MS46-P2 The taxonomy of rod-packing coordination networks (CNs)

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Figure 1. The crystal structure of $[Co_2(BDC^a)_2(BPNO^b)]$ with a parallel 1-periodic rods. ^{a} 1,4-benzene-dicarboxylate ^{b} 4,4-bipyridyl-N,N-dioxide

CNs and metal-organic frameworks (MOFs) attract a great interest due to their promising applications. MOFs possess a wide number of useful properties, e.g. adsorption and catalytic activity, magnetic susceptibility, ionic and electronic conductivity[1]. At present time,more than 18500 3-periodic CNs have been synthesized and their number is steadily growing. The combination of organic ligands,metal cations and secondary building units(SBUs) allows to obtain new coordination polymers every day. Molecular groups(clusters), chains, layers and frameworks can serve as finite and polymeric SBUs. The coordination networks constructed by rod SBUs have been called rod packing (RP) MOFs[2]. The classification of structures by a range of descriptors is of major importance for establishing correlations between structure,composition and properties and for design of new materials. Such taxonomy for RP MOFs still does not exist, and it is the main goal of our work.

Using ToposPro[3], we have extracted from CSD 5.36[4] the crystal data for 2767 RP MOFs. For each structure we have determined the number of sets of parallel rods and their mutual orientation. For each such set, the orthogonal projection has been constructed. To characterize the packing pattern, the topological type has been assigned to 2-periodic net in the orthogonal projection.

It was found that the 2658 RP MOFs consist of only one set of parallel rods. Two, three, and four sets are observed in 96, four, and one structures, respectively. Classification of the rod packings is performed in accordance to the patterns described in [2,5]. In addition, we classified the RP MOFs in more details by a series of descriptors: topological types of rod and framework, composition and coordination properties of SBUs. These values will be deposited in the knowledge database of topological and geometrical relationships in RP MOFs and they will be used for prediction of new functional RP MOFs[6].

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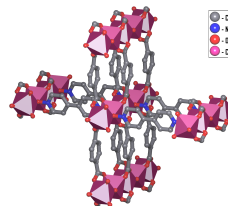6. E.V. Alexandrov,A.P. Shevchenko,A.A. Asiri,V.A. Blatov,CrystEngComm,**2015**,17,*2913*