



THE SOLSA PROJECT:

Combined techniques and databases for mineral identification



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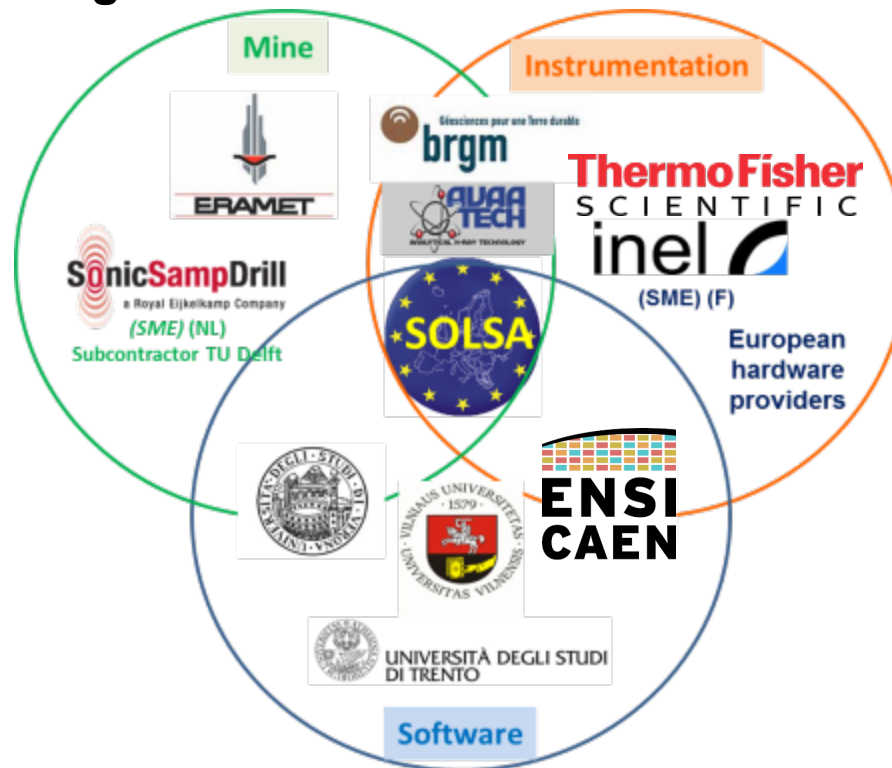
IV- CONCLUSION AND PERSPECTIVES



«Sonic Drilling coupled with Automated Mineralogy and chemistry On-Line-On-Mine-Real-Time»

Funded under the EU Programme for Research and Innovation **Horizon 2020**
The project involves the **participation of 10 partners from 4 EU countries and with almost 10 millions euro**

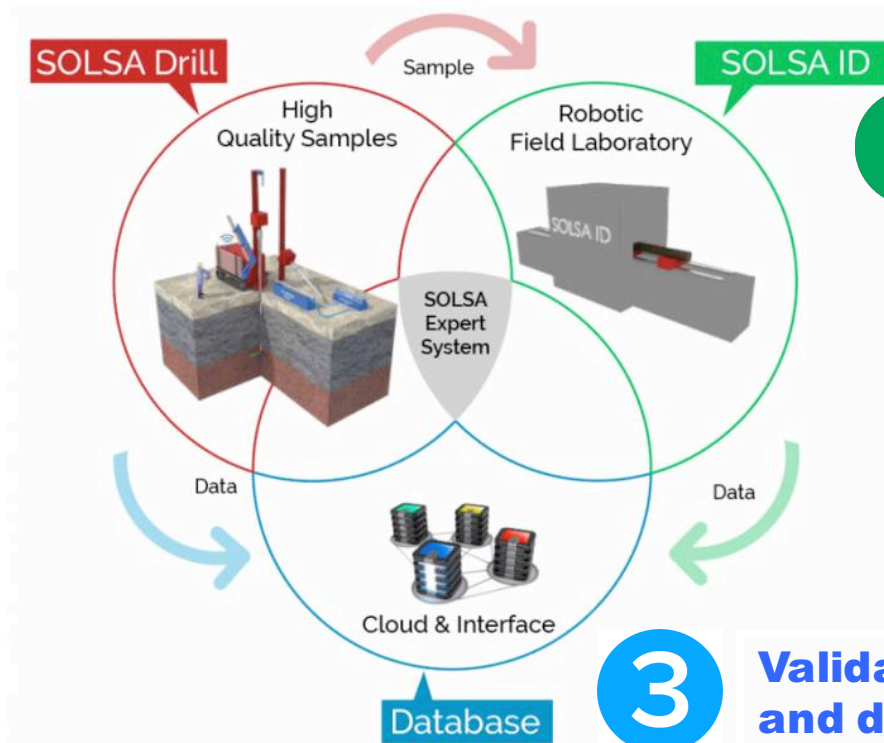
Brings together technologies from three sectors: **mining** – **instrumentation** and **software technologies**



The goal is to develop an integrated Expert System combining sonic drilling and “on-line-on-mine-in-real-time mineralogical and chemical analyses

Objectives:

1 Drilling and sampling technologies: faster, cheaper and more efficient



2 Automation of exploration tools combining *in situ* chemical and mineralogical analyzes

3 Validation, storage, interpretation and data processing

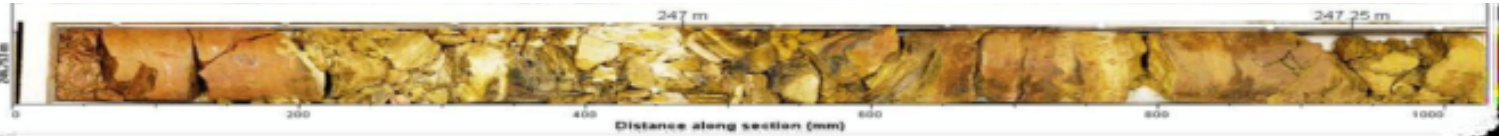
The SOLSA Expert System (1+2+3) will be validated on nickel laterites, in particular nickel laterites from the SLN's mines in New Caledonia

2

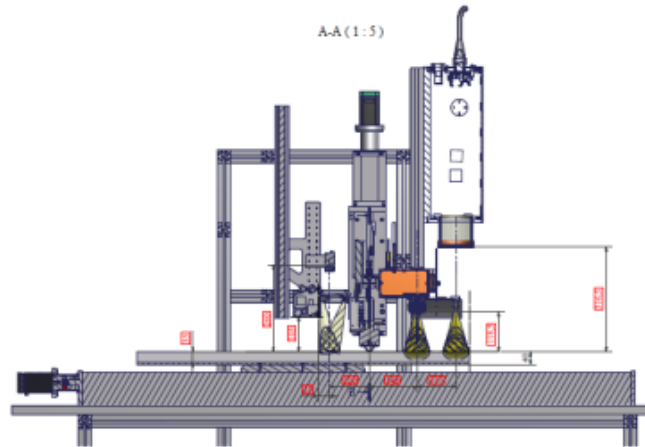
on-mine real-time

3D-Scanner Imaging

nickel laterite



profilometer, RGB camera, XRF, hyperspectral VNIR and SWIR



ThermoFisher
SCIENTIFIC

Géosciences pour une Terre durable
brgm

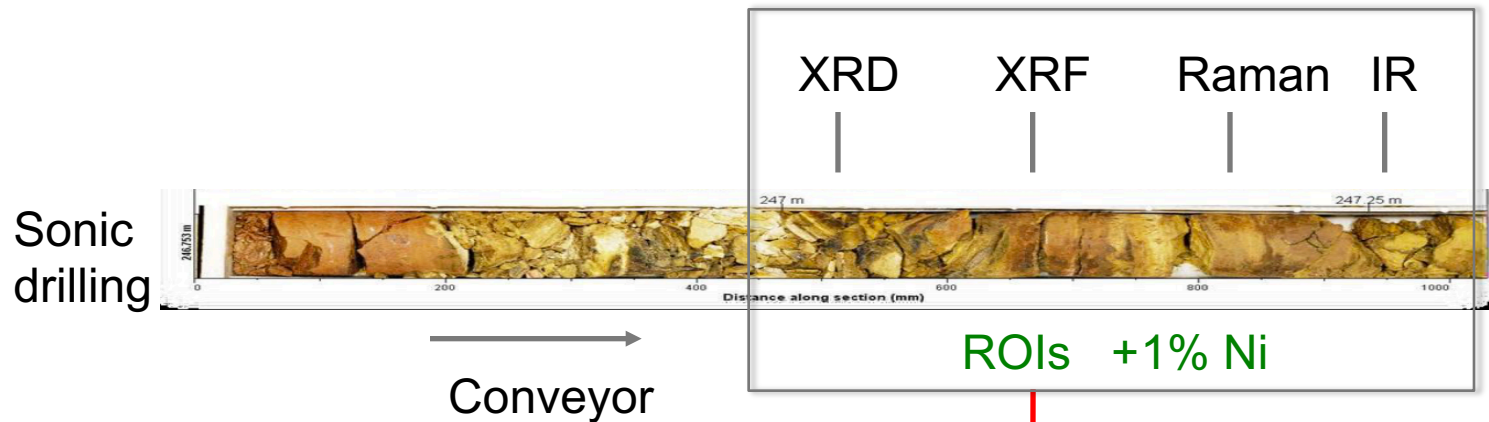


ERAMET

- Identify the main geological macroscopic characteristics (color, texture, mineralogy, key chemistry features (Fe, Ni, Cr, Co, Mn))
- To be able to identify automatically the different facies of nickel laterites.
- Define the ROIs (Region of interests, 1% Ni)

3D-Scanner Imaging
profilometer, RGB camera, XRF, hyperspectral

Sequential Acquisition (on-mine)



Chemical and phases analyzes
Microstructure, texture

The first combined system

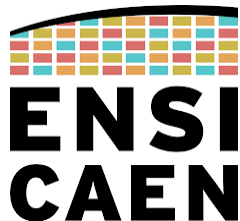
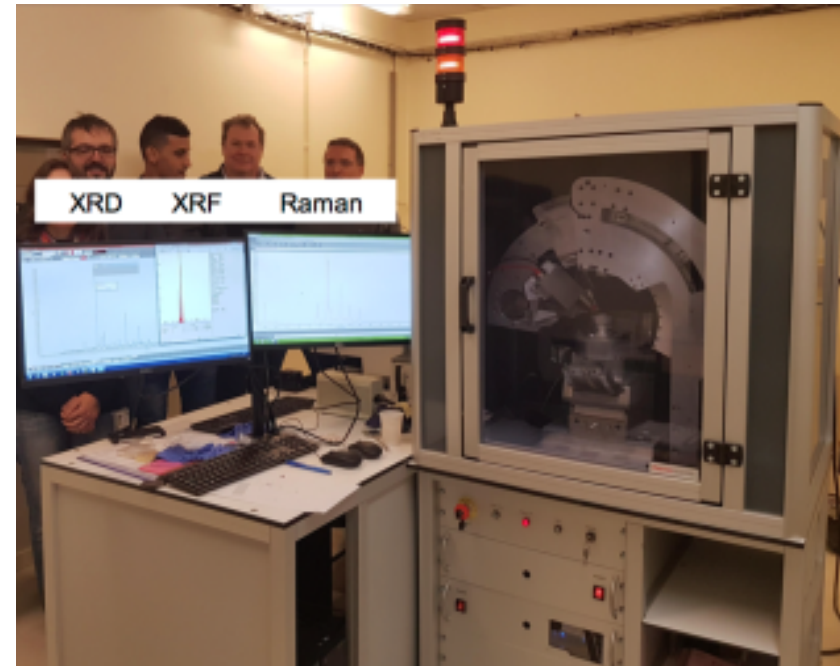
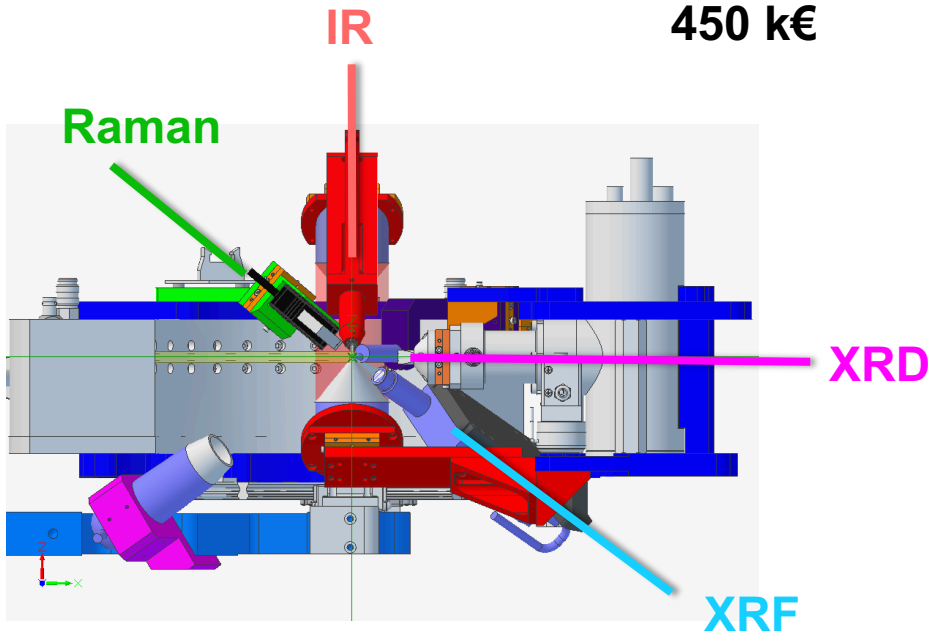
XRD - **XRF** - **Raman** - **IR**

Conception



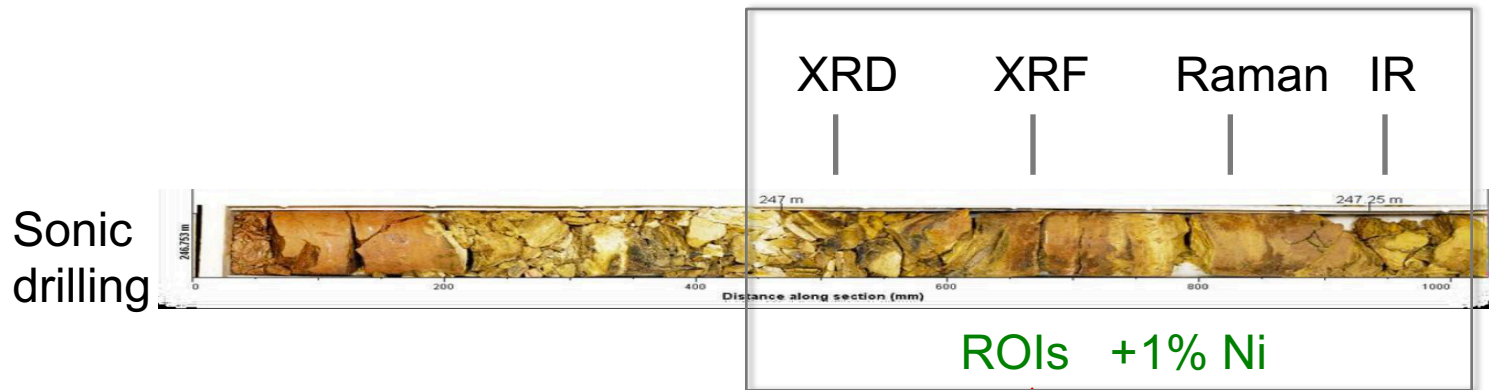
Realisation

2 years
450 k€



ThermoFisher
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COMBINED ANALYSIS



Chemical and phases analyzes
Microstructure, texture

Combined Analysis

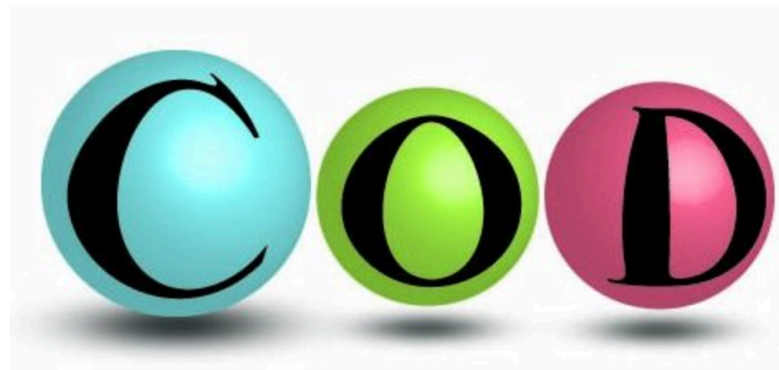
Open acces Databases:
XRD
Raman
IR

www.crystallography.net/cod/


380 000 entries



Crystallography Open Database



COD Home

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What's new? 

Accessing COD Data

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Search by structural
formula

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Manage depositions
Manage/release
prepublications

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Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding [biopolymers](#).

Including data and [software](#) from [CrystalEye](#), developed by Nick Day at the [department of Chemistry](#), the University of Cambridge under supervision of [Peter Murray-Rust](#).

All data on this site have been placed in the public domain by the contributors.

COD Advisory Board thanks [The Research Council of Lithuania](#) for their financial support of the publication "[Crystallography Open Database \(COD\): an open-access collection of crystal structures and platform for world-wide collaboration](#)",

Nucleic Acids Research. (2012) [PDF version](#)

We thank [Crystal Impact GbR](#) for their financial support of the publication "[Crystallography Open Database - an open-access collection of crystal structures](#)", *J. Appl. Crystallogr.* (2009) [PDF version](#)

Currently there are **379914** entries in the COD.

Latest deposited structure: [7228542](#) on **2017-06-26** at **09:50:13 UTC**

Full-Profile Search-Match

Diffraction pattern and sample characteristics

Upload diffraction pattern: aucun fichier sél.Structures db: mineral inorganic organic metalorganic otherAtomic elements in the sample: Threshold phase density: Threshold remove: Phases maximum number: Crystallisation: Cell parameters isotropic expansion/contraction

Experiment details

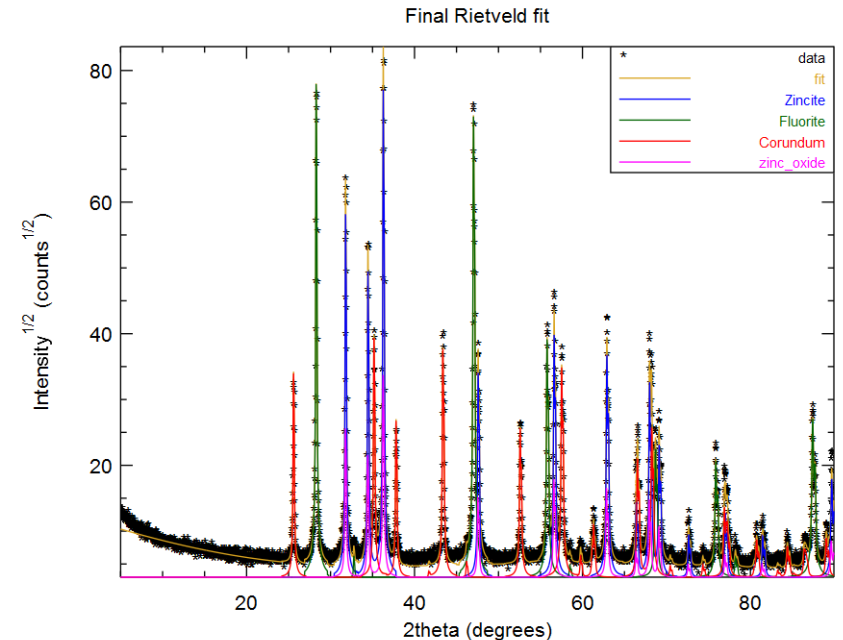
Radiation:

 X-ray tube: Other: Wavelength (Å):

Instrument geometry:

 Bragg-Brentano (theta-2theta) Bragg-Brentano (2theta only), omega: Debye-Scherrer TransmissionInstrument broadening function:

Algorithm options (Rietveld, ddm or both)

Weights type: Smooth weight: 1st weight: 2nd weight: 

Found phases and quantification:

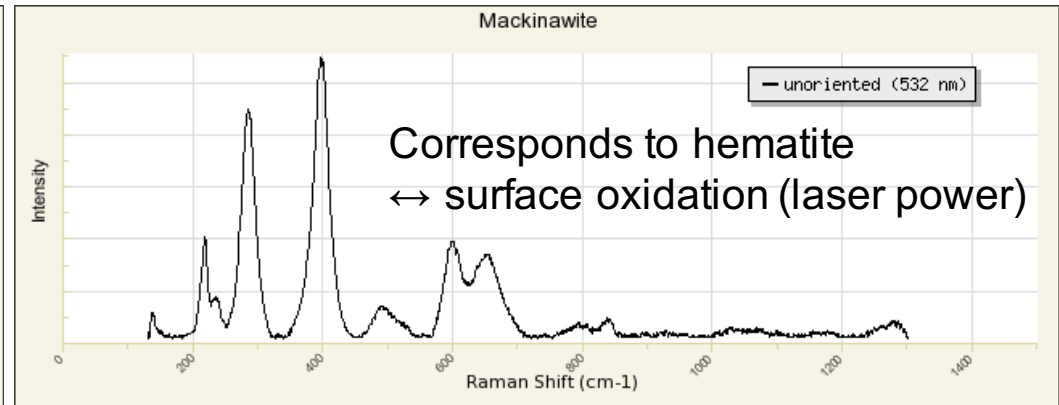
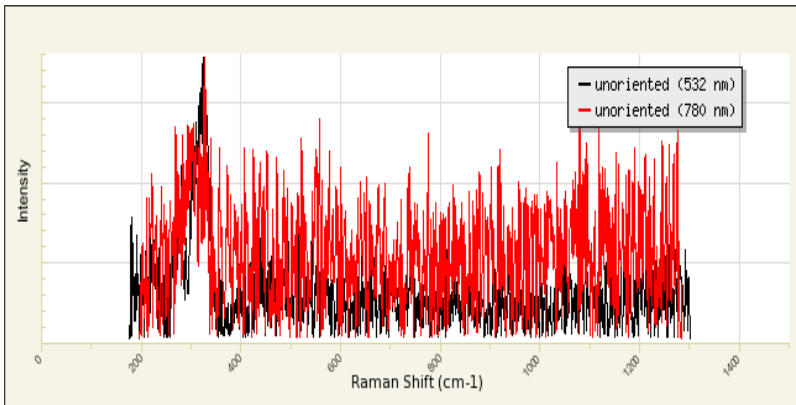
Phase ID	name	vol. (%)	wt. (%)	crystallites (Å)	microstrain
9004178	Zincite	16.8284	23.9708	2148.26	0.00028435
9009005	Fluorite	42.5522	33.9388	2117.08	0.000363147
9007498	Corundum	37.2197	37.2493	1889.82	0.000267779
2300112	zinc_oxide	3.39971	4.84114	1754.74	6.98311e-05

Final Rietveld analysis, R_w: 0.159468, Goff: 1.95869

Several open access libraries of Raman spectra exist

The RRUFF project (<http://www.rruff.info/>), dedicated to only minerals, with 13000 entries

-Some poor quality spectra without discernible vibration modes, mixture of phases



High resolution spectra will be integrated in our new ROD

Spectral data is cross-linked with the XRD data in the COD

All types of materials (organic and inorganic materials, minerals, polymers, metals, ceramics, pigments, drugs, nuclear, hazardous materials...)

All information will be present in ROD data (origin, references, authors, experiment conditions, 1 spectrum \leftrightarrow 1 phase)



Raman Open Database

ROD Home

Open-access collection of Raman spectra used for the [SOLSA H2020](#) project.

All data on this site have been placed in the public domain by the contributors.

Currently there are **1043** entries in the ROD.

Latest deposited structure: [1000660](#) on 2018-06-07 at 08:47:20 UTC



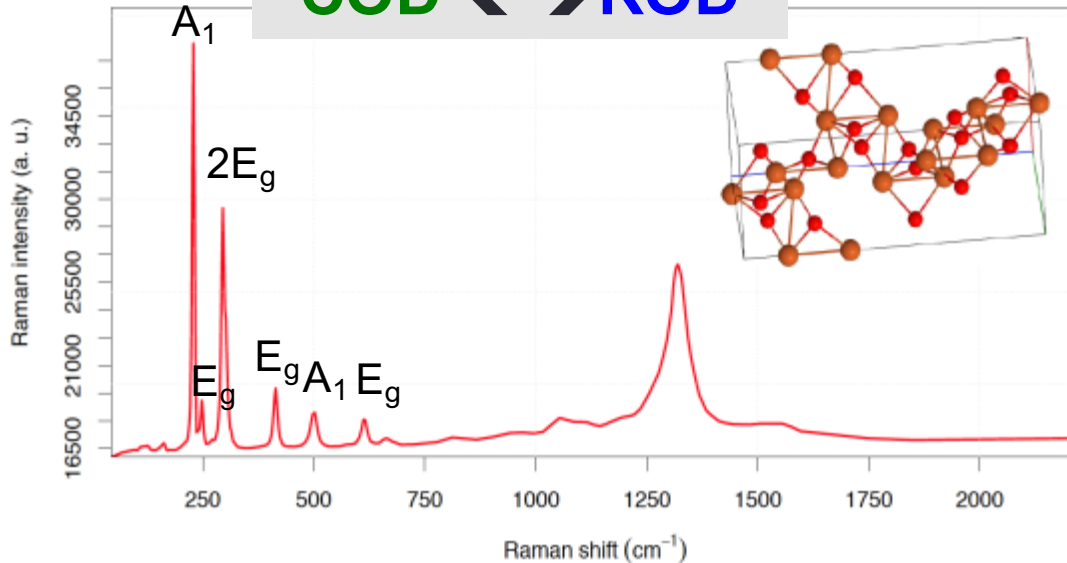
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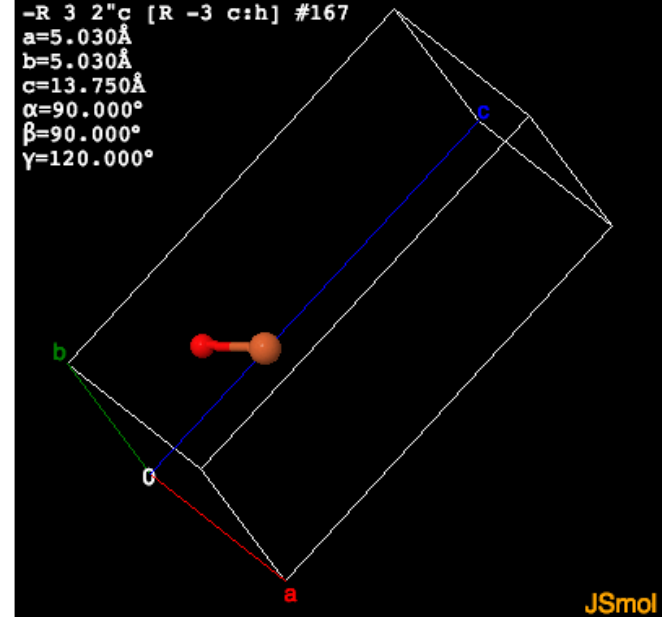
solsa.crystallography.net/rod/

Y. El Mendili, A. Merkys, S. Gražulis

COD ↔ ROD



```
-R 3 2" c [R -3 c:h] #167
a=5.030Å
b=5.030Å
c=13.750Å
α=90.000°
β=90.000°
γ=120.000°
```



JSmol

Y. El Mendili, et al, 'ROD project: First interconnected Raman-XRD open-access database for material identification worldwide'. *J. Raman. Spectrosc.* Under review

CONCLUSION

ROD brief actual state

Currently the ROD contains 1043 entries in the standard CIF format with data related to over than 700 different phases :

The ROD database is intended to provide experimental as well as **theoretical Raman spectra** from various sources.

Development and success of ROD

→ Depends completely on future contributions of the Raman community



Visit our ROD database

solsa.crystallography.net/rod/

**Thank you for your
attention**