Improvements of the polymers representation in COD using quotient graphs

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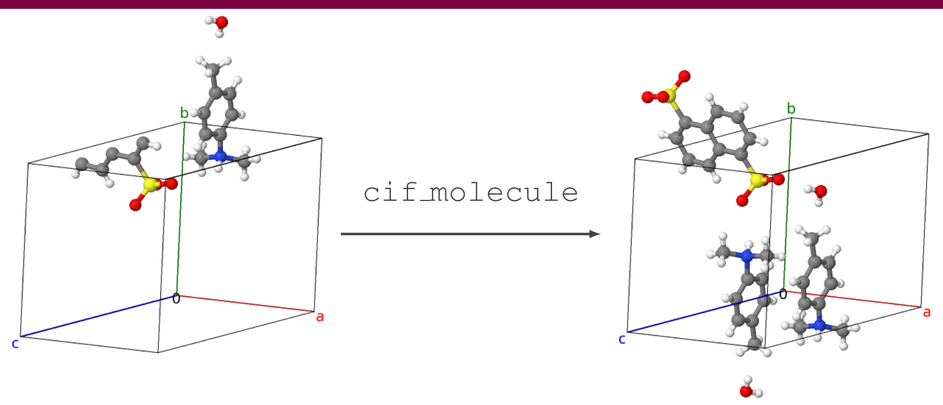
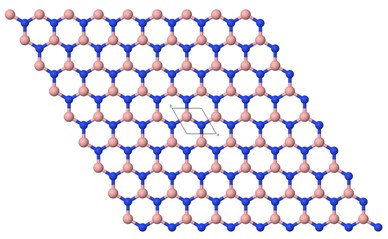
`cif_molecule` molecule reconstruction



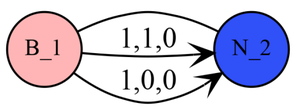
Asymmetric unit *Stoichiometrically correct molecule*

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

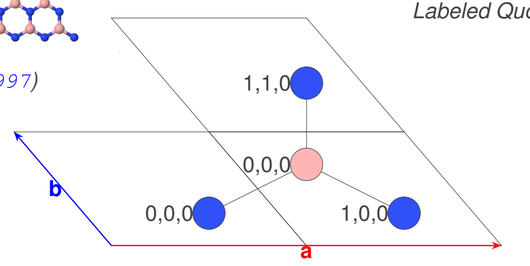
Infinite net converting to labeled quotient graph



Infinite net (COD ID 9008997)



Labeled Quotient Graph (COD ID 9008997)



Constructing Labeled Quotient Graph (LQG)

- Polymer molecules can be represented as an infinite net that spans across crystal.
- We do not know the size of the *AU* and cannot search infinitely.
- 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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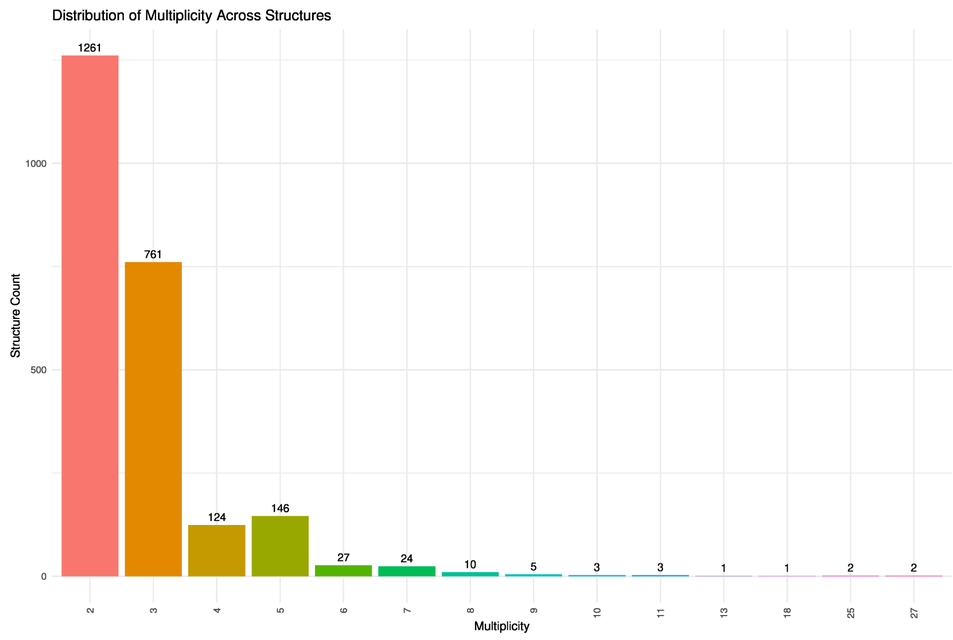
Polymer detection in the *COD*

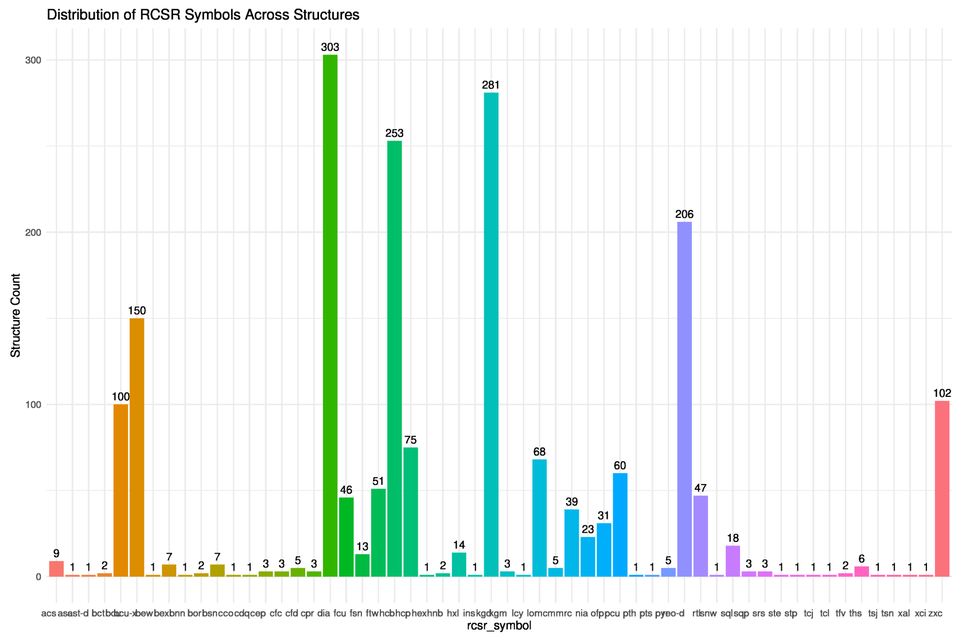
- Calculations were performed on the *Crystallography Open Database (COD)* revision *291294*. Polymers were detected and expressed as *LQG* using *cif_molecule*, *multiplicities* and *RCSR* symbols [7] were calculated using *Systre* [8]. Repository for calculations was created at `svn://databases.crystallography.lt/quotient-graphs`. Website to view results `http://polymers.crystallography.net/polymers-viewer`.
- All *CIF* outputs converted to *graphviz dot* format.
- Comparison made with calculations done on the *COD* with *cif_molecule* without *LQG* at `svn://crystallography.net/polymers-in-COD`.
- For *cif_molecule* 5 structures were not calculated (it takes long time to run).
- Multiplicity calculations were not run for 4669 files.

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`