

731

标题: Investigating the Position Isomerism Effect of Dihydroxybenzoic Acid Compounds by Terahertz Time-domain Spectroscopy

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摘要: Far-infrared vibrational absorption of a series of dihydroxybenzoic acid (DHBA) compounds with different substituted hydroxy group at different positions have been investigated using terahertz time-domain spectroscopy (THz-TDS) at room temperature. The experimental results show large difference among absorption spectra of different DHBA (2,3-DHBA, 2,4-DHBA, 2,5-DHBA, 2,6-DHBA) compounds in 0.2 similar to 2.0 THz region, which probably originated from the difference of intra-molecular and inter-molecular hydrogen bonds due to the presence of two hydroxyl group in different positions with respect to the carboxylic group in different DHBAs. All the experimental DHBAs vibrational modes showed distinct fingerprint absorption in THz region and theoretical calculation based on density functional theory (DFT) was carried out to assist the analysis and assignment of the vibrational modes. The results indicate that THz-TDS technology can not only give a new experimental method to identify and characterize the position isomerism effect of hydroxyl group between such different kinds of DHBAs from molecule-level, but also provide a useful suggestion for further assessing the possible relationships between the DHBAs vibrational properties and the effects of the substituted hydroxy group position to better know their biochemical activities in food, pharmaceutical and cosmetic fields.

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