204-091

L-TYROSINE HYDROCHLORIDE CRYSTALS UNDER HIGH PRESSURES VIA RAMAN SPECTROSCOPY

Santos, C.A.A.S.(1); Façanha Filho, P.F.(1); Dos Santos, A.O.(1); Ribeiro, L.H.L.(1); Victor, F.M.S.(1); Abreu, D.C.(1); Carvalho, J.O.(2); Soares, R.A.(1); Sousa, J.C.F.(1); Lima, R.C.(1); Cavaignac, A.O.(1); Universidade Federal do Maranhão(1); Universidade Federal do Maranhão(2); Universidade Federal do Maranhão(3); Universidade Federal do Maranhão(4); Universidade Federal do Maranhão(5); Universidade Federal do Maranhão(6); Instituto Federal do Maranhão(7); Universidade Federal do Maranhão(8); Universidade Federal do Maranhão(9); Universidade Federal do Maranhão(10); Universidade Federal do Maranhão(11);

Amino acid single crystals have been attracted researchers in recent years due to their potential applications as second harmonic generator. The goal of this work is to produce semiorganic single crystals of L-tyrosine hydrochloride (LTHCl) and verify the behavior of their vibrational normal modes under high pressures and the stability of material in these conditions extremes. The LTHCl single crystals were produced for solubilization of amino acid L-tyrosine in hydrochloric acid by slow evaporation technique of the solvent in room temperature. The technique of X-ray diffraction (XRD) and the refinement of structure by the Rietveld method were used to confirm the crystal structure. The LTHCl crystal belongs to the monoclinic crystal system having two molecules per unit cell. The refinement by the Rietveld method showed good results with Rwp = 8.49% and Rp = 6.29% with S = 1.13. Raman scattering measurements as a function of pressure was performed in a piece of crystal from the ambient pressure to 7.2 GPa and Nujol was used as pressure medium. It was observed the appearance of a weak band around 163 cm-1 between pressures of 0.5 and 1.0 GPa, which characterize an phase transition undergone by the crystal. Moreover, this band gains intensity as pressure increases while gradual decreasing relative intensity of the very strong band at 123 cm-1 for all range of pressure also was observed. In fact, almost all bands of the spectra have undergone strong decreasing up to 7.2 GPa. However, on release of pressure the crystal has reached the original phase again. Therefore, the results showed this material cannot be suitable for the application (NLO) in this range of pressure.