

# Solid Spectroscopy Data Model (SSDM-Bandlist) for the Bandlist database of the SSHADE database infrastructure

## Document Information

<b>Editor:</b>	Bernard Schmitt - IPAG, UGA-CNRS/INSU
<b>Author(s):</b>	Bernard Schmitt, Damien Albert, Manon Furrer, Philippe Bollard, Lydie Bonal, Olivier Poch
<b>Contributor(s):</b>	-
<b>Type of document:</b>	standards documentation
<b>Status:</b>	Initial version of the core
<b>Distribution:</b>	<i>Public</i>
<b>Work packages:</b>	2020-2024: VA2 VESPA (Europlanet2024-RI)
<b>Version (date):</b>	<b>0.9.2</b> (26/05/2023)
<b>File name:</b>	SSDM-bandlist_datamodel_v0.9.2
<b>Reference:</b>	Schmitt, B., Albert D., Furrer, M., Bollard P., Bonal, L., Poch, O. (2023). The Solid Spectroscopy Data Model (SSDM-Bandlist) of the bandlist database of the SSHADE database infrastructure. Version 0.9.2. <a href="https://wiki.sshade.eu/_media/ssshade/documentation/ssdm-bandlist_datamodel_v0.9.2_sshade.pdf">https://wiki.sshade.eu/_media/ssshade/documentation/ssdm-bandlist_datamodel_v0.9.2_sshade.pdf</a>

**Abstract:** The "Solid Spectroscopy Data Model" for Bandlist (SSDM-Bandlist) is a relational data model allowing a complete description of list of bands of solid materials. It includes a detailed description of the solid constituent and its species. The spectral data provided are the parameters that fully describe bands (band parameters and transition attributions).  
SSDM is the base of the SSHADE database infrastructure of spectroscopy of solids.

## Version History

Version	Date	Modified By	Description of Change
<b>v0.9.0a</b>	31/07/20	Bernard Schmitt	Initial draft version of Bandlist DataModel
v0.9.0b	21/09/20	Bernard Schmitt	Added a few KW and Enum attributes in bandlist and band
v0.9.0e	16/10/20	Bernard Schmitt	Added and changed a number of KW and Enum attributes in constituent, bandlist and band
v0.9.0f	24/10/20	Bernard Schmitt	Large changes in KW names, Enum and conditions of bandlist and band
v0.9.0g	02/11/20	Bernard Schmitt	Large addition/removel and changes in KW names, Enum and conditions of bandlist and band
<b>v0.9.1</b>	09/11/20	Bernard Schmitt	Same as v0.9.0g but with all v0.9.0g changes marks cleaned + minor changes
v0.9.1a	09/12/20	Bernard Schmitt	Minor improvements
v0.9.1b	18/12/20	Bernard Schmitt	Minor improvements
v0.9.1c	04/06/21	Bernard Schmitt	Minor improvements
v0.9.1d	30/09/21	Bernard Schmitt	Added a few KW and extended many Enum of the "Band" table
v0.9.2a	26/05/23	Bernard Schmitt	Major changes: Added several KW and condition in "Bandlist" and "Band" tables
<b>v0.9.2</b>	26/05/23	Bernard Schmitt	Same as v0.9.2a but with all v0.9.2a changes marks cleaned + minor changes

## **Disclaimer**

The information in this document is subject to change without notice. Company or product names mentioned in this document may be trademarks or registered trademarks of their respective companies.

## **All rights reserved**

The document is proprietary of the Europlanet and VAMDC consortium members. No copying or distributing, in any form or by any means, is allowed without the prior written agreement of the owner of the property rights.

This document reflects only the authors' view. The European Community is not liable for any use that may be made of the information contained herein.

## **Acknowledgements**

*Europlanet 2020 RI* (2015-2019) is funded by the European Union's "Horizon 2020" research and innovation Programme. Grant Agreement number: 654208.

*VAMDC* (2009-2012) was funded under the "Combination of Collaborative Projects and Coordination and Support Actions" Funding Scheme of The Seventh Framework Programme. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108.

*Europlanet RI* (2009-2012) was funded under the "Combination of Collaborative Projects and Coordination and Support Actions" Funding Scheme of The Seventh Framework Programme. Grant Agreement number: 228319.

**OSUG and CNRS-INSU** for their recursive supports for the early and current developments of SSDM (and the GhoSST database) since 2006 and 2013 respectively.

**CNES "Solar SystemStudies"** is also acknowledged for support through various space mission programs

## **TABLE OF CONTENT**

# 1. INTRODUCTION

## 2. GENERAL DESCRIPTION

### 2.1 Data Model Structure

The current **SSDM-spectra data model** is split in 3 main parts (+ additional existing parts of SSDM-spectra) which contain the relevant keywords to describe them and that are linked with relevant relations.

- The “**Constituent**” table which describes the “*constituents*” (minerals, synthetic solids, liquids, ...) down to their basic constitutive “*fundamental species*” (molecules, atoms, ...).
- The “**Bandlist**” table which describes the “*bandlist*” of the constituent
- The “**Band**” table which describes the “*bands*” of the bandlist, with all their parameters and attribution

### 2.2 Data Model Content

See the SSDM-spectra document

### 2.3 Tables Content Description

See the SSDM-spectra document

## 2.4 Bandlist Basic constituent Table

Root of the table: *basic\_constituent*

Data type: in 'Bandlist constituent'

Condition: if the constituent is a "basic constituent" (i.e. that can be described by one of the "fundamental solid, mineral or liquid" phases) then use this "Basic constituent" table. If not (constituent defined manually), then use the "Constituent" table.

Key-word	Type	Level	Table	Exp	Unit	Description
<i>Basic constituent index</i>						
<i>bandlist_basic_constituent_import_mode</i>	enum(text)	P [!!_m]	BL- BConst		--	Mode of import of the actual "Basic constituent" metadata  <b>Enum:</b> {first import, ignore, draft, no change, correction}  <i>Definitions:</i> see "sample_import_mode"
<i>bandlist_basic_constituent_index</i> [**][-xml]	int(10)	B [!!_g]	BL- BConst	F	--	Automatic random but unique number (ID) given to new actual basic constituent
<i>bandlist_basic_constituent_uid</i> [**]	varchar(255)	S0/S1 [!!_m]	BL- BConst	F	--	Unique identifier code (UID) given to the actual basic constituent table (to be created)  <i>Nomenclature:</i> This code name should start with 'CONST_' and be very accurately formatted in order to be simple and unique <ul style="list-style-type: none"> <li>It should be of the style 'CONST_Constituent_Phase' where 'Constituent' is a short description of the constituent that include the constituting molecules and 'Phase' describe the type of phase ('solidSO2-I', 'CH4-betaN2', ...)</li> </ul> <i>Ex:</i> 'CONST_solidCH4-II', 'CONST_clathrateSO2', 'CONST_SO2-H2Oam', 'CONST_H2S-solidSO2', 'CONST_CH4-betaN2', 'CONST_CH4-liquidN2',  <i>Notes:</i>

*bandlist\_basic\_constituent\_owner* varchar(255) U BL- F -- Link to the existing UID of the database which owns the basic constituent and manages its information  
 \_database\_uid [!\*\_][!d\_m] BConst  
 DatBas  
*Default* = 'DB\_BANDLIST'  
*Notes:*

- it will be always 'DB\_BANDLIST'
- this allows to heritate from the administration tools of databases

*bandlist\_basic\_constituent\_relevance* enum(text) U BL- -- Relevance of the basic constituent in the material  
 [-xml] [!\_d] BConst  
 [*constituent\_relevance*]  
*Enum:* {main – major}  
*Default* = 'main – major'  
*Definitions:* cf. "*constituent\_relevance*"

### ***Basic constituent arrangement***

*bandlist\_basic\_constituent\_arrangement* enum(text) U BL- -- Relative arrangement of the constituent within the material grains  
 [-xml] [!\_m] BConst  
 [*constituent\_arrangement*]  
*OpenEnum:* {single phase}  
*Default* = 'single phase'  
*Definitions:* see "*constituent\_arrangement*"  
*Notes:* see "*constituent\_arrangement*"

### ***Basic constituent name and index***

*bandlist\_basic\_constituent\_name* varchar(255) S0 BL- -- Name of the actual basic constituent  
 [!\_m] BConst  
*Note:*

- It may contain explicit info on the fundamental constituent or its variant: species name, specific abundance, and some properties of the constituent (phase, ...), origin, ....
- It is used as the title of the constituent page on the SSHADE interface

*Ex:* 'San Carlo Olivine', 'Synthetic fayalite 3% Mg', 'Water ice Ih with 0.1% CO2', ...

<i>bandlist_basic_constituent_fundamental_phase_uid</i> [*]	varchar(255)	S1/Sli0 [!!_m]	BL- BConst  Solid Miner Liquid	-- Link to the existing UID of the fundamental ‘solid’, ‘mineral’, or ‘liquid’ phase  <i>Notes:</i> - Only for fundamental ‘solid’, ‘mineral’, and ‘liquid’ phases. - The others constituents are described with the full constituent/species structure (“Constituent” table)
---	--------------	-------------------	---	---

### ***Fundamental phase variable parameters***

*Condition:* OPTIONAL block but COMPULSORY to change what is better known or different from the linked fundamental solid/mineral/liquid.

*Note:* The variable parameters are mostly used to provide more accurate composition of the actual solid/mineral/liquid: for variable solids/minerals/liquids or solid/mineral liquid/hydration series, or when solid/mineral (sub-)groups are used for ill-defined solids/minerals. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental solids/minerals for describing some related amorphous solids/minerals.

<i>bandlist_basic_constituent_solid_variables</i>	[O]	BL- BConst  Solid	VS	£: solid variable parameters  <i>Note:</i> mostly used to provide more accurate composition of the actual solid: for variable solids or solid solution/hydration series, or when solid (sub-)groups are used for ill-defined solids. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental solids for describing some related amorphous solids
---	-----	----------------------------	----	---

<i>bandlist_basic_constituent_mineral_variables</i>	[O]	BL- BConst  Miner	VMi	£: mineral variable parameters  <i>Note:</i> mostly used to provide more accurate composition of the actual mineral: for variable or solution/hydration series minerals, or when mineral (sub-)groups are used for ill-defined minerals. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental minerals for describing some related amorphous minerals.
---	-----	----------------------------	-----	--

<i>bandlist_basic_constituent_liquid_variables</i>	[O]	BL- BConst  Liquid	VL	£: liquid variable parameters  <i>Note:</i> mostly used to provide the accurate composition of the actual liquid
--	-----	-----------------------------	----	--



---

### *Constituent texture*

<i>bandlist_basic_constituent_texture</i>	enum(text)	S1b <a href="#">[m]</a>	BL- BConst	-- Internal texture of the basic constituent crystals  <i>Enum:</i> {monocrystalline, polycrystalline, cryptocrystalline, nanocrystalline, metamict, amorphous, glassy, polymeric, liquid, other, unknown}  <i>Definitions &amp; notes:</i> see “ <i>constituent_crystal_texture</i> ”
<i>bandlist_basic_constituent_comments</i>	blob	U <a href="#">[m]</a>	BL- BConst	-- Additional information on basic constituent, in particular for coating of grains: coating thickness

---

## 3. BAND LISTS – BANDS

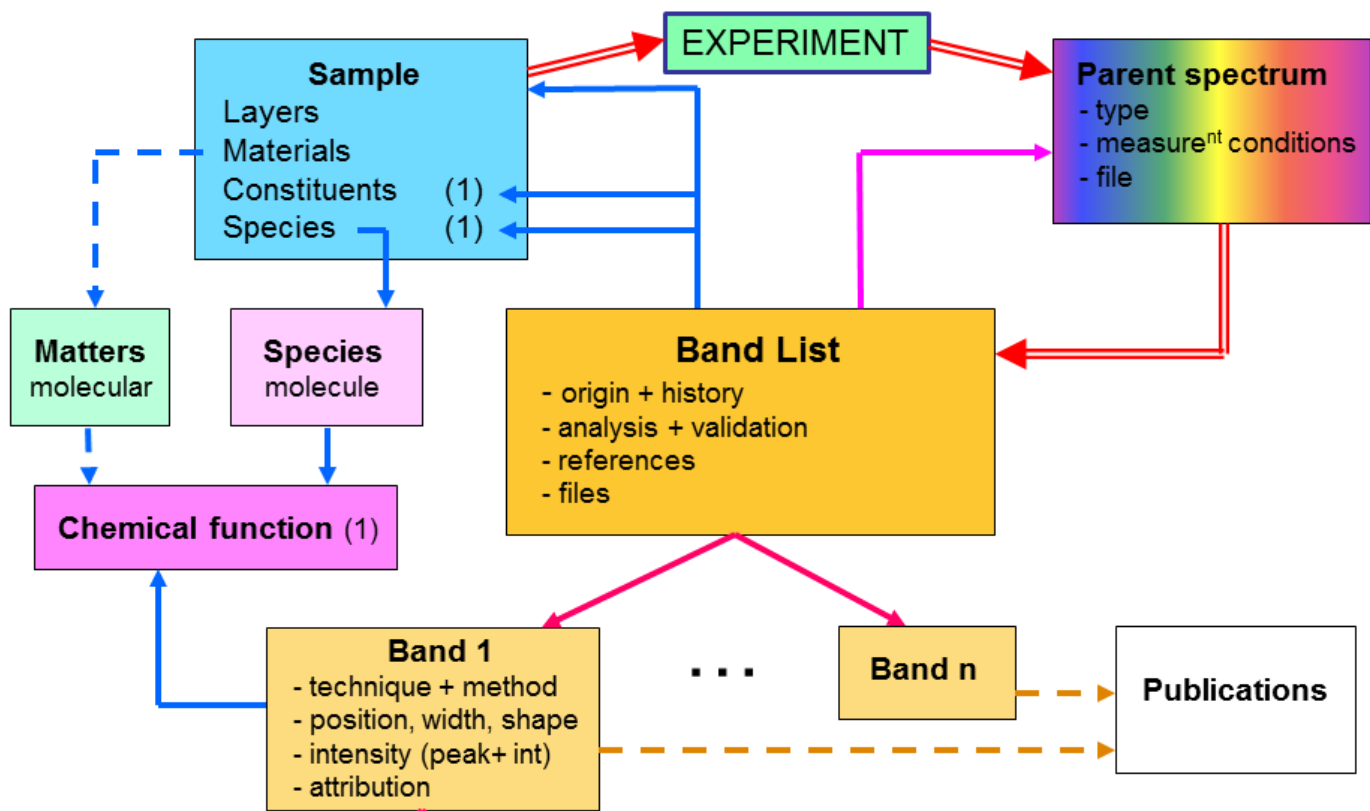
### 3.1 Description

The **band list** data base (level 5 product) contains individual information on each known vibration bands of a particular species (isotopic species) inside various solid constituents. Internal (molecular species) as well as external vibrations (phonons modes of solid) are described, as well as possible rotations. But currently we will not include electronic transitions (UV-Vis) of solids as it is probably quite difficult to define transitions and quantum numbers for these electronic transitions in solids.

So, a band list refers mostly to bands of a specific isotopic specie (but sometimes to a natural/synthetic isotopic mixture when the isotopic origin of the bands is not dicrimined in the spectra). For a given band list several values of the characteristics of a given band can be given at selected values of some physical parameters (temperature, pressure, ...).

This band information may have different and complementary origins in term of optical process and measurement type (absorption, Raman scattering, reflectance, thermal emission, fluorescence emission). One difficulty is thus to compare band characteristics coming from these different processes which may also be sensitive to the way they are measured: position (slightly sensitive), width (moderately) and intensity (strongly). As only absorption can easily provide absolute values we adopted the metric absorption coefficient (absorption) as the only absolute value while the intensity of the other type of data will be expressed as relative intensity.

This band list database is not intended to record all values taken from all spectra, but it rather needs a critical selection of relevant sets of band list of one species in selected solid constituents in well defined solid phases (e.g. CH<sub>4</sub> as pure solid phase I, same for phase II, same for liquid, diluted in N<sub>2</sub> ice (phases alpha and beta), mixed in amorphous H<sub>2</sub>O ice, ..., in clathrate hydrate type I, in mixed clathrate type II, ...)



Figures 3: Structure of Bandlist, Bands and relations with Sample and Experiment/Spectra

Currently we restrict this band list database to the “*molecular solids*” family (molecules, molecular ions, radicals and molecular chemical functions) and to molecules ad/absorbed on any type of homogeneous solid. We can also consider chemical bonds of single complex organic materials (not their mixture) and also vibration bands of molecules ad/absorbed on/in such materials. Minerals is currently out of scope of this data base (mostly because of its complexity ...) but chemical functions of their anionic radicals (OH, CO<sub>3</sub>, SO<sub>4</sub>, ...) can also be considered.

We also mostly limit this fundamental band list to pure molecular solids (i.e. solid samples with only one constituent with a single species, or its natural isotopic mixture) and to various types of solids with one or two constituents and a limited number of species (2-3) (simple molecular mixtures, binary compounds, hydrates, clathrates, simple polymers, ...) at different temperatures and in different solid phases. We also consider *molecules adsorbed on molecular solids* or *on minerals* or *on some complex but homogeneous materials* (tholins, ...), as well as *molecules absorbed or trapped inside minerals*. In all cases the band refers to a molecular species inside a single and defined constituent (even if the material has several). Data from granular mixtures or layered samples will be avoided because of the complexity to extract the contribution of a single constituent.

Note: This database is almost fully independent of the “spectra database”. It however provides links to the spectrum (or spectra) in the spectral database where the corresponding band is observed. It may also include selected bibliographic data provided that enough information on the solid sample is available.

### 3.1.1 Band Lists

*A “band list” refers to all bands of one particular isotopic species in one well defined constituent.*

Each band list is linked to **the species (molecule, ion, radical...)** which creates the band (the “primary species”). This species belong to one defined constituent (the "primary constituent") of the sample material. The sample and this constituent should be simple. For simple mixtures in a constituent the other abundant molecules are called the “secondary species”. It can be a matrix molecule in which the primary species is trapped, or the second molecule of a molecular compound, or the major isotope for minor isotopic species, or H<sub>2</sub>O for clathrates or hydrates, or the molecular solid (or mineral, ...) for adsorbed molecules, ... but it can be also a mineral on or in which the primary molecule is adsorbed/absorbed/trapped.

The band list refer to the sample that contain the primary constituent and species, and that define the composition of the constituent (compound type, abundances, ...), its state (phase, ...) and its physical properties (temperature, pressure, ...). It also refer to the spectrum/spectra from which the band list has been derived in order to know in which measurements conditions these spectra have been recorded.

Each band list is composed of a series of bands (or lines ?).

### 3.1.2 Bands

The method used to get the values of the band characteristics is first described.

Each band is then described by its position (requisite), its width, its absolute or relative peak intensity and its absolute or relative integrated intensity (over the whole band) depending which one is available. For each of them the method, accuracy, quality and an evaluation can be provided.

The band vibration type, the part of the molecule subjected to the transition (if any) and the transition assignment are then given. Each band is linked with the two states (lower and upper) of the molecule giving rise to the transition.

## 3.2 Band list Table

Root of the table: *bandlist*

Data type: 'Bandlist'

Key-word	Type	Level	Table	Exp	Unit	Description
<i>Band list import mode and indexes</i>						
<i>bandlist_import_mode</i> <i>[spectrum_import_mode]</i>	enum(text)	P [!!_m]	BandLi	--		Mode of import of the “bandlist” metadata  <b>Enum:</b> {first import, ignore, draft, no change, correction, invalidate}  <i>Constraint:</i> <ul style="list-style-type: none"> <li>- ‘invalidate’ only when at least one “band_access_right” is already ‘public’</li> <li>- ‘invalidate’ only when at least one ‘band_import_mode’ = {invalidate}</li> </ul> <i>Definitions:</i> There is 1 level of import: <ul style="list-style-type: none"> <li>- ‘first import’: during first import of the metadata and data</li> </ul> There are 3 levels of ‘no correction’: <ul style="list-style-type: none"> <li>- ‘ignore’: fully ignore this metadata table.</li> <li>- ‘draft’: used for draft (not ready to be imported). Exactly same as ‘ignore’ but duplicated for practical reasons</li> <li>- ‘no change’: when there is no change in this table (for correction in others tables) but it exist already in the database (checked)</li> </ul> There are 3 levels of correction: <ul style="list-style-type: none"> <li>- ‘correction’: used to correct/add values of metadata, links, or associated files for data already imported in the database. For bandlists it only modifies values/links/files on the current (last) version of the metadata. It should not be used to change a bandlist file (or only very minor changes).</li> <li>- ‘invalidate’: used when a bandlist is found to be mostly or fully</li> </ul>

invalid but there is currently no way to correct it and import new versions of its bands.

*Notes:*

- For 'invalidate' the “bandlist\_previous\_version\_status” and “bandlist\_previous\_version\_comments” KWs are stored with the current version and in some cases also with all the previous versions (see “bandlist\_previous\_version\_status”).

<i>bandlist_xml_filename</i> [-xml] <i>[spectrum_xml_filename]</i>	varchar(255) [virtual KW]	P [!!_vc]	BandLi	--	Name of the storage copy of the xml import file of the band list metadata ➔ determined automatically during import (from “bandlist_uid” ?)  <i>Note:</i> this file is stored in order to be able to retrieve it when it is necessary to apply corrections or import a new version of a band
<i>bandlist_index</i> [**][-xml] <i>[spectrum_index]</i>	int(10)	B [!!_g]	BandLi	F	-- Automatic random but unique number (internal ID) given to new bandlist
<i>bandlist_uid</i> [**] <i>[spectrum_uid]</i>	varchar(255)	S0 [!!_m]	BandLi	F	-- Unique identifier code (UID) given to the band list table (to be created)

*Nomenclature:*

Create this code name with ‘BANDLIST\_’ very accurately in order to be simple and unique.

It should be of the style ‘BANDLIST\_Type\_Molecule\_Constituent’, where:

- ‘Type’ is the band list type:
  - ‘ABS-R’: for ‘absorption and Raman scattering’
  - ‘REFL’: for ‘reflectance’
  - ‘THERM’: for ‘thermal emission’
  - ‘FLUO’: for ‘fluorescence emission’
- ‘Molecule’ is the general formula of the molecule (not isotopic, and not for minerals)
- ‘Constituent’ is a short description of the constituent (‘pure’, ‘N2matrix’, ...) with the phase type or number

*Note DOI:* requested in “Identifier” (for ‘bandlist’)

*Ex:*

- BANDLIST\_ABS\_CH3OH\_am-CH3OH  
for amorphous phase
- BANDLIST\_ABS\_N2\_alpha-N2  
for crystalline phases with greek letters
- BANDLIST\_ABS\_CH4\_CH4-I  
for crystalline phases with numbers
- BANDLIST\_RAMAN\_CH4\_alpha\_N2-CH4\_0-3pc  
for solid solutions
- BANDLIST\_RAMAN\_CH4\_13CD4-I  
for solids of isotopic species
- BANDLIST\_RAMAN\_Aragonite  
for minerals

<p><i>bandlist_sshade_doi</i> [-xml] <i>[experiment_sshade_doi]</i></p>	<p>varchar(255)</p>	<p>S1 <a href="#">[!_c]</a></p>	<p>BandLi</p>	<p>F</p>	<p>-- DOI of the bandlist          → automatically generated using the UID of the bandlist          ⇨ 10.26302/SSHADE.'bandlist_uid'.V'bandlist_version'  <i>Definition:</i> <a href="http://en.wikipedia.org/wiki/Digital_object_identifier">http://en.wikipedia.org/wiki/Digital_object_identifier</a>  <i>Notes:</i>          - The DOI is determined with “bandlist_uid” and ” bandlist_version”          - the prefix ‘10.26302’ has been attributed by INIST to OSUG-DC, who will manage the doi creations.          - the url of the doi is obtained by adding ‘https://doi.org/’ (note: the former standard whas ‘http://dx.doi.org/’)          - the DOI will redirect to the SSHADE page displaying the band list metadata (through a landing page)  <i>Ex:</i> 10.26302/SSHADE.BANDLIST_ABS-R_13CO_pur.V2</p>
<p><i>bandlist_sshade_url</i> [-xml] <i>[spectrum_sshade_url]</i></p>	<p>varchar(255) [Virtual KW]</p>	<p>U <a href="#">[!_c]</a></p>	<p>BandLi</p>	<p>-- Direct web link to the SSHADE band list page displaying the bandlist data and its metadata          → automatically generated and in practice not stored in database          ⇨ https://www.sshade.eu/data/ 'bandlist_uid'/'bandlist_version'</p> <p><i>Notes:</i></p>	

- can be determined by knowing the UID (not restricted to bandlist)
- can be also obtained by copying the URL when viewing a bandlist details page.

*Ex:*

[https://www.sshade.eu/data/bandlist/BANDLIST\\_ABS-R\\_13CO\\_pur](https://www.sshade.eu/data/bandlist/BANDLIST_ABS-R_13CO_pur)

<i>bandlist_owner_database_uid</i> [*] [-xml]	varchar(255)	U [!!d_m]	BandLi DatBas	F	-- Link to the existing UID of the database which owns the bandlist and manages its information (with associated bands)
--	--------------	--------------	------------------	---	---

*Default* = 'DB\_BANDLIST'

*Notes:*

- it will be always DB\_BANDLIST
- this allows to heritate from the administration tools of databases

### ***Band list description***

<i>bandlist_type</i> [ <i>spectrum_type</i> ]	enum(text)	S0 [!!_m]	BandLi	F	-- Type of band list  <b>Enum:</b> {absorption, Raman scattering, reflectance, thermal emission, fluorescence emission}
--	------------	--------------	--------	---	---

*Definitions:*

- '*absorption*': bandlist of bands with characteristics determined in absorption spectra (transmission, ATR, ...)
- '*Raman scattering*': band list with characteristics determined in Raman scattering spectra
- '*reflectance*': bandlist of bands with characteristics determined in reflectance spectra (of various types)
- '*thermal emission*': bandlist of bands with characteristics determined in thermal emission spectra
- '*fluorescence emission*': bandlist of fluorescence bands

*Notes:*

- 'absorption' band list is best defined in absorption coefficient or from optical constants spectra (converted in absorption coefficient for absolute and relative intensity) derived from transmission or ATR





[!\_m]

Notes:

- it should contain complete info on the band list type, on typical spectral ranges covered, the specie and constituent of this band list, as well as on the environment parameters (with values or range of values).
- information on possible variations of the constituent may be also given
- it will be displayed as detailed info on search result.

Ex: 'Near and Mid-IR absorption and Raman bandlist of CO2 trapped in amorphous H2O ice between 20 and 120 K.'

Note DOI:

- Recommended option as "Description / descriptionType=Abstract" (17)

### Bandlist version

- It should reflect the changes of the version if they affect at least one element of the description

---

### Band list spectral parameters

<i>bandlist_spectral_unit</i>	enum(text)	U [!_m]	BandLi	F	-- Unit of the position and width spectral parameters of the bands  <b>Enum:</b> {m-1, cm-1, angstrom, nm, micron, mm, m, km, Hz, kHz, MHz, GHz, eV, keV}  <i>Note DB:</i> band list data will be stored in the database in wavenumber "cm <sup>-1</sup> " unit whatever is the unit in which they are entered.
<i>bandlist_spectral_standard</i>	enum(text)	P [!_m]	BandLi	F	-- Medium in which the wavenumber/wavelength/frequency scale is given  <b>Enum:</b> {vacuum, air, unknown}  <i>Definitions:</i> see "parameters_instrument_spectral_standard"  ➔ conversion to vacuum reference to be done at the import of the band xml file and (if necessary) after conversion to wavenumber 'v' in cm <sup>-1</sup>  <i>Note:</i> see notes at "parameters_instrument_spectral_standard"

<i>bandlist_spectral_ranges</i>	<b>List [L1]</b>	[!!]		£: Typical spectral ranges covered by the band list
<i>bandlist_spectral_range_type</i>	varchar(255)	S0 [!!_m]	BandLi L1	-- Typical spectral range <b>Enum:</b> {gamma, hard X, soft X, EUV, VUV, UV, Vis, NIR, MIR, FIR, sub-mm, mm, cm, UHF, VHF, HF, MF, LF, VLF, ULF, SLF, ELF} <i>Definitions:</i> see “ <i>parameters_instrument_spectral_range_type</i> ” <i>Note:</i> this spectral range is indexed to an equivalence table in term of typical minimum and maximum wavenumbers/wavelength/frequency
<i>bandlist_spectral_ranges</i>	<b>List [L2]</b>	[!!]		£: Spectral ranges of the band list <i>Note:</i> they can be non-continuous ranges of list of bands due to missing data over some range (ex: ‘NIR’ and ‘FIR’, MIR missing)
<i>bandlist_spectral_range_min</i>	float	S3 [!!_m]	BandLi L2	var. Start of the spectral range of the band list <i>Unit:</i> in unit defined by “ <i>bandlist_spectral_unit</i> ” - converted in ‘cm <sup>-1</sup> ’ unit in the database but provided to user in the unit specified in SSHADE
<i>bandlist_spectral_range_max</i>	float	S3 [!!_m]	BandLi L2	var. End of the spectral range of the band list <i>Unit:</i> same as “ <i>bandlist_spectral_range_min</i> ”
<i>bandlist_spectral_comments</i>	blob	U [m]	BandLi	-- Additional information on spectral parameters: special range type, ...

### ***Band list intensity modes and units***

<i>bandlist_reference_position_electronic</i> [ <i>spectrum_reference_position</i> ]	float	U [!o_m]	BandLi	var. Reference position (wavenumber/wavelength/frequency) of the band to which the relative intensities of electronic bands are calculated <i>Condition:</i> mandatory when at least two “ <i>band_assignment_category</i> ” = ‘electronic transition’
---	-------	-------------	--------	---

*bandlist\_reference\_position\_infrared* float U BandLi  
 [!o\_m]  
 [*spectrum\_reference\_position*]

AND  
 “*band\_characteristic\_peak\_intensity\_relative*” ≠ ∅ OR  
 “*band\_characteristic\_integrated\_intensity\_relative*” ≠ ∅  
*Unit:* in unit defined by “*bandlist\_spectral\_unit*”  
 - converted in ‘cm-1’ unit in the database but provided to user in the unit specified in the export page of the web interface  
*Notes:*  
 - “*band\_characteristic\_peak\_intensity\_relative*” is set to ‘1’ at this reference position.  
 - this reference position is generally that of the peak of the strongest electronic band of the band list, or of a standard reference band.

var. Reference position (wavenumber/wavelength/frequency) of the band to which the relative intensities of infrared active bands are calculated  
*Condition:* mandatory when “*bandlist\_type*” = {absorption, Raman}  
 AND  
 when “*band\_characteristic\_peak\_intensity\_relative*” ≠ ∅ OR  
 “*band\_characteristic\_integrated\_intensity\_relative*” ≠ ∅  
*Unit:* in unit defined by “*bandlist\_spectral\_unit*”  
 • converted in ‘cm-1’ unit in the database but provided to user in the unit specified in the export page of the web interface  
*Notes:*  
 - “*band\_characteristic\_peak\_intensity\_relative*” is set to ‘1’ at this reference position.  
 - this reference position is generally that of the peak of the strongest band of the band list (preferentially the strongest fundamental vibration mode), or of a standard reference band.  
 - it is the reference for absorption bands for the ‘absorption and Raman scattering’ band list. The next KW is that for Raman.

---

***Band list constituent and specie***

A band list mostly directly refers to a fundamental phase (preferred) but in some special cases (complex constituent of interest for bandlist) it can refer to

					a constituent which need to be described.
<i>bandlist_constituent_uid</i> [*] [ <i>spectrum_band_primary_constituent_uid</i> ]	varchar(255)	Sli0+S1 b [!!_m]	BandLi BL- BConst BL- Const	F	-- Link to the existing UID of the primary “(basic) constituent” of the band list <i>Nomenclature:</i> see “ <i>bandlist_constituent_uid</i> ” <i>Notes:</i> - can be either a “ <i>basic_constituent_uid</i> ” (fundamental ‘solid’, ‘mineral’, or ‘liquid’ phase) or a “ <i>bandlist_constituent_uid</i> ” - the “band list” constituent uses the same blocs “ <i>basic_constituent</i> ” or “ <i>constituent</i> ” as sample/layer/material but it has its specific xml as there is no sample/layers/materials and several keywords are not used (abundance in material, constituent texture, ...) and some of the other have changes in mandatory and conditions and limitations in Enum lists (see “ <i>basic_constituent</i> ” and “ <i>constituent</i> ”) - the description of the constituent should reflect any range of values of composition or state (‘generic constituent’) spanned by the different, but similar, constituents used to compile that band list. These differences will be reported for each band of the band list.
<i>bandlist_constituent_primary_specie_uid</i> [*] [ <i>spectrum_band_primary_specie_uid</i> ]	varchar(255)	Sli0+S1 b [!!o_m]	BandLi Specie	F	-- Link to the existing UID of the “primary molecular specie” of the constituent of the band list <i>Condition:</i> absolute mandatory when all “ <i>bandlist_basic_constituent.mineral/solid/liquid_specie_family</i> ” = {molecule, chemical function} <i>Constraint:</i> this “ <i>bandlist_constituent_primary_specie_uid</i> ” should be one of the “ <i>bandlist_(basic_)constituent.(mineral/solid/liquid_)specie_uid</i> ” <i>Notes:</i> - This specie should be either one among the species listed in “ <i>bandlist_basic_constituent.phase_specie_uid</i> ” or “ <i>bandlist_constituent_specie_uid</i> ” - this band list contains the bands information of this specific molecular species in the above constituent. - the “ <i>bandlist_(basic_)constituent_specie_family</i> ” of this species is mostly ‘molecule’ or ‘chemical function’

- for ionic and covalent solids (salts, minerals, ...) there is no “bandlist constituent primary species” as these solids are generally made of elements making a single network (and sometimes chemical functions). So only the molecular bonds of that network will be described by directly using “*band\_transition\_chemical\_bond\_uid*”. These bonds are also described with “*bandlist\_(basic\_)constituent\_chemical\_bonds*”
- the other species of the constituent (and their state and abundance) can be found through “*bandlist\_(basic\_)constituent\_uid*”.

*bandlist\_constituent\_comments* blob U BandLi -- Additional information on the constituent (fundamental phase , ...) and on the specie (state, composition, ...)  
[m]

*Notes:*

- can describe small differences in composition and phase among the various variants of the constituent used for extracting the characteristics of the different bands of this band list
  - *Ex:* band list of CH4:beta-N2 molecular solid solution with CH4 ranging from 0.1 to 2%.
- if these differences may introduce clear changes in band characteristics it may be better to have 2 separate band lists
  - *Ex:* a bandlist for 0.1% CH3OH diluted in H2O ice, and another for 20-30% CH3OH in H2O ice
- For different phases of the constituent it is necessary to set separate band lists for each phase
  - Ex:* a band list for CH4:alpha-N2 solid and one for for CH4:beta-N2 solid.

---

***Bandlist: versions and verification***

*bandlist\_date\_created* [-xml] date S2 BandLi YYYY Date of first import or upgrade of the band list  
[*spectrum\_date\_created*] [!!\_c] -MM- DD → determined automatically by the data ingestion software.  
Initially set to the date of entry of the band list in the database (first import w. upload) and modified at each change (modification/upgrade) of the key data of a band (i.e. when at least one “*band\_import\_mode*” = ‘new version’)

<i>bandlist_date_updated</i> [-xml] <i>[spectrum_date_updated]</i>	date	S1b [!!_c]	BandLi	YYYY -MM- DD → determined automatically by the data ingestion software.	<p><i>Note:</i></p> <ul style="list-style-type: none"> <li>- each “<i>bandlist_version</i>” has its “<i>bandlist_date_created</i>” (“<i>bandlist_version.date_created</i>”)</li> <li>- in the code “<i>bandlist.date_created</i>” corresponds to “<i>bandlist_version.date_created</i>” of the first version</li> </ul> <p>Initially set to the date of entry of the band list in the database (i.e. when “<i>bandlist_import_mode</i>” = ‘first import’) and modified at each change (update) of band list metadata (i.e. when “<i>bandlist_import_mode</i>” = ‘correction’) until (not included) a new version is created, i.e, when at least one “<i>band_import_mode</i>” = ‘first import’ or ‘new version’</p>
					<p><i>Note:</i></p> <ul style="list-style-type: none"> <li>- each “<i>bandlist_version</i>” has its “<i>spectrum_date_updated</i>”</li> <li>- in the code “<i>bandlist.date_updated</i>” correspond to “<i>bandlist_version.date_updated</i>” of the last version</li> </ul>
					<p><i>Note DOI:</i></p> <ul style="list-style-type: none"> <li>- mandatory as “PublicationYear” (5) for ‘Bandlist’: it is the “<i>bandlist_date_last_updated</i>” for “<i>bandlist_version</i>” = ‘1’</li> <li>- recommended as “Date/dataType=Created” (8) for “<i>bandlist_version</i>” = ‘1’ for ‘Bandlist’</li> <li>- recommended as “Date/dataType=Updated” (8) for “<i>bandlist_version</i>” &gt; ‘1’ for ‘Bandlist’</li> </ul>
<i>bandlist_date_released</i> [-xml] <i>[spectrum_date_released]</i>	date	S1b [!!_c]	BandLi	YYYY -MM- DD → determined automatically by the interface when the first	<p>“<i>band_access_right</i>” is set to ‘public’. Initially set to the date of release of the band list and modified at each change of version of a band (i.e. when at least one “<i>band_import_mode</i>” = ‘new version’)</p>
					<p><i>Note:</i></p>

<i>bandlist_version</i> [-xml] <i>[spectrum_version]</i>	int(3)	S3 [!!c]	BandLi	<p>-- Version number of the band list data</p> <p>➔ incremented automatically by the data ingestion software when at least one “<i>band_import_mode</i>” = ‘new version’. Set to ‘1’ at first band list data ingestion and then incremented at each major change of the band list data.</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- no new version number when “<i>band_import_mode</i>” = ‘correction’</li> <li>- there could be several reasons to upgrade a s band list <ul style="list-style-type: none"> <li>✓ improvement of the data in term of band characteristics <ul style="list-style-type: none"> <li>▪ affect mostly the ‘band’ table and a few band list KW: <i>_analysis</i>, <i>_history</i>...</li> </ul> </li> <li>✓ addition of new bands <ul style="list-style-type: none"> <li>▪ affect mostly several KW of "<i>bandlist_spectral</i>" as well as KW such as <i>_title</i>, <i>_analysis</i>, <i>_history</i>...</li> </ul> </li> <li>✓ upgrade of the data to an upper product level, such as absorption coefficient, normalization of intensities, ... <ul style="list-style-type: none"> <li>▪ affect KW such as “<i>bandlist_title</i>”, <i>_type</i>, <i>_intensity_unit</i>, <i>_analysis</i>..., and can affect KW such as <i>_reference_position</i>, <i>parent_spectrum_uid</i>,...</li> </ul> </li> </ul> </li> </ul>
<i>bandlist_previous_version_status</i> <i>[spectrum_previous_version_status]</i>	enum(text)	S2 [!!o_m]	BandLi	<p>-- Validity status of the previous version of the band list</p> <p><b>Enum:</b> {obsolete version, partly invalidated version, invalidated version, partly invalidated data, invalidated data}</p> <p><i>Condition:</i> only and absolute mandatory when “<i>bandlist_import_mode</i>” = {invalidate}</p> <p>OR</p> <p>when “<i>band_import_mode</i>” = {new version, invalidate}</p> <p>AND</p> <p>when at least one “<i>band_access_right</i>” = ‘public’</p> <p><i>Constraints:</i></p> <ul style="list-style-type: none"> <li>- For “<i>band_import_mode</i>” = ‘new version’, this KW is archived with the previous version</li> <li>- For “<i>bandlist_import_mode</i>” = ‘invalidate’ OR “<i>band_import_mode</i>” = ‘invalidate’ AND “<i>bandlist_previous_version_status</i>” = {obsolete</li> </ul>



version, partly invalidated version, invalidated version} this KW is stored with the current version

- For “*bandlist\_import\_mode*” = 'invalidate' AND “*bandlist\_previous\_version\_status*” = {partly invalidated data, invalidated data} this KW is stored with the current version and all previous versions.

*Definitions:*

- ‘*obsolete version*’: This version is still scientifically valid but the new version improved at least part of the bands of the bandlist, or added new bands
- ‘*partly invalidated version*’: This version is still scientifically valid over part of the bands but errors were found that are corrected in the new version
- ‘*invalidated version*’: Errors were found over most or all the bands of this version of the bandlist that are corrected in the new version
- ‘*partly invalidated data*’: Errors were found over part of the bands of the original data, but the data cannot be corrected there. The new version of the band list has a reduced number of bands, or band characteristics. The other have been invalidated.
- ‘*invalidated data*’: An error was found over most or all the bands of the original data, but the data cannot be corrected. There is no new version of the band list. It invalidates all previous versions.

*Note SSHADE:* This status will be clearly displayed (bold) at the beginning of the page of the previous version of the bandlist (‘new version’) or on all versions for ‘invalidate’

*bandlist\_previous\_version\_comments* blob U BandLi  
 [!!o\_m]  
 [spectrum\_previous\_version\_comments]

-- Description of the reason for the change of version of the band list or for the data invalidation

*Condition:* only and absolute mandatory when “*bandlist\_import\_mode*” = {invalidate}  
 OR  
 when “*band\_import\_mode*” = {new version, invalidate}  
 AND

when at least one “*band\_access\_right*” = ‘public’

*Constraints:* same as “*bandlist\_previous\_version\_status*”

*Note SSHADE:* This comment will be clearly displayed after the status at the beginning of the page of the previous version of the bandlist

*Examples:*

- 'OBSOLETE VERSION:' ‘added FIR bands and improved MIR FWHM values in version #2’
- 'PARTLY INVALIDATED VERSION:' ‘invalidated above 3.5 μm due to error in spectral resolution. Corrected in version #2’
- 'INVALIDATED VERSION:' ‘invalidated bandlist due to a severe wavelength calibration error. Corrected in version #2’
- 'PARTLY INVALIDATED DATA:' ‘data partly invalidated due to a calibration error. Original data no more available for recalibration. No fully valid version available. ‘
- 'INVALIDATED DATA:' ‘original data of the natural molecule replaced by a bandlist for each isotope and linked to them.

---

<i>bandlist_history</i> [ <i>spectrum_history</i> ]	blob	U [cm]	BandLi
--	------	-----------	--------

- History of the bandlist import, upgrade or correction  
➔ calculated by default and added to the current text:  
”*bandlist\_date\_last\_updated*”: “*bandlist\_import\_mode*” – “*bandlist\_version*” – “*bandlist\_history*”, where “*bandlist\_history*” is the text added in the xml file.

*Note:* This KW is in “replace” = ‘no’ mode by default

*Ex:*

- '2009-12-25: first import - v1' [no text in “*bandlist\_history*”] (c)
- '2010-08-03: correction - v1: added band list publication '  
[“*bandlist\_history*” = ‘added band list publication’] (c+m)
- '2010-10-15: new version - v2: corrected errors in FWHM above 9000 cm-1'  
[“*bandlist\_history*” = ‘corrected errors in FWHM above 9000 cm-1’] (c+m)

---

### *Band list parent experiments and spectra*

---



different sources of data, ...

*Note:* details will be given for each band as the way of analysis can vary from band to band

*Note DOI:*

Recommended option as “Description / descriptionType=Method” (17)

<i>bandlist_comments</i> <i>[spectrum_comments]</i>	blob	U <i>[m]</i>	BandLi	-- General comments on the bandlist, measurements conditions or analysis
<i>bandlist_quality_flag</i> <i>[spectrum_quality_flag]</i>	enum(int)	S3 <i>[!_m]</i>	BandLi	-- Global quality flag on the band list

*Enum:* {0, 1, 2, 3, 4, 5}

*Constraint:* set to ‘0’ when “*bandlist\_import\_mode*” = ‘invalidate’.

Can have 6 quality levels from ‘0’ to ‘5’

- ‘0’: no valid data or bad data (only used to flag older invalidated versions!)
- ‘1’: low quality (only used to flag older partly invalidated versions!)
- ‘2’: medium quality
- ‘3’: good data
- ‘4’: very good data
- ‘5’: excellent data

*Notes:*

- will be evaluated over the valid spectral range taking into account its completeness and accuracy in band position, width and intensity, and transition mode attribution. Need to have some matrix of ‘completeness’ and ‘quality’ to attribute this global quality flag.
- the values ‘0’ and ‘1’ is for flagging any data that are found ‘bad’ after their import in the database and are replaced (or not) by a new version. The old ‘bad’ version is maintained in the database in order to keep track of all data which may have been used, but to clearly display a warning with “*bandlist\_previous\_version\_status*”

<i>bandlist_date_validated</i> [ <i>spectrum_date_validated</i> ]	date	S2 [!_m]	BandLi	YYYY Validation date of the version of the band list -MM- DD
<hr/>				
<i>bandlist_validators</i>	<i>List [L4]</i>			£: experimentalist(s) who processed and validated the band list
<i>bandlist_validator_experimentalist_uid</i> [*] [ <i>spectrum_validator_experimentalist_uid</i> ]	varchar(255)	S2 [!_m]	BandLi Exper L4	-- Link to the existing UID of the experimentalist(s) who processed and validated the band list
<hr/>				
<i>bandlist_documentations</i>	<i>List [L6]</i>	[O]		£: Documentations about the band list  <i>Notes:</i> - can contain compilation/analysis/review files of the band list, ... - these documentations can be downloaded or viewed inside another window of the web browser but cannot be viewed directly into SSHADE.
<i>bandlist_documentation_name</i>	varchar(255)	U [m]	BandLi L6	-- Name of the documentation about the band list  <i>Note:</i> this name will appear as the documentation title in the database  <i>Ex:</i> 'compilation of data and critical review of the 13CO2 bands in amorphous H2O ice'
<i>bandlist_documentation_filename</i>	varchar(255)	U [m]	BandLi L6	-- File name (with extension) of the documentation about the band list  <i>File formats:</i> .pdf, .png, .jpg, .gif, .tiff, .txt, ...  <i>Note:</i> this file will be imported in the database.  <i>Note xml:</i> this file should be zipped with the xml file

---

### ***Band list files***

<i>bandlist_original_data_filename</i> [ <i>spectrum_file_filename</i> ]	CS- varchar(255)	S2 [m]	BandLi	-- Name of the file (with extension) containing the original data of the band list
---	---------------------	-----------	--------	--



[[!\_c] L8

Unit: in 'cm-1'

- ➔ Calculated from the narrowest width of the selected bands
- ⇒  $\text{sampling} = \text{Mini}(\text{band\_characteristic\_width\_fwhm})/4$

*bandlist\_spectrum\_synthetic\_bands* List [L7]  
[-xml]

f: Schematic list of bands describing the band list

Note: allow to prepare the data for easy display 'as for spectra'

Definition: Each selected band is described by a triangle of peak position = "band\_characteristic\_position\_peak", center position = "band\_characteristic\_position\_center", FWHM = "band\_width" and intensity = "band\_peak\_intensity".

Condition: only for bands with "band\_characteristic\_bandlist\_nominal\_flag" = 'yes'

Note:

- this file is built only with the bands that are selected to be part of it.
- It will be used to plot the band list preview

*bandlist\_spectrum\_synthetic\_bands\_position* float P BandLi  
[-xml] [[!\_c] L7

cm<sup>-1</sup> Position of the spectral point

Unit: in 'cm-1'

Series of positions covering the whole spectral range of the band list.

➔ The synthetic spectrum is built with:

- "position\_step" =  $\text{mini}[\text{"band\_characteristic\_width\_fwhm"}]/4$
- "position(0)" = "bandlist\_spectral\_range\_min"
- "position(x)" point 'x' of the position file after x steps (with an associated intensity(x) : "bandlist\_list\_band\_intensity")
- "position(n)" = "bandlist\_spectral\_range\_max"

Notes:

*bandlist\_spectrum\_triangle\_intensity* float P BandLi  
[-xml] [[!\_c] L7

no/cm<sup>-1</sup> Value of intensity of the triangle band

Units:

- unit depends on the type of product and is stored in the database and

provided to user:

- in 'cm<sup>-1</sup>' for "bandlist\_type" = 'absorption'  
("band\_characteristic\_peak\_intensity\_abscoef")
- in ?? unit for "bandlist\_type" = 'emission'
- without unit for all other values of "bandlist\_type"  
("band\_characteristic\_peak\_intensity\_relative")

➔ The "intensity" for each selected band is given by:

1) When there is a value for both "position\_center" and "position\_peak"

- when position(x) < position\_center - width\_fwhm
- intensity(x)=0
- when position\_center - width\_fwhm < position(x) =< position\_peak  
⇒ intensity(x) = peak\_intensity \* (position(x) - position\_center + width\_fwhm)/(position\_peak - position\_center + width\_fwhm)
- when position\_peak < position(x) < position\_center + width\_fwhm  
⇒ intensity(x) = peak\_intensity \* (position(x) - position\_center - width\_fwhm)/(position\_peak - position\_center - width\_fwhm)
- when position(x) > position\_center + width\_fwhm  
⇒ intensity(x)=0

2) When there is only a value for "position\_center"

- ⇒ position\_peak = position\_center + [(width\_asymmetry\_factor - 1) / (width\_asymmetry\_factor + 1)]\*width\_fwhm/2
- Note: when " width\_asymmetry\_factor" = 1 or Ø  
⇒ position\_peak = position\_center

3) When there is only a value for "position\_peak"

- ⇒ position\_center = position\_peak - [(width\_asymmetry\_factor - 1) / (width\_asymmetry\_factor + 1)]\*width\_fwhm/2
- Note: when " width\_asymmetry\_factor" = 1 or Ø  
⇒ position\_center = position\_peak

bandlist\_spectrum\_triangle\_band\_  
intensity\_error [-xml]

float

P  
[c]

BandLi  
L7

no/cm Error (+/-) on the value of intensity  
-1

Units: in cm<sup>-1</sup> when metric absorption coefficient,  
in ?? for emission spectra . Otherwise no unit

- stored in the database in 'cm<sup>-1</sup>' (metric absorption coefficient), ?? unit



for emission spectra (TBDef) or without unit

- The “intensity\_error” for each selected band is given by:
- $$\text{intensity\_error}(x) = \text{“peak\_intensity\_abscoef\_error”} * \text{intensity}(x) / \text{peak\_intensity}$$
- or “peak\_intensity\_relative\_error” \* intensity(x) / peak\_intensity

---

*bandlist\_spectrum\_triangle\_band List [L7b]*  
*\_intensity\_isotopes [-xml]*

£: Synthetic spectrum of triangle bands for each isotope

*Condition:* only for bands with “band\_characteristic\_bandlist\_nominal\_flag” = ‘yes’

*Note:*

- this file is built only with the bands that are selected to be part of it.
- It will be used to plot the band list preview

---

*bandlist\_spectrum\_triangle\_band\_ intensity\_isotope [-xml]* float P BandLi [!!\_c] L7b

*no/cm*<sup>-1</sup> Spectrum of the sum of the intensities of all the triangle bands of a given isotope

*Units:* same as “bandlist\_list\_band\_intensity”

*Condition:* only for bands with “band\_characteristic\_bandlist\_nominal\_flag” = ‘yes’

- ⇒ summed over all the bands with the same “band\_assignment\_transition\_primary\_specie\_uid”

---

*bandlist\_spectrum\_triangle\_band\_ intensity\_total [-xml]* float P BandLi [!!\_c]

*no/cm*<sup>-1</sup> Full spectrum of the sum of the intensities of all the triangle bands

*Units:* same as “bandlist\_list\_band\_intensity”

*Condition:* only for bands with “band\_characteristic\_bandlist\_nominal\_flag” = ‘yes’

- ⇒ summed over all the bands

---

*bandlist\_spectrum\_gaussian\_bands List [L8]*  
*ds [-xml]*

£: Synthetic gaussian spectrum describing the band list

*Definition:* Each selected band is described by a Gaussian of position =

*bandlist\_spectrum\_gaussian\_band* float P BandLi  
*\_intensity [-xml]* [!!\_c] L8

*no/cm* Value of intensity of the gaussian band  
<sup>-1</sup>

Units:

- unit depends on the type of product and is stored in the database and provided to user:
  - in 'cm<sup>-1</sup>' for "*bandlist\_type*"='absorption' (*band\_characteristic\_peak\_intensity\_abscoef*)
  - in ?? unit for "*bandlist\_type*"='emission'
  - without unit for all other values of "*bandlist\_type*" (*band\_characteristic\_peak\_intensity\_relative*)

→ The "intensity" for each selected band is given by:

- when  $\text{position}(x) < \text{position\_center/peak} - 6 * \text{width\_fwhm}$  (note: coupé pour limiter le calcul)
  - ⇒  $\text{intensity}(x)=0$
- when  $\text{position\_center} - 6 * \text{width\_fwhm} < \text{position}(x) < \text{position\_center} + 6 * \text{width\_fwhm}$ 
  - ⇒  $\text{intensity}(x) = \text{peak\_intensity} * (1 / \text{width\_fwhm}) * \exp[-2.772 * ((\text{position}(x) - \text{position\_center}) / \text{width\_fwhm})^2]$
- when  $\text{position}(x) > \text{position\_center/peak} + 6 * \text{width\_fwhm}$ 
  - ⇒  $\text{intensity}(x)=0$

*bandlist\_spectrum\_gaussian\_ban* List [L7b]  
*d\_intensity\_isotopes [-xml]*

£: Synthetic spectrum of gaussian bands for each isotope

Condition: only for bands with "*band\_characteristic\_bandlist\_nominal\_flag*" =

---

*bandlist\_spectrum\_gaussian\_band\_intensity\_isotope* [-xml] float P BandLi L7b [!!\_c]

‘yes’  
*Note:*  
 - this file is built only with the bands that are selected to be part of it.  
 - It will be used to plot the band list preview

*no/cm*<sup>-1</sup> Spectrum of the sum of the intensities of all the gaussian bands of a given isotope  
*Units:* same as “*bandlist\_list\_band\_intensity*”  
*Condition:* only for bands with “*band\_characteristic\_bandlist\_nominal\_flag*” = ‘yes’  
 ⇒ summed over all the bands with the same “*band\_assignment\_transition\_primary\_specie\_uid*”

---

*bandlist\_spectrum\_gaussian\_band\_intensity\_total* [-xml] float P BandLi [!!\_c]

*no/cm*<sup>-1</sup> Full spectrum of the sum of the intensities of all the gaussian bands  
*Units:* same as “*bandlist\_list\_band\_intensity*”  
*Condition:* only for bands with “*band\_characteristic\_bandlist\_nominal\_flag*” = ‘yes’  
 ⇒ summed over all the bands

---

***Bands of band list***

*bandlist\_bands\_number* [-xml] int(10) S3 BandLi [!\_c]

*no* Number of bands of the band list  
 ➔ calculated from the list of “*band\_uid*”

*bandlist\_bands\_assignment\_number* [-xml] int(10) S3 BandLi [!\_c]

*no* Total number of different assignments of the bands of the band list  
 ➔ calculated from the sum of the maxi of “*band\_assignment\_number*” of each band

*bandlist\_bands\_characteristic\_number* [-xml] int(10) S3 BandLi

*no* Total number of different sets of characteristics of the bands of the band list  
 ➔ calculated from the sum of the maxi of “*band\_characteristics\_number*” of

[!\_c]

each band

**Band list preview**

[O]

£: parameters of the automatically generated preview plot of the selected bands of the band list (“*bandlist\_xxx\_band*”)

*Notes:*

- these parameters are optional and are used to optimize the generation of the plot
- if not specified the generation tool will do its best to optimize the plot:
  - o use “*bandlist\_spectral\_range\_min/max*” for X limits
  - o detect Ymin/max from the data and add some margin.
- However for plots that require Y log scales (ex: large spectral range over NIR-MIR) the automatic optimization is impossible due to presence of ‘0’!

*bandlist\_preview\_x\_axis*

enum(text)

P  
[m]

BandLi

-- Type of X axis in the preview plot of the selected range of the band list

**Enum:** {lin, log}

*Definitions:*

- ‘lin’: linear axis
- ‘log’: logarithmic axis

*Note xml:* the following 4 KW (“*bandlist\_preview\_x\_axis/\_unit/\_min/\_max*”) are grouped as tags of “*bandlist\_preview\_x*”: <x axis="" unit="" min="" max="" />

*bandlist\_preview\_x\_unit*

enum(text)

P  
[m]

BandLi

-- Unit of the X axis, if different from the original import unit, in which the preview is plotted

**Enum:** {m-1, cm-1, angstrom, nm, micron, mm, m, km, Hz, kHz, MHz, GHz, eV, keV}

*Note xml:* see “*bandlist\_preview\_x\_axis*”

*bandlist\_preview\_x\_min*

float

P  
[m]

BandLi

*var* Minimum value of X axis in the preview plot of the band list

- Unit: given by default by “*bandlist\_spectral\_unit*” or by

				<p>“<i>bandlist_preview_x_unit</i>” when provided</p> <p><i>Note:</i> plotted by default in the original import unit unit if no “<i>bandlist_preview_x_unit</i>”</p> <p><i>Note xml:</i> see “<i>bandlist_preview_x_axis</i>”</p>
<i>bandlist_preview_x_max</i>	float	P <a href="#">[m]</a>	BandLi	<p>var Maximum value of X axis in the preview plot of the band list</p> <ul style="list-style-type: none"> <li>• Unit: given by default by “<i>bandlist_spectral_unit</i>” or by “<i>bandlist_preview_x_unit</i>” when provided</li> </ul> <p><i>Note:</i> plotted by default in the original import unit unit if no “<i>bandlist_preview_x_unit</i>”</p> <p><i>Note xml:</i> see “<i>bandlist_preview_x_axis</i>”</p>
<i>bandlist_preview_y_axis</i>	enum(text)	P <a href="#">[m]</a>	BandLi	<p>-- Type of Y axis in which the absorption coefficient preview of the bandlist is plotted</p> <p><b>Enum:</b> {lin, log}</p> <p><i>Definitions:</i> see “<i>bandlist_preview_x_axis</i>”</p> <p><i>Note xml:</i> the following 4 KW (“<i>bandlist_preview_y_axis/_unit/_min/_max</i>”) are grouped as tags of “<i>bandlist_preview_y</i>”: &lt;y axis="" unit="" min="" max="" /&gt;</p>
<i>bandlist_preview_y_unit</i>	enum(text)	P <a href="#">[m]</a>	BandLi	<p>-- Unit of the Y axis in which the absorption coefficient preview of the bandlist is plotted</p> <p><b>OpenEnum:</b> {cm-1}</p> <p><i>Default:</i> ‘cm-1’</p> <p><i>Note:</i> currently limited to ‘cm-1’ for “<i>band_characteristic_peak_intensity_specific_abscoef</i>” and ‘no unit’ for “<i>band_characteristic_peak_intensity_relative</i>”</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- The unit of the intensity of the spectrum depends on the band list type and thus only a few pairs of conversions are allowed (or need</li> </ul>

- additional information on mass or molar solid density)
- all spectra without intensity unit: {no unit, percent, permille}  
[1 percent = 10 permille = 0.01]
  - metric absorption coefficient: {cm-1, m-1}  
[1 cm-1 = 100 m-1]
  - mass absorption coefficient: {cm2.g-1, m2.kg-1}  
[1 m2.kg-1 = 10 cm2.g-1]
  - molar absorption coefficient: {cm2.mol-1, m2.mol-1}  
[1 m2.mol-1 = 10000 cm2.mol-1]

*Note xml:* see “bandlist\_preview\_y\_axis”

<i>bandlist_preview_y_min</i>	float	P <a href="#">[m]</a>	BandLi	var Minimum value of Y axis of the absorption coefficient preview plot of the band list <ul style="list-style-type: none"> <li>• Unit: given in ‘cm-1’</li> </ul> <i>Note:</i> plotted by default in the original import unit (cm-1) if no “bandlist_preview_y_unit“ <i>Note xml:</i> see “bandlist_preview_y_axis”
<i>bandlist_preview_y_max</i>	float	P <a href="#">[m]</a>	BandLi	var Maximum value of Y axis of the absorption coefficient preview plot of the band list <ul style="list-style-type: none"> <li>• Unit: given in ‘cm-1’</li> </ul> <i>Note:</i> plotted by default in the original import unit (cm-1) if no “bandlist_preview_y_unit“ <i>Note xml:</i> see “bandlist_preview_y_axis”
<i>bandlist_preview_yrel_axis</i>	enum(text)	P <a href="#">[m]</a>	BandLi	-- Type of Y axis in which the relative intensity preview of the bandlist is plotted <b>Enum:</b> {lin, log} <i>Definitions:</i> see “bandlist_preview_x_axis” <i>Note xml:</i> the following 3 KW (“bandlist_preview_y_axis/_min/_max”) are grouped as tags of “bandlist_preview_yrel”: <yrel axis="" min="" max="" />

<i>bandlist_preview_yrel_min</i>	float	P <a href="#">[m]</a>	BandLi	- Minimum value of Y axis of the relative intensity preview plot of the band list <i>Note xml: see “bandlist_preview_yrel_axis”</i>
<i>bandlist_preview_yrel_max</i>	float	P <a href="#">[m]</a>	BandLi	- Maximum value of Y axis of the relative intensity preview plot of the band list <i>Note xml: see “bandlist_preview_yrel_axis”</i>
<i>bandlist_preview_type</i>	enum(text)	P <a href="#">[m]</a>	BandLi	-- Flag telling which plot is used as the preview, in place of the default one <b>Enum:</b> {absorption coefficient, relative intensity} <i>Definitions:</i> <ul style="list-style-type: none"> <li>- ‘<i>absorption coefficient</i>’: force the use the ‘absorption coefficient’ plot as the preview</li> <li>- ‘<i>relative intensity</i>’: force the use the ‘relative intensity’ plot as the preview</li> </ul> <i>Note:</i> the current logic for the choice os the preview is: ‘take the absorption coefficient plot as the preview if there is at lesat one data in “band_characteristic_peak_intensity_abscoef”.
<i>bandlist_preview_filename</i>	CS- varchar(255)	S2 <a href="#">[mc]</a>	BandLi	-- Name of the file containing the preview plot of the band list to be displayed ➔ plot generated automatically during import if there is no file <i>Image formats:</i> .png, .jpg, (.gif) <i>Note:</i> <ul style="list-style-type: none"> <li>- this plot will replace the automatically generated plot</li> <li>- it should include the full “bandlist_title” on top of the figure</li> <li>- image size should be preferably around HxV = 650x460 pixels (note: will be resized automatically)</li> <li>- it will be displayed in the result page for quick look at the band list results</li> </ul> <i>Note DB:</i> this file should be zipped with the “bandlist” import xml file for import.

### 3.3 Bandlist structure Table

Root of the table: *structure*

Data type: 'Bandlist'

Notes:

- This structure is used to organize the bandlist in sections and subsections, in particular when we want to separate 'absorption' bands and 'Raman' bands, and also to separate the different isotopes of a molecule.
- The bandlist, the sections and the subsections will be displayed in SSHADE in the order and with the structure defined here together with their title and the information on their type of variable parameters (band type, isotope, band transition category). The section and subsection titles are subtitles of the general title of the bandlist ("*bandlist\_title*").

Key-word	Type	Level	Table	Exp	Unit	Description
<i>Structure: sections</i>		<a href="#">[\$o_O]</a>				<p><i>Definition:</i> the "sections" is the main subdivision along one of the varying parameters.</p> <p><i>Condition:</i> strongly recommended when there are several isotopic species. Can be also used to separate electronic transitions, combination vibrations, fundamental vibrations and phonon modes.</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- when there is one varying parameters, the subdivision is done in "<i>structure_section_bands</i>" and the bands are listed in "<i>section_bands</i>"</li> <li>- when there are two varying parameters, the subdivision along the second parameter is done in "<i>structure_section_subsections</i>" and the bands are listed in "<i>subsection_bands</i>"</li> </ul>
<i>structure_sections_variable_parameter</i>	openum(text)	U <a href="#">[!_m]</a>	StructBL	--		Type of bandlist, band or constituent parameter varying between the sections of the band list.



**OpenEnum:** {no, isotope, band transition category, other}

*Definitions:*

- 'no':
- 'band type':
- 'isotope':
- 'band transition category':
- 'other':

*Note xml:* this KW is a tag at each block "structure\_sections"

*Exemples:*

- band list with 'absorption' and 'Raman scattering' bands
- constituent with several isotopes: <sup>32</sup>S<sup>16</sup>O<sub>2</sub>, <sup>33</sup>S<sup>16</sup>O<sub>2</sub>, <sup>34</sup>S<sup>16</sup>O<sub>2</sub>, <sup>32</sup>S<sup>16</sup>O<sup>18</sup>O
- band list with 'electronic transitions', 'vibration modes' and 'phonon modes'.

---

<i>structure_sections</i>	<b>List [L1]</b>	<b>[!o]</b>	
<i>structure_section_order</i> [-xml]	int(4)	P <b>[!_c]</b>	StructBL L1
<i>structure_section_title</i>	varchar(255)	U <b>[!_m]</b>	StructBL L1

£: Main sections of the band list

- Order of the sections
- determined automatically during import from the order of the "structure\_section" blocs

*Note:*

- it should be used to sort the band type, isotope, band transition category values in logical order

- Title describing the band type, isotope, or band transition category of this section of the band list

*Note:*

*Ex:*

- 'absorption bands', 'Raman bands'
- <sup>32</sup>S<sup>16</sup>O<sub>2</sub>, <sup>33</sup>S<sup>16</sup>O<sub>2</sub>, <sup>34</sup>S<sup>16</sup>O<sub>2</sub>, <sup>32</sup>S<sup>16</sup>O<sup>18</sup>O
- 'electronic transitions', 'vibration modes', 'phonon modes'

<i>structure_section_description</i>	blob	U <a href="#">[m]</a>	StructBL L1	-- Detailed description of the band type, isotope, or band transition category of this section of the band list  <i>Notes:</i>  <i>Ex:</i> <ul style="list-style-type: none"> <li>- ‘UV, Visible and infrared absorption bands of SO2 in amorphous H2O ice’</li> </ul>
--------------------------------------	------	--------------------------	----------------	--

<b><i>Structure: subsections</i></b>		<a href="#">[!O]</a>		-- <i>Definition:</i> The “subsections” are the secondary subdivision along the second varying parameter, when there are two varying parameters.  <i>Notes:</i> <ul style="list-style-type: none"> <li>– a subsection can contain either isotopes, or band transition categories</li> <li>– when there are two varying parameters, the subdivision along the second parameter is done in “<i>structure_section_subsections</i>” and the bands are listed in “subsection_bands”</li> </ul>
--------------------------------------	--	----------------------	--	---

<i>structure_section_subsections_variable_parameter</i>	openum(text)	U <a href="#">[!_m]</a>	StructBL L1	-- Type of bandlist, band or constituent parameter between the subsections of this section of the band list.  <b>OpenEnum:</b> {no, isotope, band transition category, other}  <i>Definitions:</i> see “ <i>structure_sections_variable_parameter</i> ”  <i>Note xml:</i> this KW is a tag at each block “ <i>structure_subsections</i> ”   <i>Ex:</i> see “ <i>structure_sections_variable_parameter</i> ”
---	--------------	----------------------------	----------------	--

<i>structure_section_subsections</i>	<b><i>List [L2]</i></b>	<a href="#">[!o]</a>		£: Subsections of the band list
<i>structure_section_subsection_order</i> [-xml]	int(4)	P <a href="#">[!_c]</a>	StructBL L1 L2	-- Order of the subsections <ul style="list-style-type: none"> <li>- determined automatically during import from the order of the “<i>structure_subsection</i>” blocs</li> </ul> <i>Note:</i> it should be used to sort the band type, isotope, band transition category

				values in logical order
<i>structure_section_subsection_title</i>	varchar(255)	U [!_m]	StructBL L1 L2	-- Title describing the band type, isotope, or band transition category of this subsection of the band list  <i>Note:</i> <i>Ex:</i> see “ <i>structure_section_title</i> ”
<i>structure_section_subsection_desc</i>	blob ription	U [m]	StructBL L1 L2	-- Detailed description of the band type, isotope, or band transition category of this subsection of the band list  <i>Note:</i> <i>Ex:</i> see “ <i>structure_section_description</i> ”
<hr/>				
<b><i>Structure: bands</i></b>		[!o]		<i>Note:</i> this bloc is either in the subsection or in the section bloc depending if there are, or not, subsections.  <i>Condition:</i> “ <i>structure_section_bands</i> ” mandatory when “ <i>structure_section_subsections</i> ” = ∅  <i>Condition:</i> “ <i>structure_section_subsection_bands</i> ” mandatory when “ <i>structure_section_subsections</i> ” ≠ ∅
<hr/>				
<i>structure_section_(subsection)_bands</i>	<b>List [L3]</b>			£: List of the bands
<i>structure_section_(subsection)_band_order</i>	int(4) [-xml]	P [!_c]	StructBL L1 (L2) L3	-- Order of the band in this list  - determined automatically during import from the order of the “ <i>structure_section_(subsection)_spectrum_uid</i> ”  <i>Note:</i>
<i>structure_section_(subsection)_band_uid</i>	varchar(255) [*]	U [!!_m]	StructBL Band L1	-- Link to the existing UID of the band belonging to this band list (sub)section  <i>Notes:</i> - They should be in the order you want they appear in SSHADE

(L2)  
L3

- this order should follow the increasing value of “*band\_characteristic\_position\_peak*”
  - on les range dans l’ordre croissant en cm-1 (phonons, vibrations, electronic)= FIR-MIR-NIR-Vis-UV)
  - The bands are described in the “*band*” table...
-

### 3.4 Band Table

Root of the table: *band*

Data type: in ‘Bandlist’

For “spectrum\_type” = ‘bandlist’

Key-word	Type	Level	Table	Exp	Unit	Description
<i>Band import and indexes</i>						
<i>band_import_mode</i>	enum(text)	P [!!_m]	Band	--		<p>Mode of import of the “band”</p> <p><b>Enum:</b> {first import, inherited, ignore, draft, no change, correction, new version, invalidate}</p> <p><i>Constraint:</i></p> <ul style="list-style-type: none"> <li>- ‘invalidate’ only when “<i>band_access_right</i>” is already ‘public’</li> </ul> <p><i>Definitions:</i> see “<i>bandlist_import_mode</i>” + <i>note</i>:</p> <ul style="list-style-type: none"> <li>- ‘<i>inherited</i>’: takes the “import_mode” value of the table above in the structure =&gt; “<i>band_import_mode</i>” takes the value of “<i>bandlist_import_mode</i>”.</li> <li>- ‘<i>new version</i>’: used when some values of the key band characteristics are changed.</li> </ul> <p>List of the key band characteristics:</p> <ul style="list-style-type: none"> <li>• <i>band_assignment_label</i></li> <li>• <i>band_assignment_transition_electronic_mode_label</i></li> <li>• <i>band_assignment_transition_vibration_mode_label</i></li> <li>• <i>band_assignment_transition_rotation_mode_label</i></li> <li>• <i>band_assignment_transition_phonon_mode_label</i></li> <li>• <i>band_characteristic_position_peak</i></li> <li>• <i>band_characteristic_position_center</i></li> <li>• <i>band_characteristic_width_fwhm</i></li> <li>• <i>band_characteristic_peak_intensity_abscoef</i></li> </ul>

- *band\_characteristic\_peak\_intensity\_relative*
- *band\_characteristic\_integrated\_intensity\_abscoef*
- *band\_characteristic\_integrated\_intensity\_relative*

- *'invalidate'*: used when a band is found to be fully invalid but there is no way to correct it and import a new version.

<i>band_index</i> [**] [-xml]	int(10)	B [!!_g]	Band	F	--	Automatic random but unique number (internal) given to a new band of a bandlist
<i>band_uid</i> [**]	varchar(255)	S0 [!!_m]	Band	F	--	Unique identifier code (UID) given to the band table (to be created)

*Nomenclature:*

Create this code name with 'BAND\_' very accurately in order to be simple and unique.

It should be of the style

'BAND\_Type\_(Molecule)\_Constituent\_Wavenumber(\_a)', where:

- 'Type' is the band list type:
  - 'ABS': for 'absorption'
  - 'RAMAN' for 'Raman scattering'
  - 'REFL': for 'reflectance'
  - 'THERM': for 'thermal emission'
  - 'FLUO': for 'fluorescence emission'
- 'Molecule' is the general formula of the molecule (not isotopic), only for molecular solids, or for anionic radicals
- 'Constituent' is a short description of the constituent ('CH4-ice', 'N2-matrix', 'hematite', 'forsterite-fayalite\_Fo10-30',...), with possibly some range of composition
- 'Wavenumber' the approximate wavenumber (in cm-1, or eventually wavelength in nm: then add 'nm') of the band.
- 'a' is an optional extension ('a', 'b', 'c', ...) in case of multiple bands of same primary species/bandlist at same wavelength (extracted bands)

*Ex:* for Molecular solids:

- 'BAND\_ABS\_CO\_ice\_2092'
- 'BAND\_RAMAN\_CO\_liquid\_2088'

- 'BAND\_REFL\_CO2\_matrixH2Oam\_0-5pc\_2345\_a'

*Ex:* for covalent and ionic solids:

- 'BAND\_ABS\_hematite\_2092'
- 'BAND\_RAMAN\_forsterite-fayalite\_Fo10-30\_2088'
- 'BAND\_REFL\_goethite\_2345'

<i>band_bandlist_uid</i> [*§] [-xml]	varchar(255) [Virtual Link]	B [!!_v]	Band BandLi	F	--	Link to the existing UID of the bandlist to which this band belong  <i>Note xml:</i> in practice all the bands of a band list are described in the same xml file as its band list, so no explicit reference is needed.
--------------------------------------	--------------------------------	-------------	----------------	---	----	--

### Band verification and access right

<i>band_import_verification</i> [pi] [ <i>from provider interface</i> ] [-xml] [ <i>spectrum_import_verification</i> ]	boolean [Vitual KW]	S3 [!!d_m]	Band	F	--	Verification state of an imported band  <b>BoolEnum:</b> {yes, no} or {true, false}  <i>Default:</i> 'false'/'no'  <i>Constraints:</i> <ul style="list-style-type: none"> <li>- 'false'/'no' is the only and default value when "band_import_mode" = {first import}</li> </ul> <i>Definitions:</i> <ul style="list-style-type: none"> <li>- 'false' or 'no': imported band data and metadata not yet verified in the database</li> <li>- 'true' or 'yes': band data and metadata verified in database</li> </ul> <i>Notes:</i> <ul style="list-style-type: none"> <li>- it is not a 'scientific' validation, but rather the verification of the correctness of the imported data.</li> <li>- The 'non-verified' state allows importing data in the database and taking time to fully check them online.</li> </ul> <i>Note SSHADE:</i> implemented directly in the 'provider interface' with computer controlled data access rights, not through xml.
--	------------------------	---------------	------	---	----	---

<p><i>band_access_right</i> [pi]  [<i>from provider interface</i>] [-xml]  [<i>spectrum_access_right</i>]</p>	<p>enum(text)  [Virtual KW]    [!!d_m]</p>	<p>S3    Band    F    --</p>	<p>Rights of access to the band  <b>Enum:</b> {unreleased, restricted, public}  <i>Default:</i> ‘unreleased’  <i>Constraints:</i> <ul style="list-style-type: none"> <li>- ‘unreleased’ is the only and default value when “<i>band_import_mode</i>” = {first import}</li> <li>- ‘unreleased’ and ‘restricted’ cannot be used if “<i>band_access_right</i>” has been already set to ‘public’</li> <li>- ‘public’ only when “<i>band_import_verification</i>” = ‘yes/true’</li> </ul> <i>Definitions:</i> <ul style="list-style-type: none"> <li>- ‘<i>unreleased</i>’: access only to all the ‘SSHADE managers’ and to the DB provider that imported the data.</li> <li>- ‘<i>restricted</i>’: access only to all the partner DB managers and partner DB providers</li> <li>- ‘<i>public</i>’: access to all users</li> </ul> <i>Notes:</i> <ul style="list-style-type: none"> <li>- allow to limit the access to the data first only to the SSHADE managers (and the ‘provider’ that imported the data), or to all the partner database providers, or to everybody.</li> <li>- this allows to prepare data in the database and put them online ‘public’ (or any other group restriction) only when wanted (publication of the paper ...)</li> </ul> <p><i>Note SSHADE:</i> implemented directly in the ‘provider interface’ with computer controlled data access rights, not through xml.</p> </p>
---	--	------------------------------	---

***Band: type***

<p><i>band_type</i> [-xml]</p>	<p>enum(text)  [!!c]</p>	<p>S0    Band    F    --</p>	<p>Type of band  <b>Enum:</b> {absorption, Raman scattering, reflectance, thermal emission, fluorescence emission}  <i>Defaults:</i> <ul style="list-style-type: none"> <li>- “<i>band_type</i>” = ‘absorption’ when “<i>bandlist_type</i>” = ‘absorption’</li> </ul> </p>
--------------------------------	------------------------------	------------------------------	--



- “*band\_type*” = ‘Raman scattering’ when “*bandlist\_type*” = ‘Raman scattering’
- “*band\_type*” = ‘reflectance’ when “*bandlist\_type*” = ‘reflectance’
- “*band\_type*” = ‘thermal emission’ when “*bandlist\_type*” = ‘thermal emission’
- “*band\_type*” = ‘fluorescence emission’ when “*bandlist\_type*” = ‘fluorescence emission’

Notes:

*band\_title* [-xml]  
[*spectrum\_title*]

varchar(255)

U

Band

[!!\_c]

-- Short title describing the band

➔ Calculated:

“*band\_characteristic\_position\_peak*“ (or “*\_position\_centre*“ if no value)  
 “*bandlist\_spectral\_unit*” :  
 “*band\_assignment\_label*” ‘of ‘  
 “*band\_assignment\_transition\_primary\_specie.atom\_formula*” /  
 ”.*molecule\_formula*” / ”.*chemical\_function\_formula*” ‘in’  
 “*bandlist\_constituent.basic\_constituent\_name*”

using the “*characteristic\_position*” with

“*band\_characteristic\_bandlist\_nominal\_flag*” = ‘yes’

- When there are several

“*band\_assignment\_transition\_primary\_specie.atom\_formula*” /  
 ”.*molecule\_formula*” / ”.*chemical\_function\_formula*”, put them one after the  
 other with a ‘&’ sign in between.

- When there are several “*band\_assignment*”, ”, put them one after the other  
 with a ‘ and ‘ in between.

Format: LaTeX

Notes:

Ex:

- ‘2236.2 cm<sup>-1</sup>:  $\nu_1 + 3\nu_3$  of <sup>32</sup>S<sup>16</sup>O<sub>2</sub> in solid SO<sub>2</sub>’
- ‘25620 cm<sup>-1</sup>:  $\Pi \rightarrow \Sigma$  of Fe<sup>3+</sup> & O<sup>2-</sup> in Hematite’, 300K’ (case of multiple “*band\_assignment\_transition\_primary\_specie*”)
- ‘2236.2 cm<sup>-1</sup>:  $3\nu_1$  of <sup>32</sup>S<sup>16</sup>O<sub>2</sub> and  $\nu_1 + 3\nu_3$  of <sup>33</sup>S<sup>18</sup>O<sub>2</sub> in solid SO<sub>2</sub> (case

- of multiple "band\_assignments")
- '320 cm<sup>-1</sup>: ν<sub>L</sub> in solid SO<sub>2</sub>' (case of phonon modes without "band\_assignment\_transition\_primary\_specie", only the constituent is listed)

### Band version

- will reflect the changes of the version if they affect at least one element of the title

<i>band_comments</i>	blob	U <a href="#">[m]</a>	Band	-- General comments on the band  <i>Note:</i> for exemple, detailed type of spectrum from which the characteristics of this band are derived, important sample and instrument parameters (spectral resolution, ...), ...  <i>Ex:</i> <ul style="list-style-type: none"> <li>- 'QMol quantum mechanical model used to simulate absorption and Raman spectra'</li> <li>- 'bidirectional reflectance spectrum with i=0°, e=30°'</li> </ul>
----------------------	------	--------------------------	------	---

### *Band transition assignments*

<i>band_assignments</i>	<i>List [L1]</i>	<a href="#">[!!_m]</a>	£: List of the assignments of the transitions contributing to this band  <i>Condition:</i> absolute mandatory at least one  <i>Notes:</i> <ul style="list-style-type: none"> <li>- The multiplicity allows to describe several transitions which may occur at identical or nearly identical wavelength such they cannot be easily separated and both transitions contribute to the observed 'band characteristics'.</li> <li>- The type of multiplicity is described with "band_assignment_multiplicity_type" and "band_assignment_multiplicity_degeneracy".</li> <li>- The relative contributions of the different transitions to the band (typically to its integrated intensity ~ intensity x width) is described with "band_assignment_contribution_level"</li> </ul>
-------------------------	------------------	------------------------	---

- These multiple contributions to the band can be produced either from the same primary isotope specie (accidentally degenerate band), or from different isotopes of the same (natural) primary specie (superposition of 2 bands of the same band list).
- When the accidentally degenerate or isotopically degenerate bands of the same primary specie have been separated (deconvolution, ...) two separate bands will be described in the band list with their own band characteristics. But it is worth to link them using “*band\_assignment\_multiplicity\_other\_band\_uid*”
- When another primary specie of the same constituent also contributes to the band, the band will be also described in its own band list and both bands will be linked bidirectionnally by using “*band\_assignment\_multiplicity\_other\_band\_uid*” of each band.

<i>band_assignment_number</i>	int(10)	P	Band	
		[!!_mc]		
<i>band_assignment_label</i>	varchar(255)	U	Band [Ver]	--
		[!!_m]	L1	

*no* Order number of the assignment of the band  
 ➔ set to ‘1’ “*band\_assignment\_number*” = Ø

-- Symbolic label of the band transition  
*Syntax:* LaTeX format

*Format:*

- For vibrations:  $\$a\nu_1 + b\nu_2^{dl_2} + \dots + c\nu_n^{ml_n} + eJ + fK + gKa + hKc + iL + jTx + kTy + lRx + pRy\$$  [...]
- for  $av_1 + bv_2^{dl_2} + \dots + cv_n^{ml_n} + eJ + fK + gKa + hKc + iL + jTx + kTy + lRx + pRy$  where a, b, c, d, e, f, ..., p are integers

*Ex:* ‘ $\$2\nu_1 + 3\nu_2 - T_x\$$ ’ for  $2\nu_1 + 3\nu_2 - T_x$   
 ‘ $\$R_{xy} (E_g)\$$ ’ for  $R_{xy} (E_g)$

*Notes:*

- should also include the symmetry (character) of the vibration for phonon and libration modes. Not mandatory for vibration and electronic modes.
- put ‘?’ (or ‘?+?’ for combinations) if transition is fully unknown.
- If only part is unknown, add something like ‘+?’ or ‘+?J’, ...

- Hot bands (lower state with at least one quantum number > 0) are expressed within ( ) with the ‘-‘ sign for their lower state  
*Ex:* ‘(2ν<sub>1</sub>-ν<sub>1</sub>) + 3ν<sub>2</sub> - T<sub>x</sub>’ for ν<sub>1</sub>: 1→2 ; ν<sub>2</sub>: 0→3 and T<sub>x</sub>:1→0

<i>band_assignment_symmetry_label</i>	openum(text)	SU [!_m]	Band L1	-- --	<p>Symmetry (character) of the vibration producing the band in the molecular solid structure</p> <p><i>Condition:</i> mandatory when “<i>band_assignment_category</i>” = {fundamental vibration, rotation, phonon mode}</p> <p><b>OpenEnum:</b> {A, Ag, Au, Ap, As, A1, A1g, A1u, A1p, A2, A1s, A2g, A2u, A2p, A2s, B, Bg, Bu, B1, B1g, B1u, B2, B2g, B2u, B3, B3g, B3u, E, Eg, Eu, Ep, Es, E1, E1g, E1u, E2, E2g, E2u, F, Fg, Fu, F1, F1g, F1u, F2, F2g, F2u, T, Tg, Tu, T1, T1g, T1u, T2, T2g, T2u, other, unknown}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘Ag’ = A<sub>g</sub></li> <li>- ‘Ap’ = A’</li> <li>- ‘As’ = A’’</li> <li>- ‘A1u’ = A<sub>1u</sub></li> <li>- ...</li> </ul> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>-</li> </ul>
<i>band_assignment_category</i>	enum(text)	S1 [!!_m]	Band L1	--	<p>General category of transition producing this band</p> <p><b>Enum:</b> {electronic transition, fundamental vibration, overtone vibration, combination vibration, two-phonon mode, vibron-phonon mode, rotation, overtone rotation, phonon mode, combination, other, unknown}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘<i>electronic transition</i>’: transition between electronic states</li> <li>- ‘<i>fundamental vibration</i>’: vibration in a normal mode</li> <li>- ‘<i>overtone vibration</i>’: combination of the same fundamental mode  <i>Ex:</i> 2ν<sub>1</sub> for H<sub>2</sub>O</li> <li>- ‘<i>combination vibration</i>’: combination of different fundamental vibration modes</li> </ul>

*Ex:*  $\nu_1 + \nu_3, 2\nu_1 + \nu_2$  for H<sub>2</sub>O

- ‘two-phonon mode’: mode involving the same vibration but in two different nearby molecules
- ‘vibron-phonon mode’: combination of a vibration mode with a phonon mode
- ‘rotation’: full rotation of the whole molecule (almost without perturbation from the solid)
- ‘overtone rotation’: combination of the same rotation mode
- ‘phonon mode’: normal mode involving all the atoms or molecules of a solid
- ‘combination’: other combinations of different fundamental vibration modes with rotation and/or phonon modes

*Ex:*  $\nu_R + \nu_L$

- ‘other’: other type not listed above
- ‘unknown’: unknown type of transition

*Notes:*

- see [http://en.wikipedia.org/wiki/Vibrational\\_spectroscopy](http://en.wikipedia.org/wiki/Vibrational_spectroscopy)

<i>band_assignment_method</i>	blob	U <a href="#">[m]</a>	Band L1	-- Description of the method of band transition assignment
-------------------------------	------	--------------------------	------------	--

*Ex:*

- ‘comparison with literature assignment of gas spectra’,
- ‘by determination of the interaction parameters  $X_{ij}$  from all band positions of the band list’, ...

***Band transition assignment: evaluation***

<i>band_assignment_level</i>	enum(text)	U <a href="#">[!_m]</a>	Band L1	-- Level of assignment of the specie(s) and transition(s) contributing to the band
------------------------------	------------	----------------------------	------------	--

**[Enum:](#)** {fully assigned, partly assigned, transition assigned, species assigned, uncertain assignment, not assigned}

*Definitions:*

- ‘fully assigned’: the specie(s) and transition(s) of this band are fully described (isotopic specie(s), all levels of excitation, all modes for a combination, ...).

- ‘*partly assigned*’: the isotopic specie(s) is known but the transition(s) of this band are only partly described (levels of excitation not well known, missing some contribution or missing info on some modes, ...)
- ‘*transition assigned*’: the transition(s) of this band are fully described (all levels of excitation, all modes for a combination, ...) but not the isotopic specie(s).
- ‘*species assigned*’: the isotopic specie(s) is known but the transition(s) of this band if fully unknown
- ‘*uncertain assignment*’: an assignment is proposed but it is uncertain.
- ‘*not assigned*’: neither the isotopic specie(s) nor the transition modes involved are known.

<i>band_assignment_evaluation</i>	enum(text)	S2 [!_m]	Band L1	--	Evaluation of the band assignment  <b>Enum:</b> {undefined, uncertain, validated, recommended, with caution, not recommended}  <i>Definitions:</i> see “ <i>band_characteristic_position_evaluation</i> ”
<i>band_assignment_comments</i>	blob	U [m]	Band L1	--	Comments on band transition assignment  <i>Notes:</i> <ul style="list-style-type: none"> <li>- in particular when assignment is incomplete</li> <li>- can contain detail of the band transition assignment evaluation given by the ‘Solid Band List Committee’</li> </ul> <i>Ex:</i> ‘vibration combination mode well assigned, but exact phonon mode uncertain’

---

***Band assignment: multiplicity and degeneracy***

---

<i>band_assignment_multiplicities</i>	<b>List [L2]</b>				£: List of multiplicities of contributions to this band.
<i>band_assignment_multiplicity_type</i>	enum(text)	S2 [!!_m]	Band L1 L2	-- --	Type of multiplicity of contributions to this band.  <b>Enum:</b> {no, mode degeneracy, site degeneracy, rotational structure, accidental

degeneracy, other isotopic specie, other constituent specie, other, unknown }

*Definitions:*

- ‘no’: single transition contributing to this band
- ‘mode degeneracy’: degeneracy of the transition mode of the isotopic specie (due to molecule or state symmetry)
- ‘site degeneracy’: degeneracy of the transition mode of the isotopic specie in different crystallographic sites (due to molecule or state symmetry and to site symmetry)
- ‘accidental degeneracy’: two transitions of the same isotopic specie with (nearly)equivalent energy (not due to molecule or state symmetry)
- ‘other isotope specie’: band of another isotope specie of the primary specie of this band list contributing to this band position
- ‘other constituent specie’: band of another specie of the constituent contributing to this band

*Cases:*

- ‘no’: → single assignment
- ‘mode degeneracy’: → single assignment + degeneracy (“band\_assignment\_multiplicity\_degeneracy”)
- ‘site degeneracy’: → single assignment with multiple crystallographic sites (multiple “band\_assignment\_transition\_primary\_specie\_crystal\_molecule\_sites”) + degeneracy
- ‘rotational structure’: → single assignment with multiple unresolved rotational transitions
- ‘accidental degeneracy’: → multiple assignments with same isotope specie but with different transition modes (if contributions not extracted)  
OR → multiple bands of same isotopic specie but with different transition modes (if contributions extracted) but with nearly same position.
- ‘other isotope specie’: → multiple assignments with different isotope species and possibly different transitions (if contributions not extracted)  
OR → multiple bands of different isotope species (if contributions extracted) but with nearly same position

- ‘*other constituent specie*’: → multiple bands with different constituent primary species and thus in different bandlists (when contributions extracted or not) but with same (not extracted) or nearly same position (extracted).
  - *Note*: the two bands in their respective bandlist refer one to the other through “*band\_assignment\_multiplicity\_other\_band\_uid*”
- ‘*other*’: other type of degeneracy not listed above. Explain in “*band\_assignment\_contribution\_comments*”
- ‘*unknown*’: unknown type of degeneracy

*Note*:

<i>band_assignment_multiplicity_degeneracy</i>	enum(text)	SS2	Band	F	-- --
		[!o_m]	L1		
			L2		

Degeneracy (mode, site or accidental) of the vibration mode of the isotope species producing this band

**Enum:** {no, double, triple, quadruple, double site, triple site, accidental double, accidental triple, other, unknown}

*Condition:* mandatory when “*band\_assignment\_multiplicity\_type*” = {mode degeneracy, site degeneracy, accidental degeneracy}

*Constraints:*

- = {double, triple, quadruple} only when “*band\_assignment\_multiplicity\_type*” = {mode degeneracy}
- = {double site, triple site} only when “*band\_assignment\_multiplicity\_type*” = {site degeneracy}
- = {accidental double, accidental triple} only when “*band\_assignment\_multiplicity\_type*” = {accidental degeneracy}
- when “*band\_assignment\_multiplicity\_degeneracy*” = {unknown} then “*band\_assignment\_multiplicity\_type*” should be = {mode degeneracy, site degeneracy, accidental degeneracy, unknown}

*Definitions:*

- ‘*no*’: single transition
- ‘*double*’: two similar transitions of a specie with equivalent energy (due to molecule and state symmetry)
- ‘*triple*’: three similar transitions of a specie with equivalent energy (due to molecule molecule and state symmetry)



- ‘*quadruple*’: four similar transitions of a specie with equivalent energy (due to molecule molecule and state symmetry)
- ‘*double site*’: two similar transitions of a specie in two different crystalline sites but with equivalent energy (due to site symmetry)
- ‘*triple site*’: three similar transitions of a specie in two different crystalline sites but with equivalent energy (due to site symmetry)
- ‘*accidental double*’: two different transitions of a specie with (nearly)equivalent energy (not due to molecule or state symmetry)
- ‘*accidental triple*’: three different transitions of a specie with (nearly)equivalent energy (not due to molecule or state symmetry)
- ‘*other*’: for other levels of degeneracy, other multiplicity types, or when there are several degeneracies (ex: mode and accidental). Put a comment in “*band\_assignment\_contribution\_comments*”.
- ‘*unknown*’: unknown degeneracy

*Notes:*

- Mode degeneracy (double, triple, quadruple) mostly for fundamental bands and overtones  
Ex: CH stretch of CH<sub>4</sub> => quadruple
- generally same as for “*molecule\_vibration\_degeneracy*” of the free primary molecule, but some species may change (loose) symmetry from gas to a solid compound and thus break degeneracy of some of its vibrational modes (that will split in multiple bands or band components)

*band\_assignment\_multiplicity\_o* varchar(255) U Band  
*her\_band\_uid* [\*] [!o\_m] Band  
 L1  
 L2

-- Link to the existing UID of another band contributing at the same position as this band

*Condition:* mandatory when “*band\_assignment\_contribution\_level*” = ‘extracted’

*Constraint:* this band should be one of the bands either of this band list or of the bandlist of one of the other species of the constituent of this bandlist.

*Notes:*

- When the contributions of several transitions have been extracted/separated, it is worth to link them them using this keyword.
- It can be an accidentally degenerate or an isotopically degenerate band

of the same primary specie which has been extracted (deconvolution, extraction, ...). Two separate bands will then be described in the band list with their own band characteristics.

- It can be also the band (extracted or not) of another specie of the same constituent which also contributes to the band. This band should be also described in the band list of this other specie (with same band characteristics if not extracted, with its own if extracted). But it is worth to link them using this keyword, especially if the band has not been extracted.
- If this other specie (main or impurity) does not have its own band list, then “*band\_assignment\_multiplicity\_other\_band\_uid*” cannot be filled but a comment should be written in “*band\_assignment\_contribution\_comments*”

---

*band\_assignment\_contribution\_level* enum(text) S3 Band  
 [!o\_m] L1

-- Qualitative level of contribution of this transition to the band.

**Enum:** {full, extracted, major, medium, minor, unknown}.

*Condition:* mandatory when “*band\_assignment\_multiplicity\_type*” = {accidental degeneracy, other isotope of primary specie, other constituent specie, other}

*Definitions:*

- ‘full’: this transition is the only one to contribute to the band characteristics
- ‘extracted’: the band characteristics, which have been extracted from the observed band, correspond only to this transition
- ‘major’: this transition is the major contributor to the band characteristics, in particular to the integrated intensity, and intensity
- ‘medium’: this transition has a medium contribution to the band characteristics
- ‘minor’: this transition has only a minor contribution to the band characteristics
- ‘unknown’: the contribution of this transition to the band characteristics is unknown

<i>band_assignment_contribution_comments</i>	blob	U [m]	Band L1	--	Comments on the contribution of this transition to the band characteristics <i>Notes:</i> to provide more information on how this transition contributes to the various band characteristics <i>Ex:</i> ‘wide (FWHM ~25-30 cm-1) but weak contribution to this band (integrated intensity < 10%)’
--	------	----------	------------	----	---

***Band transitions: species and its crystallographic sites***

Description of the primary specie(s) subjected to the transition, and its crystallographic site(s).

*band\_assignment\_transition\_primary\_species*     **List [L4]**

£: List of the “primary species” that produces the vibration band

<i>band_assignment_transition_primary_specie_uid</i> [*] [-]	varchar(255)	<b>Sli0+S1</b> <b>b</b> [!!o_m]	Band Specie L1 L4	[Ver]	--	Link to the existing UID of the “primary specie” subjected to the transition that produces the band <i>Condition:</i> at least one and absolute mandatory when “ <i>band_assignment_transition_electronic_mode_type</i> ” ≠ ∅ OR “ <i>band_assignment_transition_vibration_mode_type</i> ” ≠ ∅ OR “ <i>band_assignment_transition_rotation_mode_type</i> ” ≠ ∅ <i>Constraint:</i> - this specie can be: ○ an atomic specie: “ <i>atom_type</i> ”= {atom, atomic ion} ○ a molecular species: “ <i>molecule_type</i> ”= {molecule, molecular ion} ○ a chemical function: “ <i>chemical_function_type</i> ”= {mineral anionic radical} - when “ <i>bandlist_constituent_primary_specie_uid</i> ” ≠ ∅, it should be the specie of “ <i>bandlist_constituent_primary_specie_uid</i> ” or one of its isotopes ( <i>molecule_isotope_molecule_uid</i> , <i>atom_isotope_atom_uid</i> ). - when “ <i>bandlist_constituent_primary_specie_uid</i> ” = ∅, it should be one of the species of “ <i>bandlist_constituent_specie_uid</i> ”
---	--------------	---------------------------------------	----------------------------	-------	----	--

*Notes:*

- This specie may be an atom, an ion, a molecule, a molecular ion or a mineral anionic radical
- The type of specie depends both on the type of transition and on the type of solid / liquid

#### Transition modes

- For electronic transitions it will be mostly a molecule for molecular solids and one or two atoms (generally a cation and an anion, or a pair of cations) for ionic and covalent solids (salts, minerals, ...)
- For vibration transitions, the specie will be a molecule for molecular solids. For ionic and covalent solids it will be mostly described by the 2 atoms and the chemical bond(s) that vibrate, but the specie may be also a 'mineral anionic radical'.
- Rotation transition only concerns molecules but possibly also 'mineral anionic radicals'
- Phonon modes mostly concern the whole constituent and generally did not need the specie to be specified. But in some cases they may concern only the specie making up the network of the solid (e.g. H2O for a clathrate) or the major isotopic specie (e.g. <sup>12</sup>C<sup>16</sup>O<sub>2</sub> for solid CO<sub>2</sub>), the other playing the role of 'impurities'.
- Molecular solids:
  - the "(*basic\_*)constituent\_specie\_family" of this species is mostly 'molecule'
  - the specie should be either the primary (natural) species of the band list or one of its isotopes.
  - It will be the natural specie (including all isotopes) when attribution of the band to a specific isotopic specie has not yet been done.
  - It may be also the major isotopic specie of a constituent when the observed band can be safely assigned to the major isotopic specie
- Ionic and covalent solids (salts, minerals, ...):
  - the "primary species" are generally one element or two neighbor elements, but may be also an 'anionic radical'.
  - the "(*basic\_*)constituent\_specie\_family" of this species is mostly 'atom' and 'atomic ion' but may be also 'mineral anionic radicals'.

---

ary\_specie\_crystal\_molecule\_sites

band\_assignment\_transition\_primary\_specie\_crystal\_molecule\_site\_label    varchar(255)    SU    Band    F    -- --  
[£\_m]    L1  
L4  
L5a

structure

*Constraint:*

- only when “bandlist.constituent.family” = {molecular solid, molecular and covalent solid, molecular and ionic solid, complex solid}

Crystallographic site of the molecular species producing the band in the molecular solid structure

**FreeList:** see “solid\_crystal\_molecule\_site\_label”

*Constraints:*

- this site should be already described in the fundamental constituent (basic solid constituent only): “bandlist(\_basic)\_constituent.fundamental\_phase.solid\_crystal\_molecule\_site\_label
- the specie in this site of the fundamental solid (“bandlist(\_basic)\_constituent.fundamental\_phase.solid\_crystal\_molecule\_site\_specie\_uid”) should be the same as “bandlist\_constituent\_primary\_specie\_uid”

*Notes:*

- this site label refers to the corresponding site of the primary molecule of the bandlist (“bandlist\_constituent\_primary\_specie\_uid”) described by “solid\_crystal\_molecule\_site\_label” in the fundamental molecular solid defined by “bandlist\_constituent\_uid”
- when “band\_assignment\_multiplicity\_type” = ‘site degeneracy’ a band may have several contributions of the same transition mode but with the specie in several molecular crystal sites, either equivalent for this mode (true site degeneracy) or too close to be separated (pseudo site degeneracy). The different sites, if known, should be described here.

---

band\_assignment\_transition\_primary\_specie\_crystal\_sites    **List [L5b]**

£: crystallographic sites of the atomic specie producing the band in the ionic/covalent constituent structure

*Constraint:*

- only when “bandlist\_constituent.family” = {covalent network solid, ionic solid, molecular and covalent solid, molecular and ionic solid,

					covalent and ionic solid, complex solid}
<i>band_assignment_transition_primary_specie_crystal_site_label</i>	varchar(255)	US [f_m]	Band L1 L4 L5b	F	-- Crystallographic site of the atomic species producing the band in the ionic/covalent constituent structure  <b>FreeList:</b> see “ <i>solid_crystal_site_label</i> ”  <i>Constraints:</i> <ul style="list-style-type: none"> <li>- this site should be already described in the fundamental constituent (basic solid and mineral constituents only): “<i>bandlist(_basic)_constituent.fundamental_phase.solid/mineral_crystal_site_label</i>”</li> <li>- the specie in this site of the fundamental solid (“<i>bandlist(_basic)_constituent.fundamental_phase.solid/mineral_crystal_site_specie_uid</i>”) should be one of the species of “<i>bandlist_constituent_uid</i>”</li> </ul> <i>Notes:</i> <ul style="list-style-type: none"> <li>- this site label refers to the corresponding site of the atom of the constituent (“<i>band_assignment_transition_primary_specie_uid</i>”) described by “<i>solid/mineral_crystal_site_label</i>” in the fundamental ionic/covalent solid or mineral defined by “<i>bandlist_constituent_uid</i>”</li> <li>- when “<i>band_assignment_multiplicity_type</i>” = ‘site degeneracy’ a band may have several contributions of the same transition mode but with the specie in several crystal sites, either equivalent for this mode (true site degeneracy) or too close to be separated (pseudo site degeneracy). The different sites, if known, should be described here.</li> </ul>
<i>band_assignment_transition_primary_specie_sites_comments</i>	blob	U [m]	Band L1 L4		-- Comments on the sites of this specie  <i>Notes:</i> to provide more information on the sites of the species

---

### ***Band transition modes***

Description of the transition modes contributing to this transition

*Condition:* absolute mandatory at least one of the 4 types of transition:

---

---

electronic, vibration, rotation or phonon modes

---

***Band transition: electronic modes***

---

<i>band_assignment_transition_electronic_modes</i>	<b>List [L6]</b>				£: electronic transition of the atom(s) or molecule producing this band
<i>band_assignment_transition_electronic_mode_label</i>	varchar(255)	S3 [!o_m]	Band L1 L6	[Ver] --	Label including the lower and upper states of the electronic transition of the specie  <i>Condition:</i> mandatory when “ <i>band_assignment_category</i> ” = ‘electronic transition’  <i>Nomenclature:</i> cf paper Wörner and Merkt, Handbook of High-resolution Spectroscopy. 2011 John Wiley & Sons, Ltd., pp. 175-262  <i>Format:</i> LaTeX  <i>Note:</i> can also include the atoms involved in particular when there are more than one and when they are different  <i>Ex:</i> - ‘ ${}^6A_1 \sim \rightarrow {}^4E_1$ ’ for ${}^6A_1 \rightarrow {}^4E_1$ or ‘ ${}_{a^{3+}}({}^6A_1)_{b^{3+}}({}^6A_1) \sim \rightarrow {}_{a^{3+}}({}^6A_1)_{b^{3+}}({}^4T_1)$ ’ for $Fe_a^{3+}({}^6A_1) Fe_b^{3+}({}^6A_1) \rightarrow Fe_a^{3+}({}^6A_1) Fe_b^{3+}({}^4T_1)$ - ‘ ${}_{1u}O(2p) \sim \rightarrow {}_{2g}Fe(3d)$ ’ for $6t_{1u}O(2p) \rightarrow 2t_{2g}Fe(3d)$
<i>band_assignment_transition_electronic_mode_type</i>	enum(text)	S2 [!o_m]	Band L1 L6	[Ver] --	Type of electronic transition mode of the specie(s) producing this band  <b>Enum:</b> {atomic electronic transition, molecular electronic transition, crystal field, ligand-to-metal charge-transfer, intervalence charge transfer, double exciton, other, unknown}  <i>Condition:</i> mandatory when “ <i>band_assignment_category</i> ” = ‘electronic transition’  <i>Definitions:</i>

- 'atomic electronic transition': electronic transition occurring in an atomic specie
- 'molecular electronic transition': electronic transition occurring in a molecular specie
- 'crystal field': also called 'metal ligand field' transition. Transition between orbital energy states of the metal ion splitted by the crystal field generated by the ligands.
- 'ligand-to-metal charge-transfer': charge density transfer from a ligand (generally oxygen in minerals) to the central metal ion.
- 'intervalence charge transfer': process in which two metals ions in close proximity to each other in a structure transfer an electron between them (temporarily changing the oxidation state of both cations).
- 'double exciton': or 'pair excitations' is a transition involving simultaneous excitation of two metal centers with a magnetic coupling.
- 'other': other type of electronic transition not listed above. Need to provide information on this other type in "band\_assignment\_transition\_electronic\_modes\_comments"
- 'unknown': unknown type of electronic transition

Notes:

---

<i>band_assignment_transition_electronic_modes_comments</i>	blob	U <a href="#">[m]</a>	Band L1
---	------	--------------------------	------------

-- Comments on the electronic transition of the specie  
*Note:* for any additional comment on band electronic transition and involved species

---

***Band transition: vibration modes***

---

<i>band_assignment_transition_vibration_modes</i>	<b>List [L7]</b>
---	------------------

£: vibration modes of the bond or molecule producing this band

<i>band_assignment_transition_vibration_mode_label</i>	varchar(255)	S3 <a href="#">[!o_m]</a>	Band L1	<b>[Ver]</b>
--	--------------	------------------------------	------------	--------------

-- Label of the normal mode of vibration 'Vi' of the molecular specie contributing to this band

*Condition:* mandatory when "band\_assignment\_category" = {fundamental



L7

vibration, overtone vibration, combination vibration}

*Definitions:* each label is given to the modes of the free molecule following the Hertzberg rules.

*Nomenclature:*

- These normal mode of vibration labels are of the type ‘ $v_i$ ’, where ‘ $i$ ’ is an integer from 0 to  $n$ , ‘ $n$ ’ being the number of vibration modes of the molecule, given by “*molecule\_vibrations\_number*”.

*Format:* LaTeX

- ‘ $\nu_i$ ’ for  $\nu_i: 0 \rightarrow n$  from ground state
- ‘ $-\nu_i$ ’ for  $\nu_i: n \rightarrow 0$  to ground state
- ‘ $\nu_i^{dl_2}$ ’ for  $\nu_i^{dl_2}: 0 \rightarrow n$  from ground state with rotation
- ‘ $\nu_i + \nu_j$ ’ for  $\nu_i: m \rightarrow n$  for combination bands where  $i, j$  ( $i \neq j$ ),  $n, m$  are integers
- ‘ $[\nu_i + \nu_i]$ ’ for  $\nu_i: 0 \rightarrow 1$  for double phonon bands where  $i$  is an integer
- ‘ $(\nu_i - m \nu_i)$ ’ for  $\nu_i: m \rightarrow n$  for hot bands where  $i, n, m$  are integers

*Notes:*

- hot bands (lower state with at least one quantum number  $> 0$ ) are expressed within ( ) with the ‘-’ sign (without spaces) for their lower state
- double phonon transitions (absorbed by 2 nearby identical molecules) are expressed within [ ]
- put ‘?’ (‘?+?’ for combinations) if transition is fully unknown.

*Ex:*

- ‘ $3\nu_2$ ’: ‘ $3\nu_2$ ’ for  $\nu_2: 0 \rightarrow 3$
- ‘ $2\nu_1 + \nu_3$ ’: ‘ $2\nu_1 + \nu_3$ ’ for  $\nu_1: 0 \rightarrow 2$  &  $\nu_3: 0 \rightarrow 1$
- ‘ $[\nu_1 + \nu_1]$ ’: ‘ $[\nu_1 + \nu_1]$ ’ for  $\nu_1: 0 \rightarrow 1$  &  $\nu_1: 0 \rightarrow 1$
- ‘ $(2\nu_1 - \nu_1)$ ’: ‘ $(2\nu_1 - \nu_1)$ ’ for  $\nu_1: 1 \rightarrow 2$

<i>band_assignment_transition_vibration_mode_type</i>	enum(text)	S2	Band	[Ver]	--	Type of fundamental vibration mode of the bond or molecule producing this band
			L1			

[!o\_m] L7

**Enum:** {stretching, stretching sym., stretching asym., bending, bending in-p, bending out-p, bending sym., bending asym., bending sym. in-p (scissoring), bending asym. in-p (rocking), bending sym. out-p (wagging), bending asym. out-p (twisting), deformation, deformation in-p, deformation out-p, deformation sym., deformation asym., other, unknown}

**Condition:** mandatory when “band\_assignment\_category” = {fundamental vibration, overtone vibration, combination vibration}

**Definitions:**

- For fundamental vibration modes see “molecule\_vibration\_mode”

**Notes:** see:

- [http://en.wikipedia.org/wiki/Vibrational\\_spectroscopy](http://en.wikipedia.org/wiki/Vibrational_spectroscopy)
- the ‘antisym.’ modes have been depreciated and are replaced by ‘asym.’ modes

---

*band\_assignment\_transition\_vibration\_mode\_chemical\_bonds*      **List [L8]**

<i>band_assignment_transition_vibration_mode_chemical_bond_uid</i> [*] <a href="#">[molecule_vibration_chemical_bond_uid]</a>	varchar(255)	Sli2 <a href="#">[!_m]</a>	Band ChemB Molec  L1 L7 L8
--	--------------	-------------------------------	--

£: bonds or groups of atoms of the primary species or of the constituent (ionic, covalent) subjected to the transition that produces the band

-- Link to the existing UID of the bond, part of the molecule, or whole molecule, of the primary species or ionic/covalent constituent subjected to this mode of vibration

**Nomenclature:**

- the UID starts with either ‘BOND\_’, ‘MOLECPART\_’, or ‘MOLEC\_’ depending on the number of bonds involved and size of the molecule, see below.
- For bonds with H, H is the 1H atom (and not natural terrestrial isotopic mix of H) when the other atom is a specific isotope.  
*Ex:* ‘BOND\_12CH’ is ‘12C-1H’ isotopic bond  
‘BOND\_CH’ is ‘CH’ terrestrial isotopic mix of the bond

**Notes:**

- the bond (2 bonded atoms) is either:
  - o a specific isotopic bond of a pure isotopic specie
  - o a partially isotopic substituted specie
  - o but can be also a fully natural bond (mix of all isotopic bonds)

- for natural terrestrial isotopic mix of species when attribution of the band to a specific isotopic bond has not yet been done
- this description with ‘single bonds’ is mostly used for fundamental and overtone vibration bands (a single bond, a small part of the molecular species, or a small part of a covalent network) and simple vibration combinations, but limited to 3 bonds.
  - For fundamental phases these single bonds are among those described with “(basic\_ )constituent\_chemical\_bonds”
  - when more than one bond (generally 2 or 3) is involved in a single fundamental vibration mode, but not the whole molecule, or the whole network unit, a ‘molecule part’ (or its isotopic variant) should be used instead. It is mostly the case for bending, symmetric and antisymmetric stretchings, rocking, and some deformations.  
*Ex:* ‘MOLECPART\_CH3’, ‘MOLECPART\_CCdC’, ‘MOLECPART\_tCCH3’, ...
  - when a vibration mode involves the whole molecule (case of torsion, some deformations, ...) then use:
    - diatomic molecules: the bond ‘BOND\_XY’ or its isotopic variant  
*Ex:* ‘BOND\_CO’, ‘BOND\_13Cd18O’, ...
    - larger molecules: the molecule ‘MOLEC\_XYZ’ or its isotopic variant  
*Ex:* ‘MOLEC\_CH4’, ‘MOLEC\_13C16O18O’, ‘MOLEC\_CH3OH’, ...

---

<i>band_assignment_transition_vibration_modes_comments</i>	blob	U <a href="#">[m]</a>	Band L1	--	Comments on the vibration modes of the specie  <i>Note:</i> for any additional comment on vibration modes and involved species and bonds
--	------	--------------------------	------------	----	--

---

***Band transition: rotation modes***

---

<i>band_assignment_transition_rotation_modes</i>	<b><i>List [L9]</i></b>	£: rotation modes of the molecular specie producing this band
--	-------------------------	---

<i>band_assignment_transition_rotati</i>	<i>varchar(255)</i>	S3	Band	[Ver]	--	Label of the normal mode of rotation of the molecular specie contributing to this band
<i>on_mode_label</i>		[!o_m]	L1			
			L9			

*Condition:* mandatory when “*band\_assignment\_category*” = {rotation, overtone rotation}

*Nomenclature:*

- These normal mode of rotation labels are of the type ‘Rx’ (rotation) or ‘Lx’ (libration), where ‘x’ is one of the three axes (x, y, z) of the molecule ....
- ‘ $\nu_{R}$ ’: R: free rotation or hindered rotation around all axes, or one unknown axis of the molecule
- ‘ $\nu_{R_x}$ ’, ‘ $\nu_{R_y}$ ’, ‘ $\nu_{R_{xy}}$ ’, ‘ $\nu_{R_z}$ ’, ‘ $\nu_{R_{xyz}}$ ’: Rx, Ry, Rxy, Rz, Rxyz (or R): free rotation or hindered rotation around the x, y, x&y, z, all axes of the molecule, respectively
- ‘ $\nu_{L}$ ’: L: libration around all axes, or one unknown axis of the molecule
- ‘ $\nu_{L_x}$ ’, ‘ $\nu_{L_y}$ ’, ‘ $\nu_{L_{xy}}$ ’, ‘ $\nu_{L_z}$ ’, ‘ $\nu_{L_{xyz}}$ ’: Lx, Ly, Lxy, Lz, Lxyz (or L): libration around the x, y, x&y, z, all axes of the molecule, respectively

*Format:* LaTeX

- ‘ $\nu_{L_x}$ ’: for rotation around the axis x
- ‘ $\nu_{L_{xyz}}$ ’: for rotation around any of the 3 axes x, y, z

*Notes:*

- Rotation modes (mostly libration) also occurs for ‘mineral anionic radicals’
- Hot bands (lower state with at least one quantum number > 0) are expressed within ( ) with the ‘-’ sign for their lower state
- put ‘?’ if transition is fully unknown.

*Ex:*

- ‘3L<sub>x</sub>’ for L<sub>x</sub>: 0→3
- ‘(2L<sub>x</sub>-L<sub>x</sub>)’ for L<sub>x</sub>: 1→2

<i>band_assignment_transition_rotation_mode_type</i>	enum(text)	S2 [!o_m]	Band L1 L9	[Ver]	--	<p>Type of rotation mode of the molecular specie producing this band</p> <p><i>Condition:</i> mandatory when “<i>band_assignment_category</i>” = {rotation, overtone rotation}</p> <p><b>Enum:</b> {free rotation, hindered rotation, libration, other, unknown}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘<i>free rotation</i>’: full rotation of the whole molecule (almost without perturbation from the solid)</li> <li>- ‘<i>hindered rotation</i>’: = rotation of the whole molecule but with strong perturbation from the solid [%%% TBV] <ul style="list-style-type: none"> <li><i>Note:</i> ‘hindered rotation’ is also used in the literature to describe either librations or internal torsional vibrations</li> </ul> </li> <li>- ‘<i>libration</i>’: molecule with nearly fixed orientation that repeatedly rotates slightly back and forth (very strong perturbation from the solid)</li> <li>- ‘<i>other</i>’: other type of rotation modes not listed above. Need to provide information on this other type in “<i>band_assignment_transition_rotation_modes_comments</i>”</li> <li>- ‘<i>unknown</i>’: unknown type of rotation mode</li> </ul> <p><i>Notes:</i> see:</p> <ul style="list-style-type: none"> <li>- <a href="http://en.wikipedia.org/wiki/Vibrational_spectroscopy">http://en.wikipedia.org/wiki/Vibrational_spectroscopy</a></li> </ul>
--	------------	--------------	------------------	-------	----	---

<i>band_assignment_transition_rotation_modes_comments</i>	blob	U [m]	Band L1		--	<p>Comments on the rotation modes of the specie</p> <p><i>Note:</i> for any additional comment on rotation modes and involved species</p>
---	------	----------	------------	--	----	---

***Band transition: phonon modes***

<i>band_assignment_transition_phonon_modes</i>	<b>List [L10]</b>					£: transition phonon modes of the constituent solid structure
<i>band_assignment_transition_phonon_mode_label</i>	varchar(255)	S3 [!o_m]	Band L1 L10	[Ver]	--	<p>Label of the translation phonon mode of the solid contributing to this band</p> <p><i>Condition:</i> mandatory when “<i>band_assignment_category</i>” = {phonon mode}</p> <p><i>Nomenclature:</i></p>

- ‘ $\nu_{T}$ ’:  $\nu_T$  - (optic) translation mode of unknown type
- ‘ $\nu_{T(LO)}$ ’:  $\nu_{T(LO)}$  - longitudinal optic translation mode
- ‘ $\nu_{T(LOx)}$ ’:  $\nu_{T(LOx)}$ ,  $\nu_{T(LOy)}$ ,  $\nu_{T(LOz)}$  - longitudinal optic translation mode along the x, y, z axis of the crystal, respectively
- ‘ $\nu_{Tz}$ ’:  $\nu_{Tz}$  – longitudinal optic translation mode
- ‘ $\nu_{T(TO)}$ ’:  $\nu_{T(TO)}$  - transverse optic translation mode
- ‘ $\nu_{Txy}$ ’:  $\nu_{Txy}$  - transverse optic translation mode
- ‘ $\nu_{T(LA)}$ ’:  $\nu_{T(LA)}$  - longitudinal acoustic translation mode
- ‘ $\nu_{T(TA1)}$ ’:  $\nu_{T(TA1)}$  - transverse acoustic translation mode 1  
(‘ $\nu_{T(TAxy)}$ ’ ?)
- ‘ $\nu_{T(TA2)}$ ’:  $\nu_{T(TA2)}$  - transverse acoustic translation mode 2  
(‘ $\nu_{T(TAz)}$ ’ ?)

*Format:* LaTeX

- ‘ $\nu_{T}$ ’, ‘ $\nu_{T(LO)}$ ’, ...

*Notes:*

- Number of translation phonon modes (N is the number of atoms/molecules per primitive cell):
  - o acoustic: 3 (1 Longitudinal LA, 2 Transverses TA1, TA2)
  - o optic:  $3(N - 1)$  (1 Longitudinal LO, 2 Transverses TO, N-1 times)
  - o acoustic modes are generally silent (Infrared and Raman inactive)
  - o optic modes are thus only present in solids with several atoms/molecules per primitive cell
- Translation phonon modes involve all the molecular species constituting the crystal of the constituent (except impurities and minor isotopes, which are decoupled ?) and not only the primary molecular species. So, it is necessary to tell who are the other(s) main molecular specie(s) of the constituent by referring to its molecular solid structure and composition. This is done through: “*bandlist\_constituent\_uid*”.
- put ‘ $\nu_{T}$ ’ if the exact translation mode (longitudinal or transverse) is unknown.
- put ‘?’ if the phonon mode is fully unknown.

*Ex:*

- '\$\nu\_{T(LOx)}\$' for  $v_{T(LOx)} : 0 \rightarrow 1$
- '\$3\nu\_{T(LOx)}\$' for  $v_{T(LOx)} : 0 \rightarrow 3$
- '\$2\nu\_{T(LOx)} - \nu\_{T(LOx)}\$' for  $v_{T(LOx)} : 1 \rightarrow 2$

<i>band_assignment_transition_phonon_mode_type</i>	enum(text)	S2 [!o_m]	Band L1 L10	[Ver] --	<p>Type of phonon mode of the solid structure producing this band</p> <p><b>Enum:</b> {translation, longitudinal optic translation, transverse optic translation, longitudinal acoustic translation, transverse acoustic translation, other, unknown}</p> <p><i>Condition:</i> mandatory when “band_assignment_category” = {phonon mode}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘translation’: out-of-phase movements of the atoms in the lattice, but with unknown/undefined propagation direction</li> <li>- ‘longitudinal optic translation’: out-of-phase movements of the atoms in the lattice in the propagation direction</li> <li>- ‘transverse optic translation’: out-of-phase movements of the atoms in the lattice perpendicular to the propagation direction</li> <li>- ‘longitudinal acoustic translation’: coherent movements of atoms of the lattice out of their equilibrium positions in the propagation direction</li> <li>- ‘transverse acoustic translation’: coherent movements of atoms of the lattice out of their equilibrium positions perpendicular to the propagation direction</li> <li>- ‘other’: other type of phonon mode (translation) not listed above. Need to provide information on this other type in “band_assignment_transition_phonon_modes_comments”</li> <li>- ‘unknown’: unknown type of phonon mode</li> </ul> <p><i>Notes:</i> see:</p> <ul style="list-style-type: none"> <li>- <a href="https://en.wikipedia.org/wiki/Phonon#Acoustic_and_optical_phonons">https://en.wikipedia.org/wiki/Phonon#Acoustic_and_optical_phonons</a></li> </ul>
<i>band_assignment_transition_phonon_modes_comments</i>	blob	U [m]	Band L1	--	<p>Comments on the phonon modes of the constituent</p> <p><i>Note:</i> for any additional comment on phonon modes and involved species in the constituent</p>

## Band transition: resonances

<i>band_assignment_resonances</i>				
<i>band_assignment_resonances</i>	<i>List [L11]</i>	<i>[£]</i>		
				<p>£: transition modes (internal or external) with which this mode is in resonance</p> <p><i>Note:</i> in general a resonance occurs with a mode of very similar energy (wavelength) or with one of its overtone.</p>
<i>band_assignment_resonance_type</i>	varchar(255)	S2 [!o_m]	Band L1 L11	<p>-- Type of resonance of the transition mode</p> <p><i>Condition:</i> mandatory when “<i>band_assignment_resonance_band_uid</i>” ≠ {Ø, NULL}</p> <p><b>Enum:</b> {Fermi resonance, electron-phonon coupling, rotational-vibrational coupling, vibration-phonon coupling, other, unknown}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘<i>Fermi resonance</i>’: shifting of the energies and intensities of absorption bands in infrared or Raman spectra as a consequence of quantum mechanical wavefunction mixing. The two vibrations must have the same symmetries (Mulliken symbols).</li> <li>- ‘<i>electron-phonon coupling</i>’: impact of vibrations from molecular relaxations (intra-molecular modes) on site energy</li> <li>- ‘<i>rotational–vibrational coupling</i>’:</li> <li>- ‘<i>vibration-phonon coupling</i>’:</li> <li>- ‘<i>other</i>’: other type of resonance. Need to provide information on this other type in “<i>band_assignment_resonance_comments</i>”</li> <li>- ‘<i>unknown</i>’: unknown mode of resonance coupling</li> </ul> <p>See:</p> <ul style="list-style-type: none"> <li>- <a href="https://en.wikipedia.org/wiki/Fermi_resonance">https://en.wikipedia.org/wiki/Fermi_resonance</a></li> <li>- <a href="http://cleanenergywiki.org/index.php?title=Electron-Phonon_Coupling">http://cleanenergywiki.org/index.php?title=Electron-Phonon_Coupling</a></li> <li>- <a href="https://en.wikipedia.org/wiki/Rotational%E2%80%93vibrational_coupling">https://en.wikipedia.org/wiki/Rotational%E2%80%93vibrational_coupling</a></li> </ul>
<i>band_assignment_resonance_band_uid</i> [*]	varchar(255)	U	Band	-- Link to the existing UID of the band which transition mode (internal or external) is in resonance with this transition



[!o\_m] Band  
L1  
L11

*Condition:* mandatory when “*band\_assignment\_resonance\_type*” ≠ {∅, NULL}

*Notes:*

- if several transitions of the same primary isotopic species are in resonance they are thus together in one ‘polyad’
- The resonant transition may be accidental degenerate with this transition with (almost-)exactly same wavelength. It may thus either be extracted in another band (to be linked here) or not (then to be tell in “*band\_assignment\_resonance\_comments*”)
- if this transition mode belongs to another specie of the constituent, its resonant band should be already in the database to be linked, otherwise it should be specified in “*band\_assignment\_resonance\_comments*”

*band\_assignment\_resonance\_band\_assignment\_number* int(10) P Band  
[!o\_m] L1  
L11

*no* Order number of the assignment of the transition (of the band above) which is in resonance

*Condition:* mandatory when “*band\_assignment\_resonance\_band\_uid*” ≠ {∅, NULL}

*Constraint:* only when “*band\_assignment\_resonance\_band\_uid*” ≠ {∅, NULL}

*band\_assignment\_resonance\_comments* blob U Band  
[m] L1  
L11

-- Comments on the resonance with this transition

*Notes:*

- to provide more information on how this transition (and band) is in resonance with this the current transition and how it affects its band characteristics
- allow to precise which transition is in resonance when the linked band has several contributions (multiple assignments).
- also to provide info when the resonance band is not yet in the database (“*band\_assignment\_resonance\_band\_uid*” = ∅)

*Ex:* ‘in resonance with the band at 2340 cm<sup>-1</sup> of small amount of <sup>12</sup>CO<sub>2</sub> impurity in the constituent. Strongly increases its intensity (factor > 10) but only slightly shifts its position to lower wavelength (-0.3



<i>band_characteristic_constituent_texture_comments</i>	blob	U [fo_m]	Band L12	<p>-- Constituent texture, for this set of band characteristics, when it affect their values</p> <p><i>Condition:</i> compulsory when changed (or precised) compared to the values for the nominal constituent</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- mostly useful for reflectance and emission band lists</li> <li>- provide the effective values in composition and phase for this band among the range of values given for the constituent for the whole band list</li> </ul> <p><i>Ex:</i></p> <ul style="list-style-type: none"> <li>- ‘spherical grains with size range: 125-200 µm. Porosity 40%’</li> </ul>
---	------	-------------	-------------	---

***Band constituent environment parameters***

*band\_characteristic\_constituent(\_parameters\_environment)*

Environment parameters of the constituent for this set of band characteristics

£: temperature and pressure parameters

*Note xml:*

- For practical reasons it is split in 2 sub-blocs: "temperature", and "pressure"

***Constituent environment parameters: Temperature***

*band\_characteristic\_constituent(\_parameters\_environment)\_temperature* [!!\_m]

This single bloc describes the temperature conditions of the constituent

*band\_characteristic\_constituent(\_p\_e)\_temperature\_unit* enum(text) U [!!\_m] Band L12  
[sample\_temperature\_unit]

-- Unit of temperature

**Enum:** {K, C, F}

*Note DB:* all temperature data will be stored in ‘K’

*Note:* used for “*band\_characteristic\_constituent\_temperature\_value/\_error*”, “*band\_characteristic\_constituent\_formation\_temperature*”, “*band\_characteristic\_constituent\_max*”

<i>band_characteristic_constituent(_p_e)_temperature_value</i> <i>[sample_temperature_value]</i>	float	S3 <i>[!_m]</i>	Band L12	var. Effective temperature of the constituent <i>Unit:</i> in “ <i>band_characteristic_constituent_temperature_unit</i> ” - converted in ‘K’ unit in the database
<i>band_characteristic_constituent(_p_e)_temperature_error</i> <i>[sample_temperature_error]</i>	float	U <i>[!_m]</i>	Band L12	var. Absolute uncertainty on effective temperature of the constituent <i>Unit:</i> in “ <i>band_characteristic_constituent_temperature_unit</i> ” • converted in ‘K’ unit in the database
<i>band_characteristic_constituent(_p_e)_temperature_formation</i> <i>[layer_formation_temperature]</i>	float	U <i>[m]</i>	Band L12	var. Formation temperature of the constituent (for synthetic samples) <i>Unit:</i> in “ <i>band_characteristic_constituent_temperature_unit</i> ” • converted in ‘K’ unit in the database  <i>Note:</i>
<i>band_characteristic_constituent(_p_e)_temperature_max</i> <i>[sample_temperature_max]</i>	float	U <i>[!_m]</i>	Band L12	var. Maximum temperature reached by the constituent after formation <i>Unit:</i> in “ <i>band_characteristic_constituent_temperature_unit</i> ” • converted in ‘K’ unit in the database  <i>Note:</i> this maximum temperature is the highest that the constituent reached before the spectrum recording. It can be just the final temperature after constituent formation.
<i>band_characteristic_constituent(_p_e)_temperature_comments</i> <i>[sample_temperature_comments]</i>	blob	U <i>[m]</i>	Band L12	-- Comments about the temperature environment and history of the constituent  <i>Notes:</i> - when a change in temperature induces a different phase of the constituent it is necessary to set separate band lists for each phase  <i>Ex:</i> Errors on T max, annealing cycle and time, ...

---

***Constituent environment parameters: Pressure and stress***

*band\_characteristic\_constituent(parameters\_environment)\_pressur* *[O\_m]* = This single bloc describes the pressure and stress conditions of the constituent

e

<i>band_characteristic_constituent(p_e)_pressure_unit</i> [ <i>sample_pressure_unit</i> ]	U [!o_m]	Band L12	-- Unit of mechanical pressure  <b>Enum:</b> {Pa, hPa, MPa, GPa, mbar, bar, atm, torr}  <i>Condition:</i> Mandatory when “ <i>band_characteristic_constituent_pressure_value</i> ” ≠ ∅ OR “ <i>band_characteristic_constituent_pressure_formation</i> ” ≠ ∅ OR “ <i>band_characteristic_constituent_pressure_max</i> ” ≠ ∅  <i>Note DB:</i> all pressure data will be stored in ‘Pa’  <i>Note:</i> used for “ <i>band_characteristic_constituent_pressure_value/_error</i> ”, “ <i>band_characteristic_constituent_formation_pressure</i> ”, and “ <i>band_characteristic_constituent_pressure_max</i> ”
<i>band_characteristic_constituent(p_e)_pressure_value</i> [ <i>sample_pressure_value</i> ]	S3 [m]	Band L12	var. Effective mechanical pressure applied to the constituent  <i>Unit:</i> in “ <i>band_characteristic_constituent_pressure_unit</i> ” <ul style="list-style-type: none"><li>• converted in ‘Pa’ unit in the database</li></ul> <i>Note:</i> for constituent at ambient pressure => 1 bar (or 10 <sup>5</sup> Pa). For constituent under vacuum => 0 bar (or Pa).
<i>band_characteristic_constituent(p_e)_pressure_error</i> [ <i>sample_pressure_value</i> ]	U [m]	Band L12	var. Absolute uncertainty on the effective mechanical pressure applied to the constituent  <i>Unit:</i> in “ <i>band_characteristic_constituent_pressure_unit</i> ” <ul style="list-style-type: none"><li>• converted in ‘Pa’ unit in the database</li></ul>
<i>band_characteristic_constituent(p_e)_pressure_formation</i> [ <i>layer_formation_pressure</i> ]	U [m]	Band L12	var. Mechanical pressure applied to the constituent during formation  <i>Unit:</i> in “ <i>band_characteristic_constituent_pressure_unit</i> ” <ul style="list-style-type: none"><li>• converted in ‘Pa’ unit in the database</li></ul> <i>Note:</i>
<i>band_characteristic_constituent(p_e)_pressure_max</i>	U [m]	Band	var. Maximum mechanical pressure applied to the constituent after formation

<a href="#">[sample_pressure_max]</a>		L12		<p><i>Unit:</i> in “<i>band_characteristic_constituent_pressure_unit</i>”</p> <ul style="list-style-type: none"> <li>• converted in ‘Pa’ unit in the database</li> </ul> <p><i>Note:</i> this maximum pressure is the highest that the constituent reached before spectrum recording. It can be just the final pressure after constituent formation.</p>
<i>band_characteristic_constituent(_p_e)_pressure_stress_type</i> <a href="#">[sample_stress_type]</a>	enum(text) S2 [m]	Band L12	--	<p>Type of stress applied to the constituent</p> <p><b>Enum:</b> {normal uniaxial tension, normal uniaxial compression, simple shear, normal biaxial tension, normal biaxial compression, cylindrical normal tension, cylindrical normal compression, isotropic normal tension, isotropic normal compression, combined biaxial, combined triaxial, other, unknown}</p> <p><i>Definitions:</i> see “<i>sample_stress_type</i>”</p>
<i>band_characteristic_constituent(_p_e)_pressure_comments</i> <a href="#">[sample_pressure_comments]</a>	blob U [m]	Band L12	--	<p>Comments about the pressure and stress environment and history of the constituent</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- when a change in pressure induces a different phase of the constituent it is necessary to set separate band lists for each phase</li> </ul> <p><i>Ex:</i> Errors on P max, pressurization cycle and time, ...</p>

---

***Band characteristics: excitation light***

<i>band_characteristic_excitation_laser_wavelength</i>	float U [!o_m]	Band L12	nm	<p>Wavelength of the laser excitation</p> <p><i>Condition:</i> Mandatory and only when “<i>bandlist_type</i>” = {Raman scattering, fluorescence emission}</p> <p><i>Constraint:</i> Not when “<i>bandlist_type</i>” = {absorption, reflectance, thermal emission}</p> <p><i>Unit:</i> in ‘nm’</p>
<i>band_characteristic_excitation_sample_orientation_mode</i>	enum(text) U	Band L12	--	<p>Orientation mode of the axe of the incident excitation light relative to the crystalline axes of the constituent</p>

[!o\_m]

**Enum:** {oriented, unoriented, random, unknown}

*Condition:* Mandatory when “bandlist\_type” = {Raman scattering}

*Definitions:*

- ‘oriented’: the crystallographic axes of the constituent are oriented relative to the incident excitation light
- ‘unoriented’: the crystallographic axes of the constituent have no specific orientation relative to the incident excitation light
- ‘random’: the crystallographic axes of the constituent have all types of orientations relative to the incident excitation light
- ‘unknown’: possible orientation is unknown

*Notes:*

-

band\_characteristic\_excitation\_sample\_orientation varchar(255) U Band  
 [!o\_m] L12

-- Orientation of the axe of the incident excitation light relative to the crystalline axes of the constituent

*Condition:* Mandatory when “bandlist\_type” = {Raman scattering}  
 AND  
 when “band\_characteristic\_excitation\_sample\_orientation\_mode” = {oriented}

*Notes:*

-

*Ex:* ‘Laser parallel to -b\* (0 -1 0)’

band\_characteristic\_excitation\_polarization\_orientation\_mode enum(text) U Band  
 [!o\_m] L12

-- Orientation mode of the polarization of the incident excitation light relative to the crystalline axes of the constituent

**Enum:** {depolarized, polarized, unknown}

*Condition:* Mandatory when “bandlist\_type” = {Raman scattering, absorption}  
 AND  
 when “band\_characteristic\_excitation\_sample\_orientation\_mode” = {oriented}

*band\_characteristic\_excitation\_polarization\_orientation* varchar(255) U Band  
 [!o\_m] L12

*Definitions:*

- 'depolarized': the incident excitation light is not polarized
- 'polarized': the incident excitation light is linearly polarized
- 'unknown': possible polarization is unknown

*Notes:*

-- Orientation of the polarization of the incident excitation light relative to the crystalline axes of the constituent

*Condition:* Mandatory when  
 "band\_characteristic\_excitation\_polarization\_orientation\_mode" = {polarized}

*Notes:*

*Ex:* 'parallel to -c [0 0 -1]'

*band\_characteristic\_excitation\_comments* blob U Band  
 [m] L12

-- Comments about the excitation light

*Notes:*

- Can be about wavelength, polarization or orientation

*Ex:* 'two wavelength were used in the compilation: 532 and 785 nm'

---

***Band characteristics: method and fit function***

---

*band\_characteristic\_methods* List [L13] [!]

£: General methods used to get the values of the band characteristics

*Note:* allow to describe different methods for the different characteristics (position, width, intensity)

*band\_characteristic\_method\_type* enum(text) U Band  
 [!\_m] L12  
 L13

-- Method used to get the values of the band characteristics from the spectrum

**Enum:** {spectrum measurement, spectrum fit, spectrum analysis, data compilation, data extrapolation, theory, estimation, various, other, unknown}

*Definitions:*

- 'spectrum measurement': directly measured on a recorded spectrum
- 'spectrum fit': determined by a mathematical function fit of the band on



- a measured spectrum (detail to be provided in “*band\_characteristic\_method\_fit\_function\_type*” and “*\_fit\_function\_parameters*”)
- ‘*spectrum analysis*’: determined by indirect analysis methods, such as first derivative, second derivative, ...
- ‘*data compilation*’: determined by compilation of one or more published values (with no detail on characteristics determination method given, or various methods)
- ‘*data extrapolation*’: mathematical/theoretical extrapolation from values measured on other bands (ex: using harmonic frequencies and interaction parameters determined from a set of bands)
- ‘*theory*’: calculated purely theoretically (ab-initio, ...)
- ‘*estimation*’: estimation by another mean
- ‘*various*’: determined by several of the above methods. Used in particular with compilation of data from various sources
- ‘*other*’: determined by another method than the above listed methods.
- ‘*unknown*’: unknown method

<i>band_characteristic_method_description</i>	blob	U <a href="#">[m]</a>	Band L12 L13	-- Description of the method used to get the values of the different band characteristics  <i>Ex:</i> <ul style="list-style-type: none"> <li>- ‘fit of a group of bands with 5 gaussian curves from 1500 to 1580 cm<sup>-1</sup>’</li> <li>- ‘extrapolated position using the harmonic frequencies and interaction parameters obtained by fitting 17 experimental bands measured in transmission between 500 and 3500 cm<sup>-1</sup>’</li> <li>- ‘band fit of Kubelka-Munk spectrum’</li> </ul>
<i>band_characteristic_method_fit_function_type</i>	openum(text)	U <a href="#">[o_m]</a>	Band L12 L13	-- Type of function used to fit the band  <u><a href="#">OpenEnum</a></u> : {Gaussian, Voigt, Lorentzian, BWF, Doppler, other, unknown}  <i>Constraint:</i> only when “ <i>band_characteristic_method</i> ” = ‘spectrum fit’  <i>Definitions:</i> <ul style="list-style-type: none"> <li>- ‘<i>Gaussian</i>’: profile of the normal distribution (profile with 3 parameters: I, <math>\omega_0</math>, <math>\sigma^2</math>) <a href="http://en.wikipedia.org/wiki/Normal_distribution">http://en.wikipedia.org/wiki/Normal_distribution</a></li> </ul>

- $f_G(\omega) = I \cdot \exp[-(\omega - \omega_0)^2 / 2\sigma^2] / \sigma \cdot \sqrt{2\pi}$
- ‘Lorentzian’: profile of the Cauchy-Lorentz distribution (profile with 3 parameters:  $K$ ,  $\omega_0$ ,  $\Delta$ )  
([http://en.wikipedia.org/wiki/Cauchy\\_distribution](http://en.wikipedia.org/wiki/Cauchy_distribution))
  - $f_L(\omega) = K \cdot \Delta / \pi [(\omega - \omega_0)^2 + \Delta^2]$
- ‘Voigt’: convolution of a Gaussian and Lorentzian profile  
([http://en.wikipedia.org/wiki/Voigt\\_profile](http://en.wikipedia.org/wiki/Voigt_profile))
- ‘BWF’: Breit-Wigner-Fano (profile with 4 parameters:  $\omega_{BWF}$ ,  $\Gamma$ ,  $Q$ ,  $I_0$ ) (cf. Bonal 2006 thesis)
  - $F_{BWF}(\omega) = I_0 \cdot [1 + 2(\omega - \omega_0) / Q\Gamma]^2 / [1 + (2(\omega - \omega_0) / \Gamma)^2]$
- ‘Doppler’:
- ‘other’: fit with a different function than those listed above. Provide the information in “*band\_characteristic\_method\_description*”
- ‘unknown’: fit but with an unknown fit function

The type of band fit function is provided when the band position, width and/or intensities are determined using a fit of the band by a math function

<i>band_characteristic_method_fit_function_parameters</i>	blob	U <a href="#">[o_m]</a>	Band L12 L13	(var.) List of the parameters (name and symbol) of the fit function and their values (and unit) for the band
---	------	----------------------------	--------------------	--

*Definitions:*

- ‘central frequency  $\omega_0$ ’ of all profiles (Gaussian, Lorentzian, Breit-Wigner-Fano profile...)
- ‘variance  $\sigma^2$ ’ of Gaussian profile
- ‘HWHM  $\Delta_L$ ’: half width at half maximum of Lorentzian profile
- ‘FWHM  $\Delta_L$ ’: Lorentzian full width at half maximum
- ‘FWHM  $\Delta_G$ ’: Gaussian full width at half maximum
- ‘integrated intensity  $K_L$ ’ of Lorentzian profile (=  $\pi \cdot \Delta \cdot I_{\max}$ )
- ‘integrated area  $A$ ’
- ‘intensity  $I_0$ ’ of Breit-Wigner-Fano profile
- ‘broadening factor  $\Gamma_{BWF}$ ’ of Breit-Wigner-Fano profile
- ‘asymmetry factor  $Q_{BWF}$ ’ of Breit-Wigner-Fano profile (1/q is the asymmetry of the shape of the fit function)

- ...

*Format:* LaTeX can be used

*Position:*

- central frequency  $\omega_0 = \text{xxxx cm}^{-1}$

*Width*

- variance  $\sigma^2$
- Gaussian FWHM  $\Delta_G = \text{xxxx cm}^{-1}$
- Lorentzian FWHM  $\Delta_L$
- broadening factor  $\Gamma_{\text{BWF}}$
- asymmetry factor  $Q_{\text{BWF}}$

*Intensity*

- intensity  $I_0 = \text{xxxx cm}^{-1}$

*Intensity*

- integrated intensity  $K_L = \text{xxxx cm}^{-2}$
- integrated area A

*Notes:*

- For position and widths: better to use the unit defined by “*bandlist\_spectral\_unit*”
- For intensity: better to use  $\text{cm}^{-1}$  (metric absorption coefficient) or no unit (relative)
- For integrated intensity: better to use  $\text{cm}^{-2}$  (metric integrated absorption coefficient) or no unit (relative)

*Ex:* for Gaussian fit: ‘central frequency  $\omega_0 = 1254 \text{ cm}^{-1}$ ’, FWHM  $\Delta_G = 23 \text{ cm}^{-1}$ , intensity  $I_0 = 42500 \text{ cm}^{-1}$ ’

### ***Band characteristics: position***

<i>band_characteristic_overlap</i>	enum(text)	U	Band	--	Degree of overlap of the band with another band
		[!_m]	L12		<b>Enum:</b> {extracted, isolated, slightly blended, moderately blended, strongly blended, shoulder-tail, multiple, other, unknown}

*Definitions:*

- ‘*extracted*’: band extracted from a group of bands (deconvolution, ...), therefore the extracted characteristics are assumed to be its own

characteristics

- '*isolated*': band well isolated from any other band, therefore its characteristics are its own characteristics
- '*slightly blended*': band slightly overlapping another band (over the bottom of its wing), but with little effect expected on band characteristics
- '*moderately blended*': band moderately overlapping another band (up to half height), with moderate effects expected on band characteristics (limited shift in position, increase of width and contribution to peak and integrated intensities)
- '*strongly blended*': band strongly overlapping another stronger band (above half height), with strong effect expected on band characteristics (clear shift in position, increase of width and contribution to both peak and integrated intensities)
- '*shoulder-tail*': band completely overlapped by another stronger band (tail) or very strongly overlapped (shoulder), but still slightly shifted in position (no band maximum and wing of the other band seen on both sides), therefore a very strong effect is expected on band characteristics (strong shift in estimated position, increase of width and major contribution of the other band in peak and integrated intensities)
- '*multiple*': band completely overlapped by another band, with only a small shift, therefore appearing as a single band with band characteristics being the combination of those of the two underlying bands (average position and width, about sum of peak and integrated intensities)
- '*other*': other type of overlapping
- '*unknown*': unknown potential overlapping

*Note:*

- this keyword depicts the degree of overlapping of the band with another from an isolated band to one fully merged with another at exactly the same position
- it provide an estimate on how the characteristics of the band may be affected by the overlap with one or more other one(s)

*band\_characteristic\_position\_peak* enum(text) U Band  
 \_method [!!o\_m] L12

-- Method of determination of the band peak position

**Enum:** {peak, fit peak, 90%-max center, first derivative, second derivative, higher order derivative, extrapolated, calculated, estimated, various, other, unknown}

*Condition:* absolute mandatory when “*band\_characteristic\_position\_peak*” ≠ ∅

*Definitions:*

- ‘*peak*’: measured at maximum intensity
- ‘*fit peak*’: determined from peak frequency of band fit function when “*band\_characteristic\_method*” = ‘spectrum fit’
- ‘*90%-max center*’: center frequency at 90% maximum intensity (used for noisy peak)
- ‘*first derivative*’: center from position of the zero of the first derivative of the spectrum
- ‘*second derivative*’: center from position of the minimum of the second derivative of the spectrum
- ‘*higher order derivative*’: center from position of the minimum or zero of high order derivative of the spectrum
- ‘*extrapolated*’: mathematical/theoretical extrapolation of the position from values measured on other bands
  - ex: using harmonic frequencies and interaction parameters determined from a set of bands)
- ‘*calculated*’: position calculated purely theoretically (ab-initio, ...)
- ‘*estimated*’: position estimated by another mean
- ‘*various*’: peak position measured by several of the above methods. Used in particular with compilation of data from various sources
- ‘*other*’: peak position measured by another method than the above listed methods.
- ‘*unknown*’: unknown method

*Note:* difference between center and peak positions can be especially large for wide asymmetric bands. In such a case it is recommended to provide ‘peak’ or ‘90%-max center’ and also the center at half-max in “*band\_characteristic\_position\_center*”.

<i>band_characteristic_position_peak</i>	float	<b>S3</b> [!!o_m]	Band L12	[Ver]	var.	<p>Position of the peak of the band</p> <p><i>Condition:</i> absolute mandatory when “<i>band_characteristic_position_center</i>” = ∅</p> <p><i>Unit:</i> in unit defined by “<i>bandlist_spectral_unit</i>”</p> <ul style="list-style-type: none"> <li>• converted and stored in ‘cm-1’ unit in the database</li> </ul> <p><i>Note:</i> this band peak position can be determined with all spectrum types.</p> <p><i>Note xml:</i> data will be ordered in the xml file based on the increasing value of this field</p>
<i>band_characteristic_position_peak_error</i>	float	U [!!o_m]	Band L12		var.	<p>Absolute uncertainty (+/-) in the position of the band peak</p> <p><i>Condition:</i> absolute mandatory when “<i>band_characteristic_position_peak</i>” ≠ ∅</p> <p><i>Unit:</i> in unit defined by “<i>bandlist_spectral_unit</i>”</p> <ul style="list-style-type: none"> <li>• Converted and stored in ‘cm-1’ unit in the database</li> </ul> <p><i>Note:</i> Positive value, expressed as an absolute symmetric error around nominal value.</p>
<i>band_characteristic_position_center_method</i>	enum(text)	U [!!o_m]	Band L12		--	<p>Method of determination of the band center position</p> <p><b>Enum:</b> {half-max center, fit center, first derivative, second derivative, higher order derivative, extrapolated, calculated, estimated, various, other, unknown}</p> <p><i>Condition:</i> absolute mandatory when “<i>band_characteristic_position_center</i>” ≠ ∅</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- ‘<i>fit center</i>’: determined from center frequency of band fit function when “<i>band_characteristic_method</i>” = ‘spectrum fit’ (center is different from peak for the BWF profile)</li> <li>- ‘<i>half-max center</i>’: center frequency at 50% maximum intensity</li> <li>- ‘<i>first derivative</i>’: center from position of the zero of the first derivative of the spectrum</li> <li>- ‘<i>second derivative</i>’: center from position of the minimum of the second derivative of the spectrum</li> <li>- ‘<i>higher order derivative</i>’: center from position of the minimum or zero</li> </ul>

- of high order derivative of the spectrum
- ‘*extrapolated*’: mathematical/theoretical extrapolation of the position from values measured on other bands
  - ex: using harmonic frequencies and interaction parameters determined from a set of bands)
- ‘*calculated*’: position calculated purely theoretically (ab-initio, ...)
- ‘*estimated*’: position estimated by another mean
- ‘*various*’: center position measured by several of the above methods. Used in particular with compilation of data from various sources
- ‘*other*’: center position measured by another method than the above listed methods.
- ‘*unknown*’: unknown method

<i>band_characteristic_position_center</i>	float	<b>S3</b> <a href="#">[m]</a>	Band L12	<b>[Ver]</b> var.	<p>Position of the band center at half maximum intensity</p> <p><i>Unit:</i> in unit defined by “<i>bandlist_spectral_unit</i>”</p> <ul style="list-style-type: none"> <li>• converted and stored in ‘cm-1’ unit in the database</li> </ul> <p><i>Note:</i> this band center position can be determined with all spectrum types.</p> <p><i>Note:</i> useful for “<i>band_characteristic_position_peak</i>” or asymmetric bands in addition to peak position</p>
<i>band_characteristic_position_center_error</i>	float	U <a href="#">[!o_m]</a>	Band L12	var.	<p>Absolute uncertainty (+/-) of the position of the band center at half maximum intensity</p> <p><i>Condition:</i> absolute mandatory when “<i>band_characteristic_position_center</i>” ≠ ∅</p> <p><i>Unit:</i> in unit defined by “<i>bandlist_spectral_unit</i>”</p> <ul style="list-style-type: none"> <li>• converted and stored in ‘cm-1’ unit in the database</li> </ul> <p><i>Note:</i> Positive value, expressed as an absolute symmetric error around nominal value.</p>
<i>band_characteristic_position_spectral_range_type</i> [-xml]	varchar(255)	S0 <a href="#">[!_c]</a>	Band L12	--	<p>Typical spectral range of the band</p> <p><b>Enum:</b> {gamma, hard X, soft X, EUV, VUV, UV, Vis, NIR, MIR, FIR, sub-</p>

mm, mm, cm, UHF, VHF, HF, MF, LF, VLF, ULF, SLF, ELF}

Definitions: see “parameters\_instrument\_spectral\_range\_type”

→ determined from “band\_characteristic\_position\_peak“

OR with “band\_characteristic\_position\_center“ when

“band\_characteristic\_position\_peak“ = Ø

using the following ranges in cm<sup>-1</sup>:

- ‘gamma’:	10 10 <sup>9</sup> -1 10 <sup>9</sup> cm <sup>-1</sup>	0.1-10pm
- ‘hard X’:	1 10 <sup>9</sup> -50 10 <sup>6</sup> cm <sup>-1</sup>	0.01-0.2nm
- ‘soft X’:	50 10 <sup>6</sup> -1 10 <sup>6</sup> cm <sup>-1</sup>	0.2-10nm
- ‘EUV’:	1 10 <sup>6</sup> -85 000 cm <sup>-1</sup>	10-120 nm
- ‘VUV’:	85 000-50 000 cm <sup>-1</sup>	120-200 nm
- ‘UV’:	50 000-25 000 cm <sup>-1</sup>	200-400 nm
- ‘Vis’:	25 000-10 000 cm <sup>-1</sup>	400-1000 nm
- ‘NIR’:	10 000-4 000 cm <sup>-1</sup>	1-2.5 µm
- ‘MIR’:	4 000-400 cm <sup>-1</sup>	2.5-25 µm
- ‘FIR’:	400-30 cm <sup>-1</sup>	25-300 µm
- ‘sub-mm’:	30-10 cm <sup>-1</sup>	300-1000 µm
- ‘mm’:	10-1 cm <sup>-1</sup>	1-10 mm
- ‘cm’:	1-0.1 cm <sup>-1</sup>	1-10 cm
- ‘UHF’:	0.1-0.01 cm <sup>-1</sup>	0.1-1 m
- ‘VHF’:	10 <sup>-2</sup> -10 <sup>-3</sup> cm <sup>-1</sup>	1-10 m
- ‘HF’:	10 <sup>-3</sup> -10 <sup>-4</sup> cm <sup>-1</sup>	10-100 m
- ‘MF’:	10 <sup>-4</sup> -10 <sup>-5</sup> cm <sup>-1</sup>	0.1-1 km
- ‘LF’:	10 <sup>-5</sup> -10 <sup>-6</sup> cm <sup>-1</sup>	1-10 km
- ‘VLF’:	10 <sup>-6</sup> -10 <sup>-7</sup> cm <sup>-1</sup>	10-100 km
- ‘ULF’:	10 <sup>-7</sup> -10 <sup>-8</sup> cm <sup>-1</sup>	100-1 000 km
- ‘SLF’:	10 <sup>-8</sup> -10 <sup>-9</sup> cm <sup>-1</sup>	1 000-10 000 km
- ‘ELF’:	< 10 <sup>-9</sup> cm <sup>-1</sup>	> 10 000 km

Note: convertor at: <https://www.ape-berlin.de/en/calculator/>

band\_characteristic\_position\_evaluation enum(text) S2 Band  
 [!!\_m] L12

-- Evaluation of the value of band position

**Enum:** {undefined, uncertain, validated, recommended, with caution, not recommended}



*band\_characteristic\_position\_quality\_flag* [-xml] enum(text) S3 Band  
 [!!\_c] L12

-- Quality flag on band position accuracy

**Enum:** {A, B, C, D, E, undefined}

→ Calculated with Q = “position\_peak\_error” when ≠ ∅  
 ELSE

with Q = “position\_center\_error” when ≠ ∅:

- quality\_flag” = ‘A’ when  $0 \leq Q < 1$
- quality\_flag” = ‘B’ when  $1 \leq Q < 3$
- quality\_flag” = ‘C’ when  $3 \leq Q < 6$
- quality\_flag” = ‘D’ when  $6 \leq Q < 15$
- quality\_flag” = ‘E’ when  $15 \leq Q$
- quality\_flag” = ‘undefined’ when “position\_peak\_error” = ∅ AND “position\_center\_error” = ∅

*Definitions:* based on value of “*band\_characteristic\_position\_peak\_error*”

*Definitions:*

- ‘*undefined*’: unpublished value which has not been evaluated by the ‘Solid Band List Committee’
- ‘*uncertain*’: unpublished or published value that is uncertain, and that has not been evaluated by the ‘Solid Band List Committee’
- ‘*validated*’: published value that can be trusted, but that has not been evaluated by the ‘Solid Band List Committee’
- ‘*recommended*’: unpublished or published value recommended by the ‘Solid Band List Committee’
- ‘*with caution*’: unpublished or published value evaluated by the ‘Solid Band List Committee’, but with some potential problem which cannot be checked without better data available
- ‘*not recommended*’: unpublished or published value not recommended by the ‘Solid Band List Committee’ (will be mostly deleted from the database!)

*Notes:*

- The ‘validated’ label is given automatically for published data.
- The ‘recommended’, ‘with caution’, and ‘not recommended’ labels will be only attributed by the ‘Solid Band List Committee’

- 'A': 0~1 cm<sup>-1</sup> uncertainty
- 'B': 1~3 cm<sup>-1</sup> uncertainty
- 'C': 3~6 cm<sup>-1</sup> uncertainty
- 'D': 6-15 cm<sup>-1</sup> uncertainty
- 'E': 15-30 cm<sup>-1</sup> uncertainty
- 'undefined': no value of "band\_characteristic\_position\_peak\_error" and of "band\_characteristic\_position\_center\_error" is provided to assess quality.

*Note:* It is the same quality scale as the one used by the NIST Chemistry webbook.

*Note:*

<i>band_characteristic_position_comments</i>	blob	U <a href="#">[m]</a>	Band L12	--	<p>Comments on the band position and accuracy</p> <p><i>Note:</i> can contain the band position evaluation given by the 'Solid Band List Committee'</p> <p><i>Ex:</i> '90%-max center position used because flat and noisy peak'</p>
--	------	--------------------------	-------------	----	--

### ***Band characteristics: width***

<i>band_characteristic_width_method</i>	enum(text)	U <a href="#">[!o_m]</a>	Band L12	--	<p>Method of determination of band width</p> <p><b>Enum:</b> {fwhm, fit fwhm, hwhm, first derivative, extrapolated, calculated, estimated, various, other, unknown}</p> <p><i>Condition:</i> mandatory when "band_characteristic_width_fwhm" ≠ ∅</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- 'fwhm': measured full width at half maximum (FWHM) of peak intensity</li> <li>- 'fit fwhm': calculated FWHM for band characteristics obtained from a 'spectrum fit'</li> <li>- 'hwhm': measured half width at half maximum (HWHM) of peak intensity. Useful in particular when the band is blended on one side with another band, the width is then estimated on the other half side.</li> <li>- 'first derivative': width from the difference in position of the two</li> </ul>
---	------------	-----------------------------	-------------	----	---

maxima of the first derivative of the spectrum (inflection points of the band)

- ‘*extrapolated*’: mathematical/theoretical extrapolation of the width from values measured on other bands
- ‘*calculated*’: width calculated purely theoretically (ab-initio, ...)
- ‘*estimated*’: width estimated by another mean
- ‘*various*’: width measured by several of the above methods. Used in particular with compilation of data from various sources
- ‘*other*’: width measured by another method than the above listed methods.
- ‘*unknown*’: unknown method

*band\_characteristic\_width\_fwhm* float S3 Band [Ver] var. Full width at half maximum (FWHM) of the band  
[!\_m] L12

*Unit:* in unit defined by “*bandlist\_spectral\_unit*”  
 ⇒ Converted and stored in ‘cm-1’ unit in the database

*Conversion:* for narrow symmetric bands:

When “*bandlist\_spectral\_unit*” = {m-1, Hz, kHz, MHz, GHz, eV, keV}

⇒ simply convert to ‘cm-1’

When “*bandlist\_spectral\_unit*” = {angstrom, nm, micron, mm, m, km}

AND “*band\_characteristic\_position\_center*” ≠ ∅:

⇒ First convert to ‘μm’ and then convert to ‘cm-1’:

$$\Rightarrow \text{fwhm}(\text{cm-1}) = 10^4 * \text{fwhm}(\mu\text{m}) / [\text{band\_characteristic\_position\_center}(\mu\text{m})]^2$$

ELSE when “*band\_characteristic\_position\_center*” = ∅:

and “*band\_characteristic\_position\_peak*” ≠ ∅:

⇒ First convert to ‘μm’ and then convert to ‘cm-1’:

$$\Rightarrow \text{fwhm}(\text{cm-1}) = 10^4 * \text{fwhm}(\mu\text{m}) / [\text{band\_characteristic\_position\_peak}(\mu\text{m})]^2$$

⇒ FWHM(cm-1) = (equation générale)

*Note:*

- the FWHM can only be determined from spectra in ‘absorbance’, ‘absorption coefficient’, ‘**emission**’ or similar/derived spectra such

- as ‘optical constants’ but not ‘transmission’, it can also be given in ‘reflectance’, ...

*band\_characteristic\_width\_fwhm\_error* float U Band  
[!o\_m] L12

var. Absolute uncertainty (+/-) of the full width at half maximum of the band  
*Condition:* mandatory when when “*band\_characteristic\_width\_fwhm*” ≠ ∅

*Unit:* in unit defined by “*bandlist\_spectral\_unit*”

- Converted and stored in ‘cm-1’ unit in the database

*Conversion:* for narrow symmetric bands:

When “*bandlist\_spectral\_unit*” = {m-1, Hz, kHz, MHz, GHz, eV, keV}

⇒ simply convert to ‘cm-1’

When “*bandlist\_spectral\_unit*” = {angstrom, nm, micron, mm, m, km}

AND “*band\_characteristic\_position\_center*” ≠ ∅:

⇒ First convert to ‘μm’ and then convert to ‘cm-1’:

⇒  $accuracy(cm-1) = 10^4 * accuracy(\mu m) / [band\_characteristic\_position\_center(\mu m)]^2$

When “*band\_characteristic\_position\_center*” = ∅:

and “*band\_characteristic\_position\_peak*” ≠ ∅:

⇒ First convert to ‘μm’ and then convert to ‘cm-1’:

⇒  $accuracy(cm-1) = 10^4 * accuracy(\mu m) / [band\_characteristic\_position\_peak(\mu m)]^2$

⇒  $accuracy(cm-1) = (equation\ générale)$

*Note:* Positive value, expressed as an absolute symmetric error around the nominal value.

*band\_characteristic\_width\_shape* openum(text) S2 Band  
[!\_m] L12

-- Type of band shape

**OpenEnum:** {symmetric, gaussian, lorentzian, Breit-Wigner-Fano, voigt, doppler, asymmetric, asymmetric low frequency wing, asymmetric high frequency wing, shoulder, sharp shoulder, broad shoulder, low frequency tail, high frequency tail, undefined, other, unknown}

*Definitions:*

- ‘*symmetric*’: symmetric band without (or with unknown) specific shape
- ‘*gaussian*’: symmetric band with Gaussian profile
- ‘*lorentzian*’: symmetric band with Lorentzian profile
- ‘*Breit-Wigner-Fano*’: asymmetric bands shape typical of resonant scattering phenomena, that reduce to Lorentzian shape when the Fano parameter  $q = 0$ .
- ‘*voigt*’: symmetric band with Voigt profile
- ‘*doppler*’: symmetric band with Doppler profile
- ‘*asymmetric*’: asymmetric band but without one of the two specific types of asymmetry below.
- ‘*asymmetric low frequency wing*’: asymmetric band with an extended wing on the low frequency side (i.e. low wavenumber, high wavelength)
- ‘*asymmetric high frequency wing*’: asymmetric band with an extended wing on the high frequency side (i.e. high wavenumber, low wavelength)
- ‘*shoulder*’: for a band present as a shoulder (no maximum) on the wing of a stronger band
- ‘*sharp shoulder*’: for a band present as a sharp shoulder, i.e., with no maximum but with a marked change of slope on the wing of a stronger band
- ‘*broad shoulder*’: for a band present as a broad shoulder, i.e., with no maximum but with a very progressive change of slope on the wing of a stronger band
- ‘*low frequency tail*’: long tail (with no change of sign of curvature) on the low frequency side (i.e. low wavenumber, high wavelength) of a band.
- ‘*high frequency tail*’: long tail (with no change of sign of curvature) on the high frequency side (i.e. low wavenumber, high wavelength) of a band.
- ‘*undefined*’: for a band with shape difficult to define (because blending with another band, ...)
- ‘*other*’: other shape than the one described above, to be specified in “*band\_characteristic\_width\_comments*”
- ‘*unknown*’: unknown band shape

*Note:* the band shape must be determined with the spectrum in wavenumber (cm-1) or frequency (kHz, ...) unit.

<i>band_characteristic_width_asymmetry_factor</i>	float	U <a href="#">[!o_m]</a>	Band L12	no	<p>Asymmetry factor of the band shape</p> <p><i>Condition:</i> mandatory when “<i>band_characteristic_width_shape</i>” = {asymmetric, asymmetric low frequency wing, asymmetric high frequency wing}</p> <p><i>Definitions:</i></p> <ul style="list-style-type: none"> <li>- The asymmetry factor is the ratio of the HWHM (Half Width at Half Maximum) of the low frequency side (i.e. low wavenumber, high wavelength) to the HWHM on the high frequency side (i.e. high wavenumber, low wavelength).</li> <li>- A symmetric band has thus an asymmetry factor of 1 (“<i>band_characteristic_position_center</i>” = “<i>band_characteristic_position_peak</i>”)</li> <li>- An asymmetric band has a factor &gt;1 when it has a wider low frequency wing (“<i>band_characteristic_position_center</i>” = “<i>band_characteristic_position_peak</i>”), and &lt; 1 when it has a wider high frequency wing (“<i>band_characteristic_position_center</i>” = “<i>band_characteristic_position_peak</i>”).</li> </ul> <p>➔ Calcul: from “<i>band_characteristic_width_fwhm</i>”, “<i>band_characteristic_position_center</i>” and “<i>band_characteristic_position_peak</i>” when there are values for all these KW.</p> <ul style="list-style-type: none"> <li>• ‘asymmetry_factor’ = (‘width_fwhm’/2 + ‘position_peak’ - ‘position_center’) / (‘width_fwhm’/2 - ‘position_peak’ + ‘position_center’)</li> </ul> <p><i>Note:</i> the asymmetry of the band shape must be determined with the spectrum in wavenumber (cm-1) or frequency (kHz, ...) unit.</p>
<i>band_characteristic_width_asymmetry_factor_error</i>	float	U <a href="#">[m]</a>	Band L12	no	<p>Absolute uncertainty (+/-) of the asymmetry factor of the band shape</p> <p><i>Note:</i> Positive value, expressed as an absolute symmetric error around nominal value.</p>

<i>band_characteristic_width_evaluation</i>	enum(text)	S2 [!o_m]	Band L12	-- Evaluation of the value of band width <i>Enum:</i> {undefined, uncertain, validated, recommended, with caution, not recommended} <i>Condition:</i> mandatory when “ <i>band_characteristic_width_fwhm</i> ” ≠ ∅ <i>Definitions:</i> see “ <i>band_characteristic_position_evaluation</i> ”
<i>band_characteristic_width_quality_flag</i> [-xml]	enum(text)	S3 [!o_c]	Band L12	-- Quality flag on band width accuracy <i>Enum:</i> {A, B, C, D, E, undefined} → Calculated with Q = “width_fwhm_error”: <ul style="list-style-type: none"> <li>• quality_flag” = ‘A’ when <math>0 \leq Q &lt; 0.3</math></li> <li>• quality_flag” = ‘B’ when <math>0.3 \leq Q &lt; 1</math></li> <li>• quality_flag” = ‘C’ when <math>1 \leq Q &lt; 2</math></li> <li>• quality_flag” = ‘D’ when <math>2 \leq Q &lt; 5</math></li> <li>• quality_flag” = ‘E’ when <math>5 \leq Q</math></li> <li>• quality_flag” = ‘undefined’ when “width_fwhm_error” = {∅, NULL}</li> </ul> <i>Definitions:</i> based on value of “ <i>band_characteristic_width_fwhm_error</i> ” <ul style="list-style-type: none"> <li>- ‘A’: 0~0.3 cm<sup>-1</sup> uncertainty</li> <li>- ‘B’: 0.3~1 cm<sup>-1</sup> uncertainty</li> <li>- ‘C’: 1~2 cm<sup>-1</sup> uncertainty</li> <li>- ‘D’: 2~5 cm<sup>-1</sup> uncertainty</li> <li>- ‘E’: 5~10 cm<sup>-1</sup> uncertainty</li> <li>- ‘undefined’: no value of “<i>band_characteristic_width_fwhm_error</i>” provided to asses quality.</li> </ul> <i>Note:</i> Same as position quality scale used by the NIST Chemistry webbook. <i>Note:</i>
<i>band_characteristic_width_comments</i>	blob	U [m]	Band L12	-- Comments on the band width <i>Note:</i> can contain the band width evaluation given by the ‘Solid Band List Committee’ <i>Ex:</i>

- 'noisy low frequency shoulder on asymmetric band'
- 'width possibly overestimated by 5-10 cm<sup>-1</sup> due to the strong asymmetry with low frequency wing possibly due to blending with another weaker mode'

---

***Band characteristics: peak intensity***

*band\_characteristic\_peak\_intensity\_method* enum(text) U Band  
 [!o\_m] L12

-- Method of determination of band intensity

**Enum:** {peak intensity, baseline corrected peak intensity, fit intensity, extrapolated, calculated, estimated, various, other, unknown}

*Condition:* mandatory when “*band\_characteristic\_peak\_intensity\_abscoef*” ≠ {∅, NULL}

OR

when “*band\_characteristic\_peak\_intensity\_relative*” ≠ {∅, NULL}

*Definitions:*

- '*peak intensity*': intensity measured on a spectrum at maximum intensity (peak), or on the top of a shoulder
- '*baseline corrected peak intensity*': intensity measured on a spectrum at maximum intensity after baseline correction of the band. This may allow to determine the peak intensity of shoulders and of (weak) bands blended with another (stronger one)
- '*fit intensity*': calculated peak intensity obtained from the component (Gaussian, ...) of a 'spectrum fit'
- '*extrapolated*': mathematical/theoretical extrapolation of the peak intensity from values measured on other bands
- '*calculated*': peak intensity calculated purely theoretically (ab-initio, ...)
- '*estimated*': intensity estimated by another mean (isotopic abundance ration, ...)
- '*various*': intensity measured by several of the above methods. Used in particular with compilation of data from various sources
- '*other*': peak intensity measured by another method than the above listed methods. To be described in



“*band\_characteristic\_peak\_intensity\_comments*”

ex: ‘integrated intensity / width’

- ‘*unknown*’: unknown method

<i>band_characteristic_peak_intensity_abscoef</i>	float	S3 [!o_m]	Band L12	[Ver]	cm-1	Metric absorption coefficient value at band peak <i>Constraint</i> : only when “ <i>band_type</i> ” = ‘absorption’ <i>Condition #1</i> : mandatory when “ <i>band_type</i> ” = ‘absorption’ AND <i>Condition #2</i> : when “ <i>band_characteristic_peak_intensity_relative</i> ” = $\emptyset$ <i>Units</i> : <ul style="list-style-type: none"><li>• in ‘cm-1’</li></ul> <i>Notes</i> : <i>List of existing units</i> : <ul style="list-style-type: none"><li>• cm-1, m-1, cm2.g-1, m2.kg-1, mL.g-1.cm-1, cm2.mol-1, cm2.mmol-1, m2.mol-1, L.mol-1.cm-1, cm2.molec-1, m2.molec-1, cm-1.atm-1</li></ul> <i>Unit definitions</i> : <ul style="list-style-type: none"><li>- ‘cm-1’, ‘m-1’: for ‘metric absorption coefficient’ <math>\alpha_a</math> (cm<sup>-1</sup>, m<sup>-1</sup>)</li><li>- ‘cm2.g-1’, ‘m2.kg-1’, ‘mL.g-1.cm-1’: for mass absorption coefficient <math>\alpha_m</math> (cm<sup>2</sup>.g<sup>-1</sup>, m<sup>2</sup>.kg<sup>-1</sup>, mL.g<sup>-1</sup>.cm<sup>-1</sup>)</li><li>- ‘cm2.mol-1’, ‘cm2.mmol-1’, ‘m2.mol-1’, ‘L.mol-1.cm-1’: for molar absorption (or attenuation) coefficient <math>\epsilon</math> (cm<sup>2</sup>.mol<sup>-1</sup>, cm<sup>2</sup>.mmol<sup>-1</sup>, m<sup>2</sup>.mol<sup>-1</sup>, L.mol<sup>-1</sup>.cm<sup>-1</sup>)</li><li>- ‘cm2.molec-1’, ‘m2.molec-1’: for molecular absorption cross section or attenuation coefficient <math>\sigma</math> (cm<sup>2</sup>.molec<sup>-1</sup>, m<sup>2</sup>.molec<sup>-1</sup>)<ul style="list-style-type: none"><li>• Note: sometimes simply written as absorption cross section ‘cm<sup>2</sup>’, ‘m<sup>2</sup>’</li></ul></li><li>- ‘cm-1.atm-1’: for ‘*** absorption coefficient’ <math>\alpha_a</math> (cm<sup>-1</sup>.atm<sup>-1</sup>)</li></ul> <i>Unit conversions</i> : <ul style="list-style-type: none"><li>- mass absorption coefficient:<ul style="list-style-type: none"><li>• <math>\alpha_m = \alpha_a / \rho</math> with ‘<math>\rho</math>’ the density (in g.cm<sup>-3</sup>)</li></ul></li><li>- molar attenuation coefficient:</li></ul>
---	-------	--------------	-------------	-------	------	---

- $\epsilon = (\alpha_d / \rho) \cdot M / \ln(10)$  with ‘M’ the molar mass (in g.mol<sup>-1</sup>). The molar attenuation coefficient is usually decadic [ $\epsilon = A / (c \cdot \ell)$  with  $A = -\log_{10}(I/I_0)$  the absorbance,  $c$  the molar concentration (mol.cm<sup>-3</sup>),  $\ell$  the pathlength (cm).]
- molecular absorption cross section:
  - $\sigma = (\alpha_d / \rho) \cdot M / N_A$  with ‘ $N_A$ ’ the Avogadro's number (number of molecules per mole)
- \*\*\* ‘atmospheric equivalent column density’ absorption coefficient:
  - $\alpha_a = ???$

*Notes:*

- only for bands measured in absorption.
- without meaning for the othe types of bandlists

<i>band_characteristic_peak_intensity_abscoef_error</i>	float	U [!o_m]	Band L12	cm-1	<p>Absolute uncertainty (+/-) of the metric absorption coefficient intensity value at peak</p> <p><i>Condition:</i> mandatory when “<i>band_characteristic_peak_intensity_abscoef</i>” ≠ ∅</p> <p><i>Definition:</i></p> <ul style="list-style-type: none"> <li>- Positive value, expressed as an absolute error around the nominal value</li> </ul> <p><i>Units:</i></p> <ul style="list-style-type: none"> <li>• in ‘cm-1’</li> </ul>
<i>band_characteristic_peak_intensity_abscoef_specific</i>	float	S3 [m]	Band L12	[Ver] cm-1	<p>Specific metric absorption coefficient of the species at peak</p> <p><i>Constraint:</i> only when “<i>band_type</i>” = ‘absorption’</p> <p><i>Definition:</i></p> <ul style="list-style-type: none"> <li>- it is the metric absorption coefficient of the band divided by the abundance of the species producing the band</li> </ul> <p><i>Units:</i></p> <ul style="list-style-type: none"> <li>• in ‘cm-1’</li> </ul> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- in particular for isotopic species it is the metric absorption coefficient</li> </ul>

of the band divided by the isotopic abundance of the species producing the band

<i>band_characteristic_peak_intensity_abscoef_specific_error</i>	float	U [m]	Band L12	cm-1	Absolute uncertainty (+/-) in specific metric absorption coefficient at peak <i>Definition:</i> - Positive value, expressed as an absolute error around the nominal value <i>Units:</i> • in 'cm-1'
<i>band_characteristic_peak_intensity_relative</i>	float	S3 [!o_m]	Band L12	[Ver] no	Relative intensity value at band peak, compared to the peak intensity of the band occurring at a reference position <i>Condition:</i> mandatory when “ <i>band_characteristic_peak_intensity_abscoef</i> ” = ∅ <i>Definition:</i> determined as the ratio between the peak intensity of the band to that of the reference band of the same transition type (electronic, infrared or Raman). <i>Notes:</i> - provide the ratio value, not in % - the 'relative intensity' is relative to the intensity of the band situated at the position given in “ <i>bandlist_reference_position_electronic</i> ” or “ <i>bandlist_reference_position_infrared</i> ” (relative intensity = '1.0') depending on the type of transition. - This wavelength reference is generally that of the peak of the strongest band of the band list with the same type of transition (for infrared: preferentially the strongest fundamental vibration mode), or of a standard reference band - for absorption bands it is given in absorbance - for reflectance it is given in relative band depth - for emission (Raman, thermal, fluorescence) it is given in emission intensity - can also be given in parallel with “ <i>band_characteristic_peak_intensity_abscoef</i> ” when “ <i>band_type</i> ” =

'absorption'

*band\_characteristic\_peak\_intensity\_relative\_error* float U Band  
 [!o\_m] L12

*no* Absolute uncertainty (+/-) of the relative peak intensity value  
*Condition:* mandatory when “*band\_characteristic\_peak\_intensity\_relative*” ≠ ∅

*Definition:*

- Positive value, expressed as an absolute error around the nominal value

*band\_characteristic\_peak\_intensity\_strength* enum(text) S3 Band  
 [!\_m] L12

*--* Qualitative (relative) spectroscopic classification of band peak intensity

**Enum:** {ia, ew, vvw, vw, w, m, s, vs, vvs, es, unknown}

*Definitions:*

	metric abscoef (cm <sup>-1</sup> )	k & relative	rel. reflectance
- 'ia': inactive	< 0.0002	< 2e-8	< 0.0002
- 'ew': extremely weak	0.0002-0.02	2e-8~2e-6	0.0002-0.002
- 'vvw': very very weak	0.02-0.2	2e-6~2e-5	0.002-0.005
- 'vw': very weak	0.2-2	2e-5~2e-4	0.005-0.02
- 'w': weak	2-20	2e-4~2e-3	0.02-0.05
- 'm': medium	20-200	0.002~0.02	0.05-0.25
- 's': strong	200-2000	0.02~0.2	0.25-0.75
- 'vs': very strong	2e3-2e4	0.2~2	0.75-1
- 'vvs': very very strong	2e4-2e5	2-20*	1-1.25*
- 'es': extremely strong	> 2e5	> 20*	> 1.25*

*Notes:*

- mostly for absorption bands (abscoef and relative scales (=k)), but also reflectance (relative reflectance scale), fluorescence and possibly thermal emission (relative scale)
- use metric absorption coefficients (“*band\_characteristic\_peak\_intensity\_abscoef*”) when present, possibly complemented by relative intensity where missing
- typically the strongest fundamental vibration band (IR) of a molecule is ‘vs’. The strongest electronic transitions (UV) are ‘vvs’ or ‘ew’
- \*: these are values for UV bands relative to the strongest fundamental

IR vibration band

- the ranges of values for ‘*band\_characteristic\_peak\_intensity\_relative*’ are typically the same as for k, i.e. assuming that the strongest fundamental vibration band has a metric absorption coefficient in the range 5000-20000 cm<sup>-1</sup>.
- the scale for reflectance is different due to the non-linear radiative transfert (possibly also usable for thermal emission)

*band\_characteristic\_peak\_intensity\_evaluation* enum(text) S2 Band  
[!o\_m] L12

-- Evaluation of the value of band peak intensity

**Enum:** {undefined, uncertain, validated, recommended, with caution, not recommended}

*Condition:* mandatory when “*band\_characteristic\_peak\_intensity\_abscoef*” ≠ {∅, NULL}

OR

when “*band\_characteristic\_peak\_intensity\_relative*” ≠ {∅, NULL}

*Definitions:* see “*band\_characteristic\_position\_evaluation*”

*band\_characteristic\_peak\_intensity\_quality\_flag* [-xml] enum(text) S3 Band  
[!o\_c] L12

-- Quality flag on the accuracy of the band peak intensity

*Note:* will be given by the ‘Solid Band List Committee’

**Enum:** {A, B, C, D, E, undefined}

→ Calculated with  $Q = 100 * \frac{\text{“peak\_intensity\_abscoef\_error”}}{\text{“peak\_intensity\_abscoef”}}$  when “*peak\_intensity\_abscoef\_error*” ≠ ∅  
ELSE

with  $Q = 100 * \frac{\text{“peak\_intensity\_relative\_error”}}{\text{“peak\_intensity\_relative”}}$  when “*peak\_intensity\_relative\_error*” ≠ ∅

- “*quality\_flag*” = ‘A’ when  $0 \leq \text{“Q”} < 2$
- “*quality\_flag*” = ‘B’ when  $2 \leq \text{“Q”} < 5$
- “*quality\_flag*” = ‘C’ when  $5 \leq \text{“Q”} < 10$
- “*quality\_flag*” = ‘D’ when  $10 \leq \text{“Q”} < 25$
- “*quality\_flag*” = ‘E’ when  $25 \leq \text{“Q”}$
- “*quality\_flag*” = ‘undefined’ when “*peak\_intensity\_abscoef\_error*” = {∅, NULL} AND “*peak\_intensity\_relative\_error*” = {∅, NULL}

- “quality\_flag” = ‘undefined’ when “peak\_intensity\_abscoef” OR “peak\_intensity\_relative” = {Ø, NULL}

*Definitions:* based on value of  
 “band\_characteristic\_peak\_intensity\_abscoef\_error”  
 or “band\_characteristic\_peak\_intensity\_relative\_error”

- ‘A’: < 2% uncertainty
- ‘B’: 2~5% uncertainty
- ‘C’: 5~10% uncertainty
- ‘D’: 10~25% uncertainty
- ‘E’: > 25% uncertainty
- ‘undefined’: no value of  
 “band\_characteristic\_peak\_intensity\_abscoef\_error” and of  
 “band\_characteristic\_peak\_intensity\_relative\_error” is provided or can  
 be estimated to asses quality.

*Note:*

- based on the relative accuracy of band peak intensity  
 (“band\_characteristic\_peak\_intensity\_abscoef\_error” or  
 “band\_characteristic\_peak\_intensity\_relative\_error”)

<i>band_characteristic_peak_intensity_comments</i>	blob	U <a href="#">[m]</a>	Band L12	-- Comments on the band peak intensity  <i>Ex:</i> ‘absorption intensity on a strongly asymmetric peak’  <i>Note:</i> can contain the band peak intensity evaluation given by the ‘Solid Band List Committee’
--	------	--------------------------	-------------	---

***Band characteristics: integrated intensity***

<i>band_characteristic_integrated_intensity_method</i>	enum(text)	U <a href="#">[!o_m]</a>	Band L12	-- Method of determination of band integrated intensity  <b>Enum:</b> {band integrated intensity, width x peak intensity, fit integrated intensity, extrapolated, calculated, estimated, various, other, unknown}  <i>Condition:</i> mandatory when “band_characteristic_integrated_intensity_abscoef” ≠ {Ø, NULL} OR
--	------------	-----------------------------	-------------	---

when “*band\_characteristic\_integrated\_intensity\_relative*” ≠ {∅, NULL}

*Definitions:*

- ‘*band integrated intensity*’: spectrum band integration (band integral)
- ‘*width x width intensity*’: band integral obtained by the product of measured peak intensity and measured FWHM (for bands with Gaussian, Lorentzian, Voigt shapes).  
*Note:* x 0.96 for Gaussian bands, & for lorentzian
- ‘*fit integrated intensity*’: calculated integrated intensity from the component (Gaussian, ...) obtained by a ‘spectrum fit’. It will be equal to the product of the fit ‘*band\_peak\_intensity*’ and fit ‘*band\_width*’ for most types of ‘*band\_shape\_fit\_function*’.
- ‘*extrapolated*’: mathematical/theoretical extrapolation of the integrated intensity from values measured on other bands
- ‘*calculated*’: integrated intensity calculated purely theoretically (ab-initio, ...)
- ‘*estimated*’: intensity estimated by another mean (isotopic abundance ration, ...)
- ‘*various*’: intensity measured by several of the above methods. Used in particular with compilation of data from various sources
- ‘*other*’: integrated intensity measured by another method than the above listed methods.
- ‘*unknown*’: unknown method

*band\_characteristic\_integrated\_intensity\_abscoef* float

S3  
[!o\_m]

Band [Ver]  
L12

cm-2

Metric absorption coefficient integrated over the band

*Condition #1:* only when “*band\_type*” = 'absorption'

AND

*Condition #2:* mandatory when

“*band\_characteristic\_integrated\_intensity\_relative*” = ∅

*Units:*

- in ‘cm-2’

*Notes:*

*List of units:*

- cm-2, m-2, cm.g-1, m.kg-1, mL.g-1.cm-2, cm.mol-1, cm.mmol-1,

m.mol-1, cm.molec-1, m.molec-1, cm<sup>2</sup>.eV, cm<sup>2</sup>.nm, L.mol-1.cm-2, cm-2.atm-1

*Unit definitions:*

- 'cm-2', 'm-2': for 'metric integrated absorption coefficient', **A<sub>d</sub>** (cm<sup>-2</sup>, m<sup>-2</sup>)
- 'cm.g-1', 'm.kg-1', 'mL.g-1.cm-2': for mass integrated absorption coefficient, **A<sub>m</sub>** (cm.g<sup>-1</sup>, m.kg<sup>-1</sup>, mL.g<sup>-1</sup>.cm<sup>-2</sup>)
- 'cm.mol-1', 'cm.mmol-1', 'm.mol-1', 'L.mol-1.cm-2': for molar integrated absorption/attenuation coefficient, **E** (cm.mol<sup>-1</sup>, cm.mmol<sup>-1</sup>, m.mol<sup>-1</sup>, L.mol<sup>-1</sup>.cm<sup>-2</sup>)
- 'cm.molec-1', 'm.molec-1' for molecular integrated attenuation coefficient, **Σ** (cm.molec<sup>-1</sup>, m.molec<sup>-1</sup>)
- 'cm<sup>2</sup>.eV', 'cm<sup>2</sup>.nm' for molecular integrated absorption cross section (cm<sup>2</sup>.eV, cm<sup>2</sup>.nm)
  - Note: this unit is generally used only to for electronic absorption bands.
- 'cm-2.atm-1' for \*\*\* 'atmospheric column density' integrated attenuation coefficient, \*\* (cm<sup>-2</sup>.atm<sup>-1</sup>)

*Unit concordance:*

- integrated intensity unit corresponding to the peak absorption coefficient unit:
  - cm-1           =>  cm-2
  - m-1           =>  m-2
  - cm<sup>2</sup>.g-1       =>  cm.g-1
  - m<sup>2</sup>.kg-1       =>  m.kg-1
  - mL.g-1.cm-1  =>  mL.g-1.cm-2
  - cm<sup>2</sup>.mol-1     =>  cm.mol-1
  - cm<sup>2</sup>.mmol-1   =>  cm.mmol-1
  - m<sup>2</sup>.mol-1     =>  m.mol-1
  - cm<sup>2</sup>.molec-1  =>  cm.molec-1,
  - m<sup>2</sup>.molec-1   =>  m.molec-1
  - cm<sup>2</sup>(.molec-1) =>  cm<sup>2</sup>.eV or cm<sup>2</sup>.nm
  - L.mol-1.cm-1 =>  L.mol-1.cm-2



- cm-1.atm-1 => cm-2.atm-1

*Unit conversions:*

- mass integrated absorption coefficient:
  - $A_m = A_d / \rho$  with ‘ $\rho$ ’ the density (in g.cm<sup>-3</sup>)
- molar integrated attenuation coefficient:
  - $E = (A_d / \rho) \cdot M / \ln(10)$  with ‘ $M$ ’ the molar mass (in g.mol<sup>-1</sup>).  
The molar attenuation coefficient is usually decadic [ $\epsilon = A / (c \cdot \ell)$  with  $A = -\log_{10}(I/I_0)$  is the absorbance,  $c$  the molar concentration (mol.cm<sup>-3</sup>),  $\ell$  the pathlength (cm).]
- molecular integrated attenuation coefficient:
  - $\Sigma = (A_d / \rho) \cdot M / N_A$  with ‘ $N_A$ ’ the Avogadro's number (6.022 10<sup>23</sup> molec/mole)
- molecular integrated absorption cross section:

*Notes:*

- only for bands measured in absorption.
- without meaning for the othe types of bandlists

<i>band_characteristic_integrated_intensity_abscoef_error</i> float	U [!o_m]	Band L12	cm-2	Absolute uncertainty (+/-) in band intensity integrated over the band <i>Condition:</i> mandatory when “ <i>band_characteristic_integrated_intensity_abscoef</i> ” ≠ ∅ <i>Definition:</i> - Positive value, expressed as an absolute error around the nominal value <i>Units:</i> • in ‘cm-2’
<i>band_characteristic_integrated_intensity_abscoef_specific</i> float	S3 [m]	Band L12	[Ver] cm-2	Specific metric absorption coefficient of the species integrated over the band <i>Constraint:</i> only when “ <i>band_type</i> ” = 'absorption' <i>Definition:</i> - it is the metric integrated absorption coefficient of the band divided by the fractional abundance of the species producing the band <i>Units:</i>

				<ul style="list-style-type: none"> <li>• in 'cm-2'</li> </ul>
				<p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- in particular for isotopic species it is the metric integrated absorption coefficient of the band divided by the isotopic fractional abundance of the species producing the band</li> </ul>
<i>band_characteristic_integrated_intensity_abscoef_specific_error</i>	float	U [m]	Band L12	<p>cm-2 Absolute uncertainty (+/-) in specific metric absorption coefficient integrated over the band</p> <p><i>Definition:</i></p> <ul style="list-style-type: none"> <li>- Positive value, expressed as an absolute error around the nominal value</li> </ul> <p><i>Units:</i></p> <ul style="list-style-type: none"> <li>• in 'cm-2'</li> </ul>
<i>band_characteristic_integrated_intensity_relative</i>	float	S3 [!o_m]	Band L12	<p>[Ver] <i>no</i> Relative integrated band intensity, compared to the integrated intensity of the band occurring at a reference position</p> <p><i>Condition:</i> mandatory when “<i>band_characteristic_integrated_intensity_abscoef</i>” = Ø</p> <p><i>Definition:</i> determined as the ratio between the integrated intensity of the band to that of the reference band of the same transition type (electronic, infrared or Raman).</p> <p><i>Notes:</i></p> <ul style="list-style-type: none"> <li>- provide the ratio value, not in %</li> <li>- the 'relative intensity' is relative to the integrated intensity of the band situated at the position given in “<i>bandlist_reference_position_electronic</i>” or “<i>bandlist_reference_position_infrared</i>” (relative peak intensity = ‘1.0’). This wavelength reference is generally that of the peak of the strongest band of the band list (preferentially the strongest fundamental vibration mode), or of a standard reference band</li> <li>- for absorption bands it is given in integrated absorbance</li> <li>- for reflectance it is given in integrated band depth area</li> <li>- for emission (Raman, thermal, fluorescence) it is given in integrated</li> </ul>

- emission intensity
- can also be given in parallel with “*band\_characteristic\_integrated\_intensity\_abscoef*“ when “*band\_type*” = 'absorption'

*band\_characteristic\_integrated\_intensity\_relative\_error* float

U Band  
[!o\_m] L12

no Absolute uncertainty (+/-) in relative integrated band intensity

*Condition:* mandatory when “*band\_characteristic\_integrated\_intensity\_relative*” ≠ ∅

*Definition:*

- Positive value, expressed as an absolute around the nominal value

*Note:*

*band\_characteristic\_integrated\_intensity\_strength* enum(text)

S3 Band  
[m] L12

-- Qualitative (relative) spectroscopic classification of integrated band intensity

**Enum:** {ia, ew, vvw, vw, w, m, s, vs, vvs, es, unknown}

*Definitions:*

	int.abscoef (cm <sup>-2</sup> )	relative	rel. reflectance
- 'ia': inactive	< 0.002	< 2e-8	< 0.0002
- 'ew': extremely weak	0.002-0.2	2e-8~2e-6	0.0002-0.002
- 'vvw': very very weak	0.2-2	2e-6~2e-5	0.002-0.005
- 'vw': very weak	2-20	2e-5~2e-4	0.005-0.02
- 'w': weak	20-200	2e-4~2e-3	0.02-0.05
- 'm': medium	200-2000	0.002~0.02	0.05-0.25
- 's': strong	2e3-2e4	0.02~0.2	0.25-0.75
- 'vs': very strong	2e4-2e5	0.2~2	0.75-1
- 'vvs': very very strong	2e5-2e6	2-20*	1-1.25*
- 'es': extremely strong	> 2e6	> 20*	> 1.25*

*Notes:*

- mostly for absorption bands (int. abscoef and relative intensity scales), but also Raman (relative intensity scale), reflectance (relative reflectance scale), fluorescence and possibly thermal emission (relative scale)
- use metric integrated absorption coefficients

- (“*band\_characteristic\_integrated\_intensity\_abscoef*”) when present, possibly complemented by relative intensity where missing
- typically, the strongest fundamental vibration band (IR or Raman) of a molecule is ‘vs’ in absorbance. The strongest electronic transitions (UV) are ‘vvs’
- \*: these are values for UV bands relative to the strongest fundamental IR band
- the strongest fundamental vibration band has a metric integrated absorption coefficient in the range  $1e5 - 2e5 \text{ cm}^{-2}$  (extremal ex:  $\nu_1(\text{CO}) = 240000$ : vvs)
- the strongest electronic band has a metric integrated absorption coefficient in the range  $1e6 - 2e6 \text{ cm}^{-2}$  (ex:  $\text{CO} = :$  vvs)
- the scale for reflectance is different due to the non-linear radiative transfert (possibly also usable for thermal emission)

*band\_characteristic\_integrated\_intensity\_evaluation* enum(text)

S2 Band  
[!o\_m] L12

-- Evaluation of the value of band integrated intensity

**Enum:** {undefined, uncertain, validated, recommended, with caution, not recommended}

*Condition:* mandatory when

“*band\_characteristic\_integrated\_intensity\_abscoef*”  $\neq \{\emptyset, \text{NULL}\}$

OR

when “*band\_characteristic\_integrated\_intensity\_relative*”  $\neq \{\emptyset, \text{NULL}\}$

*Definitions:* see “*band\_characteristic\_position\_evaluation*”

*band\_characteristic\_integrated\_intensity\_quality\_flag* enum(text)

S3 Band  
[!\_c] L12

-- Quality flag on the accuracy of the band integrated intensity.

*Note:* will be given by the ‘Solid Band List Committee’

**Enum:** {A, B, C, D, E, undefined}

→ Calculated with  $Q = 100 * \frac{\text{“integrated\_intensity\_abscoef\_error”}}{\text{“integrated\_intensity\_abscoef”}}$  when “*integrated\_intensity\_abscoef\_error*”  $\neq \emptyset$

OR

OR

with  $Q = 100 * \frac{\text{“integrated\_intensity\_relative\_error”}}{\text{“integrated\_intensity\_relative”}}$  when “*integrated\_intensity\_relative\_error*”  $\neq \emptyset$

- “quality\_flag” = ‘A’ when  $0 \leq “Q” < 2$
- “quality\_flag” = ‘B’ when  $2 \leq “Q” < 5$
- “quality\_flag” = ‘C’ when  $5 \leq “Q” < 10$
- “quality\_flag” = ‘D’ when  $10 \leq “Q” < 25$
- “quality\_flag” = ‘E’ when  $25 \leq “Q”$
- “quality\_flag” = ‘undefined’ when  
“integrated\_intensity\_abscoef\_error” = {Ø, NULL} AND  
“integrated\_intensity\_relative\_error” = {Ø, NULL}
- “quality\_flag” = ‘undefined’ when “integrated\_intensity\_abscoef” OR  
“integrated\_intensity\_relative” = {Ø, NULL}

*Definitions:* based on value of  
“band\_characteristic\_integrated\_intensity\_abscoef\_error”  
or “band\_characteristic\_integrated\_intensity\_relative\_error”

- ‘A’: < 2% uncertainty
- ‘B’: 2~5% uncertainty
- ‘C’: 5~10% uncertainty
- ‘D’: 10~25% uncertainty
- ‘E’: > 25% uncertainty
- ‘undefined’: no value of  
“band\_characteristic\_integrated\_intensity\_abscoef\_error” and of  
“band\_characteristic\_integrated\_intensity\_relative\_error” is provided  
or can be estimated to asses quality.

*Notes:*

- based on the relative accuracy of band integrated intensity  
(“band\_characteristic\_integrated\_intensity\_abscoef\_error” or  
“band\_characteristic\_integrated\_intensity\_relative\_error”)

<i>band_characteristic_integrated_intensity_comments</i>	blob	U <a href="#">[m]</a>	Band L12	--	Comments on the band integrated intensity  <i>Ex:</i> ‘long high frequency wing not taken into account in integrated intensity (cut at 1520 cm-1)’  <i>Note:</i> can be the band integrated intensity evaluation given by the ‘Solid Band List Committee’
--	------	--------------------------	-------------	----	---

---

### ***Band preview in the bandlist***

<i>band_characteristic_bandlist_nominal_flag</i>	boolean	P [!_m]	Band	-- Flag defining if this set of band characteristics is part of the nominal band list <b>BoolEnum:</b> {yes, no} or {true, false} <i>Constraint:</i> mandatory to have a maximum of one value = ‘yes’ per band <i>Notes:</i> <ul style="list-style-type: none"> <li>- need to select a set of band characteristics (corresponding to one set of environment parameters, plus possible variations in composition of the constituent) per band, that well represents the nominal band list</li> <li>- It is best to choose the sets of environment parameters and constituent composition that are the most homogeneous in terms of temperature/pressure values and composition.</li> <li>- the set of band characteristics selected for this band will be also part of the schematic list of bands (“<i>bandlist_list_bands</i>”) and of the synthetic spectrum (“<i>bandlist_synthetic_spectrum</i>”) describing the band list.</li> <li>- it will be also part of the initial bandlist selection for the dynamic plot</li> </ul>
--	---------	------------	------	--

---

### ***Band assignment and characteristics references***

<i>band_publications</i>	<i>List [L14]</i>			£: Publications in which information on this band are published
<i>band_publication_uid</i> [*]	varchar(255)	S1b+Sli 2 [!o_m]	Band Publi L14	-- Link to the existing UID of the publications in which information on this band is published <i>Condition:</i> mandatory when “ <i>band_publication_spectrum_uid</i> ” = {Ø} AND when “ <i>band_data_publication_link</i> ” = {Ø} <i>Notes:</i> <ul style="list-style-type: none"> <li>- allow to know from which publication come the information of this band</li> <li>- these papers should be in the bibliography database, with “<i>publication_content</i>” = 'band list data'</li> </ul>



---

<i>band_publication_number</i> [-xml]	int(2)	P [c]	Band	--	Number of publications of the band ➔ calculated from “ <i>band_publication_uid</i> ” <i>Note:</i> created for internal search use to allow to pinpoint bands without reference.
<i>band_publication_comments</i>	blob	U [m]	Band	--	Comments about the band characteristics in the publications or in the linked data <i>Note:</i> for exemple which characteristics of the band is published, and in which publication ... <i>Ex:</i> ‘position and width of the band is in Grundy et al. 2002, integrated intensity in Quirico et al. 1997. Band attribution in Schmitt et al. 2017’

---