

STRUCTURAL ANALYSIS OF BUTYRIC ACID USING MATRIX ISOLATION INFRARED SPECTROSCOPY AND THEORETICAL CALCULATIONS

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Butyric acid (C₄H₈O₂) is a short-chain carboxylic acid that exhibits several conformers due to the rotational flexibility of its alkyl chain and carboxyl group. These conformers may have slightly different physicochemical properties, influencing their reactivity and interactions in various environments [1]. Understanding the structural and energetic differences between these conformers is essential for applications in chemical and biological systems [2,3]. The main goal of this work is to conduct conformational analysis of butyric acid. To accomplish this goal, high-level quantum chemical calculations and low-temperature matrix isolation infrared absorption spectroscopy in different matrices were used.

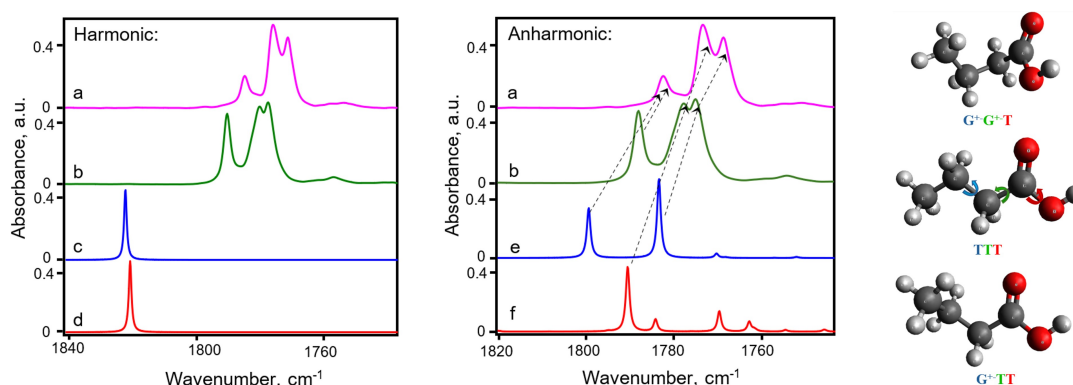


Fig.1. Infrared absorption spectra of butyric acid: (a) experimental in argon matrix, (b) experimental in neon matrix, (c) calculated TTT (harmonic), (d) calculated G \pm TT (harmonic), (e) calculated TTT (anharmonic), (f) calculated G \pm TT (anharmonic). Calculated band intensities were scaled to the experimental bands using the same factor for the all calculated spectra.

Geometry optimization and vibrational frequency calculations of possible butyric acid conformers were performed using Density Functional Theory (DFT) with the B3LYP functional and the ab initio Møller-Plesset perturbation theory (MP2), both using the cc-pVTZ basis set. Vibrational frequencies were calculated using both harmonic and anharmonic methods. Theoretical calculations identified three stable conformers of butyric acid; however, only two were experimentally observed in argon and neon matrices. Anharmonic calculations facilitated the identification of Fermi resonance bands in experimental spectra and enabled a more precise assignment of spectral bands in the C=O region. The results are presented in Fig. 1. However, in MP2 calculations, the stability order shifts when Gibbs energy is considered in energy estimations, ultimately identifying TTT as the most stable conformed.

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