PHASE TRANSITION IN THE AZITHROMYCIN INVESTIGATED THROUGH RAMAN SCATTERING

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Abstract

Azithromycin ($C_{38}H_{72}N_20_{12}$) is a pharmaceutical drug belonging to a class of antibiotics called azalides, being derivative of erythromycin A [1], and is widely used in the treatment of infectious diseases, such as toxoplasmosis and cryptosporidiosis. The azithromycin crystal can exhibits hydrated forms named which are named for monohydrate and dihydrate structures [2]. On the monohydrate form, it is known as pseudolimorph, has monoclinic symmetry with $P2_1$-space group [3]. On the other hand, the dihytrate polymorphic phase exhibits an orthorhombic symmetry with $P2_12_12_1$-space group [2]. For pharmaceutical uses, it is important to know the conformational structure of compounds in crystalline form under extreme conditions. The crystal structure of monohydrated and dihydrated azithromycin has already been previously investigated by literature [1], however from the point of view to determine its thermodynamic stability has not yet been studied. In our work, we report a study of the dihydrated azithromycin crystal (P212121-space group) using Raman scattering under high pressures. Therefore, we have performed Raman scattering experiments from the 0.0 up to 7.2 GPa to obtain spectra in the 30-3500 cm^{-1} region. From the results, we were able to observe a conformational phase transformation with pressure variation due high-pressure effects on the inter- and intramolecular vibrations of crystal through the some spectral modifications, such as discontinuities and disappearance of modes at pressure values between 3.3 and 5.5 GPa.

Keyword: Azithromycin, P hase transition , High pressures, Raman scattering.

References:

[1] J.M. Montejo-Bernardo, S. García-Granda, M.S. Bayod-Jasanada, L. Llavona-Díaz I. Llorente. Z. Kristallogr . 220 (2005) 66–73.
[2] S. Djokic, G. Kobrehel, N. Lopotar, B. Kamenar, A. Nagl, D. Mrvos. J. Chem.Res . (M)
(1988) 1239–1261.
[3] J.M. M-Bernardo, S. G-Granda, Z. Kristallogr . 222 (2007) 492–497.