

207.Title: Understanding the Terahertz Spectra of Crystalline Pharmaceuticals: Terahertz Spectroscopy and Solid-State Density Functional Theory Study of (S)-(+)-Ibuprofen and (RS)-Ibuprofen

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Abstract: The potential applications of terahertz (THz) spectroscopy in the analysis of pharmaceutical products in their crystalline state have prompted the need for a more thorough understanding of the fundamental vibrational motions contributing to the THz spectra. The detection of variations in crystal structure and the reliable assignment of observed THz absorption features can be aided by the use of solid-state density functional theory (DFT). In this study, solid-state DFT with periodic boundary conditions was used to simulate the crystalline structure and assign the experimental THz spectra (10-90 cm⁻¹) of the enantiomerically pure and racemic forms of the common pharmaceutical compound ibuprofen. The results clearly demonstrate the capabilities of DFT methodologies to accurately reproduce the THz spectra of large complicated molecular systems and provide insight into the internal and external vibrational motions that form the basis of THz spectroscopy.