2nd SSHADE partners meeting

4-5 December 2017 – IPAG, Grenoble, France

EUROPLANET 2020-RI program
VESPA JRA-5 + VA-2

Logistics

- 4th & 5th lunches: will be taken at ‘Camberra’ restaurant (5 min from here)

- Dinner **Monday 4th 19:30 @ restaurant « Caffè Forté »**
  4 place de Lavalette
  Tram B stop : « Notre-Dame Musée »

- Tuesday we start at 9:00 and end at 3:00 pm

- Dinner **Tuesday 5th 19:00 @ restaurant « L'Ardoise »**
  2 Rue Miribel
  Tram B stop : « Victor Hugo »

Dinner **Monday 4th**
19:30
@ **restaurant**
« Caffè Forté »

4 place de Lavalette

Tram B stop :
« Notre-Dame Musée »

Dinner
Tuesday 5th
19:00 @
restaurant
« L'Ardoise »

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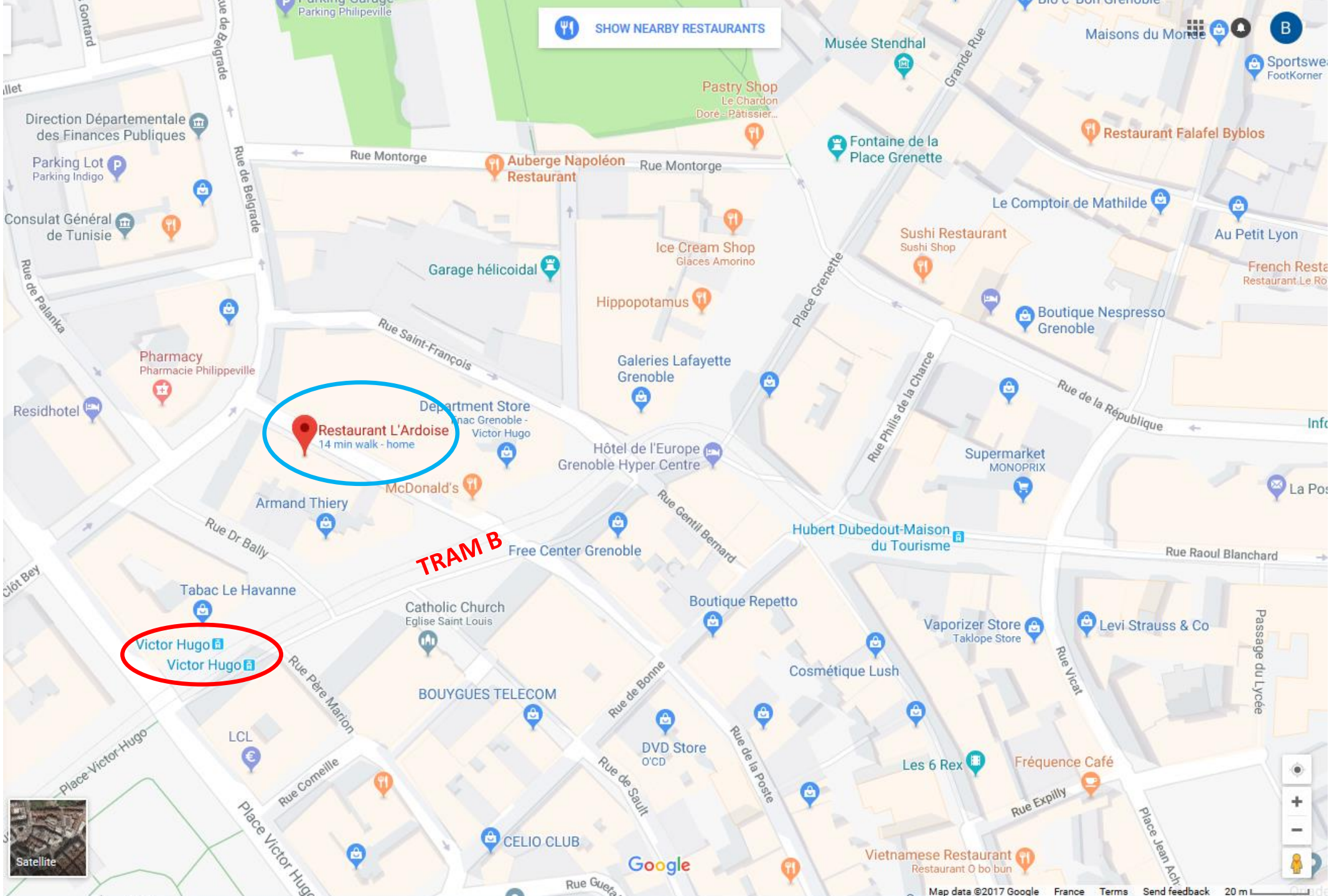


Aims of this 2nd SSHADE partners meeting

To present:

- the current state of development of the SSHADE database infrastructure
- the current state of development of the SSHADE interface
- the current state of data ingestion in the SSHADE databases
- the in-progress and future developments

To discuss and plan:

- SSHADE delivery and opening to public
- new partner's training and database filling
- SSHADE and databases sustainability
- user training – advertising SSHADE
- any question related to SSHADE and their database

SSHADE and its activity

- History
- SSHADE consortium
- Data of SSHADE
- SSHADE infrastructure
- JRA and VA activities
- Time line

A little bit of history: from past to future

- 2002: Idea ...
- 2006: Concept ...
  Content demonstrator: STSP
- 2007-2008: First “solid spectroscopy” datamodel
  Development of technical demonstrator (OSUG, ...)
- ✓ **2009-2012:** **Full developments (Europlanet + VAMDC – FP7) of:**
  SSDM (Solid Spectroscopy Data Model) and GhoSST database infrastructure
- July 2011 GhoSST functional prototype
- ✓ **25 Sept. 2012:** **GhoSST opened to the public** (v0.5 beta-version)

- 2013-2015: Continuing SSDM and GhoSST developments
  GhoSST data feeding
- ✓ **4 Feb. 2014:** **GhoSST upgrade** (v0.6)

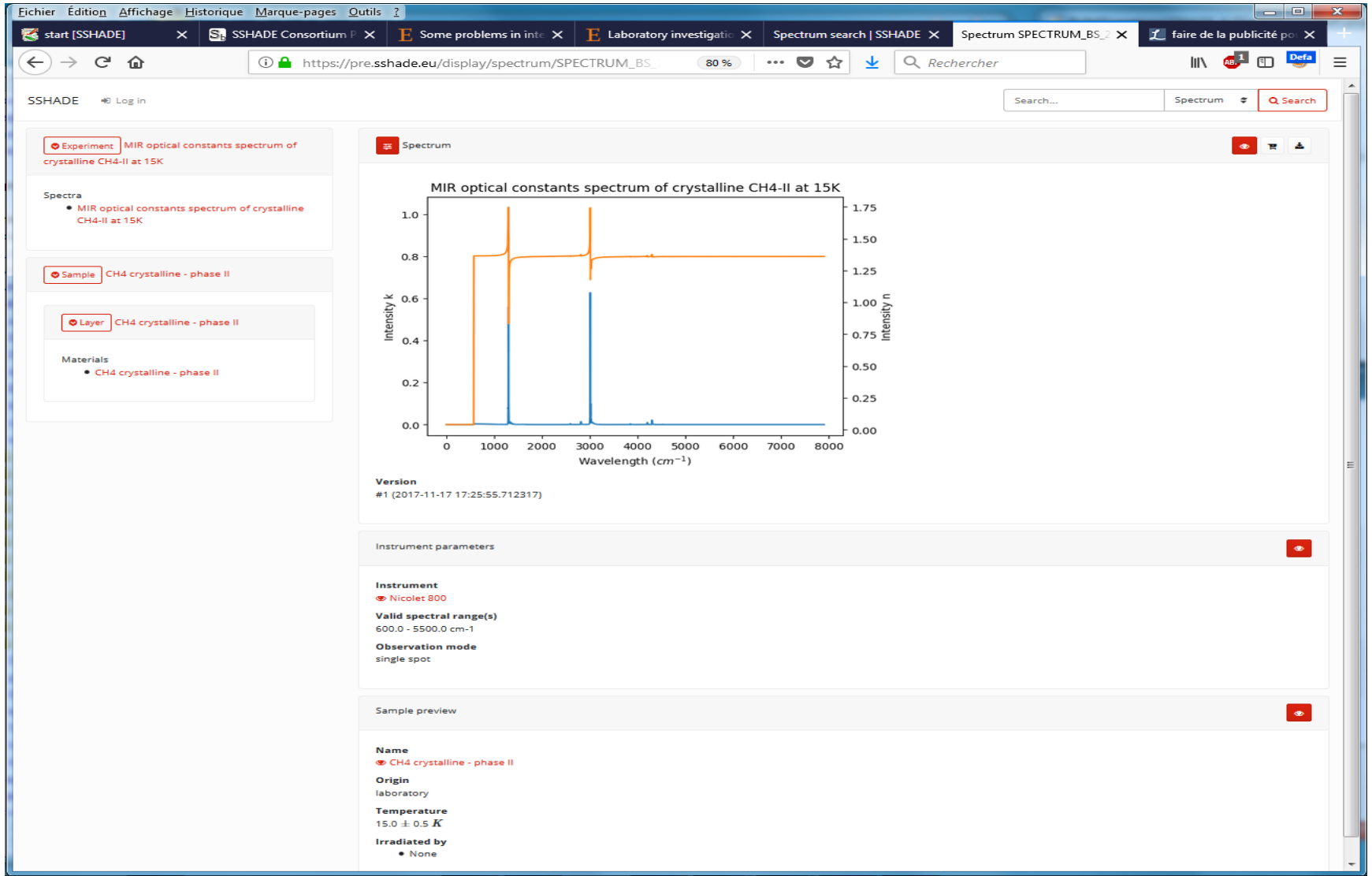
- 2014 Preparation and opening of a pre-SSHADE database
- ✓ **2015-2019:** **Development of SSHADE infrastructure under EPN@2020-RI (VESPA JRA)**
  Opening of SSHADE to participating European producers (VESPA VA)
  SSHADE online (2017)

GhoSST Web interface

- Public version of ‘old’ GhoSST accessible at: http://ghosst.osug.fr

SSHADE Web interface

- Beta version of SSHADE accessible (restricted) at: https://pre.sshade.eu



SSHADE European Consortium of Data Providers

Consortium of **20** solid spectroscopy experimental groups
in **8** European countries (F, GB, D, I, E, CH, PL, HU)
involving ~**65** peoples

Each with particular expertises on:

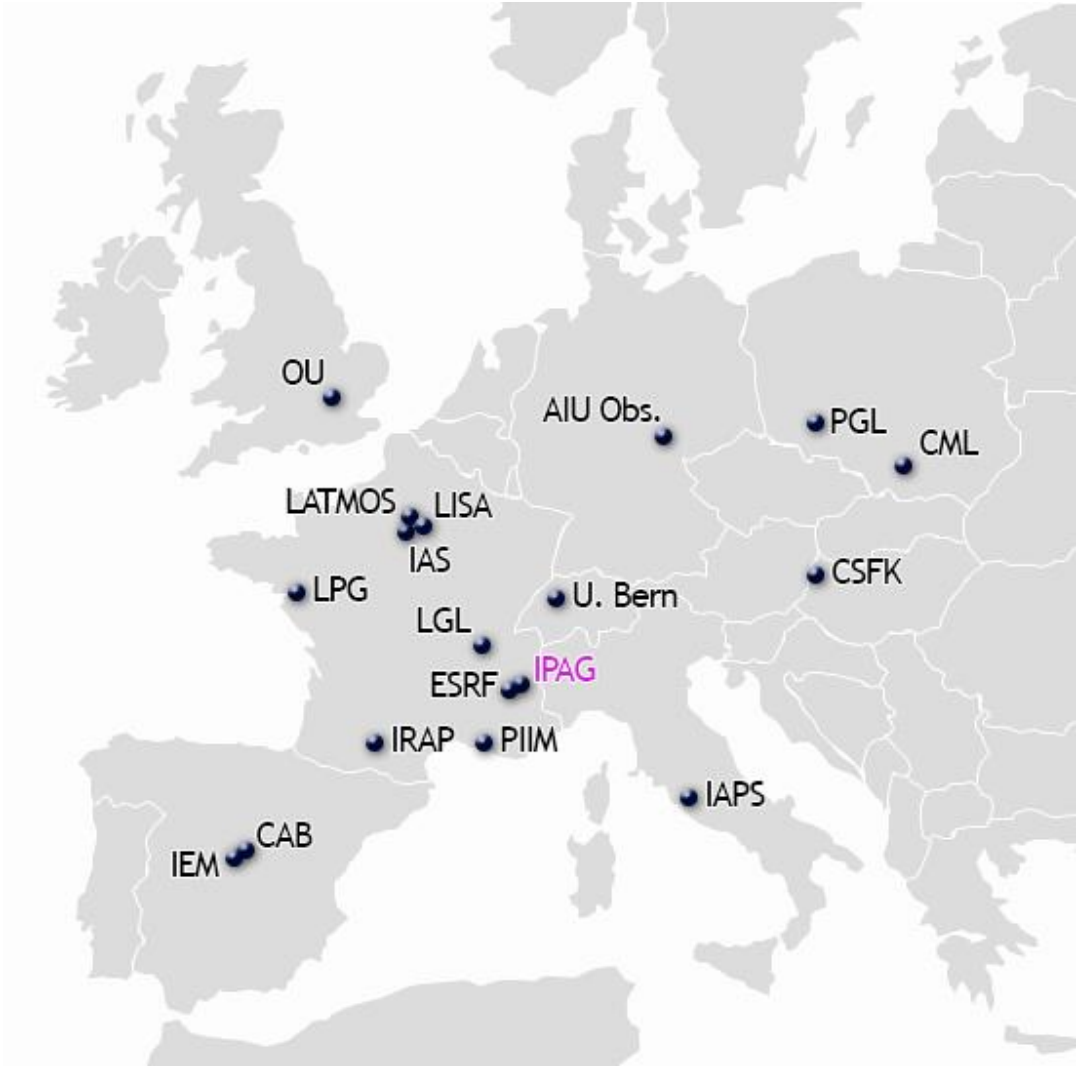
- some wavelength range
- specific techniques
- type of materials and physico-chemical conditions
- type of data and products, …

SSHADE blog : http://blog.sshade.eu

The SSHADE-Europe consortium in EPN@2020-RI

SSHADE (OSUG, Grenoble, F) (Bernard Schmitt, Philippe Bollard, Alexandre Garenne, Lydie Bonal , Damien Albert)

- **IPAG / Planéto**, Grenoble - F (Bernard Schmitt, Lydie Bonal, Alexandre Garenne)
- **Space & Planetary Science Division**, Univ. of Bern - CH (Antoine Pommerol, Olivier Poch)
- **IRAP / PEPS**, Toulouse - F (Patrick Pinet, Yves Daydou)
- **IRAP / MICMAC**, Toulouse - F (Karine Demyk , Yves Daydou)
- **Planetary Geology Lab.**, Institute of Geological Sciences – PL (Joanna Gurgurewicz)
- **IAS**, Univ. Paris-Sud - F (Rosario Brunetto, Donia Baklouti)
- **LPG**, Univ. Nantes - F (Marion Massé, Manuel Giraud)
- **AIU Observatory**, Jena - D (Harald Mutschke, Jürgen Weiprecht)
- **ESRF / FAME line**, Grenoble – EU / F (Denis Testemale, Isabelle Kieffer)
- **Clay Mineral Laboratory**, Institute of Geological Sciences – PL (Artur Kuligiewicz)
- **PIIM**, Univ. Aix-Marseille - F (Patrice Theulé)
- **Instituto de Estructura de la Materia**, Madrid – E (Vicente Timón, Miguel Angel Moreno)
- **Open University**, Milton Keynes – UK (Nigel Mason)
- **Physical Research Laboratory** , Ahmedabad – IN (Bhala Sivaraman)
- **LISA,** Univ. Paris-Est - F (Nicolas Fray)
- **Centro de Astrobiología**, INTA-CSIC – E (Guillermo Muñoz Caro)
- **LATMOS / IMPEC**, Institut Pierre Simon Laplace - F (Nathalie Carrasco)
- **IAPS**, INAF, Roma - I (Alessandra Rotundi, Vincenzo della Corte)
- **IAPS**, INAF, Roma - I (Fabrizio Capaccioni, Christian Carli)
- **LGL / ENS-Lyon** - F (Bruno Reynard, Gilles Montagnac, Razvan Caracas)
- **Konkoly Astronomical Institute** – HU (Akos Kereszturi, Ildiko Gyollai)



Data of SSHADE

- **Spectral ranges:**
  - from X-ray to mm (through UV-Vis-IR)

- **Solids:**
  - Ices (low to high pressure, low to room temperature, mixtures, matrix isolated, ...)
  - clathrates hydrates, hydrates
  - minerals (naturals and synthesized), rocs
  - organic matter (natural and synthesized), polymers, VUV
  - Extraterrestrial matter: meteorites, IDPs, ...
  - also liquids

- **Data types:**

➢ **Spectra**
  - infrared transmission spectra, absorption coefficients, optical constants
  - Raman spectra et micro-spectroscopy
  - reflectance spectra of surfaces, spectro-photometric functions
  - multispectral and multi-angular imagery of surfaces

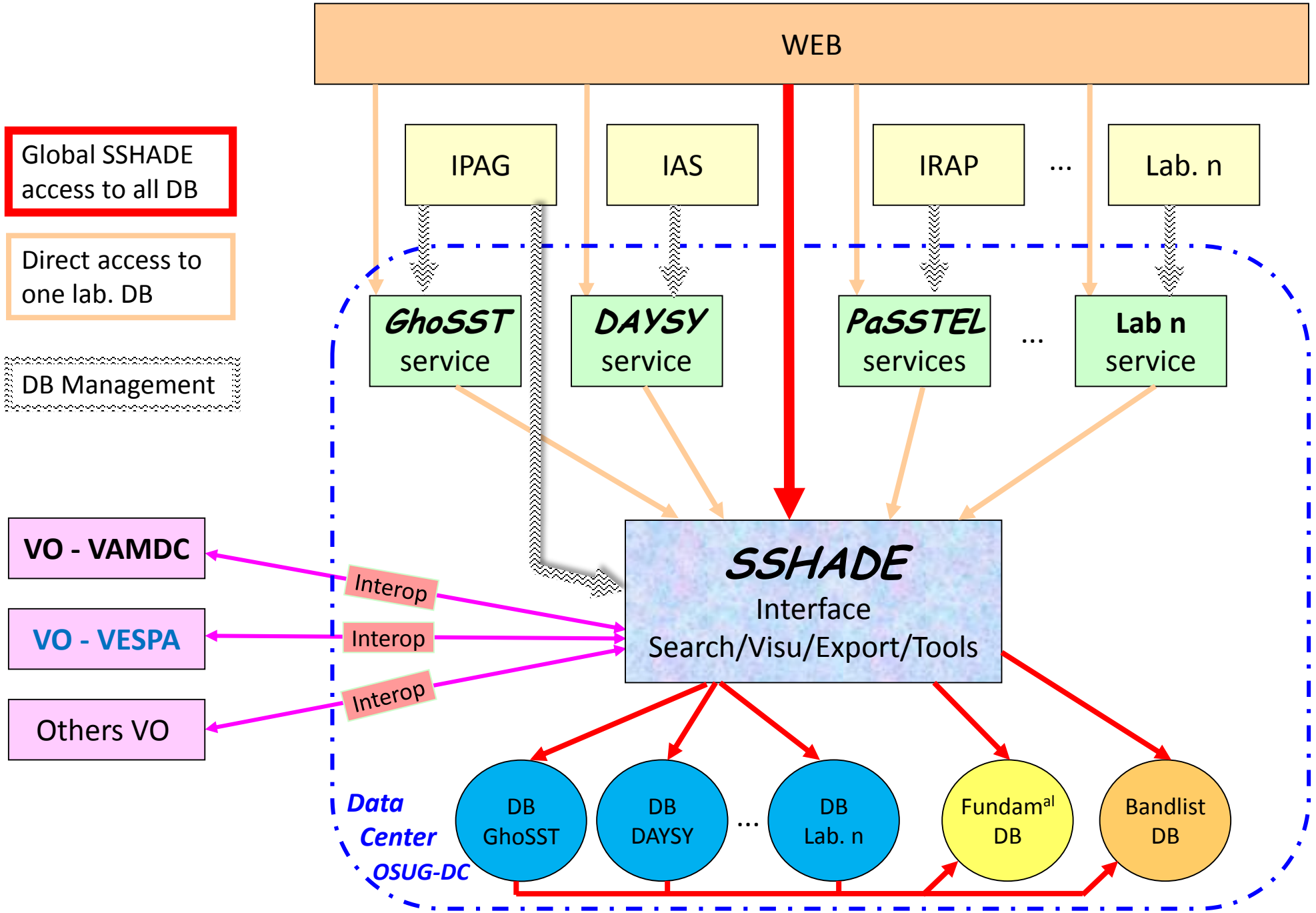
➢ **Bandlist**
  - position, width, intensity, attribution ... for molecular solids

Solid Spectroscopy data Infrastructure for European Data Providers: *SSHADE*

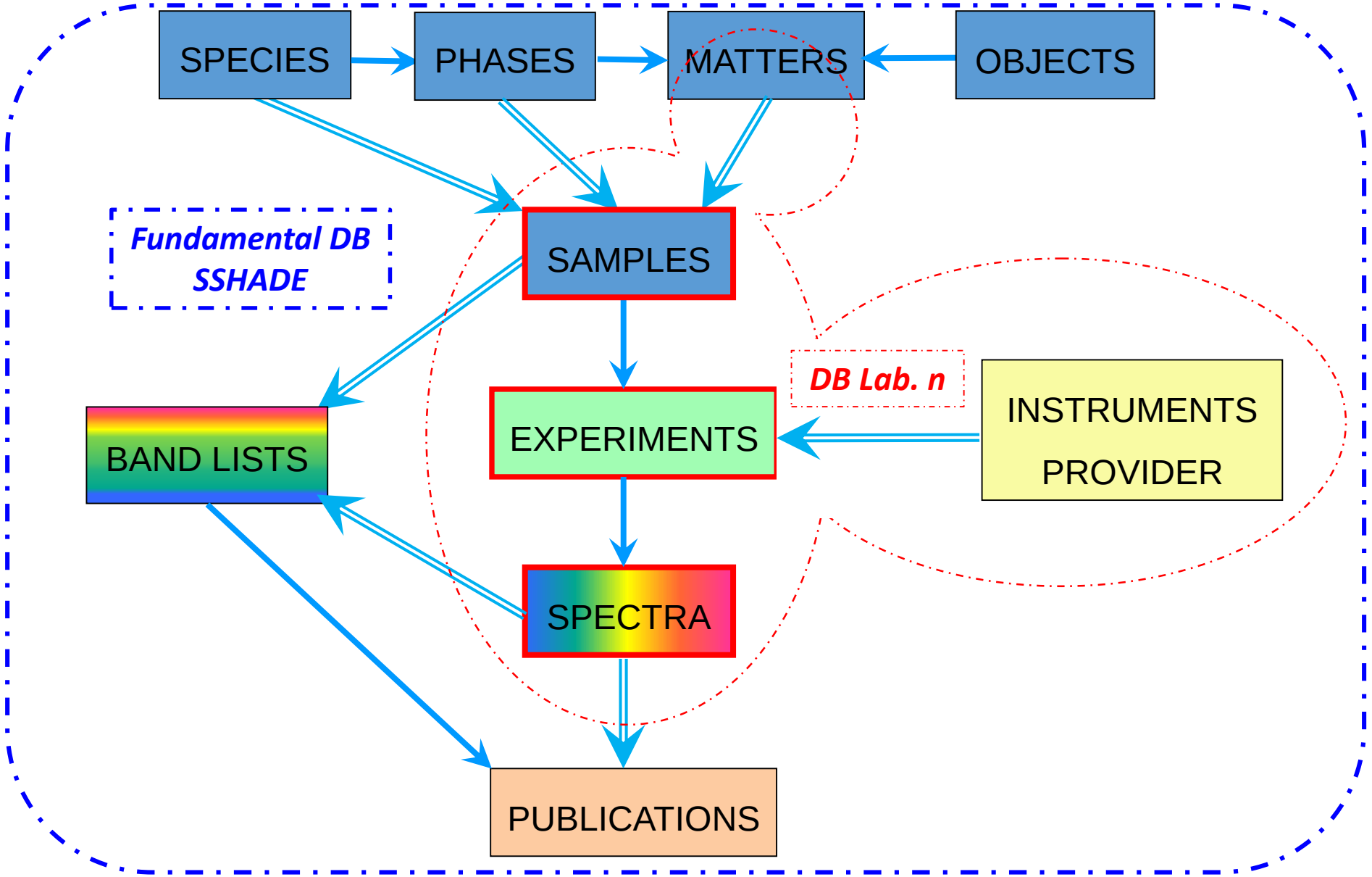
***SSHADE* :**

"Solid Spectroscopy Hosting Architecture of Databases and Expertise"

- Based on the ***GhoSST*** database developments (Europlanet + VAMDC)
  => http://ghosst.osug.fr
- Made of:
  - ✓ A 'solid spectroscopy' interface
  - ✓ A Search/Visualization/Export engine
  - ✓ A set of databases: one per group (GhoSST is one of them)
  - ✓ A common fundamental database
- All hosted at OSUG data center (OSU Grenoble – UGA *(formerly UJF)*)
- SSHADE will be a service of others VO (Europlanet-VO, VAMDC, ...)


WEB
Global SSHADE access to all DB
Direct access to one lab. DB
DB Management
IPAG
IAS
IRAP
...
Lab. n
GhoSST service
DAYSY service
PaSSTEL services
...
Lab n service
VO - VAMDC
VO - VESPA
Others VO
Interop
Interop
Interop
SSHADE
Interface
Search/Visu/Export/Tools
Data Center OSUG-DC
DB GhoSST
DB DAYSY
...
DB Lab. n
Fundamal DB
Bandlist DB

SSHADE: new SSDM structure



Europlanet 2020-RI
JRA-5 Activities (WP 11)

JRA – SSHADE infrastructure development → delivery 31st January 2018

Databases infrastructure (years 1 – 2)

- Adaptation of SSDM (data model)
- Reorganization of databases
- Rewriting data queries
- Design for easier data selection and browse
- Creation/customization of one database per Lab

Reorganization of databases

- Rewriting import parsers (year 1)
- Tools for easier data import (year 2)

VO interoperability

- with VESPA-VO and VAMDC-VO (years 2 – 3)

Europlanet 2020-RI
VA-2 Activities (WP 6)

VAA – Database feeding → delivery every year up to August 2019

Coordination of consortium

- Animation of SSHADE consortium
- Preparation and feeding of the common fundamental data of SSHADE (Years 1 - 3)
- Development of the common 'band list database' (Years 3 - 4)

Support to consortium

- 3 SSHADE consortium meetings (Years 1, 2, 4)
- Formation/training of database managers and 'feeders' (Years 1 - 3)
- Preparation of documentations and tutorials for providers
- In-situ & on-line support to each database manager

Support to users

- Tutorials & training for users at conferences (Years 3 - 4)
- Preparation of documentations and tutorials for users
- On-line support

Partners

- Preparation and feeding of spectral data and metadata

Who do what ?

SSHADE management

- *Scientific Manager*: Bernard Schmitt (IPAG)
- *Software Manager*: Damien Albert (OSUG)

SSHADE development

- *Databases development*: Philippe Bollard (IPAG)
- *VO interoperability:* Damien Albert (OSUG)
- *Databases storage*: Damien Albert + PB (OSUG Data Center, Grenoble)

Data bases feeding

- *Consortium/users support:* Alexandre Garenne + BS +LB (scientific engineer @ IPAG)
- *Fundamental data feeding* AG + Lydie Bonal + BS (science team @ IPAG)
- *Data validation, DB animation* Scientific Managers (one at each consortium group)
- *Data preparation & import* Database Managers (one at each consortium group)

SSHADE past events Time line

2015

- September — **Start of Europlanet 2020-RI**
- November — Start of SSHADE development
- December — Training database managers (session #1)

2016

- May — 1st SSHADE meeting
- May — Training database managers (session #2)
- August — 3 databases in SSHADE — **(D6.3 VAA VESPA – Y1)**
- August — **SSHADE prototype delivery** — **(D11.5 JRA VESPA)**
- October — Training database managers (session #3a) — **(D6.5 VAA VESPA – Y1)**
- November — Training database managers (session #3b)
- December — Training database managers (session #4a & 4b)

2017

- July — SSHADE 'party' (session #1 to #5)
- August — 9 databases in SSHADE — **(D6.3 VAA VESPA – Y2)**
- september — SSHADE 'party' (session #6) — **(D6.5 VAA VESPA – Y2)**
- October — Training database managers (session #5)
- December — **2nd SSHADE meeting**

SSHADE future events Time line

2018

- January — 11 databases in SSHADE
- January — **SSHADE infrastructure delivery** — **(D11.7 JRA VESPA)**
- March — Training database managers (session #6)
- March — Training users LPSC (session #1)
- April — Training users EGU (session #2)
- May — Training database managers (session #7)
- August — 14 databases in SSHADE — **(D6.3 VAA VESPA – Y3)**
- September — Training users EPSC (session #3) — **(D6.5 VAA VESPA – Y3)**
- October — Training database managers (session #8)
- October — Training users DPS (session #4)
- October — Training users ??? (session #5)

2019

- February — Training database managers (session #9)
- March — Training users LPSC (session #6)
- March — **3rd SSHADE meeting**
- April — Training users EGU (session #7) — **(D6.5 VAA VESPA – Y4)**
- June — 18 databases ingested in SSHADE
- August — **SSHADE with 18-20 databases** — **(D6.3 VAA VESPA – Y4)**
- August — **End of Europlanet 2020-RI**

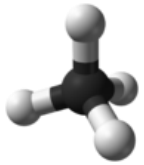
Recent SSDM Changes / Improvements

Recent SSDM Changes / Improvements (2017)

- **Sample / Constituent**
  - added options « basic constituents » in parallel to « constituent »
  - added a number of optional description & properties to ‘constituent’
- **fondamental phases:** new ! + added ‘solid’ & ‘liquid’ in addition to ‘mineral’ (added ‘polytype’)
- **Mineral matters**: extended to ‘solid matters’
- **Molecule**: added bloc with all types of ‘stereo-isomers’
- **Objects**: added extensions ‘Micrometeorites’ & ‘IDPs’
- **Spectra:** added « multi-angle data » with a single file or multiple files
  + improvements in file import options and spectrum previews

➔ Still need your inputs if something unclear !!

SSDM General Structure

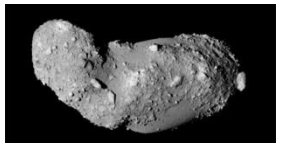


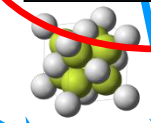
SPECIES

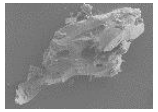
PHASES

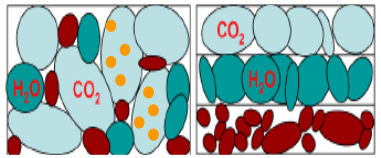
MATTERS

OBJECTS



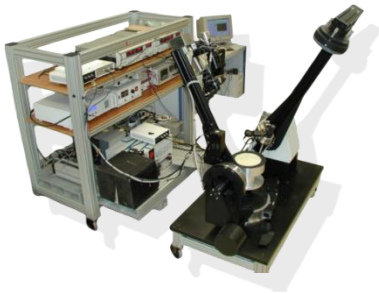


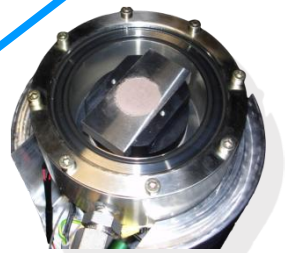




SAMPLE

INSTRUMENT



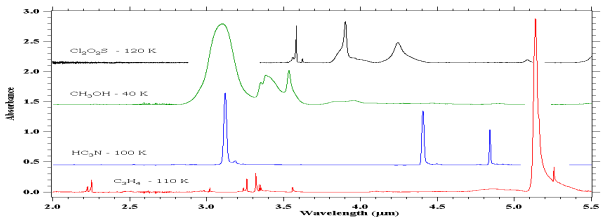


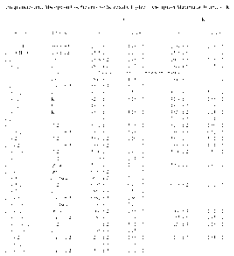
EXPERIMENT

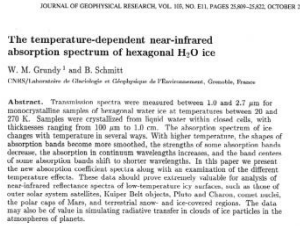
PROVIDER

BAND LIST

SPECTRA



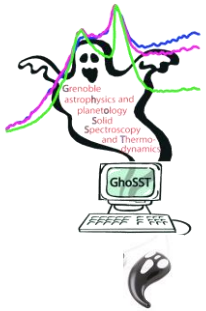




The temperature-dependent near-infrared absorption spectrum of hexagonal H_2O ice

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

PUBLICATIONS



Fundamental Phases

- **What it is?:** a single and well defined phase (or a series, or a group)
  i.e. a solid (or series of solids) with a well defined composition and crystal structure (or amorphous)

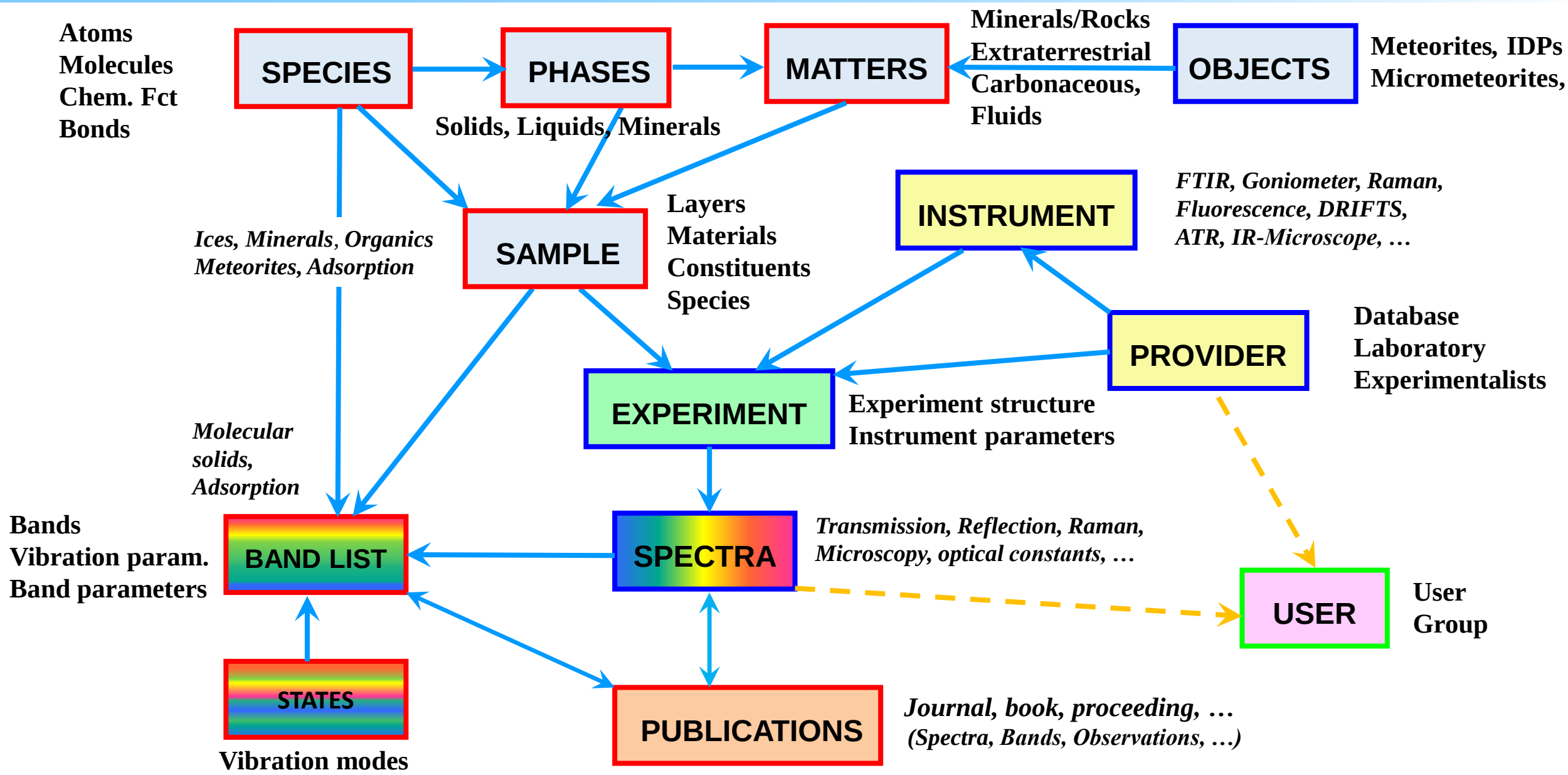
- **Why?:** * Describe one time – use many (links)
  ➔ all samples using this phase will refer to exactly the same

- **Different types:**
  - Solids (synthetics)
  - Minerals (naturals)
  - Liquids (synthetics)

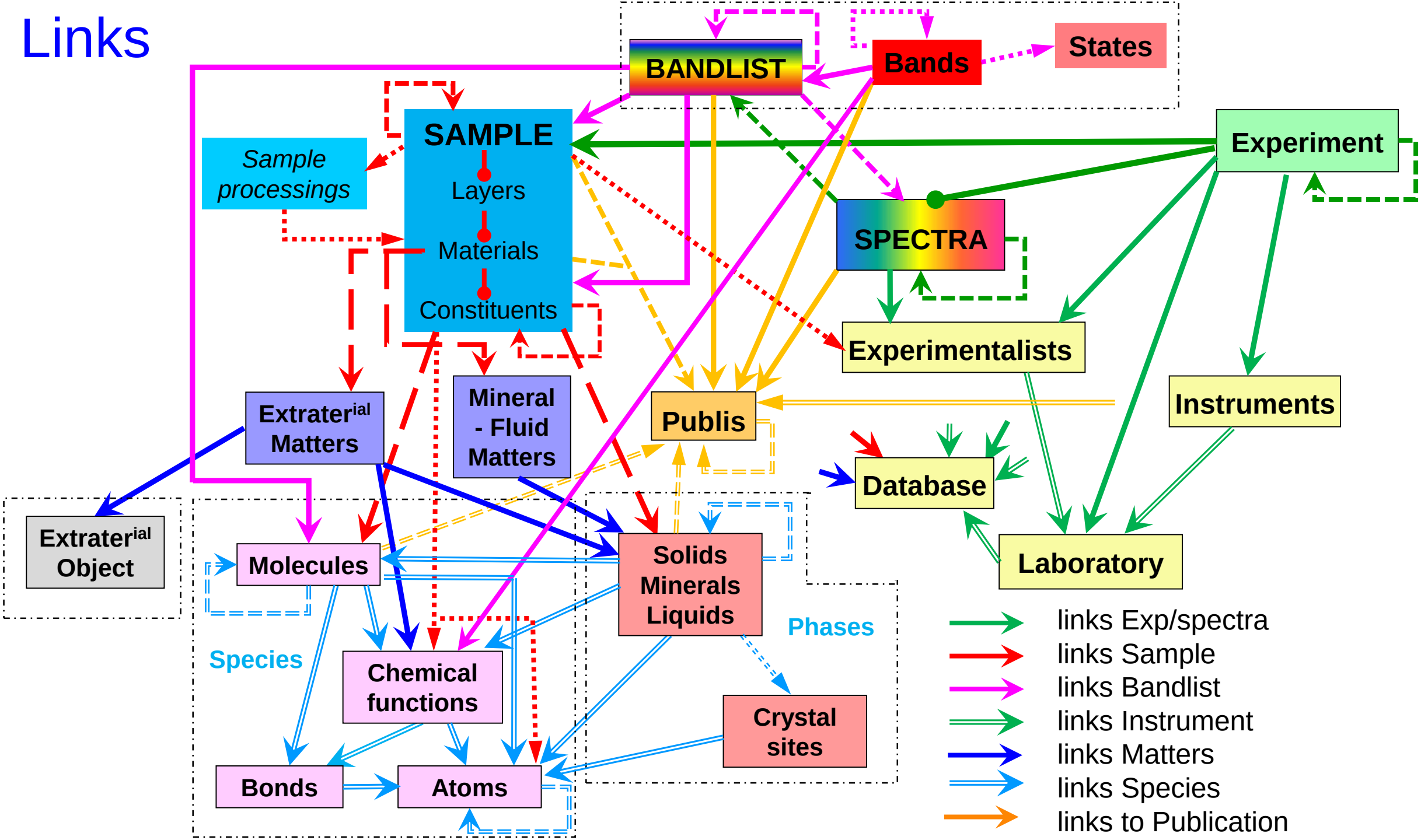
- **Provide fundamental information on the phase**
  - Common info to all phase types (name, description, composition, structure, properties ...)
  - Specific info for each phase type (classification, specific cases)
  - Composition : molecular or atomic species

- **Variable parameters** (in constituent):
  ➔ Allow to change some values of a fundamental solid, mineral or liquid phase

SSDM General Structure



Links


BANDLIST
Bands
States
SAMPLE
Layers
Materials
Constituents
Sample processings
Experiment
SPECTRA
Experimentalists
Instruments
Extraterial Matters
Mineral - Fluid Matters
Publis
Database
Laboratory
Extraterial Object
Molecules
Solids Minerals Liquids
Phases
Species
Chemical functions
Crystal sites
Bonds
Atoms
links Exp/spectra
links Sample
links Bandlist
links Instrument
links Matters
links Species
links to Publication

SSDM + SSHADE DB implementation

	SSDM	SSHADE
• Databases/Laboratories/Experimentalists:	➔ Stable	Done
• Species:		
– Atomic and Molecular	➔ Stable	Done
– Chemical bonds and functions	➔ Stable	Done
• Phases:		
– Minerals	➔ Stable	Done
– Solids, Liquids	➔ Stable	Done
• Matters:		
– Fluids	➔ Stable	Done
– Solids	➔ Stable	Done
– Extraterrestrial	➔ Stable	Done
– Carbonaceous	➔ Stable	Done
• Objects:		
– Meteorites, Cosmic Dusts, IDPs	➔ Stable	Done
• Samples: Layers/Material/Constituents	➔ Stable	Done
• Instruments/techniques:	➔ Stable	Done
• Spectra and products:	➔ Stable	Done
• Band lists (Molecular solids + adsorption)		
– Bands parameters, attributions, states	➔ TBC	TBD
– Bands parameters functions (T, P, ...)	➔ Draft	TBD
– Molecular vibration modes parameters	➔ Draft	TBD
• Publications	➔ Stable	Done

SSDM – future evolutions (2018)

- Spectra

  Multi-angle data:
  - add KW ‘spectral_observation_mode’, ‘angle_observation_mode’, ‘angle_observation_geometry’
  - simplify attributs of KW ‘spectrum_type’
  - improve import

  Spectro-images:
  - Define format of storage and import/export formats
  - Add some specific KW (but most already exists)

- Bandlist:

  List of band positions, width, intensity, transition modes … of a constituent in a defined environment (T, P, …)
  - Integrate all SSDM changes/homogeneization/simplification
  - Change ‘sample’ link to Constituent

- Band parameters

  Variation of band parameters with temperature, pressure …

- Molecular vibration modes parameters

  Harmonic frequencies and anharmonic and interaction terms of molecular species in molecular solids

Band list : bands and states

- Bands parameters
  - position (energy),
  - width, shape, …
  - intensities (peak and integrated)
  - accuracies / quality / evaluation
- Transitions assignment
  - states QN, anharmonic coefficients, …

Development of SSHADE interface

Development of SSHADE interface

Development of SSHADE interface

- For users: Login / Search / Visualization / Export
- For data providers: Detailed search, import, publication tool
- For SSHADE managers: management of database, users, groups, …., backup, special data management

➔ detail of the interface functions by Philippe

see file: SSHADE-development_2017-12-4_bollardp.pdf

➔ live demonstration of interface by Alex

➔ questions/discussion on SSHADE interface

➔ discussion on future beta testing

Development of SSHADE interface

Major changes and improvements

- Spectra search + Publications search
- Results: experiments and spectra
- Experiment / spectra structure display
- Sample structure display
- Metadata display

Spectra search

For Users

Spectra

- Simple search field ‘à la Google’
- with simple filters
  - Database
  - on Spectrum
  - on Sample

Publications

For producers

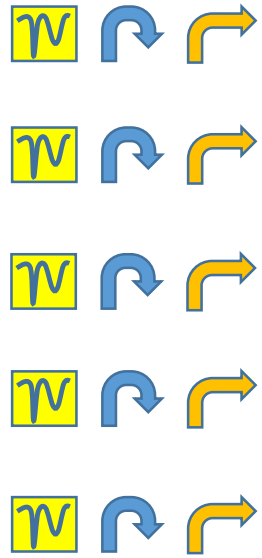
All types of data

- Fundamental species (Atoms, Chemical bonds, Chemical functions, Molecules)
- Fundamental phases (Minerals, Solids, Liquids)
- Objects (Meteorites, Micrometeorites, IDPs)
- Matters and Samples (Layers / Materials / Constituents)
- Experiments and spectral data (+ Instruments)
- Databases, Laboratories, Experimentalists
- Bibliography (Publications, Journals)
- Open Enums

Results: experiments and spectra

Spectra: 47 found

- MIR optical constants spectrum of crystalline H2O at 60K
- NIR absorption coefficient spectrum of crystalline H2O at 60K
- NIR bidirectional reflection spectra of Smectite SWy-2 [4 spectra]
- NIR transmission spectrum of amorphous H2O at 56K
- Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]



Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 47 found

Spectrum info

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Clic! => Page Spectrum

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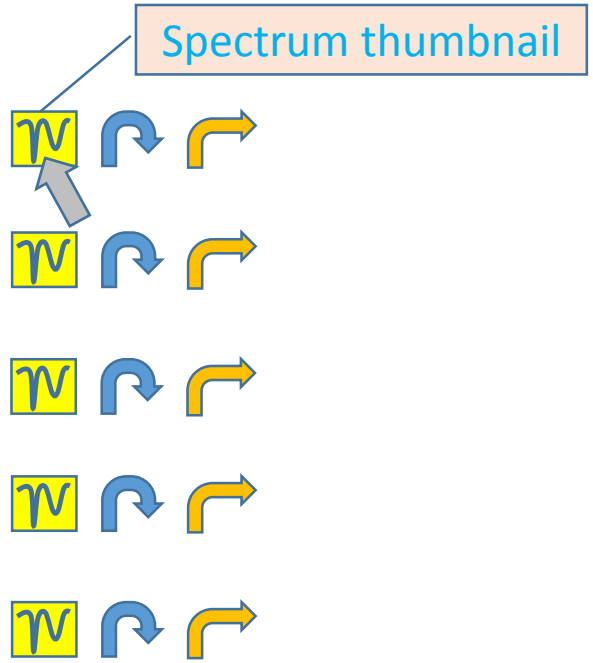

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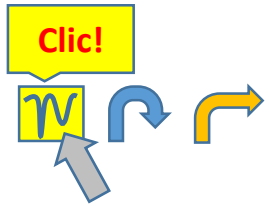
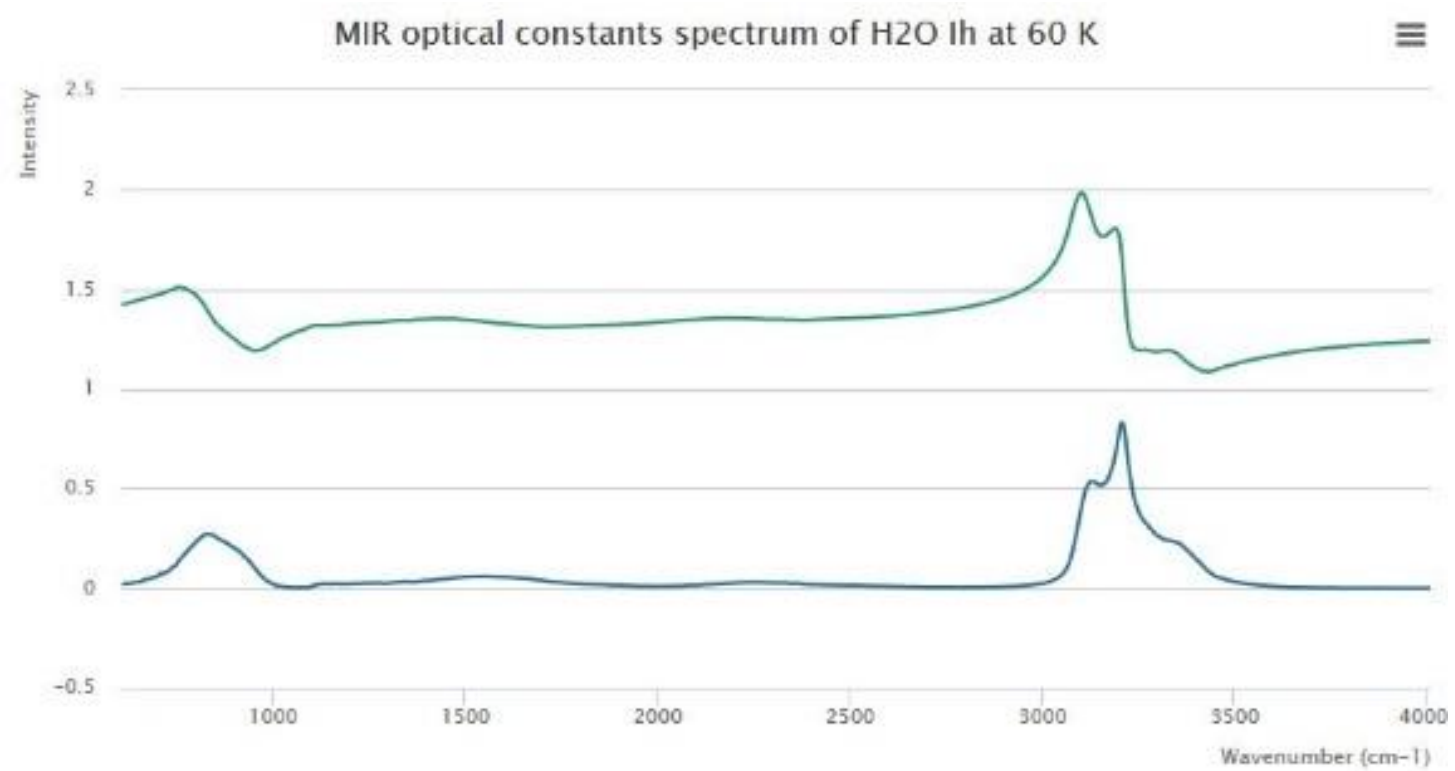
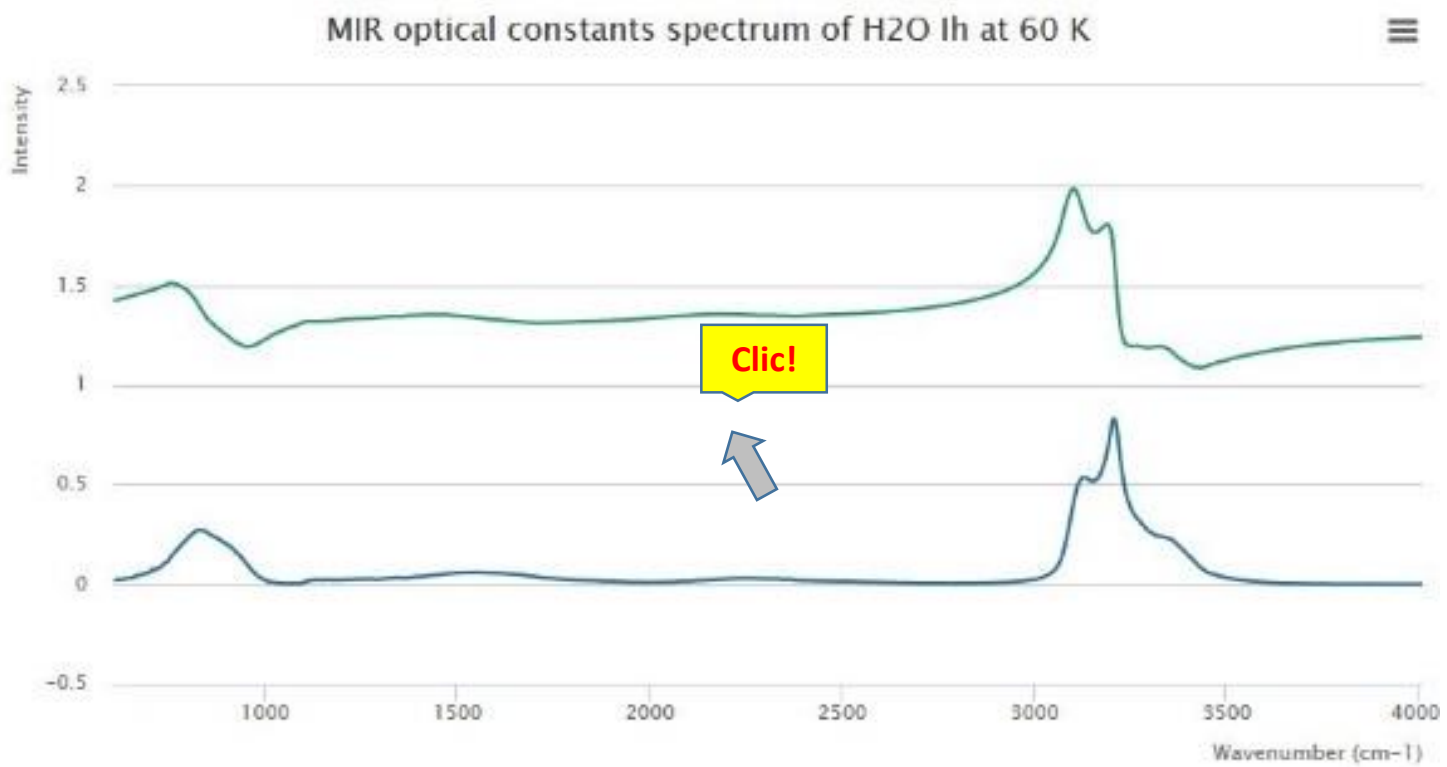




Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 47 found

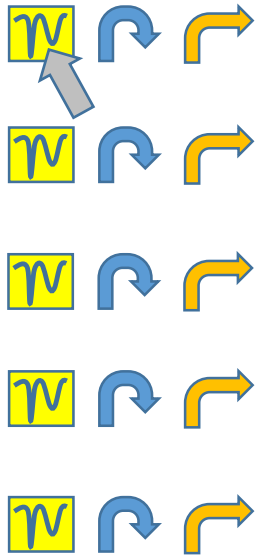
- MIR optical constants spectrum of crystalline H2O at 60K



Current Search: H2O 60K NIR MIR New Search Refine Search

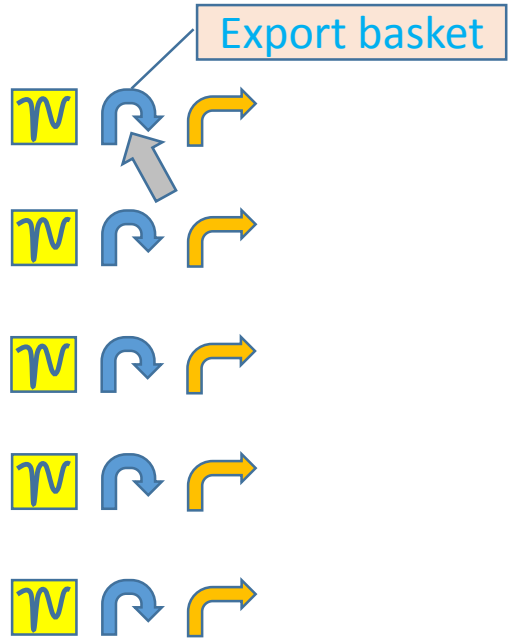
Spectra: 47 found

- MIR optical constants spectrum of crystalline H2O at 60K
- NIR absorption coefficient spectrum of crystalline H2O at 60K
- NIR bidirectional reflection spectra of Smectite SWy-2 [4 spectra]
- NIR transmission spectrum of amorphous H2O at 56K
- Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]



Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 47 found



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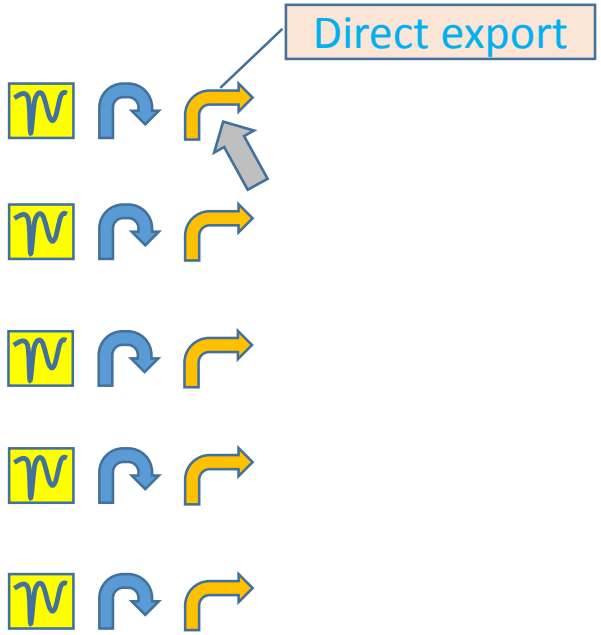
Spectra: 47 found



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Clic!

- Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra] 

Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 47 found

Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]

- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 10°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 20°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 30°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 45°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 60°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 20°, e= 10°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 20°, e= 20°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 20°, e= 30°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 20°, e= 45°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 20°, e= 60°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 30°, e= 10°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 30°, e= 20°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 30°, e= 30°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 30°, e= 45°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 30°, e= 60°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 45°, e= 10°)
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- Vis-NIR BRDF spectra of Antarctic snow (i = 45°, e= 30°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 45°, e= 45°)
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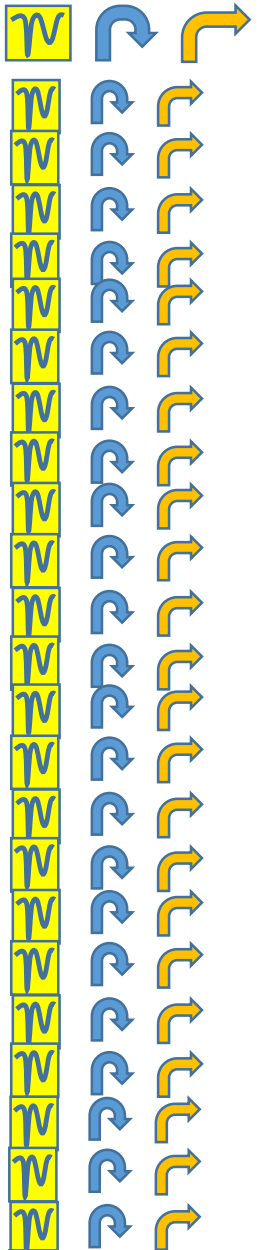
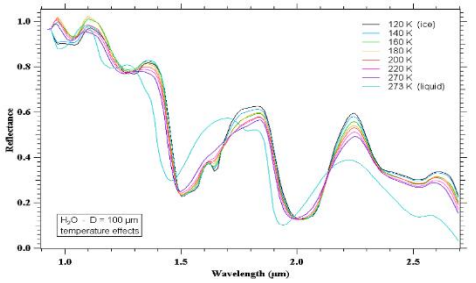
- Vis-NIR BRDF spectra of Antarctic snow (i = 60°, e= 10°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 60°, e= 20°)
- Vis-NIR BRDF spectra of Antarctic snow (i = 60°, e= 30°)





Spectra: 47 found

Clic!

Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]

- Vis-NIR BRDF spectra of Antarctic snow (i = 0°, e= 10°)
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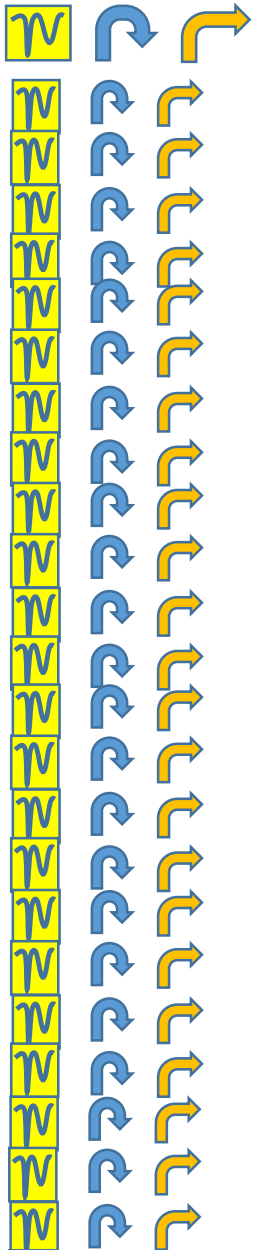

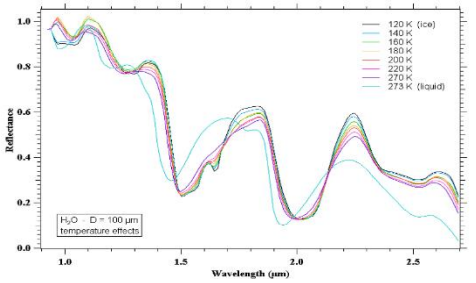

Spectra: 47 found

- MIR optical constants spectrum of crystalline H2O at 60K 
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Current Search: H2O 60K NIR MIR New Search Refine Search

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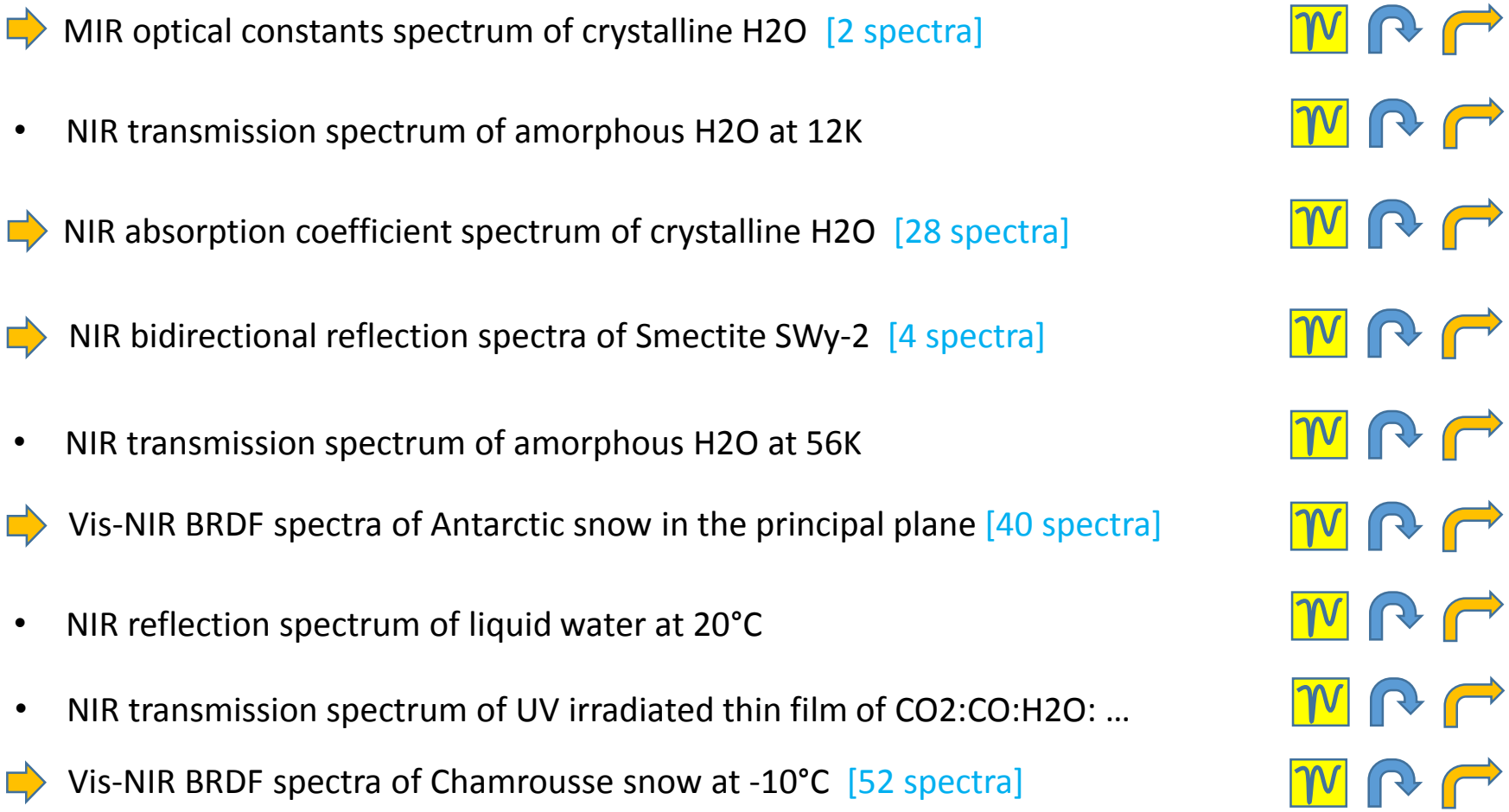
Clic!

Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 162 found

- MIR optical constants spectrum of crystalline H2O [2 spectra]
- NIR transmission spectrum of amorphous H2O at 12K
- NIR absorption coefficient spectrum of crystalline H2O [28 spectra]
- NIR bidirectional reflection spectra of Smectite SWy-2 [4 spectra]
- NIR transmission spectrum of amorphous H2O at 56K
- Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]
- NIR reflection spectrum of liquid water at 20°C
- NIR transmission spectrum of UV irradiated thin film of CO2:CO:H2O: …
- Vis-NIR BRDF spectra of Chamrousse snow at -10°C [52 spectra]
- *More …* 1 2 3



Current Search: H2O 60K NIR MIR New Search Refine Search

Spectra: 162 found

- MIR optical constants spectrum of crystalline H2O [2 spectra] 
- NIR transmission spectrum of amorphous H2O at 12K 
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- NIR transmission spectrum of amorphous H2O at 56K 
- Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra] 
- NIR reflection spectrum of liquid water at 20°C 
- NIR transmission spectrum of UV irradiated thin film of CO2:CO:H2O:CH3OH=1:1:0.1:0.05 mixture at 125 K
- Vis-NIR BRDF spectra of Chamrousse snow at -10°C [52 spectra] 
- *More …* 1 2 3

Current Search: ■ H2O □ 60K ■ NIR ■ MIR New Search Refine Search

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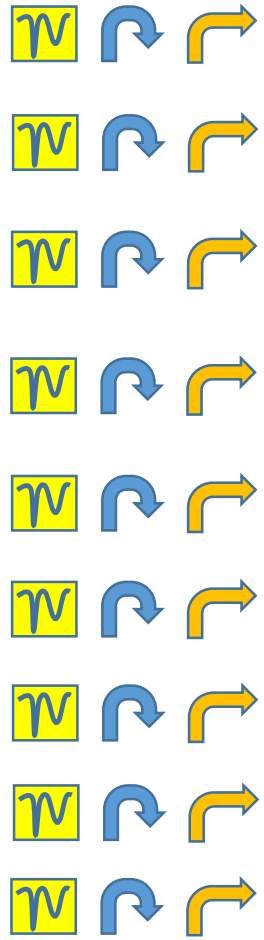

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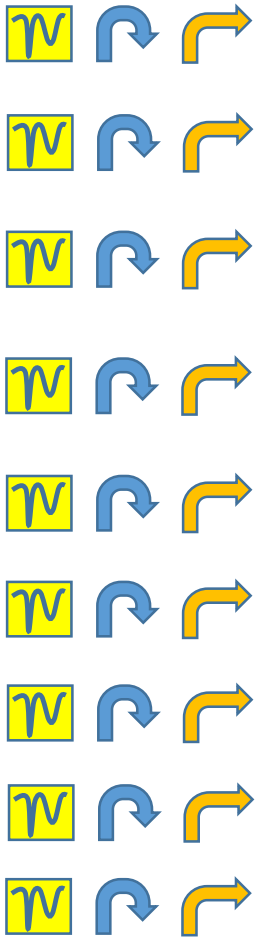

Clic!

=> Page Search (reseted)

Current Search: ■ H2O □ 60K ■ NIR ■ MIR

New Search

Refine Search

Spectra: 162 found

- MIR optical constants spectrum of crystalline H2O [2 spectra]
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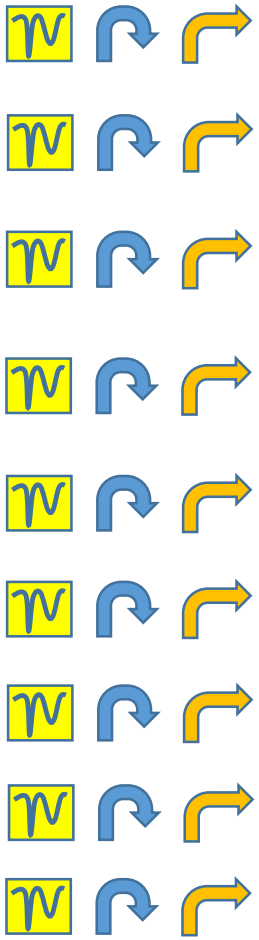


Page Search (keep current choices) <= **Clic!**

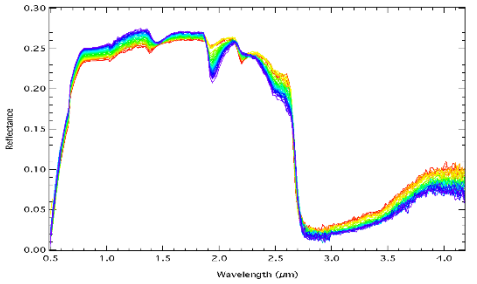
Current Search: ■ H2O □ 60K ■ NIR ■ MIR New Search Refine Search

Experiment / spectra structure display

Spectra: 162 found

- ⊞ MIR optical constants spectrum of crystalline H2O [2 spectra]
- NIR transmission spectrum of amorphous H2O at 12K
- ⊞ NIR absorption coefficient spectrum of crystalline H2O [28 spectra]
- ⊟ NIR bidirectional reflection spectrum of Smectite SWy-2 [4 spectra]
  - NIR bidirectional reflection spectrum of Smectite SWy-2 (0-25µm grains) at 60 K
  - NIR bidirectional reflection spectrum of Smectite SWy-2 (25-50µm grains) at 60 K
  - NIR bidirectional reflection spectrum of Smectite SWy-2 (50-100µm grains) at 60 K
  - NIR bidirectional reflection spectrum of Smectite SWy-2 (100-250µm grains) at 60 K

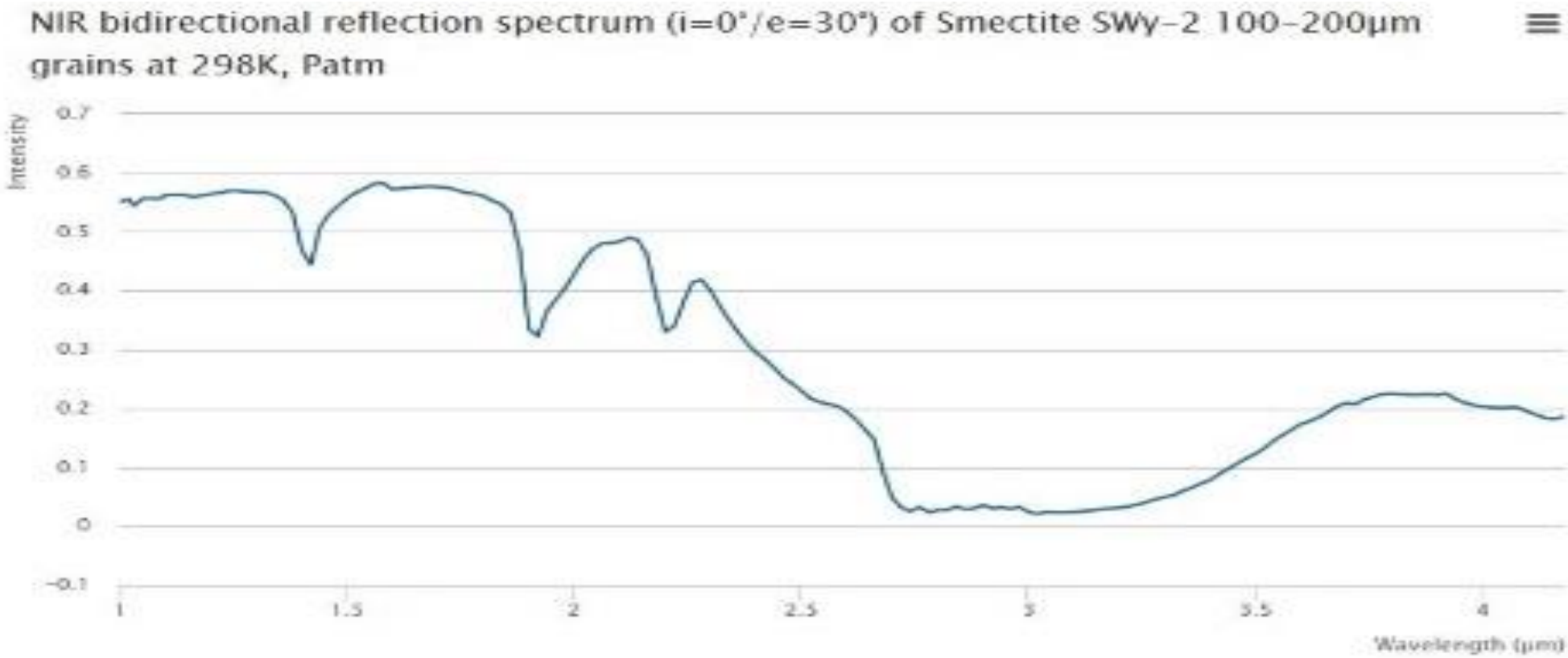
Clic!



- NIR transmission spectrum of amorphous H2O at 56K
- ⊞ Vis-NIR BRDF spectra of Antarctic snow in the principal plane [40 spectra]
- NIR reflection spectrum of liquid water at 20°C
- *More …* 1 2 3

Current Search: ■ H2O □ 60K ■ NIR ■ MIR New Search Refine Search

Spectrum preview



Database	GhoSST, SSTONE	
Instrument(s)	Spectro-gonio radiometer SHADOWS	
Spectrum type	bidirectional reflectance	
Version	#1 (2014-08-11)	[version n (last_updated #n)]
Valid spectral range(s)	400 – 1050 nm; 1100 – 2500 nm	[spectral_range_min / _max; …]
Observation geometry	i = 0°; e = 30°; az = 0°	
Observation mode	single spot	

Sample preview

Name	Na-Montmorillonite SWy-2 - 100-200 mic grains
Origin	natural terrestrial, commercial
Texture	earthy
Thickness	1 ± 0.1 mm
Temperature	293 ± 1 K
Pressure	1 ± 0.05 bar
Stress	normal compression
Fluid	Dry atmospheric air, 98% - H_2O, 2 ± 0.2 % - CO_2, 0.05 ± 0.01 %
Irradiated by	VUV photons, 12 eV

Publications

A. Pommerol, B. Schmitt, 2008, Journal of Geophysical Research – Planets, 113, E10, 33p

P. Beck et al., 2009, Journal of Geophysical Research – Planets, 115, E17, 22p

Results

Experiment NIR reflectance of Na-Montmorillonite SWy-2, with different grain sizes and temperatures

Variables: sample texture, temperature

Sub-Experiment NIR reflectance of Na-Montmorillonite SWy-2, 100 – 200 µm with different temperatures

Variable: temperature

Spectra

- NIR reflectance of Na-Montmorillonite SWy-2, 100 – 200 µm at 320 K
- NIR reflectance of Na-Montmorillonite SWy-2, 100 – 200 µm at 298 K
- NIR reflectance of Na-Montmorillonite SWy-2, 100 – 200 µm at 250 K

Sub-Experiment NIR reflectance of Na-Montmorillonite SWy-2, 200 – 500 µm with different temperatures

Variable: temperature

Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Materials

Parent Matter: Swy-2

- Na-Montmorillonite with adsorbed and interlayer water 71 w%
- Quartz – 7.8 w%

Results

Experiment NIR reflectance of Na-Montmorillonite SWy-2, with different grain sizes and temperatures

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Clic!

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- NIR ref
- NIR ref

Description: Near IR (0.8-5.5 µm) bidirectional reflectance at temperatures 250, 298 and 320 K of Na-Montmorillonite SWy-2, grains size range: 200 – 500 µm

Sub-Experiment NIR reflectance of Na-Montmorillonite SWy-2, 200 – 500 µm with different temperatures

Variable: temperature

Spectra

- NIR reflectance of Na-Montmorillonite SWy-2, 200 – 500 µm at 320 K
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Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Materials

Results

Experiment NIR reflectance of Na-Montmorillonite SWy-2, with different grain sizes and temperatures — *Variables: sample texture, temperature*

Sub-Experiment NIR reflectance of Na-Montmorillonite SWy-2, 100 – 200 µm with different temperatures — *Variable: temperature*

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Clic!

Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Materials

Results

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Layers Na-Montmorillonite SWy-2 - 200-500 mic grains – Layer #1

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Clic!

Experiment NIR reflectance of Na-Montmorillonite SWy-2, with different grain sizes and temperatures

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Sample Na-Montmorillonite SWy-2 - 200-500 mic grains

Layers Na-Montmorillonite SWy-2 - 200-500 mic grains – Layer #1

Materials

Results

Sample structure display

Experiment NIR reflectance of Na-Montmorillonite with different grain sizes and temperat

Sample Na-Montmorillonite SWy-2 - 200-500 mic grains

Layers Na-Montmorillonite SWy-2 - 200-500 mic grains – Layer #1

Materials

Clic!

arent Matter: Swy-2

- Na-Montmorillonite with adsorbed and interlayer water 71 w%
- Quartz – 7.8 w%
- Plagioclase – 12 w%
- Gypsum – 1 w%
- Calcite – 0.7 w%
- Orthopyroxenes – 1.4 w%

- H2O ice – 20 w%

Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Materials

Parent Matter: Swy-2

Na-Montmorillonite with adsorbed and interlayer water 71 w%

Constituents

- Na-Montmorillonite – 100 w%
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Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Clic!

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Experiment NIR reflectance of Na-Montmorillonite SWy-2 with different grain sizes and temperatures

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Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Experiment NIR reflectance of Na-Montmorillonite SWy-2 with different grain sizes and temperatures

---

Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Clic!

Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Clic!

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- Interlayer water - 1.4 w% sorbed
- Quartz – 7.8 w%
- Plagioclase – 12 w%
- Gypsum – 1 w%
- Calcite – 0.7 w%
- Orthopyroxenes – 1.4 w%

Sample preview

Name	Na-Montmorillonite SWy-2 - 100-200 mic grains
Origin	natural terrestrial, commercial
Texture	earthy
Thickness	1 ± 0.1 mm
Temperature	293 ± 1 K
Pressure	1 ± 0.05 bar
Stress	normal compression
Fluid	Dry atmospheric air, 98% - H_2O, 2 ± 0.2 % - CO_2, 0.05 ± 0.01 %
Irradiated by	VUV photons, 12 eV

Publications

A. Pommerol, B. Schmitt, 2008, Journal of Geophysical Research – Planets, 113, E10, 33p

P. Beck et al., 2009, Journal of Geophysical Research – Planets, 115, E17, 22p

Sample

UID

Name	Na-Montmorillonite SWy-2 - 100-200 µm grains

⊞ Owner of sample

⊞ Origin of sample

⊞ *Image*

⊟ *Physical characteristics*

Thickness	1 ± 0.1 mm
Diameter	30 mm
Volume	710 mm^3
Mass	1.35 ± 0.08 g
Surface roughness	polished
Texture	earthy
Substrate material	aluminum anodized black
Comments	blabla bla

⊞ *Sample Environment: Temperature*

⊞ *Sample Environment: Hydrostatic pressure*

⊞ *Sample Environment: Fluid*

Sample

- *Sample Environment: Mechanical stress*
- *Sample Environment: Irradiation*
- *Documentation & Publications*
- *Layers in sample*
- *Sample processings*

Sample

UID

Name	Na-Montmorillonite SWy-2 - 100-200 µm grains

Clic!

Owner of sample

Origin of sample

Image

Physical characteristics

Thickness	1 ± 0.1 mm
Diameter	30 mm
Volume	710 mm^3
Mass	1.35 ± 0.08 g
Surface roughness	polished
Texture	earthy
Substrate material	aluminum anodized black
Comments	blabla bla

Sample Environment: Temperature

Sample Environment: Hydrostatic pressure

Sample Environment: Fluid

Sample

UID

Name Na-Montmorillonite SWy-2 - 100-200 µm grains

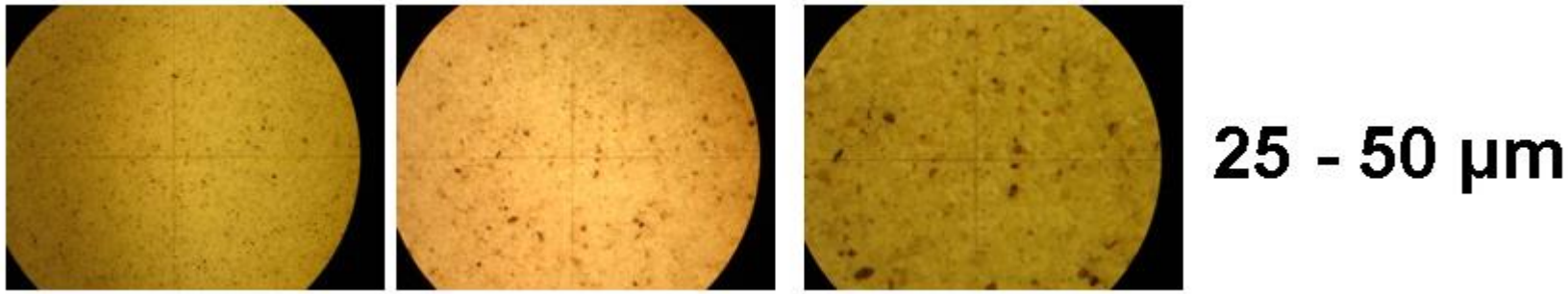
Owner

Database GhoSST, SSTONE
Experimentalists Pierre Beck, Olivier Poch
Date 2017-11-13

Origin

Provider IPAG
Parent sample Na-Montmorillonite SWy-2
Generic sample yes
Original samples Na-Montmorillonite SWy-2 - 100-150 µm grains
Na-Montmorillonite SWy-2 - 150-200 µm grains
Previous sample Na-Montmorillonite SWy-2 - 100-200 µm grains

Image



Picture of the sample Na-Montmorillonite SWy-2 - 25-50 µm grains

Sample

UID

Sample Environment: Temperature

Temperature	293 ± 1 K
Time at T	20 ± 1 min
Temperature max	293 ± 1 K
Time at Tmax	125 min
Comments	blabla bla

Sample Environment: Hydrostatic pressure

Pressure	1 ± 0.05 bar
Time at P	20 ± 1 min
Pressure max	100 ± 0.5 bar
Time at Pmax	125 min
Comments	blabla bla

Sample Environment: Fluid

Type	molecular gas
Fluids	dry atmospheric air, 98 ± 0.2 %
	H_2O, 2 ± 0.2 %
	CO_2, 0.05 ± 0.01 %
Fluid temperature	293 ± 1 K
Fluid pressure	1 ± 0.05 bar
Fluid pH	5.3 ± 0.1
Time at T, P, pH	20 ± 1 min
Comments	blabla bla

Sample

UID

Documentation

Frozen samples

Publications

A. Pommerol, B. Schmitt, 2008, Journal of Geophysical Research – Planets, 113, E10, 33p

P. Beck et al., 2009, Journal of Geophysical Research – Planets, 115, E17, 22p

Layers in sample

Number	2
Arrangement	homogeneous mixing
Layers	#2: H2O frost, 1 mm
	#1: Na-Montmorillonite SWy-2 - 100-200 µm grains, 20 mm

Sample processings

Sample Na-Montmorillonite SWy-2 - 100-200 mic grains

Layers Na-Montmorillonite SWy-2 - 100-200 mic grains – Layer #1

Materials

Parent Matter: Swy-2

Na-Montmorillonite with adsorbed and interlayer water 71 w%

Constituents

Clic!

- Na-Montmorillonite – 100 w%
- Adsorbed water - 7.2 w% sorbed
- Interlayer water - 1.4 w% sorbed
- Quartz – 7.8 w%
- Plagioclase – 12 w%
- Gypsum – 1 w%
- Calcite – 0.7 w%
- Orthopyroxenes – 1.4 w%

Constituent

Name Truc Much

Type

Constituent abundance in Material

Arrangement single phase
Mass 1.85 ± 0.05 g
Mass Fraction 0.56 ± 0.04

Constituent sorption

Chemical composition

Formula CH_3-$(CH_2)_4$-CH=COOH•4(H_2O)
Chemical formula CH3-(CH2)4-CH=COOH•4(H2O)
Elemental formula C7 O6 H21
Hydration yes
Hydration number 4
Isotope mixture type terrestrial abundance

Species

Chemical functions and bonds

Crystallography & texture

Properties

The SSHADE Wiki

The SSHADE Wiki (and Blog)

https://wiki.sshade.eu

Documentation for the user:

- SSHADE interface manual, tutorial, user cases, …
- Papers from SSHADE
- Description of all databases
  - Samples and spectra, instruments, papers, …

Documentation for the provider :

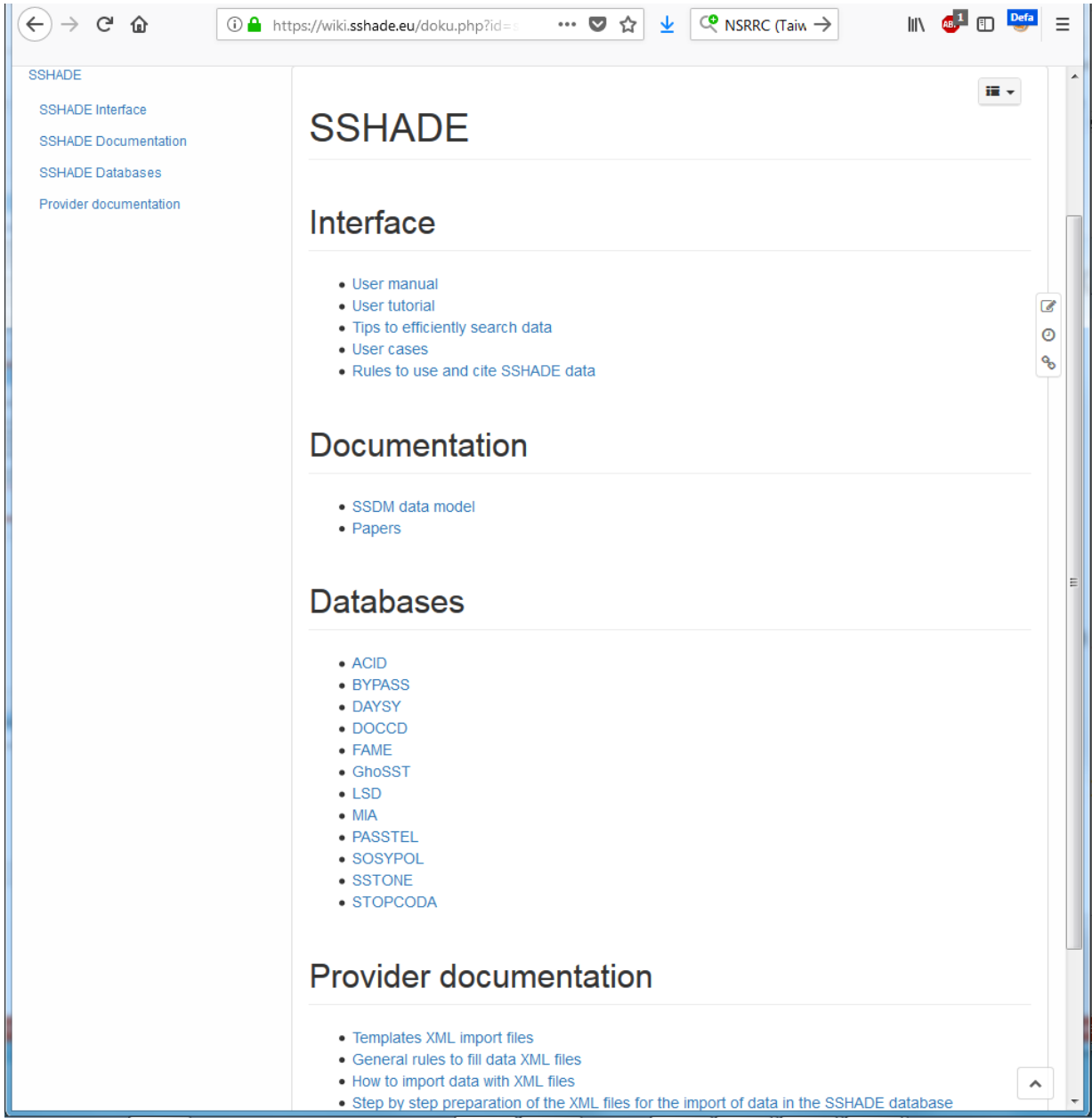
(restricted access: same login as SSHADE)

- SSDM data model
- XML import templates (up-to-date), customized …
- Import manual, tutorials, …

SSHADE blog : https://blog.sshade.eu

- To move to Wiki (description, consortium partners, …)
- To move to SSHADE front page (news, …)

Databases: need for a private area ?



The SSHADE Wiki

Still to be done before delivery:

By SSHADE team

- SSDM data model: to be updated to v0.8.4
- XML import templates (up-to-date) : OK
- Import manual, tutorials, … : to be updated
- Documentation for the user (user manual, citation rules): to be updated

By each partner

- Description of all active databases

➔ to be filled for each database with data (before 15th january)

Development of SSHADE VO

Development of SSHADE VO

Development of SSHADE Virtual Observatory (VO) access for VESPA

- Provide VO search on a limited number of main metadata
  (species name/formula, spectral type, T, …)
- Allow to retrieve the data (spectra) and some metadata for displaying in VO

➔ details of VO and proto demonstration by Damien

see file: *OSUG-VO SSHADE-VO_2017-12_D-Albert.pdf*

➔ questions/discussion on SSHADE VO

The DOI in SSHADE

The DOI in SSHADE

At 4 levels

- SSHADE — 10.5072/SSHADE
- each database — 10.xxxx/SSHADE."database_acronym"
  ex: 10.5072/SSHADE.GhoSST
- each experiment — 10.xxxx/SSHADE."database_acronym"."experiment_uid"
  ex: 10.5072/SSHADE.GhoSST.EXP_BS_20161109_001
- each Bandlist: — 10.xxxx/SSHADE."bandlist_uid"
  ex: 10.5072/SSHADE.BANDLIST_H2O_125K

DOI will redirect to a 'landing page' => SSHADE page, or the data page

➔ will be implemented only after delivery

The DOI in SSHADE

The DOI

- will be automatically created during an experiment import

- create a standardized data reference from the data
  - Creator (PublicationYear): Title. Publisher. Identifier

  or
  - Creator (PublicationYear): Title. Version. Publisher. ResourceType. Identifier

  ➔ equivalence with SSDM

  - Database: ‘database creators’ (creation_year), SSHADE / ‘database_acronym’: ‘database_name’, SSHADE (OSUG-DC), Database, 10.5072/SSHADE.’database_acronym’

    Ex: Schmitt B., Albert D., Bollard Ph., Bonal L. (2012), SSHADE / GhoSST: Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamic database, SSHADE (OSUG-DC), Database, 10.5072/SSHADE.GhoSST

  - Experiment: ‘experimentalists’ (record year), ‘experiment_title’, version 2, SSHADE (OSUG-DC) / "database_acronym", Experiment, 10.5072/SSHADE.’database_acronym’.’experiment_uid’

    Ex: Beck P., Quirico E., Bonal L. (2016) NIR reflectance of Na-Montmorillonite SWy-2, with different grain sizes and temperatures. version 2. SSHADE (OSUG-DC) / GhoSST, Experiment, 10.5072/SSHADE.GhoSST.EXP_BS_20161109_001

Data ingestion in SSHADE and its databases

State of data ingestion in SSHADE and its databases

- SSHADE
  - Fundamental Species:
    - ✓ Atoms, molecules, chemical bonds, chemical functions
  - Fundamental Phases:
    - ✓ minerals, solids, liquids
  - Reference Matters
  - Objects:
    - ✓ Meteorites, Cosmic Dusts, IDPs
  - Publications, Journals

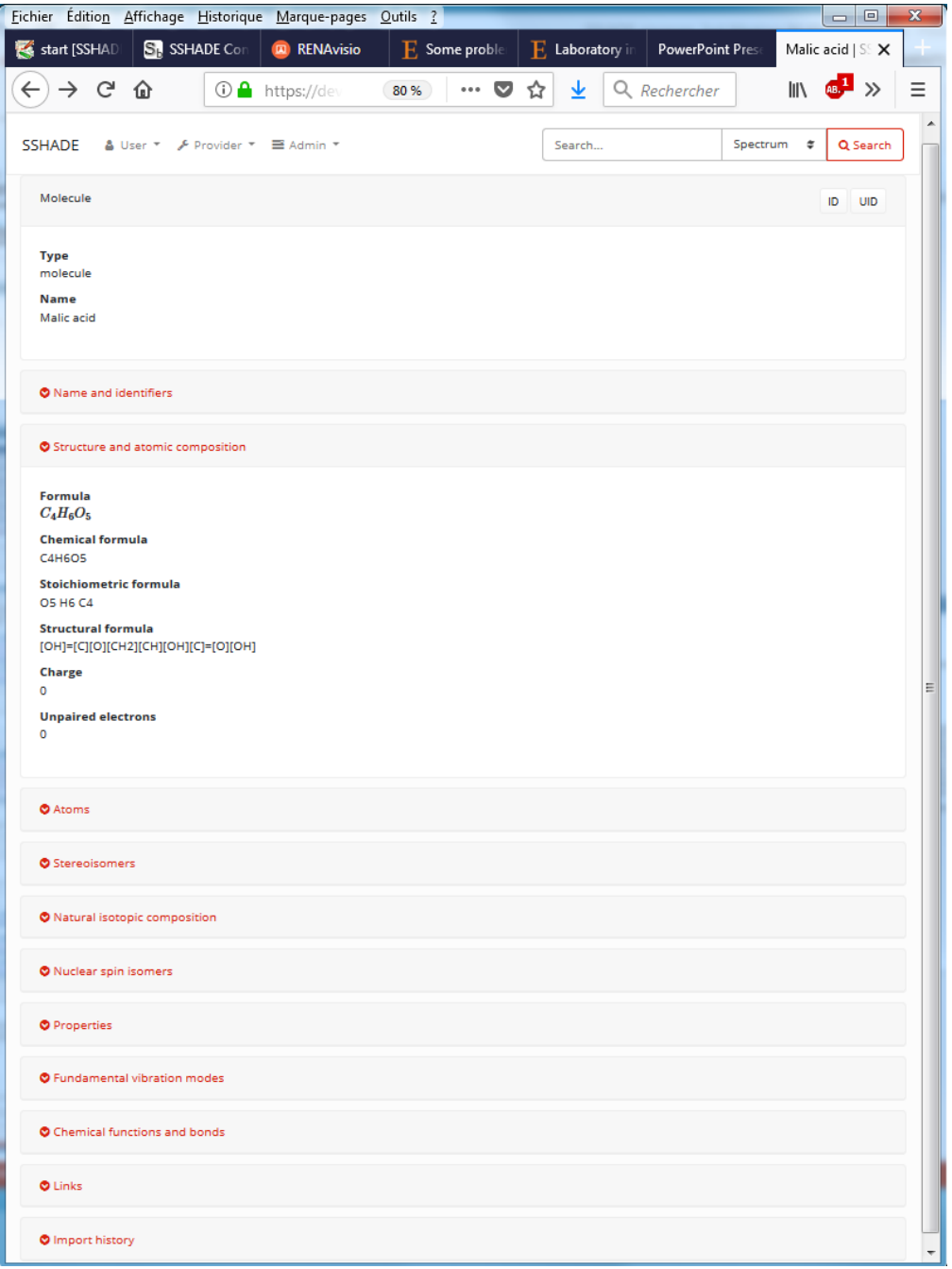
- SSHADE databases
  - Database, laboratory, experimentalists, Instruments-techniques
  - Local Matters, Samples
  - Experiments & Spectra
  - Publications

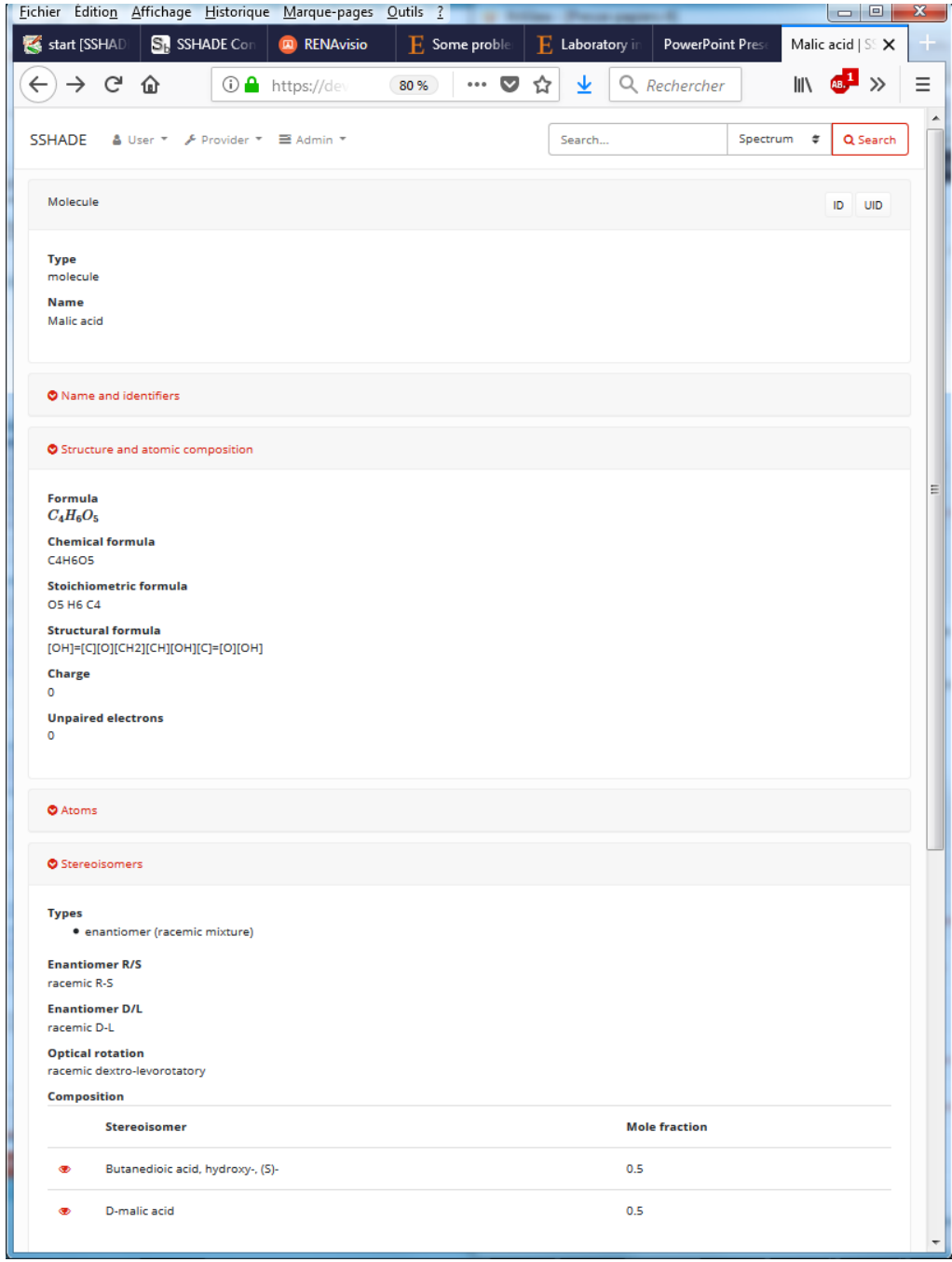
State of data ingestion in SSHADE and its databases

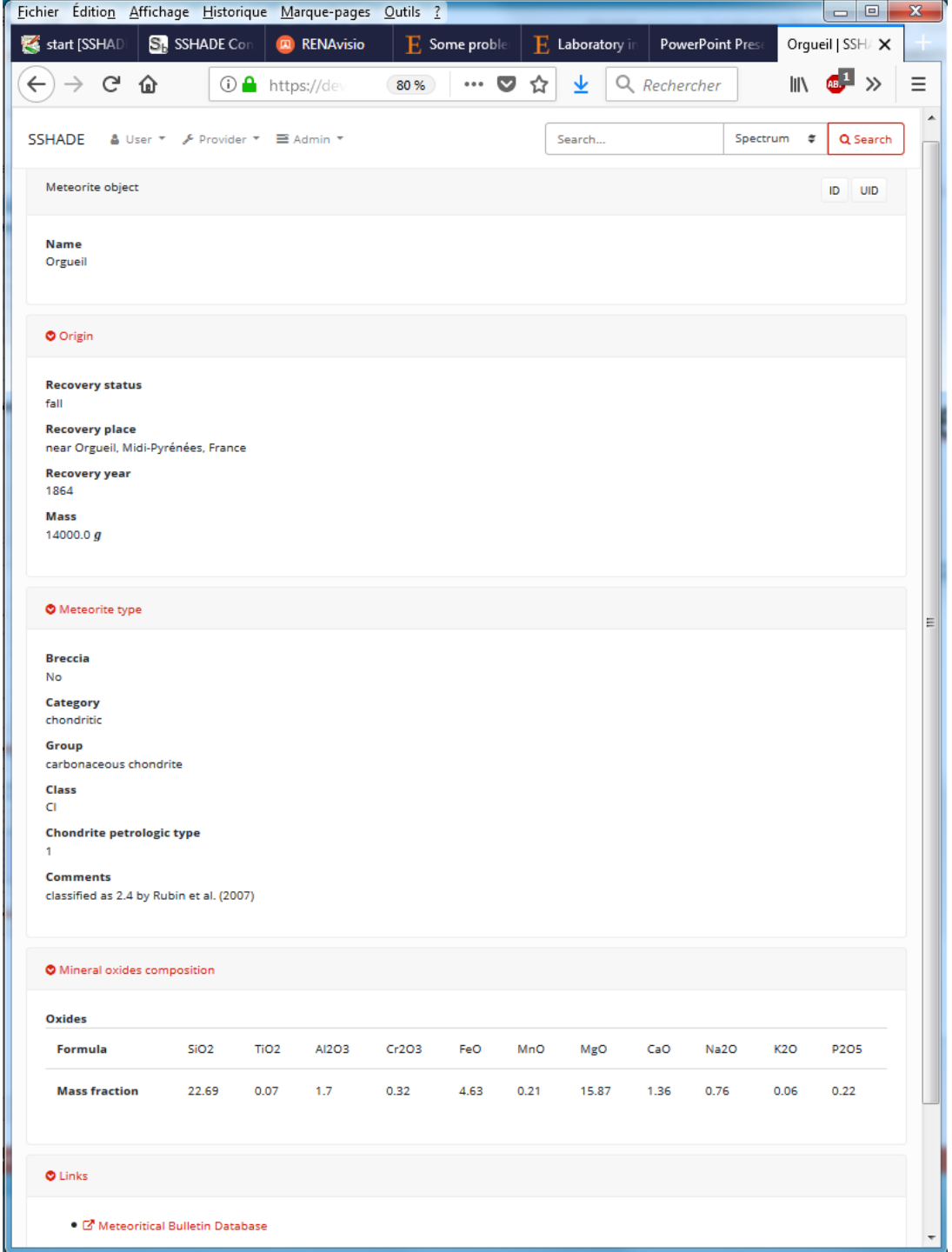
	Dec. 2017
Species	
• Atoms	141
• Chemical bonds	192
• Chemical Functions	51
• Molecules	116
Phases	
• Minerals	169
• Solids	46
• Liquids	8
Objects	
• Meteorites	94
• Micrometeorite	11
• IDPs	0
TOTAL	828

	Dec. 2017
Databases	
• Databases	12
• Laboratories	34
• Experimentalists	72
• Instruments-techniques	82
Matters	
• Fluid	38
• Solid	57
• Mineral	64
• Carbonaceous	4
• Extraterrestrial	59
Publications	
• Journals	44
• Publications	174
TOTAL	640

Molecule


SSHADE
User
Provider
Admin
Search...
Spectrum
Search
Molecule
ID
UID
Type
molecule
Name
Malic acid
Name and identifiers
Structure and atomic composition
Formula
$C_4H_6O_5$
Chemical formula
C4H6O5
Stoichiometric formula
O5 H6 C4
Structural formula
[OH]=[C][O][CH2][CH][OH][C]=[O][OH]
Charge
0
Unpaired electrons
0
Atoms
Stereoisomers
Natural isotopic composition
Nuclear spin isomers
Properties
Fundamental vibration modes
Chemical functions and bonds
Links
Import history


SSHADE
User
Provider
Admin
Search...
Spectrum
Search
Molecule
ID
UID
Type
molecule
Name
Malic acid
Name and identifiers
Structure and atomic composition
Formula
$C_4H_6O_5$
Chemical formula
C4H6O5
Stoichiometric formula
O5 H6 C4
Structural formula
[OH]=[C][O][CH2][CH][OH][C]=[O][OH]
Charge
0
Unpaired electrons
0
Atoms
Stereoisomers
Types
enantiomer (racemic mixture)
Enantiomer R/S
racemic R-S
Enantiomer D/L
racemic D-L
Optical rotation
racemic dextro-levorotatory
Composition
Stereoisomer
Mole fraction
Butanedioic acid, hydroxy-, (S)-
0.5
D-malic acid
0.5


Fichier Édition Affichage Historique Marque-pages Outils ?
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Some proble
Laboratory in
PowerPoint Pres
Orgueil | SSH
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80 %
Rechercher
SSHADE
User
Provider
Admin
Search...
Spectrum
Search
Meteorite object
ID
UID
Name
Orgueil
Origin
Recovery status
fall
Recovery place
near Orgueil, Midi-Pyrénées, France
Recovery year
1864
Mass
14000.0 g
Meteorite type
Breccia
No
Category
chondritic
Group
carbonaceous chondrite
Class
CI
Chondrite petrologic type
1
Comments
classified as 2.4 by Rubin et al. (2007)
Mineral oxides composition
Oxides
Formula SiO2 TiO2 Al2O3 Cr2O3 FeO MnO MgO CaO Na2O K2O P2O5
Mass fraction 22.69 0.07 1.7 0.32 4.63 0.21 15.87 1.36 0.76 0.06 0.22
Links
Meteoritical Bulletin Database

Meteorite

Fichier Édition Affichage Historique Marque-pages Outils ?

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https://dev 80 % Rechercher

SSHADE User Provider Admin Search... Spectrum Search

Publication ID UID

Short reference
Pommerol and Schmitt, 2009, Icarus, 204, 114 - 136

Title
Water sorption on Martian regolith analogs: thermodynamics and near-infrared reflectance spectroscopy

Authors

Names
- A. Pommerol
- B. Schmitt
- P. Beck
- O. Brissaud

Abstract and keywords

Abstract
The near-infrared reflectance spectra of the martian surface present strong absorption features attributed to hydration water present in the regolith. In order to characterize the relationships between this water and atmospheric vapor and decipher the physical state of water molecules in martian regolith analogs, we designed and built an experimental setup to measure near-IR reflectance spectra under martian atmospheric conditions. Six samples were studied that cover part of the diversity of Mars surface mineralogy: a hydrated ferric oxide (ferrihydrite), two igneous samples (volcanic tuff, and dunite sand), and three potential water rich soil materials (Mg-sulfate, smectite powder and a palagonitic soil, the JSC Mars-1 regolith stimulant). Sorption and desorption isotherms were measured at 243 K for water vapor pressure varying from 10-5 to ~0.3 mbar (relative humidity: 10-4 to 75%). These measurements reveal a large diversity of behavior among the sample suite in terms of absolute amount of water adsorbed, shape of the isotherm and hysteresis between the adsorption and desorption branches. Simultaneous in situ spectroscopic observations permit a detailed analysis of the spectral signature of adsorbed water and also point to clear differences between the samples. Ferric (oxy)hydroxides like ferrihydrite or other phases present in palagonitic soils are very strong water adsorbent and may play an important role in the current martian water cycle by allowing large exchange of water between dust-covered regions and atmosphere at diurnal and seasonal scales.

Keywords
spectroscopy, spectro-gonio radiometer, thermodynamics, sample cell, bidirectional reflection, bidirectional reflectance spectra, band position, band intensity, band integrated intensity, fluid process, adsorption, near-IR, mineral, palagonite JSC Mars-1, ferrihydrite, smectite Swy-2, dunite, basaltic volcanic tuff, epsomite - magnesium sulfate, H2O, Mars

Contents
instrument-technique, sample, material-matter, spectral data, thermodynamic data, planetary sciences

Journal

Year
2009

Journal
Icarus

Volume
204

Number
1

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https://dev 80 % Rechercher

SSHADE User Provider Admin Search... Spectrum Search

Journal

Year
2009

Journal
Icarus

Volume
204

Number
1

Pages
114 - 136

Pages number
23

Publication

Type and state

Type
journal

Document type
article

Publication state
published

Access right
publisher copyright

Links

Doi
10.1016/j.icarus.2009.06.013

Url
http://dx.doi.org/10.1016/j.icarus.2009.06.013

Bibcode - ADS
2009Icar..204..114P

ADS Url
http://adsabs.harvard.edu/abs/2009Icar..204..114P

File
pommerol09-Icarus-204-114.pdf

Import history

Date	Mode	XML filename	SSDM Version	Import file
2017-07-04 10:12:21.350653	first import	publications_Articles_89-09_IPAG_v070a.xml	0.8.4	Download

State of data ingestion in SSHADE databases

Database	Matters	Samples	Experiments	Spectra
BYPASS	4	5	1	9
DAYSY	2	5	4	20
DOCCD	11	42	4	36
FAME	8	31	25	60
GhoSST	86	340	51	471
LSD	63	130	33	145
MIA	0	1	1	1
PaSSTEL	15	12	13	18
SOSYPOL	2	73	15	269
SSTONE	6	146	6	146
STOPCODA	14	12	3	56
Total	**211**	**797**	**156**	**1231**

Dec. 2017

11 Databases:

- Samples 797
- Experiments 156
- Spectra 1231

TOTAL 2184

GRAND TOTAL 3652 files

Spectrum

Fichier Édition Affichage Historique Marque-pages Outils ?

start [SSHADE] | SSHADE Consortium Partners | RENAvisio | Some problems in interpreta | Laboratory investigations of T | PowerPoint Presentation - Wright | Spectrum SPECTRUM_BS_20130103_001

https://dev.sshade.eu/display/spectrum/SPECTRUM_BS_20130103_001 80 %

SSHADE User Provider Admin

Search... Spectrum Search

Experiment: NIR optical constant spectra of CH4 in solid solution in alpha and beta-N2 at 5 different temperatures (35K - 43K)

Sub-Experiment: NIR Optical constants spectrum of CH4 (normalized to 100%) in solid solution in beta-N2 crystal at different temperatures

- Spectrum: NIR Optical constants spectrum of CH4 (normalized to 100% and with corrected continuum) in solid solution in beta-N2 crystal at 43 K
- Spectrum: NIR Optical constants spectrum of CH4 (normalized to 100% and with corrected continuum) in solid solution in beta-N2 crystal at 41 K
- Spectrum: NIR Optical constants spectrum of CH4 (normalized to 100% and with corrected continuum) in solid solution in beta-N2 crystal at 38 K
- Spectrum: NIR Optical constants spectrum of CH4 (normalized to 100% and with corrected continuum) in solid solution in beta-N2 crystal at 36.5 K

Sub-Experiment: NIR Optical constants spectrum of CH4 (normalized to 100%) in solid solution in alpha-N2 crystal at 35 K

- Spectrum: NIR Optical constants spectrum of CH4 (normalized to 100%) in solid solution in alpha-N2 crystal at 35 K

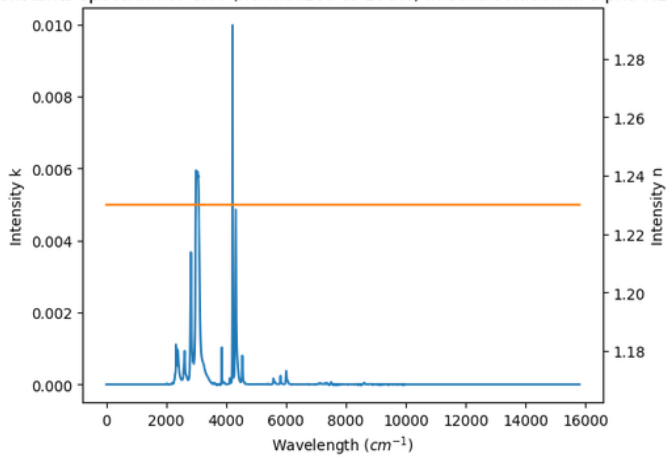
Sample: CH4 in alpha-N2 crystalline

Layer: #1

- CH4:N2 crystalline solid solution - alpha phase

Spectrum ID UID

NIR Optical constants spectrum of CH4 (normalized to 100%) in solid solution in alpha-N2 crystal at 35 K



Version
#1 (2017-12-01 17:25:04.027932)

Instrument parameters ID UID

Instrument
Nicolet 800

Valid spectral range(s)
2520.0 - 2985.0 cm-1 ; 3090.0 - 10000.0 cm-1

Observation mode
single spot

Sample preview ID UID

Name
CH4 in alpha-N2 crystalline

Origin
laboratory

Temperature
35.0 ± 0.3 K

Fluid
- CH_4, 0.001 ± 5e-05
- N_2, 0.999 ± 5e-05

Future of data ingestion in SSHADE and its databases

- SSHADE common databases
  - continue to ingest Fundamental Species & Phases and Objects
  - add some Reference Matters, Publications, Journals
    - ➔ On request of the databases
  - Band list => critical review and selection

- Trained SSHADE partner databases
  - continue to fill with Samples (+ Matters), Experiments & Spectra, Publications
    - ➔ focuses on published data (publication link)

- To be trained SSHADE partner databases
  - start with Database, Laboratory, Experimentalists, Instruments-techniques
  - then with Samples (+ Matters), Experiments & Spectra, Publications

Band list : bands and states

- Bands parameters
  - position (energy),
  - width, shape, …
  - intensities (peak and integrated)
  - accuracies / quality / evaluation
- Transitions assignment
  - states QN, anharmonic coefficients, …

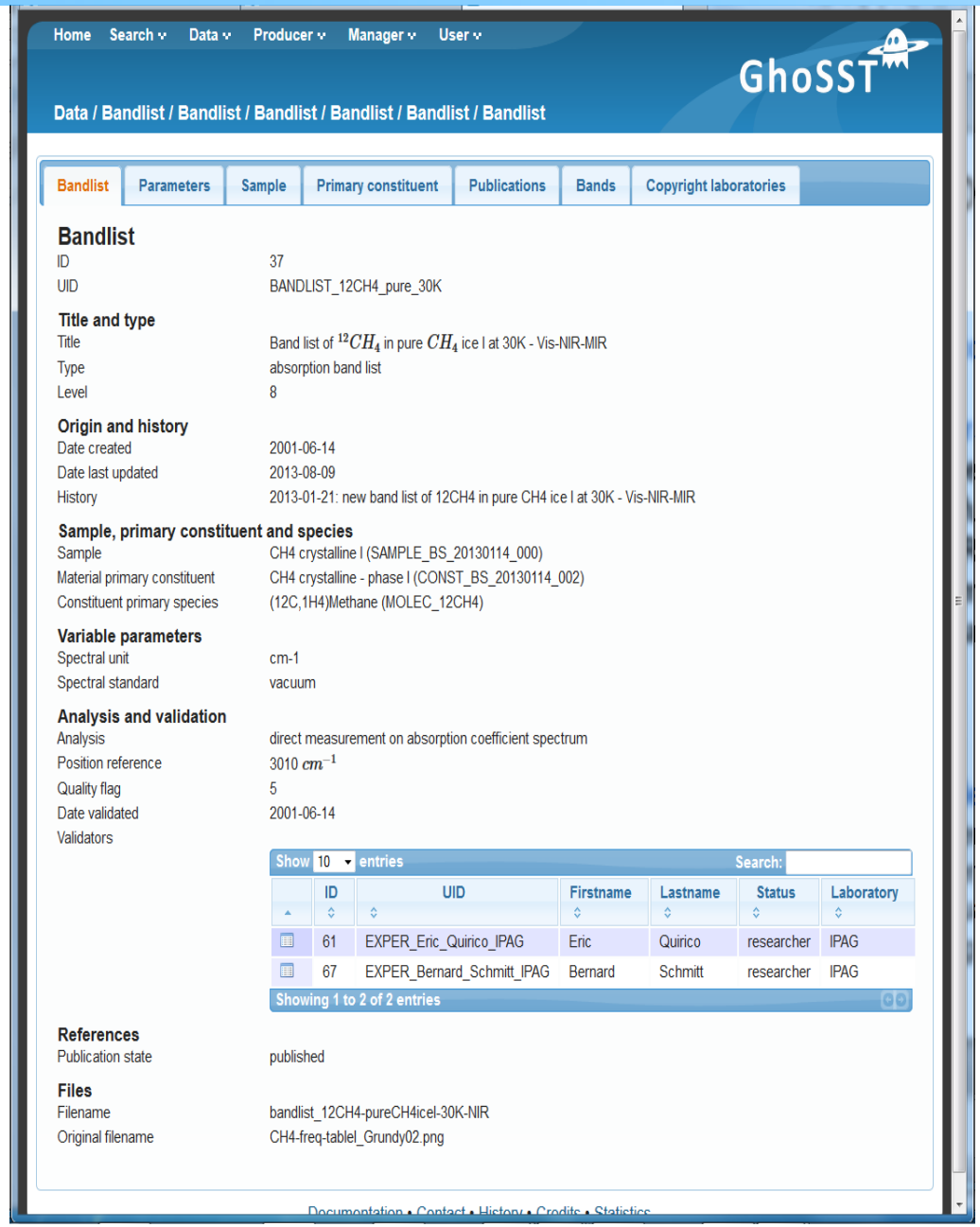
Review the available data for molecular solids

- Partner's data (see examples in 'old GhoSST')
- Publications

  => critical review and selection

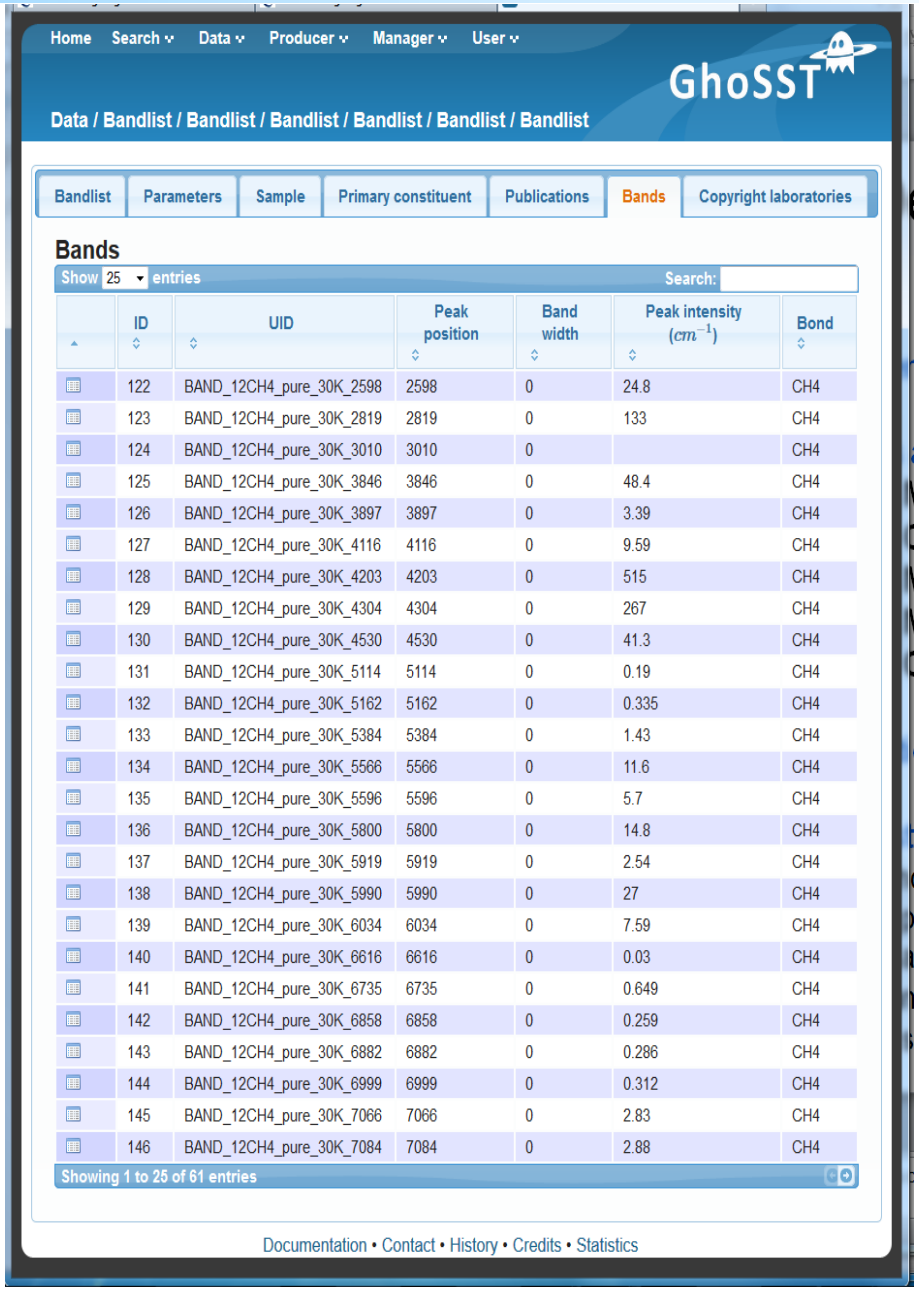
  => selection committee ? (➔ 2019)

Band lists and Bands



'old GhoSST':

- 15 bandlists
- 167 bands



SSHADE infrastructure delivery

SSHADE infrastructure delivery to Europe (JRA 5)

To be delivered:

- To Europlanet: 23th January 2018
- To Europe: 31st January 2018
- Open to public 1st February 2018

Document

- SSDM
- SSHADE infrastructure
- Interfaces and tools (users, providers, managers)
- Partner's databases and their contents ➔ need your input (5-6 lines on DB content)
- Documentation: manuals, tutorials, … (Blog, Wiki, …)

Interface

- Data search(s)
- Spectra and metadata visualization
- Data export
- Tools

SSHADE infrastructure delivery to Europe (JRA 5)

To be done before delivery:

- active database: ➔ Check if you have 'non-published' data
- still inactive database: ➔ provide a name and acronym for your database

Will be done soon after:

- activate the DOI
- activate the data access control and validation procedure

You can do:

- Web page at your institution web site
  - start setting up a web page on SSHADE and your database
    - describing SSHADE (we will provide a small common text for SSHADE + logos, …)
    - describing your database
    - with a link to SSHADE
    - a 'first search windows' (that will redirect to SSHADE) will be provided later

Future SSHADE delivery to Europe

To be delivered:

- SSHADE infrastructure 31st January 2018 **(D11,8 JRA5 VESPA – Y1 & Y2)**
- Filling of infrastructure **(D6.3 VA2 VESPA – Y3 & Y4)**
- Training of providers and users **(D6.5 VA2 VESPA – Y3 & Y4)**

Final delivery: 31st August 2019 **SSHADE with 18-20 databases**

Less than 18 databases = failure *(we will assess this point beginning 2019)*

➔ need to rapidly found other(s) (we have a list…)

Documents to be delivered

- Delivery reports
- Documentation: manuals, tutorials, …
- Blog, Wiki, …

SSHADE future events Time line

2018

- January — 11 databases in SSHADE
- January — **SSHADE infrastructure delivery** — **(D11.7 JRA VESPA)**
- March — Training database managers (session #6)
- March — Training users LPSC (session #1)
- April — Training users EGU (session #2)
- May — Training database managers (session #7)
- August — 14 databases in SSHADE — **(D6.3 VAA VESPA – Y3)**
- September — Training users EPSC (session #3) — **(D6.5 VAA VESPA – Y3)**
- October — Training database managers (session #8)
- October — Training users DPS (session #4)
- October — Training users ??? (session #5)

2019

- February — Training database managers (session #9)
- March — Training users LPSC (session #6)
- March — 3rd SSHADE meeting
- April — Training users EGU (session #7) — **(D6.5 VAA VESPA – Y4)**
- June — 18 databases ingested in SSHADE
- August — **SSHADE with 18-20 databases** — **(D6.3 VAA VESPA – Y4)**
- August — **End of Europlanet 2020-RI**

SSHADE advertising

Advertise SSHADE by various ways

- Mail footers with web address
  - ➔ all SSHADE partners
- Flyer
  - ➔ to be sent by mail
- Newsletters
  - ➔ need to list all national and international newletters
- Conferences
  - ➔ SSHADE poster to post at all conferences
- Web Medias (FaceBook, ...)
- Stickers …
- Shirts …
  - ➔ need Logo, drawing and a catching slogan
- Other ideas ? …

Partner’s training

Partner’s training (past)

Trained partners

10.5 already trained :

- AIU (Jena, G)
- CML (Krakow, PL)
- FAME/ESRF (Grenoble, F)
- IAS (Orsay, F)
- IEM (Madrid, E) [partly]
- IRAP PEPS+MICMAC (Toulouse, F)
- LPGN (Nantes, F)
- PGL (Wroclaw, PL)
- PIIM (Marseille, F)
- Unibe (Bern, CH)

Partner's 'SSHADE Party'

How

- 2-3 full days at partner lab or in Grenoble

Aim

- Help to prepare and ingest one set of data for the different types of sample / experiment
- Build specialized matter / sample / experiment templates for these types of experiments

Result

- Seems to have strongly helped and motivated the partners for data ingestion.
- We will continue with the new ones, after training.

SSHADE past events Time line

2015

- September — **Start of Europlanet 2020-RI**
- November — Start of SSHADE development
- December — Training database managers (session #1)

2016

- May — 1st SSHADE meeting
- May — Training database managers (session #2)
- August — 3 databases in SSHADE — **(D6.3 VAA VESPA – Y1)**
- August — **SSHADE prototype delivery** — **(D11.5 JRA VESPA)**
- October — Training database managers (session #3a) — **(D6.5 VAA VESPA – Y1)**
- November — Training database managers (session #3b)
- December — Training database managers (session #4a & 4b)

2017

- July — SSHADE 'party' (session #1 to #5)
- August — 9 databases in SSHADE — **(D6.3 VAA VESPA – Y2)**
- september — SSHADE 'party' (session #6) — **(D6.5 VAA VESPA – Y2)**
- October — Training database managers (session #5)
- December — 2nd SSHADE meeting

Partner's training + party (future)

Partners to be trained

- AGC (HU)
- CAB (Madrid, E)
- IAPS (Rome, I: 2 groups)
- IEM (Madrid, E): to be completed
- OU (Milton Keynes, GB) + PRL (Ahmedabad, IN)
- LATMOS (Guyancourt, F)
- LGL (Lyon, F)
- LISA (Céteil, F)

➔ training program to be defined

- 3 or 4 sessions in 2018 (2 partners each time)
- 1 session in 2019

➔ will send doodle to organize 2018 + option for 2019 (small DB)

Database implementation by partners

- Training session of managers (2.5 - 3 days)

- Define Who do what in your lab (which part of the work, …)
- Define your feeding plans (which data, …)

- Preparation of basic information and metadata
  - Database
  - Laboratory
  - Experimentalists
  - Instruments
  - Publications

Database implementation by partners

- Preparation of fundamental data
  - Provide list of fundamental data to be used:
    - Molecules,
    - Minerals, solids, (liquids)
    - Meteorite, Micrometeorites, IDPs
    - Standard matters
  - Contribute to document them ➔ we will prepare them before

- Preparation of spectral data and metadata
  - Local matters
  - Samples
  - Experiments
  - Spectra

Discussion / Questions on database implementation

- ask questions ??

SSHADE future events Time line

2018

- January — 11 databases in SSHADE
- January — **SSHADE infrastructure delivery** — **(D11.7 JRA VESPA)**
- March — Training database managers (session #6)
- March — Training users LPSC (session #1)
- April — Training users EGU (session #2)
- May — Training database managers (session #7)
- August — 14 databases in SSHADE — **(D6.3 VAA VESPA – Y3)**
- September — Training users EPSC (session #3) — **(D6.5 VAA VESPA – Y3)**
- October — Training database managers (session #8)
- October — Training users DPS (session #4)
- October — Training users ??? (session #5)

2019

- February — Training database managers (session #9)
- March — Training users LPSC (session #6)
- March — 3rd SSHADE meeting
- April — Training users EGU (session #7) — **(D6.5 VAA VESPA – Y4)**
- June — 18 databases ingested in SSHADE
- August — **SSHADE with 18-20 databases** — **(D6.3 VAA VESPA – Y4)**
- August — **End of Europlanet 2020-RI**

SSHADE and databases sustainability

SSHADE and databases sustainability

SSHADE development team employment in 2018-2019

- Damien Albert (development): permanent, part time
- Philippe Bollard (development): contract full time => 02/2019 + ...
- Alexandre Garenne (support): contract full time => 12/2018 + ...
- Lydie Bonal (support): permanent, part time (Astronome service)
- ?? (support): 2nd permanent (Astronome service)

Labellisation of SSHADE infrastructure (+ french databases) by INSU/CNRS

4 December 2017 !

=> sustainability of infrastructure (by OSUG)

=> sustainability of French databases

=> more money from INSU ?, OSUG ?, other OSUs?

=> additional positions (support / development) ?

Tasks of SSHADE @ IPAG

SSHADE infrastructure development

- SSDM (data model) for Bandlist + improvement multi-angle/imagedata
- Import tools for Bandlist, tools for users
- SSHADE interface improvements (visualization) + Band list
- VO interoperability (with VESPA, VAMDC, …)

Coordination of consortium

- Continue preparation of common fundamental data of SSHADE
- Development of the common ‘band list database’ (compilation, critical review…)

Support to partners consortium

- Training of database managers + SSHADE party
- Completion of documentations and tutorials for providers
- On-line support

Support to users

- Tutorials & training for users at conferences
- Preparation of documentations and tutorials
- By-mail support

Tasks of the Scientific Managers and Database Managers

Scientific manager

- define which data will by provided to the database
- scientific validation of data
  ➔ responsible of the scientific content of its database
- animation of his data base
- contribution to the common « Band list » database

Database manager

- prepare and test import files (all types)
- import data (sample, spectra, matters) + corrections
- report bugs, data errors and improvements
- Help in beta testing of infrastructure

SSHADE and databases sustainability

up to end program and beyond …

SSHADE

- maintain/improve SSDM
- continue to improve the interface and tools
- need to keep active the users/providers access to the SSHADE infrastructure
- should ensure database partners training and support
- should ensure users training and support
- provide a repository for the data of the Europlanet TNA visits (spectroscopy)

All databases

- need to keep 1-2 active Scientific/Database manager(s)
- continue to feed their database
- Animate their database (news, posters/presentation, …), advertisements …
- Sign (your institution) a memorandum to maintain/develop their database at ‘best effort’

Users training

Users training

Future training sessions for users

at major planetary and astrophysics conferences:

- LPSC, EPSC, DPS
- EGU, AGU, …
- ???

1-2 SSHADE team member at each …

➔ participation of partners ?

➔ Provide us with a list of your 2018 conferences

Document for users

- SSHADE manual, Tutorials
- Users cases => Video
- …

SSHADE future events Time line

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2019

- February — Training database managers (session #9)
- March — Training users LPSC (session #6)
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- April — Training users EGU (session #7) — **(D6.5 VAA VESPA – Y4)**
- June — 18 databases ingested in SSHADE
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- August — **End of Europlanet 2020-RI**

Summary of Managers actions

Managers actions (active database)

Active databases

before delivery: (before 15th january)

- Check if you have ‘non-published’ data in SSHADE that you don’t want to be public now (tell us!)
- Continue to ingest Samples, Experiments & Spectra, Publications

  ➔ focuse on published data

For SSHADE delivery document

- Description of your database and its current content (sample/spectra) ➔ (5-8 lines)
- Sign a memorandum to maintain/develop your database at ‘best effort’ (to be sent)

For Wiki

- Description of your database
- Description of typical sample / spectra type (only those already in SSHADE)
  note: You can add a separate part describing the future data you intend to put in SSHADE
- Instruments, cells, techniques

Managers actions (active database)

Active databases

after delivery:

- Provide a list the national and international newletters you know + link + contact
- Provide a list of your 2018 conferences (for help in user training/advertising)
- Provide a list of fundamental data (not yet present in SSHADE) needed in the coming months
- Validate your data when validation procedure will be ready
- Report any error in SSHADE data (Fundamental species / phases / objects / Publication / …)
  or in other databases
- Contribute to beta-testing of user / provider interface
- Create a Web page on SSHADE and your database at your institution web site
  - describing SSHADE (we will provide a small common text for SSHADE + logos, …)
  - describing your database, with a link to SSHADE
  - a ‘first search windows’ (that will redirect to SSHADE) will be provided later

Managers actions (future database)

Future databases

before delivery:

- Provide a name and an acronym for your database
- Answer the Doodle for 2018 training program (to be sent soon)

after delivery:

- Provide a list the national and international newletters you know + link + contact
- Provide a list of fundamental data you need for your future database
- Contribute to beta-testing of user interface

Future reports and meeting

Prepare contributions to reports for deliveries for VESPA VA

- Task 2. Enlarging content (beneficiaries) => SSHADE and database filling
- Task 5. Dissemination & Sustainability => SSHADE and database sustainability
- Task 6. Training => Users and SSHADE databases manager training

- D6.13: 3rd VESPA Training Session reports (month 33) => May 2018
- D6.8: 3rd VESPA Annual report (month 36) => August 2018

- 3th (and last) SSHADE meeting will be around may-june 2019

- D6.15: 4th VESPA Training Session reports (month 42) => February 2019
- D6.10: 2nd set of standards documentation (= SSDM) (month 46) => June2019
- D6.14: 4th VESPA Annual report (month 48) => August 2019

- Contribution to the final Europlanet report (month 48) => August 2019