New terephthalate 3D-MOF based on Y_6 cluster

V. Tsonis[a], P. Oikonomopoulos[a], G. S. Papaefstathiou[a]

[a]*Laboratory of Inorganic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Zografou GR-15771, Greece*

e-mail: vastsonis@chem.uoa.gr

MOFs are crystalline, porous materials that consist of metal ions or clusters (SBUs) connected by organic molecules acting as bridging ligands. These create 2 or 3 – dimensional coordination networks which are of great scientific importance due to their pores being able to absorb various molecules, and thus have multiple applications. UiO-66 is one of the most well-known MOFs in the field of coordination chemistry. It is formed by 12-coordinated Zr_6 clusters that are bridged by the dianions of terephthalic acid (BDC).[1] What sets it apart from most other MOFs is its porous network which results in a high surface area and exceptional thermal stability, as well as the ability to use various BDC derivatives (usually NH_2-BDC), making it highly modular.[2]

In our laboratory we have been working a lot with isophthalic acid, since no MOFs have been reported to utilize it alongside the Zr_6 cluster. Thus, we wondered what would happen if we combined both isophthalic and terephthalic acid, intending for them to simultaneously react with the hexanuclear cluster. The difference is that Yttrium was used instead of Zirconium to form the hexanuclear cluster, as it is easier to obtain single crystals with it. As a result, we obtained a new MOF based on the Y_6 clusters which are bridged only by terephthalates, whereas the isophthalic acid acts as a modulator. Its role seems to lead to a new structure, depending on the reaction conditions as well, while some of the other products we obtained were known structures such as the Yttrium analogues of UiO-66.

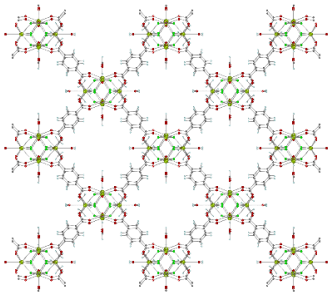

Figure 1: The 3D crystalline structure of the new Y-MOF down the crystallographic axis a.

References:

[1] B. Mu, J. Winarta, B. Shan, S. M. Mcintyre, L. Ye, C. Wang, J. Liu, Cryst. Growth Des. 2020, 20, 2, 1347–1362

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