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标题: Detection of POPs in soil by using terahertz time-domain spectroscopy

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摘要: The terahertz transmission spectra of three different persistent organic pollutants (POPs) (aldrin, dieldrin, and endrin) are measured by using terahertz time-domain spectroscopy (THz-TDS) in the terahertz region of 0.2-1.8THz. The spectral dependence of the absorption for individual three kinds of POPs is extracted from the transmission data. Computational chemistry using the B3LYP density functional method is used to study structure and internal rotations in POPs, where results strongly suggest that frequencies of the POPs internal rotor correspond to the observed spectra. The absorption coefficient for the soil/aldrin mixture is 19.64cm(-1) at 1.41THz, 20.91cm(-1) at 1.57THz, 13.69cm(-1) at 1.78THz. For soil/dieldrin mixture, the frequency positions of prominent absorption features at 1.29, 1.4 and 1.56THz are observed. The absorption coefficient for the soil/dieldrin mixture is 16.73cm(-1) at 1.29THz, 18.85cm(-1) at 1.4THz, 24.5cm(-1) at 1.56THz. There exhibits three strong absorption peaks coefficient of the soil/endrin mixture at the frequency of 1.58THz and 1.67THz. The absorption coefficient of the soil/endrin mixture is 6.24cm(-1) at 1.58THz, 12.58cm(-1) at 1.67THz. There is reasonably good agreement between theory and experiment. The results show that the THz-TDS can be used to study POPs in soil quality evaluation or safety inspection further.

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作者关键词: Terahertz; terahertz time-domain spectroscopy; aldrin; dieldrin; endrin; B3LYP; density functional method; persistent organic pollutants; POPs

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