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Title:Terahertz absorption spectra of benzene-1,2-diol, benzene-1,3-diol and benzene-1,4-diol
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Abstract:The terahertz spectra (8-128 cm⁻¹) of three structural isomers have been measured using terahertz time-domain spectroscopy at room temperature. Substantial differences among these THz spectra have been found and implied that THz-TDS is an excellent tool to identify isomers. Numerical calculation based on solid-state density functional theory has been carried out and assigned the observed THz features theoretically. Good agreement between the calculated and experimentally measured spectra for benzene-1,2-diol and benzene-1,3-diol has been achieved. According to the calculated results, it is found that the measured THz spectra of these two isomers mainly originate from intermolecular vibrations.
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