Using COD and TCOD, searching and getting data

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USNC/Cr Database Workshop 2022

Family of open-access structural databases

Database	Records	License	URL	Est.
COD	490 000	public domain	https://www.crystallography.net/cod/	2003
PCOD	1 000 000	public domain	https://www.crystallography.net/pcod/	2003
MPOD	300	public domain	http://mpod.cimav.edu.mx/	2010
TCOD	2 600	public domain	https://www.crystallography.net/tcod/	2013
ROD	1 100	public domain	https://solsa.crystallography.net/rod/	2017

COD entry

- Describes a single crystal structure
- Has provenance record
- May be accompanied by diffraction data
- Is assigned permanent 7-digit identifier

Deposition types in the COD

- Published material:
  - harvested journal supplements
  - donated collections
  - individual depositors
- Prepublication material
- Personal communications

Entry information card

Contents:

- 3D structure preview
- links to download files
- links to other databases
- bibliographic data
- cell parameters
- contents (name, formula, SMILES)
- space group information
- experiment details
- version history

Example:

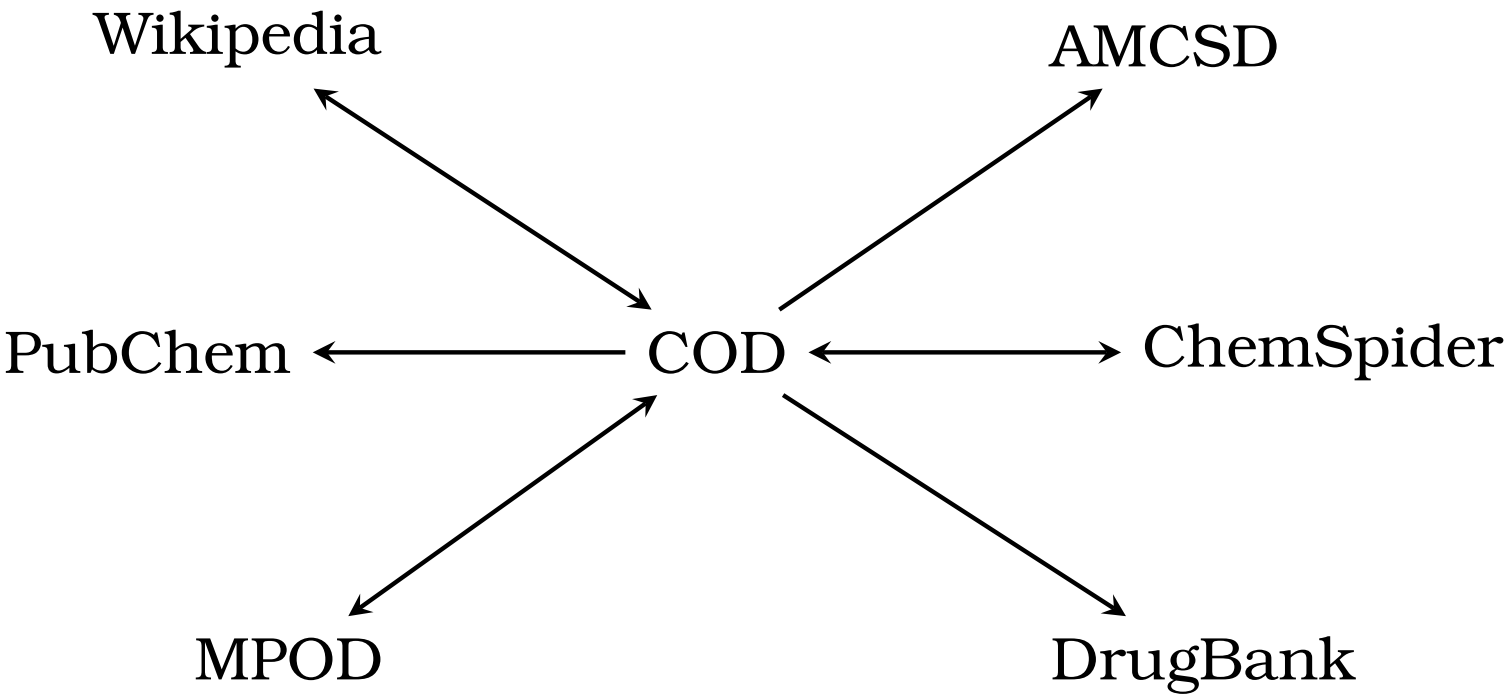
`https://www.crystallography.net/cod/4308000.html`

Crystallographic Information File/Framework (CIF)

COD and TCOD uses CIF v1.1

- ASCII-based human-readable text
- Data storage:
  - key-value pairs
  - tables
- 3D viewers:
  - Avogadro
  - Jmol
- I/O software libraries:
  - codcif, CIF API (C)
  - ciftools-java (Java)
  - PyCifRW, pycodcif (Python)

Links with other databases



Data versioning

Changes:

- are recorded
- get stable sequential identifiers
- are accompanied by log messages
- can be viewed

Curation

Curation

- Deposition time fixes
- (Semi-)automated fixes
- Manual curation

Deposition time fixes

- Fix CIF syntax errors
- Reformat or estimate space group
- Reformat summary chemical formula
- Calculate cell volume
- Exclude unknown or placeholder CIF data items
- Convert temperature values
- Perform various other fixes

Unusual entries

COD entries regarded unusual:

- duplicate entries (≈ 4500, e.g., 1000018)
- theoretical structures (≈ 600, e.g., 2100167)
- entries without coordinates (≈ 240, e.g., 1000195)
- retracted structures (≈ 150, e.g., 2015946)

Validation database

- Uses CIF dictionaries to check data conformity
- Updated periodically
- Provides insight into most frequent issues

Table of validation issues:

`https://sql.crystallography.net/db/cod_validation/validation_issue`

Vaitkus et al., 2021

Querying COD

Search methods:

- bibliography
- cell parameters
- cell contents
- substructure by SMILES
- substructure by drawn fragment

Response formats:

- human-readable HTML
- database ID list
- CIF URL list
- CSV
- archive of matching files

Download the whole COD. Quarterly releases

Links

- Link for the most recent release:

  `https://www.crystallography.net/cod/archives/cod-cifs-mysql.tgz`

- Older releases:

  `https://www.crystallography.net/cod/archives/<YEAR>/data/`

Contents

- coordinate files
- SQL table data

Sizes of 2021-10-16 release

- TAR GZ – 17 GB
- TAR XZ – 12 GB
- ZIP – 18 GB

Individual entry access

Whole file tree for browsing:

`https://www.crystallography.net/cod/cif`

Download individual entry

- coordinate file

  `https://www.crystallography.net/cod/<ID>.cif`
- diffraction data

  `https://www.crystallography.net/cod/<ID>.hkl`
- coordinate file at specified revision

  `https://www.crystallography.net/cod/<ID>.cif@<revision>`

Download the whole COD. *Rsync*

Rsync access

```
$ mkdir cif hkl
$ rsync -aq --delete rsync://www.crystallography.net/cif/ cif/
$ rsync -aq --delete rsync://www.crystallography.net/hkl/ hkl/
```

(for verbose mode, replace `-q` with `-v`)

Advantages:

- Subsequent `rsync` executions will fetch updates
- Network traffic is kept minimal

Access with *Subversion*

Checkout (downloads uncompressed COD CIF collection)

```
$ export LC_TIME=en_US.UTF-8 # Fix locale
$ svn checkout svn://www.crystallography.net/cod/cif
```

Fetch updates

```
$ svn up cif/
```

Go back to specific revision (here 1234)

```
$ svn up cif/ -r1234
```

Examining changes with *Subversion*

Get contents of CIF file in revision 12345

```
$ svn cat svn://www.crystallography.net/cod/cif/1/00/00/1000000.cif -
    r12345
```

Get change of CIF file in revision 91932

```
$ svn diff svn://www.crystallography.net/cod/cif/1/00/00/1000000.cif -
    c91932
Index: 1000000.cif
===================================================================
--- 1000000.cif (revision 91931)
+++ 1000000.cif (revision 91932)
@@ -348,3 +348,4 @@
 N2 H2C O6 1_655 .89 1.88 2.750(5) 164.8
 N2 H2D O4 2_645 .89 2.05 2.869(5) 153.3
 N2 H2E O7 1_655 .89 1.98 2.861(6) 170.9
+_journal_paper_doi 10.1107/S0108270100008532
```

RESTful API for querying the COD

Documentation:

`https://wiki.crystallography.net/RESTful_API/`

Fetch entries describing cucurbiturils from year 2017, in CSV format

```
$ curl https://www.crystallography.net/cod/result -F text=cucurbituril
    -F format=csv -F year=2017
```

SQL access

Connection details:

- Server: `sql.crystallography.net`
- Database: `cod`
- User: `cod_reader`

Explanation of fields in `data` table:

`https://wiki.crystallography.net/cod_mysql_schema/`

SQL access (*cont.*)

Find five most voluminous MOFs

```
$ mysql -h sql.crystallography.net cod -u cod_reader -e "select file,
    commonname, vol from data where commonname like \"%MOF%\" order by
    vol desc limit 5"
+---------+-------------+--------+
| file    | commonname  | vol    |
+---------+-------------+--------+
| 4120255 | bio-MOF-102 | 425902 |
| 4120254 | bio-MOF-101 | 238778 |
| 4109100 | MOF-HTB'    | 148818 |
| 4111295 | mesoMOF-1   | 122163 |
| 4109099 | MOF-HTB     | 110988 |
+---------+-------------+--------+
```

OPTIMADE interface

Select ternary structures having C, Si, Ge or Sn, but not having Pb

```
$ curl -L https://www.crystallography.net/cod/optimade/structures -F '
    filter=elements HAS ANY "C", "Si", "Ge", "Sn" AND NOT elements HAS
    "Pb" AND elements LENGTH 3'
```

Andersen et al., 2021

Theoretical Crystallography Open Database (TCOD)

- Has 8-digit identifiers
- Contains computational details
- Embeds files used in computations

Merkys et al., 2017

Acknowledgments

COD Advisory Board

Saulius Gražulis
Andrius Merkys
Daniel Chateigner
Robert T. Downs
Werner Kaminsky
Armel Le Bail
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