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标题: Terahertz and mid-infrared spectroscopy of benzene-1,2-diol
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来源出版物: JOURNAL OF MOLECULAR SPECTROSCOPY 卷: 281 页: 13-17 DOI: 10.1016/j.jms.2012.09.005 出版年: NOV 2012
在 Web of Science 中的被引频次: 0
被引频次合计: 0
引用的参考文献数: 34
摘要: The terahertz (THz) and mid-infrared (MIR) spectra of benzene-1,2-diol in the solid state have been modeled by density functional theory (DFT). Calculations of the vibrational spectra based on the optimized geometries provided a good fit to the observed spectra, and a more reasonable spectral reproduction has been achieved than those in previous work. For THz spectrum, the simulation based on the varied unit cell dimension has clearly shown that THz spectral reproduction is affected by the temperature change of unit cell. For MIR spectrum, band assignments are reported in terms of potential-energy distribution (PED). which differ to those previously reported for benzene-1,2-diol in some respects. (c) 2012 Elsevier Inc. All rights reserved.
入藏号: WOS:000311771200004
语种: English
文献类型: Article
作者关键词: Terahertz; IR spectroscopy; Density functional theory; Benzene-12-diol
KeyWords Plus: FUNCTIONAL PERTURBATION-THEORY; TIME-DOMAIN SPECTROSCOPY; VIBRATIONAL-SPECTRA; CATECHOL; PYROCATECHOL; HYDROQUINONE; RESORCINOL; SOLIDS; CASTEP; MODES
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出版商: ACADEMIC PRESS INC ELSEVIER SCIENCE
出版商地址: 525 B ST, STE 1900, SAN DIEGO, CA 92101-4495 USA
Web of Science 类别: Physics, Atomic, Molecular & Chemical; Spectroscopy
研究方向: Physics; Spectroscopy
IDS 号: 046NH
ISSN: 0022-2852
29 字符的来源出版物名称缩写: J MOL SPECTROSC
ISO 来源出版物缩写: J. Mol. Spectrosc.
来源出版物页码计数: 5