

## IId06-005

Synthesis, characterization, and crystal structure analysis of a Mn(II) complex with phenanthroline and maleate ligands

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Development of complexes constituted of chelating agents as ligands bonded to transition metal ions has been the object of study of several research projects, due to their stability and potential biological activities. In this work, a crystal was obtained with a complex formation from Mn(II) with phenanthroline and malonate ligands, via slow evaporation of the solvent. Phenanthroline becomes an interesting bidentate ligand, with a rigid structure and two N atoms that can bond to the metal ion. Mn(II) is the third most abundant transition metal, being essential for human health, since it can help in urea metabolism and autophagy. The material obtained was characterized by X-ray diffraction (XRD) associated with Rietveld refinement, Fourier Transform Infrared Spectroscopy (FTIR) and Differential Scanning Calorimetry (DSC). XRD showed peaks of a very crystalline structure. The Rietveld refinement shows that the complex crystallized in a triclinic system with a P1 space group, containing two molecules per unit cell (Z = 2) and the following refined lattice parameters: a = 8.128(8) Å, b = 8.170(3) Å, c = 13.636(6) Å, Alpha = 80.940(3)°, Beta = 87.063(5)°, Gamma = 78.121(5)°, and V = 875.010(7) Å3. The FTIR showed the characteristic vibrational modes of 1,10-phenanthroline, maleic acid and bands with weak intensity corresponding to the stretching and deformation of the Mn-O and Mn-N bonds, cofirming the formation of the coordination complex. The DSC thermogram shows a physical endothermic event related to the dehydration process of free water molecules. The results suggest that the synthesis of the crystalline complex was successful, allowing for future physical, chemical, and biological characterizations, with additional publications, J. M. Yang, Z. H. Zhou, H. Zhang, H. L. Wan, S. J. Lu, Inorg. Chim. Act., v. 358, p. 1841, 2005. I. Kani, O. Atlier, K. Güven, J. Chem. Sci. v. 128, n. 4, p. 523, 2016. B. H. Toby, Pow. Diffract., v. 21 p. 67, 2006.