# Anharmonicity and spectra–structure correlations in MIR and NIR spectra of crystalline menadione (vitamin $K_3$).

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Streszczenie

Mid-infrared (MIR) and near-infrared (NIR) spectra of crystalline menadione (vitamin $K_3$) were measured and analyzed with aid of quantum chemical calculations. The calculations were carried out using the harmonic approach for the periodic model of crystal lattice and the anharmonic DVPT2 calculations applied for the single molecule model. The theoretical spectra accurately reconstructed the experimental ones permitting for reliable assignment of the MIR and NIR bands. For the first time, a detailed analysis of the NIR spectrum of a molecular system based on a naphthoquinone moiety was performed to elucidate the relationship between the chemical structure of menadione and the origin of the overtones and combination bands. In addition, the importance of these bands during interpretation of the MIR spectrum was demonstrated. The overtones and combination bands contribute to 46.4% of the total intensity of menadione in the range of 3600–2600 $cm^{-1}$. Evidently, these bands play a key role in shaping of the C-H stretching region of MIR spectrum. We have shown also that the spectral regions without fundamentals may provide valuable structural information. For example, the theoretical calculations reliably reconstructed numerous overtones and combination bands in the 4000–3600 and 2800–1800 $cm^{-1}$ ranges. These results, provide a comprehensive origin of the fundamentals, overtones and combination bands in the NIR and MIR spectra of menadione, and the relationship of these spectral features with the molecular structure.

Słowa kluczowe

near-infrared (NIR), mid-infrared (MIR) spectroscopy, overtones, combination bands, anharmonicity, periodic boundary system, menadione, vitamin K3

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