The Crystallography Open Database

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Kaunas, OpenCon 2016

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Data Sharing and Reproducible Research

. . . the imperative

- "/. . . / research which yields nonsignificant results is not published. Such research being unknown to other investigators may be repeated independently until eventually by chance a significant result occurs /. . . / the literature of such a field consists in substantial part of false conclusions" [Sterling, 1959]
- in $< 1/2$ of the microarray publications, analyses are not reproducible due to lack of data/protocols/software [Ioannidis et al., 2009]
- "If you use p = 0.05 to suggest that you have made a discovery, you will be wrong at least 30% of the time. If, as is often the case, experiments are underpowered, you will be wrong" **most of the time**[1]. [Colquhoun, 2014]

[1] Emphasis mine. S.G.

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Data Sharing in Crystallography

Started quite early

- **1948 Acta Cryst. (IUCr)** The Acta Crystallographica journal was launched, *all coordinates were printed in journal articles, and Acta Crystallographica published the structure factors as well*
- **1965 CSD (CCDC)** *The CCDC was established at the Department of Chemistry, Cambridge University /. . . / about 2000 structures published before 1965 were gradually incorporated into the developing database*
- **1971 PDB** *In June 1971, the two communities attended the Cold Spring Harbor Symposium on Quantitative Biology (Cold Spring Laboratory Press, 1972)*

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Problems with access to data

Proprietary licensing causes a lot of headache in the XXI century...

- CCDC Access Structures Terms and Conditions: “These services must not be used to systematically download or redistribute these structures, data or associated information. Programmatic access to these services is not permitted.”
  (https://summary.ccdc.cam.ac.uk/about-this-service, last accessed 2016-11-24)
- “In the specific case of the article in question,/. . . / a small molecule 3-D structure predictor and Web server (COSMOS) /…/ [t]he CCDC vigorously intervened to prevent distribution of such a tool. The statement in the CCDC’s letter that “express permission was immediately granted” is simply false. A dozen librarians and other staff from the University of California (UC) had to intervene under the threat of losing a system-wide license to the CSD.” [Baldi, 2011]

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The COD project

But what if crystallographers work together to establish a public domain database with all relevant crystallographic data? This would not only overcome the current situation with 'fragmented' databases, it would also prevent for becoming dependent from monopolists.

What would be needed?

1. A small team of engaged scientists with some experience in database and software design to coordinate the project.

2. The authors (i.e. the scientific community = YOU) who provides the project with database entries (note, that if you have'nt sold your experimental results exclusively, you are free to distribute the data to such a database, even if they have already been part of a publication - and a lot of good data have never been published).

3. Free software a) for maintaining the database, b) for data evaluation and calculation of derived data (e.g. calculated powder pattern from crystal structures for search-match purposes), c) for browsing and retrieval.

gemstonede (Dr. Michael BERNDT) Fri Feb 14, 2003 1:26 pm

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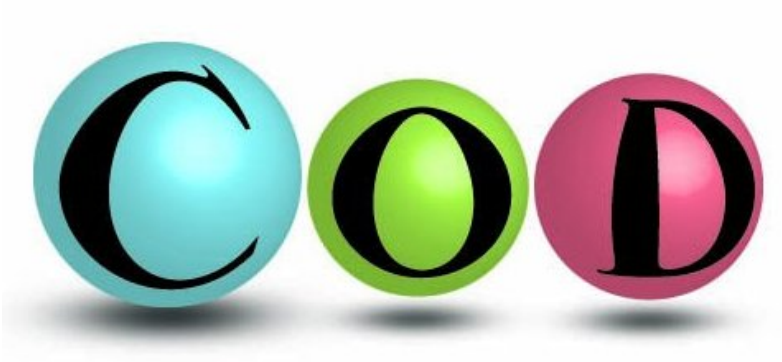
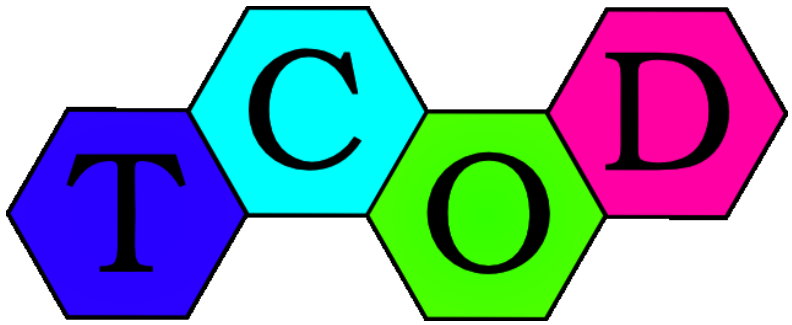
Open Crystallographic Databases

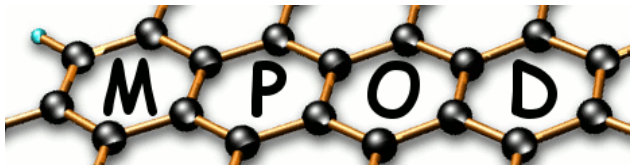
COD, TCOD, PCOD, MPOD, ...



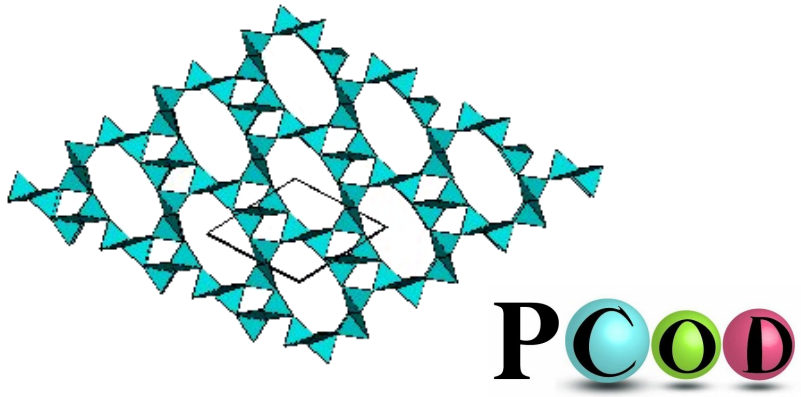
http://www.crystallography.net/cod
$>$ 367 000 entries (ready to grow $> 10^6$?)



http://www.crystallography.net/tcod
$>$ 2000 entries (ready to grow to $>$ 350 000?)



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



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

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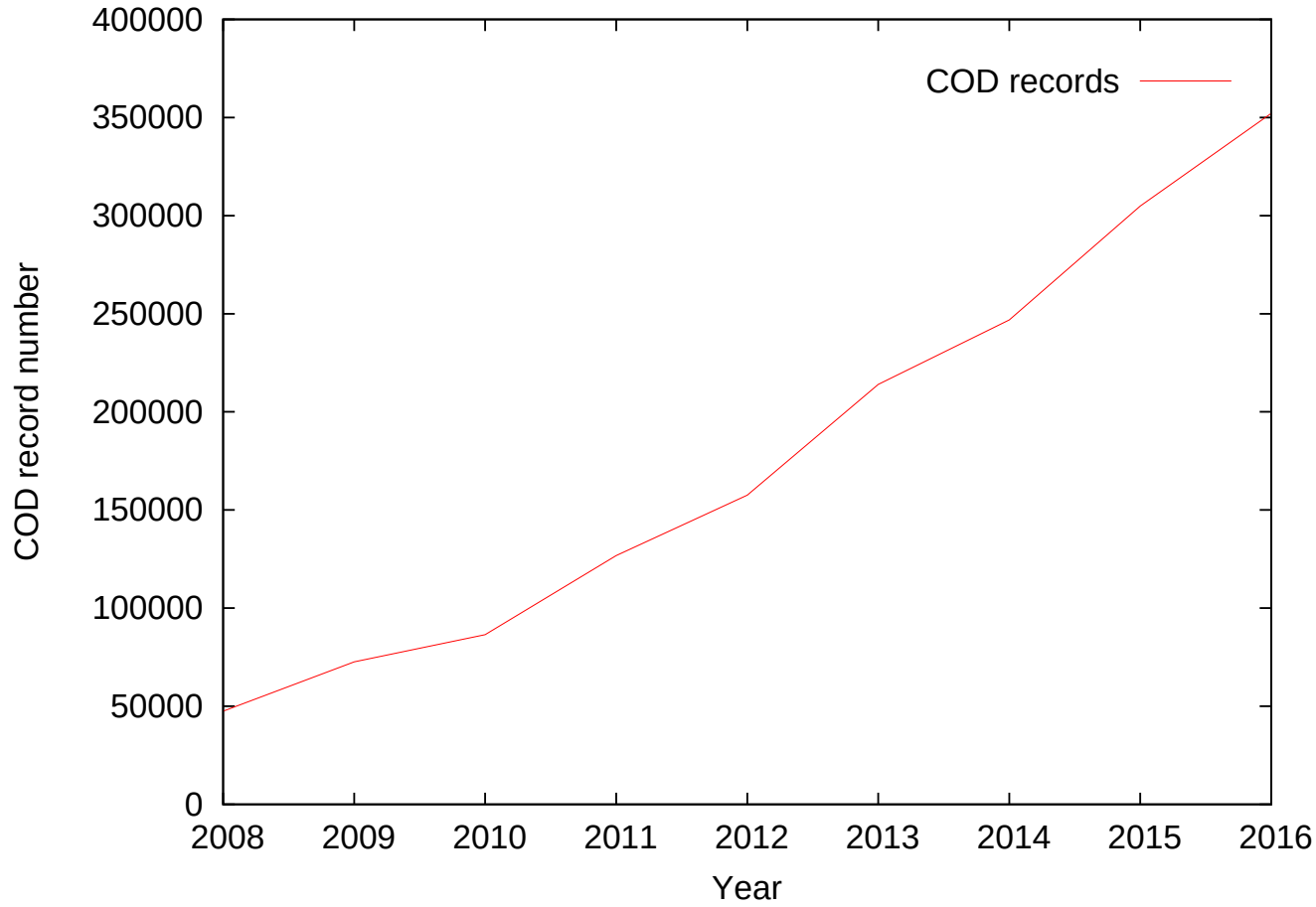
COD 13 years later

COD increased 7-fold; currently contains over 367000 records (Sept. 2016)



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Common framework: the CIF

The Crystallographic Interchange Framework (CIF) is developed and curated by the International Union of Crystallography (IUCr).
`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)
```

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Description of semantics

CIF dictionaries

```
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_.
;
```

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TCOD dictionary contents

The most basic data names

- `cif_tcod.dic`: ver. 0.008, last update 2015-06-16, 107 data names;
- `cif_dft.dic`: ver. 0.019, last update 2016-04-13, 87 data names.

e.g. (same as NOMAD atom_forces?):

```
data_tcod_atom_site_residual_force
loop_ _name
'_tcod_atom_site_resid_force_Cartn_x'
'_tcod_atom_site_resid_force_Cartn_y'
'_tcod_atom_site_resid_force_Cartn_z'
# ... some names omitted for brevity
_type numb
_units eV/\%A
_units_detail 'electronvolts per Angstroem'
_definition
;
These data items describe residual forces on atoms in the final
structure. For a converged computation of a stable structure these
...
;
```

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New developments: CIF2

- Support of Unicode (UTF-8) [Bernstein et al., 2016];
- Array data (including multidimensional arrays);
- Data hashes (key–value pairs);
- Computer readable semantics definitions (in a multiparadigm language dREL):

```
    _units.code                         angstroms_cubed
    _method.expression
;
    With v as cell_vector
        _cell.volume = v.a * ( v.b ^ v.c )
;
```

http://oldwww.iucr.org/iucr-top/cif/ddlm/dREL_spec_20071013.html

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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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COD query examples

Web, REST, SQL

- Via the WWW interface – go for “search” in:
  - http://www.crystallography.net/cod
  - http://www.crystallography.net/tcod
  - http://www.crystallography.net/pcod
- Via the **stable** URLs (REST):
  - http://www.crystallography.net/cod/2000000.cif
  - http://www.crystallography.net/tcod/10000002.cif
  - 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
                date between "2013-01-01" and
                             "2014-12-31" and
                formula regexp " C[0-9]* "
                order by vol desc limit 10'
    ```

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    ```

COD applications

- SOLSA
  - http://www.solsa-mining.eu/
- AiiDA [Pizzi et al., 2016]
  - http://www.aiida.net/
- COSMOS [Sadowski and Baldi, 2013]
  - http://cdb.ics.uci.edu/
- FPSM [Boullay et al., 2014], MAUD [Boullay et al., 2012]
  - http://fpsm.radiographema.com/
  - http://maud.radiographema.eu/
- DataWarrior
  - http://www.openmolecules.org/datawarrior/
- MolView
  - http://molview.org/
- search-match (Bruker, PANalytical, Rigaku)
- ... and more!

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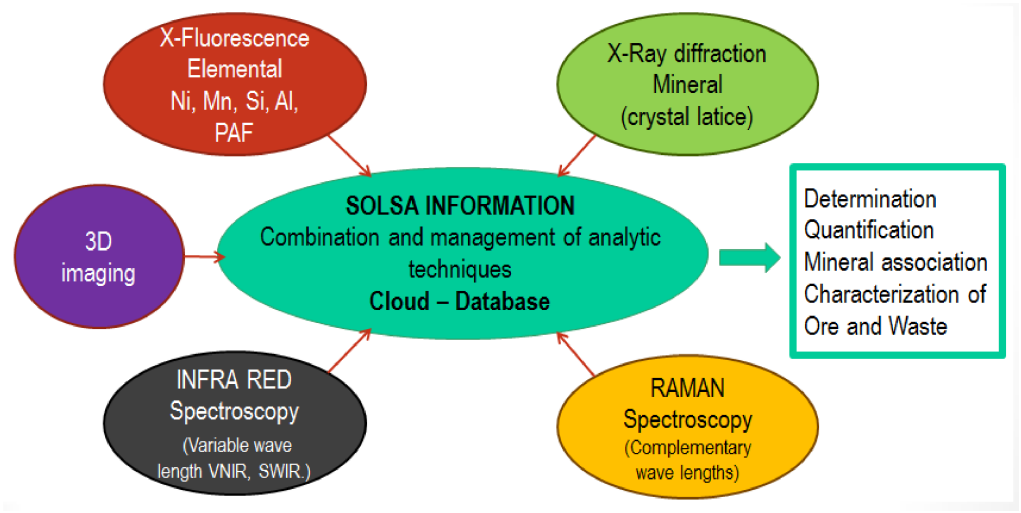
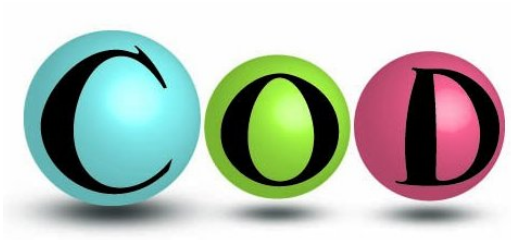
SOLSA project and COD



$\Leftrightarrow$



COD will be used in SOLSA for:

- mineral identification;
- subsequent data dissemination.

SOLSA data flow diagram courtesy Monique Le Guen, ERAMET.

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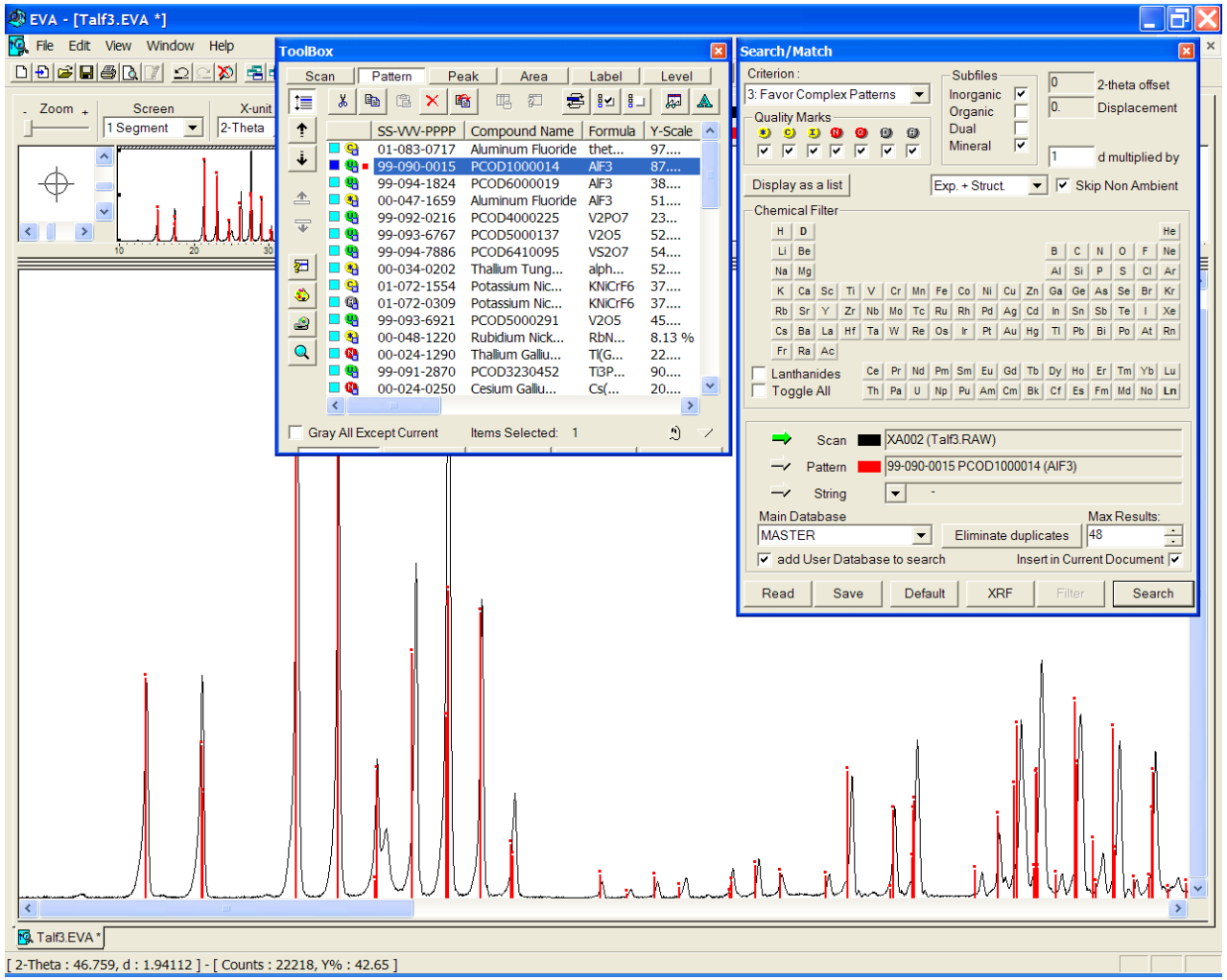
Use of *COD databases

Search-match identification of the materials



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

Courtesy Armel Le Bail
[Le Bail, 2008]

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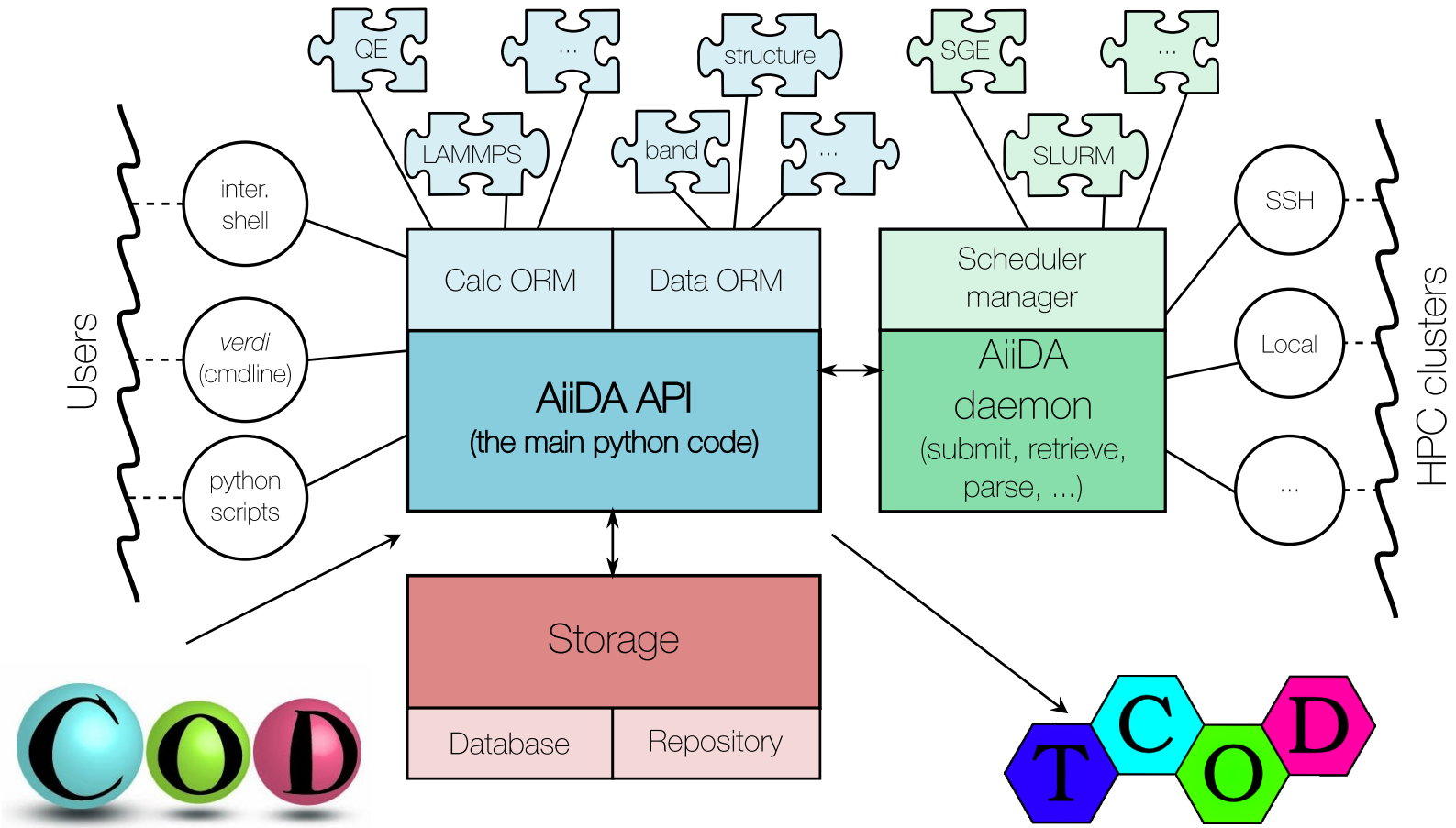
COD, TCOD and AiiDA link



Courtesy AiiDA developers [Pizzi et al., 2016]

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*COD data citation

The Research Data Alliance has just published and endorsed **recommendations** from the RDA Working Group on Data Citation:
https://www.rd-alliance.org/groups/data-citation-wg.html

COD data can be cited in several ways:

- Using a data reference URI:

> Srivastava, R. C.; Klooster, W. T.; Koetzle, T. F. "Neutron Structures of Ammonium Fluoroberyllate" (1999) *The Crystallography Open Database*, rev. 176759, the COD Advisory Board (eds.), http://www.crystallography.net/cod/2002926.cif. [Retrieved 2016-09-21 16:48 EEST]

- Using a "landing page" URI:

> Srivastava, R. C.; Klooster, W. T.; Koetzle, T. F. "Neutron Structures of Ammonium Fluoroberyllate" (1999) *The Crystallography Open Database*, rev. 176759, the COD Advisory Board (eds.), http://www.crystallography.net/cod/2002926.html. [Retrieved 2016-09-21 16:48 EEST]

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*COD data citation (2)

COD data can be cited in several ways:

- Using a data reference URI **with explicit revision**:

> Srivastava, R. C.; Klooster, W. T.; Koetzle, T. F. "Neutron Structures of Ammonium Fluoroberyllate" (1999) *The Crystallography Open Database*, rev. 176759, the COD Advisory Board (eds.), http://www.crystallography.net/cod/2002926.cif@176759. [Retrieved 2016-09-21 16:48 EEST]

- Using a content-negotiable URI (with or without explicit revision):

> Srivastava, R. C.; Klooster, W. T.; Koetzle, T. F. "Neutron Structures of Ammonium Fluoroberyllate" (1999) *The Crystallography Open Database*, rev. 176759, the COD Advisory Board (eds.), http://www.crystallography.net/cod/2002926. [Retrieved 2016-09-21 16:48 EEST]

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*COD metadata

COD metadata are available in RDF format:

http://www.crystallography.net/cod/2002926.rdf

`examples/data/2002926-example.rdf`:

```
<?xml version="1.0"?>
<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
         xmlns:cod="http://www.crystallography.net/cod/doc/rdf/">
  <rdf:Description rdf:about=
        "http://www.crystallography.net/cod/2002926.html">
    <cod:Rall>0.0476</cod:Rall>
    <cod:Robs>0.0476</cod:Robs>
    <cod:Z>8</cod:Z>
    <cod:Zprime>2</cod:Zprime>
    <cod:a>15.017</cod:a>
    <cod:acce_code>BK0051</cod:acce_code>
    <cod:alpha>90</cod:alpha>
    <cod:author>Srivastava, R. C.</cod:author>
    <cod:author>Klooster, W. T.</cod:author>
    <cod:author>Koetzle, T. F.</cod:author>
    <cod:b>5.876</cod:b>
    <cod:beta>90</cod:beta>
    <cod:c>10.418</cod:c>
    <cod:calcformula>Be F4 H8 N2</cod:calcformula>
    <cod:celltemp>163</cod:celltemp>
    <cod:chemname>ammonium tetrafluoroberyllate</cod:chemname>
    <!-- Some content omitted for brevity ... -->
  </rdf:Description>
</rdf:RDF>
```

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Database **request** citation

- Data requests (searches) should get their persistent identifiers to hide the underlying mechanism:

  http://www.crystallography.net/cod/query/123456
  $\rightarrow$
  http://www.crystallography.net/cod/result?text=perovskite

- Data requests (searches) should be re-runnable on new and old versions of the database:

  http://www.crystallography.net/cod/query/567890
  $\rightarrow$
  http://www.crystallography.net/cod/result?text=perovskite&dbrev=112233

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Software citations?

FORCE11 recommendations:

Should software be cited? (Yes!) Recommendations published in [Smith et al., 2016]

- TCOD dictionaries contain data items for versions and names of programs and libraries – additional data items for unique identifiers should be provided;
- How deep do we need to cite software? Compiler? OS? CPU? How reproducible will these be?

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Interlinked data in COD

Crystallography Open Database

COD Home
Home
What's new?

Accessing COD Data
Browse
Search
Search by structural formula

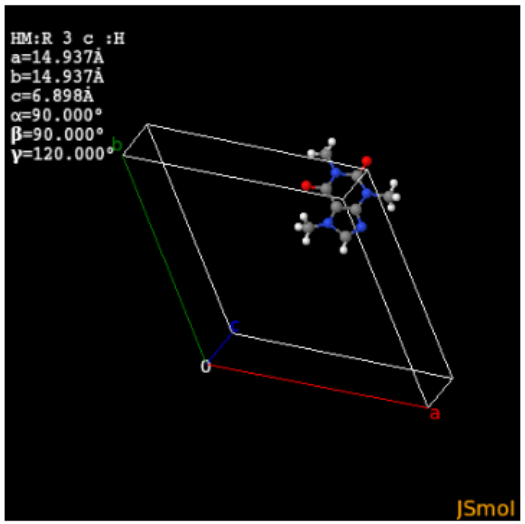
Add Your Data
Deposit your data
Manage depositions
Manage/release prepublications

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

Information card for 2100202

2100201 << **2100202** >> 2100203

Preview



Display in Jmol

Coordinates	2100202.cif
Original IUCr paper	HTML
External links	ChemSpider; DrugBank; PubChem; Wikipedia

▾ **Structure parameters**

```
select * from wikipedia_x_cod
+----+--------------+---------+-------------+
| id | ext_id       | cod_id  | relation_id |
+----+--------------+---------+-------------+
|  1 | Ibuprofen    | 2006278 |           1 |
|  2 | Caffeine     | 2100202 |           1 |
|  3 | Serotonin    | 2019147 |           1 |
|  4 | Pristinamycin| 1000001 |           1 |
|  5 | Cucurbituril | 1516465 |           1 |
|  6 | Rubrene      | 1516682 |           1 |
+----+--------------+---------+-------------+
```

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VU Institute of Biotechnology	**QM community**	**COD Advisory board**
	Björkman	Daniel Chateigner
Virginijus Siksnys	Torbjörn	Robert T. Downs
(*head of the dept.*)	Stefaan Cottenier	Werner Kaminsky
	Nicola Marzari	Armel Le Bail
Andrius Merkys	Giovanni Pizzi	Luca Lutterotti
Antanas Vaitkus	Lubomir Smrcok	Peter Moeck
	Linas Vilčiauskas	Peter Murray-Rust
	Chris Wolverton	Miguel Quirós

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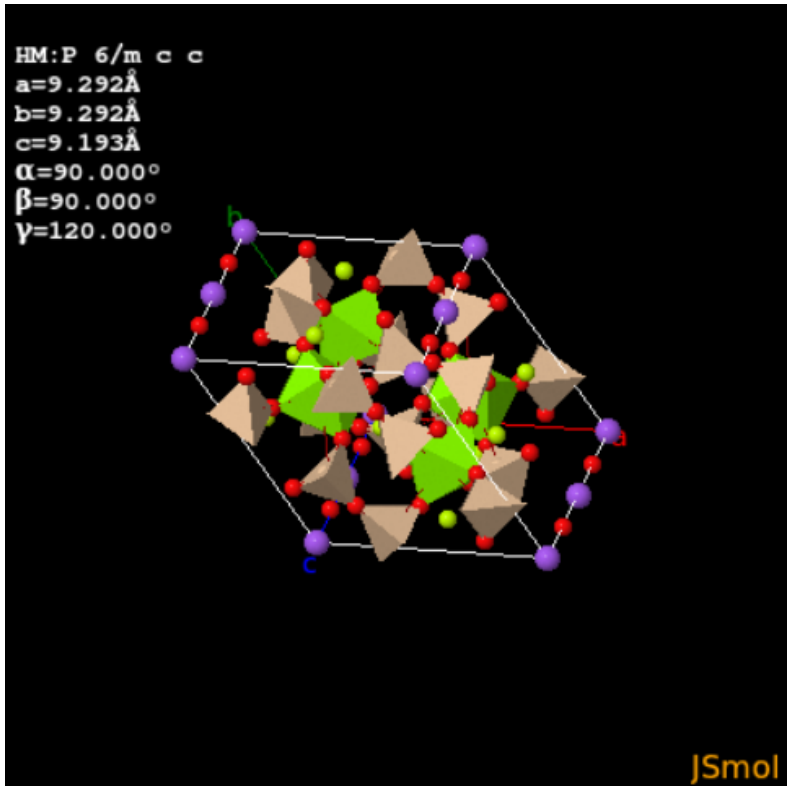
This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Thank you!

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



http://www.crystallography.net/5000095.html

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Data-driven high-throughput prediction of the 3-D structure of small molecules: review and progress. A response to the letter by the Cambridge Crystallographic Data Centre.
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Fast microstructure and phase analyses of nanopowders using combined analysis of transmission electron microscopy scattering patterns.
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PeerJ Computer Science, 2:e86.

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Publication decisions and their possible effects on inferences drawn from tests of significance — or vice versa.
Journal of the American Statistical Association, 54:30–34.

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