Poster

A new chiral metal-organic framework with spiranes

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Chiral MOF materials are being intensively studied for specific applications such as chiral recognition, separation and catalysis. One of the main challenges of their preparation is to find suitable chiral linkers with proper size and rigidity. Spiranes are aliphatic molecules that contain at least two rings with only one common atom. This structure gives these twisted molecules exceptional stiffness. In addition, substituted spiranes can possess axial chirality, making them ideal candidates as components of chiral frameworks.

Using spiranes as chiral carbocyclic spirolinkers a new homochiral IRMOF structure, WIG-5 was prepared [1]. First the enantiopure (R)-spiro[3.3]heptane-2,6-dicarboxylic acid was synthetized than used in the reaction with zinc nitrate hexahydrate in dimethyl formamide (DMF), to prepare the MOF crystals by solvothermal method. WIG-5 crystallizes in the $P2_12_12_1$ space group, its structure is composed of tetranuclear $Zn_4O(CO_2)_6(DMF)_2$ SBUs at the vertices and (*R*)-spiro[3.3]heptane-2,6-dicarboxylic acid linkers at the edges. Similar to MOF-5, WIG-5 has a **pcu** underlying network topology and tetranuclear zinc-containing SBUs. The coordination of two DMF molecules to the SBUs results in the formation of a distorted MOF-5-like structure and two additional non-coordinating DMF molecules are present in the voids. The crystal structure is built up of two interpenetrating 3D polymer networks (Fig.1.) and contains narrow pore channels that can be accessed only by small molecules with $R \leq 1.67$Å. Here we also compare the main features of the crystal structures of three similar MOF materials with similar sized rigid linkers: therephtalic acid, cubane dicarboxylate [2, 3] and this spirane compound.

The single crystals of WIG-5 with dimensions from 100 μm up to a millimeter show birefringence, enabling potential non-linear optical applications of the new spirane-based homochiral MOF structure.

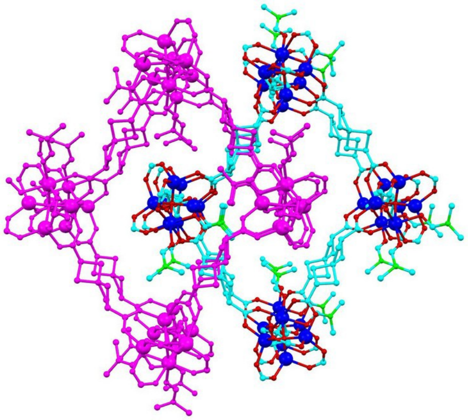

Figure 1. Interpenetrating network of WIG-5.

[1] Földes, D., Kováts, É., Bortel, G., Kamarás, K., Tarczay, G., Jakab, E., Pekker, S. (2022) *Journal of Molecular Structure* **1257**, 132538

[2] Földes, D., Kováts, É., Bortel, G., Klébert, S., Jakab, E., Pekker, S. (2020) *ChemRxiv*. doi:10.26434/chemrxiv.11854389.v1

[3] Macreadie, L.K., Mensforth, E.J., Babarao, R., Konstas, K., Telfer, S.G., Doherty, C.M., Tsanaktsidis, J., Batten, S.R., Hil, M.R. (2019) *Journal of the American Chemical Society*, **141**, 3828–3832.