Biologinių makromolekulių rentgenostruktūrinė analizė

Saulius Gražulis

Vilnius, 2019

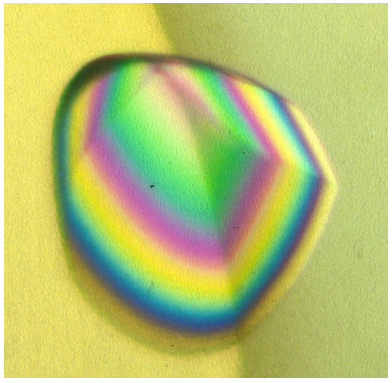
Vilniaus universiteto Biotechnologijos institutas

Kristalai

Gražūs, ar ne?

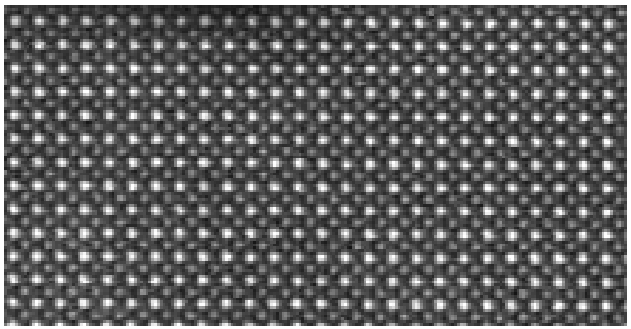
Piritas, CarlesMillan - CC BY-SA 3.0

Kvarcas, JJ Harrison
CC BY-SA 2.5

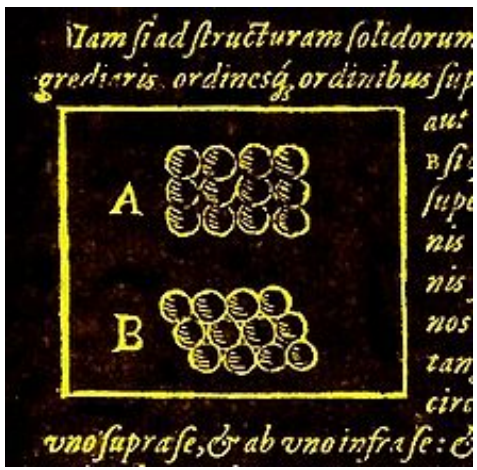


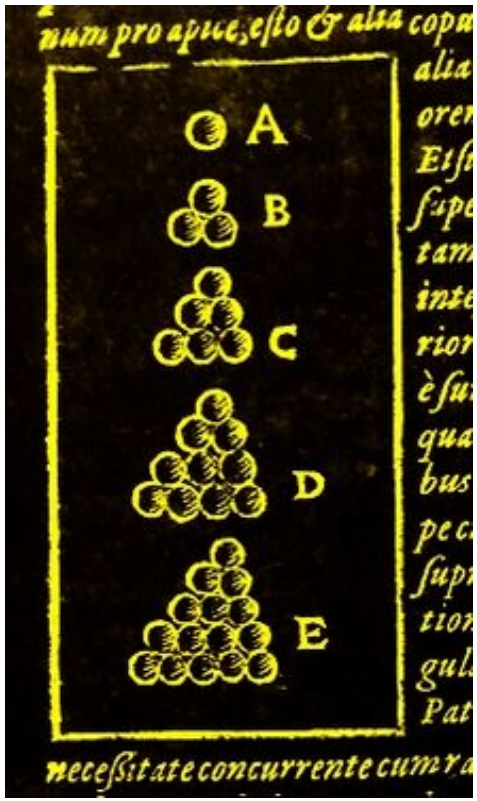
Cfr10I baltymas, S.G.

Kristalo formos paaiškinimas

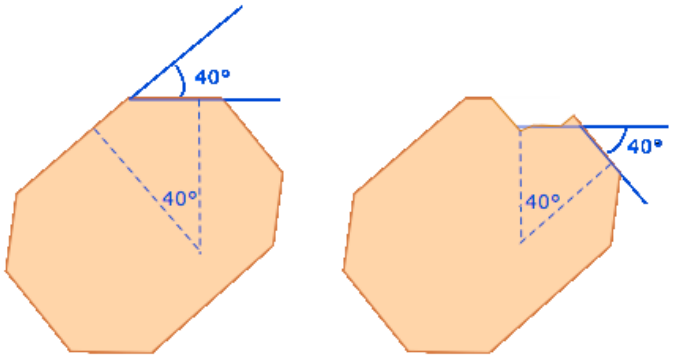


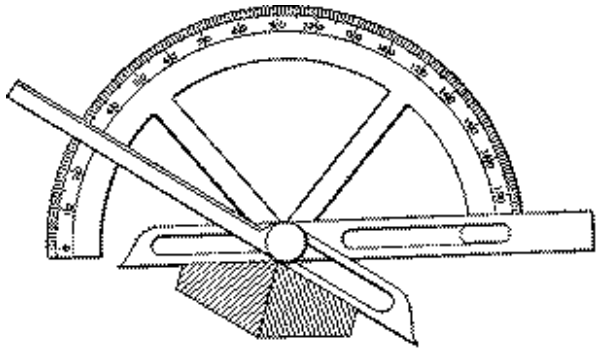
Johannes Kepler, 1611 m. “Strena Seu de Nive Sexangula” (A New Year’s Gift of Hexagonal Snow)





Kampų pastovumo dėsnis

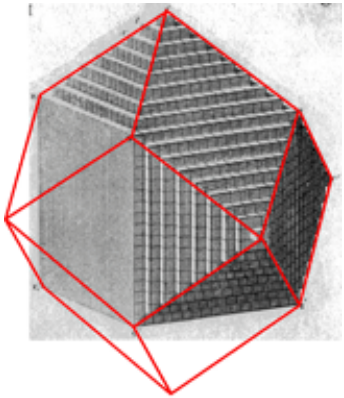




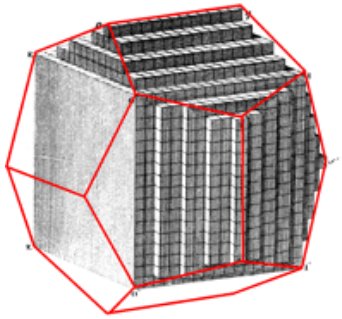
Nicolas Steno, 1669 m. “De solido intra solidum naturaliter contento”

Paveiksliukai iš
http://www.chem1.com/acad/webtext/states/crystals-ext.html

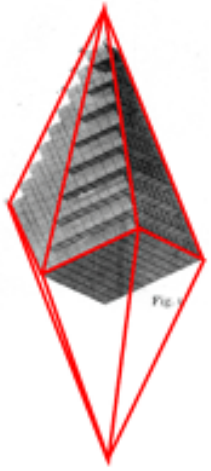
Vidinė kristalų struktūra



Rhomb-dodecahedron



Pentagon-dodecahedron



Scalenohedron

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

Paveiksliukai iš
http://xrayweb.chem.ou.edu/notes/symmetry.html

Ką mes norėtume žinoti?

?

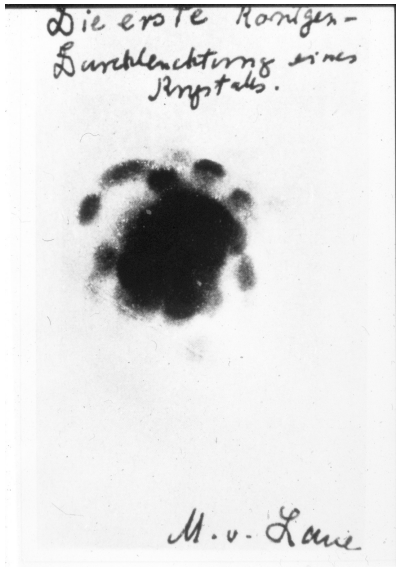
Ką mes norėtume žinoti?

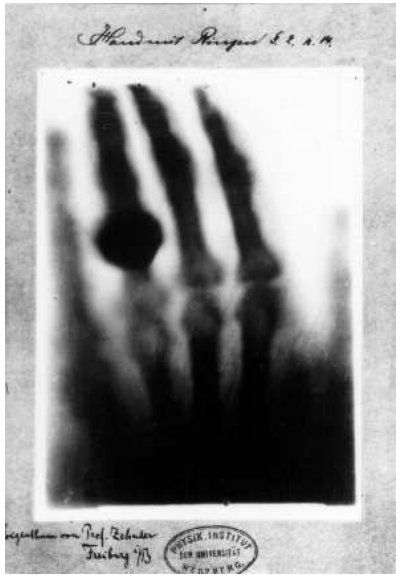
Medžiagų savybės

- Gryni cheminiai junginiai turi pastovią sudėtį, nepriklausomai nuo jų gavimo būdo *(Prusto dėsnis)*
- Grynų medžiagų savybės iš esmės priklauso nuo atomų susijungimo jose tvarkos *(Butlerovo dėsnis)*

Rentgeno spinduliai

Wilhelm Conrad Röntgen Pirmoji fizikos Nobelio premija, 1901 m.

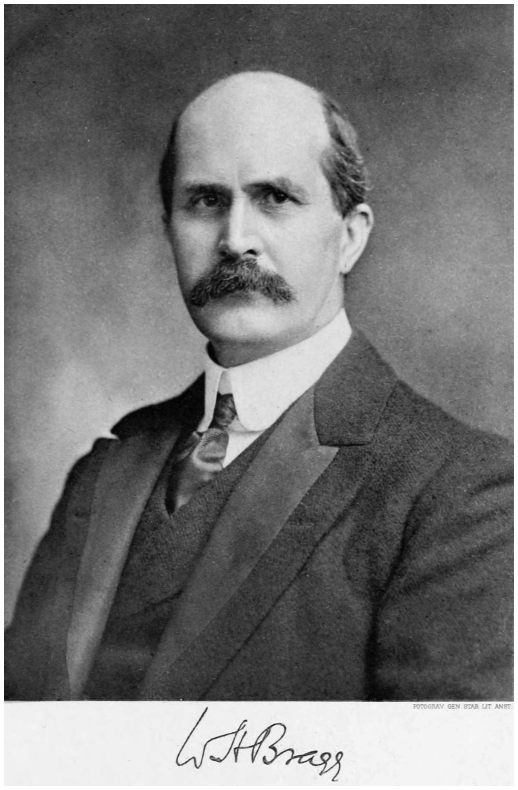




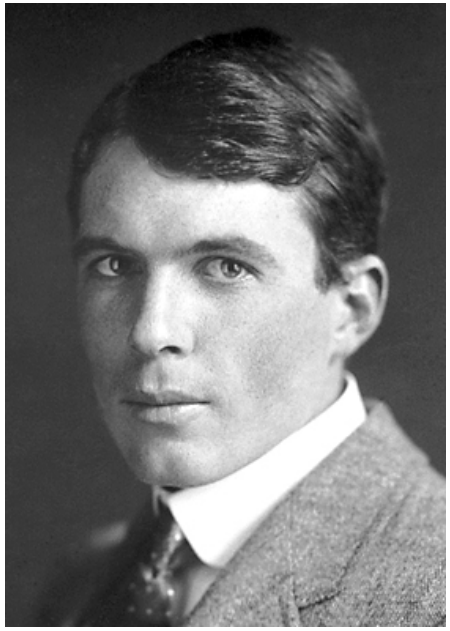
Max von Laue, Nobelio premija, 1914 m.

Rentgeno spindulių sklaidymo paaiškinimas

Tėvas ir sūnus Bregai



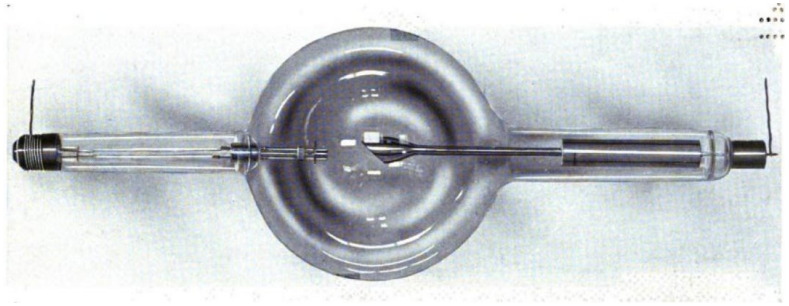
Sir William Henry Bragg OM KBE PRS



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

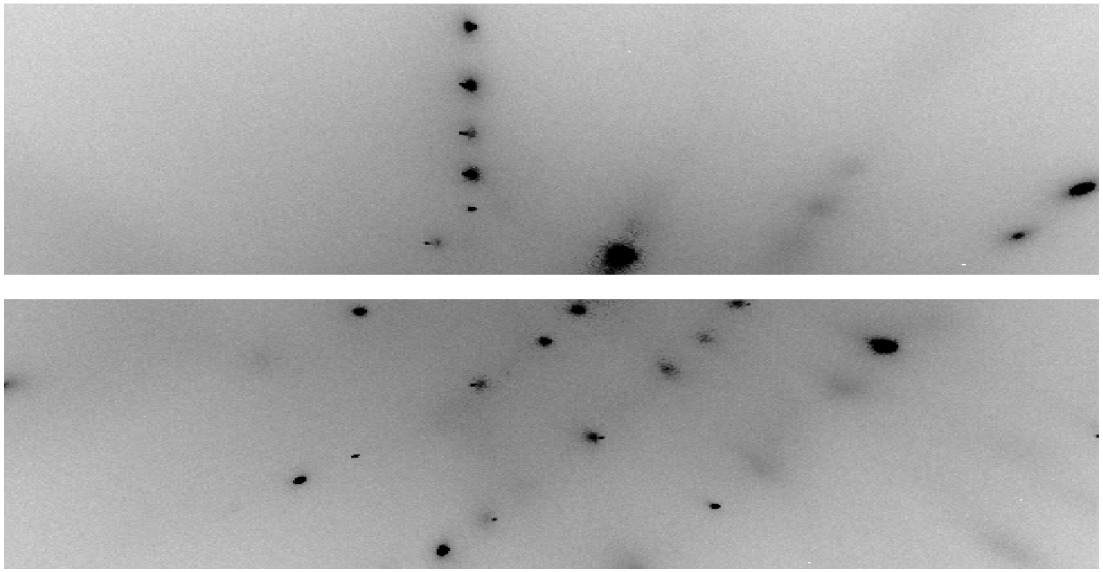
Fizikos Nobelio premija, 1915 m.

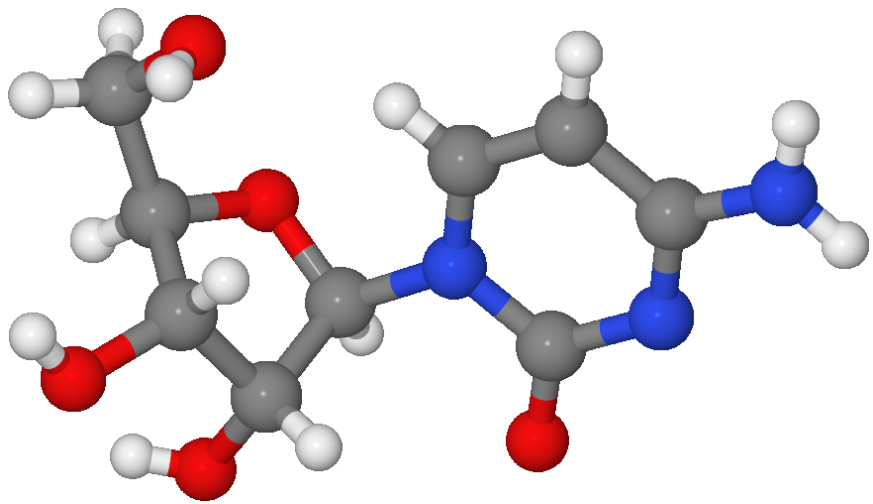
Rentgeno spindulių vamzdeliai ir difraktometrai



Rentgeno spindulių sklaidymas

Molekulių struktūros nustatymas





Sunkumai gaunant duomenis

Nuosavybinės DB licenzijos XXI a. – tai nuolatinis galvos skausmas...

- 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]

COD projektas

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).

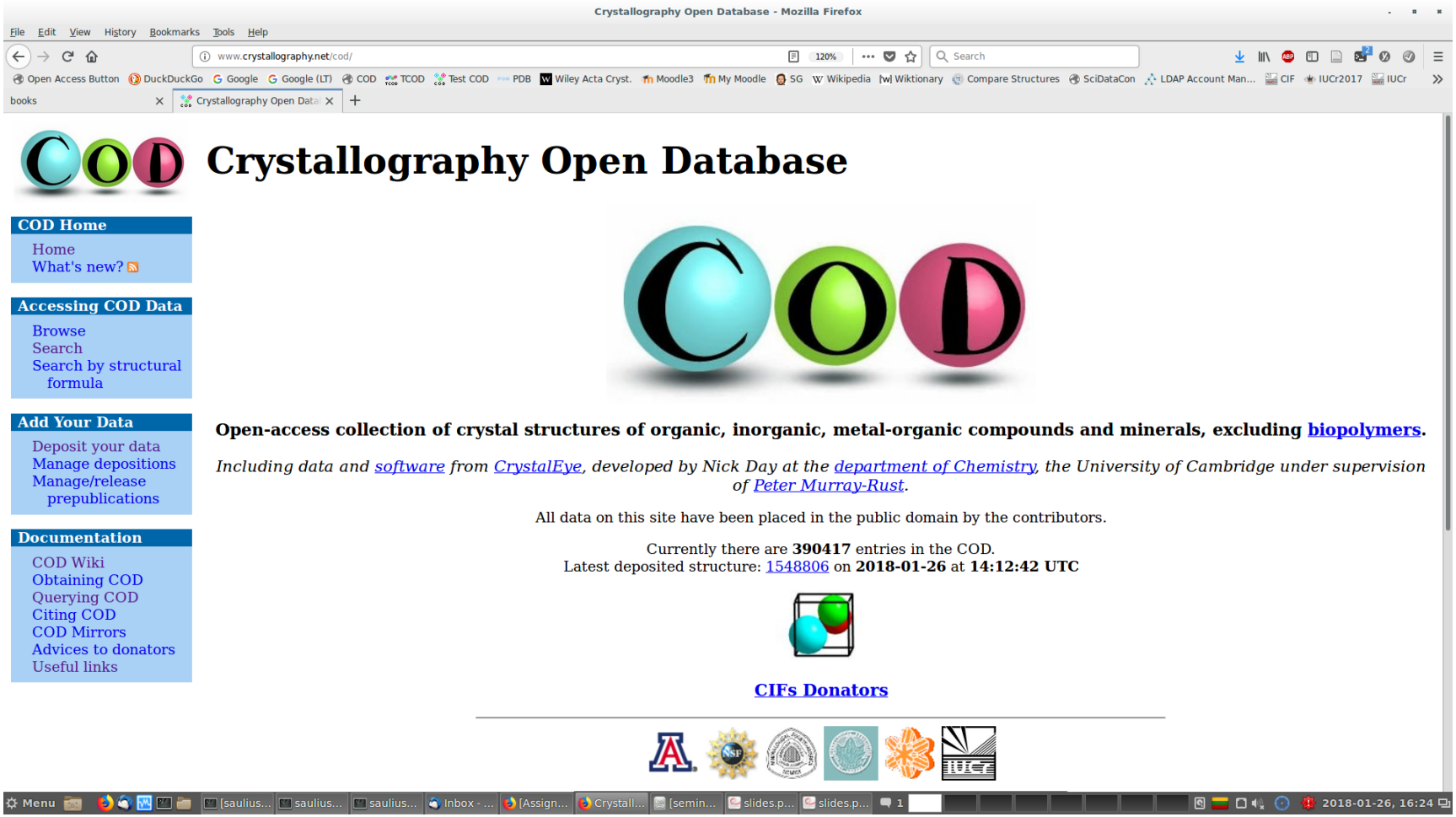
3. Free software a) for maintaining the database, b) for data evaluation and calculation of derived data (e.g. calculated powder pattern from crystal structures for search-match purposes), c) for browsing and retrieval.

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

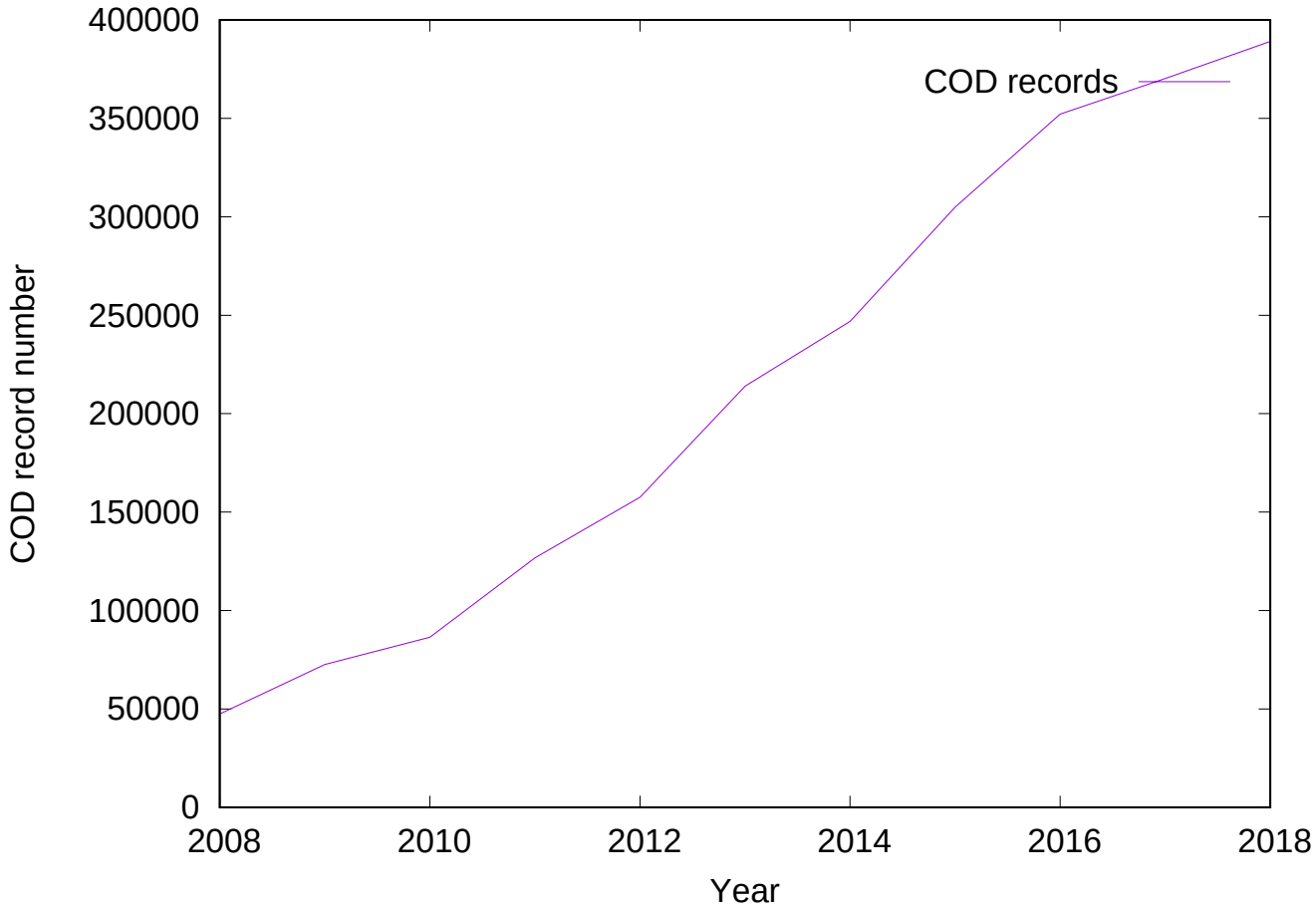
Atvira duomenų bazė COD

The Crystallography Open Database

http://www.crystallography.net/cod

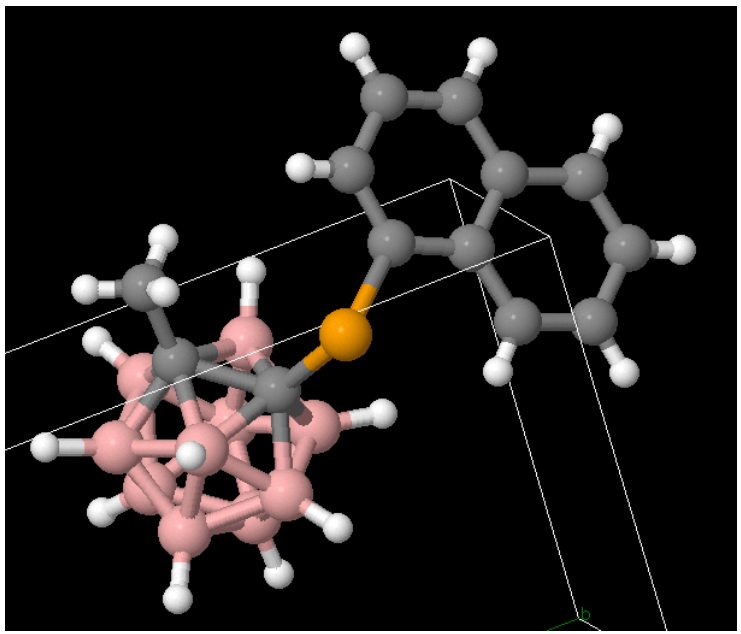


COD augimas

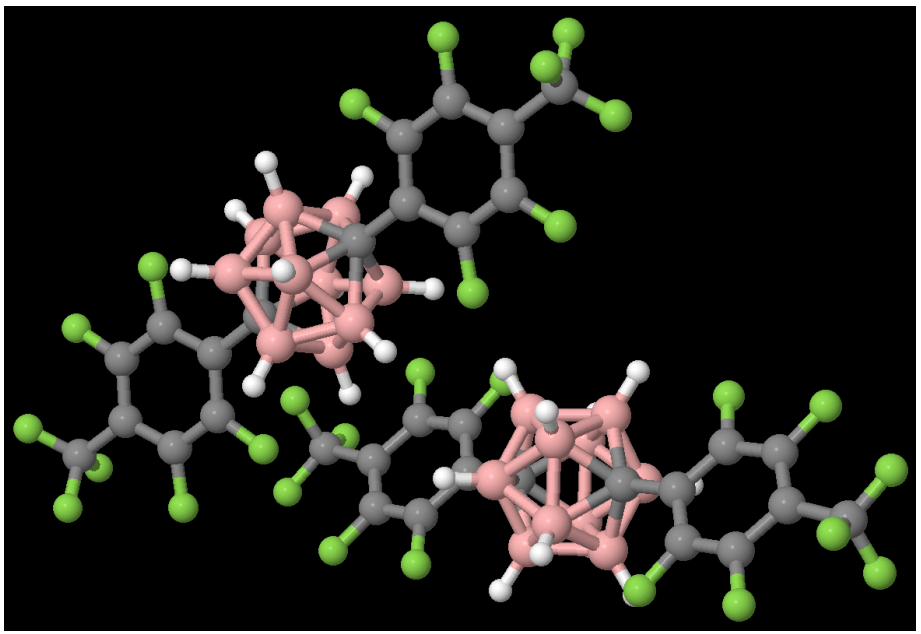

COD records
COD record number
Year
400000
350000
300000
250000
200000
150000
100000
50000
0
2008
2010
2012
2014
2016
2018

Karboranai

6-valentė anglis?



COD 7015488



COD 7015654

Crystallography Open Database

COD Home
- Home
- What's new?

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

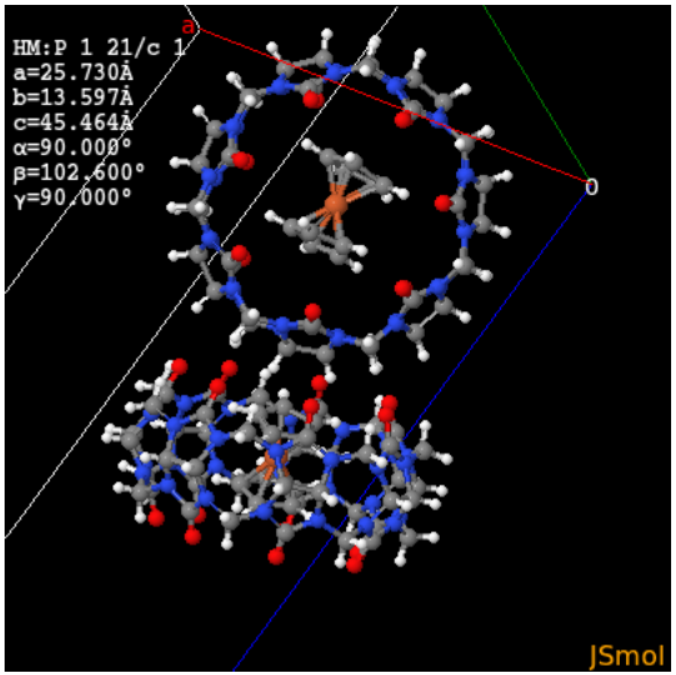
Add Your Data
- Deposit your data
- Manage depositions
- Manage/release prepublications

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

Information card for entry 4111922

4111921 << **4111922** >> 4111923

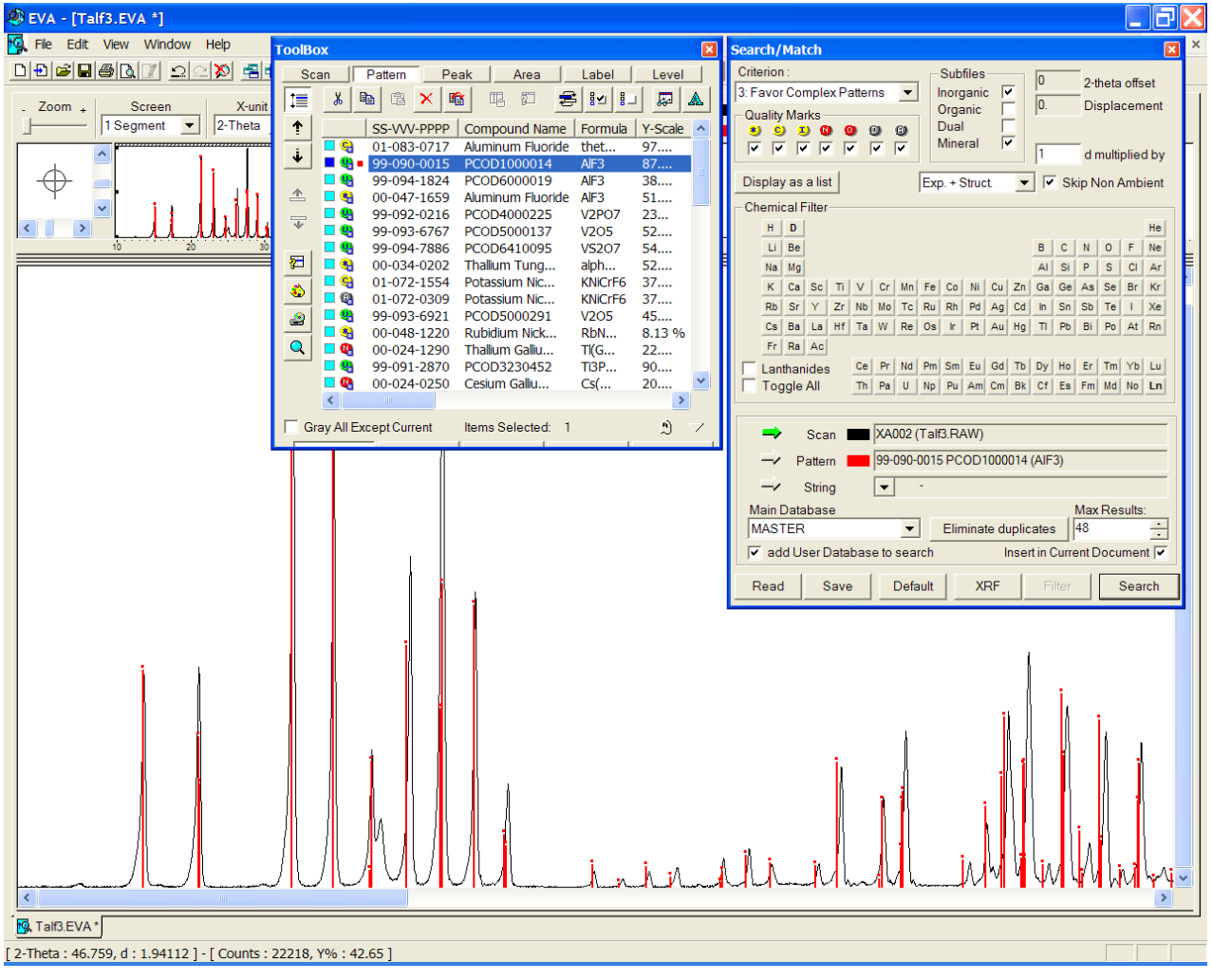
Preview



COD 4111922

COD duomenų bazės panaudojimas

Medžiagų identifikavimas



Paveiksliuku pasidalino Armel Le Bail [Le Bail, 2008]

Padėkos

VU Biotechnologijos institutas

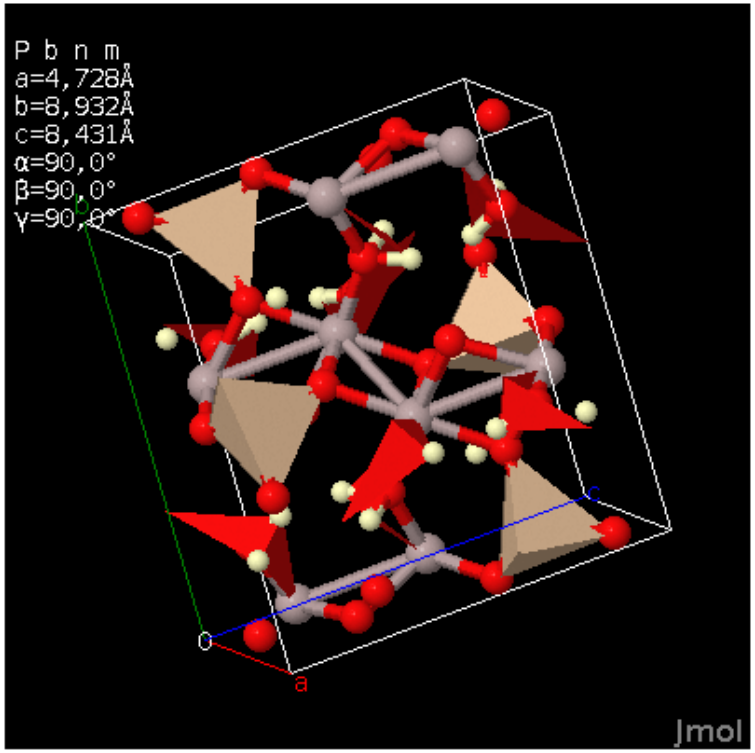
Virginijus Siksnys (*skyriaus vadovas*)

Andrius Merkys
Antanas Vaitkus

COD Taryba (Advisory board)

Daniel Chateigner
Robert T. Downs
Werner Kaminsky
Armel Le Bail
Luca Lutterotti
Peter Moeck
Peter Murray-Rust
Miguel Quirós

Ačiū!



Coordinates	2207377.cif
Original IUCr paper	HTML

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

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

Nuorodos 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.