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Application of terahertz spectroscopy and theoretical calculation in dimethylurea isomers investigation

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Abstract

The characteristic absorption spectra of two structural isomers of dimethylurea (DMU) in 0.6~1.8 THz region have been measured using terahertz time-domain spectroscopy (THZ-TDS) at room temperature. Significant differences have been found between their terahertz spectra and implied that the THZ-TDS is an effective means of identifying structural isomers. To simulate their spectra, calculations on single molecule and cluster of 1,1-DMU and 1,3-DMU were performed, and we found that the cluster calculations using DFT-D3 method are better to predict the experimental spectra. Using the normal mode as displacements in redundant internal coordinates and the GaussView program, most observed THz vibrational modes are assigned to bending and rocking modes related to the intermolecular hydrogen bonding interactions, and twisting mode of ethyl groups. The different spectral features of two isomers mainly arise from different intermolecular hydrogen bonds resulting from different atom arrangements in molecules and different molecule arrangements in crystals. Using the reduced-density-gradient (RDG) analysis, the positions and types of inter-

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