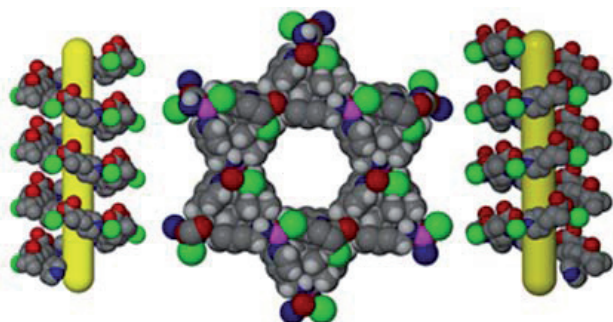


MS87.P11

Acta Cryst. (2011) A67, C752**Homochiral metal organic framework with *unh*-Topology**Subash Chandra Sahoo, Tanay Kundu, and Rahul Banerjee, *Physical/Materials Chemistry Division, National Chemical Laboratory, Pune 411008, (India)*. E-mail: sc.sahoo@ncl.res.in

Four new homochiral metal organic frameworks using amino acid derived links as a pure chiral precursor named, $[Zn(l/d\text{-Val-Py})(X)](H_2O)$ (**1-4**), $[X = Cl^-$ (**1,3**), Br^- (**2,4**)] have been synthesized from aqueous media via solvothermal route and characterized by single-crystal X-ray diffraction. Structural analysis reveals that a 3D MOF with a 1D channel in the direction of c-axis were formed having a pore aperture of $\sim 13\text{\AA}$. All the structures form a rare zeolitic topology i.e. *unh* type, which is not reported so far in the literature. The guest water molecule sits inside the 1D channel in a helical fashion and can be removed without affecting the crystal structure as revealed from TGA analysis. The anions used in these reaction systems (either from metal or ligand source) play a crucial role in formation of 3D structure. The structures with desired topology forms only when the ligand source is either pure *l* or *d* but in from the racemic. Applications of these chiral MOFs towards catalytic or chiral separations under process in our lab. Owing to the importance of chiral MOFs for various applications as shown by Web lin et.al and others¹⁻³, we believe that the successful synthesis of these four chiral MOFs form a easy chiral source like amino acids, will open up new vistas in the search for useful applications.



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Keywords: porous, homochiral, zeolitic

MS87.P12

Acta Cryst. (2011) A67, C752**1D and 2D Zn(II) and Cd(II) sulfates with bipyridine and dioxime ligands**Eduard B. Coropceanu,^a Lilia Croitor,^b Anatolii V. Siminel,^b Victor Ch. Kravtsov,^b Marina S. Fonari,^b ^a*Institute of Chemistry Academy of Sciences of R. Moldova, Academy str., 3 MD2028, Chisinau, (Moldova)*. ^b*Institute of Applied Physics Academy of Sciences of R. Moldova, Academy str., 5 MD2028, Chisinau, (Moldova)*. E-mail: ecoropceanu@yahoo.com

Nowadays extensive researches contribute to elaborating low-dimensional coordination compounds with the wheel-and-axle (WAA) geometry which similar to 3D metal-organic frameworks (MOFs) are capable to accommodate small molecules [1-3]. Being in line with these investigations we report herein the products of interaction of Zn(II) or

Cd(II) sulfate with 4,4'-bipyridine (bpy) or 4,4'-bipyridinethane(bpe) in the presence of 1,2-cyclohexanedionedioxime (NioxH₂) which represent four novel polymeric compounds with the compositions $\{[Zn(H_2O)_6][Zn(SO_4)_2(H_2O)_2(bpy)][Zn(SO_4)(H_2O)_3(bpy)]\}_n$ (**1**), $\{[Zn(SO_4)(NioxH_2)(bpy)] \cdot 0.5H_2O \cdot DMF\}_n$ (**2**), $[Zn(SO_4)(NioxH_2)(bpe)]_n$ (**3**), and $[Cd(SO_4)(NioxH_2)(bpe)]_n$ (**4**) [4]. All compounds are characterized by spectroscopic techniques and single crystal X-ray method. Compound **1** crystallizes in the triclinic non-centrosymmetric *P1* (No.1) space group. The bpy molecules as bridging ligands generate two types of linear chains, differing by the number of sulfate anions and water molecules coordinated to the metal center. The adjacent chains are arranged in a cross-like fashion at the midpoints of the bpy ligands and form the rhombic channels along the *a*-axis. The $[Zn(H_2O)_6]^{2+}$ cations are located within the structure channels and serve as structure-directing templates. The hydrogen bonds between the coordinated water molecules and sulfate anions contribute to the crystal stability. The chiral layer coordination polymer built up from the helices of the same handedness is the robust structural motif in **2-4**. The NioxH₂ bulky ligand and the tetrahedral sulfate anion impose the asymmetry around the metal center that provides an access to the chiral structural motifs in the form of porous layers. Although compounds **3** and **4** were isolated in the same crystallization conditions, the layers of opposite chirality constitute the achiral (**3**, sp. gr. *P2₁/n*), and the layers of the same chirality result in chiral (**4**, sp. gr. *P2₁2₁2₁*) architectures. The mode of sulfate-anion coordination to the metal center makes main impact on the dimensionality of the final coordination compounds, while the differences in the metal radii for Zn(II) and Cd(II) atoms and in the conformation of the bidentate bipyridine ligands prove to be not decisive for the final architecture resulting in the formation of supramolecular isomers differing by the packing of the similar layers. The low packing efficacy of **2-4** with the WAA structure topology provides the possibility of small molecules inclusion in the interlayer space. All compounds reveal blue luminescent properties.

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Keywords: cadmium(II), zinc(II), chirality

MS87.P13

Acta Cryst. (2011) A67, C752-C753**Synthesis and crystal structure of a new cadmium coordination polymer with 2-(pyrazol-1-yl)-2-thiazoline (PyTn)**R. Pedrero-Marín, F. Luna-Giles, A. Bernalte-García, F. J. Barros-García, E. Viñuelas-Zahinos, P. Torres-García, *Organic and Inorganic Chemistry Department, Universidad de Extremadura, Badajoz (Spain)*. E-mail: rospema@unex.es

We report here the synthesis and crystal structure of the coordination polymer $[Cd(\mu\text{-Cl})_2(PyTn)]_n$. For the synthesis of this compound, ethanol-water solutions of $CdCl_2 \cdot 2.5H_2O$ and PyTn [1] (1:1 ratio) were mixed, precipitating a white solid that was recrystallized from water. Colourless, plate crystals were obtained by slow evaporation of the solvent.

Unit cells are orthorhombic [$a = 7.315(1)\text{\AA}$, $b = 9.083(1)\text{\AA}$, $c = 29.698(1)\text{\AA}$, $V = 1973(3)\text{\AA}^3$, space group *Pca2₁*, $Z = 8$], each one