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Terahertz spectroscopic investigation of gallic acid and its monohydrate

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Abstract: The low-frequency spectra of gallic acid (GA) and its monohydrate were investigated by terahertz time-domain spectroscopy (THz-TDS) in the range of 0.5 to 4.5 THz. The dehydration process of GA monohydrate was monitored on-line. The kinetic mechanism of the dehydration process was analyzed depending on the THz spectral change at different temperatures. The results indicate that the diffusion of water molecule dominates the speed of the entire dehydration process. Solid-state density functional theory (DFT) calculations of the vibrational modes of both GA and its monohydrate were performed based on their crystalline structures for better interpreting the experimental THz spectra. The results demonstrate that the characterized features of GA mainly originate from the collective vibrations of molecules. And the interactions between GA and water molecules are responsible for THz fingerprint of GA monohydrate. Multi-techniques including differential scanning

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