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Experimental and theoretical investigations of tartaric acid isomers by terahertz spectroscopy and density functional theory

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Abstract: **The terahertz (THz) absorption spectra of L-, D-, and DL-tartaric acid have been measured in the frequency range from 0.2 to 2.0 THz by terahertz time-domain spectroscopy (THz-TDS). The characteristic absorption peaks of these three tartaric acid isomers were obtained, which showed remarkable difference between enantiomers (L- and D-tartaric acid) and the racemic compound (DL-tartaric acid) in their peak frequencies. In parallel with the experimental study, theoretical calculations on isolated-molecule and unit cell of tartaric acids using density functional theory (DFT) were also performed for simulating the experimental THz spectrum features, which were in good agreement with the experimental data. Results demonstrate that THz-TDS can distinguish the tiny diversity between tartaric acid chiral isomers and its racemic compound, and provided an effective method for molecular identification in biological and biomedical engineering.**

Keywords: **Terahertz time-domain spectroscopy; Density functional theory; Tartaric acids; Isomer**

1. Introduction

Terahertz (THz) wave with wavelength between microwave and infrared is a segment of electromagnetic wave, which develops slowly due to lack of effective generation and detection techniques in a long time. Recently, in pace with the breakthrough of ultrafast laser technology, which provides stable and reliable radiation source for the generation of THz waves, and enables THz technology to get a rapid development [1-3]. Terahertz time-domain spectroscopy (THz-TDS) is an effective means of detecting material spectra information in the THz region by employing ultrafast laser technology. It has a comparative high signal-to-noise ratio and a wider frequency band, and can be used to detect material composition and subtle structure changes [4-7]. Walther *et al* [8] firstly investigated the spectra of three retinal isomers (all-trans, 9-cis and 13-cis retinal) by THz-TDS, which discovered that obvious differences between the low-frequency vibrational spectra of these three isomers, and demonstrates that the feasibility of using THz-TDS to analyze the molecular structure of the isomers and the mechanism of the vibrational modes.

Density functional theory (DFT) is a quantum chemical calculation method, which is rapidly becoming a “standard tool” for diverse materials modeling problems in chemistry, physics, geology, materials science, and other disciplines [9]. This

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