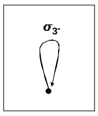

Non-Redundant Graph Representation of Polyhedral Networks

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Infinite networks of coordination polyhedra in crystal structures can be finitely represented by so-called quotient graphs or direction-labeled graphs, when detailed information on the way polyhedra are connected is not of interest [1],[2]. These finite graphs are obtained from periodic nets by graph folding based upon translational symmetries.
Taking all given symmetries into account this proceeding can be generalized such that so-called symmetry-labeled graphs are obtained [3].
Redundancy can be avoided in this representation form by checking whether edges exist which may be generated by applying symmetry operations to other edges.

A similar proceeding can be applied to polyhedra graphs [4] . In these graphs, nodes represent geometrical or topological views of polyhedra. Edges represent connections between polyhedra with polyhedra vertices involved in the connections as labels. A suitable denotation of faces in topological views allows to reflect the main characteristics of a given polyhedral network when polyhedra are assumed to be rigid bodies.
In both cases, the minimal graph forms are well-suited for enumeration processes since they allow to avoid the generation of isomorphic graphs in an early stage. A further application is the improvement of indexes supporting the efficient search for isomorphic substructures in large collections of crystal structures

Literature:

[1] Chung S.J., Hahn T., Klee W.E., *Acta Cryst.*, 1984, A40, 42-50.
[2] Goetzke K., Klein H.-J., Kandzia P., *Lect. Notes Comp. Sc.*, 1988, 314, 242-254.
[3] Klein H.-J., *Math. Modelling and Scientific Computing*, 1996, 6, 325-330.
[4] Klein H.-J., *Proc. 16th Int. Conf. SSDBM*, 2004, 255-264.

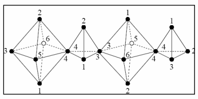
Non-redundant graph representation

Nodes: Representing coordination polyhedra as sets of faces.
Different modes:
- *topological view* (eventually including information on symmetries)
- *geometrical view* (including coordinates of vertices).

Edges: Labeled with pairs of vertex numbers.

Polyhedra graph

Face-oriented representation of polyhedra:



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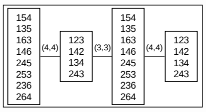
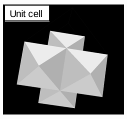
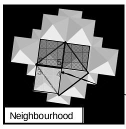
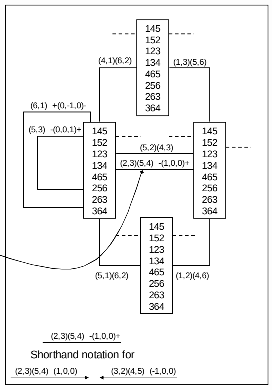


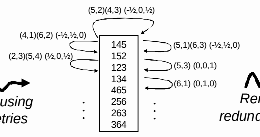






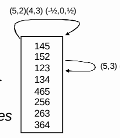
Direction-labeled polyhedra graph

Folding using symmetries



Symmetry-labeled polyhedra graph

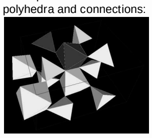
Removing redundant edges



Reduced symmetry-labeled polyhedra graph

Nodes: Representing coordination polyhedra with central atom in the asymmetric unit.
Edges: Directed and labeled with pairs of vertex numbers and symmetry operations.

Example with two kinds of polyhedra and connections:



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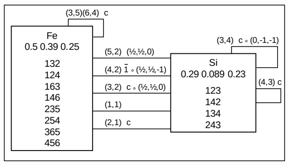
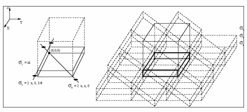


Space-group oriented enumeration of graphs

- space-group
- neighbourhood (x,y,z) of asymmetric unit
- kinds of nodes in
  - asymmetric unit (*from-to*)
  - unit cell (*maximal*)
- linkedness (corner, edge, face sharing)
- dimensionality (0,1,2,3)
- Wyckoff positions allowed for nodes (letter)
- special properties (ring sizes, pattern of polyhedra,...)



Enumeration parameters

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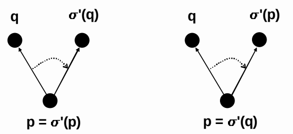
- *Generate possible labels for edges between nodes representing Wyckoff positions of the space-group (including loops).*
- *Remove edges not in conformity with parameters.*
- *Construct classes of labeled edges closed under implication by symmetries.*
- *Use representatives of classes for the enumeration process.*

Implication of edges by symmetries:

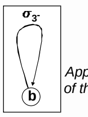


In case of loops: q = σ(p)

Example

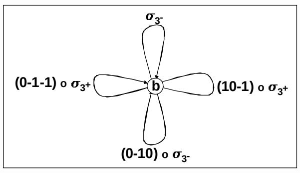
- space-group $P3_21$1
- first neighbourhood in x,y, second neighbourhood in z
- one tetrahedron in asym. unit
- corner sharing
- dimensionality 3
- Wyckoff position b

One out of four isomorphic graphs in the result of enumeration:



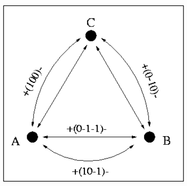
Reduced sl-graph

Applying symmetries of the space-group to edges

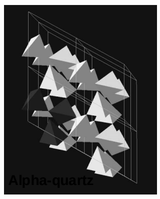


Complete sl-graph

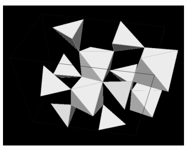
Unfolding by application of space-group symmetries



Embedding (center of gravity, simulated annealing)

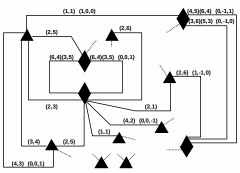


Searching for isomorphic substructures in a large set of model structures

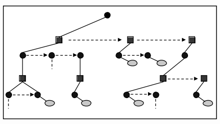


Model structure (in $Cm\bar{3}m$)

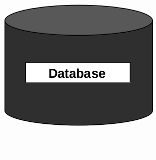
Generate polyhedra graph

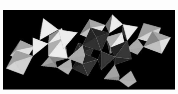


Determine chains up to some fixed length and organize them together with the chains of all other model structures in an ordered prefix tree; use symmetry information to avoid redundancy



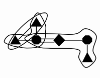
Store the index together with the data of model structures





Substructure marked for search

Determine a covering of the substructure by chains



Use the index to find candidate model structures for embedding the substructure topologically

Check possibility for geometric embedding; analyze similarity