Raw data and external links in the Crystallography Open Database

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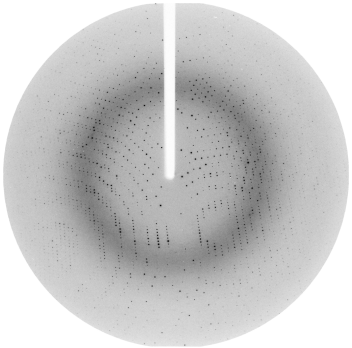
https://www.crystallography.net/cod/archives/2025/slides/2025-Poznan-ECM35/slides.pdf

Id: slides.tex 3115 2025-08-29 05:16:21Z saulius August 29, 2025

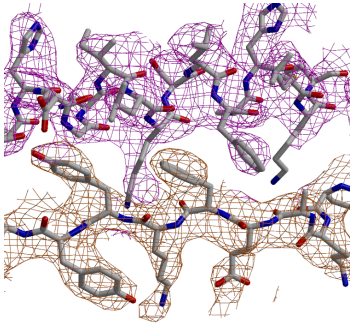
The crystallographic workflow

Data reduction steps

Detector signal → Iobs (Fobs) data → Atomic coordinates



⇒



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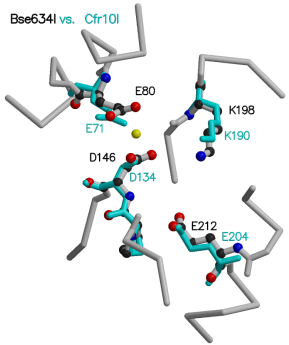


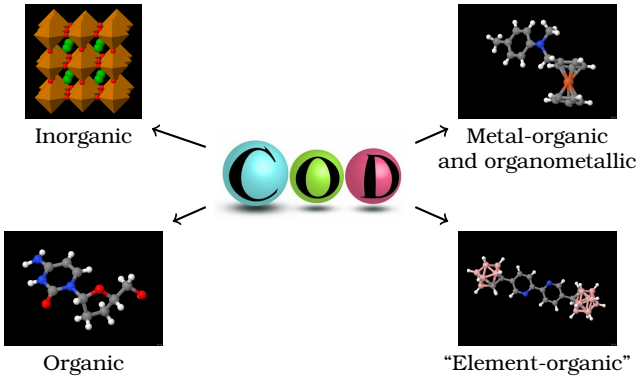
Most crystallographic databases store the last two. Today, we start linking with the first one.

What is the Crystallography Open Database (COD)

A brief intro

(Gražulis, Chateigner, et al. 2009; Gražulis, Daškevič, et al. 2012)

https://www.crystallography.net

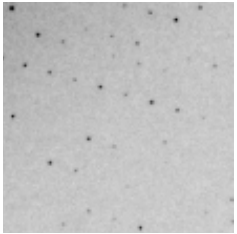


As of 2025-08-22:

527276 entries

Value of raw data

Verification, improvement, unintended reuse



- Verify and validate the findings;
- Ensure reproducible computations;
- Reuse raw data for (unintended) purposes (multiple lattices, sattelite reflections, non-Bragg scattering, machine studies, reflection shape...);
- Improve structures with better software/methdods;
- Teaching :)

Challenges with the raw data

Size, formats, net traffic

- Volume of raw data (orders of magnitude larger than even F_{obs})
- Many different data formats, some proprietary;
  - Good news: IUCr CBF
  - Good news: NeXUS & the Gold Standard (Bernstein et al. 2020)!
- Long transfer times;
- Political reasons...

Storages of XRD data

World wide repositories

- ProteinDiffraction;
- SBGrid;
- XRDa;
- Zenodo (?!) (e.g. https://zenodo.org/records/15992324, https://zenodo.org/records/12794355)
- National and institutional archives (?!)

The COD SQL data schema + COD CIF dictionary;

data

Field	Type	Key
file	int(7) unsigned	PRI
a	double unsigned	MUL
siga	float unsigned	
b	double unsigned	MUL
sigb	float unsigned	
c	double unsigned	MUL
sigc	float unsigned	
...	...	...

XRDa_x_COD

Field	Type	Key
id	int(11)	PRI
cod_id	int(7) unsigned	MUL
ext_id	int(11)	MUL
relation_id	int(11)	MUL

relations

Field	Type	Key
id	int(11)	PRI
name	varchar(255)	
description	text	

Similar schemas: Star schema:
(Apeh 2024)

Example of the COD data record raw data link

XRDa as an example

https://www.crystallography.net/cod/3000497.html

COD Home
Home
What's new?

Accessing COD Data
Browse
Search
Search by structural formula

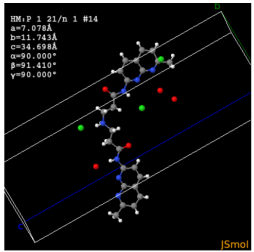
Add Your Data
Deposit your data
Manage depositions
Manage/release prepublications

Documentation
COD Wiki
Obtaining COD
License
Privacy and GDPR
Querying COD
Citing COD
COD Mirrors
Advice to donators
Useful links

Information card for entry 3000497

3000496 << **3000497** >> 3000498

Preview



Coordinates	3000497.cif
Original paper (DOI)	HTML
External links	XRDa

▾ Structure parameters

Formula	C24 H26 Cl3 N7 O5
Calculated formula	C24 H26 Cl3 N7 O5
Authors of publication	Kawamoto, Akihiro; Kojima Chojiro; Kurisu, Genji; Nakane, Takanori; Nakatani Kazuhiko; Sakurabayashi Shuhei
Journal of publication	Journal of the American Chemical Society
Year of publication	2025
a	7.078 Å
b	11.743 Å
c	34.698 Å
α	90°
β	91.41°
γ	90°

(Sakurabayashi et al. 2025)

XRDa side

Links to the COD :)

https://xrda.pdbj.org/entry/335

Entry information

Entry ID:	XRD-00335
Entry title:	MicroED dataset of ND
Entry type:	Electron Diffraction
XRD entry authors:	Shuhei Sakurabayashi; Kyoko Furuita; Takeshi Yamada; Noriaki Sugiura; Makoto Nomura; Takanori Nakane; Akihiro Kawamoto; Genji Kurisu; Yohei Miyanoiri; Toshimichi Fujiwara; Kazuhiko Nakatani; Chojiro Kojima
Entry:	Download (141.85 GB)
XRDa entry DOI:	10.51093/xrd-00335
CCDC entry:	2350096
Crystallography Open Database entry:	3000497
Citation DOI:	10.1021/jacs.4c17538

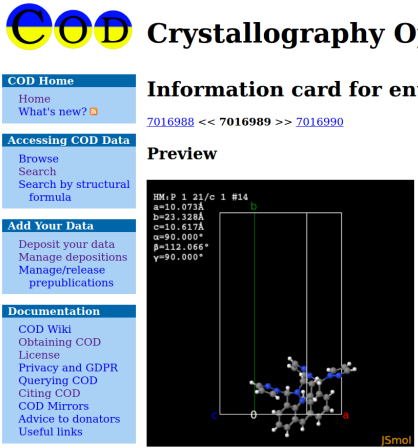
A side note: links with other data sources

Pubchem as an example

pubchem_x_cod

id	ext_id	cod_id
120396	101539687	7016989
99284	168336540	4135255
18081	168304792	1554891
147524	25198875	7155506
134464	168350383	7104999

169 593 rows
(Vaitkus et al. 2023)



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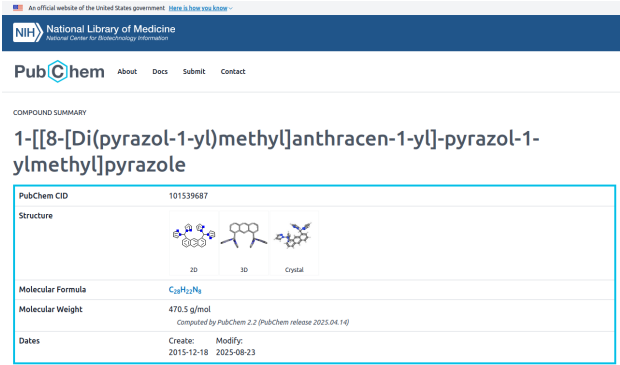


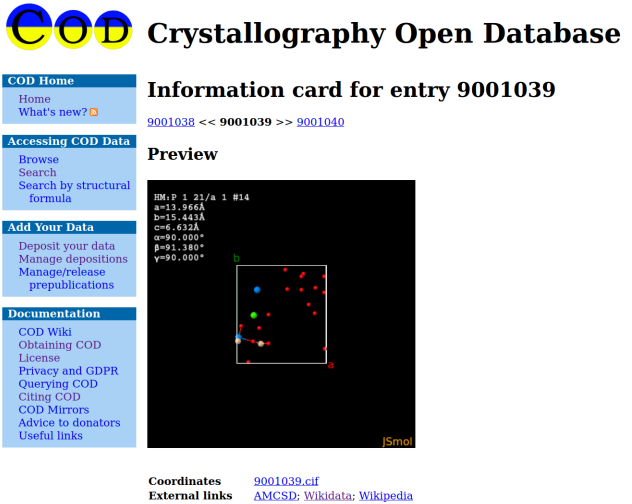
A side note: links with other data sources

Wikidata as an example

wikidata_x_cod

id	ext_id	cod_id
145	Q423494	9001039
2	Q1067912	9017917
150	Q182264	9001030
14	Q3649812	9000094
111	Q19861259	2105051

76 rows



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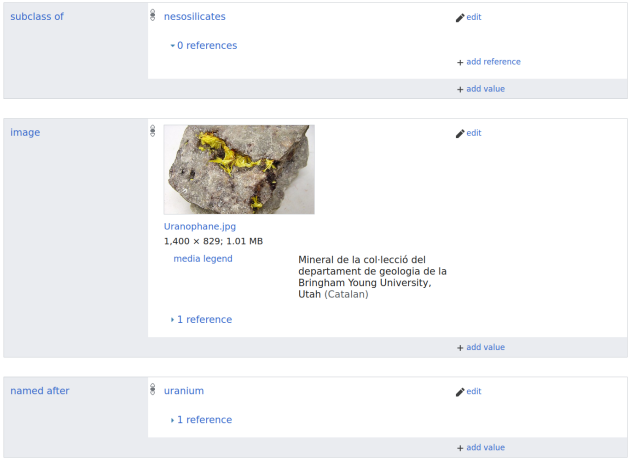

Relation types

Different relations for different records

Relation “ontology”: the `relations` table;

id	name	description	...
1	RELATED	THE CIF is related in some way to the ext	...
2	DIRECTLY_DERIVED	The CIF file was generated directly from	...
3	INDIRECTLY_DERIVED	Related by name, but not confirmed as the	...
4	SIMILAR_TO	It shares some characteristics but wasn’t	...

CIF data source

Data flows from CIF to SQL (and never in reverse direction!)

From the COD 3000497 entry:

```
loop_
_cod_related_entry_id
_cod_related_entry_database
_cod_related_entry_code
_cod_related_entry_description
1 XRDA 00335 10.51093/xrd-00335
```

CIF data source

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From the COD 3000497 entry:

```
loop_
_cod_related_entry_id
_cod_related_entry_database
_cod_related_entry_code
_cod_related_entry_description
1 XRDA 00335 10.51093/xrd-00335
```

From the COD 7016989 entry:

```
loop_
_cod_related_entry_id
_cod_related_entry_database
_cod_related_entry_code
1 AMCSD 0001061
2 Wikidata Q423494
3 Wikipedia Uranophane
```

Encoding in CIFs

Using COD CIF dictionary

```
data_cod_related_entry_code
_name                                  '_cod_related_entry_code'
_category                              cod_related_entry
_type                                  char
_list                                  both
# ...
_definition
;
 The unique identifier of the related entry assigned by the
 related database (see _cod_related_entry_database).
;
```

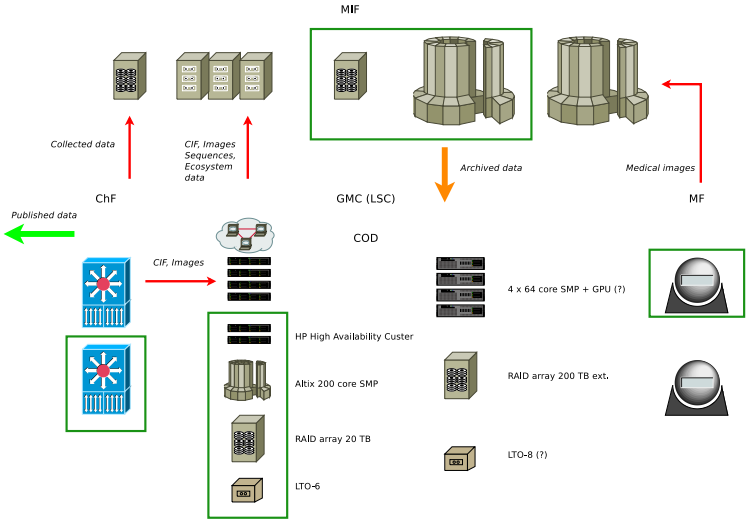
IUCr ImgCIF

Direct links to frames

https://github.com/COMCIFS/imgCIF.git

- Should in principle permit direct links to X-ray frames;
- Still work in progress (recent commit: `Date: Mon Apr 28 09:55:40 2025 +1000`);
- No tags in Git ...;
- Still in flux (already has deprecated items);

Infrastructure



Conclusions

- Simple link tables let us find Raw diffraction images;
- The method is general and suitable for other data as well;
- Predicates enable more precise descritpion of the links;
- More advanced methods that are under development (e.g. ImgCIF) are compatible with the proposed links;

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Rickard Armiento

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Miguel Quirós

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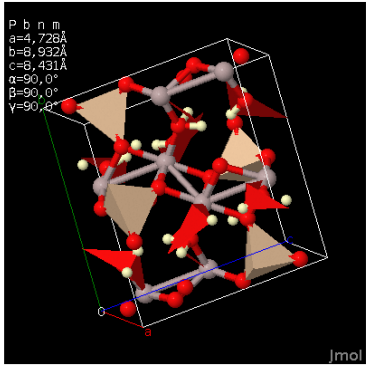
Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

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

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

References I

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