

FA4-MS10-P01**Topological Analysis of MOFs with Entanglements of 2-Periodic Structural Groups.**

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273 metal-organic frameworks (MOF) with entanglements of two-periodic structural groups (layers) were found by a comprehensive analysis of the Cambridge Structural Database using the program package TOPOS [1]. 163 Parallel and 108 inclined catenated layers were observed and in only in one case both modes of entanglement are realized together. TOPOS tools were applied to consider simplified representations of the structural groups as nets, where the nodes correspond to metals and/or centers of gravity of polydentate ligands. The most widespread type of topology of the layers in the simplified nets is the square net 44-sql (161 compounds); 65 MOFs have the topology of the honeycomb net 66-hcb; the third place is occupied by the topology 4.82-fes (13 cases). A strong correlation was found between the coordination type of ligand, the coordination number of central atom and the global topology of the net. Thus, in 146 compounds with the underlying topology of the square net, metal is connected to four bridge ligands. Out of them, in 122 compounds all the bridge ligands are bidentate, and in 83 compounds metal has coordination number six being connected to four bidentate-bridge and two monodentate dangled ligands. Among the compounds with the honeycomb type of topology the most frequent local topology is formed by three bidentate-bridge and two bidentate terminal (coordination number of metal is seven). It was shown, that the results obtained can be used to design the crystals containing tangled two-periodic structural groups.

Keywords: topology; entanglement; metal-organic frameworks

FA4-MS10-P02**Local and Global Topology of Two-Dimensional Structural Groups.**

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The analysis of local and global topology of two-dimensional metal-organic frameworks (MOF) in the crystal structures of 1303 coordination compounds of zinc, cadmium, copper and silver was made with the program package TOPOS (<http://www.topos.ssu.samara.ru>) [1]. 198 different types of global topologies (2D nets) were found, with the most frequent topology corresponding to square net 4⁴-sql (39,5%), followed by honeycomb net 6³-hcb (16,9%) and 4.8²-fes (7%).

The most widespread (12%) local topology of metal centers conforms to the coordination of two bidentate bridge and two monodentate terminal ligands, moreover, almost in all such cases (95%) they result in the 4⁴-sql global topology. Thus, in two-dimensional MOFs the topology of coordination centers severely determines the global topology of the net. At the same time, a given global topology can correspond to a number of local topologies to be distinguished by denticity of the ligands. We propose a general classification for these nets, where polyatomic ligands are contracted into unstructured centers of a new simplified net keeping the connectivity of the initial net. As a result, various methods of coordination of complexing atoms can be described within the same topological type of the simplified net and related to its global topology.

We have discussed the capabilities of this approach to predict the topological motifs in coordination polymers at the specified complexing atoms and ligands with a given denticity.

[1] Blatov V.A., *IUCr CompComm Newsletter*, 2006, 7, 4.

Keywords: topological aspects of structure; classification of crystal structures; computer analysis

FA4-MS10-P03**Fluorine and Crystals Disorder.**

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Fluorine atoms are typically located at the periphery of organic molecules and, when bonded to neutral groups, are characterized by very weak intermolecular interactions with any kind of atom. Consequently, perfluorocarbon derivatives (PFCs) have lower boiling point compared with hydrocarbons having comparable molecular weight and very low friction coefficient; they are also hydrophobic and lipophobic and are poorly miscible with many organic solvents. Partially fluorinated molecules show similar trends as a function of the number of fluorine atoms. Weak intermolecular interactions mean crystallization problems, too. Plastic phases, liquid crystals, amorphous glasses and structural disorder are common in fluorinated compounds. Long PFCs show steric hindrance between fluorine atoms bonded in position 1,3 on the carbon chains; their stable conformation is then helical, distorted *all-trans*, with a pitch of 27-30 C-C bonds; near always the two enantiomeric helices are found in the same crystallographic site as disordered groups. The present work will show how common this disorder is and how frequently it is ignored, also in molecules with small fluorinated residues such as -CF₃. Asking for X-CF₃ (X any atom) under the conditions *No error, Not polymer, No ions, No powder structures*, we found 8752 hits from CCDC (version November, 2008); they became 6117 with *No disorder* and 3204 also with