

Poster Presentation

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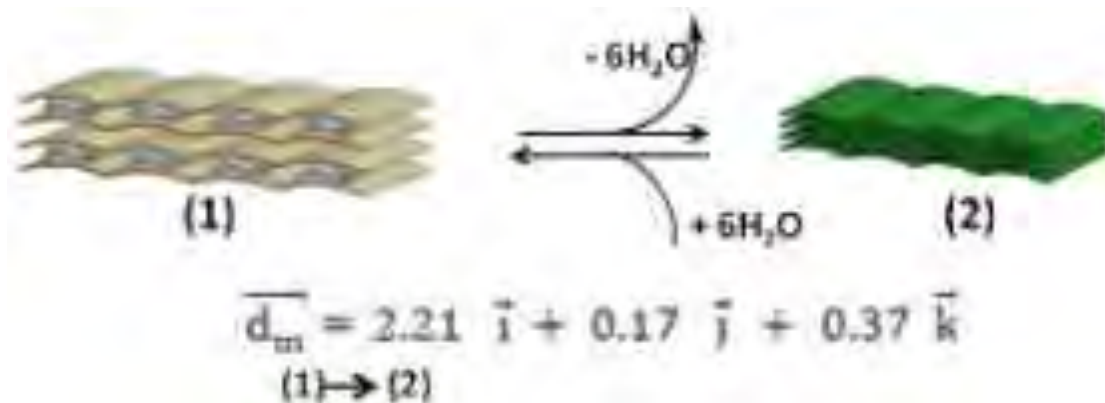
Dynamic porous property in a new heterometallic supramolecular compound

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Supramolecular compounds have attracted considerable interest to chemists, physicists and materials scientists due to their fascinating structures and potential applications as porosity [1-3] but one of the most appealing aims today, is to build multifunctional compounds. We are interested to rationalize the synthesis of porous heterometallic compounds by self-assembly via hydrogen bonds. In this communication, we present a stacked 2D Catena- $\{Co(amp)_3Cr(ox)_3 \cdot 6H_2O\}$ (amp = 2-picolyamine, ox=oxalate). It is built by layers in which both $(Co(amp)_3)^{3+}$ (D) and $(Cr(ox)_3)^{-}$ (A) ionic units are linked in a repeating DADADA...pattern along both the a and c axis with four and two hydrogen bonds respectively. These layers host very well resolved dodecameric discrete ring water clusters (R12) built by six independent molecules located around the centrosymmetric Wyckoff position's of the P21/n space group in which the compound crystallizes. The clusters are ranged along the [001] direction, occupy 807.6 \AA^3 (23.9%) of the unit cell and have a chair conformation via 10 hydrogen bonds. The dehydration process of the compound occurs in one step around 77°C and the dehydrated compound remains crystalline although all framework atoms move by 2.25 \AA along a mean vector ($d_m = 2.21 \text{ i} + 0.17 \text{ j} + 0.37 \text{ k}$) during the process. The unit cell is then reduced by 12.34 % along a, 12.22% along b and 2.03% along c reducing V by 22.03%. By exposure to air, the regeneration of the compound needs 90 min, following the first kinetic Avrami's model.

[1] C.-C. Wang, C.-T. Yeh, Y.-T. Cheng, et al., *CrystEngComm*, 2012, 14, 4637-4643, [2] A. C. Soegiarto, A. Comotti, M. D. Ward, et al., *J. Am. Chem. Soc.*, 2010, 132, 14603-14616, [3] M. S. Deshpande, A. S. Kumbhar, V. G. Puranik, et al., *Cryst. Growth Des.*, 2008, 8, 1952-1960



Keywords: hydrogen bonds, dynamic porous property, Single Crystal and Powder diffraction