MS31-P07 | Breathing Metal-Organic Frameworks Based On Flexible Inorganic Building Units

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Bismuth is a fairly inexpensive heavy metal and its compounds generally have low toxicity (i.e. significantly less than NaCl) and have been used as active pharmaceutical ingredients (APIs) for centuries. Despite these features, few nanoporous metal-organic frameworks (MOFs) have been built using bismuth cations. Our ongoing investigations on bismuth-MOFs have repeatedly shown framework flexibility. Typically, the breathing effect in MOFs (the reversible opening and closing of the framework as a response to its environment) is permitted by a flexible range of bond angles between the metal cation and the ligand. Through a combination of electron diffraction [1-3] and X-ray powder diffraction, we established that different mechanisms are responsible for the dynamic features in bismuth-based systems.

We have recently developed a new MOF, SU-100, containing Bi_2O_{12} inorganic building units (IBUs). Unlike most other breathing MOFs, flexibility of SU-100 is largely attributed to deformations of the IBU made possible by the flexible coordination geometry around the Bi(III) cations. We have also developed novel pseudo-polymorphs of the API bismuth subgallate [4], one of which is a breathing MOF. Two types of metal-ligand interactions are observed, strong and rigid chelation, as well as weaker interactions which give rise to framework flexibility.

[1] Nannenga, B.L. *et al.* (2014) *Nat. Methods*, **11**, 927-931.
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[3] Cichocka M.O. et al. (2018) *J. Appl. Crystallogr.* **51**, 1652-1661.
[4] Wang, Y. *et al*. (2017) *Chem. Commun.*, **53**, 7018-7021.