

NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features.

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Near-infrared spectroscopy (NIRS) is an effective analytical/quality control tool in various appliances, i.e. in phytopharmaceutical industry. While multivariate analysis gives NIRS the desired level of analytical performance it lacks in providing deeper physical insights. Quantum mechanical (QM) simulation of NIR spectra is becoming feasible for complex molecules in the present days. The usefulness of QM simulation in NIRS surpasses that in IR region as NIR spectra are intrinsically complex as a result of anharmonic effects; yet QM investigations in NIRS remain rare due to practical limitations. QM provides detailed band assignments, far exceeding the capability of classical spectroscopic methods, but also offers unveiling the influential factors in the chemometric models. In the present work we investigate NIR spectrum of thymol, a constituent of Thymi herba used in traditional medicine. Experimental part compares the NIR spectra of thymol in solid state, melted (neat liquid) and in CCl₄ solutions of different concentrations. The analysis unveils the spectral regions of strongly varying sensitivity level to the sample state; two regions (6000–5600cm⁻¹ and 4490–4000cm⁻¹) are identified as remaining largely invariant under the sample state. The band assignments and plotted density of modal contribution visualize generalized and categorized NIR spectra forming factors of thymol. A principle relationship with the regression coefficients plot is established, demonstrating that the NIR bands which retain high insensitivity to the intermolecular interactions give the most influence in the PLS regression model of thymol.

Słowa kluczowe

NIRS, Spectra simulation, Thymol, 5-Methyl-2-(propan-2-yl)phenol, phase transition, Thymi herba, Phytopharmaceuticals, Overtones, Combination bands

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