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

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Crystals of L-Arginine H₃PO₄ 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 (C6H14N4O2) Faga Lab of a purity of 99.6% and PM=174.20, and fosforic acid (H3PO4) 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 H3PO4, pH of the solution of L-Arginine was of 11,3 and at the time of adding H3PO4 2.6. the reason of the second distilled solution was of 50mL of water, 10,5 g of L-Arginine and 3.1mL of H3PO4, pH of the solution of L-Arginine was of 11,3 and at the time of adding the H3PO4 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:

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

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 -, NH³⁺) 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. 5. Structure simulation built from XRD results



Fig. 6. AFM image of the LAP nanocrystals