MS33-P120 - LATE | THE CRYSTALLINE SPONGE METHOD FOR THE STRUCTURAL DETERMINATION OF NON-CRYSTALLINE COMPOUNDS USING METAL ORGANIC FRAMEWORK

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The crystalline sponge method [1,2] allows the absolute structural determination of non-crystalline compounds such as powder, amorphous solid, liquid, volatile matter or oily state. It involves using a porous framework material such as metal-organic frameworks (MOFs) as crystalline sponge, into which non-crystalline compounds in the solution can be soaked and arrange themselves in a regular pattern with the help of specific interactions between MOF pores and the guests. Thus, allowing molecular structure determination of non-crystalline compounds along with the framework via single crystal X-ray diffraction.

We are focused on structure determination of terpenoids into the pores of $[\{(Znl_2)_3(tris(4-pyridyl)-1,3,5-triazine)_2 \cdot x(solvent)_n]$ MOF or crystalline sponge. In this work, we present two novel inclusion compounds with geraniol and θ -damascone in the pores $[\{(Znl_2)_3(tris(4-pyridyl)-1,3,5-triazine)_2 \cdot x(solvent)_n]$ crystalline sponge along with the experimental details and showing guest-host interactions.

[1] Y. Inokuma, S. Yoshioka, J. Ariyoshi, T. Arai, Y. Hitora, K. Takada, S. Matsunaga, K. Rissanen and M. Fujita, *Nature*, 2013, **501**, 262–262.

[2] M. Hoshino, A. Khutia, H. Xing, Y. Inokuma and M. Fujita, *IUCrJ*, 2016, **3**, 139–151.