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标题: THz spectroscopic investigation of chlorotoluron by solid-state density functional theory
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摘要: The terahertz time-domain spectrum (THz-TDS) of chlorotoluron has been simulated and assigned with solid-state density functional theory (DFT) in the range of 0.5-2.2 THz. The calculations based on the hybrid density functionals B3LYP and PW91 are performed to analyze the origins of observed spectral features in chlorotoluron THz spectra of solid-state forms using the software package CRYSTAL09. The computed THz spectrum of the B3LYP provides better agreements with observed THz spectral characters. Moreover, all the experimental THz absorption peaks are assigned utilizing the B3LYP method. (C) 2012 Elsevier B.V. All rights reserved.

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