

Poster Presentation

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Structural elucidation of multi-cation arrangements in metal-organic frameworks.

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Metal-organic frameworks, MOFs, comprising multiple metal cations [1] have been shown to be of interest as they might exhibit different and/or enhanced properties compared to their single-metal counterparts. For example, it has been proved that it is possible to tune the heterogeneous catalytic activity of solid solution MOFs in complex multicomponent reactions by adjusting the selected metal ratios [2].

Herein, we report a series of isostructural MOFs prepared by the combination of multiple metal elements, and the same organic linker. Zinc, cobalt, manganese, and calcium have been selected and combined using different molar ratios, to produce porous MOFs where the distribution of the metal cations in the inorganic secondary building units (SBUs) is controllable. The structure of the resulting MOFs has been determined with the combination of single crystal X-ray, and powder neutron diffraction, along with electron microscopy and spectroscopic techniques. Thus, variations in lattice parameters and symmetry have been observed, and determined to be related to the occupation of the different cations within the inorganic SBUs. Furthermore, temperature variable powder neutron diffraction experiments show that these changes might be triggered by temperature variations, and are determined by the selected cation molar ratios.

[1] Wang, L. J. et al. Inorg. Chem. 2014, 53, 5881

[2] Aguirre-Diaz, L. M. et al. J. Am. Chem. Soc. 2015, 137, 6132

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