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Title:Spectral analysis of nitrofurantoin in the terahertz frequency range
Authors:Kang, Xu-Sheng (1); Hou, Di-Bo (1); Zhang, Guang-Xin (1); Chen, Xi-Ai (1); Yue, Fei-Heng (1); Huang, Ping-Jie (1); Zhou, Ze-Kui (1)
Author affiliation:(1) Department of Control Science and Engineering, Zhejiang University, Hangzhou 310027, China; (2) City College, Zhejiang University, Hangzhou 310015, China; (3) China Jiliang University, Hangzhou 310018, China
Corresponding author:Hou, D.-B.(houdb@zju.edu.cn)
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Abstract:The present article measured the absorption coefficient spectra and refractive index spectra of nitrofurantoin original drug, which is one kind of nitrofuran drugs, in the terahertz frequency range from 0.2 to 1.8 THz using terahertz time-domain spectroscopy. The results showed that there exist a number of characteristic absorption peaks of nitrofurantoin with different intensity in the range and the absorption coefficient spectra can be used to identify nitrofurantoin. The article also simulated absorption coefficient spectra of nitrofurantoin molecule within 0.2~1.8 THz using density functional theory by Gaussian software, and vibrational modes of some peaks in the experimental absorption coefficient spectra were analyzed and identified. The results show that the experimental absorption peaks at 1.25 and 1.60 THz correspond with the theoretical peaks at 1.30 and 1.67 THz, and these experimental peaks were caused by intramolecular vibrational modes of nitrofurantoin.
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