

Synthesis and Rietveld refinement of MeMOF-74 (Me = Co, Zn, Mg and Ni)

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In the porous material Science, Metal Organic framework (MOF) are intensely studied, among other qualities, for has the tailorable pores suitable for applications like gas separation and storage, catalysis and so on. For definition the MOF's are porous coordination networks, with void pores, formed by metallic sites organized in secondary building units (SBU) connected by organic linkers. The geometrical variety of the SBU's result in different topologies and a variety of pores with different sizes (from micro- to mesopores). In particular, the MeMOF-74 (Me = Co, Zn, Mg e Ni) has a hexagonal structure with unidimensional porosity, where the metal cations are connected to 6 oxygens exhibiting a SBU with straight helical form. In this work, high quality powder X ray diffraction pattern of MeMOF74 (Me = Co, Ni, Zn and Mg) were investigated using the Rietveld refinement method. This analysis was used to compare the influence of metal on the local geometry of secondary building units (SBU) and to study the influence of bimetallic sites on the structure.

Keywords: Metal Organic Framework, Rietveld, x-ray diffraction, Crystal.