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Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids : near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid.

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Quantum chemical reproduction of entire NIR spectra is a new trend, enabled by contemporary advances in the anharmonic approaches. At the same time, recent increase of the importance of NIR spectroscopy of biological samples raises high demand for gaining deeper understanding of NIR spectra of biomolecules, i.e. fatty acids. In this work we investigate saturated and unsaturated medium-chain fatty acids, hexanoic acid and sorbic acid, in the near-infrared region. By employing fully anharmonic density functional theory (DFT) calculations we reproduce the experimental NIR spectra of these systems, including the highly specific spectral features corresponding to the dimerization of fatty acids. Broad range of concentration levels from $5{\cdot}10^{-4}$M in CCl_4 to pure samples are investigated. The major role of cyclic dimers can be evidenced for the vast majority of these samples. A highly specific NIR feature of fatty acids, the elevation of spectral baseline around 6500-4000cm^{-1}, is being explained by the contributions of combination bands resulting from the vibrations of hydrogen-bonded OH groups in the cyclic dimers. Based on the high agreement between the calculated and experimental NIR spectra, a detailed NIR band assignments are proposed for hexanoic acid and sorbic acid. Subsequently, the correlations between the structure and NIR spectra are elucidated, emphasizing the regions in which clear and universal traces of specific bands corresponding to saturated and unsaturated alkyl chains can be established, thus demonstrating the wavenumber regions highly valuable for structural identifications.

Słowa kluczowe

NIR, Fatty acids, Anharmonic DFT, Hexanoic acid, Sorbic acid

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