X-ray crystallography of biological macromolecules

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Vilnius, 2019

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Crystals

They are beatiful, aren't they?

Pyrite, by CarlesMillan - CC BY-SA 3.0

Quartz, by JJ Harrison
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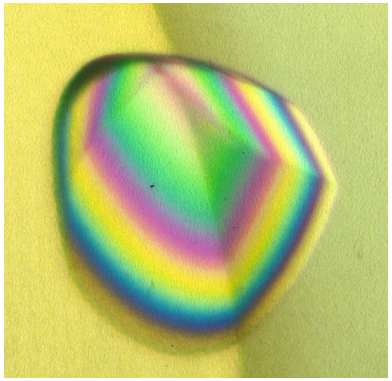
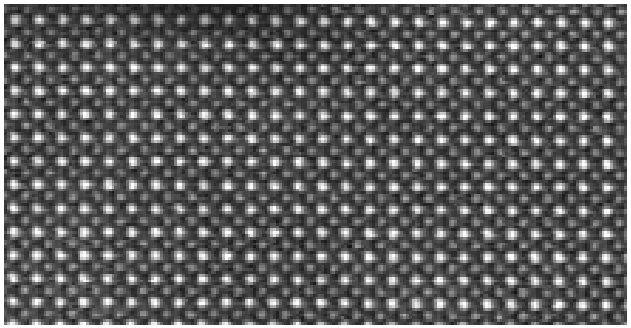
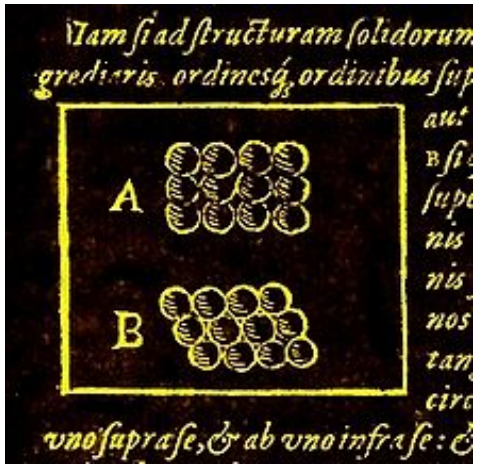


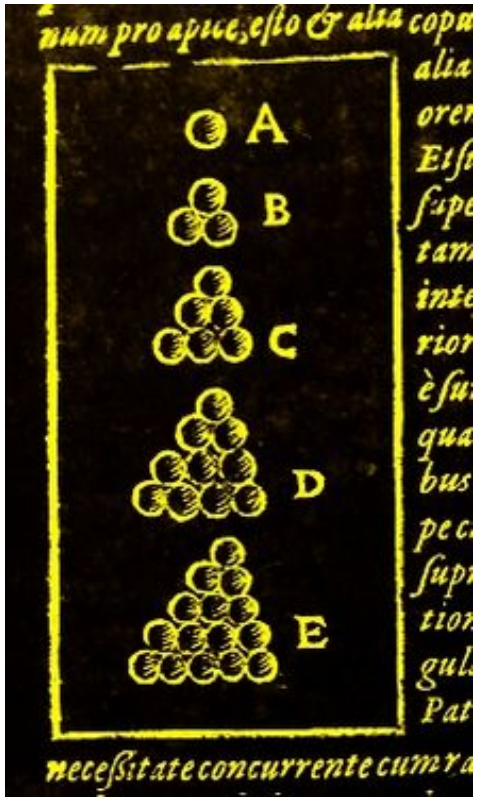
Cfr10I protein, by S.G.

Explanation of the crystal form

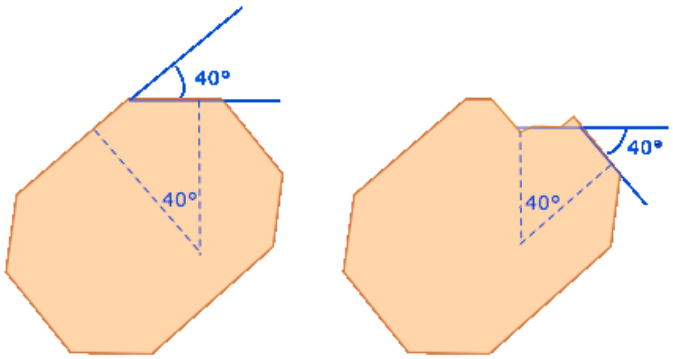


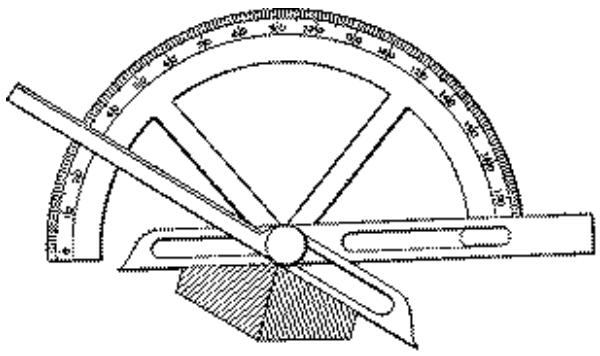
Johannes Kepler, year 1611 “Strena Seu de Nive Sexangula” (A New Year’s Gift of Hexagonal Snow)





The law of constant angles

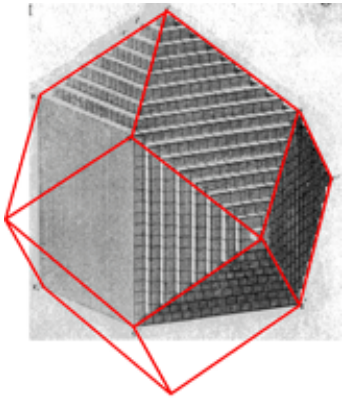




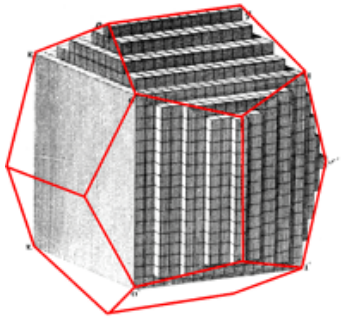
Nicolas Steno, year 1669 “De solido intra solidum naturaliter contento”

Images taken from
http://www.chem1.com/acad/webtext/states/crystals-ext.html

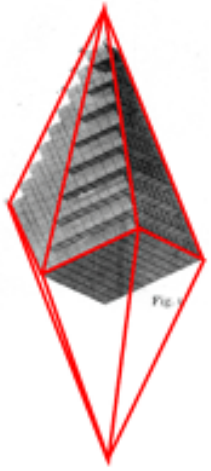
The inner structure of crystals



Rhomb-dodecahedron



Pentagon-dodecahedron



Scalenohedron

René Just Haüy Traité de minéralogie
(5 vols, 1801)

Images taken from
http://xrayweb.chem.ou.edu/notes/symmetry.html

What would we like to know?

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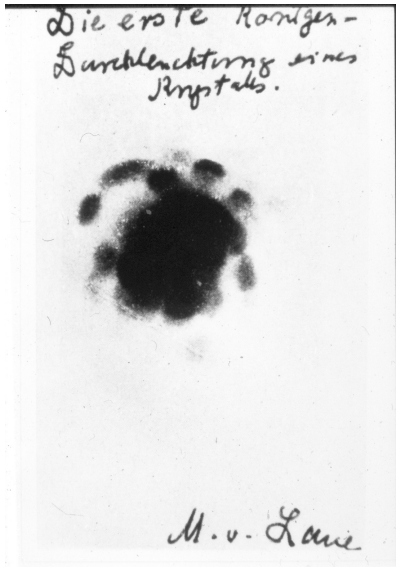
What would we like to know?

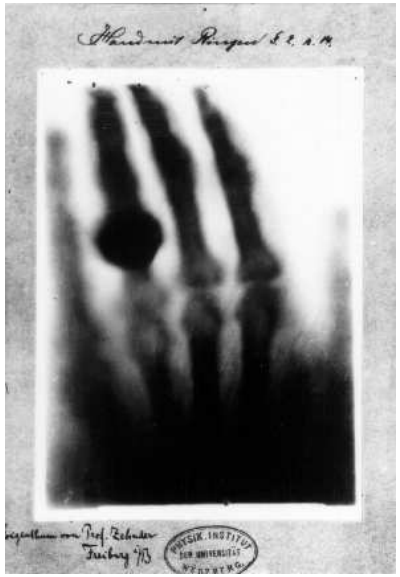
Material properties

- A given chemical compound always contains its component elements in fixed ratio (by mass) and does not depend on its source and method of preparation *(Proust's law)*
- Chemical compounds are not a random cluster of atoms and functional groups, but rather had a definite order defined by the valency of the atoms composing the molecule *(Butlerov's law)*

X-rays

Wilhelm Conrad Röntgen The first Nobel prize in physics, 1901

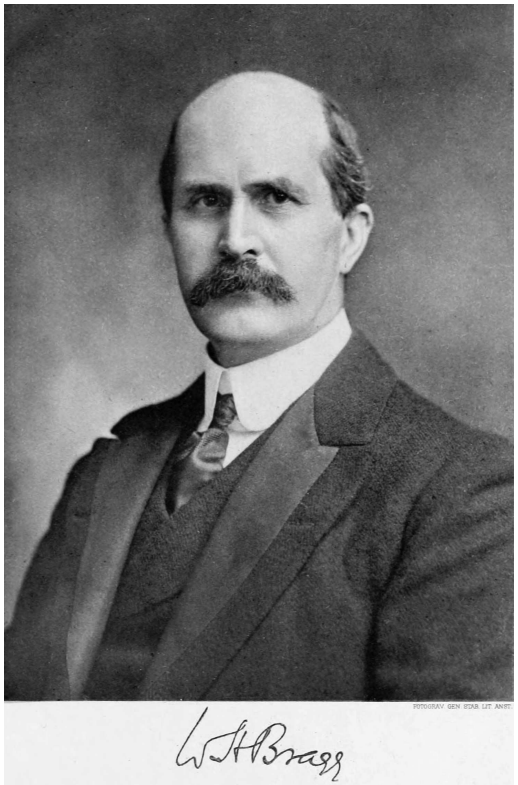




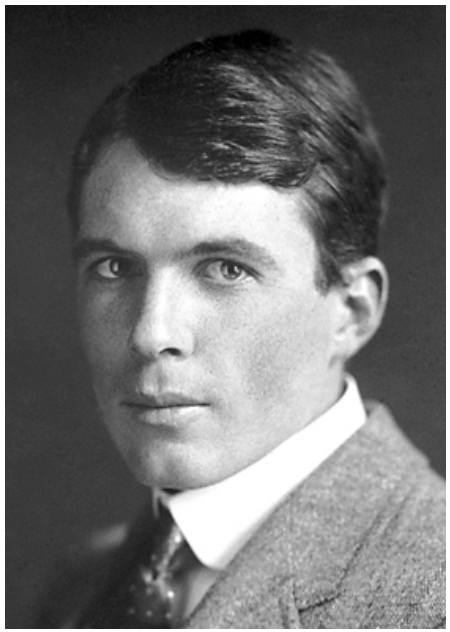
Max von Laue, Nobel prize, 1914

Explanation of X-ray diffraction

William and Lawrence Bragg, father and son



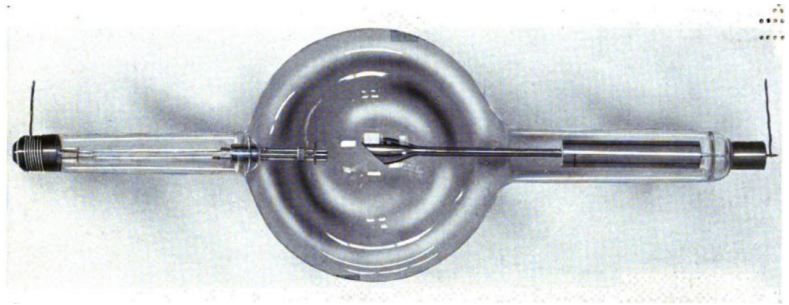
Sir William Henry Bragg OM KBE PRS



Sir William Lawrence Bragg, CH, OBE, MC, FRS

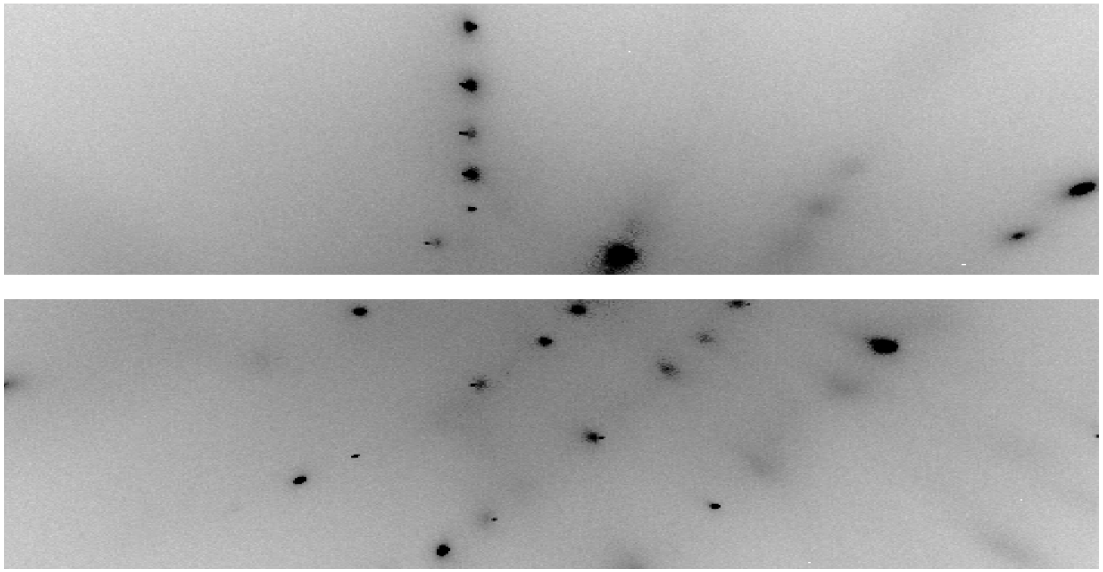
Nobel prize in physics, 1915.

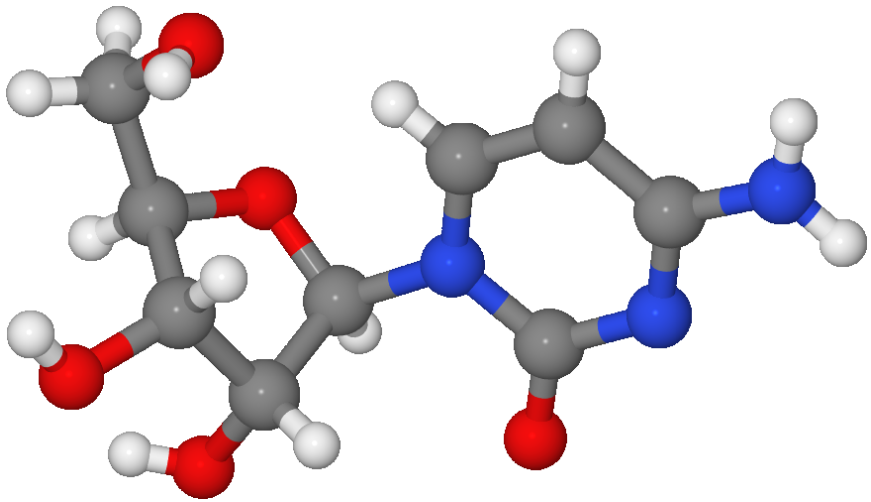
X-ray tubes and diffractometers



X-ray diffraction

Molecular structure determination





Difficulties obtaining data

Proprietary licenses – a constant 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 2018-02-09)
- “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).

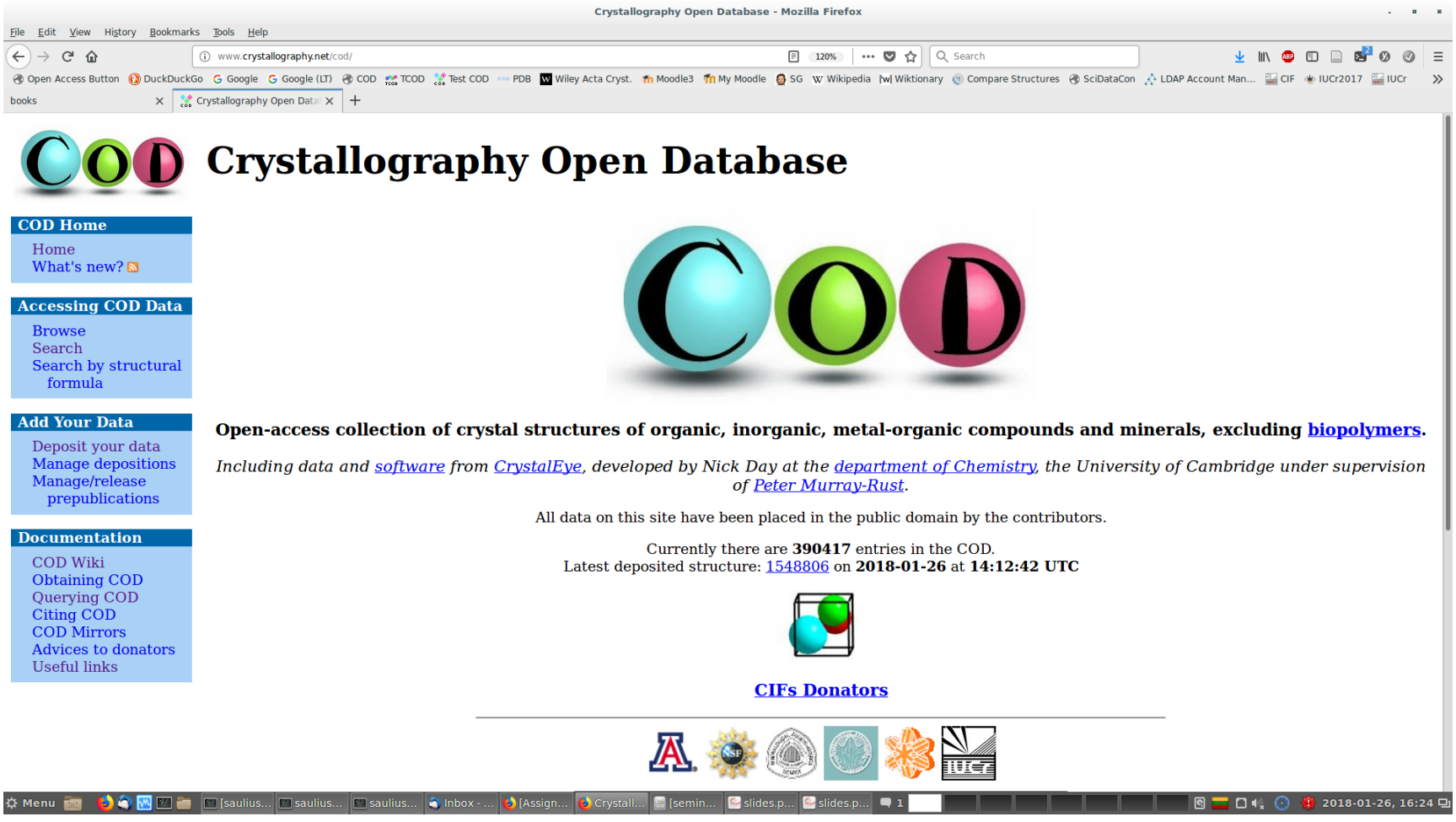
3. Free software a) for maintaining the database, b) for data evaluation and calculation of derived data (e.g. calculated powder pattern from crystal structures for search-match purposes), c) for browsing and retrieval.

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

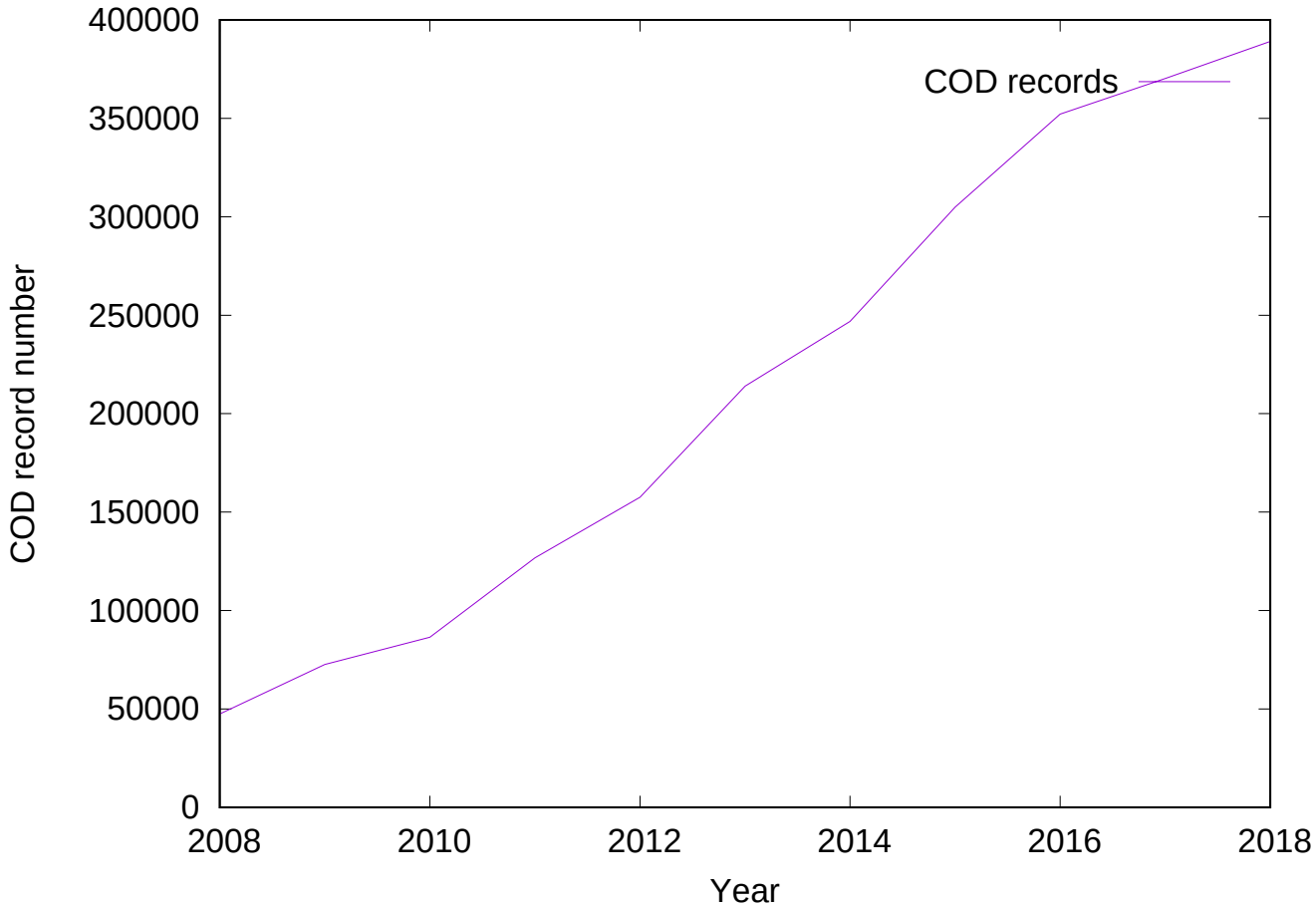
The COD

The Crystallography Open Database

http://www.crystallography.net/cod



COD growth


COD records
COD record number
Year
400000
350000
300000
250000
200000
150000
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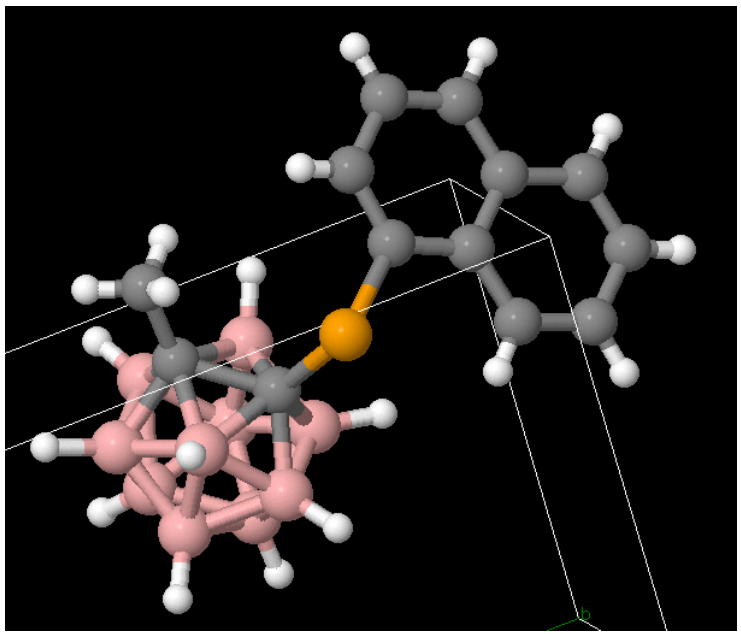
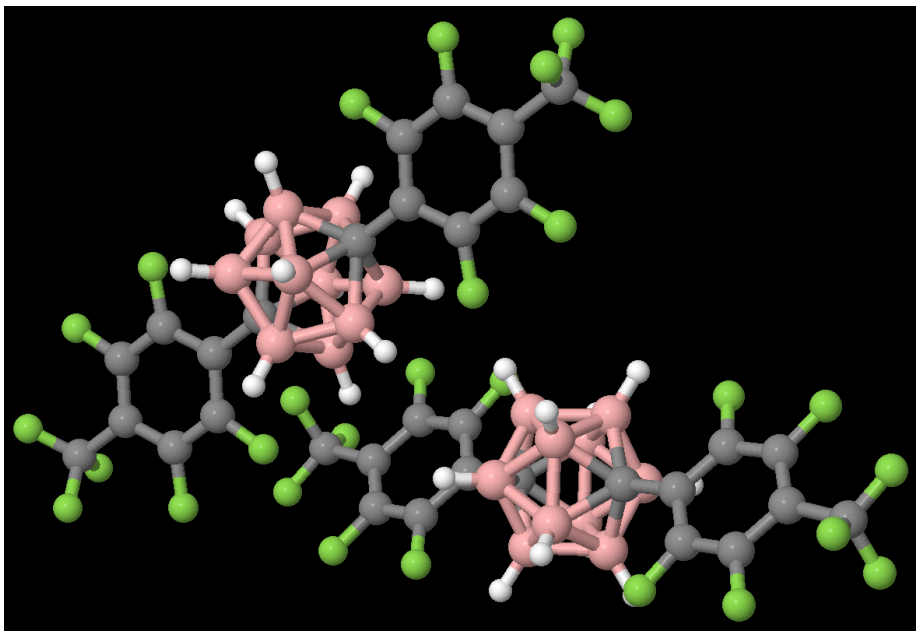
50000
0
2008
2010
2012
2014
2016
2018

Carboranes

6-valent carbon?



COD 7015488



COD 7015654

Crystallography Open Database

COD Home
- Home
- What's new?

Accessing COD Data
- Browse
- Search
- Search by structural formula

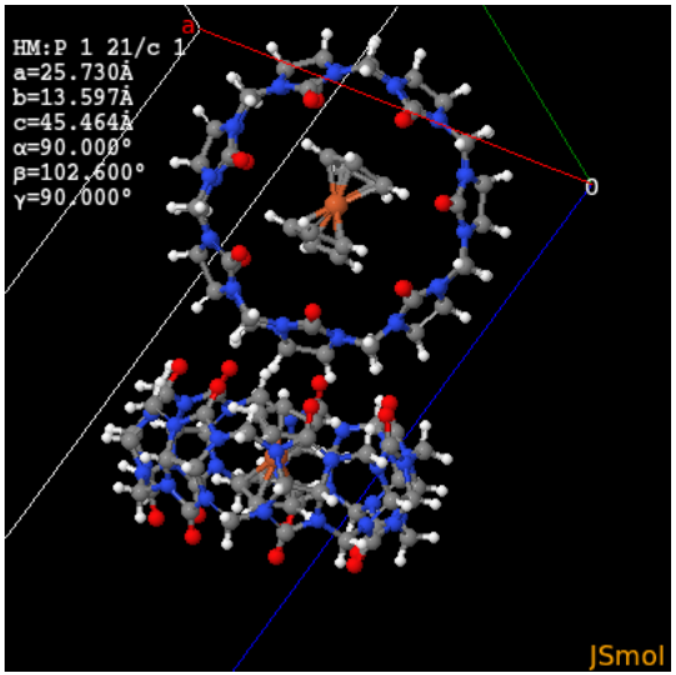
Add Your Data
- Deposit your data
- Manage depositions
- Manage/release prepublications

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

Information card for entry 4111922

4111921 << **4111922** >> 4111923

Preview



COD 4111922

Applications of the COD

Material identification

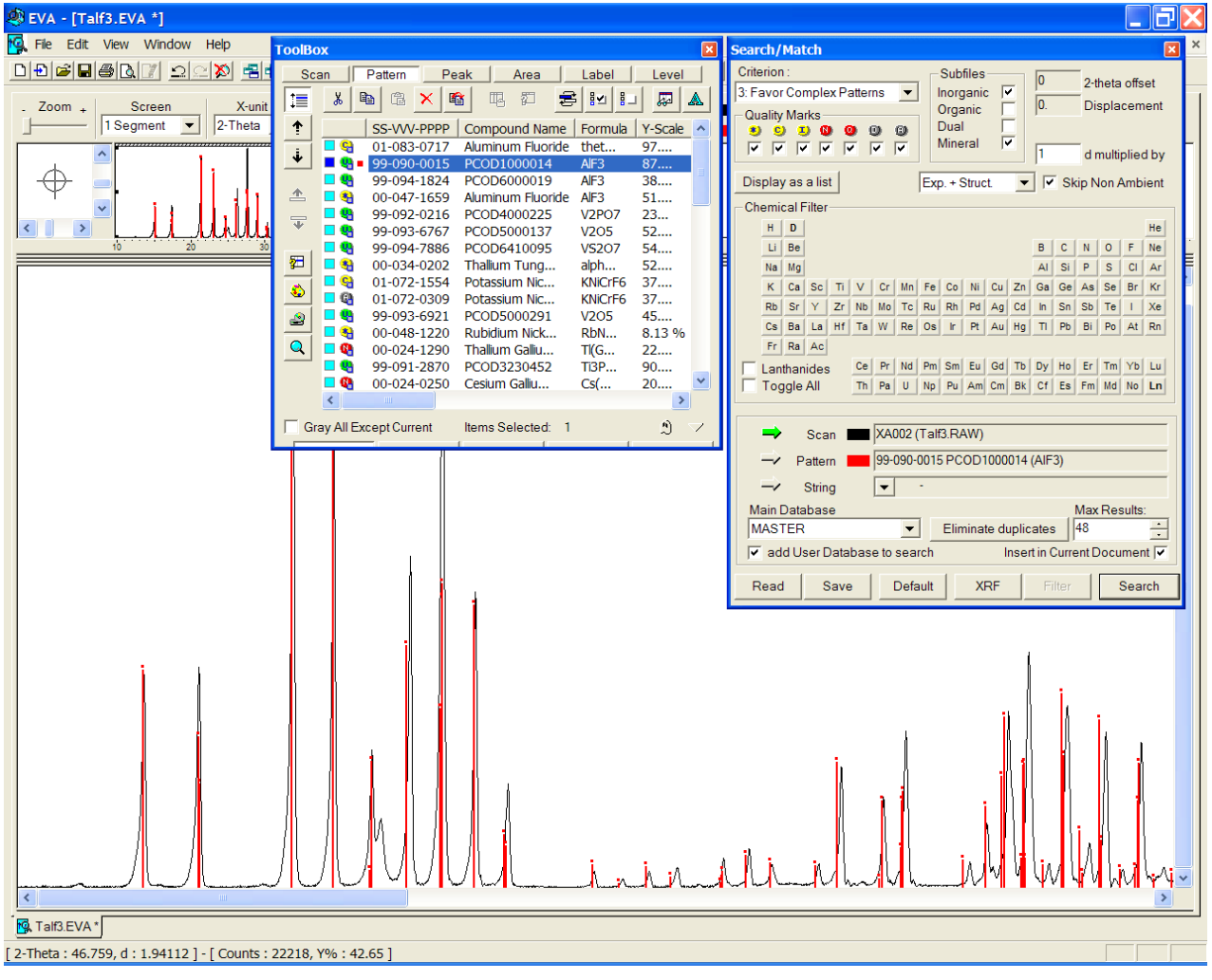


Image courtesy
Armel Le Bail
[Le Bail, 2008]

Acknowledgements

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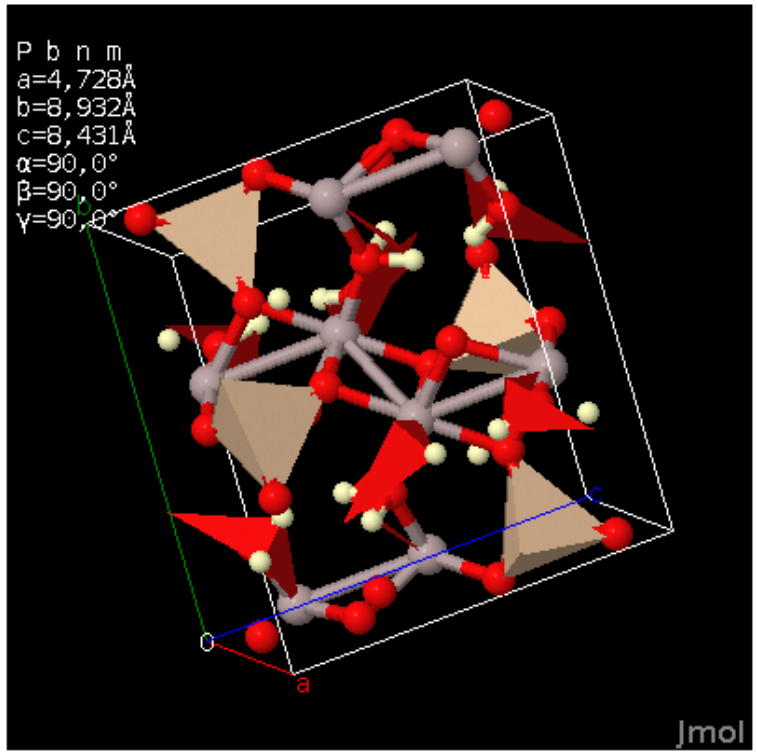
Werner Kaminsky
Armel Le Bail
Luca Lutterotti
Peter Moeck
Peter Murray-Rust
Miguel Quirós

Ačiū! Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

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

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

References I

Baldi, P. (2011).
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.
Journal of chemical information and modeling, 51:3029.

Le Bail, A. (2008).
Frontiers between crystal-structure prediction and determination by powder diffractometry.
Powder Diffraction Suppl., pages S5–S12.