

# SSHADÉ-Band List: the new database of spectroscopy band list of solids

(on-line 1st October 2021)

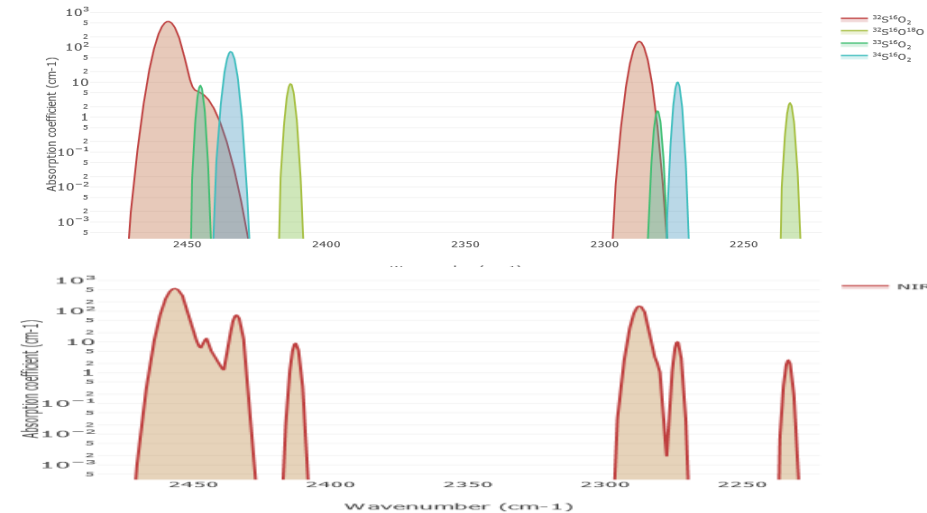
[www.sshade.eu](http://www.sshade.eu)

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Show  entries

Position (cm <sup>-1</sup> )	Width (cm <sup>-1</sup> )	Relative intensity	Strength	Transition mode	Isotope	Bond	Mode type
50.5 ± 0.25	5 ± 1	0.00055	w	$\nu_T - (E_u)$ $\nu_T - (T_u)$	<sup>12</sup> C <sup>16</sup> O <sup>12</sup> C <sup>18</sup> O		other other
86 ± 0.25	13 ± 1	0.00026	w	$\nu_{22}$	<sup>12</sup> C <sup>18</sup> O		other libration
2039.9 ± 0.1	1.3 ± 0.15	-	-	$\nu_3$	<sup>13</sup> C <sup>16</sup> O	<sup>13</sup> C ≡ <sup>16</sup> O	stretching
2064.5 ± 0.3	1.4 ± 0.2	-	-	$\nu_3$	<sup>13</sup> C <sup>17</sup> O	<sup>13</sup> C ≡ <sup>17</sup> O	stretching
2088.5 ± 0.5	1.6 ± 0.5	0.0035	m	$\nu_3$	<sup>12</sup> C <sup>18</sup> O	<sup>12</sup> C ≡ <sup>18</sup> O	stretching
2092.5 ± 0.7	1.4 ± 0.4	0.015	s	$\nu_3$	<sup>13</sup> C <sup>16</sup> O	<sup>13</sup> C ≡ <sup>16</sup> O	stretching
2112 ± 0.2	1.2 ± 0.3	0.00064	w	$\nu_3$	<sup>12</sup> C <sup>17</sup> O	<sup>12</sup> C ≡ <sup>17</sup> O	stretching
2139 ± 0.7	2.5 ± 1	1	vvs	$\nu_3$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching
2209 ± 1	42.5 ± 2	0.00478413068844807	m	$\nu_1 + \nu_{2,3}$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching other libration
4054.9 ± 0.2	4.7 ± 0.2	1.85e-07	vw	2 $\nu_3$	<sup>13</sup> C <sup>16</sup> O	<sup>13</sup> C ≡ <sup>16</sup> O	stretching
4150.8 ± 0.5	2.5 ± 0.1	1.65e-05	w	2 $\nu_3$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching
4158.1 ± 0.2	2.3 ± 0.2	6.8e-05	w	2 $\nu_3$	<sup>13</sup> C <sup>16</sup> O	<sup>13</sup> C ≡ <sup>16</sup> O	stretching
4198.3 ± 0.2	2.6 ± 0.1	3.2e-06	vw	2 $\nu_3$	<sup>12</sup> C <sup>17</sup> O	<sup>12</sup> C ≡ <sup>17</sup> O	stretching
4252 ± 1.1	2.7 ± 0.7	0.0086	s	2 $\nu_3$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching
4278.7 ± 0.5	5.4 ± 0.3	3e-05	w	$\nu_1 + \nu_3$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching
4317 ± 1.3	44 ± 1.5	3.6e-05	w	2 $\nu_1 + \nu_{2,3}$	<sup>12</sup> C <sup>16</sup> O	<sup>12</sup> C ≡ <sup>16</sup> O	stretching other



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# 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)

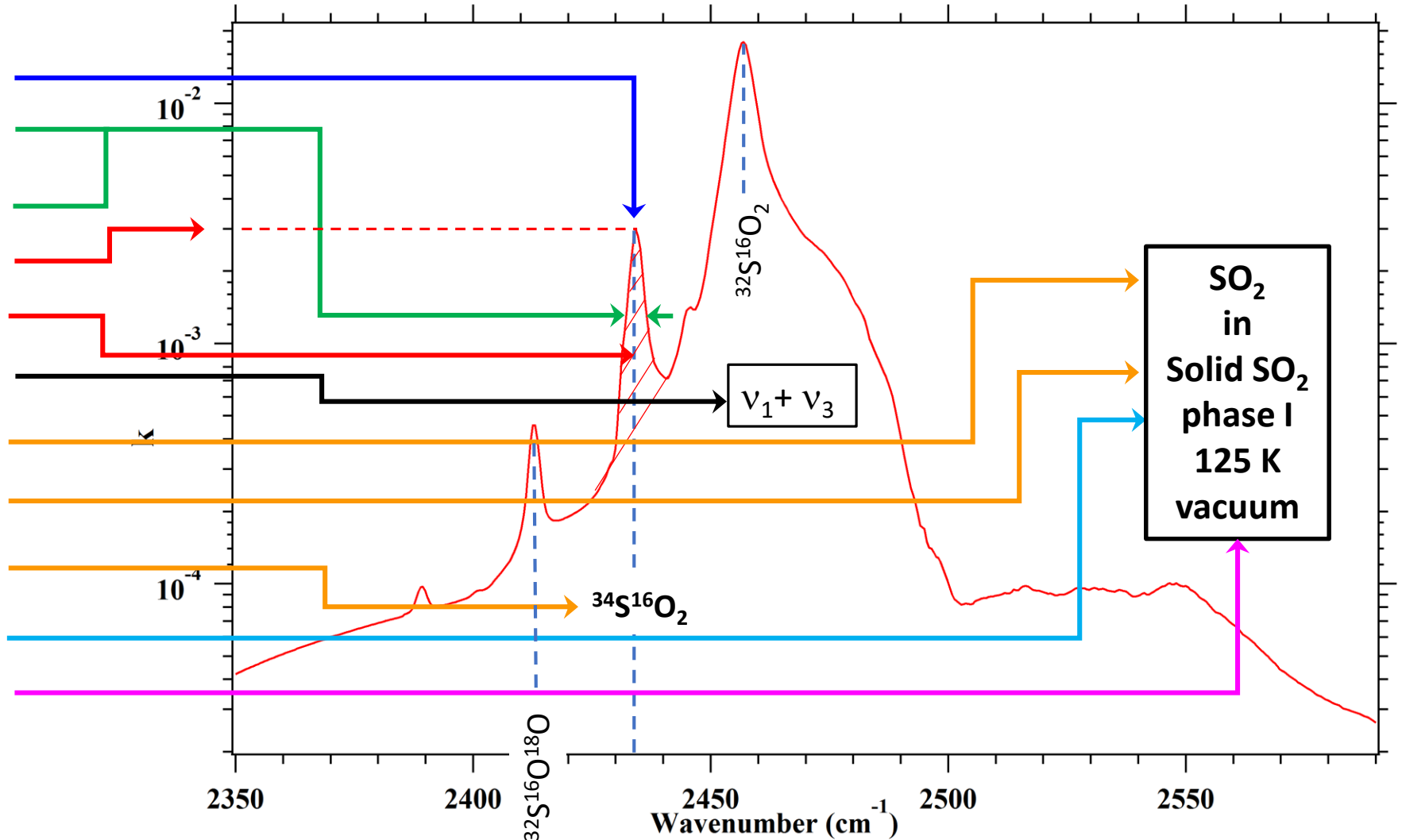
- ✓ includes the bands of all isotopes (sub-bandlists)
- ✓ can be provided for different environments (T, P, ...)

# Band list of solids: band parameters

## Bands parameters

Spectral range : from VUV to Far-IR

- Band parameters**
- Position (energy)
  - Width
  - Shape
  - Peak intensity
  - Integrated intensity
  - Vibration mode
- Constituent**
- Molecule
  - Constituent
  - Isotope
  - Phase
  - Environment cond.
- Quality**
- Accuracies
  - Quality / evaluation



# 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 lists search

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

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...

Filters

By Band

Type: in absorption

Band position min: >= 2400 cm-1

Band position max: <= 2450 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

Options

Results

5 bands

# Band list & bands: dynamic display tool

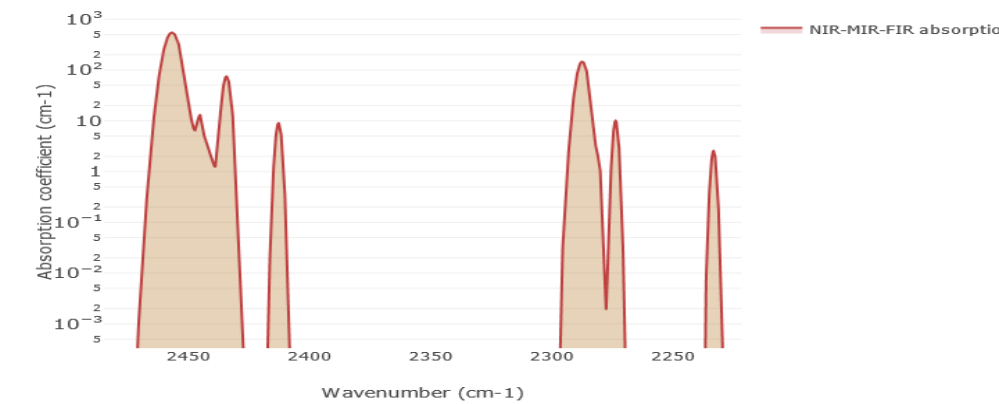
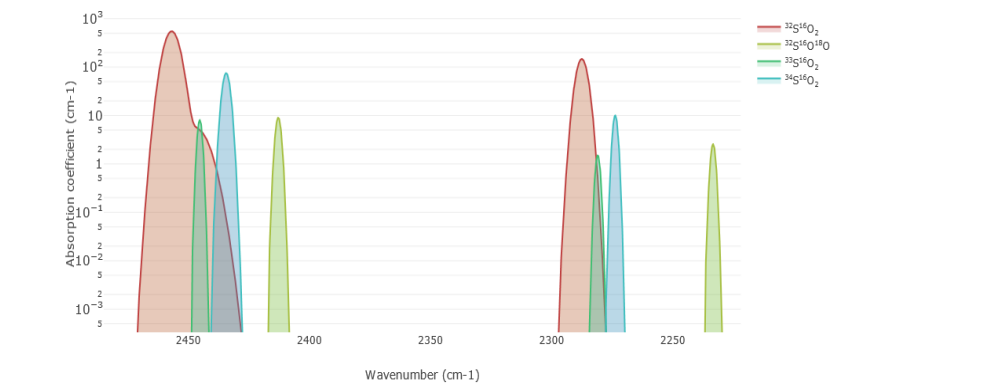
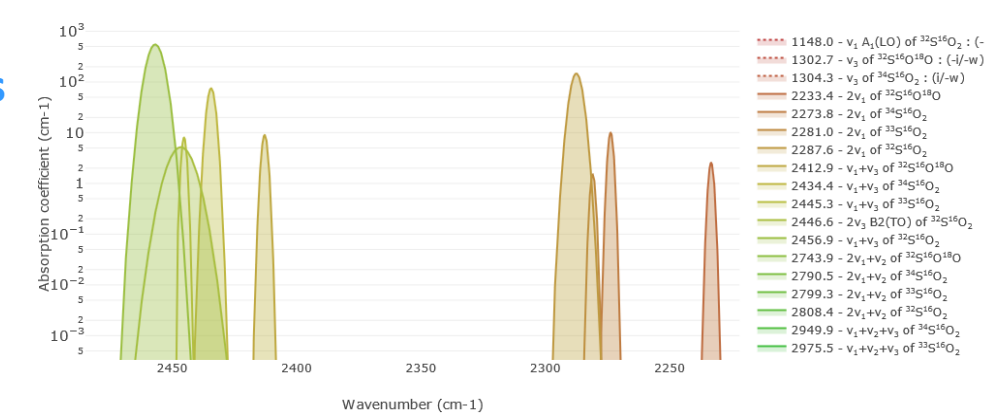
The screenshot shows a web-based interface for displaying absorption bands. At the top, there's a search bar with the text "Spectrum" and "Write your keywords here". Below this, there are tabs for "Bandlist" and "Constituent". The main content area is titled "VUV-NIR-MIR-FIR absorption band list of CO in pure solid alpha-CO". It features a "Dynamic plot" showing relative intensity versus wavenumber (cm-1) on a logarithmic scale. The plot displays several absorption bands, with a prominent one at 4319 cm-1. A legend on the right lists various isotopes and their corresponding colors. Below the plot, there are controls for "Position" (12C16O, 4319.09), "Title", "Data" (Individual bands, Sum all bands, Sum bands by isotopes, Sum bands for an individual isotope: 12C16O), "Intensity" (Relative intensity), "Representation" (Simple, Gaussian, Peaks), "Draw options" (Draw line, Fill area, Line width, Fill opacity, Colors, Range, Saturation, Lightness), and "Data" (Unit, Range, X Axis, Y Axis, Legend).

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 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 Spectrum Write your keywords here c

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  $a^3\Pi_u \leftarrow X^1\Sigma^+$  system

Sub-Bandlist Vibration modes

Sub-Bandlist Phonon modes

Help Data Bernard Schmitt

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		$a^3\Pi_u \leftarrow X^1\Sigma^+(2,0)$	$^{12}C^{16}O$	$^{12}C- \equiv ^{16}O^+$	intervalence charge transfer stretching	double site
50150 ± 25	504 ± 10	0.5		$a^3\Pi_u \leftarrow X^1\Sigma^+(1,0)$	$^{12}C^{16}O$	$^{12}C- \equiv ^{16}O^+$	intervalence charge transfer stretching	double site
48400 ± 25	563 ± 10	1		$a^3\Pi_u \leftarrow X^1\Sigma^+(0,0)$	$^{12}C^{16}O$		intervalence charge transfer	double site
6390 ± 1	43 ± 2	5.5e-07	vw	$3\nu_1 + \nu_{4,T}$	$^{12}C^{16}O$	$^{12}C- \equiv ^{16}O^+$	stretching other	
6337.8 ± 0.8	3.7 ± 0.2	3.1e-05	vw	$3\nu_1$	$^{12}C^{16}O$	$^{12}C- \equiv ^{16}O^+$	stretching	
6258 ± 0.5	3.7 ± 0.2	1.2e-08	vw	$3\nu_1$	$^{12}C^{17}O$	$^{12}C- \equiv ^{17}O^+$	stretching	
6199 ± 0.6	3.6 ± 0.2	3e-07	vw	$3\nu_1$	$^{18}C^{16}O$	$^{18}C- \equiv ^{16}O^+$	stretching	
6188.4 ± 0.5	3.7 ± 0.3	6.5e-08	vw	$3\nu_1$	$^{12}C^{18}O$	$^{12}C- \equiv ^{18}O^+$	stretching	

- ✓ **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<sub>4</sub>, CO, CO<sub>2</sub>, N<sub>2</sub>, SO<sub>2</sub>, NH<sub>3</sub>, CH<sub>3</sub>OH, 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)



# SSHAE-BL

