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标题: Vibrational frequencies of anti-diabetic drug studied by terahertz time-domain spectroscopy
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来源出版物: APPLIED PHYSICS LETTERS 卷: 100 期: 14 文献号: 143702 DOI: 10.1063/1.3700808 出版年: APR 2 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: 18
摘要: By using terahertz time-domain spectroscopy, the absorption spectra of seven anti-diabetic pills have been investigated. For gliquidone, glipizide, gliclazide, and glimepiride, an obvious resonance peak is found at 1.37 THz. Furthermore, to overcome the limit of density functional theory that can analyze the normal mode frequencies of the ground state of organic material, we also present a method that relies on pharmacophore recognition, from which we can obtain the resonance peak at 1.37 THz can be attributed to the vibration of sulfonylurea group. The results indicate that the veracity of density functional theory can be increased by combining pharmacophore recognition. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.3700808]
入藏号: WOS:000302567800080
语种: English
文献类型: Article
KeyWords Plus: DENSITY; EXCHANGE; SPECTRA
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出版商: AMER INST PHYSICS
出版商地址: CIRCULATION & FULFILLMENT DIV, 2 HUNTINGTON QUADRANGLE, STE 1 N O 1, MELVILLE, NY 11747-4501 USA
Web of Science 分类: Physics, Applied
学科类别: Physics
IDS 号: 922SG
ISSN: 0003-6951
29 字符的来源出版物名称缩写: APPL PHYS LETT
ISO 来源出版物缩写: Appl. Phys. Lett.
来源出版物页码计数: 4