TEMPERATURE-DEPENDENT STUDY DODECANOIC ACID BY RAMAN SPECTROSCOPY AND DFT CALCULATIONS

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Abstract

Fatty acids are organic compounds constituted from carbon chains being that an isolated molecule has one carboxylic group and one methyl radical [1]. Such acids can be found abundantly in nature as part of the chemical composition f several Amazon vegetable oils and have received great attention in the fields of chemistry industries, pharmaceutics, medicine, cosmetic, food, among others [2,3]. Due to its importance, it is necessary a better comprehension of their physical properties under low-temperature conditions. In our work, we study the thermodynamic behavior of dodecanoic acid (lauric-acid) crystal when submitted to low temperatures using Raman spectroscopy. The Raman spectra were measured in the 30–3000 cm−1 range on cooling from 300 up to 38 K. From the analysis of bands behavior and lattice- and internal-vibration modes, we observe that crystal undergoes a conformational phase transition. This phase transition is connected with possible modifications in the dimeric conformation through hydrogen bond changes within the unit cell. In addition, density functional theory calculations were also performed to assign all Raman- and infrared-active modes for a better interpretation of the experimental data at room temperature.

Keywords: Dodecanoic acid, Phase transformation, Raman spectroscopy, DFT calculations

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