Synthesis and Characterization of L-Arginine H3PO4 Nano-Crystals with Non-Linear Optical Properties

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Crystals of L-Arginine H_3PO_4 with potential non-linear properties have been grown from aqueous solution by slow evaporation method at room temperature and controlled pH. These Crystals were characterized by UV-VIS, FTIR, AFM and XRD powder diffraction technique. Ultraviolet-Visible, show a highly transparent window to 275-1100 nm. Infrared, IR spectra confirm the chemical constituents and functional groups are present in the crystals [1] and AFM technique confirm their sizes around 20 nm. A discussion about the atomic and electronic structure and its simulation are presented here.

The reagents used for the preparation of the LAP solution were: L-Arginine ($C_6H_{14}N_4O_2$) Faga Lab of a purity of 99.6% and PM=174.20, and fosforic acid (H_3PO_4) J.T-Baker at 85.1%. The first solution was prepared with 50mL of distilled water, 10,5 g of L-Arginine and 4.9mL of H_3PO_4, pH of the solution of L-Arginine was of 11,3 and at the time of adding H_3PO_4 2.6. the reason of the second distilled solution was of 50mL of water, 10,5 g of L-Arginine and 3.1mL of H_3PO_4, pH of the solution of L-Arginine was of 11,3 and at the time of adding the H_3PO_4 change to 4,3 both systems they stayed in constant agitation during the preparation, once ready were let rest to room temperature, soon when appearing formation of small crystals retirement a drop and placed in microscope substrate , observed the formation of a gel in the equal solution of pH 2.6

The possible reaction that happens is the following one:

$$NH_2NHCNH(CH_2)_3CH(NH_2)COOH + H_3PO_4 \rightarrow (NH_2)_2CNH(CH_2)_3CH(NH_3)+COO\text{-}H_2PO_4$$

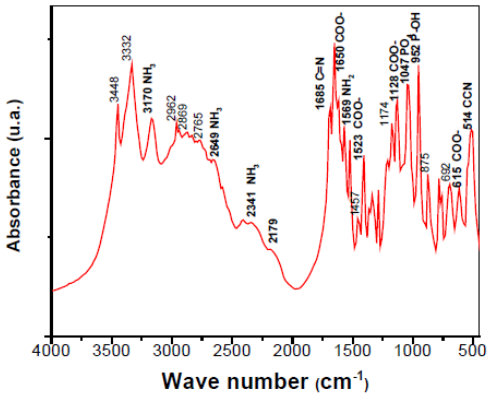
The growth method of nanocrystals by the evaporation technique at room temperature generated crystals LAP with a stable combination ionic amino acid-compound that was verified by using different techniques. FTIR in Fig. 1 shows the radical groups of the L-Arginine. Also the presence of a dipole molecule was confirmed (COO -, NH^{3+}) that favored to the formation of the crystalline structure. Analyzing the spectra of UV-Vis [2] in Fig. 2 the material do not present electronic transitions, in the rank of 275 to 1100nm which indicate that is a good candidate for non-linear effects under radiation of 1064 nm. The thermal analysis shows to a maximum temperature of exhibition by 1 hour 120°C for LAP, in which the crystal present thermal stability and conserve their crystalline structure (Fig. 3), it is verified with the study by X-ray diffraction, Fig. 4, where the conservation of the initial crystalline structure of the crystal is detected. Figure 5 displays a simulation of the structure built starting from the parameters obtained by the X-ray diffraction and

Rietveld fit. Finally in Figure 6 appears an AFM image of the LAP nanocrystal where is appreaciable its monolitic growth.

References

[1] Wei Wu, Cheng Ye and Dong Wang, Arkivoc, II: 59-69. 2003

[2] R. T. Bailey, et al. J. Phys D: Appl. Phys. 24:135-145 1991.



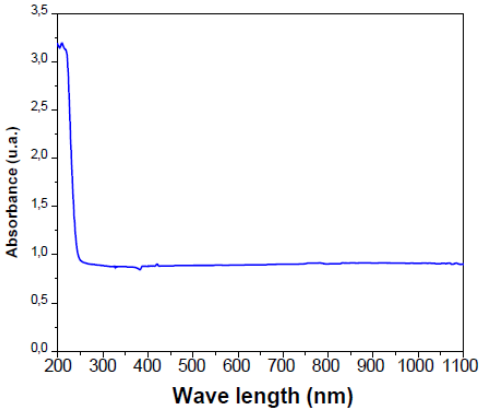
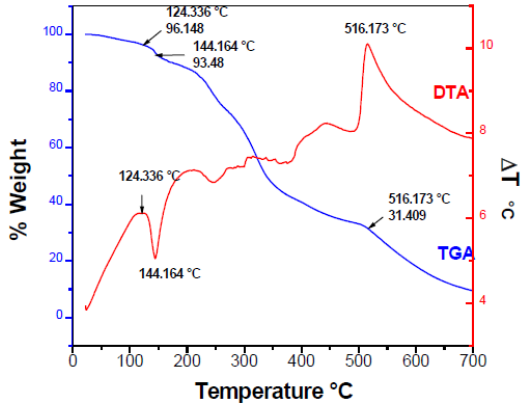


Fig. 1. IR spectrum of LAP showing its functional groups Fig. 2. UV-vis spectrum of LAP



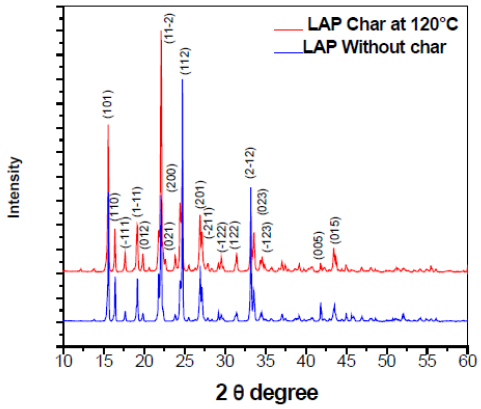
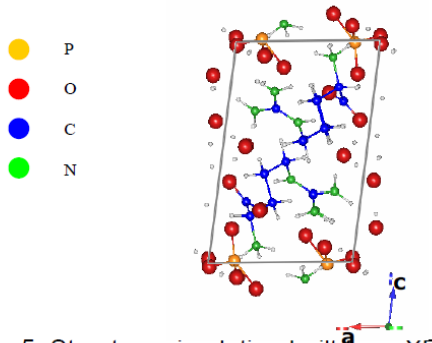


Fig. 3. DTA-TGA spectrum of LAP taken at 1hour Fig. 4. A comparison between XRD patterns



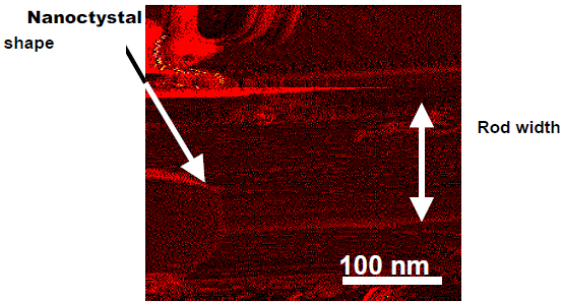


Fig. 5. Structure simulation built from XRD results Fig. 6. AFM image of the LAP nanocrystals