

MS33-03 | RULES FOR DESIGNING ROD METAL-ORGANIC FRAMEWORKS: A TOPOLOGICAL APPROACH

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We present a comprehensive geometrical-topological taxonomy of 1869 metal-organic frameworks with rod secondary building units (rod MOFs) retrieved from the Cambridge Structural Database. First taxonomy of Rod MOFs was presented in [1]. Our new classification was performed with automatic tools implemented in the ToposPro program package (<https://topospro.com/>). As a result, a knowledge database that contains information on geometrical and topological properties of the MOFs and building units (ligands, linkers and rods) was created. A number of descriptors were identified for ligands (chemical formula, molecular graph, coordination mode), rods (rings, points of extension, topological type, shape), linkers (chemical formula, molecular graph, coordination number) and frameworks (rods orientations, underlying nets). Rod MOFs were arranged according to their complexity (the number and type of constituent components and value of numerical descriptors) and a number of correlations between descriptors were identified.

We have shown that these rules are useful for screening and designing rod MOFs, in particular, chemically and mechanically stable crystalline materials with „breathing“ behavior upon adsorption.

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[1] Schoedel A., Li M., Li D., O’Keeffe M., Yaghi O. M. *Chem. Rev.*, 2016, 116, 12466