple import of your own data in your user space
- ✓ Comparison with SSHADE spectra (conversion in same wavelength unit, ...)
- ✓ Comparison between spectra of different experiments

- **Improvement of ‘Search bar’ tool:**

- ✓ Synonyms, plural, equivalent and derived terms, generic terms, ...
- ✓ Graphie variants, English/US, ...
- ✓ filtering of ‘sample impurities’ (materials & constituents), ...

- **Polarization spectra:**

- ✓ Import of Stokes parameters (I, Q, U, V)
- ✓ Visualization, export