20 years of the COD: disseminating crystallographic data

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Grenoble, 2024

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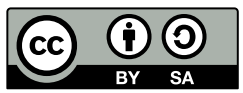
Id: slides2-policy.tex 2882 2024-09-25 04:53:12Z saulius September 25, 2024



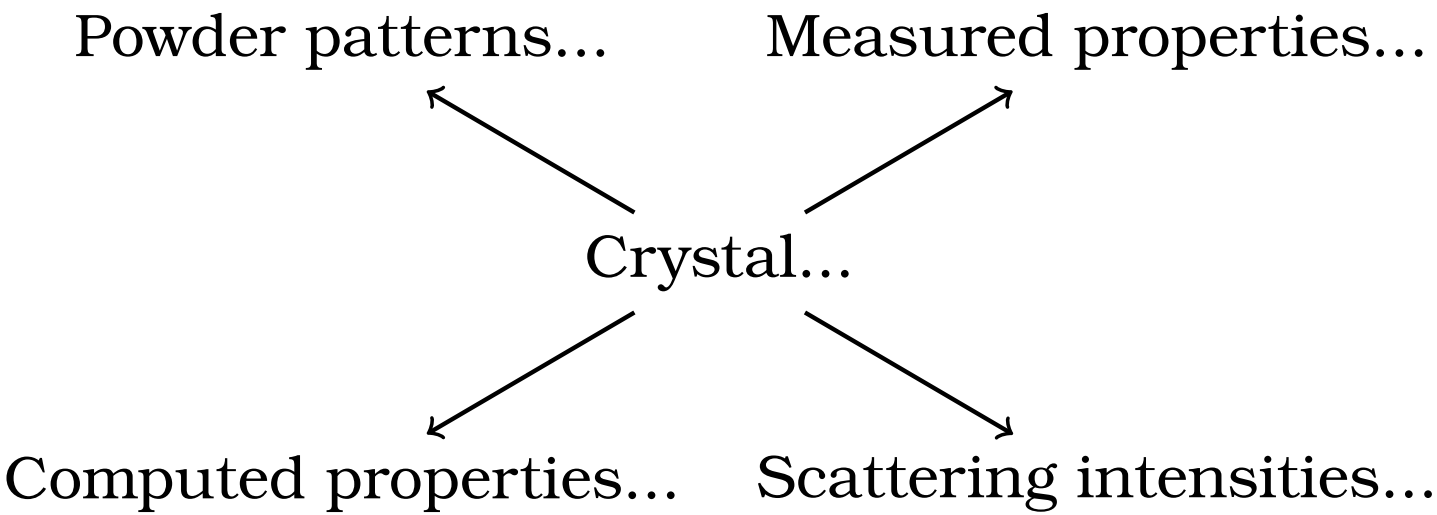
Overview of the talk

- What is COD (with some history);
- COD contents and data curation principles;
- Recent developments with the COD;
- Software for COD data;
- Future prospects;

https://www.crystallography.net/archives/2024/slides/NOBUGS-Talk/slides2-policy.pdf

The importance of crystallographic data

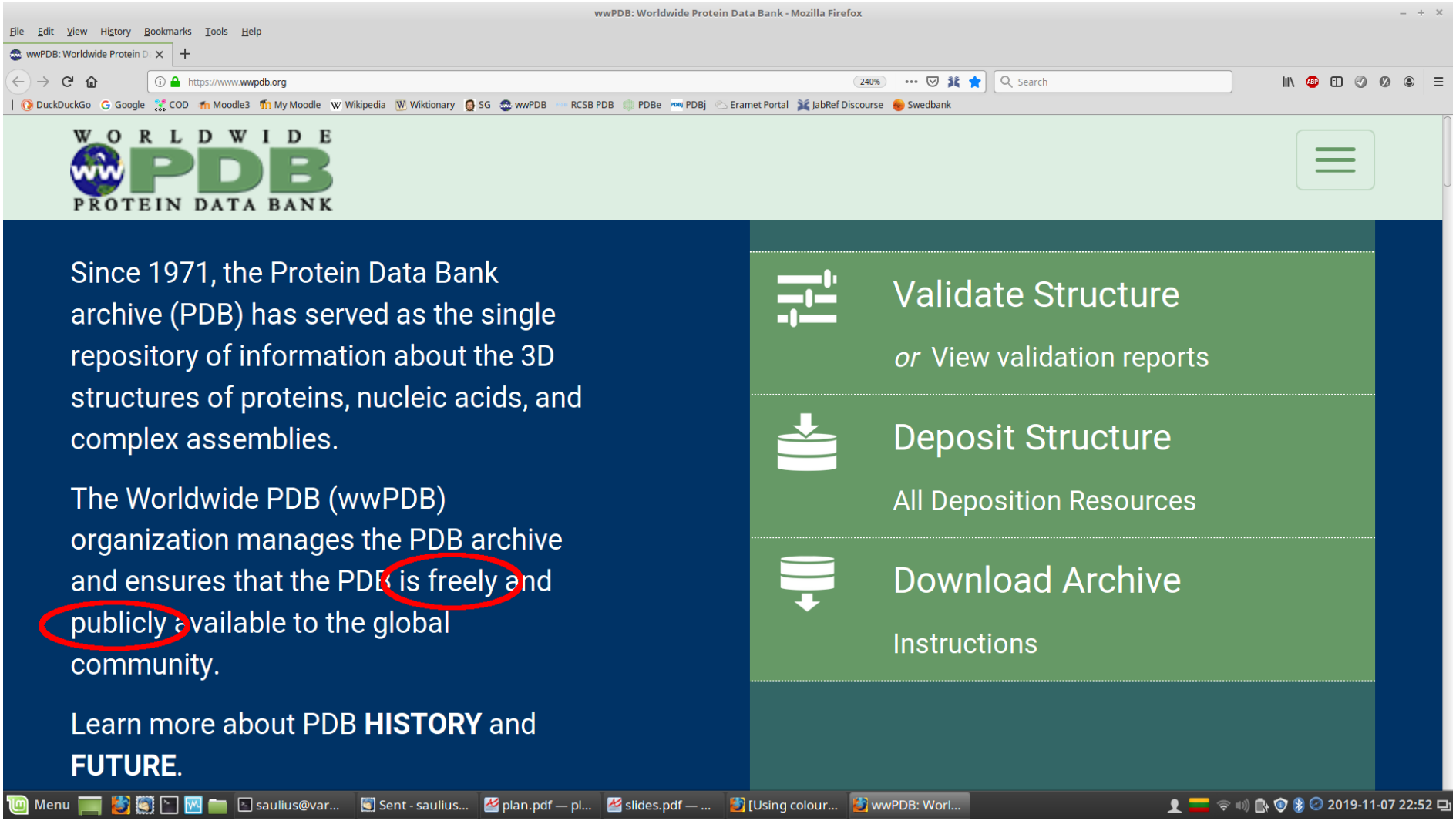
All observations *must* be compatible with crystallographic models.



Things to do with Open Data

Crystal structures
- Drug design
- Material property prediction
- Teaching
- Citizen science
- Machine learning models
- ...

PDB is just fine!



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://www.ccdc.cam.ac.uk/access-structures-terms/, last accessed 2024-09-20)
- “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)

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

The Crystallography Open Database (COD)

https://www.crystallography.net/cod

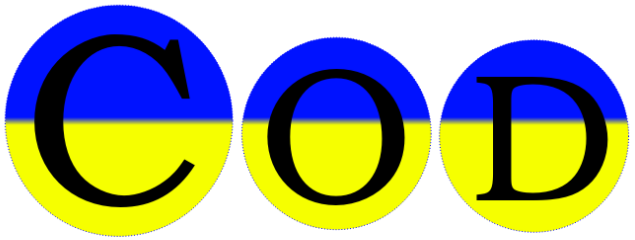
Crystallography Open Database

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
- License
- Privacy and GDPR
- Querying COD
- Citing COD
- COD Mirrors
- Advice 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 **509888** entries in the COD.
Latest deposited structure: 7159763 on **2024-01-11** at **01:32:14 UTC**

CIFs Donators

Advisory Board

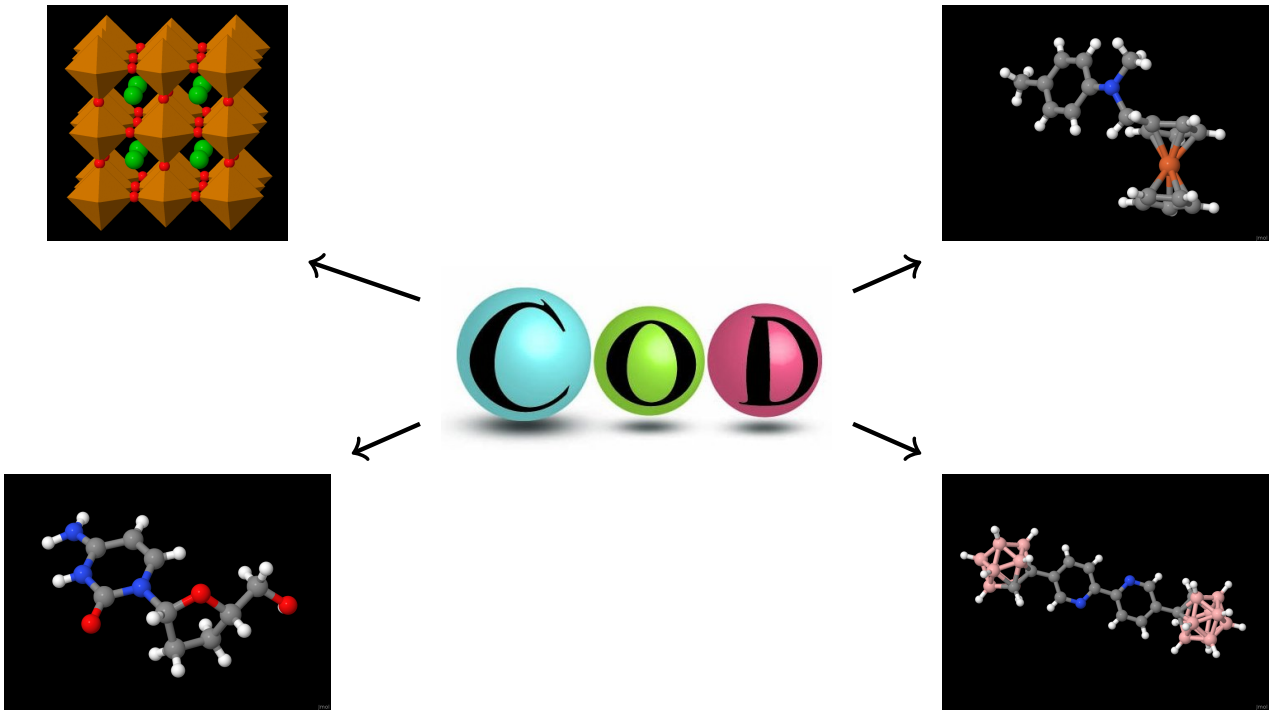
Daniel Chateigner, Xiaolong Chen, Marco Ciriotti,
Robert T. Downs, Saulius Gražulis, Werner Kaminsky, Armel Le Bail, Luca Lutterotti,
Yoshitaka Matsushita, Andrius Merkys, Peter Moeck, Peter Murray-Rust, Miguel Quirós Olozábal,
Hareesh Rajan, Antanas Vaitkus, Alexandre F.T. Yokochi

If you find bugs in the COD or have any feedback, please contact us at
cod-bugs@ibt.lt

Top of the page

COD contents

https://www.crystallography.net/cod



509 888 records as of 2024-01-11, available under **CC0 License**

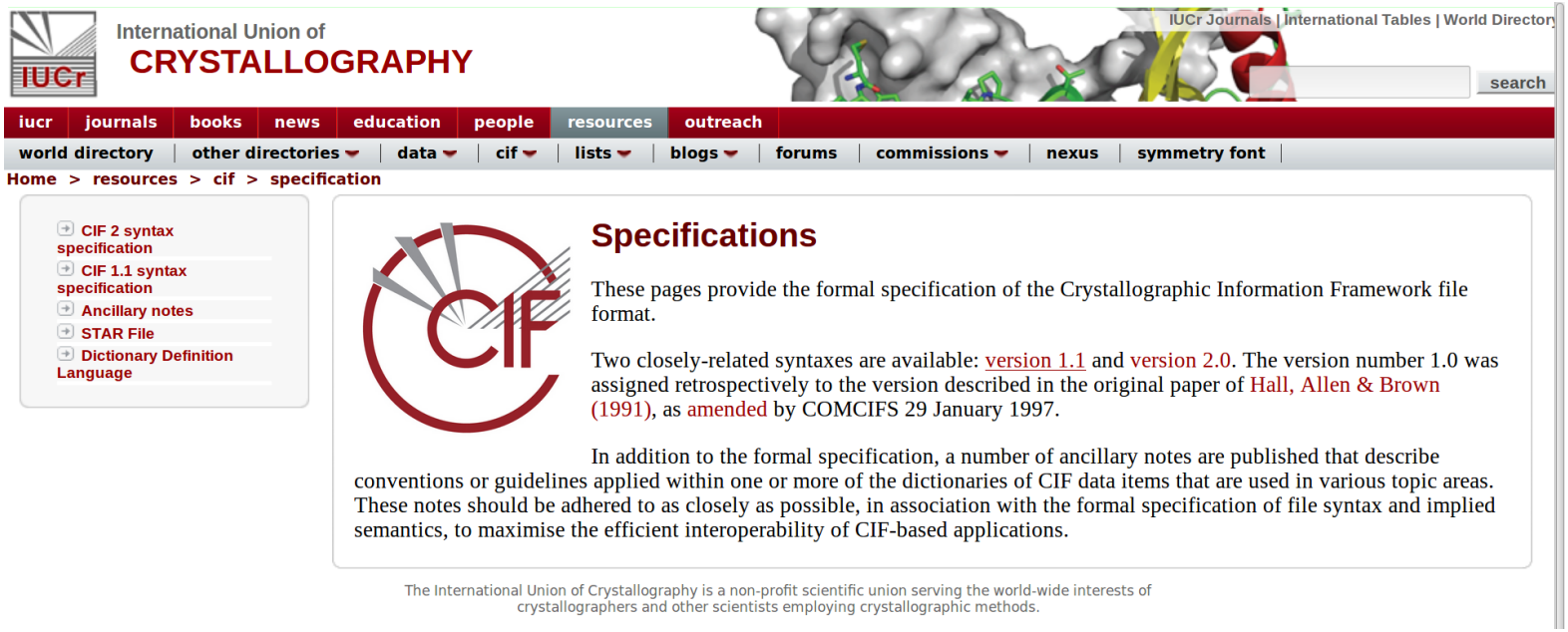
All data are presented in a standardised, machine-readable form (Gražulis et al. 2009; Gražulis et al. 2012).

COD data sources

- Peer-reviewed publications;
- Preprints, dissertations;
- Depositions by crystallographers (pers. comm., pre-publ.);
- Other databases; notably **AMCSD**, maintained by the group of Robert Downs (Downs et al. 2003; Rajan et al. 2006)

https://rruff.geo.arizona.edu/AMS/amcsd.php

CIF for the COD



(Hall et al. 1991; Bernstein et al. 2016)

The Crystallographic Interchange File/Framework (CIF):

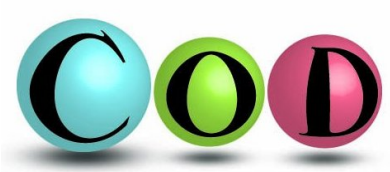
- Provides standard means for data publishing and exchange;
- Is suitable for archiving;
- Is maintained by the IUCr;

Accessing the COD

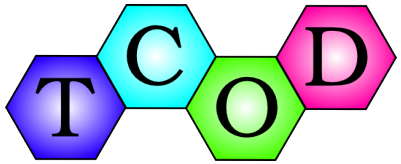
COD data can be accessed:

1. Via the Web page:
   https://www.crystallography.net/cod/7159763.html
2. Via the COD REST API:
   https://www.crystallography.net/cod/7159763.cif
   https://www.crystallography.net/cod/result?text=perovskite
3. Via the OPTIMADE API (Andersen et al. 2021):
   https://www.crystallography.net/cod/optimade/structures?filter=elements+HAS+"U"
4. Via SQL:
   ```
   mysql -u cod_reader -h sql.crystallography.net cod -e \
   'select file from data where formula = "- H2 O -"'
   ```
5. By downloading to your computer using Subversion, `rsync` or simple Web download:
   https://wiki.crystallography.net/howtoobtaincod

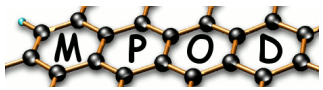
COD “sisters”



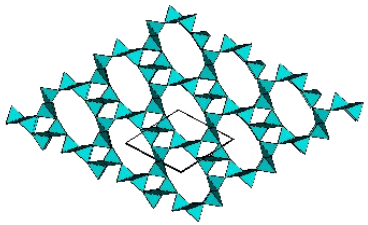
http://www.crystallography.net/cod
$>$ 500 000 entries



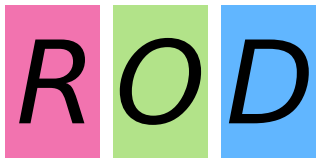
http://www.crystallography.net/tcod
$>$ 7400 entries (ready to grow to $>$ 10^7?)



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



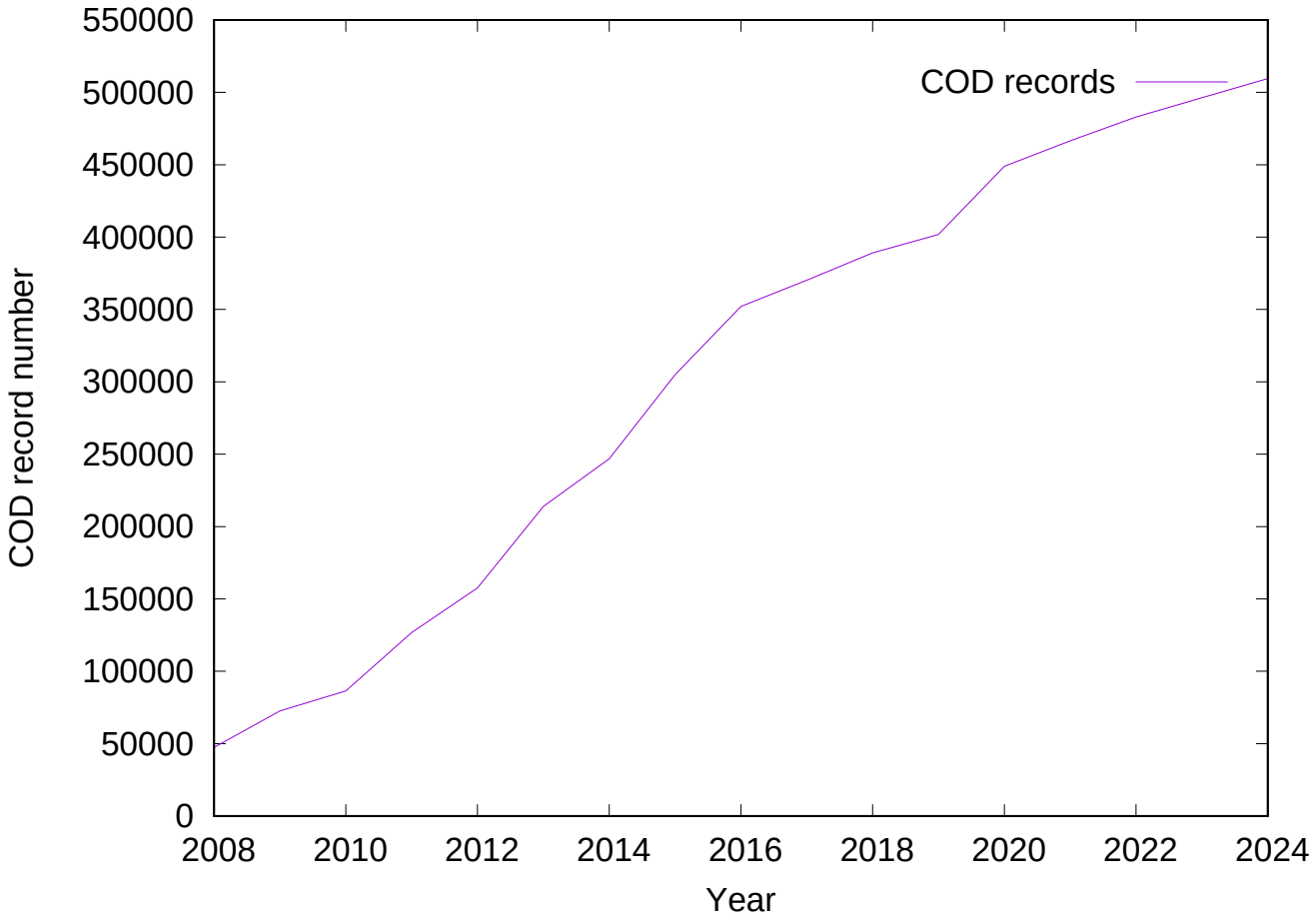
http://www.crystallography.net/pcod
$>$ 10^6 entries (ready to grow to $>$ 10^8?)



http://solsa.crystallography.net/rod/
$>$ 1100 entries

(Gražulis et al. 2009; Gražulis et al. 2012; Pepponi et al. 2012; Fuentes-Cobas et al. 2017; Mendili et al. 2019)

COD growth


COD records
COD record number
Year
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
2008
2010
2012
2014
2016
2018
2020
2022
2024

COD Data Curation

Data curation in the COD:

```
svn log -r283960 --diff svn://www.crystallography.net/cod/cif/9
```

```
--- 00/15/9001556.cif (revision 283959)
+++ 00/15/9001556.cif (revision 283960)
@@ -68,8 +68,24 @@
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
{+_atom_site_type_symbol+}
{+_atom_site_attached_hydrogens+}
Fe 0.25000 0.25000 0.25000 0.00490 {+Fe 0+}
O-H1 0.50000 0.17800 0.30800 0.00100 {+O 1+}
O-H2 0.19500 0.19000 0.50000 0.00100 {+O 1+}
O-H3 0.31800 0.50000 0.32300 0.00100 {+O 1+}
Wat 0.00000 0.50000 0.50000 0.00640 {+O 2+}
/.../
```

COD data curation

Inputs from COD users

Thomas Dortmann (2013), PANalytical, "`COD-minerals.xlsx`":

> *The entries that now have the mineral name are minerals, the rest are not.*

$> 3\,500$ unique mineral names assigned 104 "atypical" names[1].

Update (2024):

$> 4\,257$ unique mineral names, 566 "atypical" names

[1] Not matching the RE `/^[A-Z][-a-zA-Z ()]+$/`

COD versioning

Essential for reproducibility

All COD changes are tracked in a Subversion repository.

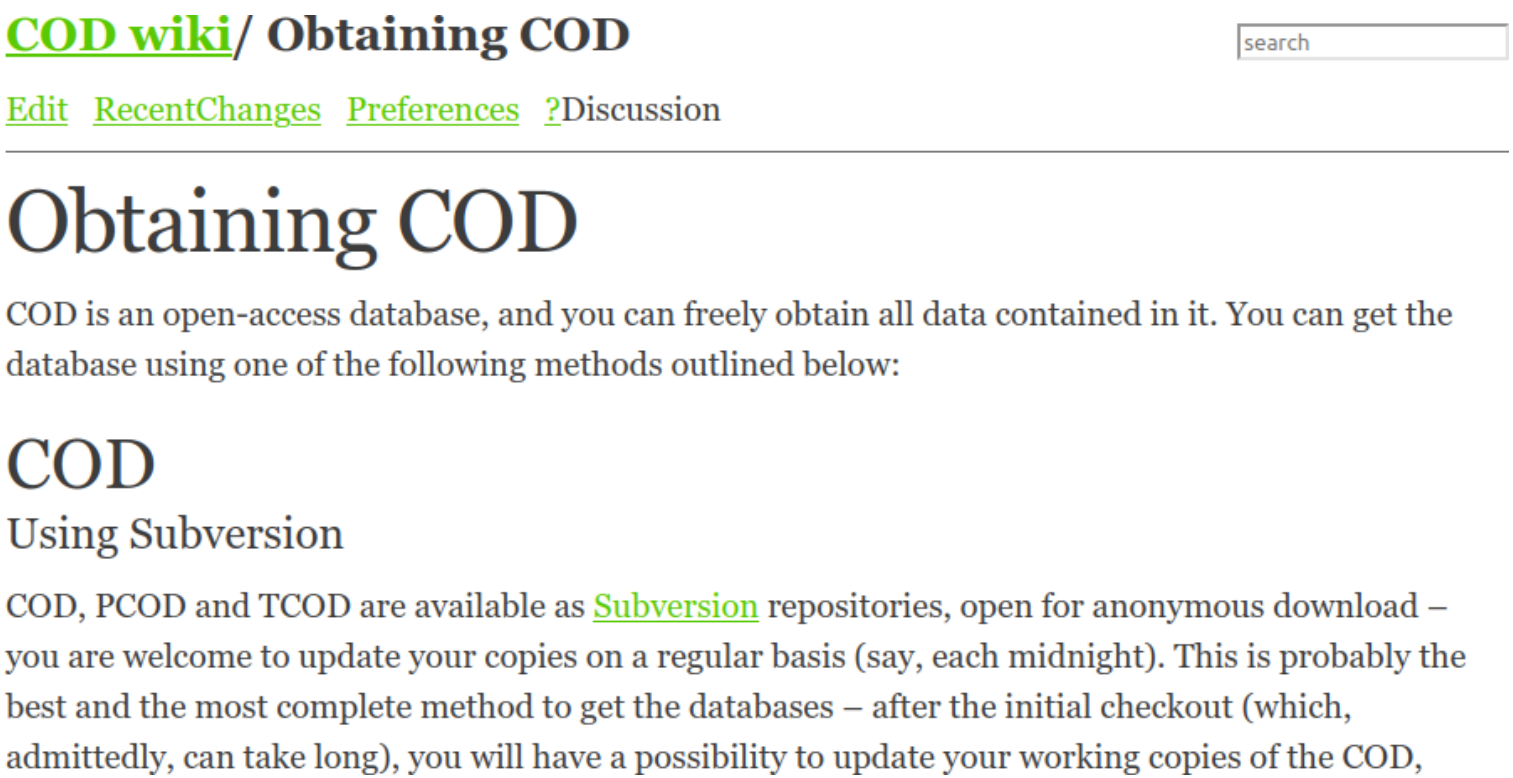
▾ Version history

Revision	Date	Message	Files
277834 (current)	2022-09-14	cif/ Added space group information derived from the space group operation list using the 'cif_filter' program.	2000000.cif
199748	2017-08-14	cif/2/00/00/ (antanas@echidna.ibt.lt) Removing 43 symmetrically equivalent atoms in entry 2000000.	2000000.cif

- The latest revision has a stable URI:
  https://www.crystallography.net/cod/2000000.cif
- A URI with a specific revision allows to reconstruct the *specific byte stream*:
  https://www.crystallography.net/cod/2000000.cif@199748

COD Data Checkout

https://wiki.crystallography.net/howtoobtaincod/



COD wiki/ Obtaining COD

search

Edit RecentChanges Preferences ?Discussion

Obtaining COD

COD is an open-access database, and you can freely obtain all data contained in it. You can get the database using one of the following methods outlined below:

COD

Using Subversion

COD, PCOD and TCOD are available as Subversion repositories, open for anonymous download – you are welcome to update your copies on a regular basis (say, each midnight). This is probably the best and the most complete method to get the databases – after the initial checkout (which, admittedly, can take long), you will have a possibility to update your working copies of the COD,

Partial COD checkout

Saves your disk space and time :)

Recommended: partial checkout of the COD SVN working copy:

```
$ svn co --depth empty svn://crystallography.net/cod
$ cd cod
$ svn up --set-depth infinity cif/
$ svn up --set-depth infinity hkl/
$ svn up --set-depth infinity smi/

$ svn up --set-depth exclude hkl/
```

COD validation and deposition Web site

https://www.crystallography.net/cod/deposit
https://www.crystallography.net/cod/initiate_deposition.php

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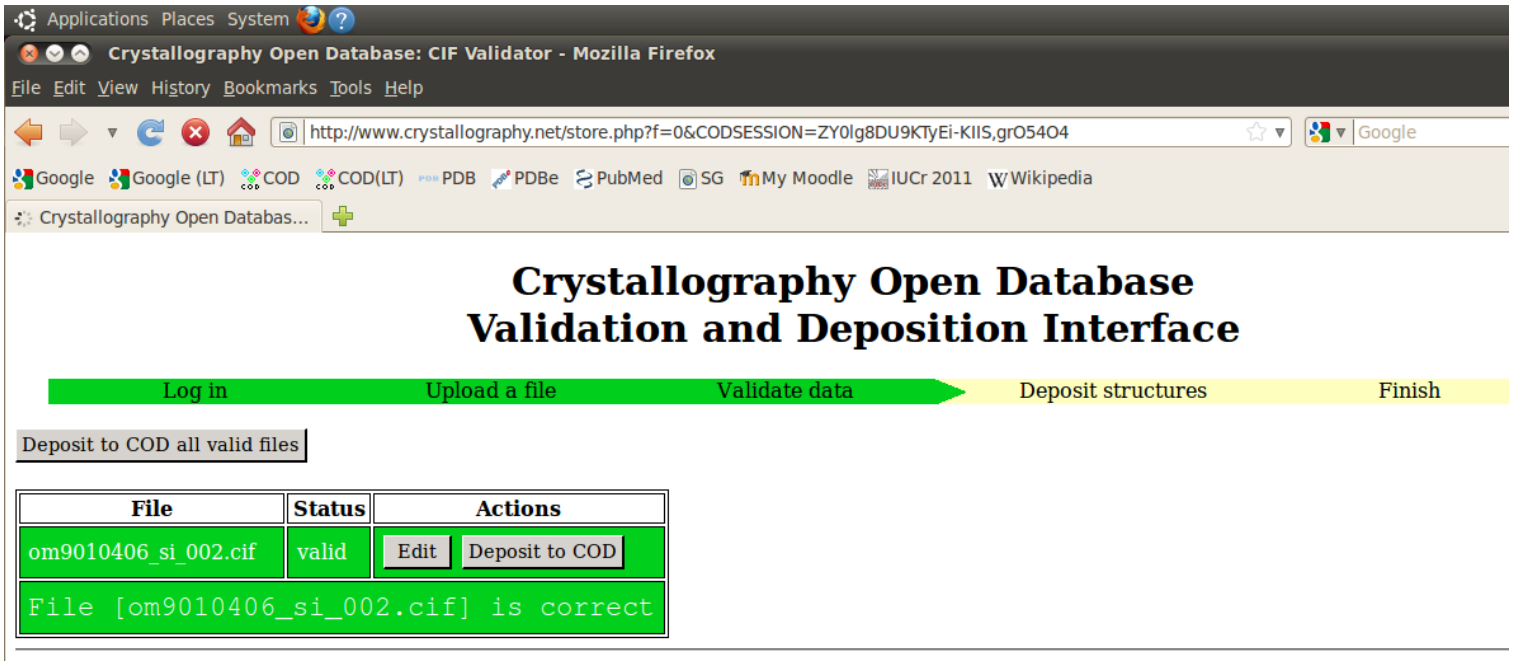


COD data validation

COD data validation policies:

1. Syntactic checks:
   ```
   $ cifparse 7234818.cif
   ```
2. Semantic validation (against dictionaries)
   ```
   $ cif_validate -D cif_core.dic 7234818.cif
   ```
3. Database-specific checks
   ```
   $ cif_cod_check 7234818.cif
   ```

Commands from the `cod-tools` package:
svn://cod.ibt.lt/cod-tools
https://github.com/cod-developers/cod-tools

COD entry checks – IUCr criteria checks

- Checks on prepublications and Personal communications;
- Checks on published structures;
- *Statistics of structures in the database*

IUCr data validation criteria (Version: 2000.06.09,
ftp://ftp.iucr.ac.uk/pub/dvntests or
ftp://ftp.iucr.org/pub/dvntests)

COD entry checks – IUCr criteria checks

- Checks on prepublications and Personal communications;
- Checks on published structures;
- *Statistics of structures in the database*

IUCr data validation criteria (Version: 2000.06.09, ftp://ftp.iucr.ac.uk/pub/dvntests or ftp://ftp.iucr.org/pub/dvntests)

```
cif_cod_check 3000424.cif
```

```
/usr/bin/cif_cod_check: 3000424.cif data_3000424: NOTE, data item
    '_refine_ls_R_factor_gt' value '0.1120' is > 0.1.
/usr/bin/cif_cod_check: 3000424.cif data_3000424: NOTE, data item
    '_refine_ls_wR_factor_ref' value '0.3195' is > 0.25.
/usr/bin/cif_cod_check: 3000424.cif: NOTE, 2 NOTE(s) encountered.
```

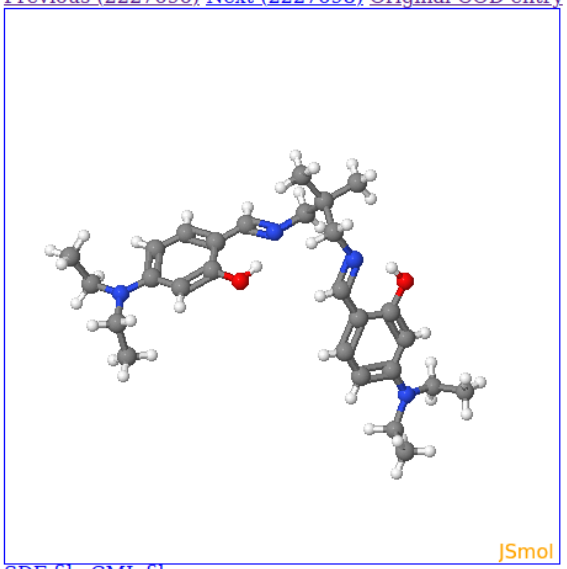
COD deposition types

1. Published structure
   - Must have full bibliography or at least DOI;
   - Assumed to be peer-reviewed, no IUCr checks enforced;
2. Pre-publication
   - Can be on-hold until publication (default 6 months, extendable);
   - IUCr checks performed and enforced;
3. Personal communication
   - Becomes public immediately;
   - IUCr checks performed and enforced;

COD chemical repertoire

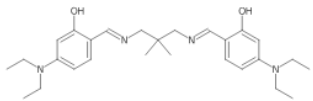
http://molecules.crystallography.net/

Previous (2227696) Next (2227698) Original COD entry



SDF file CML file

Reduced structural formula



Reduced canonical SMILES:

CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC **(x1)** PubChem

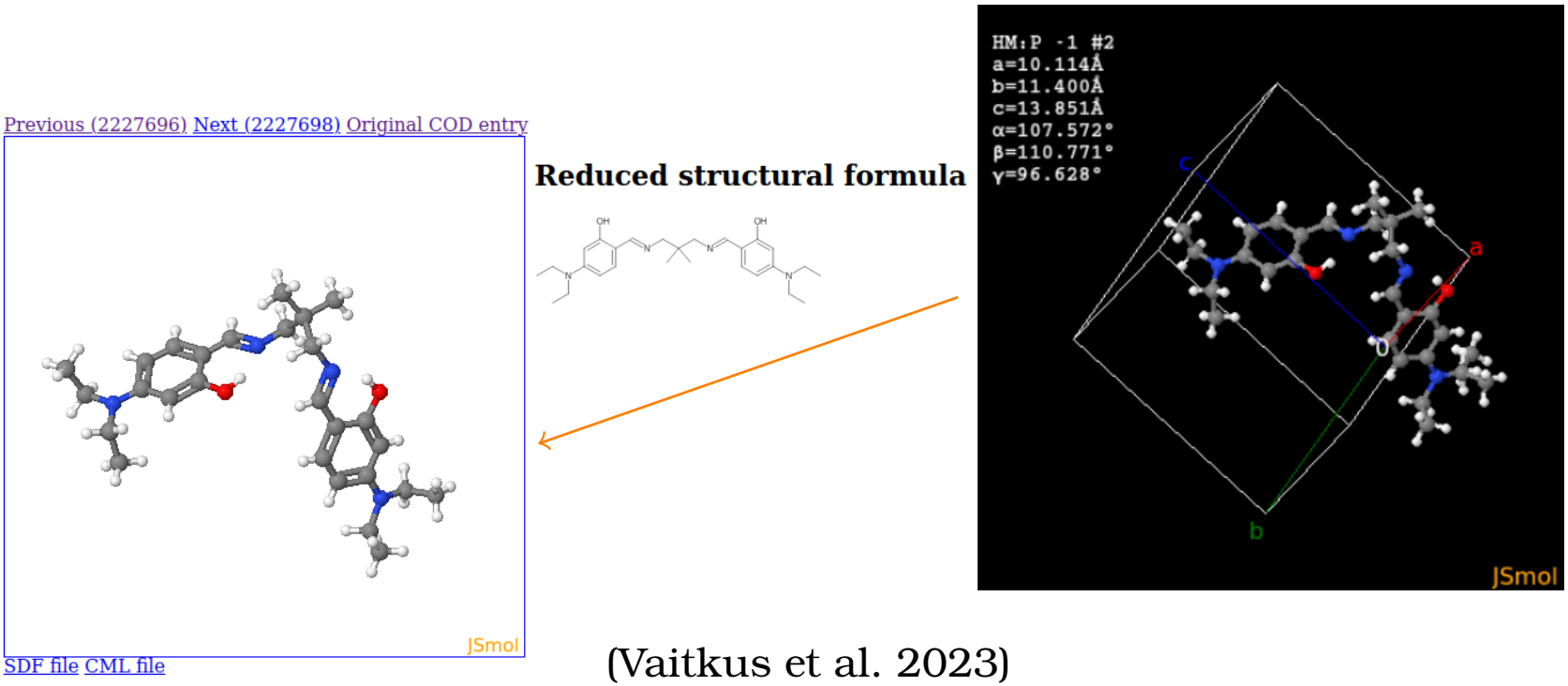
Unique components

SMILES	InChI
CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC	InChI=1S/C27H40N4O2/c1-7-30(8-2)23-13-11-21(25(32)15-23)17-28-19-27(5,6)2 /h11-18,32-33H,7-10,19-20H2,1-6H3/b28-17+,29-18+

See also poster by Merkys et al. (https://bit.ly/3BKZ5vG)

COD chemical repertoire

http://molecules.crystallography.net/



(Vaitkus et al. 2023)

Reduced canonical SMILES:

CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC **(x1)** PubChem

Unique components

SMILES	InChI
CCN(c1ccc(c(c1)O)/C=N/CC(C/N=C/c1ccc(cc1O)N(CC)CC)(C)C)CC	InChI=1S/C27H40N4O2/c1-7-30(8-2)23-13-11-21(25(32)15-23)17-28-19-27(5,6)2(/h11-18,32-33H,7-10,19-20H2,1-6H3/b28-17+,29-18+

See also poster by Merkys et al. (https://bit.ly/3BKZ5vG)

COD chemical repertoire

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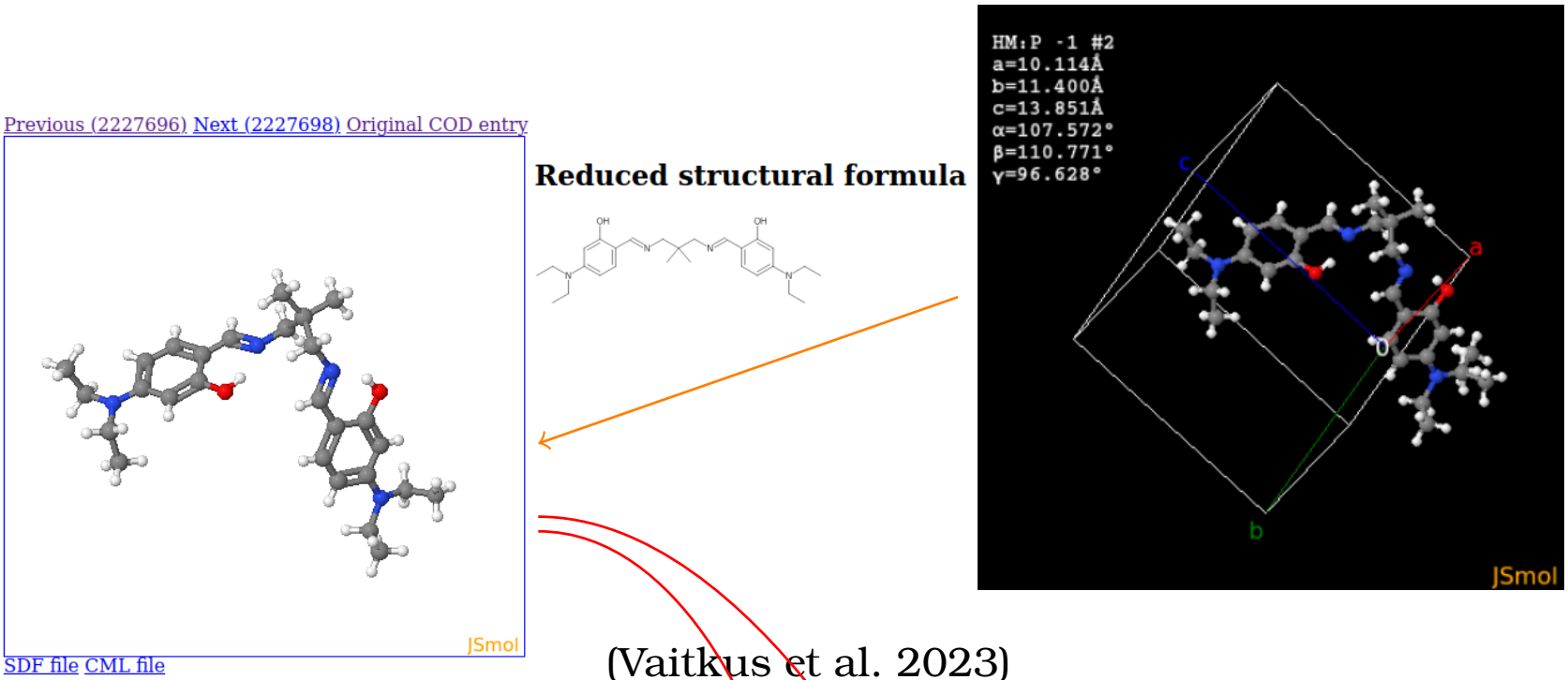


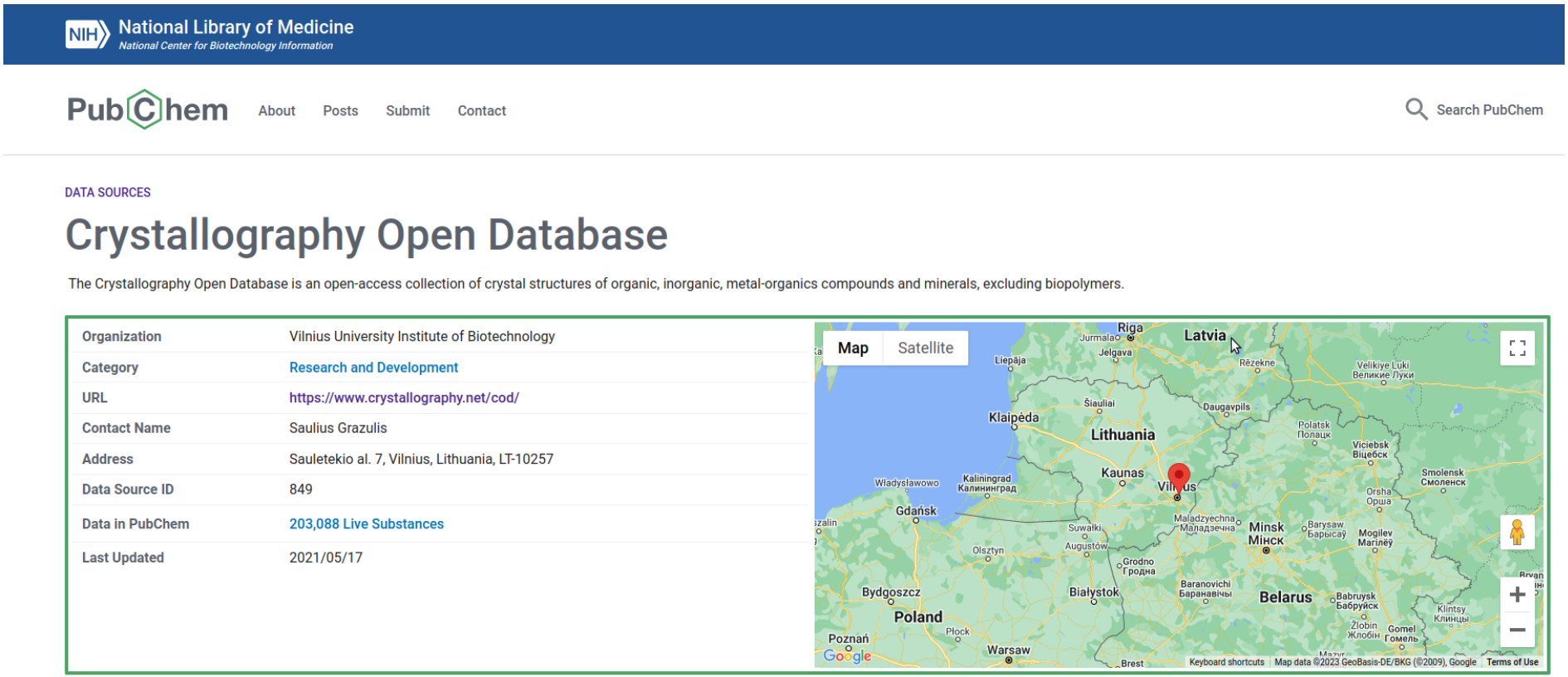
(Vaitkus et al. 2023)

See also poster by Merkys et al. (https://bit.ly/3BKZ5vG)

COD use cases

COD and PubChem

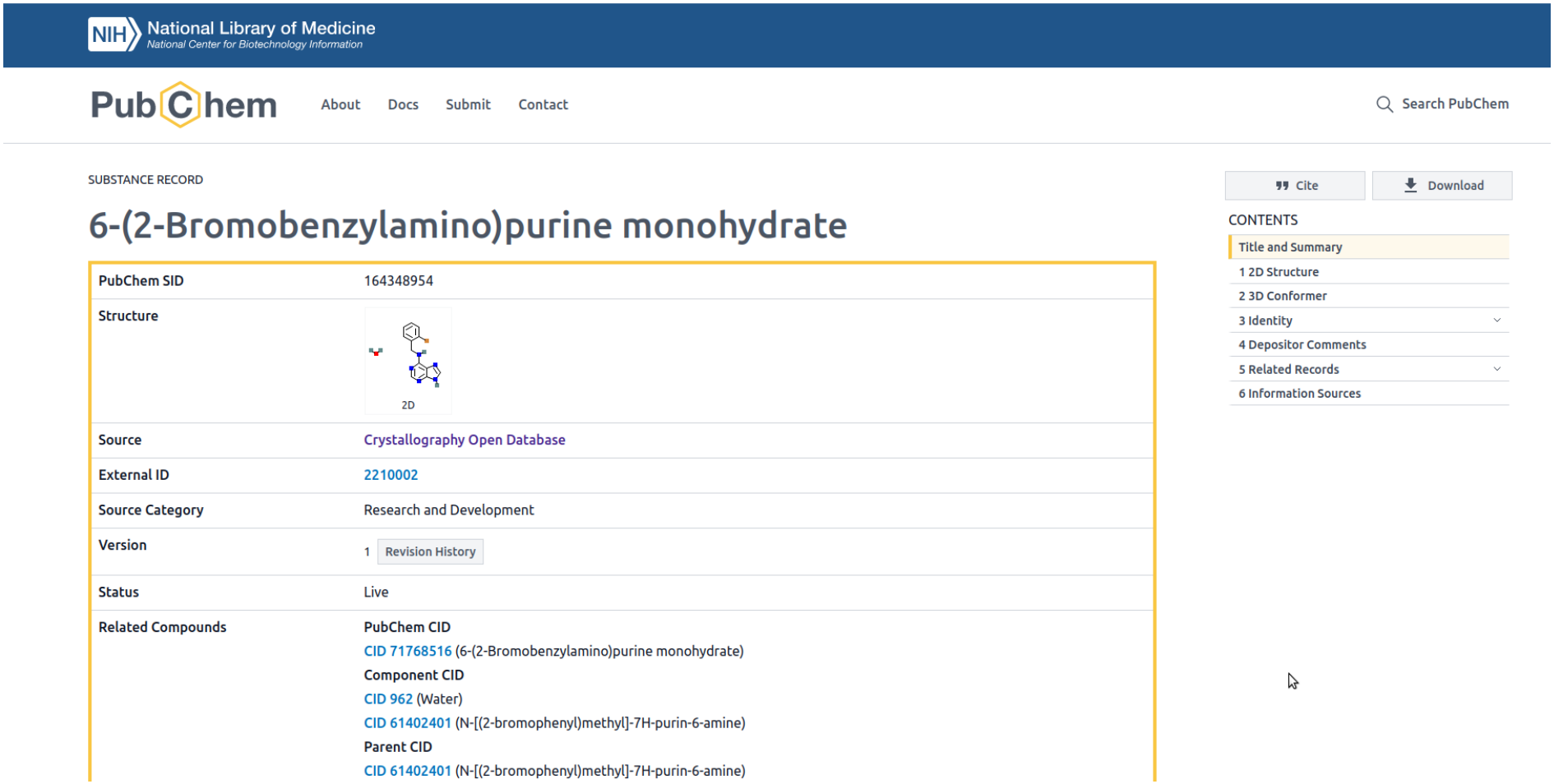
https://pubchem.ncbi.nlm.nih.gov/source/849



COD use cases

COD and PubChem

https://pubchem.ncbi.nlm.nih.gov/substance/164348954

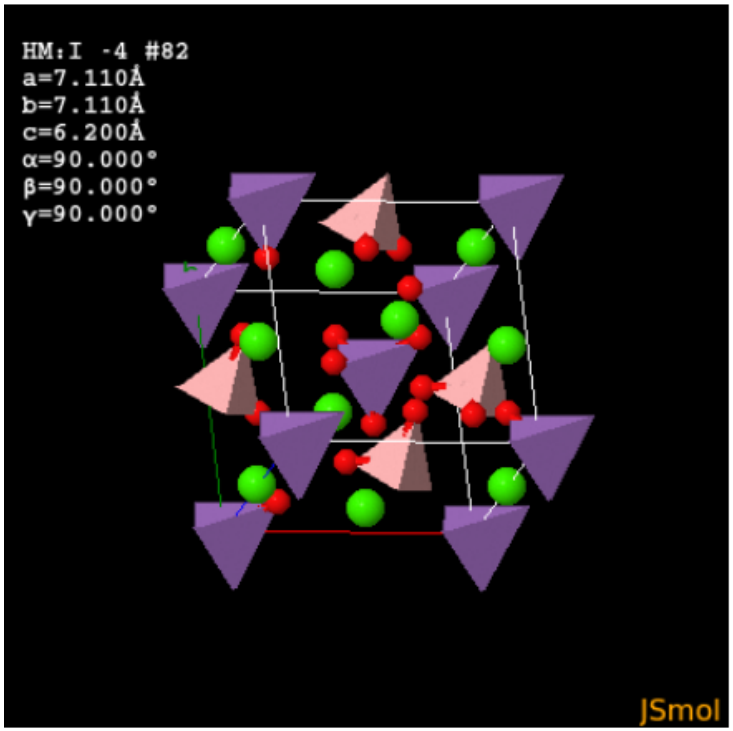


Data cross-referencing

External links

Links to external databases are implemented and populated:

- Implemented: AMCSD, Wikidata, Wikipedia, MPOD, ChemSpider;
- Planned: PubChem, **raw diffraction data**;



Coordinates 9016740.cif
External links AMCSD; Wikidata; Wikipedia

Interlinked data in COD

Crystallography Open Database

COD Home
Home
What's new?

Accessing COD Data
Browse
Search
Search by structural formula

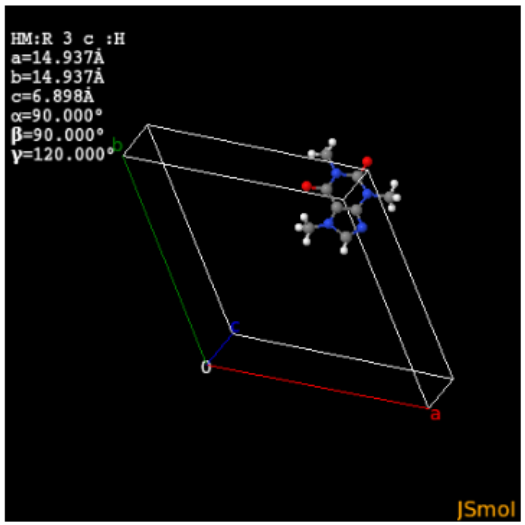
Add Your Data
Deposit your data
Manage depositions
Manage/release prepublications

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

Group theory in Ada/SPARK

examples/group_theory.ads

```
pragma Spark_Mode (On);

generic
   type Element is private;
   Identity : Element;
   with function "*" (E, F: Element) return Element is <>;
```

```
   function Is_Closed_On_Multiplication (G : Group) return Boolean
   is (for all E of G =>
         (for all F of G => (Belongs_To (E*F, G))))
     with Ghost;

   function All_Elements_Have_Inverses (G : Group) return Boolean
   is (for all E of G => Has_Inverse (E, G))
     with Ghost;

   function Is_Group (G : Group) return Boolean
   is (Has_Identity (G) and then
         All_Elements_Have_Inverses (G) and then
         Is_Closed_On_Multiplication (G)
      )
     with Ghost;
```

(Petrauskas et al. 2022)

Automatic compilation of proven code

Ada and SPARK

examples/make_group.ads

```
8     type Ring_Element is mod 37;
```

```
29    function Build_Group (E : Ring_Element) return Group
30      with
31      Post => Is_Group (Build_Group'Result);
```

gnatprove -P main.gpr --report=all make_group.adb

```
make_group.ads:23:14: info: postcondition proved
make_group.ads:27:14: info: postcondition proved
make_group.ads:31:14: info: postcondition proved
group_theory.ads:16:15: info: postcondition proved, in instantiation at make_group.ads:16
```

```
saulius@tasmanijos-velnias spacegroups/ $ ./run_make_group 8
(1, 8, 27, 31, 26, 23, 36, 29, 10, 6, 11, 14)

saulius@tasmanijos-velnias spacegroups/ $ ./run_make_group 7
(1, 7, 12, 10, 33, 9, 26, 34, 16)
```

Why Ada/SPARK?

1. Durable design – first designed in 1983!
2. Modern language – latest standard is Ada 2022;
3. Mostly backwards compatible;
4. Good F/LOSS compiler available – GNAT;
5. Ada is statically very strictly typed;
6. Programs are easy to read (Level (Ada) > Level (C));
7. Ada & SPARK have a rich type system;
8. Language level concurrent programming;
9. Produces fast optimised native code, links with any language;
10. Not controlled by any private company;

(Amiard et al. 2022)

Why is Ada not popular (yet)?

1. The language is complex and difficult to implement;
2. No good compilers in the 1990's;
3. Procured by the DOD, used for "war fighting software";
4. Poor academic outreach in the 20th century;

(National Research Council 1997)

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A code example

From https://github.com/sauliusg/decode-Hall-symbol: `examples/decode_hall.adb`

```
Build_Group (Symmetry_Operators, N_Symmetry_Operators);

-- Add centering and inversion matrices:

declare
   M : Positive := N_Symmetry_Operators;
   New_Symmetry_Operator : Symmetry_Operator;
begin
   for I in 1..N_Inversions loop
      for C in 1..N_Centering loop
         if I /= 1 or else C /= 1 then
            for S in 1..N_Symmetry_Operators loop
               New_Symmetry_Operator :=
                 Symmetry_Operators (S) * Centering (C) * Inversions (I);
               if not Has_Symmetry_Operator (Symmetry_Operators, M,
                                             New_Symmetry_Operator) then
                  M := M + 1;
                  Symmetry_Operators (M) := New_Symmetry_Operator;
               end if;
            end loop;
         end if;
      end loop;
   end loop;
   N_Symmetry_Operators := M;
end;
```

Compile and use it!

From https://github.com/sauliusg/decode-Hall-symbol:

```
$ decode_hall '-P 2ab'
```

```
saulius@starta slides/ $ decode_hall '-P 2ab'
X,Y,Z
-X+1/2,-Y+1/2,Z
-X,-Y,-Z
X+1/2,Y+1/2,-Z
```

Where to go further?

- Collect more structures;
- Find all papers with crystal structures;
- Write reliable, readable software;
- Apply machine learning;
- Expand the community – **your contributions are invaluable!**

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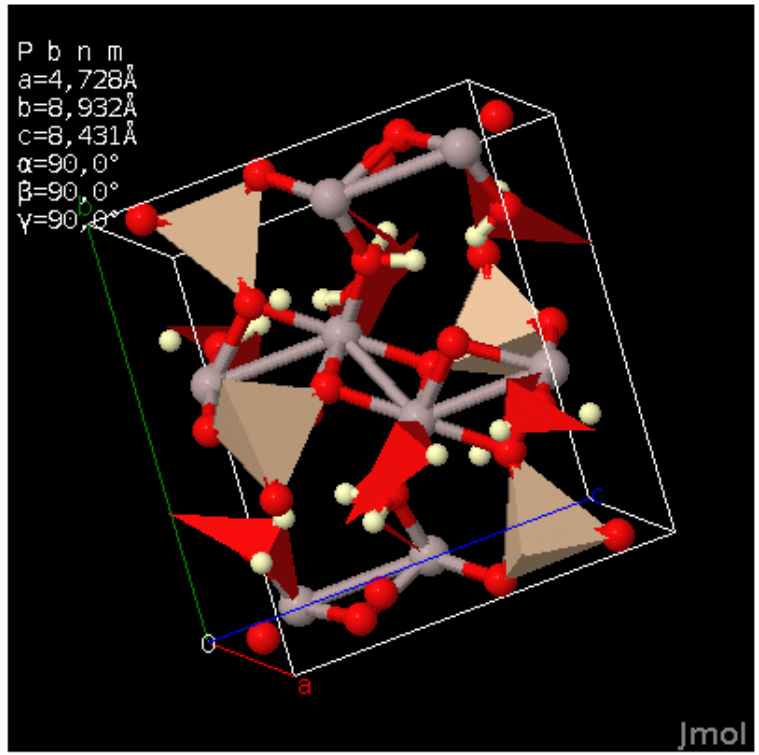
Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

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

http://www.crystallography.net/2207377.html

https://www.crystallography.net/archives/2024/slides/NOBUGS-Talk/slides2-policy.pdf

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