# F/LOSS for Open Science: Crystallography Open Database

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"Galaktika", 2013

Vilnius University Institute of Biotechnology


# Free software (r)evolution

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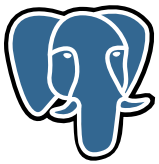

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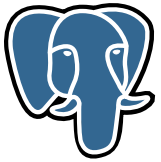
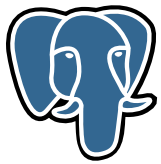


# Free software (r)evolution

- A set of tools to achieve our goals
- A set of ideas how to collaborate







# Applicability of open source principles to scientific investigations

Science is an open endeavour:

- it is based on open discussion and substantial criticism;
- it is based on publication of the results;
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- based on the **reuse** of the results

# The origins of COD

## SDPD mailing list:
## Open crystallographic database - a role for whom?

```
> When crystallographers will be tired to buy all these fragmented
> databases, maybe they will do something. A role for IUCr ? If not, a
> role for whom ?
```

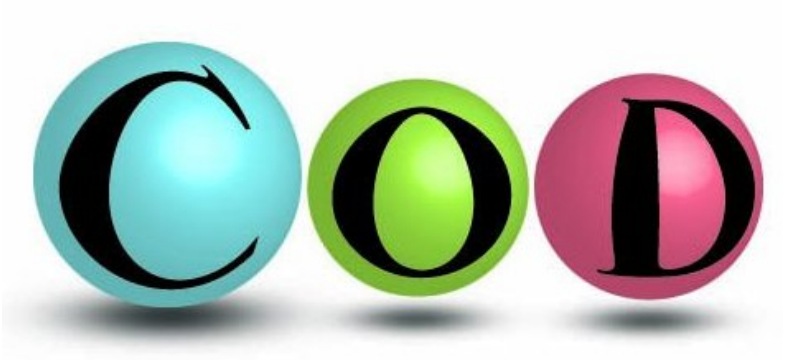
armellebail (Armel Le Bail) Wed Feb 12, 2003 7:24 pm

```
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

# Crystallography Open Database

## A grass-root initiative




http://www.crystallography.net/

- Total ≈**217 000** records
- **179** registered users
- **23** depositors (deposited at least one structure)
- In year 2012:
  - >**56 000** new structures uploaded (**26 000** more than last year)
  - **16** active depositors (who deposited at least one structure in 2012)

# Contents and access

# Crystallography Open Database

**COD Home**

Home
What's new?

**Accessing COD Data**

Browse
Search

**Add Your Data**

Deposit your data
Manage depositions
Manage/release prepublications

**Documentation**

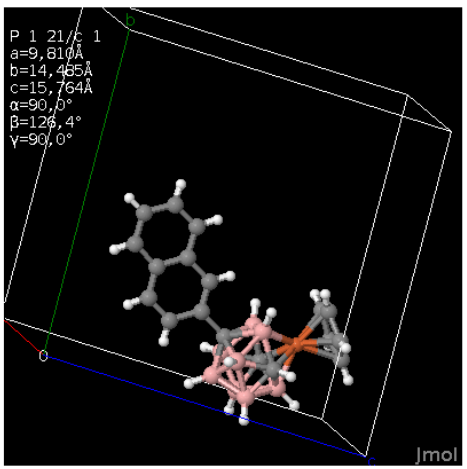
COD Wiki
Obtaining COD
Citing COD
COD Mirrors
Advices to donators

## CIF Information Card

## Information card for 4079785

4079784 << **4079785** >> 4100000

### Preview

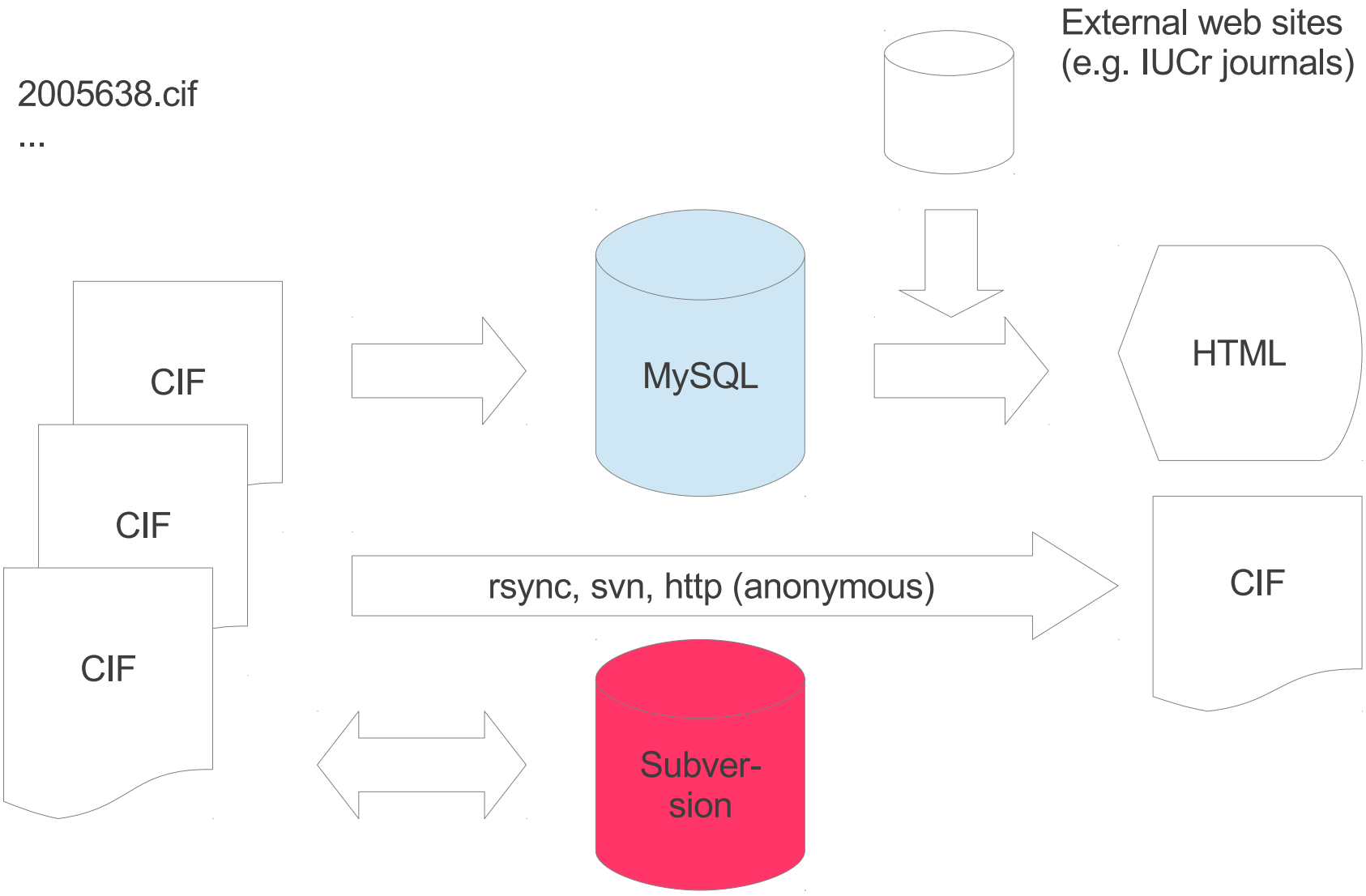



**Coordinates** 4079785.cif

### Structure parameters

| | |
|---|---|
| Formula | - C18 H22 B8 Fe - |
| Calculated formula | - C18 H22 B8 Fe - |
| Title of publication | Three Isomers of Aryl-Substituted |
| Authors of publication | Bakardjiev, Mario; Štíbr, Bohumil; |
| Journal of publication | Organometallics |
| Year of publication | 2013 |
| Journal volume | 32 |
| Journal issue | 2 |
| a | 9.81 ± 0.0006 Å |
| b | 14.4851 ± 0.0009 Å |

# Implementation



# Possible uses

- Protein model refinement
- Data validation
- Search for a “black swan”

H = “All swans are white” (the usual case)

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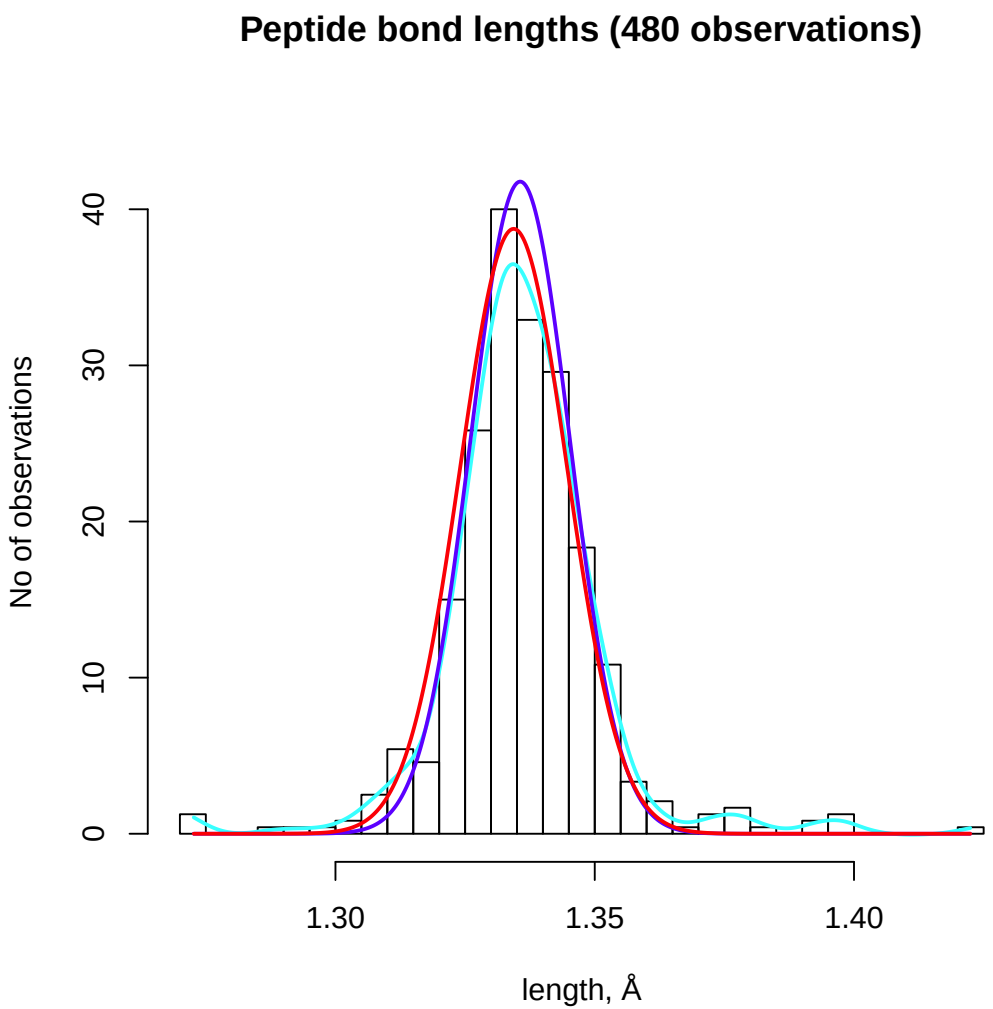
# Example:
## Peptide bonds



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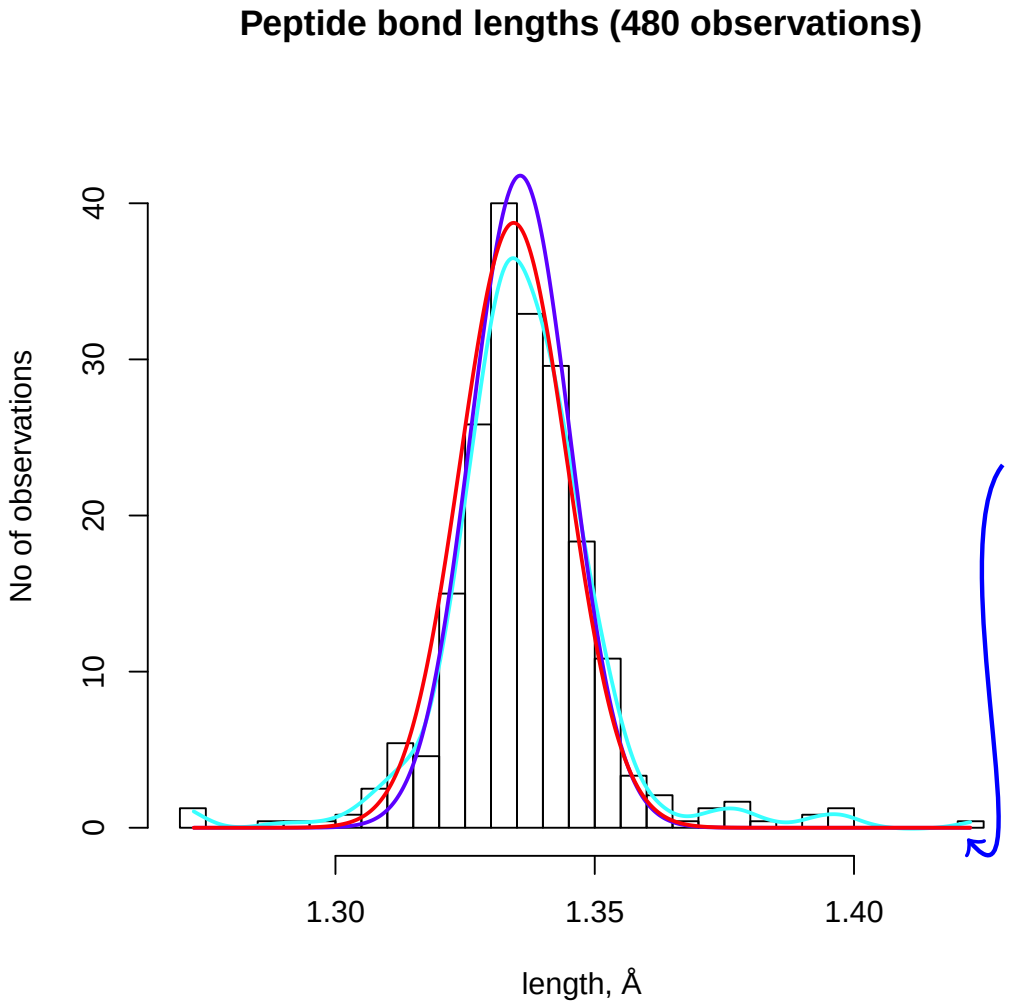


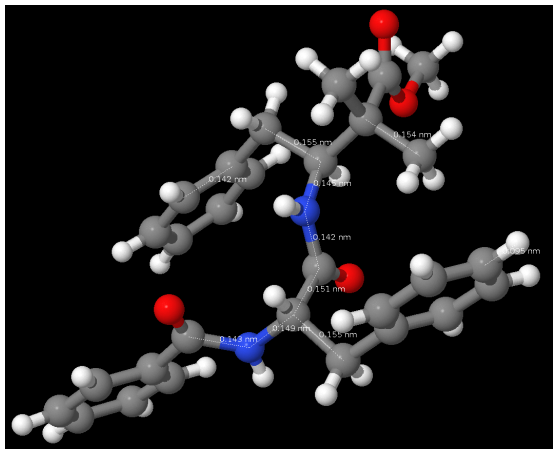

COD 4024607, $l = 1.4224$ Å

# Example:
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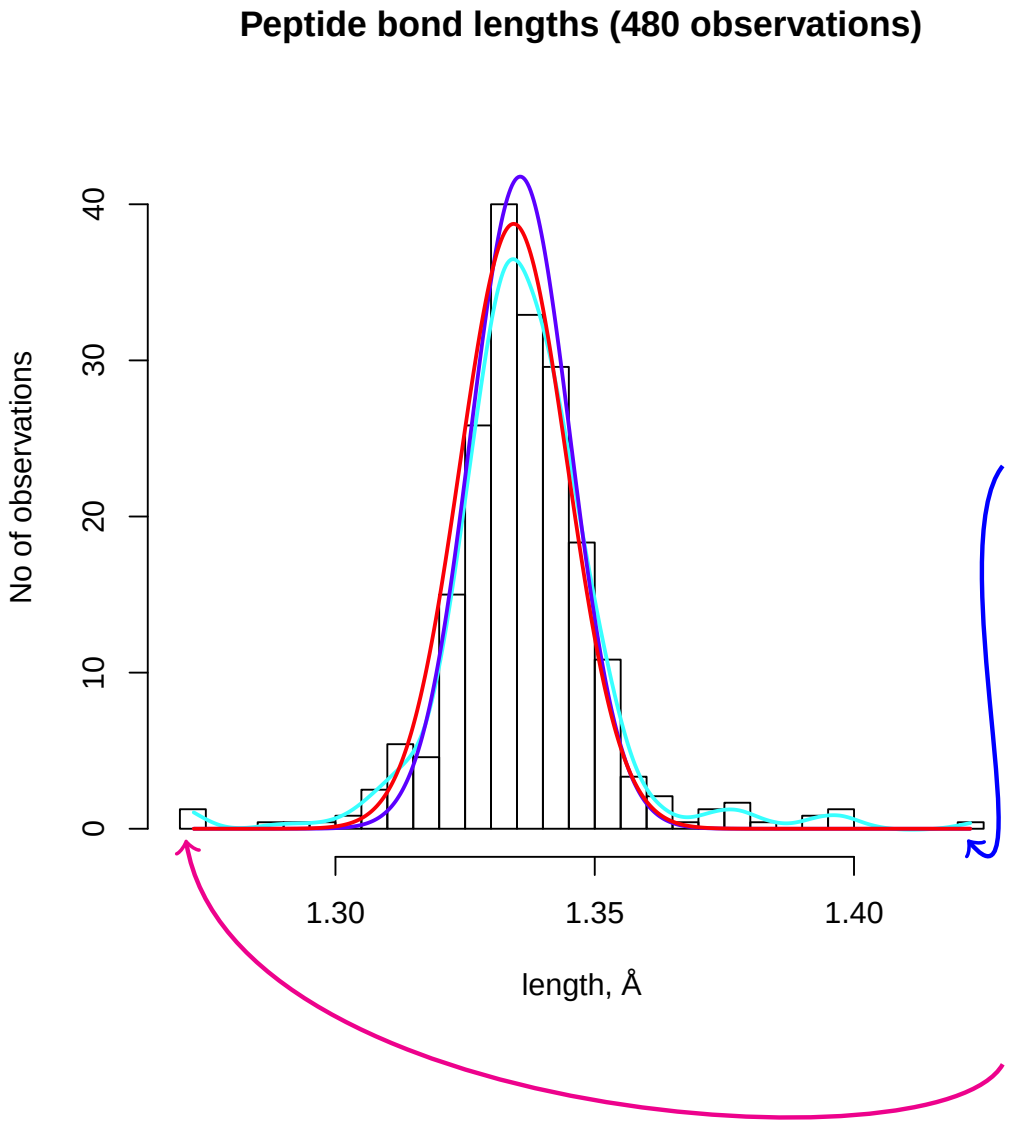


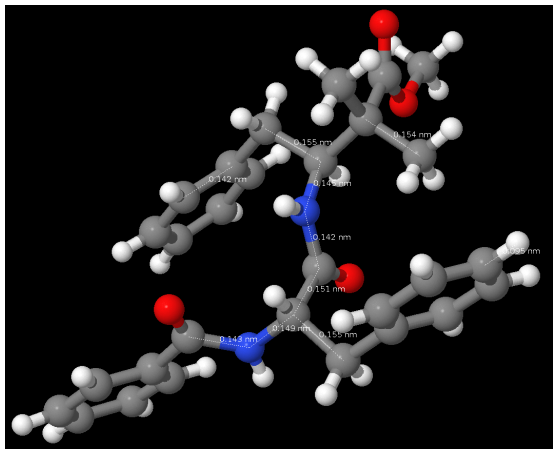

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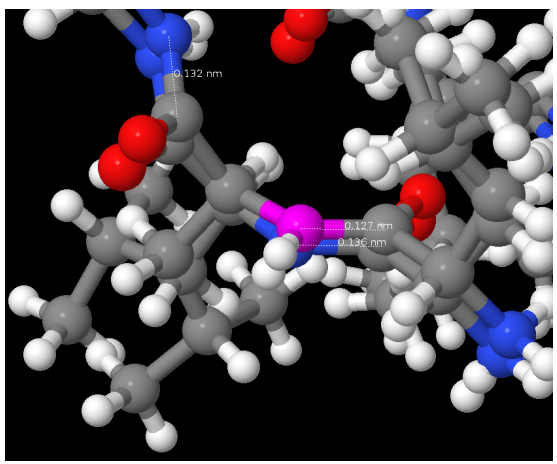

COD 7203041, $l = 1.2727$ Å

# Another example:

## Carbon with valence 6 (!?)

We observe carbons (atoms of type “C”) with **6** neighbours at a covalent distance in our database.(?)

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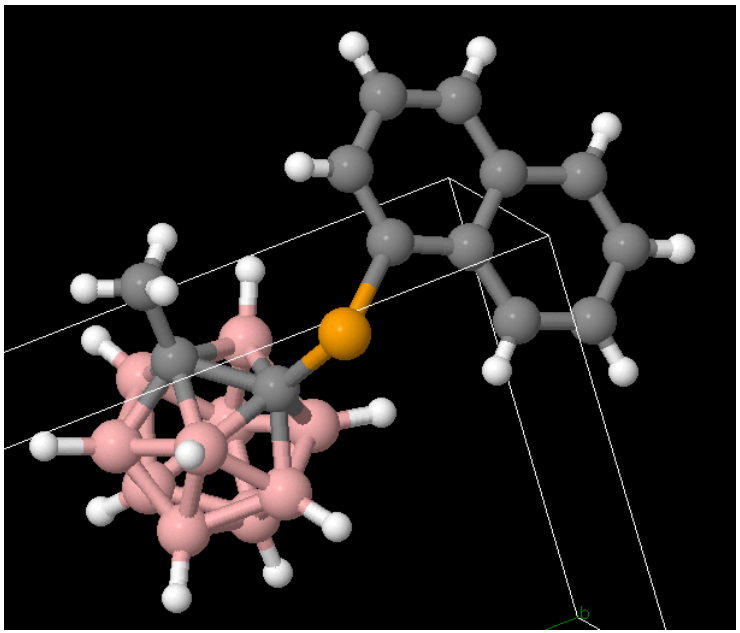
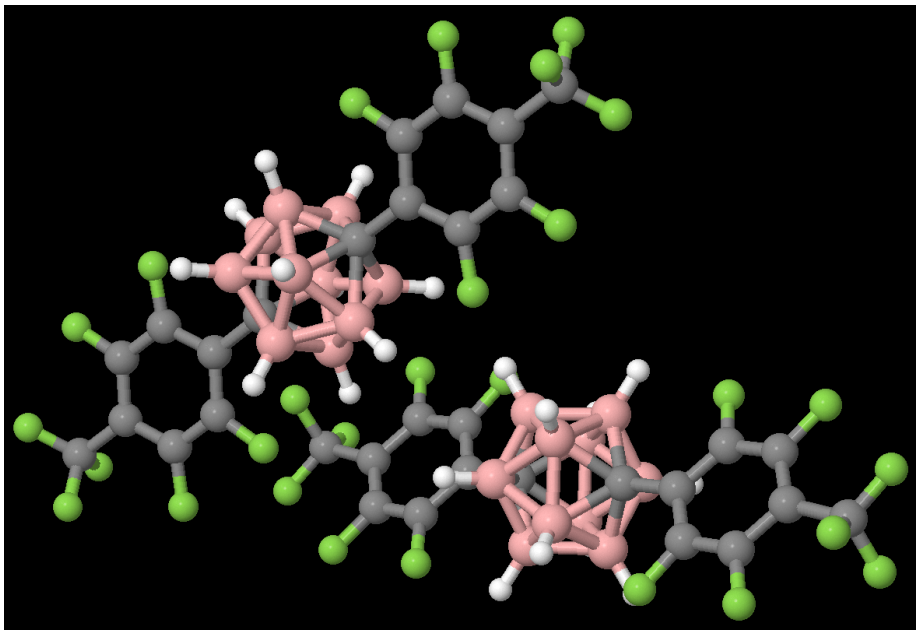


COD 7015488



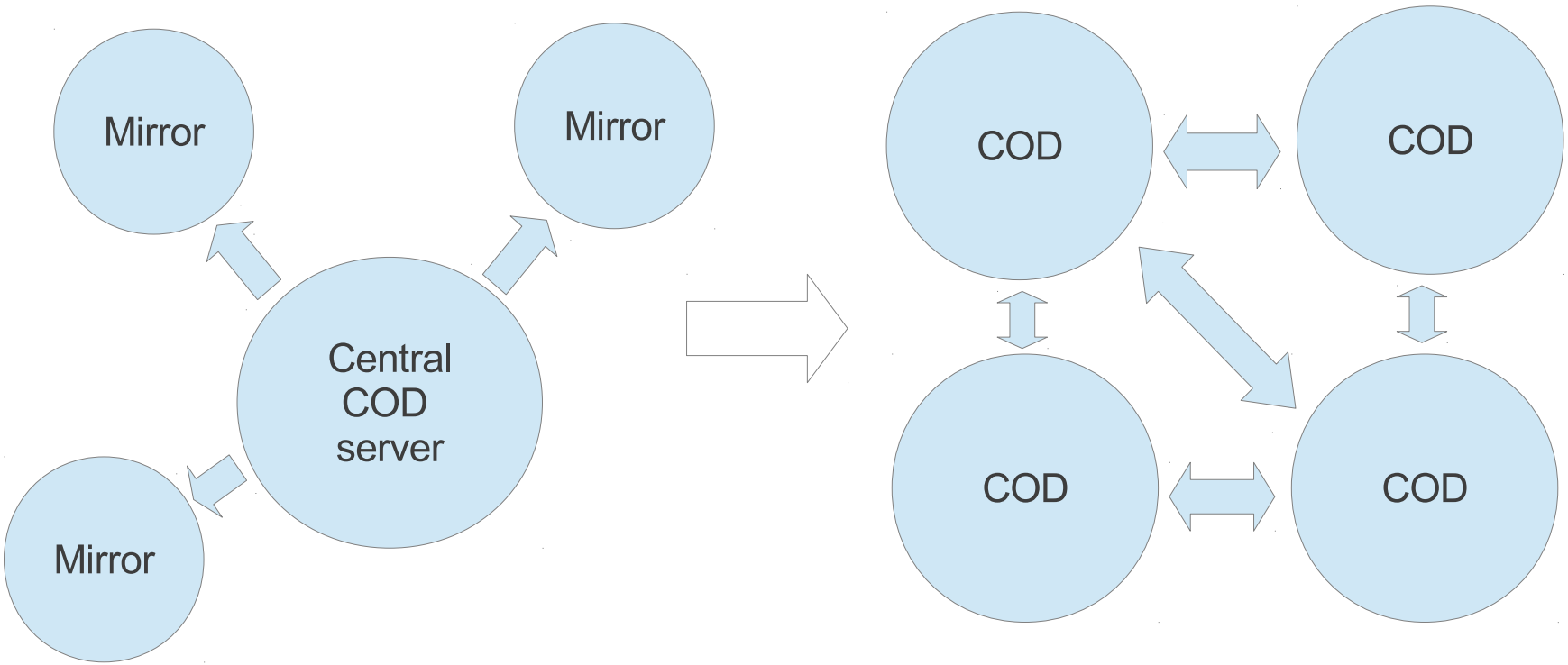
COD 7015654

# Applications

New materials (e.g. semiconductors)

New medicines

# A workbench for scientists from the whole world



# Thank you!