83
Accession number:20114914584727
Title:Modeling the THz spectrum of the bentazon
Authors:Wang, Huali (1); Wang, Qiang (1)
Author affiliation:(1) Department of Quality and Safety Engineering, China Jiliang University, Hangzhou 310018, China
Corresponding author:Wang, Q.(qiangwang@cjlu.edu.cn)
Source title:Chinese Optics Letters
Abbreviated source title:Chin. Opt. Lett.
Volume:9
Issue:11
Issue date:November 2011
Publication year:2011
Article number:110011
Language:English
ISSN:16717694
Document type:Journal article (JA)
Publisher:Science Press, 18,Shuangqing Street,Haidian, Beijing, 100085, China
Abstract:Terahertz (THz) spectra of bentazon are determined within the range of 0.3-2.4 THz at room temperature. Density functional methods are used to compute the THz spectra using three different programs: Gaussian03 for isolated-molecule form, DMol3 and CRYSTAL09 for solid-state forms. Among the three, the computed THz spectrum of CRYSTAL09 shows better bond length and angle agreements with X-ray experimental results, and corresponds with observed THz experiment spectral characteristics. The isolated-molecule vibrational mode values are less by half than those derived from solid-state calculations. The last five peak positions of the two solid-state computations coincide with each other. Moreover, all the experimental THz absorption peaks are assigned by utilizing CRYSTAL09.
Number of references:18