

Investigation of Temperature Dependence of Terahertz Spectra of Amino Acids

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In this paper, we employ terahertz Time Domain Spectroscopy (THz-TDS) combined with temperature-tuned system to measure the temperature dependence of terahertz spectroscopic features of various amino acids, such as β -Alanine, L-Tyrosine, L-Glycine, L-Asparagine and so on. We investigate the absorption frequencies of amino acids at different environmental temperatures, in order to study the temperature dependence of THz spectra. The measured absorption spectra are compared with the results simulated by Density Function Theory (DFT) using hybrid functional B3LYP with basis set of 6-31 G (d). In the theoretical simulations, we vary the ambient temperatures of samples to observe the shift of absorption peak. The discrepancy between simulation and experiment results originates from that the molecular structure used in the simulation is gas phase molecular model, which is different from crystal structure.