Development of a Solid Spectroscopy Data Model (SSDM)

GhoSST

"Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service

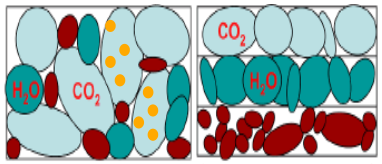
Bernard Schmitt, Damien Albert
and the SSDM Expert group*

Laboratoire de Planétologie de Grenoble (future IPAG), CNRS / UJF

Observatoire OSUG des Sciences de l'Univers de Grenoble

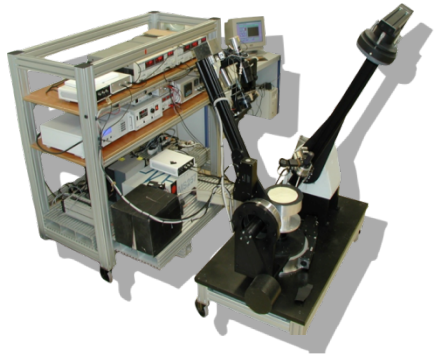
Laboratoire de Planétologie Grenoble

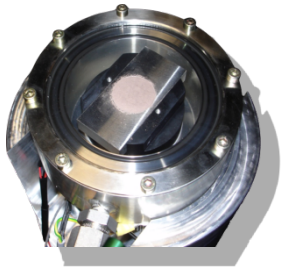
SSDM general structure



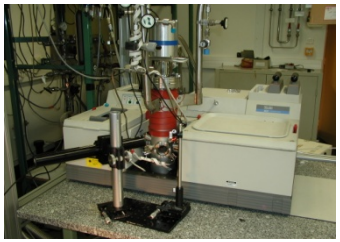
SAMPLE

INSTRUMENT

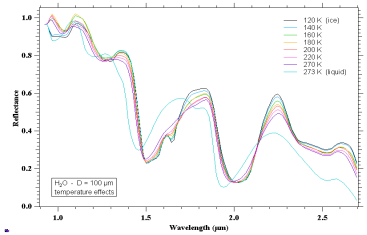




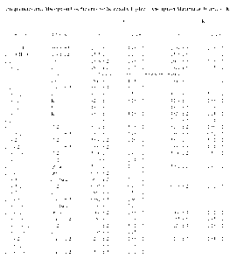
EXPERIMENT



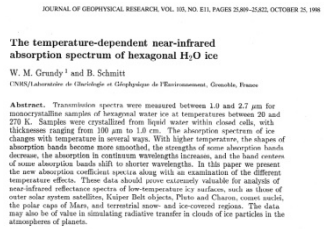
SPECTRA



BAND LIST



REFERENCES



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The temperature-dependent near-infrared absorption spectrum of hexagonal H_2O ice

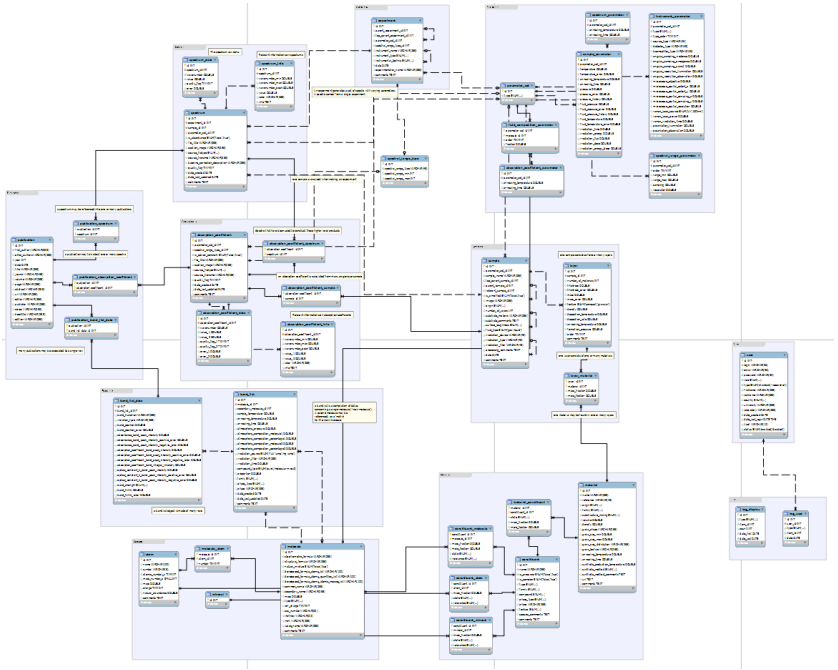
W. M. Grundy [1] and B. Schmitt

CNRS/Laboratoire de Glaciologie et Géophysique de l'Environnement, Grenoble, France

Abstract. Transmission spectra were measured between 1.0 and 2.7 µm for nanocrystalline samples of hexagonal water ice at temperatures between 20 and 270 K. Samples were crystallized from liquid water within closed cells, with thicknesses ranging from 100 µm to 1.0 cm. The absorption spectrum of ice changes with temperature in several ways. With higher temperature, the shapes of absorption bands become more smoothed, the strengths of some absorption bands decrease, the absorption in continuum wavelengths increases, and the band centers of some absorption bands shift to shorter wavelengths. In this paper we present the new absorption coefficient spectra along with an examination of the different temperature effects. These data should prove extremely valuable for analysis of near-infrared reflectance spectra of low-temperature icy surfaces, such as those of outer solar system satellites, Kuiper Belt objects, Pluto and Charon, comet nuclei, the polar caps of Mars, and terrestrial snow- and ice-covered regions. The data may also be of value in simulating radiative transfer in clouds of ice particles in the atmospheres of planets.

Solid Spectroscopy Data Model

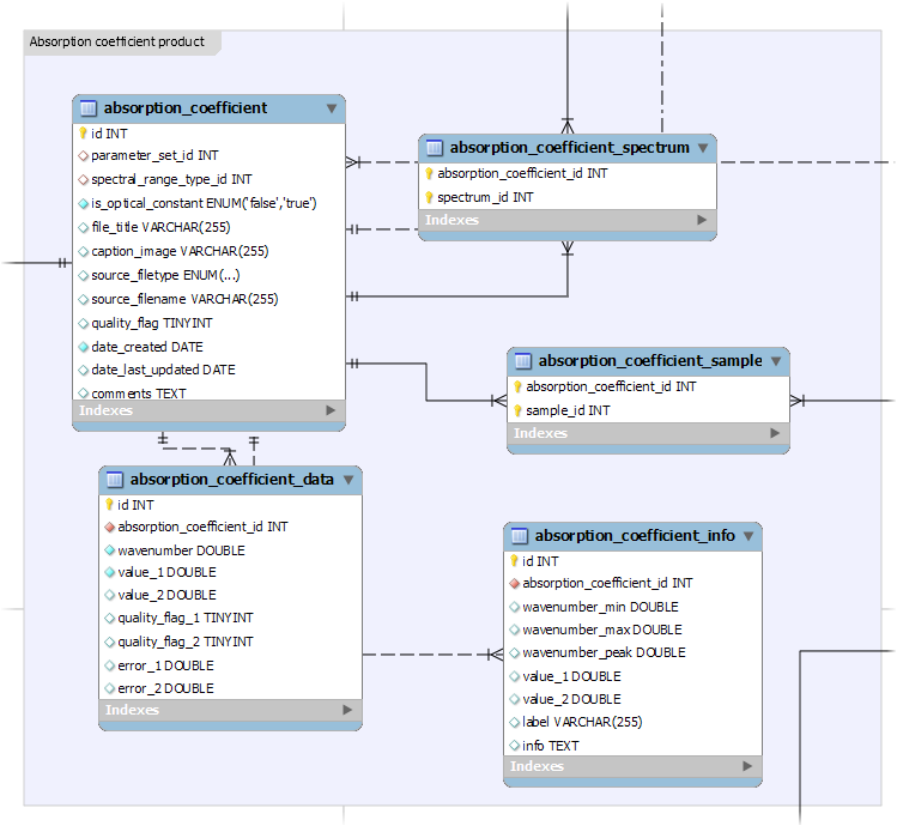
- Relational database advantages
  - Permits to store a wide range of parameters variations in experiments.
  - Experiment samples can handle complex structures (multiple layers / materials / constituents / precursors).
  - Samples and experiments can have a relation to a parent sample/experiment, enabling full history for those.
  - At term for an advanced use every parameters could be searchable.
- Molecule database identification standards available in SSDM :
  - InChIKey (International Chemical Identifier).
  - CAS Registry Number (Chemical Abstracts Service).
  - IUPAC Name



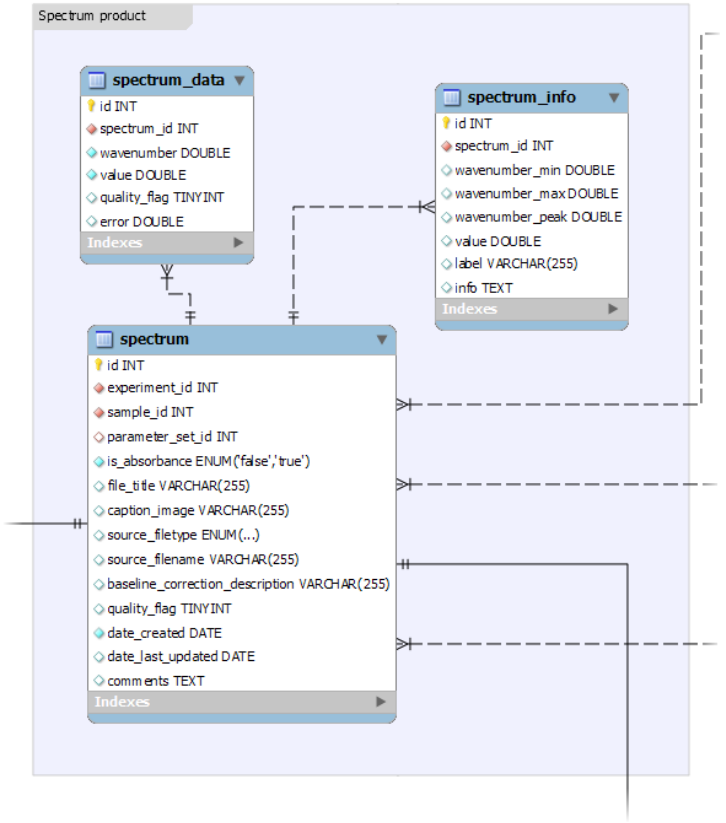
SSDM Overview

Spectrum data model

- Spectrum « meta-data » in single table
- Spectrum data stored in database
- Additional spectrum informations displayable

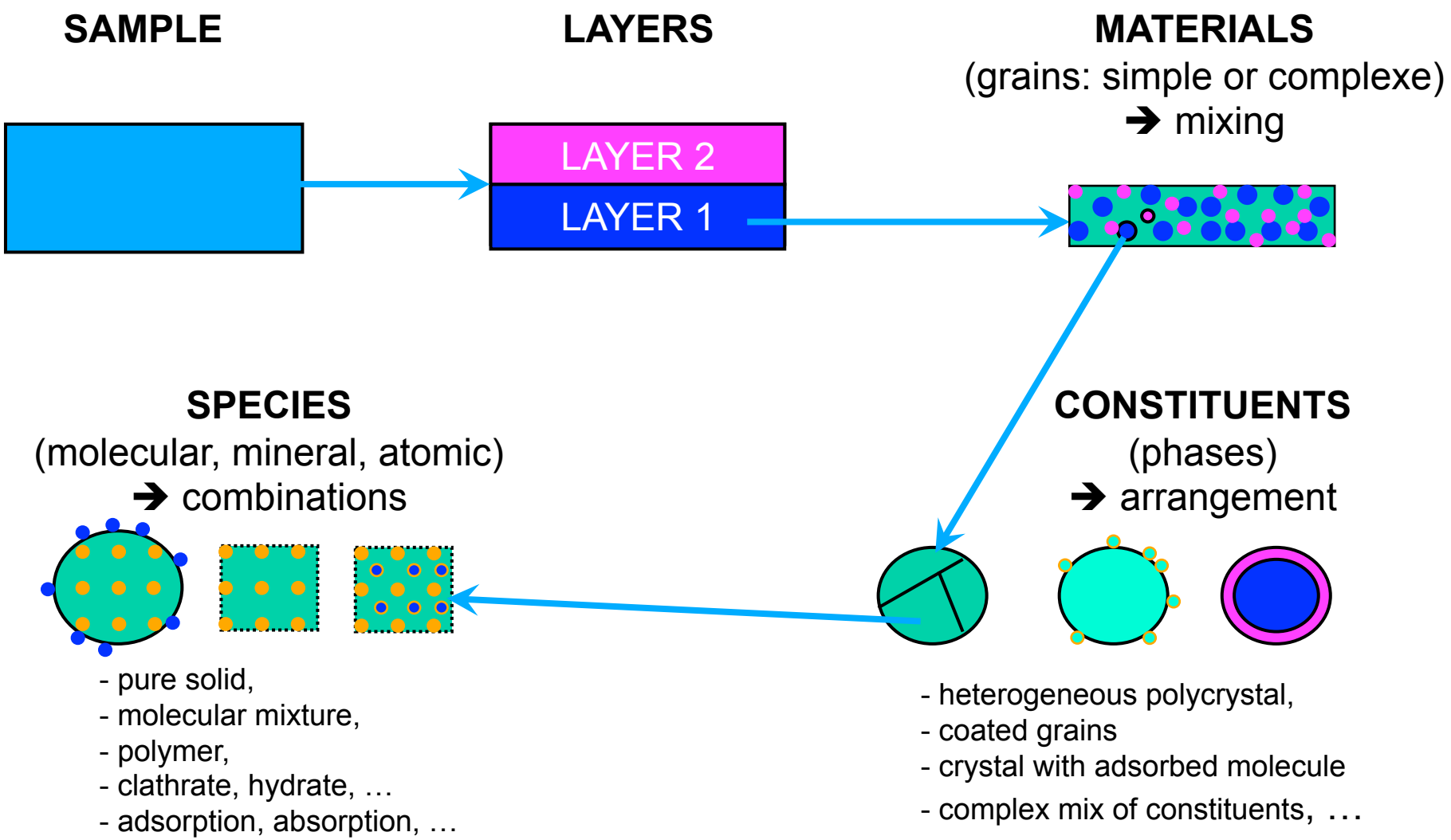


Absorption coefficient tables



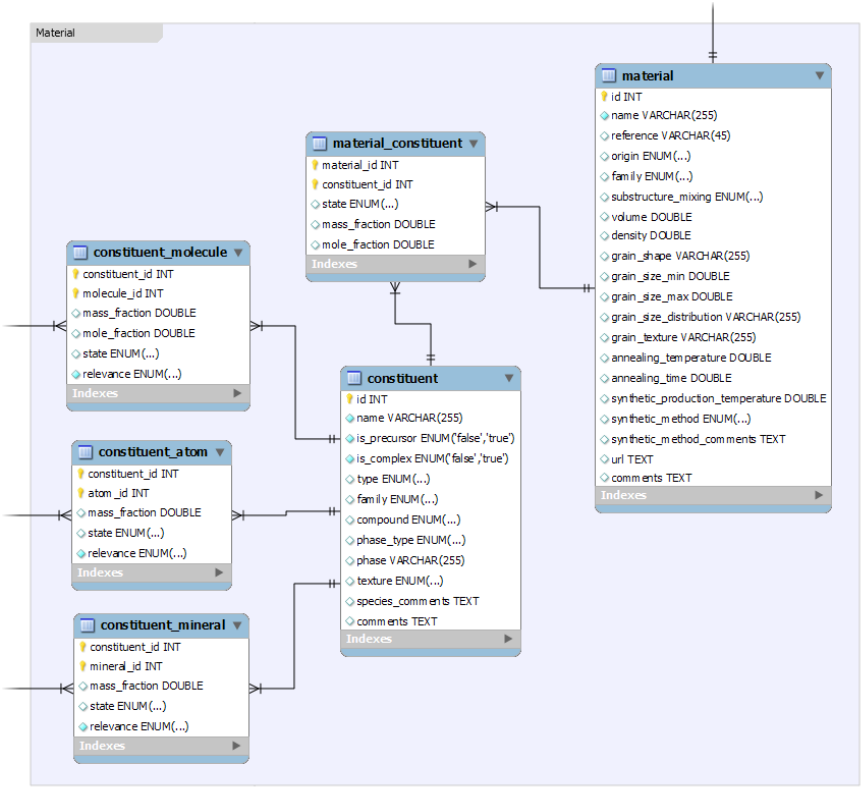
Spectrum tables

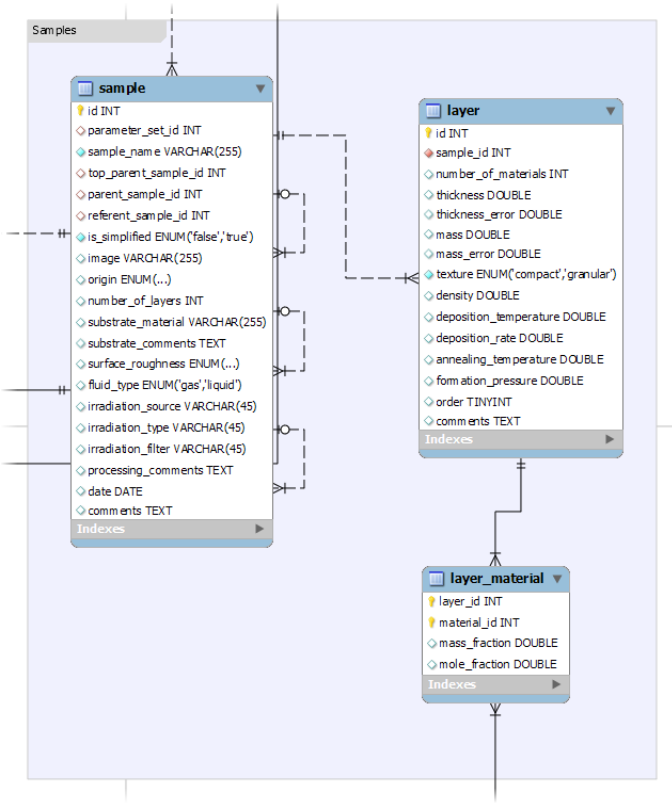
Sample scientific description



Sample & Material model

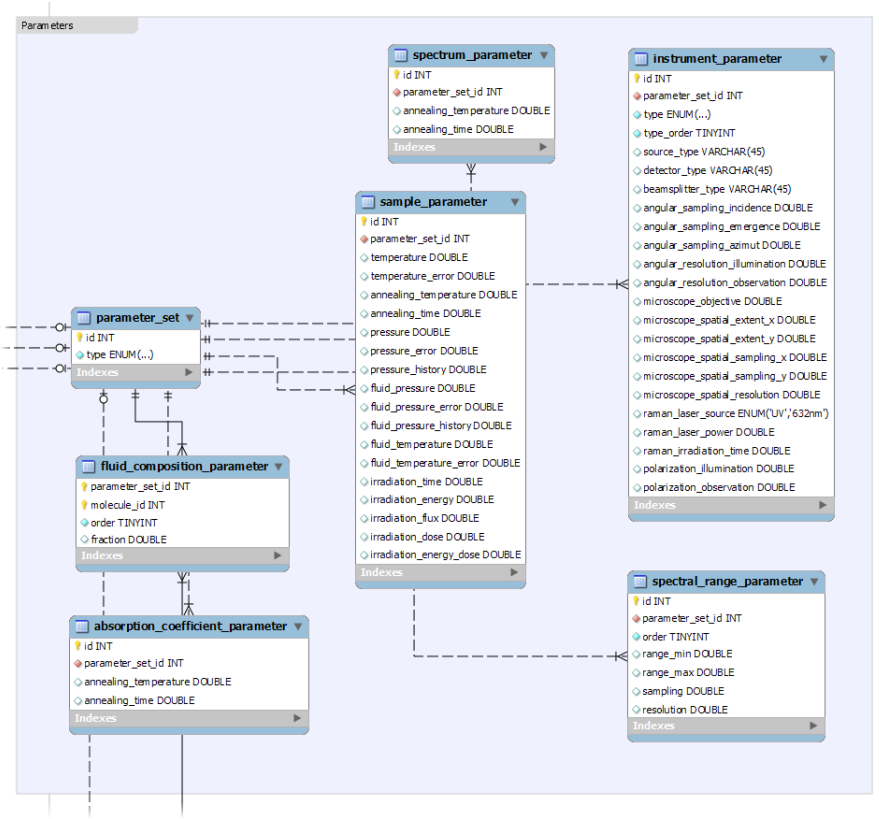
- Heavy relational tables
- Handle all of the scientific description specificities





Parameters set model

- Parameters set are a way to store the same meta-datas for different objects
- Static values are stored in the object table
- More versatile solution, but difficult to handle simply with datamining tools
- Necessity of an interoperability layer with communication protocols



Import XML Schema

- Ensures valid XML documents
- Human-readable errors

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema">
    <!-- EXPERIMENT ========================================================================================== -->
    <xs:complexType name="experiment">
        <xs:all>
            <xs:element name="parent_experiment_index"      type="xs:unsignedLong"            minOccurs="0"/>
            <xs:element name="instrument_name"              type="xs:string"/>
            <xs:element name="instrument_type">
                <xs:simpleType>
                    <xs:restriction                         base="xs:string">
                        <xs:enumeration                     value="FTIR spectrometer"/>
                        <xs:enumeration                     value="spectrogoniometer"/>
                        <xs:enumeration                     value="Raman"/>
                        <xs:enumeration                     value="IR microscope"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="instrumental_technic">
                <xs:simpleType>
                    <xs:restriction                         base="xs:string">
                        <xs:enumeration                     value="transmission"/>
                        <xs:enumeration                     value="reflection"/>
                        <xs:enumeration                     value="reflection spectroscopy"/>
                        <xs:enumeration                     value="BRDF"/>
                        <xs:enumeration                     value="spectrometry"/>
                        <xs:enumeration                     value="microscopy"/>
                        <xs:enumeration                     value="fluorescence"/>
                        <xs:enumeration                     value="ATR"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="date"                         type="xs:date"/>
            <xs:element name="experimentator_name"          type="xs:string"/>
            <xs:element name="spectral_range_type"          type="xs:string"/>
            <xs:element name="comments"                                                   minOccurs="0"/>
            <!-- parameters -->
            <xs:element name="parameters"                                                 minOccurs="0">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="instrument"       type="instrument_parameter"   minOccurs="0"/>
                        <xs:element name="spectral_range"   type="spectral_range_parameter"   minOccurs="0"   maxOccurs="unbounded"/>
                    </xs:sequence>
                    <xs:attribute name="type"               fixed="experiment"            use="required"/>
                </xs:complexType>
            </xs:element>
        </xs:all>
    </xs:complexType>
    <!-- SAMPLE ============================================================================================== -->
    <xs:complexType name="sample">
        <xs:all>
            <xs:element name="sample_name"/>
            <xs:element name="parent_sample_index"              type="xs:unsignedLong"                minOccurs="0"/>
            <xs:element name="parent_sample_ref"                type="xs:integer"                     minOccurs="0"/>
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            <xs:element name="is_simplified"                    type="xs:boolean"                     minOccurs="0"/>
            <xs:element name="image"                            type="xs:string"                      minOccurs="0"/>
            <xs:element name="origin"                                                                 minOccurs="0">
                <xs:simpleType>
                    <xs:restriction                             base="xs:string">
                        <xs:enumeration                         value="natural"/>
                        <xs:enumeration                         value="synthetic"/>
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                        <xs:enumeration                         value="generic"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="substrate_material"               type="xs:string"                      minOccurs="0"/>
            <xs:element name="substrate_comments"                                                     minOccurs="0"/>
            <xs:element name="surface_roughness"                                                      minOccurs="0">
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```

Import XML Templates

- Can be produced by hand or automated
- Doesn’t reflect all the complexity of the relational model

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

Specific notes :
    - Spectrum datas can be given in this XML file, or in corresponding source_filename data file. Remove <spectrum_datas> if not needed

General notes :
    - Most of the tags are optional, remove unnecessary ones.
    - Enumeration type must contain one item of the list given in brackets.
    - Tags marked as multiple can be copied if needed.
    - If used, order must be unique by tag.
    - Indexes are references from the SSDM, you have to look for the index beforehand.
-->
<import>
    <experiment>
        <parent_experiment_index></parent_experiment_index>
        <instrument_name></instrument_name>
        <instrument_type></instrument_type><!-- {FTIR spectrometer,spectrogoniometer,Raman,IR microscope} -->
        <instrumental_technic></instrumental_technic><!-- {transmission,reflection,reflection spectroscopy,BRDF,spectrometry,microscopy.
        <date></date>
        <experimentator_name></experimentator_name>
        <spectral_range_type></spectral_range_type>
        <parameters type="experiment"><!-- cf. parameters doc -->
            <instrument></instrument>
            <spectral_range></spectral_range><!-- multiple -->
        </parameters>
    </experiment>
    <sample></sample><!-- cf. sample template -->
    <spectrum><!-- multiple -->
        <is_absorbance></is_absorbance><!-- {true,false} -->
        <source_filename></source_filename>
        <source_filetype></source_filetype><!-- {nicolet,ascii-ni,ascii-simple} -->
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        <baseline_correction_description></baseline_correction_description>
        <quality_flag></quality_flag>
        <comments></comments>
        <sample_index></sample_index>
        <parameters type="spectrum"><!-- cf. parameters template -->
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            <sample></sample>
            <instrument type="" order="1"></instrument><!-- multiple -->
            <spectral_range order="1"></spectral_range><!-- multiple -->
            <atmospheric_composition order="1"></atmospheric_composition><!-- multiple -->
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        <spectrum_infos>
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        <spectrum_datas>
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</import>
```