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Title:Terahertz spectroscopic investigation of elaidic acid

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Abstract:The optical properties of elaidic acid in the THz band were investigated by using THz time-domain spectroscopy (THZ-TDS). The absorption and refractive index spectra in the frequency range from 0.5 to 2.5 THz were obtained at room temperature under nitrogen atmosphere, and the results show that elaidic acid had some characteristic absorption peaks, and the average refractive index of the sample was 1.43. The structure and vibrational frequencies of elaidic acid molecule in the THz range were simulated by the B3LYP algorithm of density functional theory, and the THz characteristic absorption peaks of elaidic acid molecule were identified by using Gaussian View software. The results show that the experimental and theoretical results agree in general, and the observed absorption peaks in the THz range were mainly caused by the intramolecular and intermolecular vibrations jointly. At the same time, the fingerprint spectra of elaidic acid in the THz band verify that the time-domain terahertz spectroscopy can be used to detect oleic acid, and this study provides a new experimental method for the detection of trans fatty acids in food.