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标题: Terahertz Time-Domain Spectroscopy of Alpha Endosulfan Persistent Organic Pollutant
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摘要: Frequency-dependent absorption coefficient spectrum and refractive index spectrum of alpha endosulfan, a kind of persistent organic pollutants, are presented in the terahertz frequency region by terahertz (THz) time-domain spectroscopy (TDS). The spectral features in the THz region have a number of unique characteristic absorption peaks. The result demonstrates that THz-TDS is a promising method to identify materials. Then we adopted density functional calculation method to analyze theoretic absorption coefficients of single alpha endosulfan molecule within 0. 2 similar to 2 THz. The results show that absorption peaks at 1. 68, 1. 91 THz in theoretical calculation correspond to 1. 7, 1. 88 THz in the experiment. Finally, vibrational modes and approximate assignments were discussed, showing that these matched peaks are caused by intramolecular vibrational modes of alpha endosulfan. Others might be related to intermolecular vibrational modes or combined vibrational modes.
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