MS33-P122 - LATE | USING METAL ORGANIC FRAMEWORKS TO DETERMINE THE CRYSTAL STRUCTURES OF NON-CRYSTALLINE COMPOUNDS

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Publication of the crystalline sponge (CS) method by Fujita *et al.* in 2013[1] provided a major advancement in the structural elucidation of non-crystalline compounds using single crystal X-ray diffraction. This method involves soaking a metal-organic framework (MOF) in a solution of the target compound, the target can then enter the MOF pores where it is ordered and held in place by host-guest intermolecular interactions. The most commonly used crystalline sponge, $\{[(ZnX_2)_3(TPT)_2].x(\text{solvent})\}_n$ (TPT = 2,4,6-Tri(4-Pyridyl)-1,3,5-triazine), is limited by the size (8 x 5 $Å^2$) and the hydrophobic nature of the pores, therefore, alternative MOFs are needed to overcome these limitations.

In this work, novel inclusion complexes of a fungicide and herbicide are reported within the pores of the host $\{[(ZnBr_2)_3(TPT)_2].x(CHCl_3)\}_n$. Additionally, simple aromatic compounds were successfully encapsulated into a copper-based MOF which was investigated as a crystalline host due to the hydrophilic nature of the MOF, suitable pore sizes (24 Å x 9.6 Å and 12.7 Å x 12.7 Å) and low symmetry space group ($P2_1/c$).