

*Transformation of achiral to chiral structure, its applications in catalysis*Purna Chandra Rao¹, Sukhendu Mandal¹¹School Of Chemistry, IISER-TVM, Trivandrum, India

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The chirality is an important research area in biology and materials science due to their rich application and similarity to natural phenomena. The research on the targeted synthesis of homochiral materials is eminent for their applications in enantioselective separation, nonlinear optics, catalysis, and magnetism.[1] Generally, enantiopure starting reagents produce homochiral materials. The applications of these materials are hindered due to the cost effectiveness of enantiopure reagents. Even chiral materials can be synthesized from achiral reagents where chirality can be generated either through spontaneous resolution or by chirality induction. Separation and crystallization of homochiral materials from achiral units still remains an unexplored area. Symmetry breaking can induce chirality in the final structure by affecting the nucleation or crystal growth. The example of induced chirality through symmetry breaking where the final product does not contain any chiral unit is very rare. This process has an advantage compared to spontaneous resolution due to the enantiopure product formation, whereas spontaneous resolution produces opposite handedness or racemic twins. There are several reports on chiral symmetry breaking, but the proper mechanism or factors responsible for this are not very clear. According to Kondepudi et al., during the stirring of the reactions mixture, secondary crystal nuclei may rapidly clone the parent structure. This is known as chiral autocatalysis. Once the cloned structure formed, it leads to the formation of enantiopure crystals. It is also predicted that supramolecular interactions like H-bonding or π - π stacking may induce the symmetry breaking.

The structural transformation of flexible metal-organic frameworks (MOFs) through dehydration/desolvation or rehydration/resolution has gained much interest in gas adsorption due to breathing behavior. Transformation has vital role in various applications. Commonly, structural transformation was happening through external stimuli (like thermal treatment, mechanical grinding) involve breaking and reforming of bonds. Metal organic frameworks (MOFs) or Coordination polymers (CPs) are crystalline materials have eminent role in several applications like magnetism, gas adsorption, sensing and catalysis etc.[2]

In this work, we have isolated two copper-based coordination polymers through solvent diffusion and solvothermal methods using copper salt, furan dicarboxylic acid (FDC), 4, 4'-bipyridine (bpy) in MeOH/ethylene glycol, and water solvents. Compound 1 is adopting P21/c space group and adopts a one-dimensional wire like structure with a free carboxylate anion. Compound 2 crystallizes in chiral space group P65. This is a three-dimensional structure with helical chains. This helicity might be the reason for chiral generation and symmetry breaking. We have converted compound 1 to compound 2 using grinding, followed by a solvothermal method. The circular dichroism data of 2 showed that it is an enantioenriched compound. We have shown that compound 2 is a very good catalyst for chemo- and regioselective enamination reaction and for azide-alkyne Huisgen cycloaddition, respectively. [3]

[1] Morris, R. E. & Bu, X. (2010). Nat. Chem. 2, 353-361.

[2] Halcrow, M. A. (2013). Chem. Soc. Rev. 42, 1784-1795.

[3] Rao, P. C. et al. (2016). Inorg. Chem. 55, 12669-12674.



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