Novel Chiral MOFs Constructed by both Mixed Metals and Dicarboxylate Ligands. 

Keywords: cyanide complexes, molecular magnets, crystal engineering

Novel Chiral MOFs Constructed by both Mixed Metals and Dicarboxylate Ligands. Zakarane Amghouz, Laura Roces, José R. García, Santiago García-Granda, Badredine Souhail, Luis Mafra, Faniian Shi, João Rocha, *Departamento de Química Física y Analítica y Química Orgánica e Inorgánica, Universidad de Oviedo, Spain. †Departement de Chimie, Faculté des Sciences, Université Abdelmalek Essaâdi, Tétouan, Morocco. ‡Department of Chemistry, CICECO, University of Aveiro, Portugal.

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Metal–Organic Frameworks (MOFs), also known as coordination polymers, materials composed of metal ions or metal clusters as nodes and multifunctional organic linkers, are currently one of the most active and attractive research fields in the materials science, owing to their wide variety of fascinating architectures and topologies, and their wide range of potential applications in gas storage and separation, catalysis, magnetism, luminescence, and so on. Those properties provide many possibilities to construct attractive multifunctional materials. The design of chiral MOFs attracts much attention recently because of their potential applications in asymmetric catalysis and chiral separation [1,2]. Nevertheless, the attempts for construction of chiral lanthanides-based MOFs are still rare [3,4] and even more challenging than those based on transition metals. Herein, we will confine ourselves to report two novel chiral Yttrium-based MOFs with fascinating architectures, as first example up to now, of chiral structure containing both mixed Y(III)-Na(I) metals and chiral flexible-achiral rigid dicarboxylate ligands, obtained as single phase under hydrothermal conditions. Their structures were solved by single crystal XRD, and characterized by 13 C CPMAS NMR, thermal analyses (TG-MS and DSC) and X-ray thermodiffractometry. The crystallographic data of the complexes is given below: C_{11}H_{9}CoN_{7}O_{2}, monoclinic C2/c, a=14.469(2), b=9.161(1) Å, c=12.658(1) Å, β=122.10(1)°, Z=4, D=1.655Mg/m 3. (Data/parameters)= 1459/106, I>2σ →0.0371, 0.1229, GOF=1.142, Δρ_{max}→0.680, -0.408 e.Å -3, λ=0.71073 Å.

Two New Co(II) Complexes with NNN Type Pyrazol Ligands (Mat2006–01997, Factoría de Cristalización Consolider Ingenio 2010 and FPI grant BES-2007-14340), and FEDER founding, is acknowledged.

Figure 26: (A) Synthesis of Bis-2,6(3,5-dimethylpyrazol-1-yl)pyridine (dmpp) and cyanate ions, however, the result was not as expected, mononuclear Co(II) complexes were obtained instead. In this study, Bis-2,6(Pyrazol-1-yl)pyridine (pp) and Bis-2,6-(3,5-dimethylpyrazol-1-yl)pyridine (dmpp) have been used to obtain, two completely different complexes. The complex synthesized with Bis-2,6(Pyrazol-1-yl)pyridine (pp) is a neutral one in which Co(II) ion is coordinated by the three nitrogens of the organic ligand and the oxygens of cyanate group. The complex synthesized with bis-2,6(3,5-dimethylpyrazol-1-yl)pyridine (dmpp) on the other hand, is an ionic complex in which the organic ligand and one Co(II) ion forms the cationic sphere and the anionic sphere is found to be [Co(OCN)]_4^2-.

Keywords: Chiral MOFs, Hydrothermal Synthesis, Structural Determination


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