The Crystallography Open Database – new perspectives

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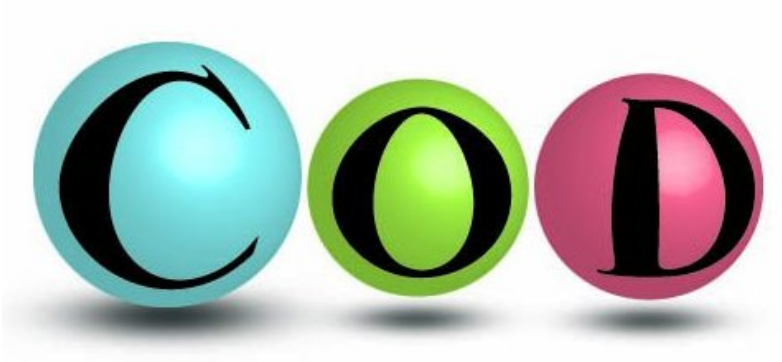
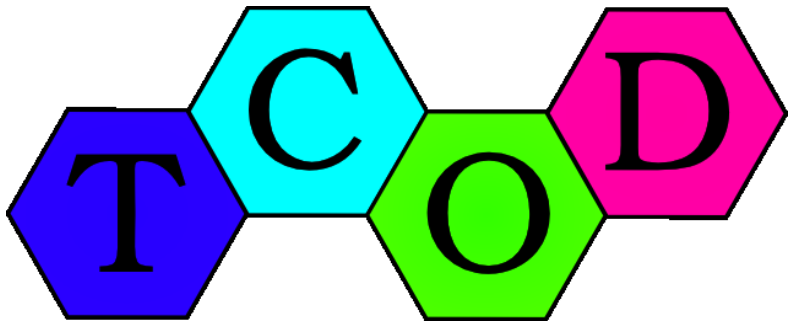
Open Crystallographic Databases

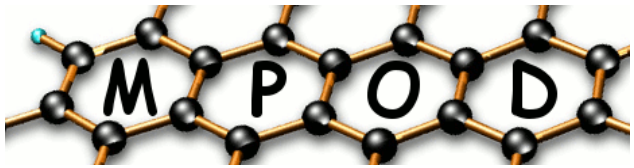
COD, TCOD, PCOD, MPOD, ...



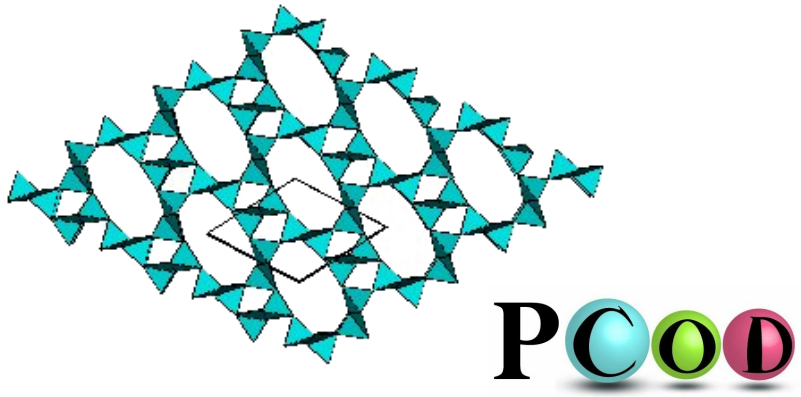
http://www.crystallography.net/cod
> 367 000 entries (ready to grow > 10^6?)



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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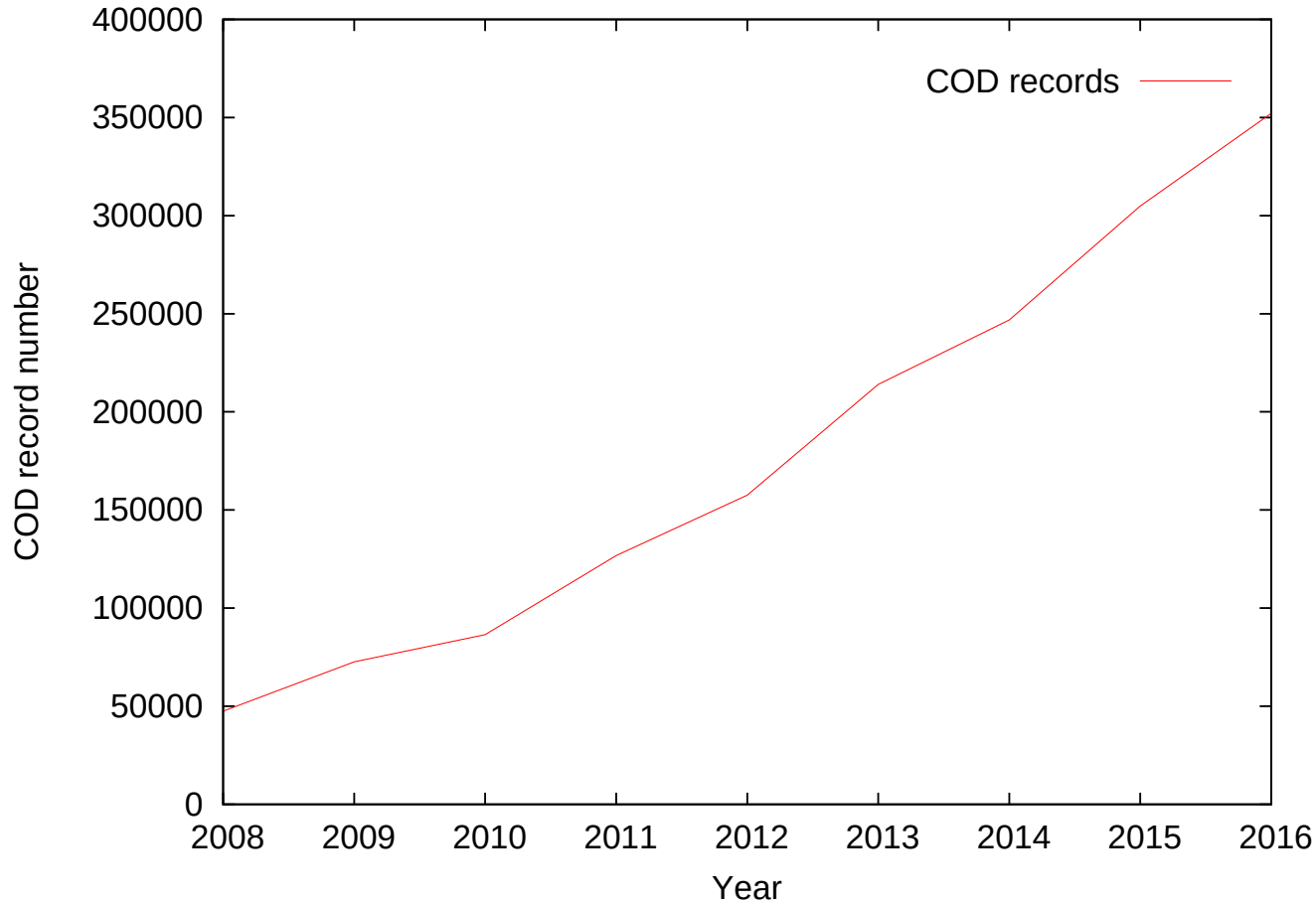
COD 13 years later

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



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Commong 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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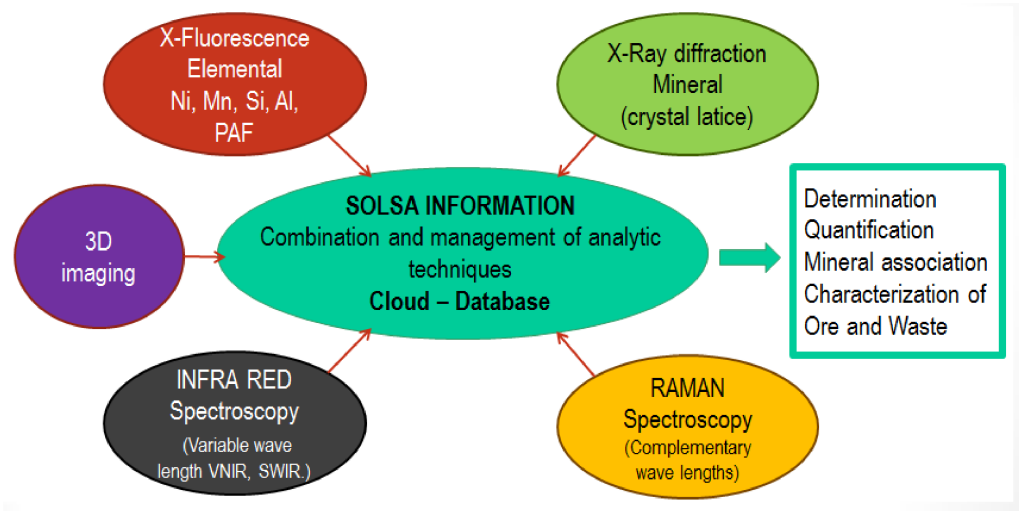
SOLSA project and COD



$\Leftrightarrow$

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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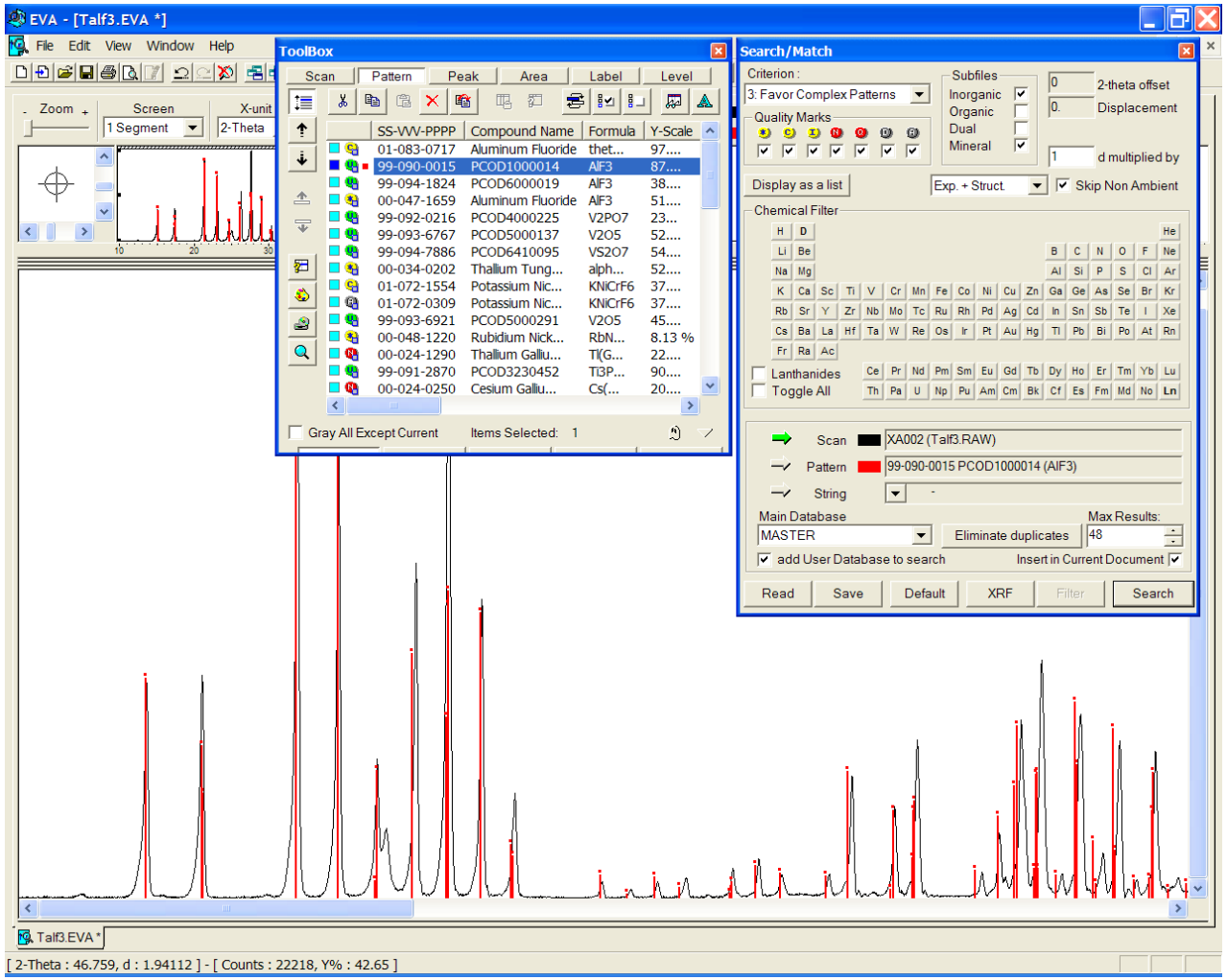
Use of *COD databases

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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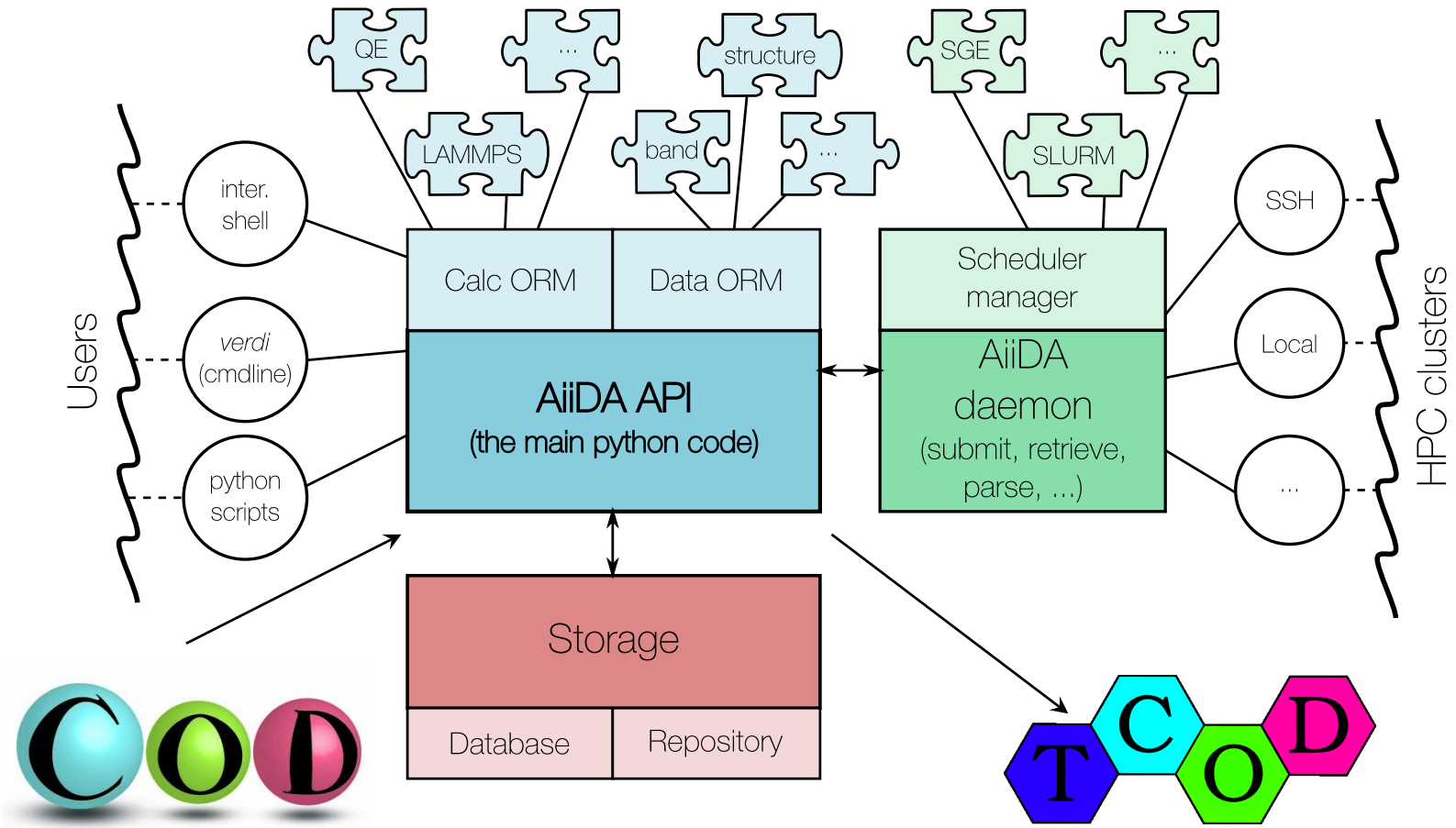
COD, TCOD and AiiDA link



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

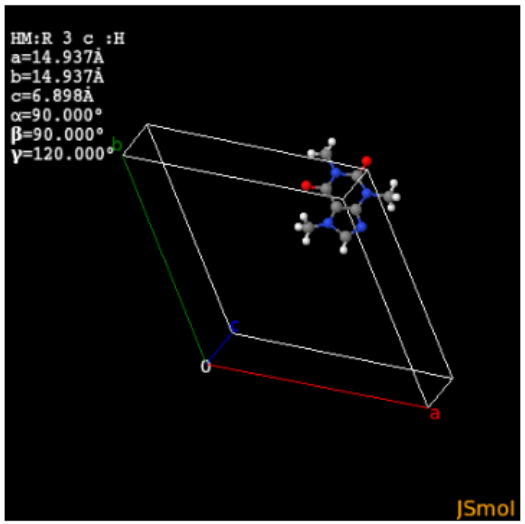
Add Your Data
Deposit your data
Manage depositions
Manage/release prepublications

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

```
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 |
+----+--------------+---------+-------------+
```

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

▾ **Structure parameters**

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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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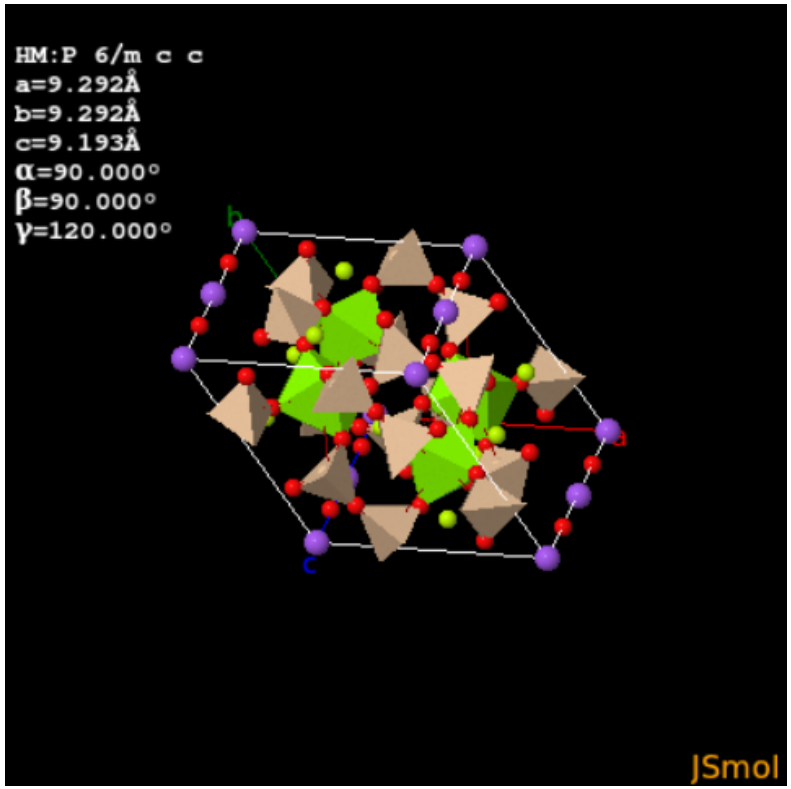
Thank you!

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



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

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