Improvements of the polymers representation in COD using quotient graphs

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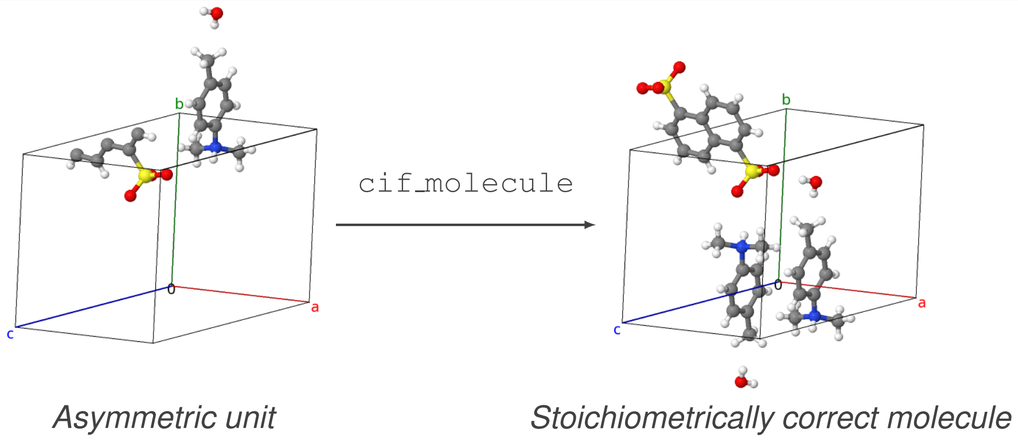
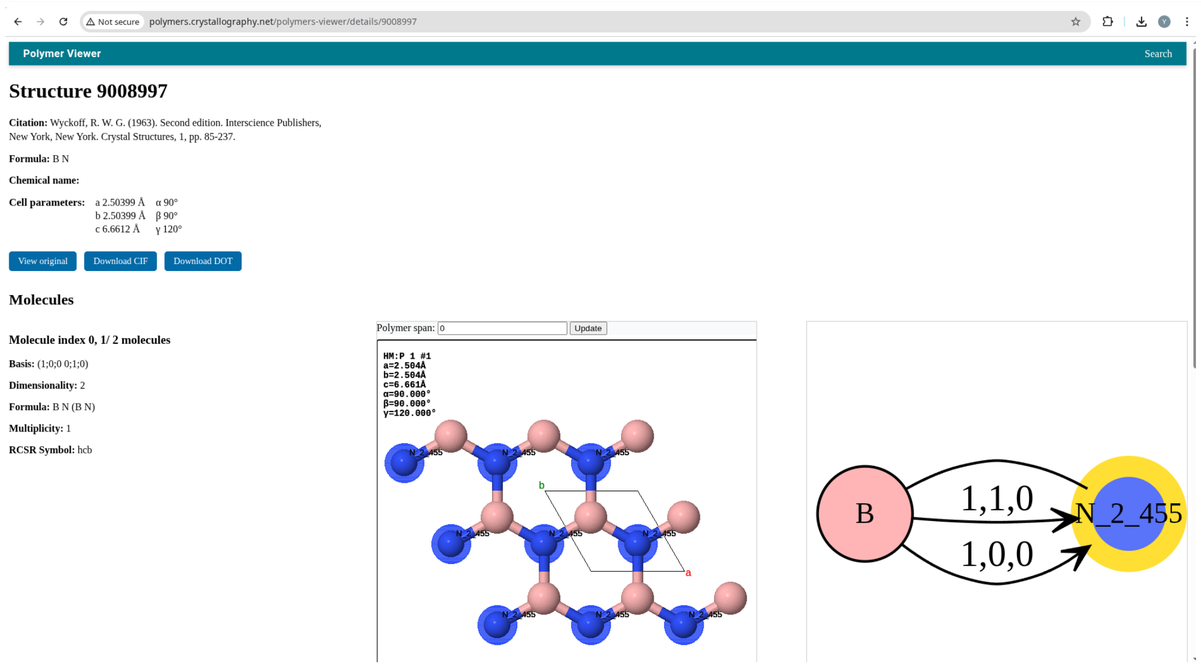
`cif_molecule` molecule reconstruction



Asymmetric unit *Stoichiometrically correct molecule*

- Reconstructs molecule from the *asymmetric unit (AU)*.
- Preserves stoichiometry.
- Part of the open-source `cod-tools` package [1].

Infinite net converting to labeled quotient graph



Web view with JSmol view and Labeled Quotient Graph (COD ID 9008997)

- To create a finite representation of an infinite net, we use *Labeled Quotient Graphs (LQG)* [2].
- Algorithm for constructing *LQG* from an infinite net:
  1. Choose a coordinate system, select basis vectors.
  2. Assign initial labels to the original vertices $(0, 0, 0)$.
  3. If the net has an edge from point $P(m, n)$ to point $R(p, q) \Rightarrow$ there is a directed edge in *LQG* with label $(p - m, q - n)$ from P to R.

Implementation of the *LQG* in `cif_molecule`

- Polymer representation as *LQG* was implemented in the *cif_molecule* and was made available in *cod-tools* release *3.11.0* [3].
- *LQG* information was added to the *cif_molecule* output expressed using *topoCIF* dictionary data items. This allows *LQG* recognition by existing software like *Jmol* [4].
- *LQG* is used to calculate dimensionality of infinite molecules [5].
- Additional programs introduced:
  - *cif2qg* to convert *LQG* from *CIF* to other formats like *graphviz* [6].
  - *cif_polymer_multiplicity* to calculate *multiplicity* [5] of a polymer (how many identical molecules in the crystal are self penetrated).
- Stoichiometry is preserved in reconstructed molecules. No more need to specify `--max-polymer-span` and `--max-polymer-atoms` parameters for infinite molecules.

References

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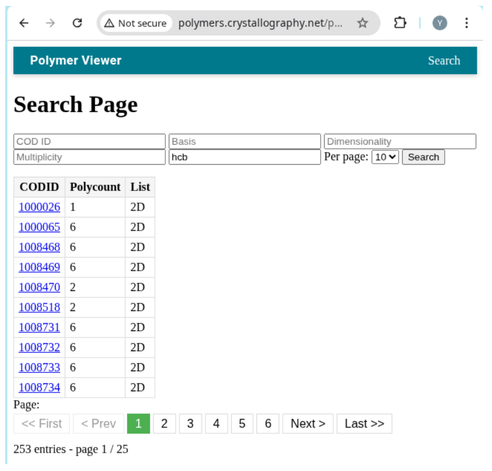
Polymer detection in the *COD*

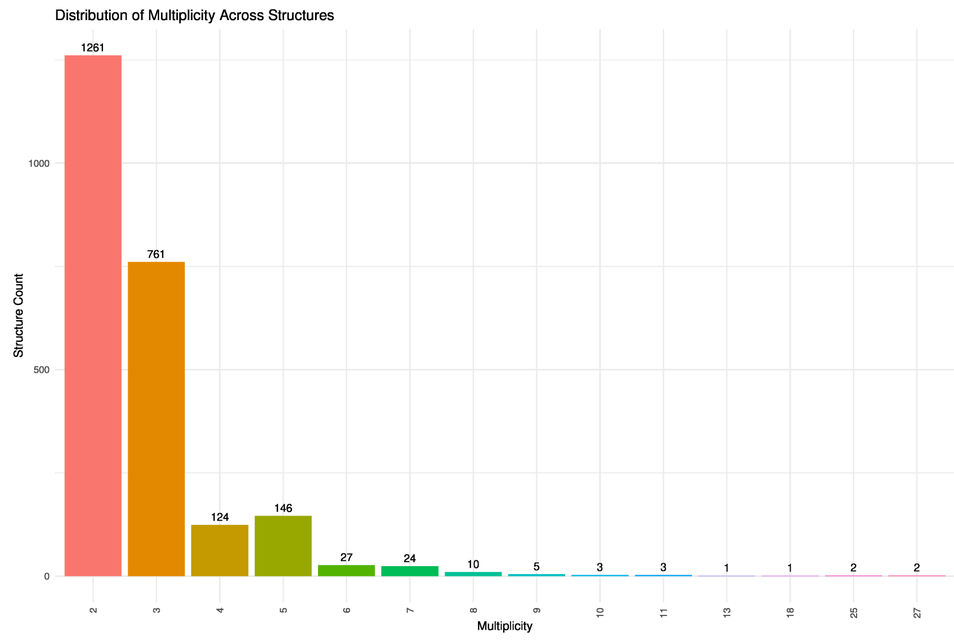
- Calculations were performed on the *Crystallography Open Database (COD)* revision *291294*.
- *multiplicities* and *RCSR* symbols [7] were calculated using *Systre* [8].



Search page of the website.

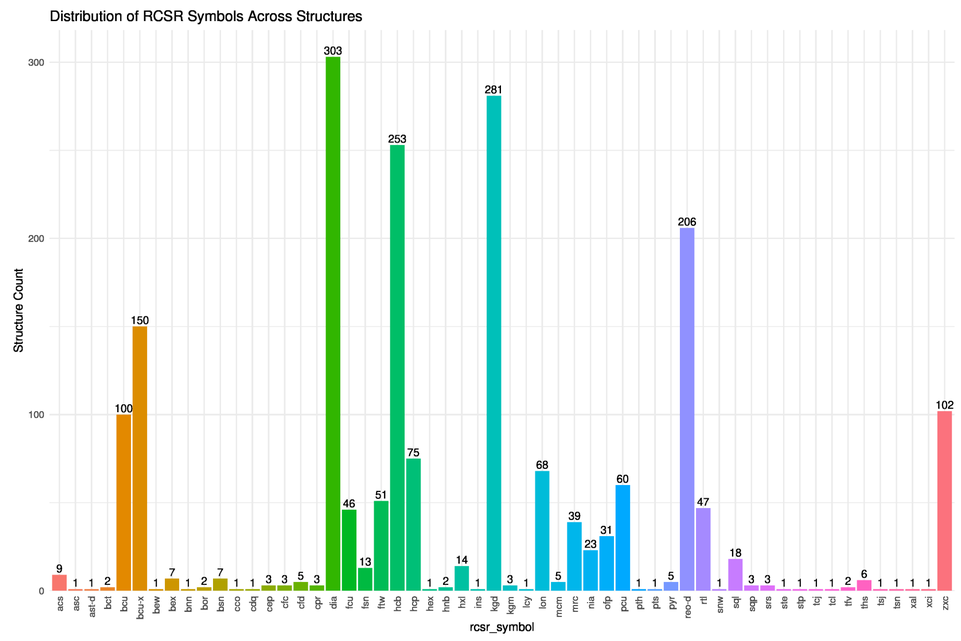
- Repository for calculations using *make* was created at `svn://databases.crystallography.lt/quotient-graphs`.
- Website to view results `http://polymers.crystallography.net/polymers-viewer`.

Multiplicities in the COD



- 2370 polymers were identified as *self-penetrated*, majority of structures have 2 molecules in the crystal.

RCSR symbols in the COD



- *Systre* identified 56 unique *RCSR* symbols. Most common are **hcb**, **dia**, and **kgm**.

Conclusions

- *LQG* allows creating finite representation of infinite polymers.
- Polymers and their dimensionality are correctly identified using *cif_molecule* with *LQG*.
- Output using *topoCIF* dictionary data items allows using *LQG* in other software.

Yaroslav Rozdobudko has no conflict of interest.
Antanas Vaitkus has no conflict of interest.
Andrius Merkys has no conflict of interest.
Saulius Gražulis has no conflict of interest.

On-line version of the poster: `https://bit.ly/4j4wO6x`