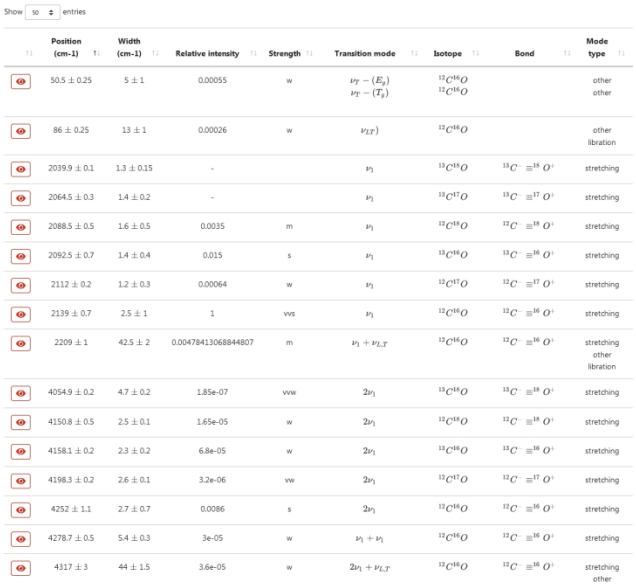
SSHADE-Band List:

the new database of spectroscopy band list of solids



Show 50 entries

	Position (cm-1)	Width (cm-1)	Relative intensity	Strength	Transition mode	Isotope	Bond	Mode type
	50.5 ± 0.25	5 ± 1	0.00055	w	$\nu_T - (E_g)$ $\nu_T - (T_g)$	$^{12}C^{16}O$ $^{12}C^{16}O$		other other
	86 ± 0.25	13 ± 1	0.00026	w	$\nu_{LT})$	$^{12}C^{16}O$		other libration
	2039.9 ± 0.1	1.3 ± 0.15	-		ν_1	$^{13}C^{18}O$	$^{13}C-{}^{18}O$	stretching
	2064.5 ± 0.3	1.4 ± 0.2	-		ν_1	$^{13}C^{17}O$	$^{13}C-{}^{17}O$	stretching
	2088.5 ± 0.5	1.6 ± 0.5	0.0035	m	ν_1	$^{12}C^{18}O$	$^{12}C-{}^{18}O$	stretching
	2092.5 ± 0.7	1.4 ± 0.4	0.015	s	ν_1	$^{13}C^{16}O$	$^{13}C-{}^{16}O$	stretching
	2112 ± 0.2	1.2 ± 0.3	0.00064	w	ν_1	$^{12}C^{17}O$	$^{12}C-{}^{17}O$	stretching
	2139 ± 0.7	2.5 ± 1	1	vvs	ν_1	$^{12}C^{16}O$	$^{12}C-{}^{16}O$	stretching
	2209 ± 1	42.5 ± 2	0.0047841306884807	m	$\nu_1 + \nu_{LT}$	$^{12}C^{16}O$	$^{12}C-{}^{16}O$	stretching other libration
	4054.9 ± 0.2	4.7 ± 0.2	1.85e-07	vvw	$2\nu_1$	$^{13}C^{18}O$	$^{13}C-{}^{18}O$	stretching
	4150.8 ± 0.5	2.5 ± 0.1	1.65e-05	w	$2\nu_1$	$^{12}C^{18}O$	$^{12}C-{}^{18}O$	stretching
	4158.1 ± 0.2	2.3 ± 0.2	6.8e-05	w	$2\nu_1$	$^{13}C^{16}O$	$^{13}C-{}^{16}O$	stretching
	4198.3 ± 0.2	2.6 ± 0.1	3.2e-06	vw	$2\nu_1$	$^{12}C^{17}O$	$^{12}C-{}^{17}O$	stretching
	4252 ± 1.1	2.7 ± 0.7	0.0086	s	$2\nu_1$	$^{12}C^{16}O$	$^{12}C-{}^{16}O$	stretching
	4278.7 ± 0.5	5.4 ± 0.3	3e-05	w	$\nu_1 + \nu_3$	$^{12}C^{16}O$	$^{12}C-{}^{16}O$	stretching
	4317 ± 3	44 ± 1.5	3.6e-05	w	$2\nu_1 + \nu_{LT}$	$^{12}C^{16}O$	$^{12}C-{}^{16}O$	stretching other

(on-line 1st October 2021)

www.sshade.eu

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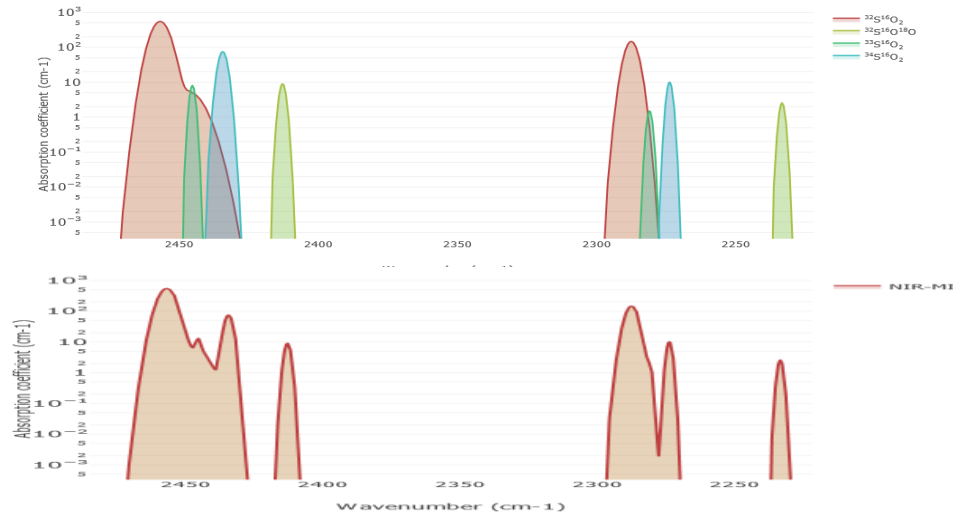


Bernard Schmitt, Manon Furrer, Damien Albert, Philippe Bollard,
Maria Gorbacheva, Lydie Bonal, Olivier Poch
(UGA / CNRS, IPAG, OSUG)

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) of astrophysical interest

  ➔ To help **identify absorption or emission bands from solids** observed in various astrophysical environments or in laboratory simulations …

  ➔ 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**

➔ Will provide the tools to **Import / Search / Visualize / Export** Band lists & Bands

- **Definition:**

Bandlist = List of band parameters and vibration modes of a **molecule** in a simple molecular **constituent** (2-3 species maxi), or of a **mineral** with a well-defined **phase** and **composition** (fixed or small range)

  ✓ includes the bands of all isotopes (sub-bandlists)

  ✓ can be provided for different environments (T, P, …)

Band list of solids: band parameters

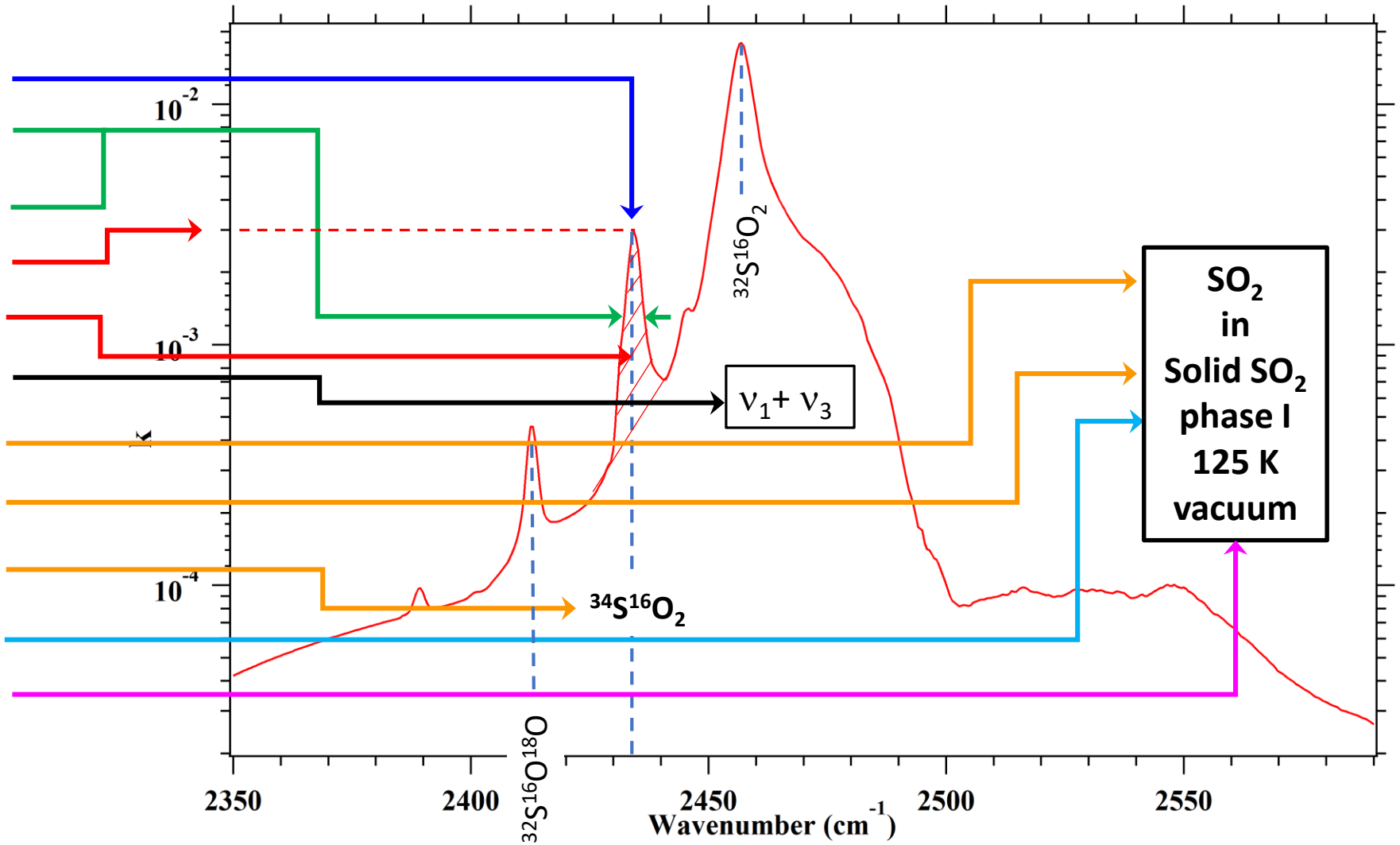
Bands parameters

Band parameters
- Position (energy)
- Width
- Shape
- Peak intensity
- Integrated intensity
- Vibration mode

Constituent
- Molecule
- Constituent
- Isotope
- Phase
- Environment cond.

Quality
- Accuracies
- Quality / evaluation

Spectral range : from VUV to Far-IR



Band lists & Bands: search interfaces

- Search: combination between a ‘search bar’ and a set of specialized filters

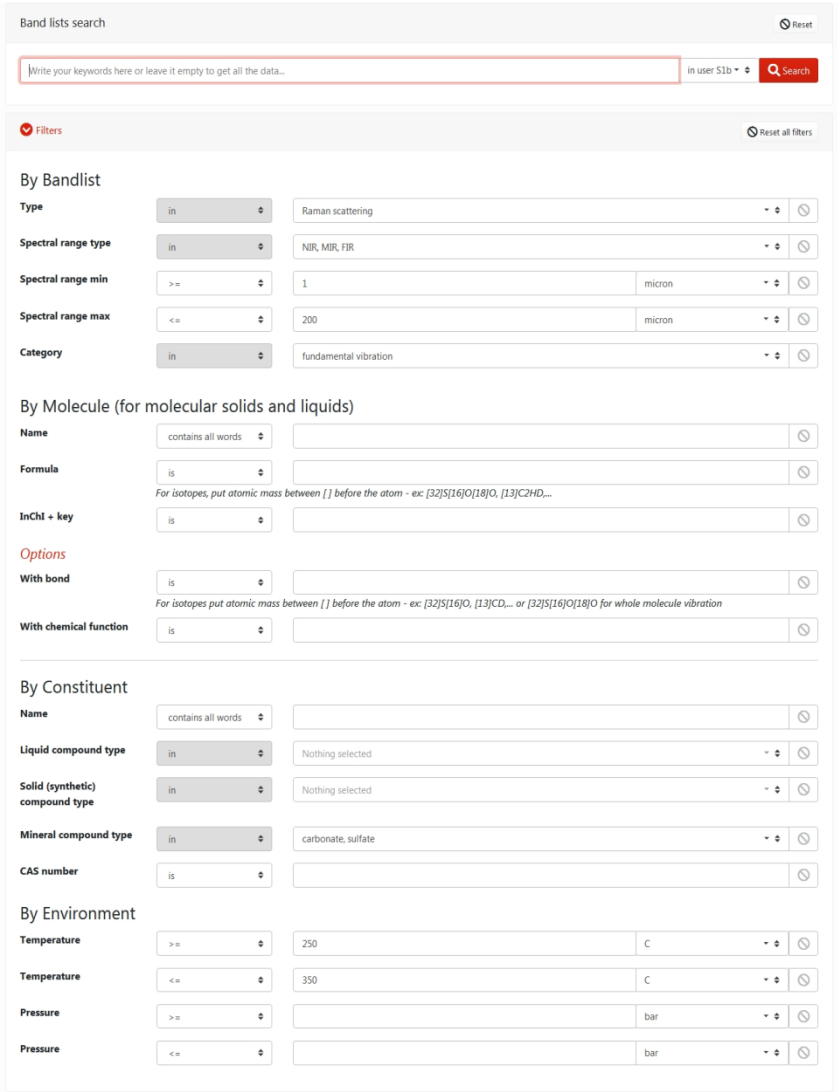
Band list:

Type and spectral range

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

Constituent *(ice, mineral, organic…)*

Environment *(T, P)*

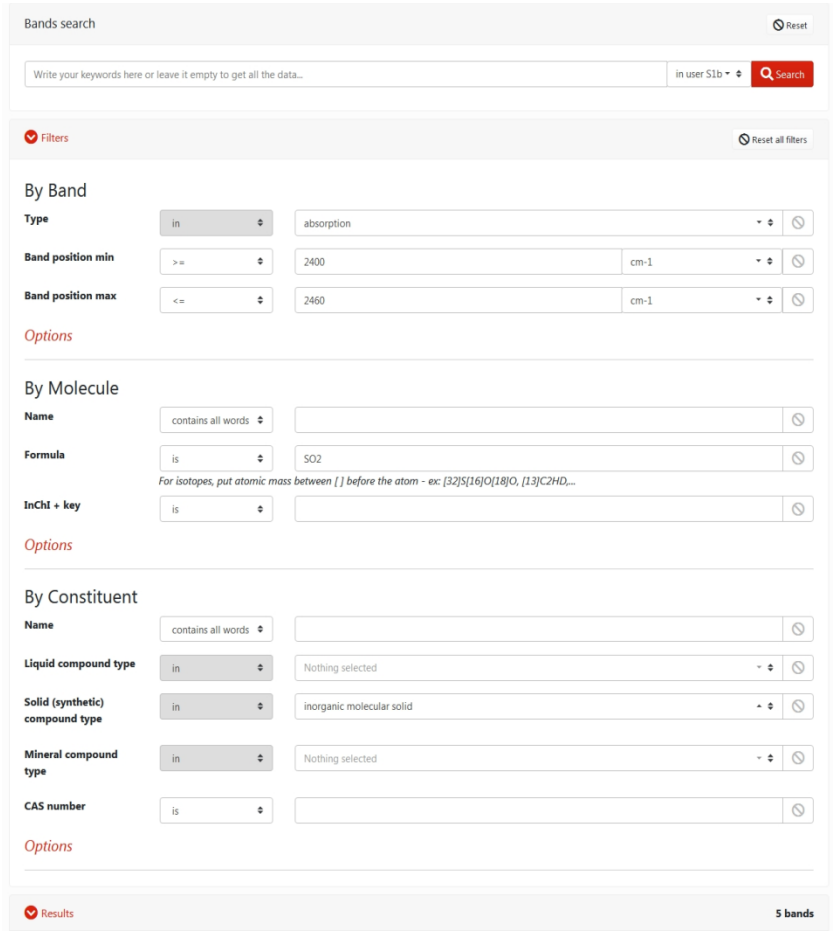


Band:

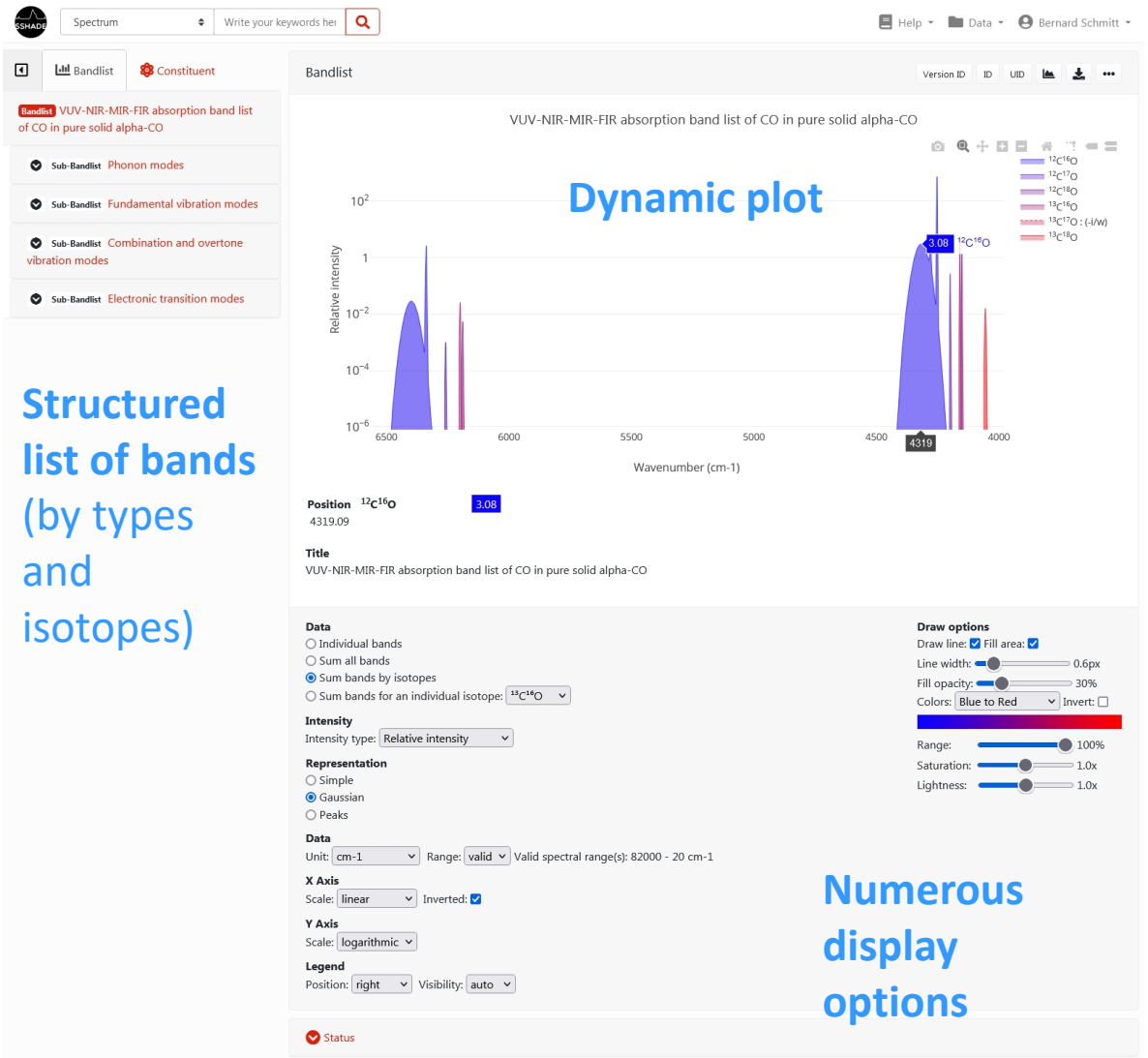
Wavelength, intensity, width…

Molecule, bond *(molecular solid/liquid)*

Constituent *(ice, mineral, organic…)*



Band list & bands: dynamic display tool

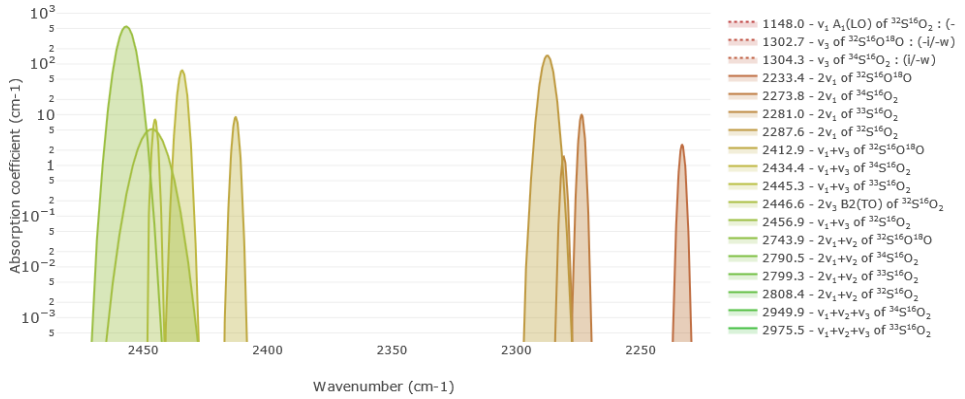


Structured list of bands (by types and isotopes)

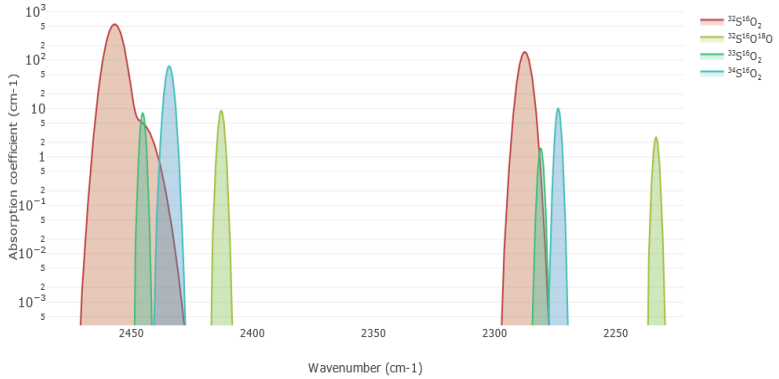
Numerous display options

Band list plot options

- Individual bands



- Sum of bands for each isotope

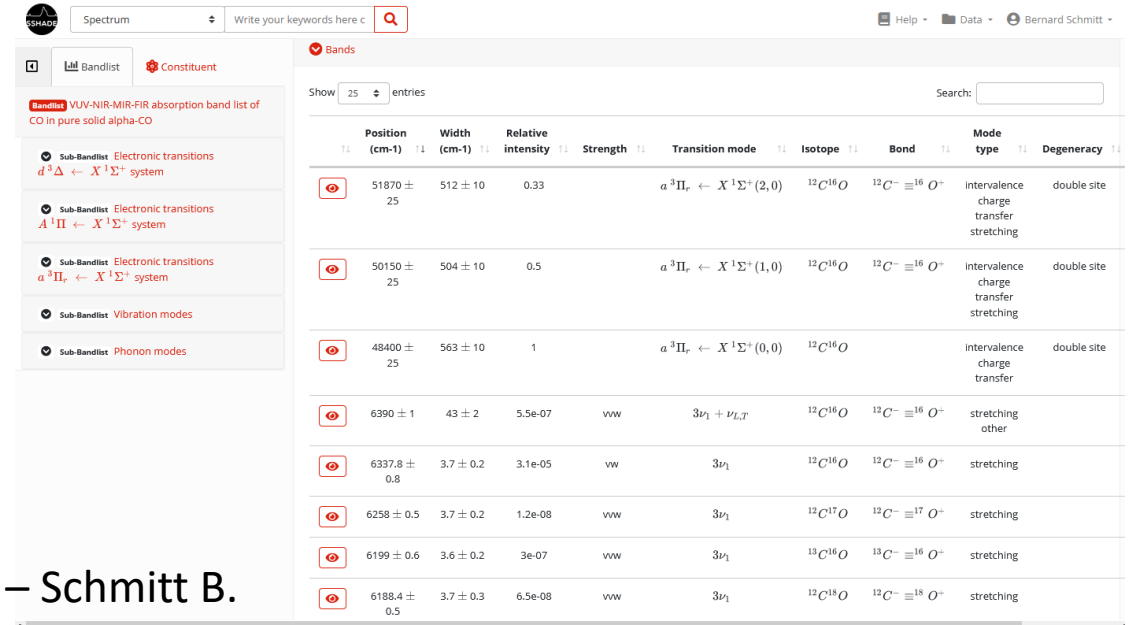


- Sum of bands of whole band list

Export

Export content:

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



SSHADE-BL content

✓ **Critical compilation** of all available publications on a solid
✓ **+ analysis of SSHADE-Spectra data**

Prototype:

Online: 1st October 2021

with > 25 band lists
> 600 bands

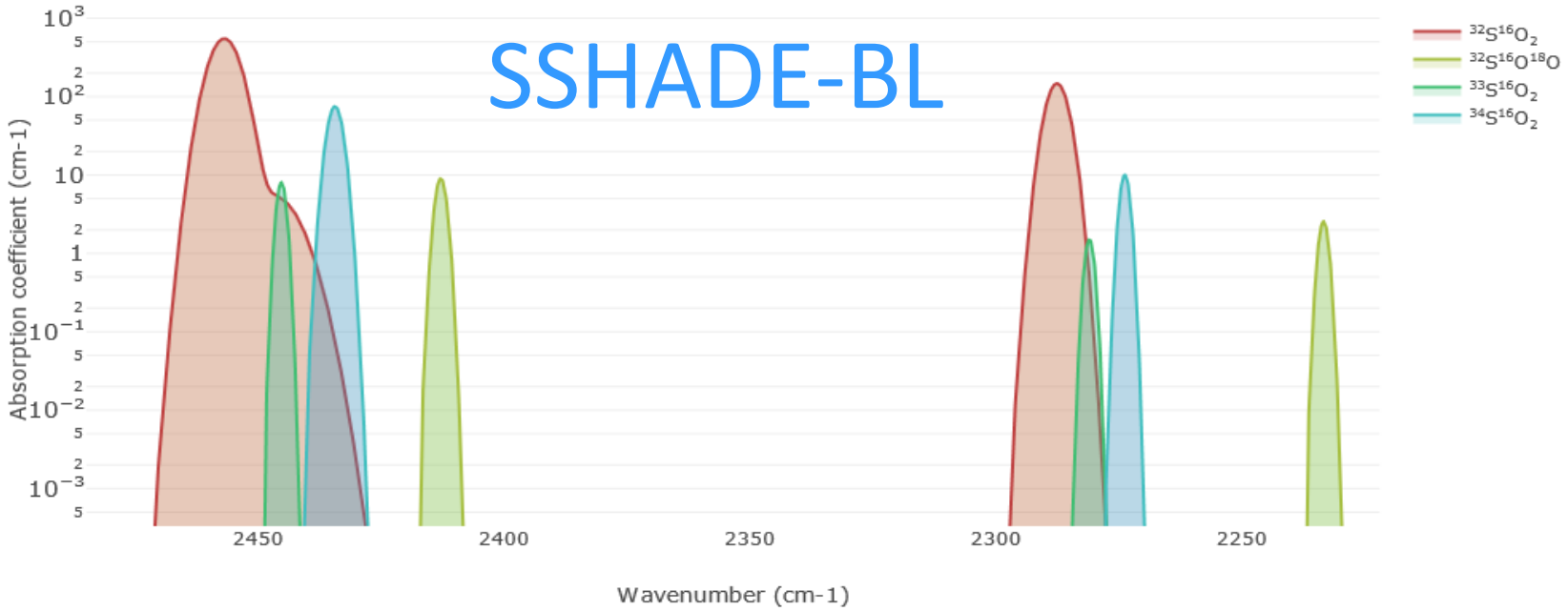
- Absorption and Raman
- Ices (CH_4, CO, CO_2, N_2, SO_2, NH_3, CH_3OH, nitriles…)
- Minerals (carbonates, …)

Final version:

Online: 1st February 2023

with > 70 band lists
> 1500 bands

Developed in the frame of the *Europlanet-2024 RI program*
(*Horizon 2020 research and innovation programme grant* N° 871149)


SSHADE-BL
Absorption coefficient (cm-1)
Wavenumber (cm-1)
2450
2400
2350
2300
2250
$^{32}S^{16}O_2$
$^{32}S^{16}O^{18}O$
$^{33}S^{16}O_2$
$^{34}S^{16}O_2$