SOLSA

Open linked databases in the mining industry

Saulius Gražulis

Kaunas, OpenCon 2017

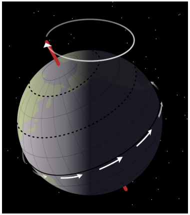
Vilnius University Institute of Biotechnology

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Data importance

Hipparchus (c. 190 – c. 120 BCE)

- measured the longitude of Spica and Regulus and other bright stars
- compared his measurements with data from his predecessors, Timocharis and Aristillus, who lived ≈**100** years before him,
- discovered what is now called *the precession of the equinoxes*



By NASA, Public Domain

(Wikipedia, see also articles on Timocharis and Aristyllus)

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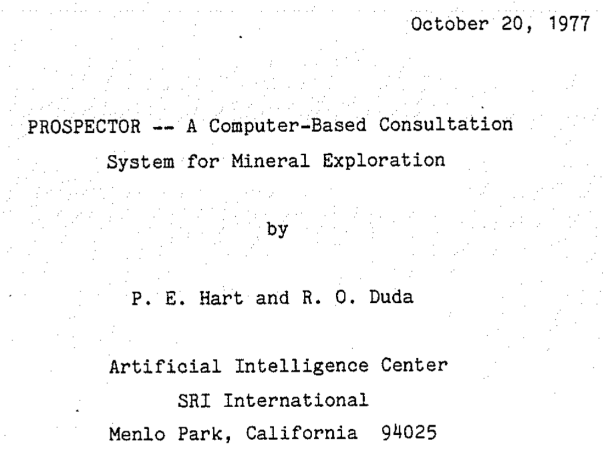
Data and AI systems for geology

[Hart and Duda, 1977]



October 20, 1977

PROSPECTOR -- A Computer-Based Consultation
System for Mineral Exploration

by

P. E. Hart and R. O. Duda

Artificial Intelligence Center
SRI International
Menlo Park, California 94025

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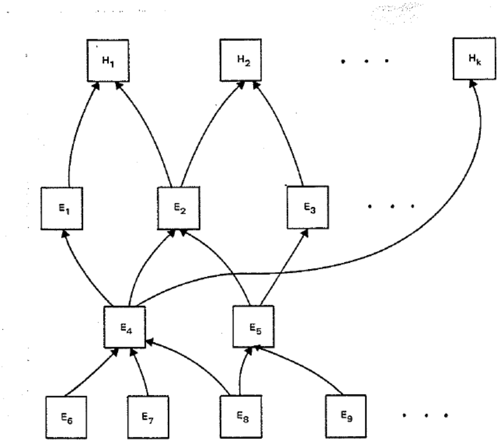
The PROSPECTOR network of inference

[Hart and Duda, 1977]



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Data kinds in the SOLSA project

Sonic drilling in Ni laterites
courtesy of Eijkelkamp SonicSampDrill

Discover SOLSA

http://solsa-mining.eu/

- Crystal structures (COD)
- Raman spectra (ROD)
- Hyperspectral images (HOD)

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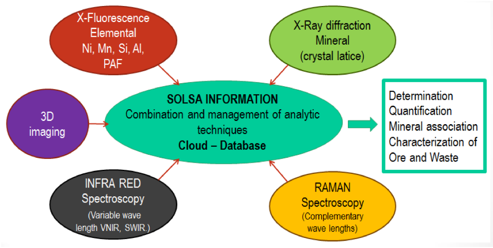
SOLSA project, COD and ROD



X-Fluorescence
Elemental
Ni, Mn, Si, Al,
PAF

X-Ray diffraction
Mineral
(crystal latice)

3D
imaging

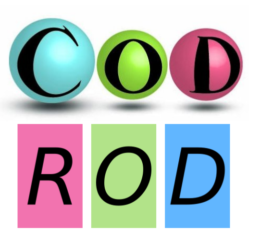
SOLSA INFORMATION
Combination and management of analytic techniques
Cloud – Database

INFRA RED
Spectroscopy
(Variable wave length VNIR, SWIR.)

RAMAN
Spectroscopy
(Complementary wave lengths)

Determination
Quantification
Mineral association
Characterization of
Ore and Waste

⇔



COD and other open databases will be used in SOLSA for:

- mineral identification;
- subsequent data dissemination.

SOLSA data flow diagram courtesy Monique Le Guen, ERAMET.

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Requirements for long-term data archiving and reuse

- Platform independence
  - Text-based formats (ASCII, UTF-8)
- Software independence
- Network-transparency
  - Standard, open protocols (W3C http)
  - Standard, open data carrier formats (JSON, XML, CIF).
  - RESTful servers
- Machine-readable semantics
  - Dictionaries, schemas
- Durability
  - Persistent identifiers
  - Open data principles
  - FAIR principles

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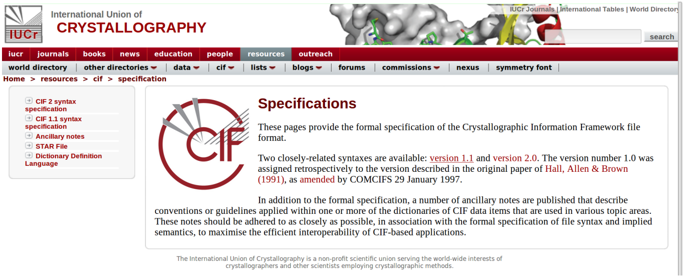
Data exchange in crystallography



Specifications

These pages provide the formal specification of the Crystallographic Information Framework file format.

Two closely-related syntaxes are available: version 1.1 and version 2.0. The version number 1.0 was assigned retrospectively to the version described in the original paper of Hall, Allen & Brown (1991), as amended by COMCIFS 29 January 1997.

In addition to the formal specification, a number of ancillary notes are published that describe conventions or guidelines applied within one or more of the dictionaries of CIF data items that are used in various topic areas. These notes should be adhered to as closely as possible, in association with the formal specification of file syntax and implied semantics, to maximise the efficient interoperability of CIF-based applications.

The International Union of Crystallography is a non-profit scientific union serving the world-wide interests of crystallographers and other scientists employing crystallographic methods.

[Hall et al., 1991]

The Crystallographic Interchange File/Framework (CIF):

- Provides standard means for data publishing and exchange;
- Is suitable for data archiving and publishing;
- Is maintained by the IUCr;

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CIF for scientific data

examples/data/2100858-head.cif:

```
data_2100858
loop_
_publ_author_name
'Buttner, R. H.'
'Maslen, E. N.'
_publ_section_title
;
 Structural parameters and electron difference density in BaTiO~3~
;
_journal_issue                  6
_journal_name_full              'Acta Crystallographica Section B'
_journal_page_first             764
_journal_page_last              769
_journal_volume                 48
_journal_year                   1992
_chemical_compound_source       'synthetic, from a mixture of KF:KMoO4:BaTiO3'
_chemical_formula_sum           'Ba O3 Ti'
_chemical_formula_weight        233.24
_symmetry_cell_setting          tetragonal
_symmetry_space_group_name_Hall 'P 4 -2'
_symmetry_space_group_name_H-M  'P 4 m m'
_cell_angle_alpha               90.0
_cell_angle_beta                90.0
_cell_angle_gamma               90.0
_cell_formula_units_Z           1
_cell_length_a                  3.9998(8)
_cell_length_b                  3.9998(8)
_cell_length_c                  4.0180(8)
```

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Controlled vocabularies

examples/dictionaries/cif-core-example.cif:

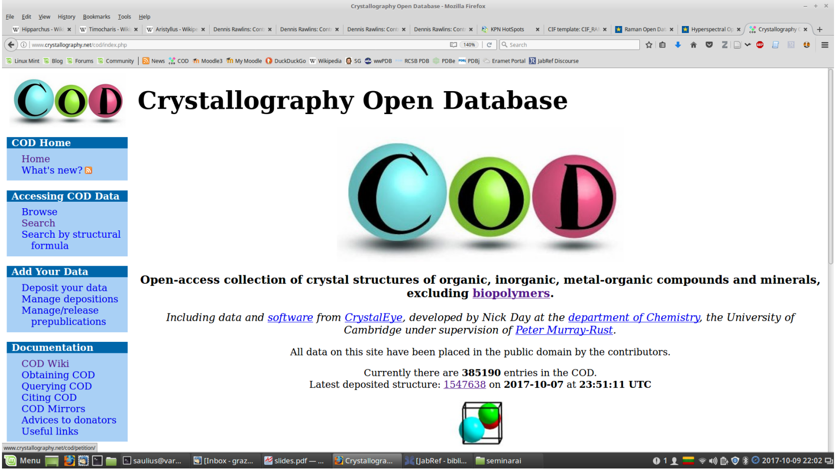
```
data_cell_length_
    loop_ _name                ’_cell_length_a’
                               ’_cell_length_b’
                               ’_cell_length_c’
    _category                    cell
    _type                        numb
    _type_conditions             esd
    _enumeration_range           0.0:
    _units                       A
    _units_detail              ’angstroms’
    _definition
;              Unit-cell lengths in angstroms corresponding to the structure
               reported. The values of _refln_index_h, *_k, *_l must
               correspond to the cell defined by these values and _cell_angle_
               values. The values of _diffrn_refln_index_h, *_k, *_l may not
               correspond to these values if a cell transformation took place
               following the measurement of the diffraction intensities. See
               also _diffrn_reflns_transf_matrix_.
;
```

This project has received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement No 689868.

Crystallographic data

The Crystallography Open Database

http://www.crystallography.net/cod



Crystallography Open Database

COD Home

Home
What's new?

Accessing COD Data

Browse
Search
Search by structural formula

Add Your Data

Deposit your data
Manage depositions
Manage/release prepublications

Documentation

COD Wiki
Obtaining COD
Querying COD
Citing COD
COD Mirrors
Advices to donators
Useful links

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.

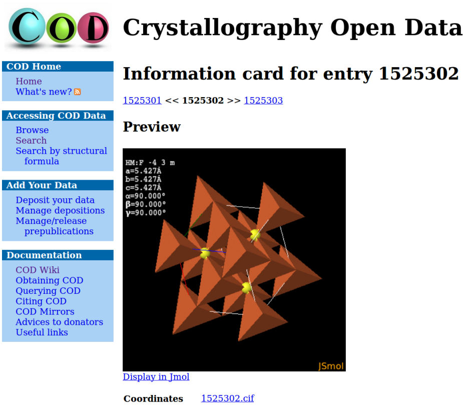
Currently there are **385190** entries in the COD.
Latest deposited structure: 1547638 on **2017-10-07** at **23:51:11 UTC**

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

A COD crystal structure page example

Sphalerite

http://www.crystallography.net/cod/1525302.html



Crystallography Open Database

COD Home

- Home
- What's new?

Accessing COD Data

- Browse
- Search
- Search by structural formula

Add Your Data

- Deposit your data
- Manage depositions
- Manage/release prepublications

Documentation

- COD Wiki
- Obtaining COD
- Querying COD
- Citing COD
- COD Mirrors
- Advices to donators
- Useful links

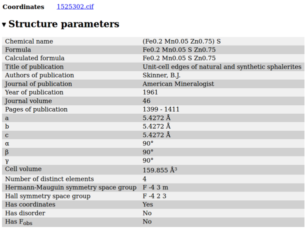
Information card for entry 1525302

1525301 << **1525302** >> 1525303

Preview

Display in Jmol

Coordinates 1525302.cif



Coordinates 1525302.cif

▾ Structure parameters

Chemical name	(Fe0.2 Mn0.05 Zn0.75) S
Formula	Fe0.2 Mn0.05 S Zn0.75
Calculated formula	Fe0.2 Mn0.05 S Zn0.75
Title of publication	Unit-cell edges of natural and synthetic sphalerites
Authors of publication	Skinner, B.J.
Journal of publication	American Mineralogist
Year of publication	1961
Journal volume	46
Pages of publication	1399 - 1411
a	5.4272 Å
b	5.4272 Å
c	5.4272 Å
α	90°
β	90°
γ	90°
Cell volume	159.855 Å^3
Number of distinct elements	4
Hermann-Mauguin symmetry space group	F -4 3 m
Hall symmetry space group	F -4 2 3
Has coordinates	Yes
Has disorder	No
Has F_{obs}	No

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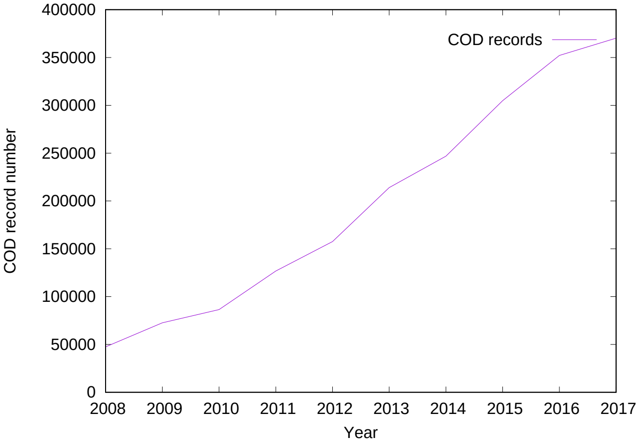
COD persistence

COD is on-line for 13 years, increased 7-fold over the last 8 years; currently contains over 385 000 records (October 2017):



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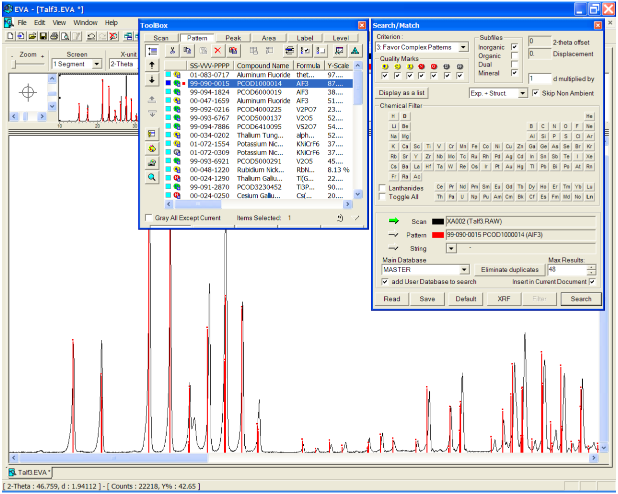
Use of COD and PCOD databases

Search-match identification of the materials



1 Segment
2-Theta

SS-VVV-PPPP	Compound Name	Formula	Y-Scale
01-083-0717	Aluminum Fluoride	thet...	97....
99-090-0015	PCOD1000014	AlF3	87....
99-094-1824	PCOD6000019	AlF3	38....
00-047-1659	Aluminum Fluoride	AlF3	51....
99-092-0216	PCOD4000225	V2PO7	23....
99-093-6767	PCOD5000137	V2O5	52....
99-094-7886	PCOD6410095	VS2O7	54....
00-034-0202	Thallium Tung...	alph...	52....
01-072-1554	Potassium Nic...	KNiCrF6	37....
01-072-0309	Potassium Nic...	KNiCrF6	37....
99-093-6921	PCOD5000291	V2O5	45....
00-048-1220	Rubidium Nick...	RbN...	8.13 %
00-024-1290	Thallium Galliu...	Tl(G...	22....
99-091-2870	PCOD3230452	Ti3P...	90....
00-024-0250	Cesium Galliu...	Cs(...	20....

□ Gray All Except Current   Items Selected: 1

Criterion : 3: Favor Complex Patterns

Quality Marks: ☑ ☑ ☑ ☑ ☑ ☑ ☑

Subfiles: Inorganic ☑ Organic □ Dual □ Mineral ☑

0 2-theta offset

0. Displacement

1 d multiplied by

Exp. + Struct.   ☑ Skip Non Ambient

□ Lanthanides

□ Toggle All

Scan: XA002 (Talf3.RAW)

Pattern: 99-090-0015 PCOD1000014 (AlF3)

String: -

Main Database: MASTER

Max Results: 48

☑ add User Database to search

Insert in Current Document ☑

[2-Theta : 46.759, d : 1.94112] - [Counts : 22218, Y% : 42.65]

A **predicted** phase from PCOD could be identified in experimental data.

Courtesy Armel Le Bail [Le Bail, 2008]

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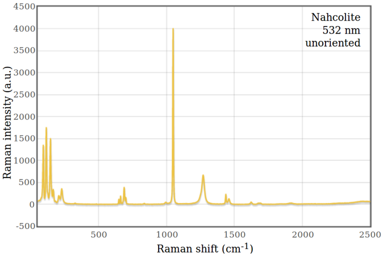
Ramano spectroscopy

us-tech.co.za



ROD 3500101

- the method is very fast
- requires comprehensive, high quality database

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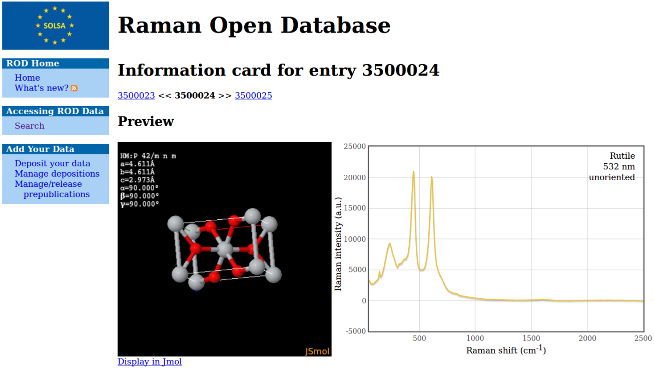
Raman spectroscopy data

The Raman Open Database

http://solsa.crystallography.net/rod



ROD Home

Home

What's new?

Accessing ROD Data

Search

Add Your Data

Deposit your data

Manage depositions

Manage/release prepublications

Raman Open Database

Information card for entry 3500024

3500023 << **3500024** >> 3500025

Preview

Display in Jmol

Data records contributed to the ROD by Yassine El Mendili

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

ROD data files

ROD uses CIF syntax

examples/data/3500024-head.rod:

```
#------------------------------------------------------------------------------
#$Date: 2017-10-05 18:15:36 +0300 (Thu, 05 Oct 2017) $
#$Revision: 219 $
#$URL: svn://172.16.1.102/rod/cif/3/50/00/3500024.rod $
#------------------------------------------------------------------------------
#
# This file is available in the Raman Open Database (ROD),
# http://solsa.crystallography.net/rod/
#
# All data on this site have been placed in the public domain by the
# contributors.
#
data_3500024
loop_
_publ_author_name
'El Mendili, Y'
_publ_section_title
;
 SOLSA communication to ROD
;
_journal_name_full               'Personal communication to ROD'
_journal_year                    2017
_chemical_compound_source        'commercial powder Prolabo pur'
_chemical_formula_structural     'O2 Ti'
```

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The ROD dictionary

ROD uses controlled CIF vocabulary

http://solsa.crystallography.net/rod/cif/dictionaries/cif_raman_0.1.1.dic
http://solsa.crystallography.net/rod/cif/dictionaries/cif_rod_0.1.0.dic

`examples/dictionaries/raman-example.dic`:

```
save__raman_measurement_device.direction_polarization
    _definition.id                 '_raman_measurement_device.direction_polarization'
# ... some text omited for brevity ...
    _definition.update             2017-04-10
    _description.text
;
    The direction polarization of the measurement device.
;
# ...
    loop_
    _enumeration_set.state
    _enumeration_set.detail
    unoriented
;
 Unoriented.
;
    Z(XX)Z
;
 Laser polarized parallel to the x axis; analyzer set to pass the x axis
 polarized light.
;
```

ROD dictionaries coded by Antanas Vaitkus

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Semantic versioning of the ROD dictionaries

- ROD dictionaries undergo semantic versioning:
  - Bug-fix releases (1.2.x) are compatible backwards and forward;
  - Minor releases (1.x) are backwards compatible;
  - Incompatible changes will be marked by major releases (1.x → 2.x);

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COD query examples

Web, REST, SQL

- Via the WWW interface – go for “search” in:
  - http://www.crystallography.net/cod
  - http://solsa.crystallography.net/rod
  - http://solsa.crystallography.net/hod
- Via the **stable** URLs (REST):
  - http://www.crystallography.net/cod/2000000.cif
  - http://solsa.crystallography.net/rod/3500021.rod
  - http://solsa.crystallography.net/rod/3500021.html
  - http://www.crystallography.net/cod/result?text=perovskite
- Via the **views** of the SQL database:

```
mysql -u cod_reader cod -h www.crystallography.net\
    -e ’select file, a, b, c, vol, formula
        from data where
            year between 2013 and
                         2014 and
            formula regexp " C[0-9]* "
            order by vol desc limit 10’
```

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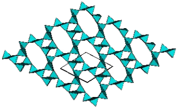
Open Crystallographic Databases

COD, TCOD, PCOD, MPOD, ROD, HOD ...

http://www.crystallography.net/cod
$>$ 385 000 entries (ready to grow $> 10^6$?)

http://www.crystallography.net/tcod
$>$ 2500 entries (ready to grow to $> 10^7$?)

http://mpod.cimav.edu.mx/
$>$ 300 entries



http://www.crystallography.net/pcod
$>$ 10^6 entries (ready to grow to $> 10^8$?)

http://solsa.crystallography.net/rod/
$>$ 120 entries

HOD

http://solsa.crystallography.net/hod/
TBA...

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COD accessibility

COD is a **fully open-access database**. All records are available under public domain designation.

Provided access methods are:

- Web search
- URLs constructed from stable identifiers
- RESTful interfaces
- Full data download

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Hyperspectral image database (HOD)

http://solsa.crystallography.net/hod

A “hybrid” approach necessary due to large size of raster data:

- Metadata and image headers stored in CIF;
- Raster data stored as “raw” binaries;

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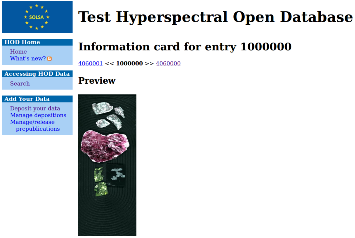
HOD record example

examples/hod/1000000-head.cif:

```
data_1000000
loop_
_[local]_description
'ENVI File'
'Created [Wed Jun 08 12:34:07 2016]'
_[local]_wavelength_units           Nanometers
loop_
_hyper_bands.default
220
227
253
_hyper_bands.lines                  937
_hyper_bands.number                 288
_hyper_bands.samples                384
_hyper_file.byte_order              0
_hyper_file.data_type               4
_hyper_file.type                    ENVI_Standard
_hyper_header.offset                0
_hyper_header_file.contents
;ENVI
description = {
  ENVI File, Created [Wed Jun 08 12:34:07 2016]}
samples = 384
lines   = 937
```

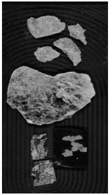


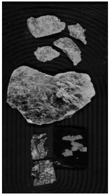
Test Hyperspectral Open Database

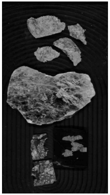
Information card for entry 1000000

4060001 << 1000000 >> 4060000

Preview





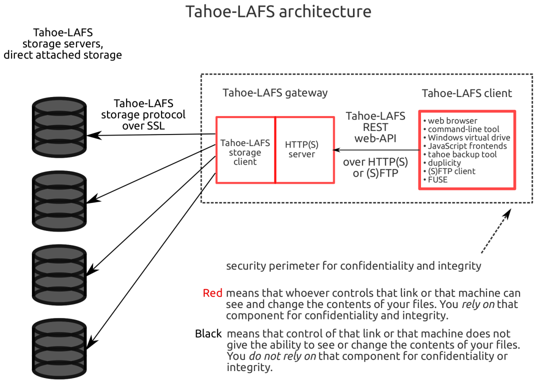


This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

SOLSA Large File Store

Suitable, e.g., for images

Uses Tahoe-LAFS (https://tahoe-lafs.org) as a back-end [Selimi and Freitag, 2014]:



Tahoe-LAFS architecture

Tahoe-LAFS storage servers, direct attached storage

Tahoe-LAFS storage protocol over SSL

Tahoe-LAFS gateway

Tahoe-LAFS storage client

HTTP(S) server

Tahoe-LAFS REST web-API

over HTTP(S) or (S)FTP

Tahoe-LAFS client

- web browser
- command-line tool
- Windows virtual drive
- JavaScript frontends
- tahoe backup tool
- duplicity
- (S)FTP client
- FUSE

security perimeter for confidentiality and integrity

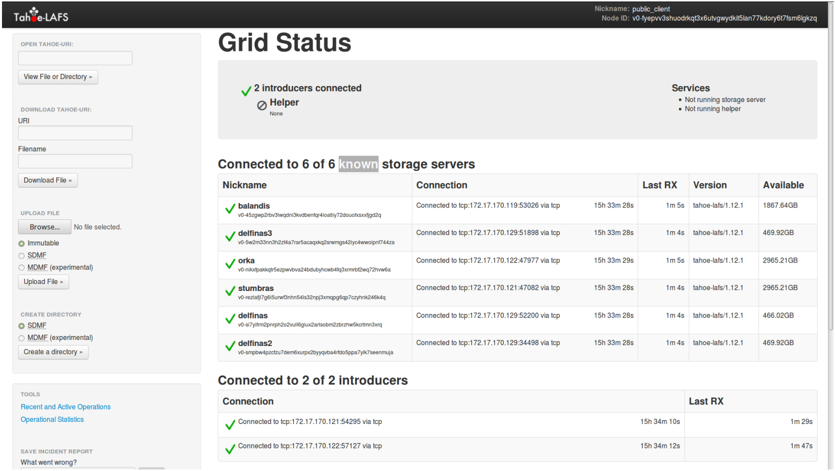
Red means that whoever controls that link or that machine can see and change the contents of your files. You *rely on* that component for confidentiality and integrity.

Black means that control of that link or that machine does not give the ability to see or change the contents of your files. You *do not rely on* that component for confidentiality or integrity.

Quoted from https://tahoe-lafs.org/trac/tahoe-lafs

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Tahoe LAFS Grid for SOLSA



Nickname: public_client
Node ID: v0-fyepvv3shuodrkqt3x6utvgwydkit5lan77kdory6t7fsm6lgkzq

Grid Status

✓ 2 introducers connected

⊘ Helper
None

Services
- Not running storage server
- Not running helper

Connected to 6 of 6 known storage servers

Nickname	Connection	Last RX	Version	Available
✓ **balandis** v0-45zgwp2rbv3lwqdni3kvdbenfqr4ioatiiy72douofxsxxfjgd2q	Connected to tcp:172.17.170.119:53026 via tcp 15h 33m 28s	1m 5s	tahoe-lafs/1.12.1	1867.64GB
✓ **delfinas3** v0-5w2m33nn3h2zf4a7rar5acaqxkq2srwmgs42iyc4wwolpnf744za	Connected to tcp:172.17.170.129:51898 via tcp 15h 33m 28s	1m 4s	tahoe-lafs/1.12.1	469.92GB
✓ **orka** v0-nikxfpakkqtr5ezpwvbva24bdubyhcwb4fq3xrmrbf2wq72hvw6a	Connected to tcp:172.17.170.122:47977 via tcp 15h 33m 29s	1m 5s	tahoe-lafs/1.12.1	2965.21GB
✓ **stumbras** v0-rezlafjl7g6i5urwf3nhn54ls32npj3xmqpg6qp7czyhnk246k4q	Connected to tcp:172.17.170.121:47082 via tcp 15h 33m 28s	1m 4s	tahoe-lafs/1.12.1	2965.21GB
✓ **delfinas** v0-si7yifrm2pnrph2o2vull6giux2arlsobm2zbrzhw5kcrtmn3xrq	Connected to tcp:172.17.170.129:52200 via tcp 15h 33m 28s	1m 4s	tahoe-lafs/1.12.1	466.02GB
✓ **delfinas2** v0-smpbw4pzcfzu7dem6xurpx2byyqvba4rfdo5ppa7ylk7seenmuja	Connected to tcp:172.17.170.129:34498 via tcp 15h 33m 28s	1m 4s	tahoe-lafs/1.12.1	469.92GB

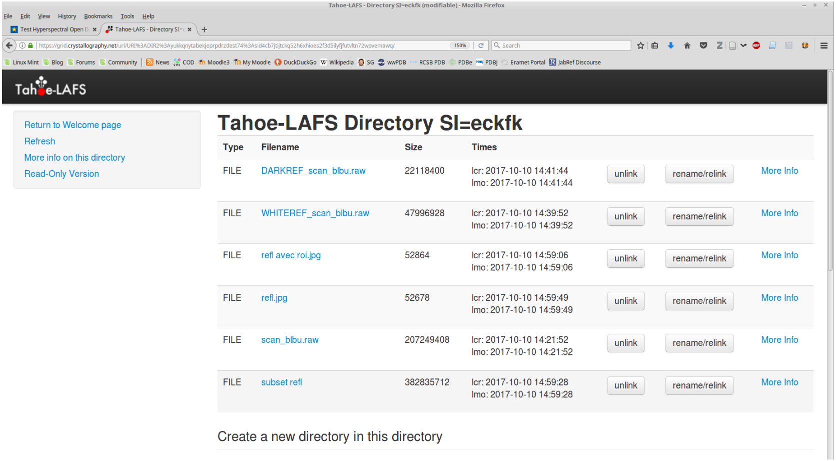
Connected to 2 of 2 introducers

Connection	Last RX
✓ Connected to tcp:172.17.170.121:54295 via tcp 15h 34m 10s	1m 29s
✓ Connected to tcp:172.17.170.122:57127 via tcp 15h 34m 12s	1m 47s

Tahoe-LAFS for SOLSA set up by Erikas Raginis

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

HOD files on the Tahoe LAFS grid


Tahoe-LAFS - Directory SI=eckfk (modifiable) - Mozilla Firefox
File Edit View History Bookmarks Tools Help
Test Hyperspectral Open D
Tahoe-LAFS - Directory SI=
https://grid.crystallography.net/uri/URI%3ADIR2%3Ayukkqnytabekjeprpdrzdest74%3Asld4cb7jtijtckq52h6xhioes2f3d5ilyfjfutvltn72wpvemawq/
150%
Search
Linux Mint
Blog
Forums
Community
News
COD
Moodle3
My Moodle
DuckDuckGo
Wikipedia
SG
wwPDB
RCSB PDB
PDBe
PDBj
Eramet Portal
JabRef Discourse
Tahoe-LAFS
Return to Welcome page
Refresh
More info on this directory
Read-Only Version

Tahoe-LAFS Directory SI=eckfk

Type	Filename	Size	Times			
FILE	DARKREF_scan_blbu.raw	22118400	lcr: 2017-10-10 14:41:44 lmo: 2017-10-10 14:41:44	unlink	rename/relink	More Info
FILE	WHITEREF_scan_blbu.raw	47996928	lcr: 2017-10-10 14:39:52 lmo: 2017-10-10 14:39:52	unlink	rename/relink	More Info
FILE	refl avec roi.jpg	52864	lcr: 2017-10-10 14:59:06 lmo: 2017-10-10 14:59:06	unlink	rename/relink	More Info
FILE	refl.jpg	52678	lcr: 2017-10-10 14:59:49 lmo: 2017-10-10 14:59:49	unlink	rename/relink	More Info
FILE	scan_blbu.raw	207249408	lcr: 2017-10-10 14:21:52 lmo: 2017-10-10 14:21:52	unlink	rename/relink	More Info
FILE	subset refl	382835712	lcr: 2017-10-10 14:59:28 lmo: 2017-10-10 14:59:28	unlink	rename/relink	More Info

Create a new directory in this directory

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HOD (large) data retention policy

A managed data phase-out policy possible:

- Keep data that are:
  - The first of their kind;
  - The best of their kind;
  - The most often used/cited;
  - A small but representative test set (for software);
- Apply lossy compression to older records (×20 fold possible)
- Discard data for other records, leave just (aggregated) metadata;

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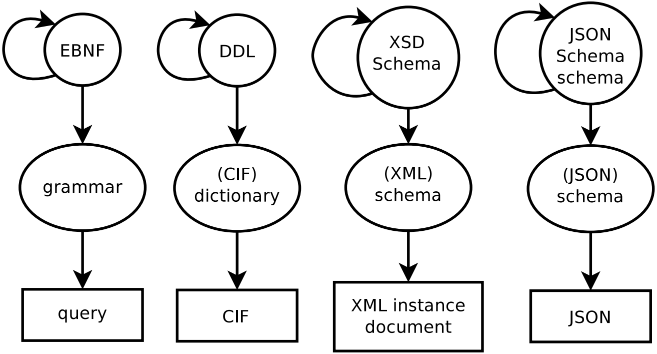
Common pattern of self-describing data definitions



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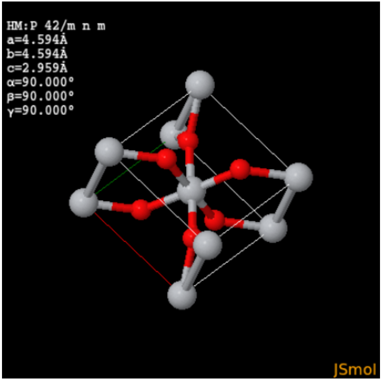
Thank you!

http://en.wikipedia.org/wiki/Rutile

Rob Lavinsky, iRocks.com – CC-BY-SA-3.0



```
HM:P 42/m n m
a=4.594Å
b=4.594Å
c=2.959Å
α=90.000°
β=90.000°
γ=90.000°
```

http://www.crystallography.net/9015662.html

A path to freedom: GNU → Linux → Ubuntu+Debian → MySQL → R → Perl → LaTeX → TikZ → Beamer

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The fun of REST

RESTful queries [Fielding, 2000]:

- Programming language, transfer protocol **independent**
- GET queries should be null-potent (do not change anything; always provide the same result for the same query);
- POST/PUT queries should be idempotent (the same query executed several times should have the same result as just one query).

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