

Growth and Structural properties of L-Asparagine Monohydrate

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The L-Asparagine is an amino acid involved in the metabolic control of cell functions in nerve and brain tissue. Its monohydrate form ($C_4H_8O_3N_2 \cdot H_2O$) was grown by slow evaporation method by using a seed within a saturated solution to promote the growth of larger crystals, normally oriented in the [001] direction. It crystallizes in the orthorhombic structure, space group $P2_12_12_1$ with 4 molecules per unit cell. The structural characterization of the L-asparagine monohydrate crystal was performed in the Philips X'Pert MRD equipment, using CuK_{α} radiation, a graphite monochromator for diffracted beam, 0.02° steps and 4 sec/step of counting time. The measured powder pattern was refined through the Rietveld method (PC-GSAS software) by using the necessary literature crystallographic data (Verbist, Lehmann, Koetzle and Hamilton, *Acta Cryst.* (1972) **B28**, 3006.). The refinement has provided a very good fit with a R_{wp} factor of 6.87% and lattice parameters $a = 5.572(3) \text{ \AA}$, $b = 9.796(6) \text{ \AA}$ and $c = 11.773(8) \text{ \AA}$ which are in good agreement (order of 0.3%) with the published values. Since we have obtained very good L-asparagine monohydrate single crystals, it is our original plan to use them in the measurement of the piezoelectric coefficients of this amino acid through X-ray diffraction measurements, particularly the method based on the X-ray multiple diffraction technique (Avanci, Cardoso, Girdwood, Pugh, Sherwood and Roberts, *Phys. Rev. Lett.* (1998) **81**(24), 5426). (This work was financed by CNPq, CAPES and FAPESP).