Phase Transition in all-trans-β-Carotene Crystal: Temperature-Dependent Raman Spectra

Kleber José Rosário da Silva, Waldomiro Paschoal Jr., Ezequiel A. Belo, Sanclayton G. C. Moreira
Universidade Federal do Pará, Brazil

In this study, we studied the stability of an all-trans-β-carotene single crystal using Raman spectroscopy with line excitation at 632.8 nm, in the temperature range 20–300 K. The Raman spectra exhibit clear modifications in the spectral range of the lattice and internal vibrational modes. The temperature dependence of the most intense vibrational modes ν1(1511 cm\(^{-1}\)) and ν2(1156 cm\(^{-1}\)) that are related to the C=C and C—C stretching vibrations of the polyene chain, respectively, shows an upward shift on the Raman modes. This behavior is similar to that stated in the theoretical work of Wei-Long Liu et al. We conclude that the all-trans-β-carotene crystal undergoes a temperature-induced phase transition at approximately 219 K. This transition is interpreted as a rotation experienced by β-ring groups at each end of the all-trans-β-carotene molecule around the dihedral angle. At low temperatures, the new molecular configuration affects the sliding plane of the space group C2h5 (P21/n), and the phase transition leads to an unchanged monoclinic structure; however, the original space group is possibly lowered to the space group C2. In the temperature range 200–220 K, the spectral ratio (S) of the integrated intensities of the spectral modes around the symmetric and asymmetric stretching wavenumbers of the methyl group (CH\(_3\)) changes as a function of temperature in agreement with the phase transition. Furthermore, according to phase transition undergone by the all-trans-β-carotene, the thermal results obtained by differential scanning calorimetry show an exothermic process that occurs near the transition temperature assigned by the Raman spectra.