New Zn MOFs, topological relationships.

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The worldwide researchers’ attention in design and synthesis of new kinds of coordination networks and metal organic frameworks (MOFs) “on demand” is continuously increasing due to the wide range of the potential applications of these materials: heterogeneous catalysis, separation of mixtures, gas storage, drug delivery, energy and luminescent devices... As properties depend strongly on the structure of the material, when designing new materials focused on desired properties, it is important to take into account the convolution of the properties of the central cationic atom and the ones from the chosen ligand, leading to a periodic crystal structure. As an extension of our previous work on Zn MOFs with the bent ligand 2,2-Bis(4-carboxyphenyl)hexafluoropropane (L1 from now on) and trying to increase the pore size of one compound synthetized by our research group some years ago, Zn(C17O4H8F6)6 [3] we present here a polymorph: [Zn(C4O3H3F3)2] [Zn2(HL1)3(L1)0.5] [ZnO(HL1)pyrazol] with an interesting interpenetrated structure, and [Zn(C6O4H4N6)] in which the ligand does not take part in the framework. By replacing L1, with 4,4’-(Hexafluoroisopropylidene)diphthalic anhydride L2 two new MOFs: [Zn3(H2O)(HL2)2][H2O]0.36, and [Zn2O(HL2)1.5 (C6H12N2)1.5], were obtained. Comparisons with that previously reported by Zou et al. [5] [Zn2(C6O3H6F6)3] will be established. Complete synthetic and crystallographic details of the five new compounds will also be shown.

Keywords: Zn MOFs; crystal structure; topology.

Solid-State Structural Transformations from 2D Interdigitated Layers to 3D Interpenetrated Structures. Raghavender Medishetty, Prof. Jagadese J. Vittal, Department of Chemistry, National University of Singapore, 3, Science Drive 3, Singapore 117543 E-mail: raghavender@nus.edu.sg

Crystal engineering of coordination driven functional materials with multidimensional architectures is of interest for the past two decades. This is due to wide range of applications like gas storage, separation, catalysis. Of these interdigitating two-dimensional (2D) coordination polymers have been found to exhibit dynamic behavior, gate opening properties, provide platform for various surface conversions and selective guest trapping. In addition to the expansion/shrinkage of the 2D layered structures by the guest molecules, the transformation between the 2D and 3D frameworks is expected to lead to large differences in their structural and functional behaviors. Such solid-state transformations can be achieved by heat, light, guest removal or uptake. We are interested to fine tune the photo-reactivity of the interdigitated 2D coordination polymeric sheets. We are interested in fine tuning the photo-reactivity of the interdigitated 2D coordination polymeric sheets. In our recent work,[1] we describes a novel photo-induced solid-state transformation of a 2D interdigitated coordination polymer to a 3D interpenetrated structure. Interestingly, one of the two 2D structures investigated, one was accompanied by Single crystal to Single crystal (SCSC) manner, which seem to be unprecedented. Probably for the first time, we used a photo reactive terminal ligand which leads to a photo induced solid state transformation to higher dimensional network structure. This provides a new route to synthesize a 3D coordination polymer by non-self-assembly method using a retrosynthetic approach.

Fig. 1. Schematic diagram shows the structural transformation of 2D interdigitated layer to 3D MOF.

Keywords: isostuctural ligands · metal-organic frameworks · photo cycloaddition · single-crystal-to-single-crystal transformation.