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PII:	S1386-1425(18)30760-1
DOI:	doi:10.1016/j.saa.2018.07.096
Reference:	SAA 16365
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	18 January 2018
Revised date:	28 July 2018
Accepted date:	30 July 2018

Please cite this article as: R.M.C.S. Diniz, C.E.S. Nogueira, C.C. Santos, F.S.M. Sinfrônio, F.F. de Sousa, A.S. de Menezes , Structural, vibrational and thermal studies on bis(l-glutaminato)copper(II). Saa (2018), doi:10.1016/j.saa.2018.07.096

Structural, Vibrational and Thermal Studies on Bis(L-Glutaminato)Copper(II)

R. M. C. S. Diniz[a], C. E. S. Nogueira[b], C. C. Santos[a], F. S. M. Sinfrônio[c], F. F. de Sousa[d], A. S. de Menezes[a]

[a] *Departamento de Fìsica, Universidade Federal do Maranhão, São Luís-MA, 65080-805, Brazil*

[b] *Universidade Regional do Cariri, Crato-CE, 63105-000, Brazil*

[c] *Departamento de Engenharia Elétrica, Universidade Federal do Maranhão, São Luís-MA, 65080-805,Brazil*

[d] *Instituto de Ciências Exatas e Naturais, Universidade Federal do Pará, Belém-PA, 66075-110, Brazil*

Abstract

Copper(II) complexes of amino acids have been widely studied as potentials medicines and dietary supplementation, so the knowledge about the metal-ligand sites, thermal stability and behavior of these complexes is an important subject of study. Although the Raman spectroscopy could help to elucidate the nature of the interactions into crystal there are only few information about vibrational study of this compound in the literature and no data depending on the temperature. In addition, there is no temperature-dependent X-ray diffraction study of this material. We report here Raman Spectroscopy and Powder X-ray Diffraction measurements, both as a function of temperature and as a way of studying the thermal stability of the material. After the synthesis of the sample and confirmation of its crystal structure by Powder X-ray Diffraction, Raman measurements were performed in the 70–3600 cm^{-1} spectral region as a function of temperature from 10 up to 300 K. Some peaks become more evident during the cooling, due to a decrease in width and an increase in intensity. There is a discontinuity in the wavenumbers evolution around 110 K, that should be associated with a conformation of the structure. Optimized geometry and vibrational frequencies were obtained by means of Density Functional Theory and for the first time the analysis of the vibrational modes was done in terms of the Potential Energy Distribution. X-ray diffraction measurements as a function of temperature and Rietveld refinement showed discontinuities in the lattice parameters and degradation around 493 K (at air atmosphere) and 513 K (under vacuum). These results were corroborated by the thermal analysis which indicates that the compound is stable up to 493 K.