



*Journées ASOV  
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## SSHADE-BL : Développement d'une nouvelle base de données de 'liste de bandes des solides'



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

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# Band lists: Aims

- Provide a data base containing the **list of electronic, vibration and phonon bands of various solids** of astrophysical interest.
  - Ices
  - Simple organics
  - Minerals
- ➔ 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**
- ➔ Provide the tools to Import / Search / Visualize / Export
  - Bandlist & Bands
- Developed in the frame of the *Europlanet-2024 RI program* (EU H2020-RI N° 871149)

# Band list of solids: definition

- **Bandlist:**

List of band parameters and vibration modes of:

- a **molecule** in a simple molecular **constituent** (2-3 species maxi)
- a **mineral** or a **ionic/covalent solid**

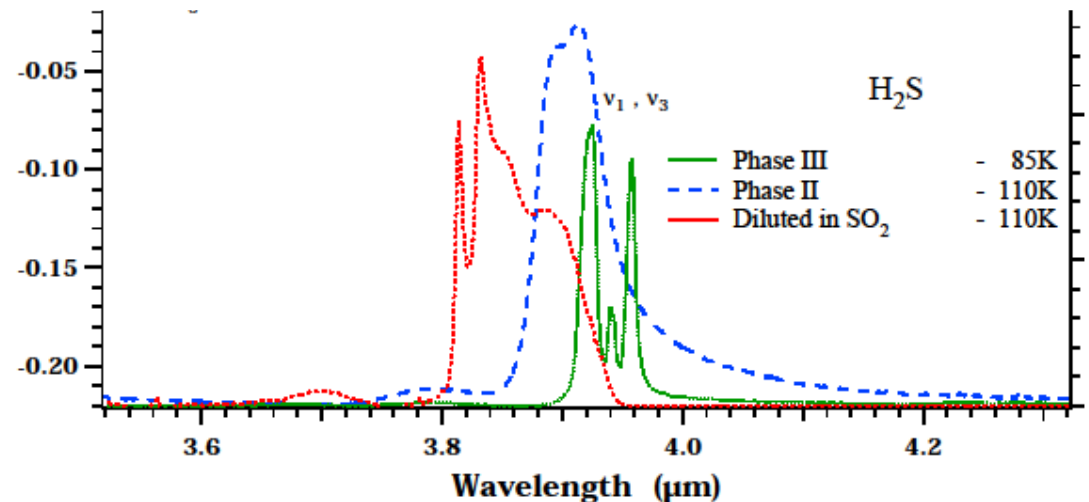
with a defined **phase** and **composition** (fixed or small range)

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

## Exemples

**H<sub>2</sub>S** in:

- solid H<sub>2</sub>S – phase II
- solid H<sub>2</sub>S – phase III
- H<sub>2</sub>S in crystalline solid SO<sub>2</sub>
- H<sub>2</sub>S in amorphous H<sub>2</sub>O
- H<sub>2</sub>S clathrate hydrate



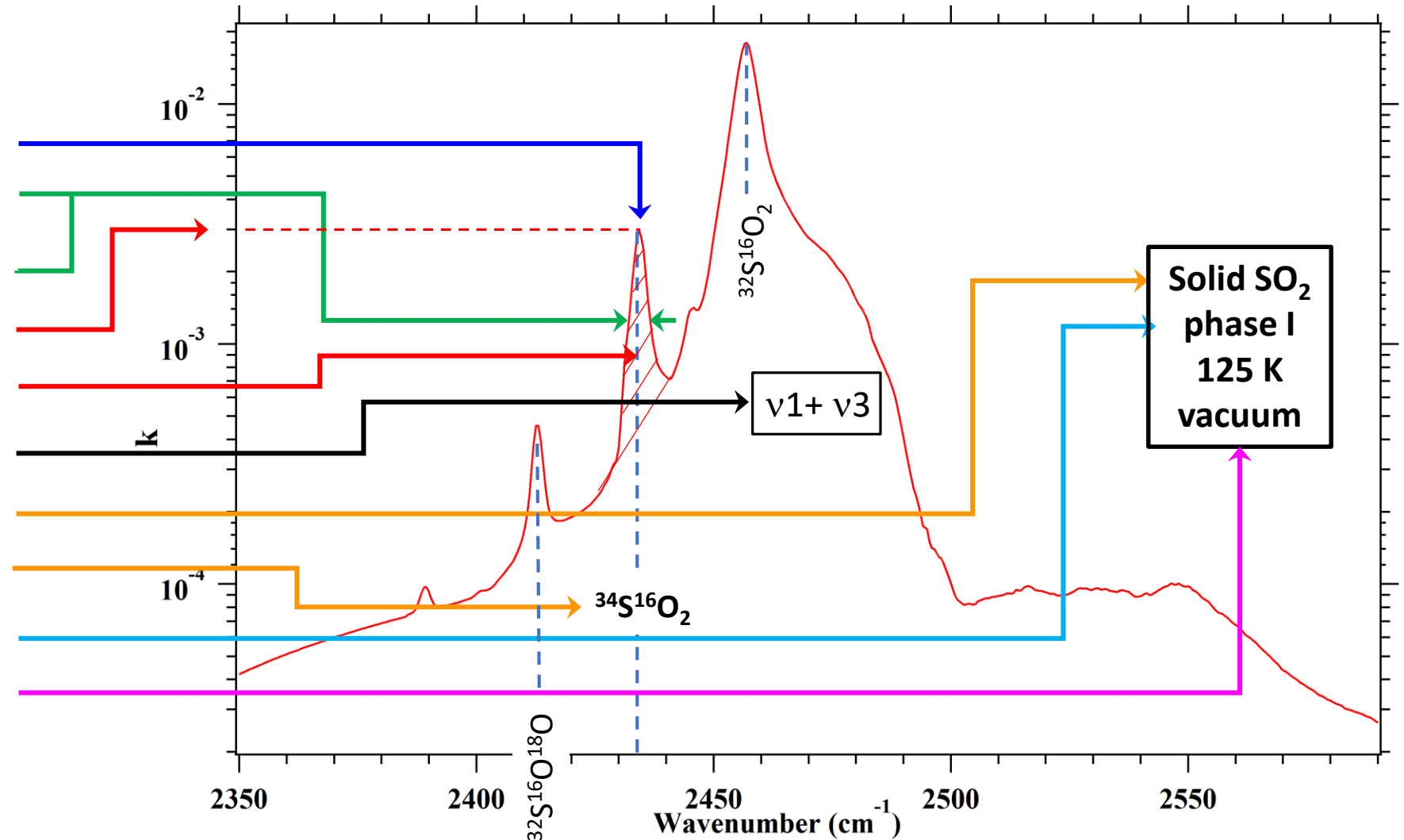
# Band list of solids: parameters

- Bands:
  - Specie(s) assignment
    - molecule, atom, ion, isotopic species, ...
  - Transition assignment(s)
    - Electronic, vibration or phonon mode(s), resonances, ...
    - (but no quantum number: not the practice for solids)
  - Band parameters
    - position (energy),
    - width, shape, ...
    - intensities (peak and integrated)
    - accuracies / quality / evaluation
    - in different environments (T, P)

# Band list of solids: band parameters

## Bands parameters

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



# Band lists and Bands

- Crystalline  $\alpha$ -CO

SSHADE Spectrum   Help Data Bernard Schmitt

**Bandlist**  Bandlist  Constituent

**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  entries Search:

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

# Band lists and Bands

- Crystalline  $\beta$ -CH<sub>3</sub>CN

SSHADE Spectrum Write your keywords here c

Help Data Bernard Schmitt

Bandlist Constituent

Bandlist NIR-MIR-FIR absorption band list of CH<sub>3</sub>CN in solid beta CH<sub>3</sub>CN

Sub-Bandlist Combination-overtone vibration modes

Sub-Bandlist Fundamental vibration modes

Sub-Bandlist Phonon modes

Bands

Show 50 entries Search:

	Position (cm <sup>-1</sup> )	Width (cm <sup>-1</sup> )	Relative intensity	Strength	Transition mode	Isotope	Bond	Mode type	Degeneracy
	1036 ± 0.5	-	-		$\nu_7$ (E)	CH <sub>3</sub> CN	-C ≤ H <sub>3</sub>	bending antisym. in-p (rocking)	
	1032 ± 0.5	-	-		$\nu_7$ (E)	<sup>13</sup> CH <sub>3</sub> CN	- <sup>13</sup> C ≤ H <sub>3</sub>	bending antisym. in-p (rocking)	
	918 ± 0.5	-	-		$\nu_4$ (A1)	CH <sub>3</sub> CN	≡ C - C ≤	stretching	
	915 ± 0.5	-	-		$\nu_4$ (A1)	CH <sub>3</sub> <sup>13</sup> CN	≡ <sup>13</sup> C - <sup>12</sup> C ≤	stretching	
	163 ± 1	-	-		$\nu_{L_{xy}}$ (E)	CH <sub>3</sub> CN		libration	
	141 ± 1.5	-	-		$\nu_{L_{xy}}$ (E)	CH <sub>3</sub> CN		libration	
	129.5 ± 2	-	-		$\nu_{L_{xy}}$ (E)	CH <sub>3</sub> CN		libration	
	129.5 ± 2	-	-		$\nu_T$	CH <sub>3</sub> CN		unknown	
	393.5 ± 0.5	-	-		$\nu_8$ (E)	CH <sub>3</sub> CN	≥ C - C ≡ N	bending	

# Development of the 'band list database of solids'

## Europlanet-2024 RI (2020-2024)

- |   |               |            |
|---|---------------|------------|
| ➤ Development of bandlist datamodel                               | (Done)        | B. Schmitt |
| ➤ Development of bandlist database                                | (Done)        | M. Furrer  |
| ➤ Development of:   |               |            |
| • Import / validation tool  | (Done)        | M.F.       |
| • Search tool   | (Done)        | M.F.       |
| • Visualization tool (data + metadata)                            | (Done)        | D. Albert  |
| ➤ Export tool   | (In progress) | D.A.       |
| • DOI generation  | (To be done)  | D.A.       |
| ➤ VO interoperability (VESPA, VAMDC, ...)                         | (To be done)  | D.A.       |
| ➤ Filling of the database   | (In progress) | B.S.       |
| ➔ Review the available data for molecular solids and minerals ... |               |            |

Prototype (online) ➔ August 2021

'Finalized' version ➔ end 2022



# Band lists data model: SSDM-BL

## **SSDM-BL:** Solid Spectroscopy Data Model for Band List

- Description of the 'solid constituent'
  - same as SSDM, but simplified
- Description of the 'Bandlist'
  - type (absorption, Raman, fluo, ...)
  - constituent and primary species (for molec. solids)
  - spectral units...
  - version, history, ...
  - link to 'parent spectra'
  - analysis, quality flag, ...
  - preview

# Band lists data model: SSDM-BL

## SSDM-BL: Solid Spectroscopy Data Model for Band List

- Description of the 'Bands'

- **Assignments** (multiple)
  - Multiplicity, degeneracy, resonances
  - Transition
    - label, type
    - species, crystal site and symmetry
    - bond (for molec. solids)
  - Evaluation
- **Characteristics** (multiple)
  - environnement: T, P
  - position peak / center + error
  - width, shape + error
  - Peak intensity (absolute / relative) + error
  - Integrated intensity (absolute / relative) + error
- **Publications** (in the SSHADE publi database)

# Band lists: import tool

- Solid constituent, Bandlist & bands: XML files

```
1 <?xml version="1.0" encoding="UTF-8"?>
2 <!--
3 Data type : Bandlist
4
5 CH3CN in solid beta CH3CN
6 -->
7 <import type="bandlist" ssdm_version="0.9.1"
8   xmlns="http://sshade.eu/schema/import"
9   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
10  xsi:schemaLocation="http://sshade.eu/schema/import http://sshade.eu/schema/i
11
12 <bandlist><!-- multiple -->
13 <!-- BAND LIST IMPORT MODE AND INDEXES -->
14 <import_mode>correction</import_mode> <!-- **ABS MANDATORY** Mode of import
15 <uid>BANDLIST_ABS_CH3CN_beta-CH3CN</uid> <!-- **ABS MANDATORY to CREATE** Un
16
17 <!-- BAND LIST DESCRIPTION -->
18 <type>absorption</type> <!-- **ABS MANDATORY** Type of band list. Enum: {abs
19 <title>NIR-MIR-FIR absorption band list of CH3CN in solid beta CH3CN</title>
20 <description><![CDATA[NIR-MIR-FIR absorption band list of $CH_3CN$ and isotc
21
22 <!-- BANDLIST: SPECTRAL RANGES -->
23 <parameters_spectral> <!-- **ABS MANDATORY** -->
24 <unit>cm-1</unit> <!-- **ABS MANDATORY** Unit of the position and width
25 <standard>vacuum</standard> <!-- **ABS MANDATORY** Medium in which the w
26 <range_types> <!-- **ABS MANDATORY at least one** -->
27 <type>NIR</type> <!-- multiple --> <!-- **ABS MANDATORY** Typical spe
28 <type>MIR</type>
29 <type>FIR</type>
30 </range_types>
31 <ranges> <!-- **ABS MANDATORY at least one** -->
32 <range><!-- multiple -->
33 <min>90</min> <!-- **ABS MANDATORY** Start of the spectral range
34 <max>4450</max> <!-- **ABS MANDATORY** End of the spectral range
35 </range>
36 </ranges>
37 <comments><![CDATA[]]></comments> <!-- Additional information on spectra
38 </parameters_spectral>
39
40 <!-- BANDLIST: INTENSITY MODES AND UNITS -->
41 <reference_position>
42 <electronic></electronic> <!-- **MANDATORY for electronic bands when ban
43 <infrared></infrared> <!-- **MANDATORY for infrared and Raman bands when
44 </reference_position>
45
46 <!-- BAND LIST: CONSTITUENT AND SPECIE -->
47 <constituent>
48 <uid>CONST_solid_beta_CH3CN</uid> <!-- **ABS MANDATORY** LINK to the exi
49 <primary specie uid>MOLEC CH3CN</primary specie uid> <!-- **ABS MANDATORY
```



The screenshot shows the SSHADE web interface. At the top, there is a search bar with the text "Spectrum" and "Write your keywords here c". Below the search bar, there are several navigation icons: a home icon, a user icon, a settings icon, and a help icon. A "Documentation" link is visible. A prominent red "Import" button is located in the top right corner. Below the navigation icons, there is a "Provider Import" section. It features a file input field containing the filename "bandlist\_ABS\_CH3CN\_beta-CH3CN\_v091c.xml" and a "Browse" button. Underneath, there is an "Options" section with the following settings: "Simulation mode" is checked, "Ignore missing resources" is unchecked, and "Data validation" is checked. At the bottom, there is a "Debug options" section with three unchecked checkboxes: "Ignore fixed OpenEnum values", "Skip faulty files instead of stopping on first error", and "Bypass Elasticsearch indexation".

# Band lists: user search tool + results

- Bandlists of specific solids with various criteria

SSHADE Band list Write your keywords here c Q

Help Data Bernard Schmitt

Band lists search Reset

absorption in user 51b Search

Filters Reset all filters

**By Bandlist**

Type in absorption

Spectral range type in UV, Vis, NIR, MIR, FIR

Spectral range min >= 200 cm-1

Spectral range max <= 30000 cm-1

Category in fundamental vibration, overtone vibration, combination vibration

**By Molecule (for molecular solids and liquids)**

Name contains all word: acetonitrile

Formula is [13]CH3CN  
For isotopes, put atomic mass between [ ] before the atom - ex: [32]S[16]O[18]O, [13]C2HD,...

InChI + key is WEVYAHXRMPXWCK-UHFFFAOYSA-N

**Options**

With bond contains any CN CC  
For isotopes put atomic mass between [ ] before the atom - ex: [32]S[16]O, [13]CD, or [32]S[16]O[18]O for whole molecule vibration

With chemical function is CH3

**By Constituent**

Name contains all word: acetonitrile

Liquid compound type in Nothing selected

Solid (synthetic) compound type in nitrile

Mineral compound type in Nothing selected

CAS number is

**By Environment**

Temperature >= 80 K

Temperature <= 150 K

Pressure >= bar

Pressure <= 5 bar


Results 2 band lists

NIR-MIR-FIR absorption band list of CH3CN in solid beta CH3CN [42 bands]

NIR-MIR-FIR absorption band list of CH3CN in solid amorphous CH3CN [20 bands]

# Bands: user search tool

- Bands with various spectral and composition criteria

 Spectrum

Help Data Bernard Schmitt

### Bands search

in user 51b

### Filters

#### By Band

Type	in	<input type="text" value="absorption"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
Band position min	>=	<input type="text" value="2250"/>	<input type="text" value="cm-1"/>	<input type="button" value="v"/>
Band position max	<=	<input type="text" value="2500"/>	<input type="text" value="cm-1"/>	<input type="button" value="v"/>
<b>Options</b>				
Band width min	>=	<input type="text" value="5"/>	<input type="text" value="cm - 1"/>	<input type="button" value="v"/>
Band width max	<=	<input type="text" value="25"/>	<input type="text" value="cm - 1"/>	<input type="button" value="v"/>
Band strength min	>=	<input type="text" value="m"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
Band strength max	<=	<input type="text" value="vs"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
Transition category	in	<input type="text" value="fundamental vibration, combination vibration"/>	<input type="button" value="v"/>	<input type="button" value="x"/>
Transition mode	in	<input type="text" value="Nothing selected"/>	<input type="button" value="v"/>	<input type="button" value="x"/>

### By Molecule

Name	contains all word:	<input type="text" value="acetonitrile"/>	<input type="button" value="v"/>
Formula	is	<input type="text" value="CH3CN"/>	<input type="button" value="v"/>
<small>For isotopes, put atomic mass between [ ] before the atom - ex: [32]S[16]O[18]O, [13]C2HD,...</small>			
InChI + key	is	<input type="text" value="WEVYAHXRMPXWCK-UHFFFAOYSA-N"/>	<input type="button" value="v"/>
<b>Options</b>			
With bond	is	<input type="text"/>	<input type="button" value="v"/>
<small>For isotopes put atomic mass between [ ] before the atom - ex: [32]S[16]O, [13]CD,.... or [32]S[16]O[18]O for whole molecule vibration</small>			

---

### By Constituent

Name	contains all word:	<input type="text"/>	<input type="button" value="v"/>	
Liquid compound type	in	<input type="text" value="Nothing selected"/>	<input type="button" value="v"/>	
Solid (synthetic) compound type	in	<input type="text" value="nitrile"/>	<input type="button" value="v"/>	
Mineral compound type	in	<input type="text" value="Nothing selected"/>	<input type="button" value="v"/>	
CAS number	is	<input type="text"/>	<input type="button" value="v"/>	
<b>Options</b>				
Temperature	>=	<input type="text" value="80"/>	<input type="text" value="K"/>	<input type="button" value="v"/>
Temperature	<=	<input type="text" value="150"/>	<input type="text" value="K"/>	<input type="button" value="v"/>
Pressure	>=	<input type="text"/>	<input type="text" value="bar"/>	<input type="button" value="v"/>
Pressure	<=	<input type="text" value="5"/>	<input type="text" value="bar"/>	<input type="button" value="v"/>

# Bands: results

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

Results 60 bands

Show  entries Search:

	Position (cm-1)	Width (cm-1)	Strength	Assignment	Type	Isotope	Molecule/Atom	Constituent	Temperature (K)	Pressure (bar)
	51870 ± 25	512 ± 10	-	$a^3\Pi_r \leftarrow X^1\Sigma^+(2,0)$	absorption	$^{12}\text{C}^{16}\text{O}$	CO	alpha-CO	20	-
	50150 ± 25	504 ± 10	-	$a^3\Pi_r \leftarrow X^1\Sigma^+(1,0)$	absorption	$^{12}\text{C}^{16}\text{O}$	CO	alpha-CO	20	-
	48400 ± 25	563 ± 10	-	$a^3\Pi_r \leftarrow X^1\Sigma^+(0,0)$	absorption	$^{12}\text{C}^{16}\text{O}$	CO	alpha-CO	20	-
	6390 ± 1	43 ± 2	vww	$3\nu_1 + \nu_{L,T}$	absorption	$^{12}\text{C}^{16}\text{O}$	CO	alpha-CO	21	-
	6337.8 ± 0.8	3.7 ± 0.2	vw	$3\nu_1$	absorption	$^{12}\text{C}^{16}\text{O}$	CO	alpha-CO	20	-
	6258 ± 0.5	3.7 ± 0.2	vww	$3\nu_1$	absorption	$^{12}\text{C}^{17}\text{O}$	CO	alpha-CO	21	-
	6199 ± 0.6	3.6 ± 0.2	vww	$3\nu_1$	absorption	$^{13}\text{C}^{16}\text{O}$	CO	alpha-CO	21	-
	6188.4 ± 0.5	3.7 ± 0.3	vw	$3\nu_1$	absorption	$^{12}\text{C}^{18}\text{O}$	CO	alpha-CO	21	-

# 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: display tools

SSHADE Spectrum Write your keywords here

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**Bandlist** Constituent

**Bandlist** NIR-MIR-FIR absorption band list of SO2 in pure solid SO2-I

Sub-Bandlist **Combination-overtone vibration modes**

Sub-Bandlist **Fundamental vibration modes**

### NIR-MIR-FIR absorption band list of SO2 in pure solid SO2-I

Position **BAND\_ABS\_SO2\_SO2-I\_3874.57\_I\_3883.V1** **0.04** **BAND\_ABS\_SO2\_SO2-I\_3890.V1** **0.38** **BAND\_ABS\_SO2\_SO2-I\_3912.V1** **0.07** **BAND\_ABS\_SO2\_SO2-I\_3936.V1** **2.45**

**Title**  
NIR-MIR-FIR absorption band list of SO2 in pure solid SO2-I

**Data**  
 Individual bands  
 Sum all bands  
 Sum bands by isotopes  
 Sum bands for an individual isotope: MOLEC\_32S16O2

**Intensity**  
Intensity type: Absorption coefficient

**Representation**  
 Simple  
 Gaussian  
 Peaks

**Data**  
Unit: cm-1 Range: valid Valid spectral range(s): 5100 - 500 cm-1

**X Axis**  
Scale: linear Inverted:

**Y Axis**  
Scale: logarithmic

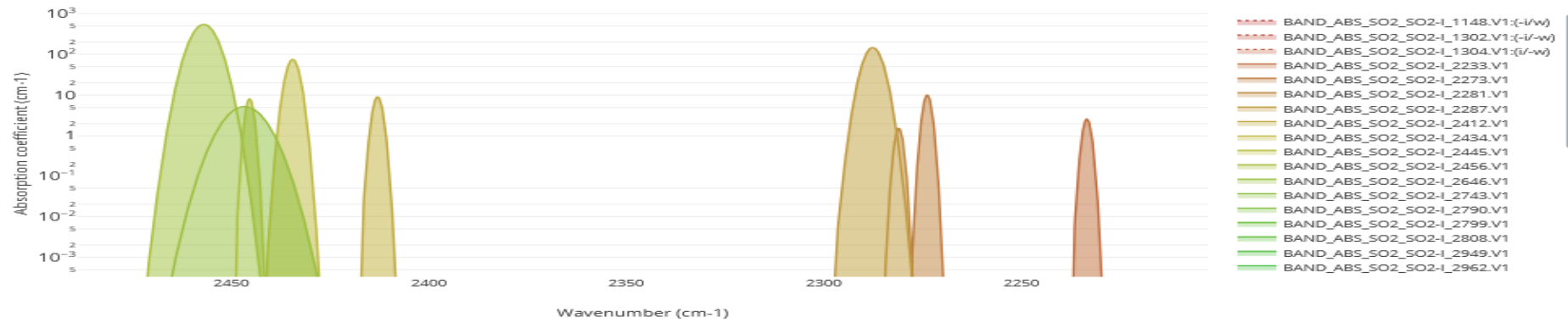
**Legend**  
Position: right Visibility: show

**Draw options**  
Draw line:  Fill area:   
Line width: 1.8px  
Fill opacity: 30%  
Colors: SSHADE Invert:   
Saturation: 1.0x  
Lightness: 1.0x

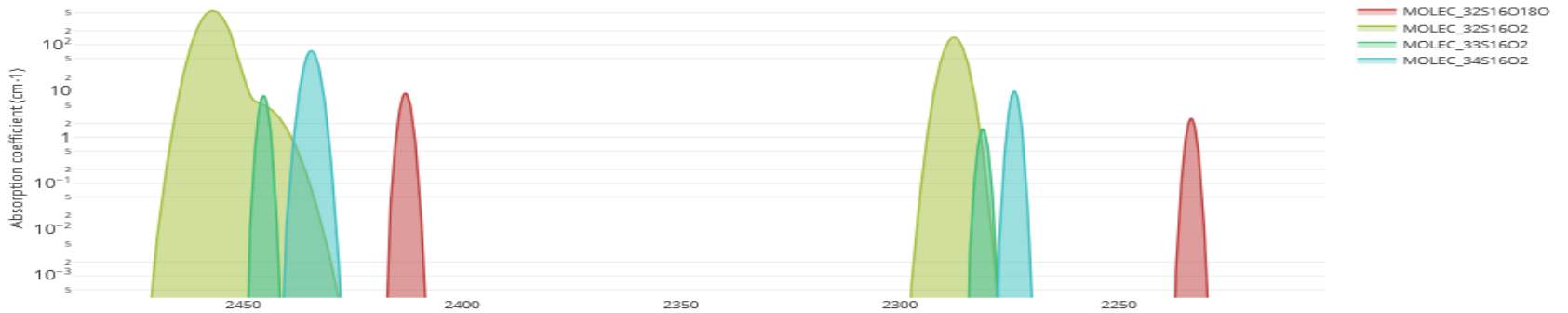


# Band list & bands: display tools

- Individual bands



- Sum of bands of each isotope

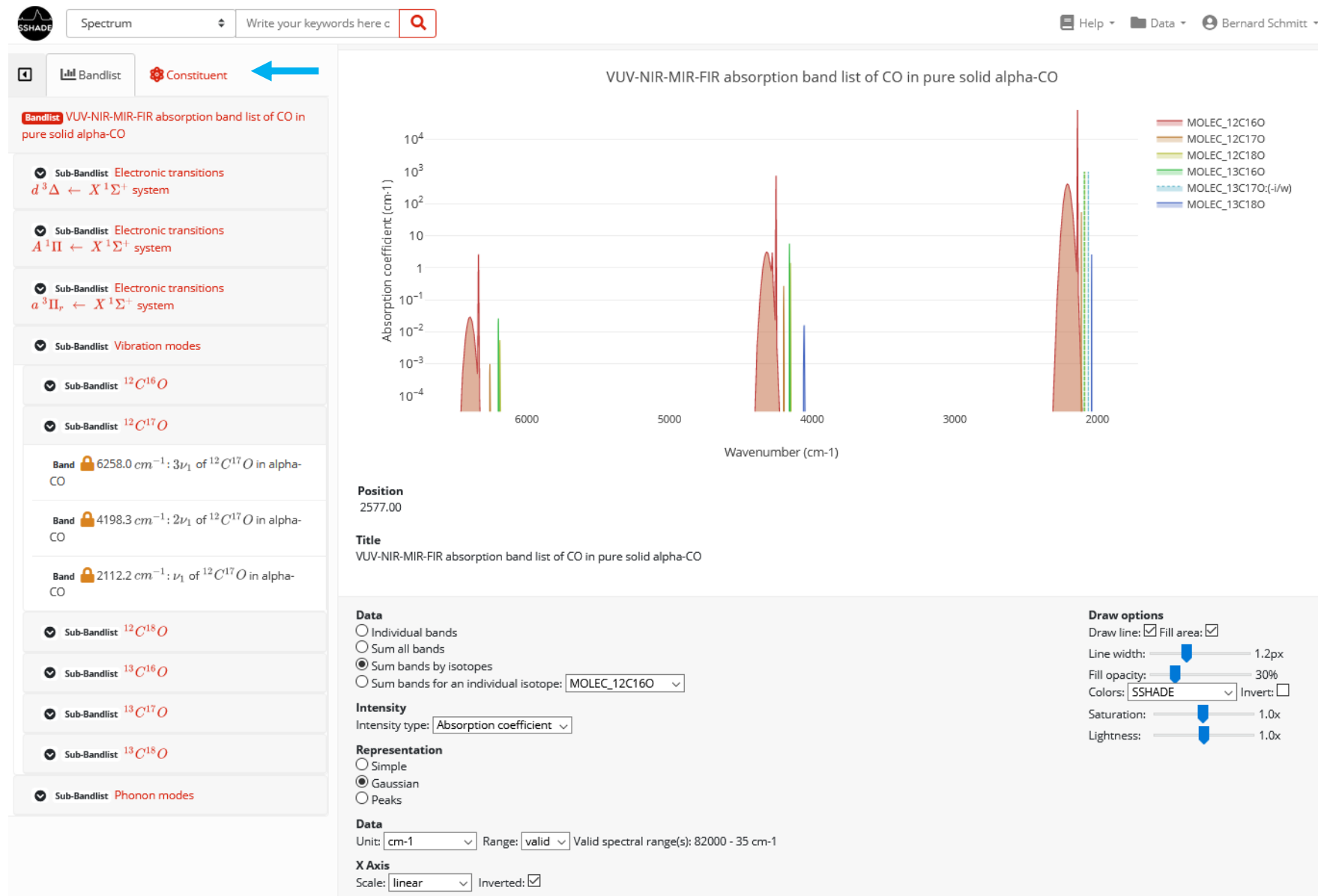


- Sum of bands of whole bandlist





# Band list & bands: organisation of the bands

- Constituent
- Electronic bands
- Vibration modes
  - By isotope
- Phonon modes



# Band list & bands: Metadata

Spectrum  




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Bandlist Constituent

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  $^{12}\text{C}^{16}\text{O}$
- Sub-Bandlist  $^{12}\text{C}^{17}\text{O}$**
- Band  $6258.0\text{ cm}^{-1}; 3\nu_1$  of  $^{12}\text{C}^{17}\text{O}$  in alpha-CO
- Band  $4198.3\text{ cm}^{-1}; 2\nu_1$  of  $^{12}\text{C}^{17}\text{O}$  in alpha-CO
- Band  $2112.2\text{ cm}^{-1}; \nu_1$  of  $^{12}\text{C}^{17}\text{O}$  in alpha-CO**
- Sub-Bandlist  $^{12}\text{C}^{18}\text{O}$
- Sub-Bandlist  $^{13}\text{C}^{16}\text{O}$
- Sub-Bandlist  $^{13}\text{C}^{17}\text{O}$

## Band

Unverified  Unreleased Version ID ID UID   

**Title**  
 $2112.2\text{ cm}^{-1}; \nu_1$  of  $^{12}\text{C}^{17}\text{O}$  in alpha-CO

**Band type**  
absorption

**Type**  
absorption

**Assignments summary**

Assignment	Mode	Isotope	Molecule/Atom	Bond	Multiplicity	Degeneracy	Contribution	Resonance
$\nu_1$	stretching	$^{12}\text{C}^{17}\text{O}$	$\text{CO}$	$^{12}\text{C} \equiv ^{17}\text{O}^+$	no			

**Characteristics summary**

Peak position (cm-1)	Center position (cm-1)	Width (cm-1)	Shape	Asymmetry factor	Peak intensity (cm-1)	Peak intensity relative	Peak strength	Integrated intensity (cm-2)	Integrated intensity relative	Integrated strength	Temperature (K)	Pressure (bar)
$2112.2 \pm 0.3$	$1.2 \pm 0.2$		gaussian		$55 \pm 5$	0.00064	m	$64 \pm 6.5$	0.00026	vw	23	

**Band assignment #1**

**Assignment**

**Label**  
 $\nu_1$

# Band list & bands: export tools

- Export tool : **in development**
  - Export full bandlist with all bands data (table) and metadata
  - In several formats (ascii, VOTable, FITS ...)
- Tool to customize export
  - Export units
  - Spectral range, ...
  - Data and file format

# Band lists: DOI

- DOI
  - One DOI per bandlist
  - generate a data reference
    - The SSHADE bandlist committee (2021): NIR-MIR-FIR absorption band list of CH<sub>3</sub>CN in solid beta CH<sub>3</sub>CN. Version 1. SSHADE (OSUG Data Center). Dataset/Band list Data. doi: [10.21362/SSHADE/BANDLIST\\_ABS\\_CH3CN\\_beta-CH3CN](https://doi.org/10.21362/SSHADE/BANDLIST_ABS_CH3CN_beta-CH3CN)
- DOI generation: **to be implemented**
  - Mapping of SSDM-BL with DataCite schema
    - To be upgraded (**in progress**)
  - Tool for automatic DOI submission request:
    - already developed for spectra
    - Activated when data pushed to 'public'

# Band lists: data compilation

## Review the available data for molecular solids and the minerals

- SSHADE consortium partner's data
- Publications
  - Many many papers scattered in the literature (> 10 000 ...)
    - Physics, chemistry, astrophysics, optics, material science, geophysics, geology, mineralogy, ...
    - Ex: spectrum of pure solid  $\alpha$ -CO : > 30 papers ! (1961-2020...)
- First selection :
  - ~ 50 simple and pure molecular solids (H<sub>2</sub>O, CO, SO<sub>2</sub>, CH<sub>4</sub>, ... C<sub>6</sub>H<sub>6</sub>, CH<sub>3</sub>CN, ... )
  - ~ 50 simple 'unique' minerals (fayalite, forsterite, hematite, salts ...)

=> **critical review of all parameters**

→ **selection** (→ 2020-...)

=> selection committee ?

# Bandlist: V.O.

## → To be developed

- Interoperability layer for VESPA
  - already exist for spectra
- Mapping SSDM-BL with EPN-TAP
  - Partly done
- Definition of the search KeyWords
  - Subset of user search KW
- Implementation

→ To be online in 2022

→ See you at next ASOV meeting !!!

**VESPA**  
Virtual European Solar and Planetary Access

Form Query  
EPN-TAP Services Custom Service

Back To Services Results  
Results in service SSHADE

**SSHADE - SSHADE spectra library**  
SSHADE is an infrastructure for Solid Spectroscopy hosting a set of specialized databases provided by several research groups. SSHADE distributes spectral and photometric data (transmission, reflectance, optical constants, Raman, etc) obtained by various spectroscopic techniques over the whole electromagnetic spectrum but mostly covering the X, UV, Vis, Near/Mid/Far-IR, and sub-mm ranges. The measured samples include ices, minerals, rocks, organic, carbonaceous materials, and liquids — including field samples, synthesized and extraterrestrial materials. A dedicated search/visualization/export interface is available at <https://www.sshade.eu>. Information on SSHADE and its databases can be found at <https://wiki.sshade.eu/>

**Credits:**  
Creators: Damien Albert, Philippe Bollard  
Contributors: IPAG/CNRS, SSHADE partners, Bernard Schmitt  
Publisher: OSUG Data Center

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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

Plotting tools  
TOPCAT  
Aladin  
SPLAT  
CASSIS  
3DView

Example queries  
Saturn in March 2012

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