Growth and thermal-structural study of 1,10-phenanthroline monohydrated crystal

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The 1,10-phenanthroline (Phen) it is a chelating bidentate ligand that plays an important role in coordination chemistry and its use is classic with transition metal ions [1]. Several cytotoxic metal complexes have been developed in recent years based on the Phen ligand; however, few studies report the unique properties of this heteroaromatic compound [2]. In order to solve this problem, here we carry out a comprehensive study of the structural, vibrational and thermal properties of Phen. The crystals were synthesized from the solvent slow evaporation method in deionized water, using 0.1 mol/L of the starting compound. After seven days, the needle-shaped crystals were obtained with average dimensions of 0.38 × 0.17 × 0.13 cm^3 (L x W x H). X-ray powder diffraction (PXRD) shows that the sample crystallizes in a hexagonal structure (P32-space group), containing nine molecules per unit cell (Z= 9). In addition, thermogravimetry (TG) and differential thermal analysis (DTA) showed that the Phen crystal presents three endothermic events. The first is dehydration at 368 K, a conformational change at 392 K, and decomposition at 535 K. Motivated by these thermal-structural phenomena observed on the TG-DTA curves, PXRD measurements as a function of temperature was performed to analyze and determine the new structural phases. The Le Bail method was used to identify the system and space group of the anhydrous form of Phen crystals. The results obtained made it better to understand the Phen ligand''s physical and chemical properties.

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References

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