MS19-P6 A knowledge database for intermetallics: the collection of Topological Types of Nanoclusters

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The main goal of our work was to develop a database containing information on structural building units in intermetallics. We have applied a universal method based on the strict algorithm of searching for the multi-shell onion-like primary nanoclusters that assemble the intermetallic compounds [1]. This "Nanoclustering" procedure was implemented in the program package ToposPro [2]. Using the information on more than 27,000 crystal structures of intermetallics from the ICSD and Pearson's Crystal Data, we have created the *Topological Types of Nanoclusters* (TTN) collection. The TTN collection contains 1006 polyhedral and 1016 multishell nanoclusters as local configurations of atoms and as primary nanoclusters in intermetallics. To illustrate the possibility of the TTN collection we have considered icosahedron-based intermetallics. Altogether, 319 ordered intermetallic compounds with centered icosahedra as primary nanoclusters were fully investigated. As a result, we have found correlations between topological parameters and chemical composition of those intermetallics. In particular, the A@M12 composition is realized in 87 compounds of which 84 assemble into **bcu-x** (body-centered cubic) motif. We have collected the distributions on chemical composition, symmetry and topological parameters in a knowledge database. It is shown that the knowledge database can be used to find possible motifs of assembling building units in intermetallics, and further, to predict new possible intermetallic compounds.

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Keywords: intermetallics, topology

MS19-P7 Rod packing nets in 3-periodic metal-organic frameworks

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The main goal of our work is creating the strict and useful taxonomy for packings of rods into metal-organic frameworks. The classification of rod-packings by the set of robust descriptors and establishing the correlations between their crystal structure and composition is very important task for design of new MOFs and prediction of their properties [1]. Using ToposPro [2] we found rod packings in 5132 coordination polymers (26.9% from the overall list of 3D coordination polymers). These structures analyzed with cluster representation gives 4805 simplified chains that consist of one set of parallel rods (only in one direction); 309 contain two sets of rods in two different directions; 16 - three directions; 2 - four directions. Classification is carried out in according with 14 types of packings described by O'Keeffe and coworkers [1, 3]. For more detailed classification we used topological type of underlying net of the structure to characterize the global topology, as well composition and coordination of ligands and bridging groups in rods to describe the local topology. The values of these descriptors will be stored in the "Knowledge database" of MOFs and can efficiently be used by "Expert system" for prediction of new MOFs with the specified set of properties and crystal structure composition [4].

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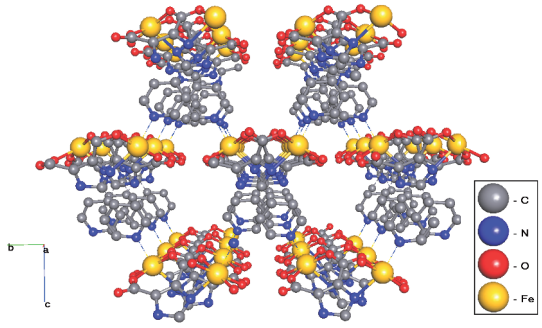

Figure 1. The parallel 1-periodic rods in 3-periodic crystal structure of $\{[Fe(HPIDC)^a(H_2O)]\cdot 2H_2O\}_n$ (some valence bond changed to hydrogen bonds). ^{a}2-(pyridin-4-yl)-1H-imidazole-4,5-dicarboxylate

Keywords: Metal-organic frameworks, topological classification, rod packings, topology of crystal structure