Last developments of GhoSST and its Solid Spectroscopy Data Model

The SSHADE project

Bernard Schmitt, Damien Albert, Philippe Bollard, Lydie Bonal, Maria Gorbacheva, P. Beck, E. Quirico and the SSDM Expert group*

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Gho SSDM T HADE

Solid Spectroscopy Data Bases

SSDM: *the Data Model*

SSHADE: *the Hosting Architecture of Databases*

GhoSST: *the first Database in Grenoble for Astrophysics and Planetology*

European projects: *IDIS/Europlanet* & VAMDC (2009-2012)

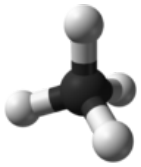
Laboratory spectroscopic databases for solids :

- ***Develop a Solid spectroscopy data model (SSDM)***
- ***Generate a first new database with IPAG data (GhoSST)*** covering :
  - UV-to-FIR transmission spectroscopy of ices and simple organics
  - UV-to-NIR bidirectional reflection spectroscopy of solid surfaces (planetary materials; minerals and ices, meteorites, organics, adsorption, processed, …)
  - IR, Raman and Fluorescence micro-spectrometry (minerals, meteorites, organics…)
  - Band list of molecular solids and adsorbed molecules

➔ **public version of GhoSST delivered: 25th September 2012**

- ***Develop a generic database infrastructure*** *(SSHADE)* (+ some tools) for spectroscopic data of solids *(to be available to other data producers, in a second step).*

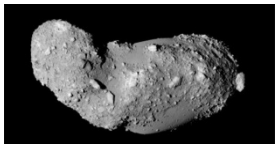
SSDM General Structure

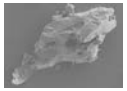


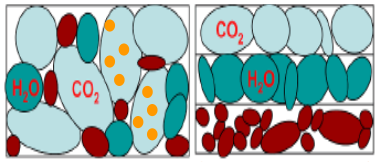
SPECIES

MATTERS

OBJECTS

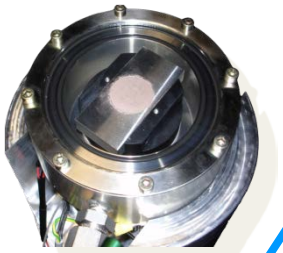




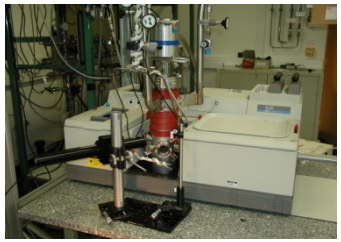


SAMPLE

INSTRUMENT

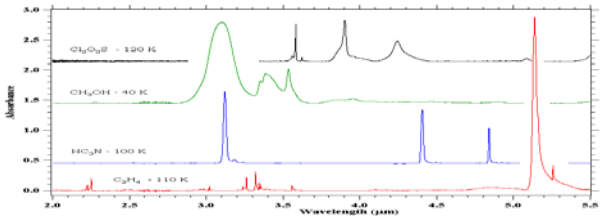


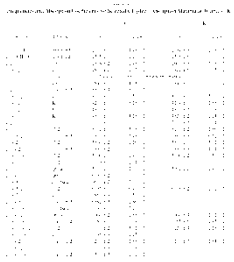
EXPERIMENT



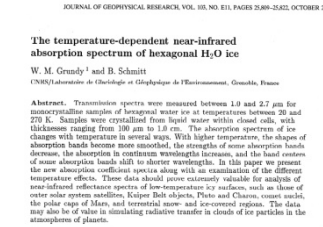
BAND LIST

SPECTRA





PUBLICATIONS



JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 103, NO. E11, PAGES 25,809–25,822, OCTOBER 25, 1998

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 monocrystalline 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.

Development of SSDM Datamodel

(v 0.6)

* **Improvements of core Data Model** (species/samples/instruments/spectra)

* **Species and Matters:**
  - **Mineral species**
  - **Chemical functions**
  - **Mineral & Rock matters**
  - **Meteorite matters & meteorite objects**
  - **Organic matters**

* **Publications**

* **Band list data model : bands and states**
  - Bands parameters
    - position (energy), width, shape, intensities (peak and integrated)
    - accuracy / quality / evaluation
  - Transitions assignment
    - states QN, ...

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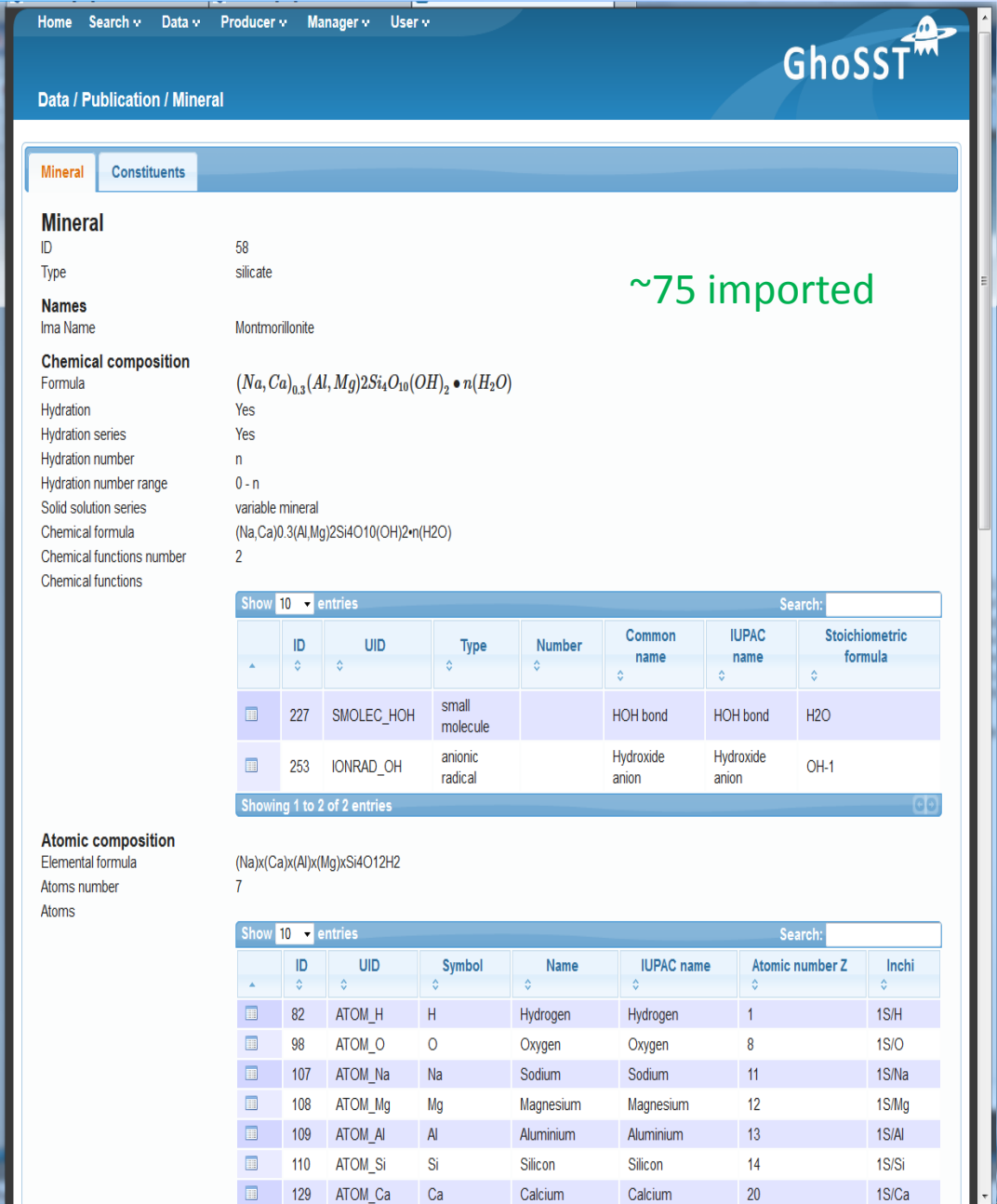
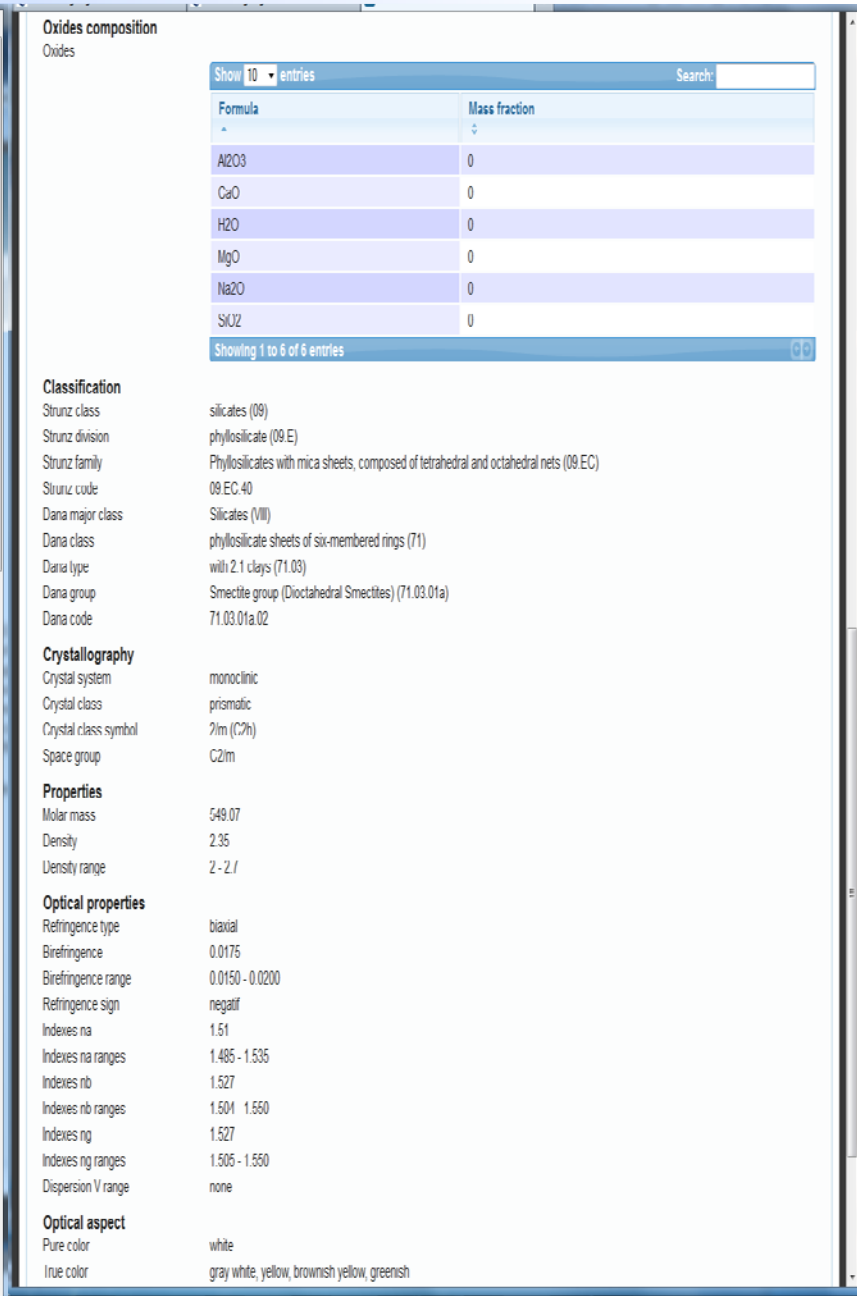
Minerals


Home
Search
Data
Producer
Manager
User
GhoSST
Data / Publication / Mineral
Mineral
Constituents
Mineral
ID 58
Type silicate
~75 imported
Names
Ima Name Montmorillonite
Chemical composition
Formula $(Na,Ca)_{0.3}(Al,Mg)2Si_4O_{10}(OH)_2 \bullet n(H_2O)$
Hydration Yes
Hydration series Yes
Hydration number n
Hydration number range 0 - n
Solid solution series variable mineral
Chemical formula (Na,Ca)0.3(Al,Mg)2Si4O10(OH)2•n(H2O)
Chemical functions number 2
Chemical functions
Show 10 entries
Search:
ID
UID
Type
Number
Common name
IUPAC name
Stoichiometric formula
227 SMOLEC_HOH small molecule HOH bond HOH bond H2O
253 IONRAD_OH anionic radical Hydroxide anion Hydroxide anion OH-1
Showing 1 to 2 of 2 entries
Atomic composition
Elemental formula (Na)x(Ca)x(Al)x(Mg)xSi4O12H2
Atoms number 7
Atoms
Show 10 entries
Search:
ID
UID
Symbol
Name
IUPAC name
Atomic number Z
Inchi
82 ATOM_H H Hydrogen Hydrogen 1 1S/H
98 ATOM_O O Oxygen Oxygen 8 1S/O
107 ATOM_Na Na Sodium Sodium 11 1S/Na
108 ATOM_Mg Mg Magnesium Magnesium 12 1S/Mg
109 ATOM_Al Al Aluminium Aluminium 13 1S/Al
110 ATOM_Si Si Silicon Silicon 14 1S/Si
129 ATOM_Ca Ca Calcium Calcium 20 1S/Ca


Oxides composition
Oxides
Show 10 entries
Search:
Formula
Mass fraction
Al2O3 0
CaO 0
H2O 0
MgO 0
Na2O 0
SiO2 0
Showing 1 to 6 of 6 entries
Classification
Strunz class silicates (09)
Strunz division phyllosilicate (09.E)
Strunz family Phyllosilicates with mica sheets, composed of tetrahedral and octahedral nets (09.EC)
Strunz code 09.EC.40
Dana major class Silicates (VIII)
Dana class phyllosilicate sheets of six-membered rings (71)
Dana type with 2:1 clays (71.03)
Dana group Smectite group (Dioctahedral Smectites) (71.03.01a)
Dana code 71.03.01a.02
Crystallography
Crystal system monoclinic
Crystal class prismatic
Crystal class symbol 2/m (C2h)
Space group C2/m
Properties
Molar mass 549.07
Density 2.35
Density range 2 - 2.7
Optical properties
Refringence type biaxial
Birefringence 0.0175
Birefringence range 0.0150 - 0.0200
Refringence sign negatif
Indexes na 1.51
Indexes na ranges 1.485 - 1.535
Indexes nb 1.527
Indexes nb ranges 1.501 1.550
Indexes ng 1.527
Indexes ng ranges 1.505 - 1.550
Dispersion V range none
Optical aspect
Pure color white
True color gray white, yellow, brownish yellow, greenish

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(v 0.6)

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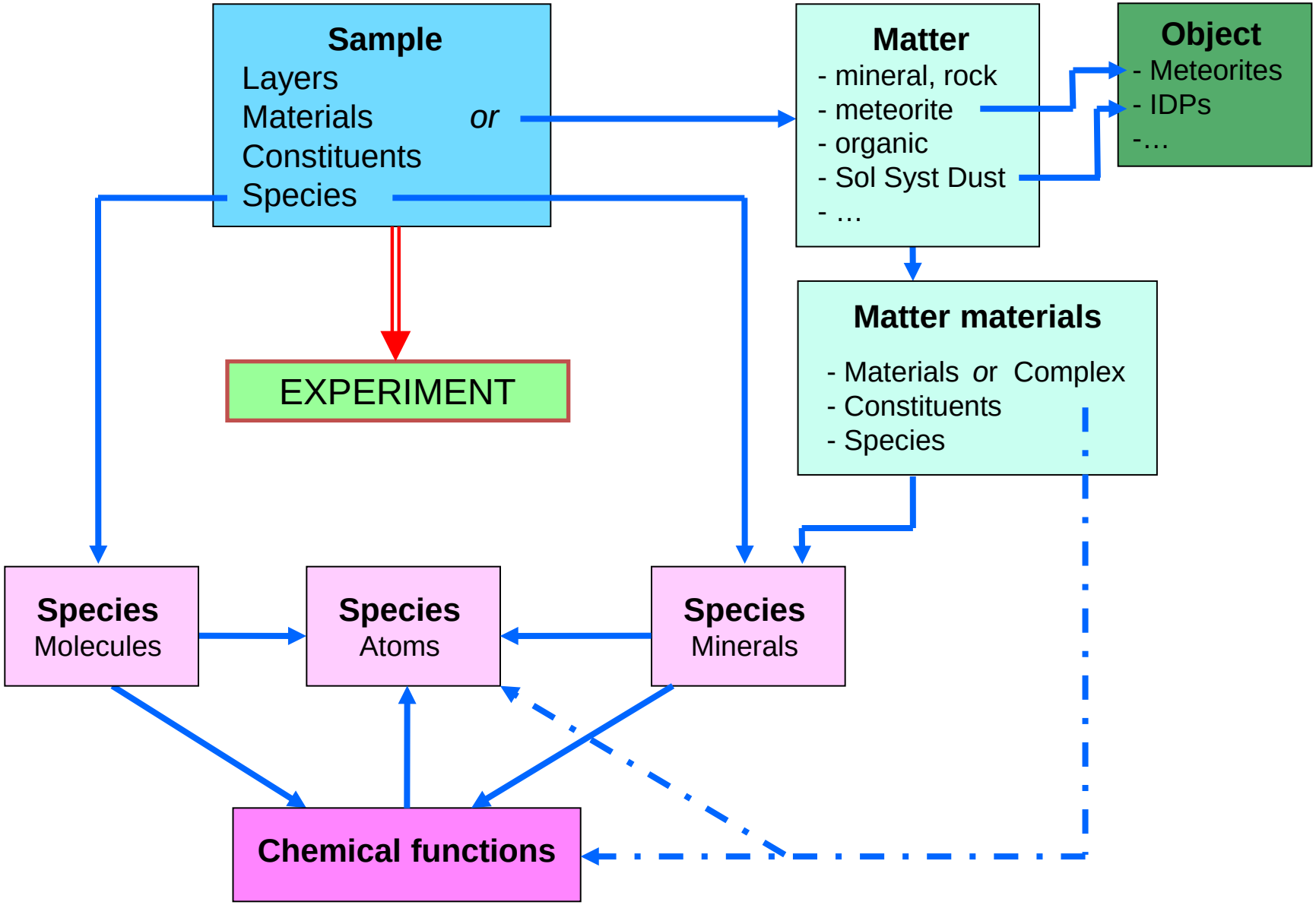
Sample – Species – Matters & Objects



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Publications

Home Search Data Producer Manager User

GhoSST

Data / Publication

Publication | Cited publications

Publication

ID	104
UID	PUBLI_Schmitt_2003
Authors	**B. Schmitt**, S. Rodriguez
Year	**2003**
Title	Possible identification of local deposits of Cl2SO2 on Io from NIMS/Galileo spectra

77 imported

Type and access

Type	journal
Document type	article
State	published
Access rights	publisher free

Content

Abstract	Starting from the recent discovery of chlorine ions in Io's plasma torus, we searched for evidence of Cl-bearing species at the surface of the satellite. We have identified Cl2SO2, with possible contribution by ClSO2, as candidates for the absorber(s) of the 3.92 μm band locally present in NIMS/Galileo spectra of the reddish deposits south of Marduk's volcanic center. Low-temperature laboratory measurements of the infrared spectra of several Cl and S-bearing molecules in the solid state, coupled with radiative transfer modeling, first allowed us to select four candidate molecules. Their abundance and stability at Io's surface have been tested through formation, condensation, and destruction scenarios using volcanic and atmospheric models completed with chemical and thermodynamical data. In particular, the sublimation rates of solid Cl2SO2 and SO2 have been measured to study the selective condensation of these species. Cl2SO2 diluted at ~1% in a millimeter thick layer of solid SO2 is the favorite candidate for the 3.92 μm band. We strongly favor a formation process of this molecule by heterogeneous reaction of Cl atoms on SO2 ice condensing on plume particles or at Io's surface. The high Cl2SO2 abundance observed implies that a Cl-rich volcanic eruption ([Cl - (Na + K)]/S > 0.015) occurred at Marduk. ClSO2 is a potential additional contributor to the band. Pure H2S is safely discarded as it is extremely unstable at Io's surface but an upper limit of 0.01% is derived for H2S diluted in SO2. Finally, chemical constraints allow us to firmly exclude H2S2. We also suggest that Cl2S may be an alternative explanation for the reddish coloration of some volcanic deposits.
Keywords	spectroscopy, thermodynamics, transmission, absorbance spectra, optical constants spectra, band position, near-IR, molecular solid, ice, Cl2SO2, SO2, H2S, radiative transfer simulation, surface, Io
Contents	sample, spectral data, thermodynamic data, planetary sciences, spectral data use,

Document

Journal	Journal of Geophysical Research - Planets
Acronym	JGR E
Volume	108
Issue	E9
First page	5104
Last page	5122
Pages number	19

Links

Pdf	schmitt03-JGRE-108-5104.pdf
Doi	10.1029/2002JE001988
Url	http://dx.doi.org/10.1029/2002JE001988
ADS Url	http://adsabs.harvard.edu/abs/2003JGRE..108.5104S

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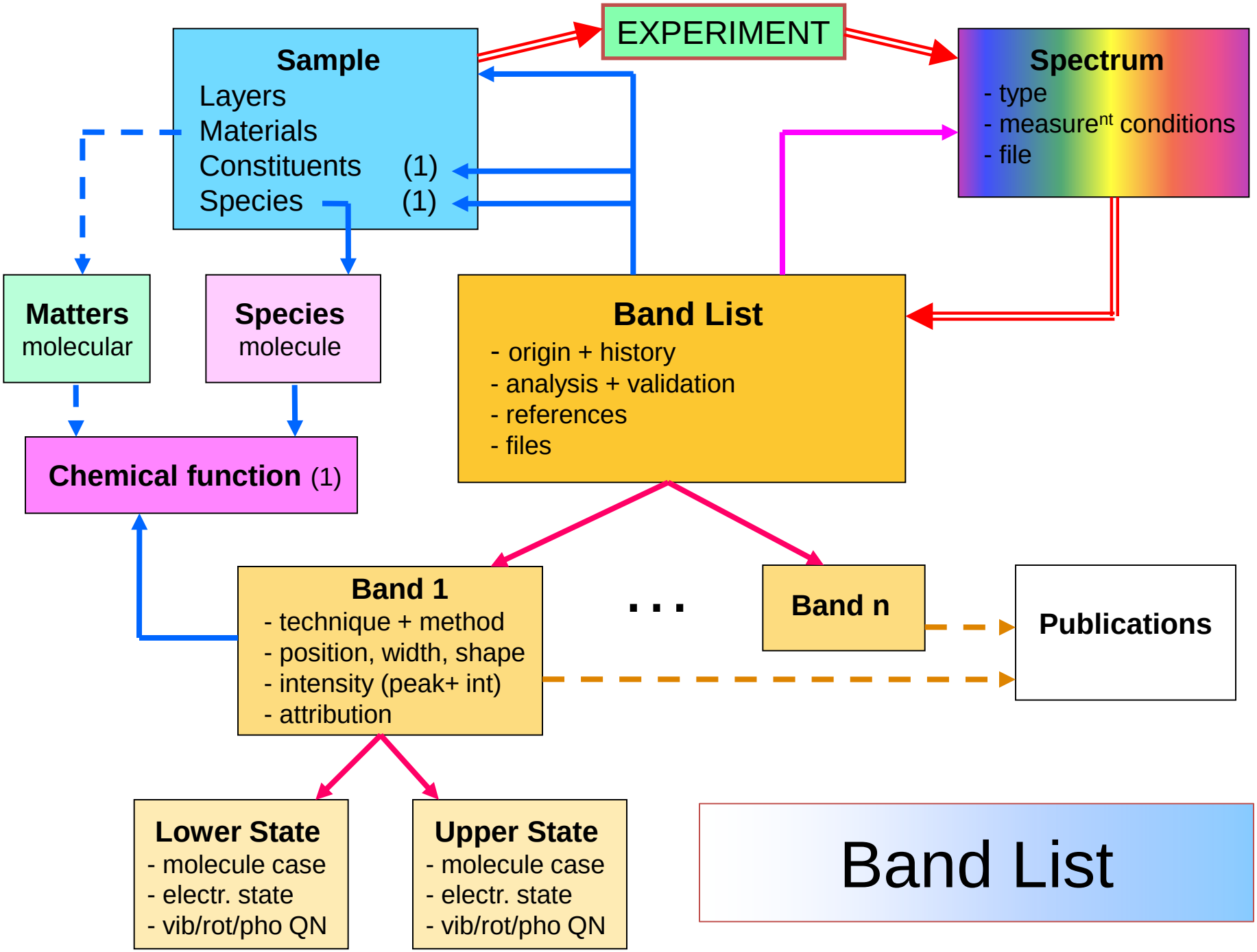
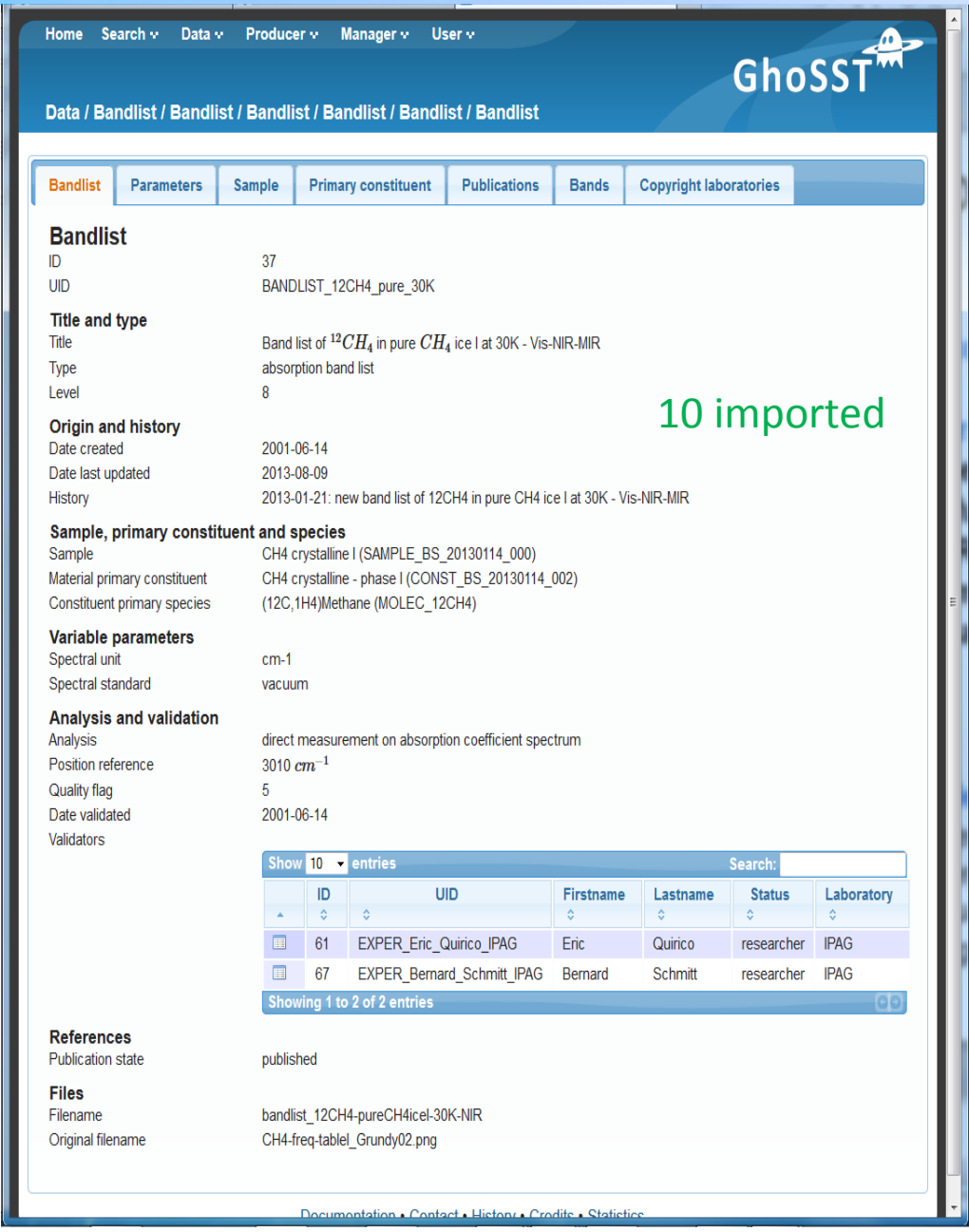

EXPERIMENT
Sample
Layers
Materials
Constituents (1)
Species (1)
Spectrum
- type
- measurent conditions
- file
Matters
molecular
Species
molecule
Band List
- origin + history
- analysis + validation
- references
- files
Chemical function (1)
Band 1
- technique + method
- position, width, shape
- intensity (peak+ int)
- attribution
. . .
Band n
Publications
Lower State
- molecule case
- electr. state
- vib/rot/pho QN
Upper State
- molecule case
- electr. state
- vib/rot/pho QN
Band List

Band list and Bands



Development of GhoSST interface

import / search /vizualization / export / ... : still lot of developments in progress

GhoSST

Data / Experiment / Sample / Layer

Layer

ID 47

Layer organization in sample

Order	1
Type	granular
Comments	small mechanical pressure when sample was flattened with a spatula

Layer physical characteristics

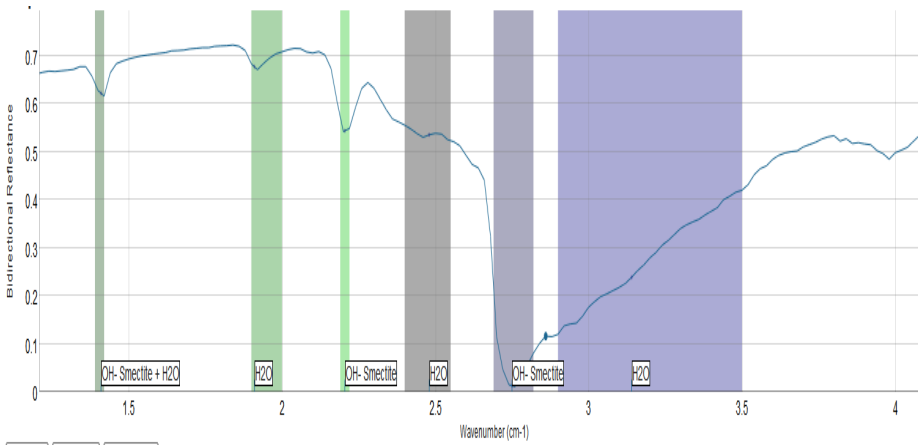
Thickness (mm)	1
Thickness error (mm)	0.1
Texture	loose granular
Porosity	0.53
Density (g/cm3)	0.65

Layer formation conditions

Deposition conditions	manual deposition
Deposition temperature (K)	300
Annealing temperature (K)	443

Layer materials mixing

Number of materials 4



Sample

Sample name and references

ID	48
Sample name	H2O adsorbed on Smectite - 243K
Date	2008-02-01
Comments	Sample temperature error is mostly due to possible vertical temperature gradient in the sample. Temperature reading accuracy and stability is 0.1K - Fluid error depicts estimated therma cell - H2O saturation pressure at 243K is 0.37mb

Sample physical characteristics

Surface roughness	low
Thickness	1 mm

Sample layers organization

Number of layers	1
Layer addition	The sample holder is filled to rim with the non-compacted sample powder and then flattened with a spatula to obtain a smooth surface with limited powder compaction

Sample substrate

Substrate material aluminum anodized black

Sample processings

Processing type	fluid
Temperature (K)	243.1
Annealing temperature (K)	443
Pressure (bar)	0

More details...

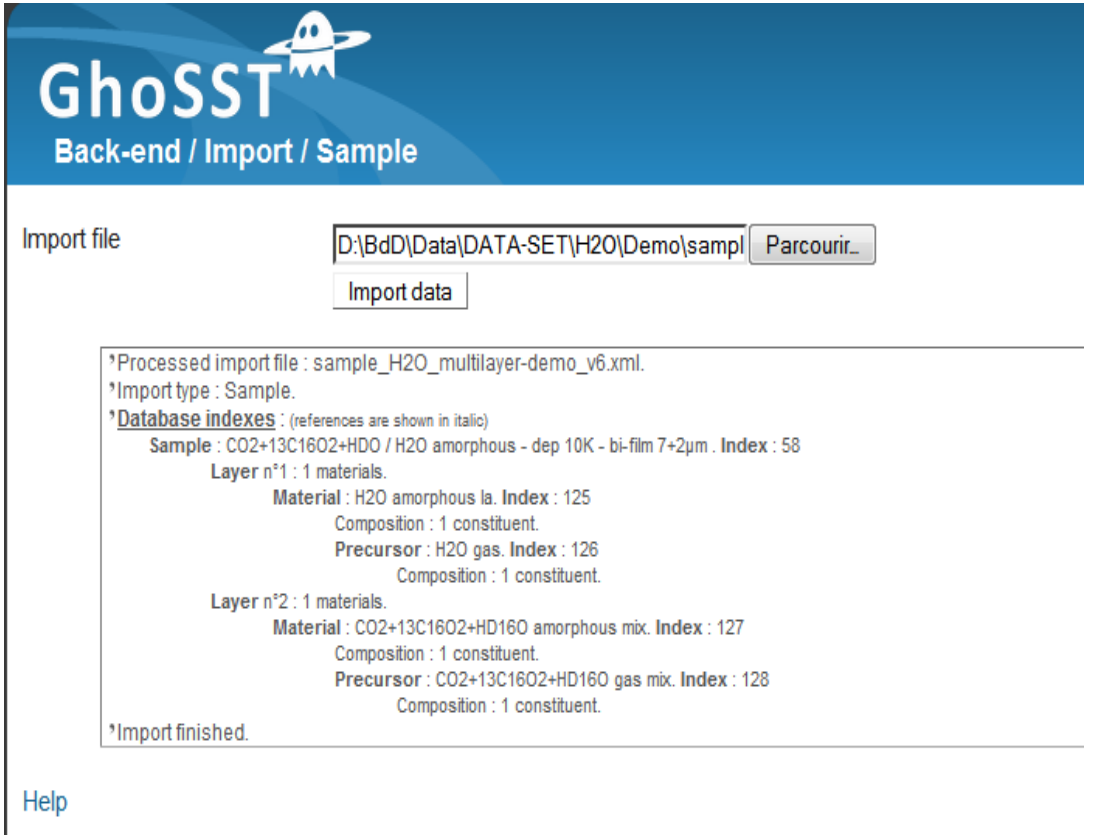
Materials

Actions	ID	Name	Matter origin	Matter family	Mole fraction	Mass fraction
View	85	Smectite with adsorbed H2O	terrestrial	mineral		0.75
View	86	Quartz	terrestrial	mineral		0.08
View	87	Feldspar	terrestrial	mineral		0.16
View	88	Gypsum	terrestrial	mineral		0.01

IMPORT for DATA PRODUCERS

Developed:

- xml templates for each data type
- import tools + validators
- control interface
- import history
- import documentation
- import tutorials

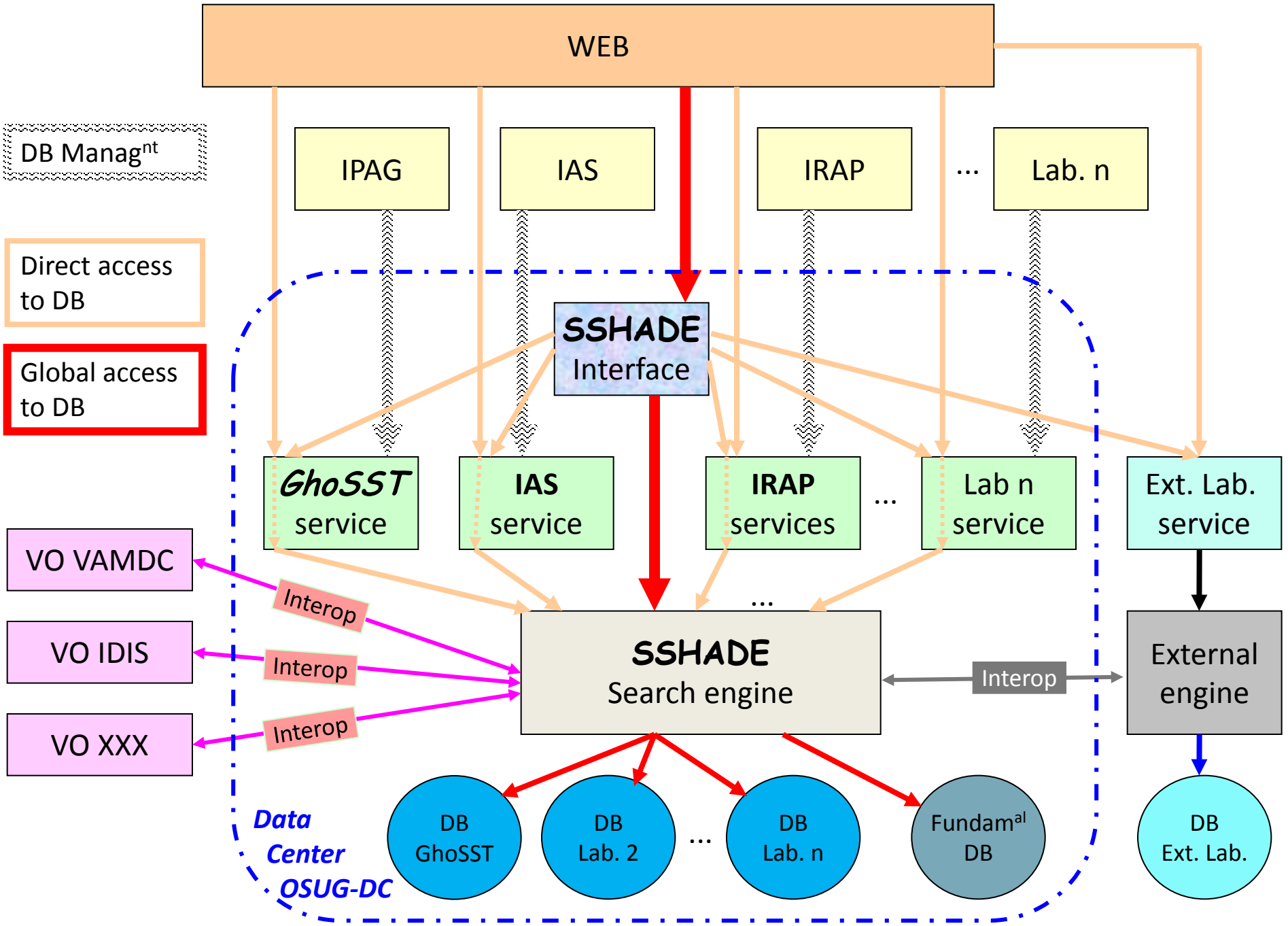


Hosting Solid Spectroscopy data of other Data Providers: *SSHADE*

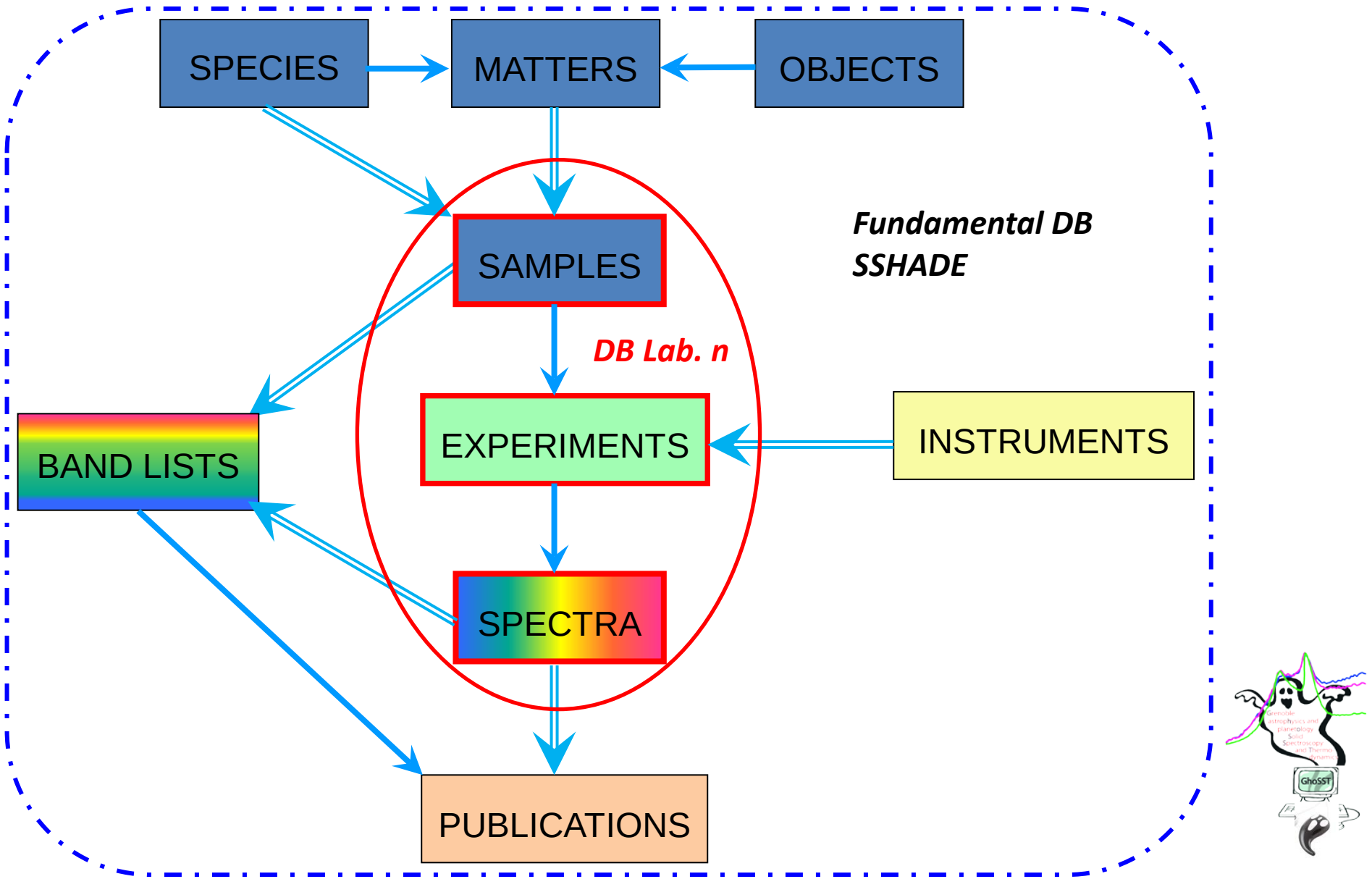
***SSHADE* :**

"Solid Spectroscopy Hosting Architecture of Databases and Expertise"

- Solid Spectroscopy interface
- A database per laboratory
- Also direct link to each individual DB interfaces
- All databases and engines hosted at OSUG data center (OSU Grenoble - UJF)
- SSHADE will be a client of others VO (IDIS, VAMDC, ...)
- Possible to link to other external Solid Spect. databases (need interoperability layer with SSDM)


WEB
DB Managnt
IPAG
IAS
IRAP
...
Lab. n
Direct access to DB
Global access to DB
SSHADE Interface
GhoSST service
IAS service
IRAP services
...
Lab n service
Ext. Lab. service
VO VAMDC
VO IDIS
VO XXX
Interop
Interop
Interop
...
SSHADE Search engine
Interop
External engine
DB GhoSST
DB Lab. 2
...
DB Lab. n
Fundamal DB
DB Ext. Lab.
Data Center OSUG-DC

SSHADE: new SSDM Structure



SSHADE Project

- **VAMDC/EPN** (2009-2012)
  - Development of SSDM and GhoSST (with SSHADE compatibility in head)
  - Test of data ingestion by others laboratories

- **In progress:**
  - 2012: proposition of SSHADE to INSU/CNRS w. 5 French laboratories
  - 2013: GhoSST get label from INSU/CNRS
    Recommendation from INSU/CNRS to develop SSHADE
    Funding asked on French side (OSUG, INSU/CNRS, ASOV, CNES)
  - 10/2013: 1st meeting of SSHADE-France (IPAG, Grenoble)
  - 11/2013: 1st meeting of SSHADE-Europe (OU, Milton Keynes)

- **Project:**
  - **2014: start development of SSHADE infrastructure**
  - **2014/15: start 2-3 new DataBases** (to be selected)
  - European funding: *Horizon 2020* call ?

look at Video: « GhoSST user case »