

[s9.m31.p3](#) **Searching for Substructures in Polyhedral Topologies of Inorganic Crystal Structures.** [Hans-Joachim Klein](#), *Inst. f. Informatik u. Prakt. Mathematik, Universität Kiel, Germany. E-mail: [hjk@is.informatik.uni-kiel.de](mailto:hjk@is.informatik.uni-kiel.de)*

**Keywords: Coordination polyhedra; Polyhedra graphs; Isomorphic substructures**

When large collections of crystal structures are studied at the level of coordination polyhedra, advanced facilities for searching related figures formed by polyhedra are of interest. Well-known indexing techniques based upon predefined sets of rigid substructures such as rings, for instance, are in general difficult to apply in connection with inorganic crystal structures because of the large variety of chemical elements and patterns which have to be taken into account. Hence we have built a system based upon a representation of polyhedral topologies by graphs which uses an indexing technique not referring to special substructures but to paths in graphs. For any finite cluster of polyhedra it allows to find all possible embeddings into polyhedral topologies of a given set of crystal structures. Embeddings found at the topological level can be checked for geometric conformity with the cluster afterwards. In the representation of polyhedral topologies by so-called *polyhedra graphs*, a coordination polyhedron is represented as a single node and a connection between two polyhedra as a labelled line. With each node an ordered face representation of the corresponding polyhedron is associated. This pure topological view is generated by numbering the vertices of the polyhedron and by collecting these numbers for every face in a unique way (e.g., in clockwise order). For every pair of neighbouring polyhedra sharing a vertex, an edge, or a face the corresponding nodes of the graph are connected by a line which is labelled with the pairs of numbers of polyhedral vertices involved in the connection. This graph form allows to distinguish chains of edge-sharing pyramids, for example, even if they are identical up to the orientation of some apices. Finite graph representations can be obtained for infinite topologies by folding infinite polyhedra graphs appropriately. Depending on the intended usage of the graph representation, additional information such as symmetries or coordinates can be assigned to the nodes. For topological embedding, however, this information is not relevant. Let a finite input cluster  $C$  of polyhedra and a polyhedra graph  $P$  of a crystal structure be given.  $C$  is *topologically embeddable* into  $P$  if the polyhedra graph of  $C$  is isomorphic to a subgraph of  $P$  containing with each pair of nodes all lines between these nodes in  $P$ . To deal with the computational complexity of the subgraph isomorphism problem, the structures of a given collection are preprocessed and an index is built based upon a path enumeration for the polyhedra graphs of all structures. Using prefix trees and a fixed interval for the lengths of paths to consider, a space-saving indexation can be achieved. For the graph of the input cluster a minimal line covering by paths is determined and applied for search. This technique allows to search for substructures efficiently even in large collections of data. A web interface has been realized such that the searching functionality can be accessed on-line [1]. It is possible to mark polyhedra in a three-dimensional interactive display of a structure and to search for one or all possible topological embeddings in a given database. Qualifying structures are visualized with substructures highlighted appropriately. New structures can be added by submitting structure data as a HTML form or as a CIF file.

[1] CRYSTANA:  
<http://www.is.informatik.uni-kiel.de/~hjk/Crystana>

[s9.m31.p4](#) **Variable Temperature Experiments Performed Using Automated In-House Software.** [Mark Light](#), Simon Coles and Michael Hursthouse, *School of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, UK. E-mail: [light@soton.ac.uk](mailto:light@soton.ac.uk)*

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Variable temperature experiments have, in the past, involved a large amount of operator input and effort. As a result many interesting results may have been missed or found only as a result of serendipity. In Southampton this situation has been addressed by the development of in-house software to perform such variable temperature experiments in a fully automated manner. The code is written in PYTHON and utilises the ability of a Kappa CCD to talk to a cryostream, and the accessibility of the *collect* [1] data collection modules, classes and functions. The user is able to select the start and end temperatures (going either up or down), the ramp step and rate and a wait time to allow the cryostream to stabilise. Thus it is possible to easily study any crystalline sample over a range of temperatures (80-500K) with no human interaction. The types of experiment that can be carried out include thermal dehydration of compounds such as zeolites, parametric studies to look for effects like negative thermal expansion, phase transition location, and investigation of temperature dependant ion migration. Many of these utilise the capability of the cryostream plus to go up in temperature above ambient, as well as down. As an example a phase transitions can be located by automatically running a series of unit cell determinations over a selected range of temperatures. Once located it can be studied in more detail in full data collection mode via either a preset or calculated strategy. This poster will present the software and a series of results obtained using it.

[1] "Collect" data collection software, Nonius B.V., 1999.