Journées ASOV
On-line – 22 March 2021

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

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**

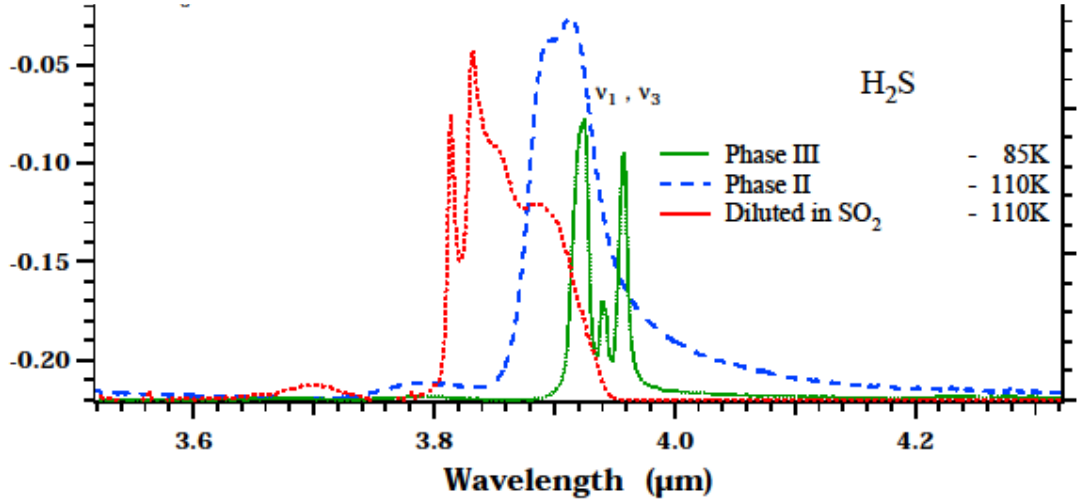
  with a defined **phase** and **composition** (fixed or small range)

  ✓ includes bands of all isot opes (sub-bandlists)
  ✓ for different environments (T, P, …)

Exemples

H_2S in:

- solid H_2S – phase II
- solid H_2S – phase III
- H_2S in crystalline solid SO_2
- H_2S in amorphous H_2O
- H_2S 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)

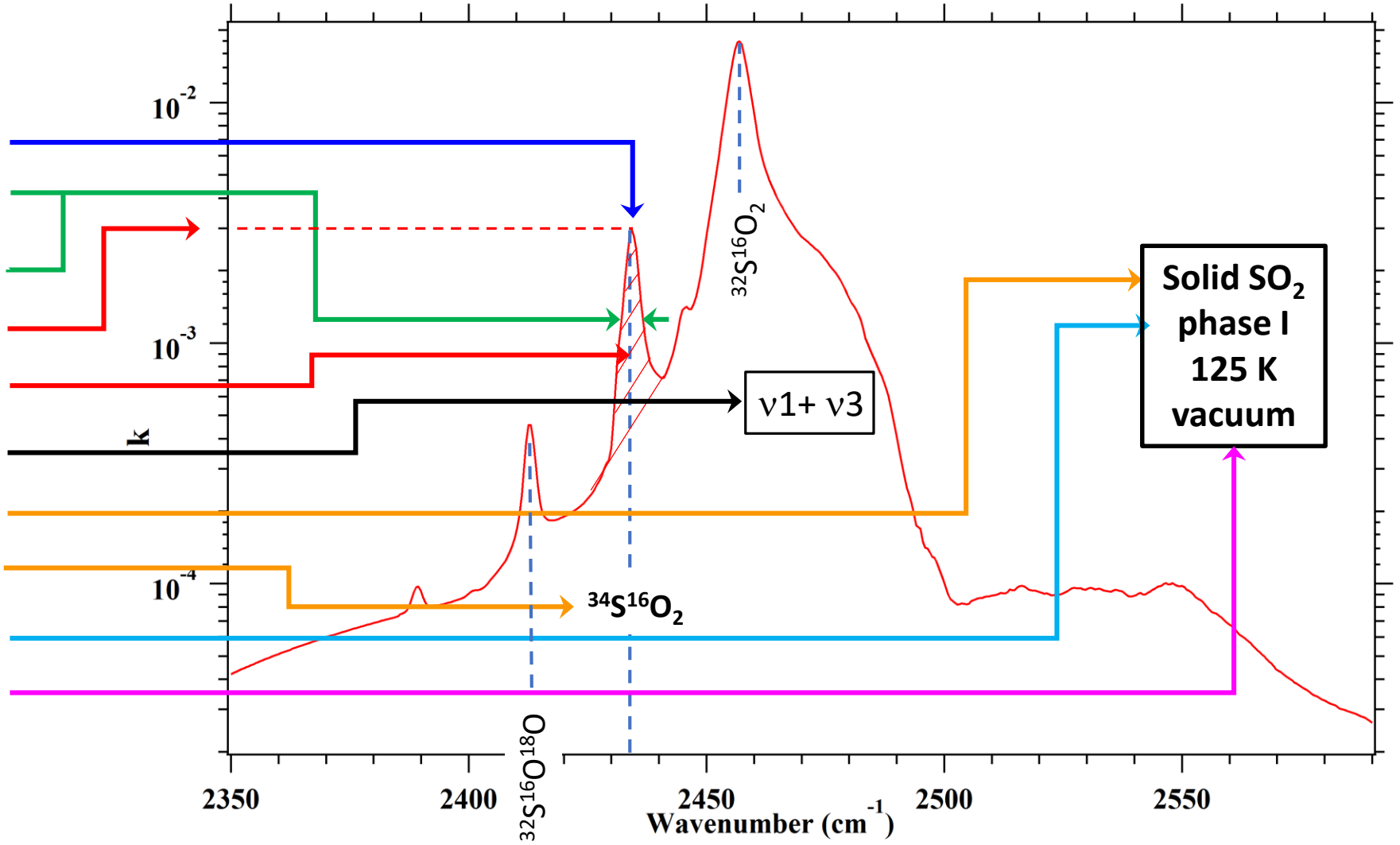
Band list of solids: band parameters

Bands parameters

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

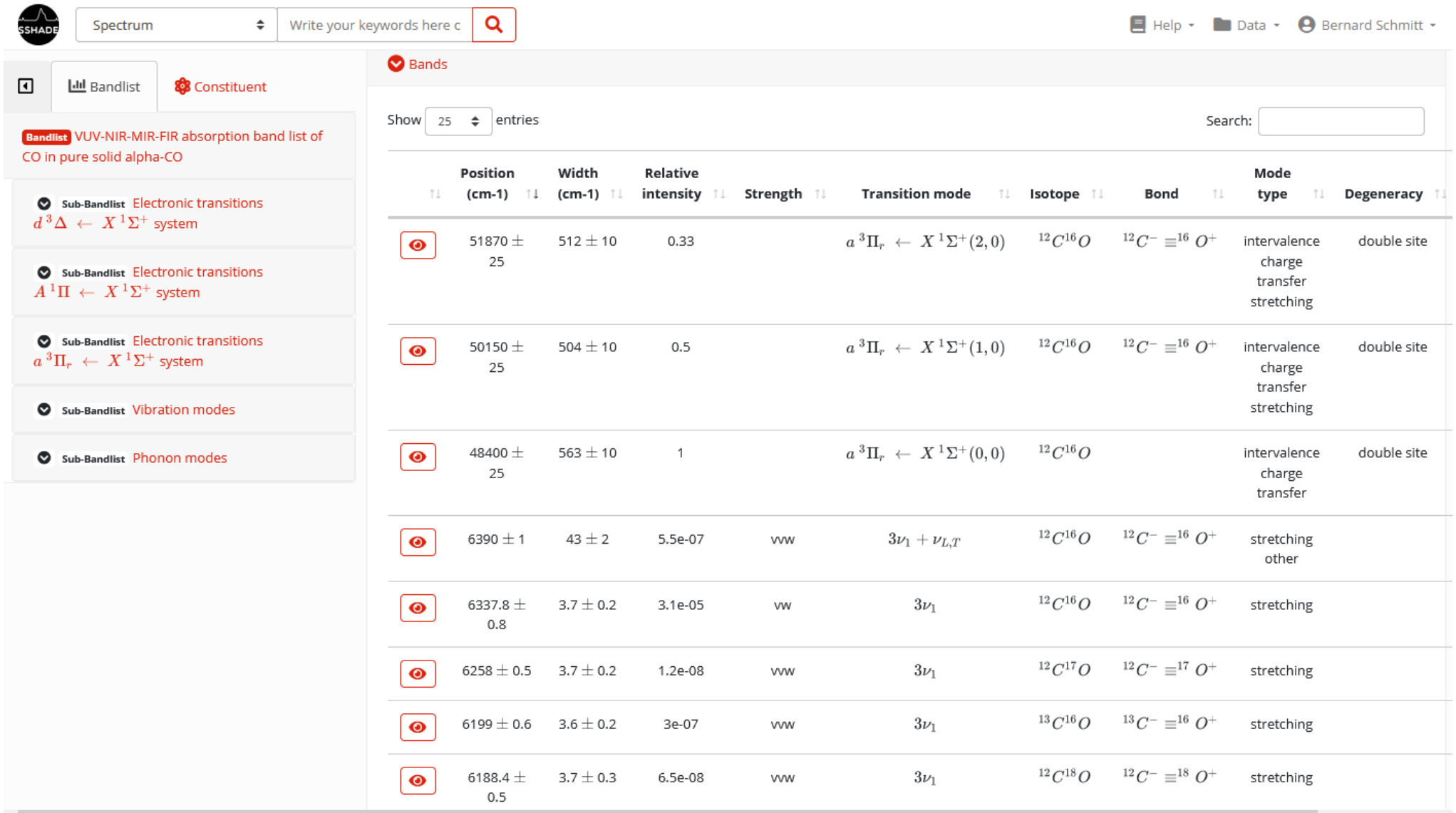
Constituent
- Molecule
- Isotope
- Phase
- Environment cond.

Quality
- Accuracies
- Quality / evaluation



Band lists and Bands

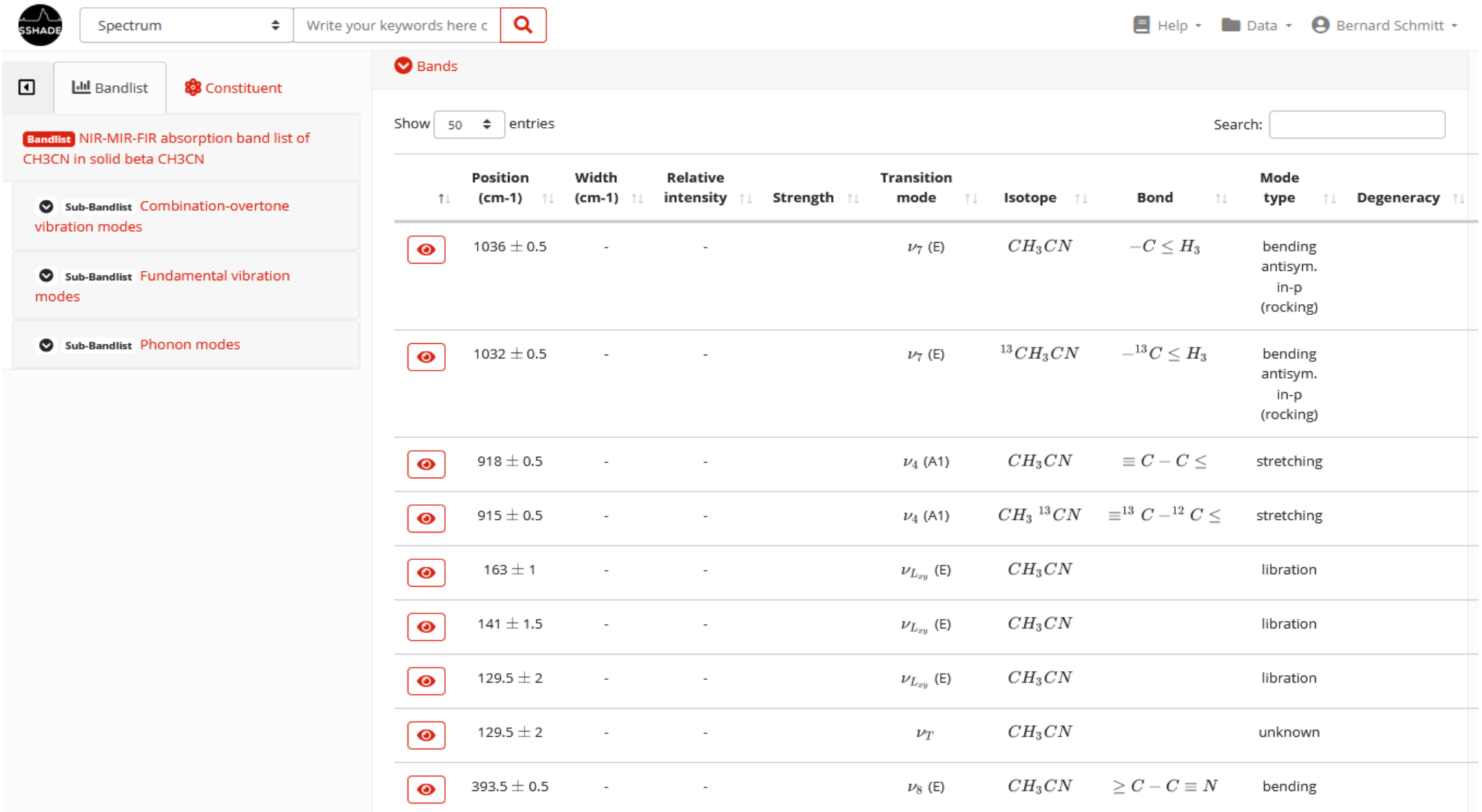
- Crystalline α-CO



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

Band lists and Bands

- Crystalline β-CH3CN



	Position (cm-1)	Width (cm-1)	Relative intensity	Strength	Transition mode	Isotope	Bond	Mode type	Degeneracy
	1036 ± 0.5	-	-		ν_7 (E)	CH_3CN	$-C \leq H_3$	bending antisym. in-p (rocking)	
	1032 ± 0.5	-	-		ν_7 (E)	$^{13}CH_3CN$	$-^{13}C \leq H_3$	bending antisym. in-p (rocking)	
	918 ± 0.5	-	-		ν_4 (A1)	CH_3CN	$\equiv C - C \leq$	stretching	
	915 ± 0.5	-	-		ν_4 (A1)	$CH_3\ ^{13}CN$	$\equiv^{13} C -^{12} C \leq$	stretching	
	163 ± 1	-	-		$\nu_{L_{zy}}$ (E)	CH_3CN		libration	
	141 ± 1.5	-	-		$\nu_{L_{zy}}$ (E)	CH_3CN		libration	
	129.5 ± 2	-	-		$\nu_{L_{zy}}$ (E)	CH_3CN		libration	
	129.5 ± 2	-	-		ν_T	CH_3CN		unknown	
	393.5 ± 0.5	-	-		ν_8 (E)	CH_3CN	$\geq C - C \equiv N$	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.
• Seach 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

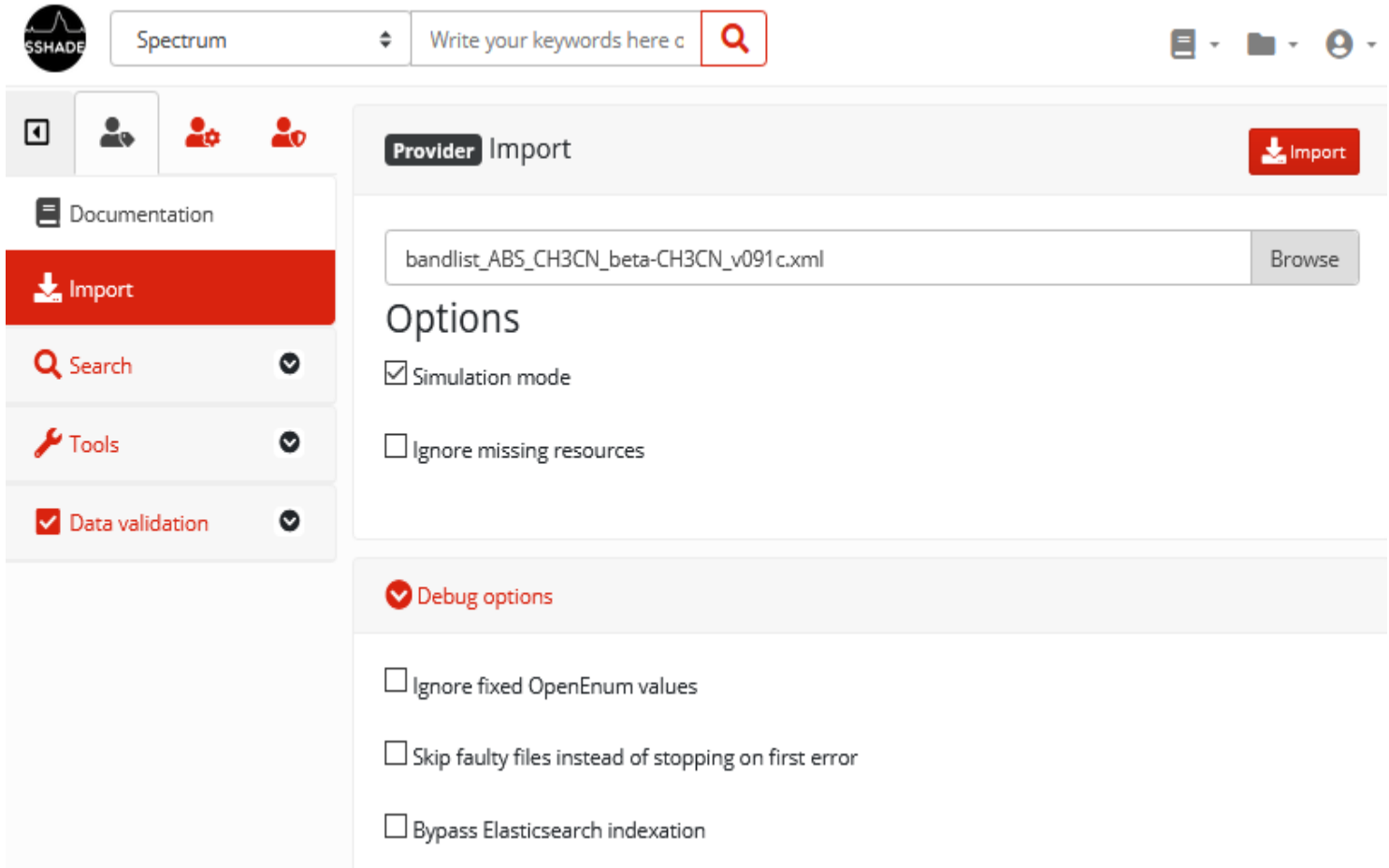
- Description of the ‘Bands’
  - **Assignments** (multiple)
    - Multiplicity, degeneracy, resonances
    - Transition
      - label, type
      - species, crystal site and symmetry
      - bond (for molec. solids)
    - Evaluation
  - **Characteristics** (multiple)
    - environnement: T, P
    - position 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

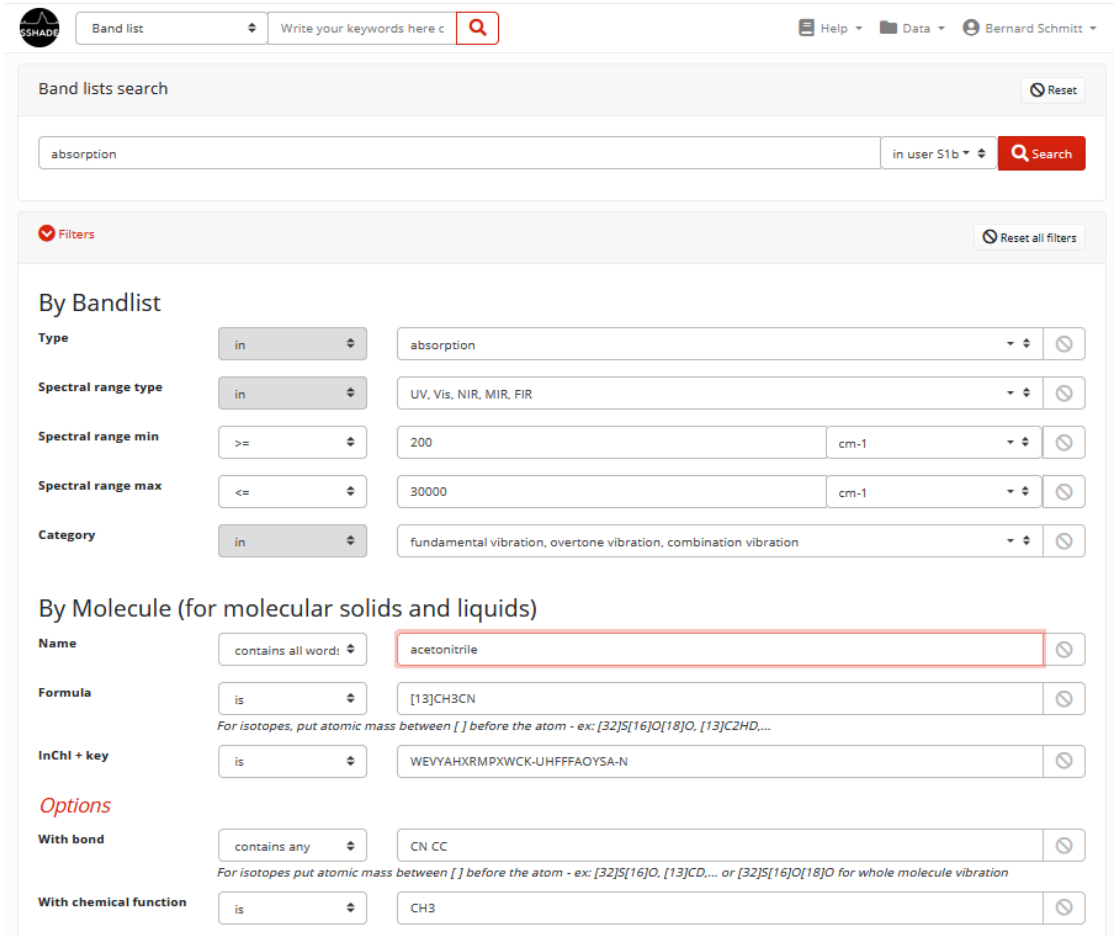
bandlist_ABS_CH3CN_beta-CH3CN_v091c.xml

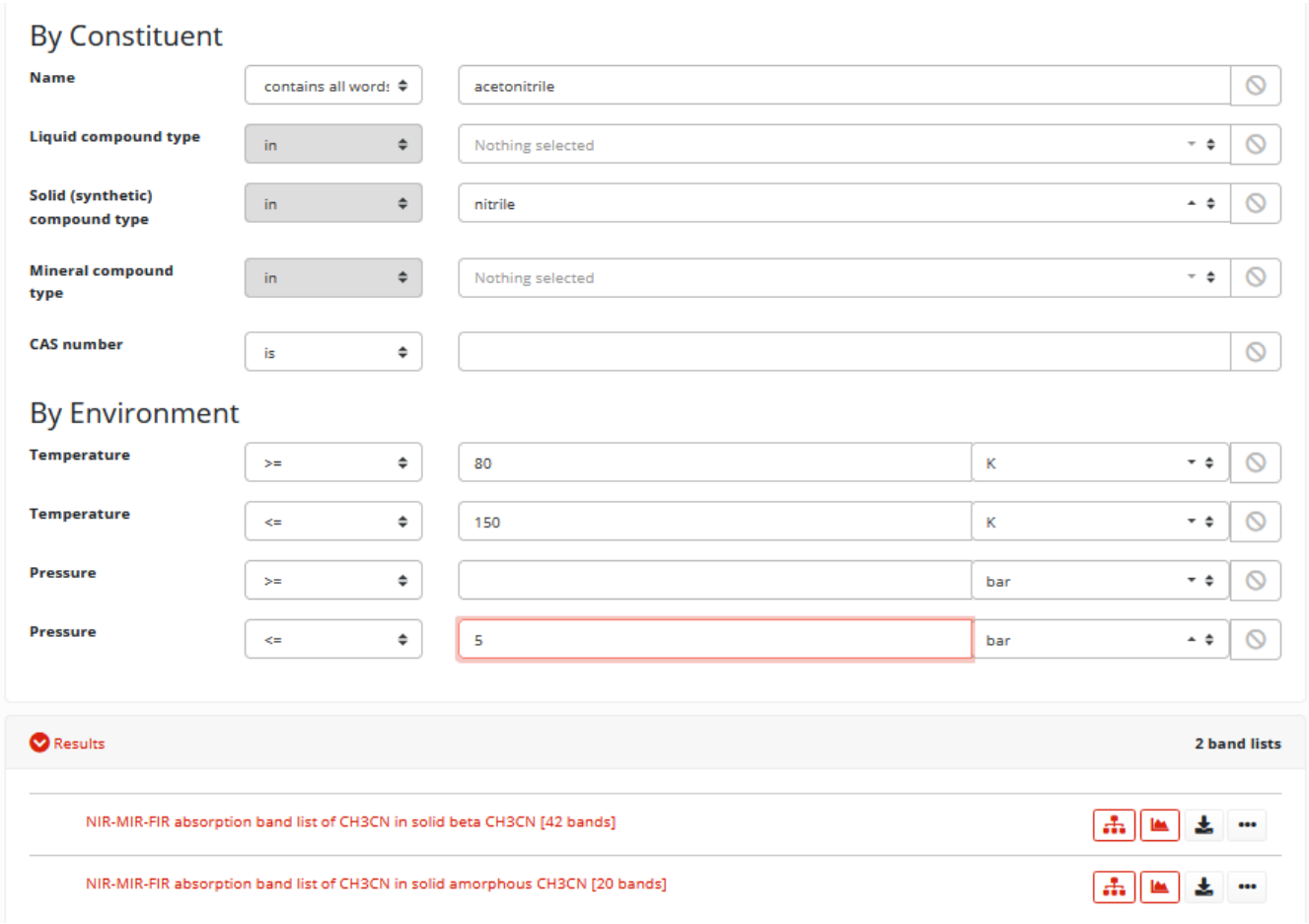
```xml
<?xml version="1.0" encoding="UTF-8"?>
<!--
Data type : Bandlist

CH3CN in solid beta CH3CN
-->
<import type="bandlist" ssdm_version="0.9.1"
        xmlns="http://sshade.eu/schema/import"
        xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
        xsi:schemaLocation="http://sshade.eu/schema/import http://sshade.eu/schema/i

    <bandlist><!-- multiple -->
    <!-- BAND LIST IMPORT MODE AND INDEXES -->
        <import_mode>correction</import_mode> <!-- **ABS MANDATORY** Mode of import
        <uid>BANDLIST_ABS_CH3CN_beta-CH3CN</uid> <!-- **ABS MANDATORY to CREATE** Un

    <!-- BAND LIST DESCRIPTION -->
        <type>absorption</type> <!-- **ABS MANDATORY** Type of band list. Enum: {abs
        <title>NIR-MIR-FIR absorption band list of CH3CN in solid beta CH3CN</title>
        <description><![CDATA[NIR-MIR-FIR absorption band list of $CH_3CN$ and isotc

    <!-- BANDLIST: SPECTRAL RANGES -->
        <parameters_spectral> <!-- **ABS MANDATORY** -->
            <unit>cm-1</unit> <!-- **ABS MANDATORY** Unit of the position and width
            <standard>vacuum</standard> <!-- **ABS MANDATORY** Medium in which the w
            <range_types> <!-- **ABS MANDATORY at least one** -->
                <type>NIR</type><!-- multiple --> <!-- **ABS MANDATORY** Typical spe
                <type>MIR</type>
                <type>FIR</type>
            </range_types>
            <ranges> <!-- **ABS MANDATORY at least one** -->
                <range><!-- multiple -->
                    <min>90</min> <!-- **ABS MANDATORY** Start of the spectral range
                    <max>4450</max> <!-- **ABS MANDATORY** End of the spectral range
                </range>
            </ranges>
            <comments><![CDATA[]]></comments> <!-- Additional information on spectra
        </parameters_spectral>

    <!-- BANDLIST: INTENSITY MODES AND UNITS -->
        <reference_position>
            <electronic></electronic> <!-- **MANDATORY for electronic bands when ban
            <infrared></infrared> <!-- **MANDATORY for infrared and Raman bands when
        </reference_position>

    <!-- BAND LIST: CONSTITUENT AND SPECIE -->
        <constituent>
            <uid>CONST_solid_beta_CH3CN</uid> <!-- **ABS MANDATORY** LINK to the exi
            <primary_specie_uid>MOLEC_CH3CN</primary_specie_uid> <!--  $$**ABS MANDA
```



Band lists: user search tool + results

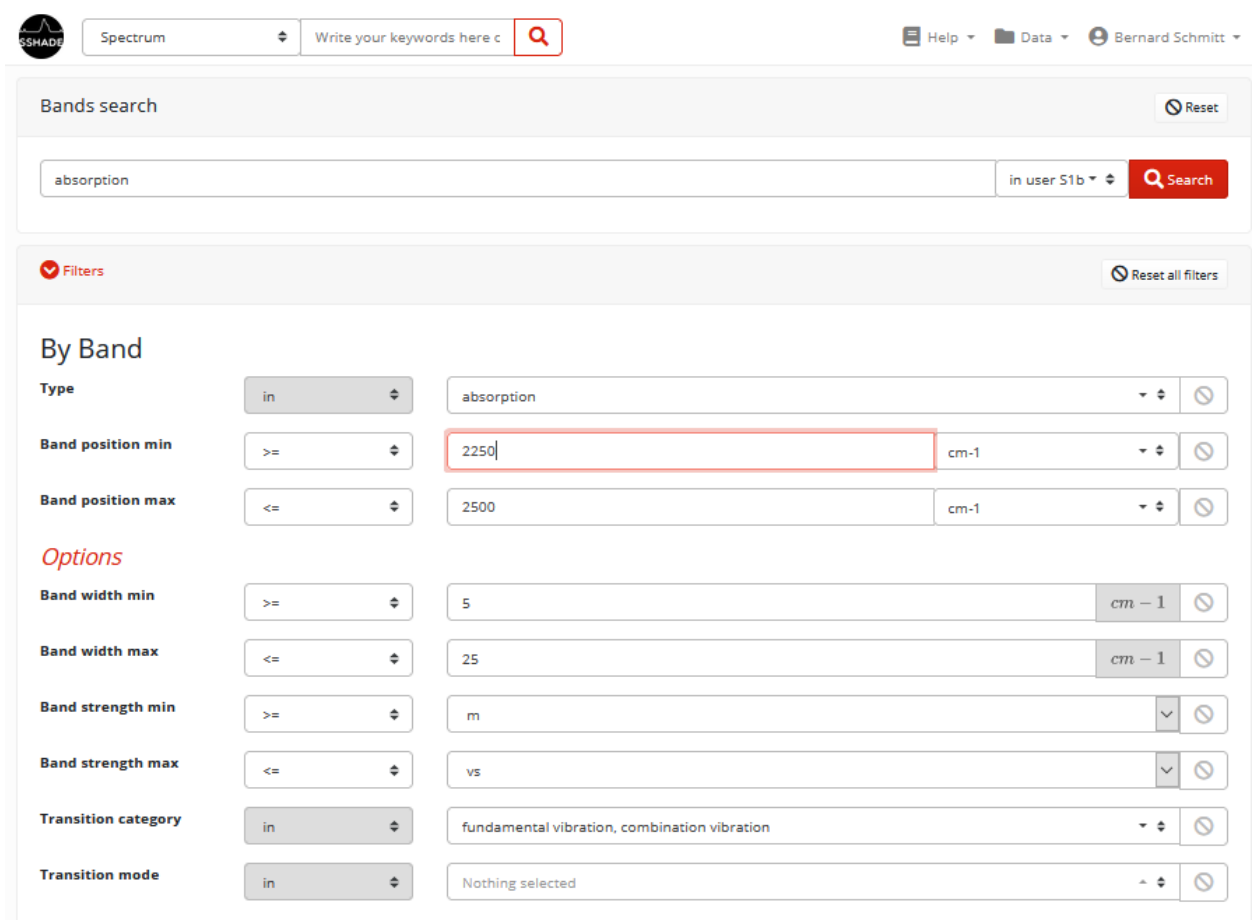
- Bandlists of specific solids with various criteria

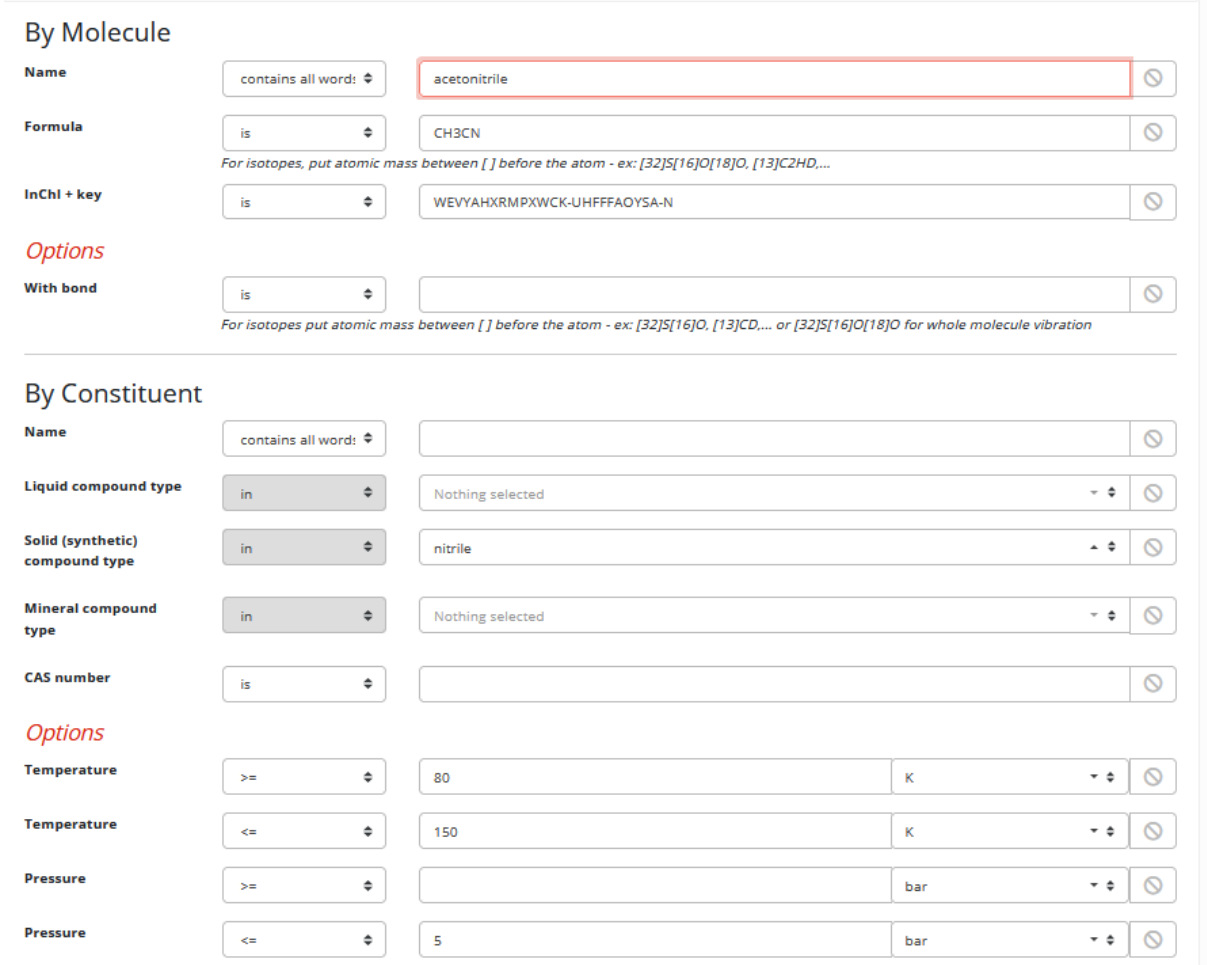




Bands: user search tool

- Bands with various spectral and composition criteria





Bands: results

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

Results — 60 bands

Show 25 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	$^{12}C^{16}O$	CO	alpha-CO	20	-
50150 ± 25	504 ± 10	-	$a\,^3\Pi_r \leftarrow X\,^1\Sigma^+(1,0)$	absorption	$^{12}C^{16}O$	CO	alpha-CO	20	-
48400 ± 25	563 ± 10	-	$a\,^3\Pi_r \leftarrow X\,^1\Sigma^+(0,0)$	absorption	$^{12}C^{16}O$	CO	alpha-CO	20	-
6390 ± 1	43 ± 2	vvw	$3\nu_1 + \nu_{L,T}$	absorption	$^{12}C^{16}O$	CO	alpha-CO	21	-
6337.8 ± 0.8	3.7 ± 0.2	vw	$3\nu_1$	absorption	$^{12}C^{16}O$	CO	alpha-CO	20	-
6258 ± 0.5	3.7 ± 0.2	vvw	$3\nu_1$	absorption	$^{12}C^{17}O$	CO	alpha-CO	21	-
6199 ± 0.6	3.6 ± 0.2	vvw	$3\nu_1$	absorption	$^{13}C^{16}O$	CO	alpha-CO	21	-
6188.4 ± 0.5	3.7 ± 0.3	vvw	$3\nu_1$	absorption	$^{12}C^{18}O$	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

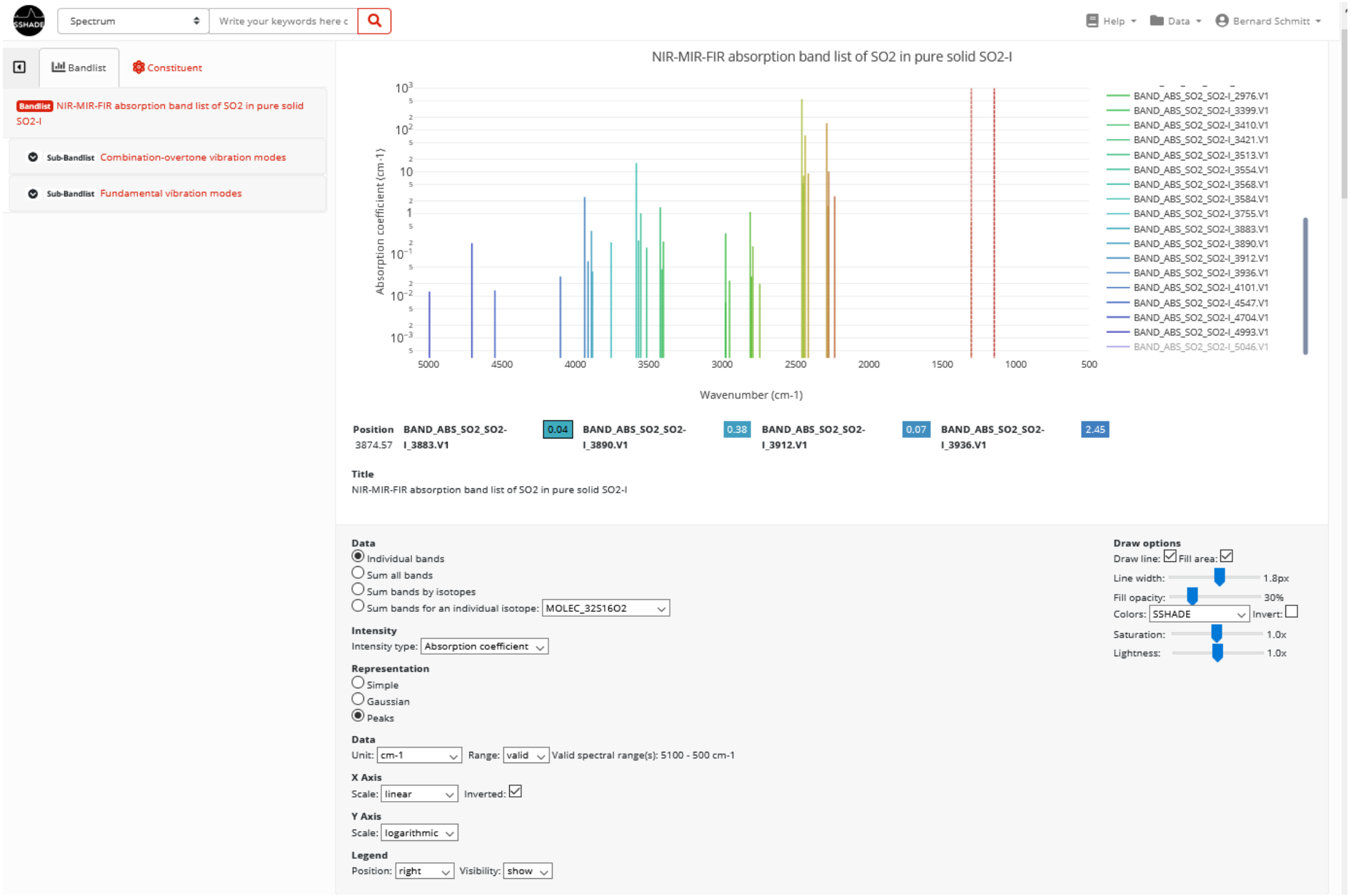
- Absorption coefficient
- Relative intensity

Representation

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

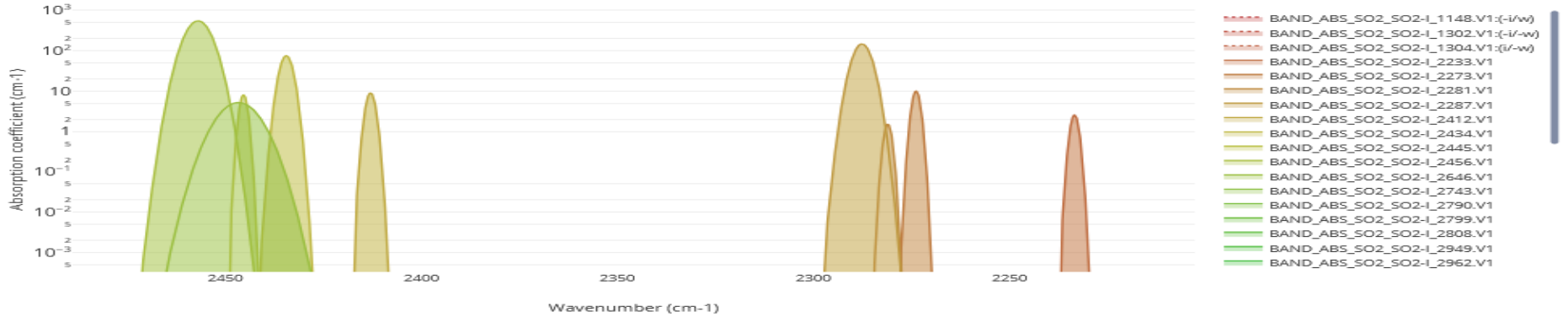
✓ Manage missing data on width and/or intensity

Band list & bands: display tools



Band list & bands: display tools

- Individual bands

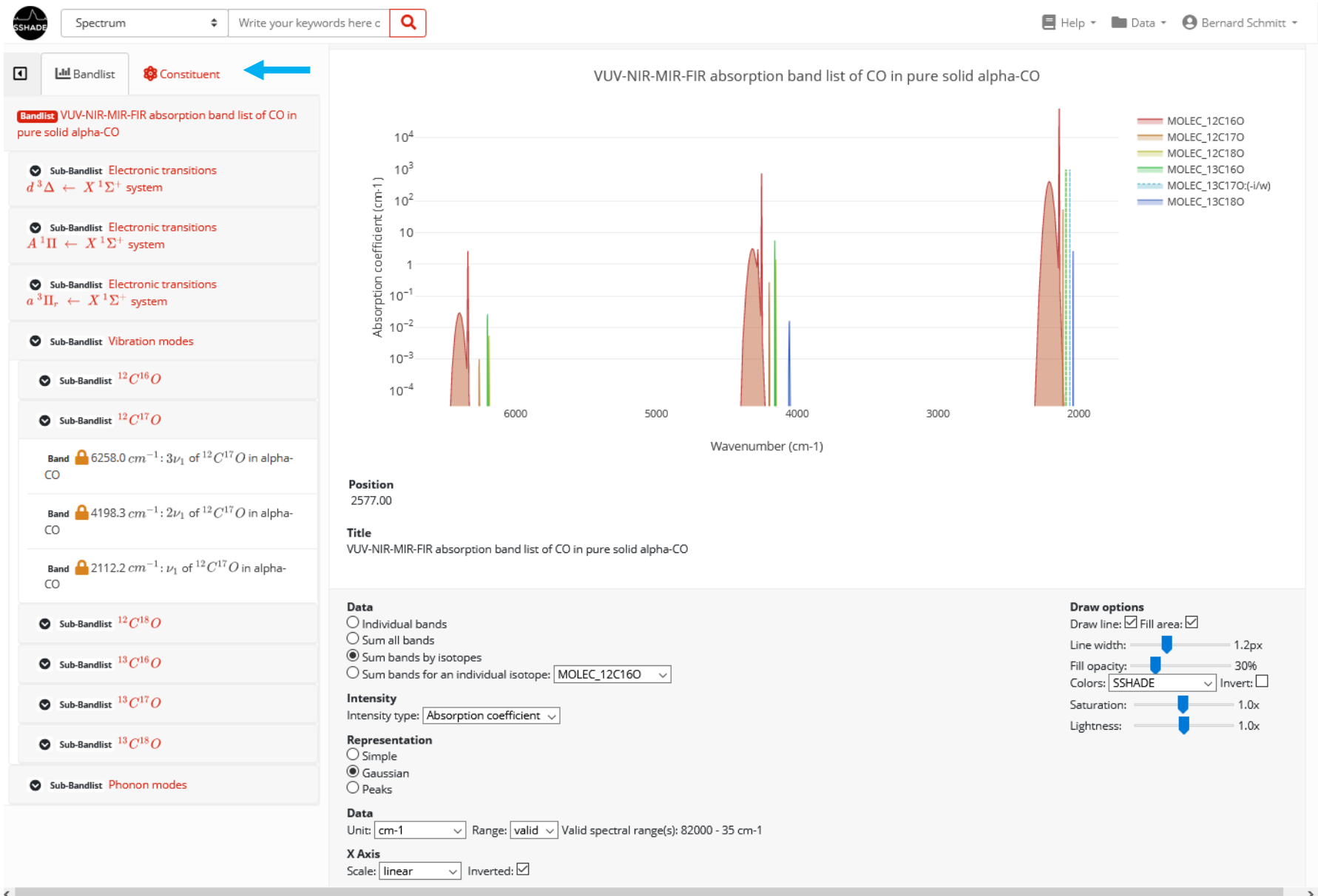


- Sum of bands of each isotope

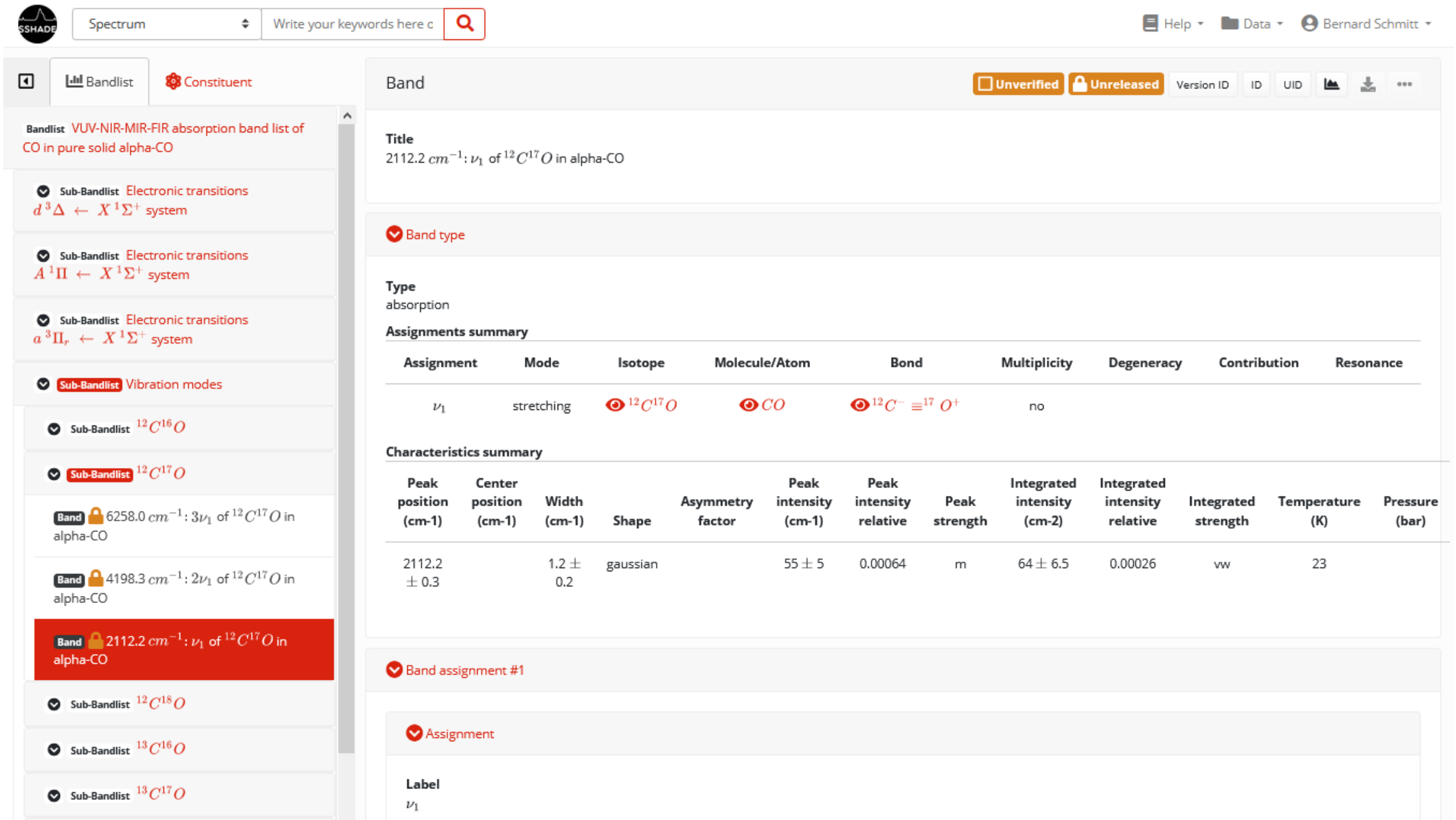
- Sum of bands of whole bandlist

Band list & bands: organisation of the bands

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



Band list & bands: Metadata



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 commitee (2021): NIR-MIR-FIR absorption band list of CH3CN in solid beta CH3CN. Version 1. SSHADE (OSUG Data Center). Dataset/Band list Data. doi: 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 α-CO : > 30 papers ! (1961-2020…)
- First selection :

  ~ 50 simple and pure molecular solids (H2O, CO, SO2, CH4, … C6H6, CH3CN, …)

  ~ 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 !!!