

MS35-P03**Solvomorphism in the active pharmaceutical ingredient bismuth subgallate: microporous 1D, 2D and 3D coordination polymers**

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Bismuth is heaviest nonradioactive metal, yet its compounds generally have very low toxicity and have been used as active pharmaceutical ingredients (APIs) for nearly three centuries. Bismuth subgallate, a compound comprising of Bi³⁺ cations and the organic ligand gallic acid, has been used in medical applications since at least the 1890s for its antimicrobial, hemostatic, astringent, and deodorizing properties. The material has been used in wound therapy and the treatment of gastrointestinal disorders, and is still used as the API in several over-the-counter drugs today. Yet, despite its century-long use in medical applications, the crystal structure of bismuth subgallate long remained elusive due to complications that arise from its small crystal size.

We recently determined the crystal structure of bismuth subgallate, using continuous rotation electron diffraction. The technique, which is performed in a transmission electron microscope (TEM), allows for the fast acquisition of 3D diffraction data on crystals with diameters on the nanometer length scale.[1] The very fast data acquisition of 3D data, which takes 1-3 minutes in total, is essential for minimizing beam damage to the crystals. Structure determination of bismuth subgallate revealed that the material is a microporous 1D coordination polymer.[2] Knowledge of the structure led to the discovery of new properties of the materials. Gas sorption experiments indicated a high selectivity for CO₂/N₂ gas separation; the crystal structure was observed to be rather robust for a coordination polymer and remains intact even after stirring the material in HCl solution (pH = 2) and phosphate buffered saline solution for at least several hours. Two novel solvomorphs of bismuth gallate were also synthesized and their structures were also solved by continuous rotation electron diffraction. One is a 3D framework structure consisting of bismuth-oxo rods, while the other consists of the same rods but condensed into layers resulting in a 2D layered crystal structure.

References:

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MS35-P04**Design of new bi- and tri-periodic indium MOFs and their catalytic activity in the Strecker and Ugi multicomponents reactions**

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Metal-organic Frameworks (MOFs) are a type of materials made of the combination of organic linkers and metal centres. [1] Our group has extensively carried out research focused on the design and preparation of MOFs with group 13-elements, which have shown great potential in the field of heterogeneous catalysis. [2] In particular, indium-MOFs have shown remarkable activity as Lewis-acid catalysts for multicomponent reactions (MCRs) such as Strecker and Ugi reactions (involving the reaction of ketones, amines and cyanides in the former, and aldehydes, amines, carboxylic acids and cyanides in the later). With the use of In-MOFs, these MCRs can be carried out in one step and under Green conditions by reducing the amount of solvent, at room temperature, and reaching high yields. We have prepared three different MOFs with the combination of indium and the tritopic linker 1,3,5-Tris(4-carboxyphenyl)benzene (H₃btb), denoted InPF-110, InPF-50, and InPF-51. InPF-110 exhibits a mesoporous, three-periodic structure formed by trimetric inorganic secondary building unit with the metal centres in octahedral coordination environment. This MOF, which allows the diffusion of multiple substrate inside the pores, has demonstrated exceptional activity in the Strecker reaction. On the other hand, InPF-50 and InPF-51 exhibit two periodic structures with entangled layers. Presence of metal centers with low coordination number, large number of accessible open-metal sites, and presence of Lewis basic centers result in excellent catalytic activity of these MOFs in the Ugi reaction.

References:

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