Application of terahertz spectroscopy and theoretical calculation in dimethylurea isomers investigation

Yonghong Zhao, Zhi Li, Jianjun Liu, Tao Chen, Huo Zhang, Binyi Qin, Yifang Wu

PII: S1386-1425(17)30950-2
DOI: doi:10.1016/j.saa.2017.11.040
Reference: SAA 15622

To appear in:

Received date: 9 October 2017
Revised date: 10 November 2017
Accepted date: 18 November 2017

Please cite this article as: Yonghong Zhao, Zhi Li, Jianjun Liu, Tao Chen, Huo Zhang, Binyi Qin, Yifang Wu, Application of terahertz spectroscopy and theoretical calculation in dimethylurea isomers investigation, (2017), doi:10.1016/j.saa.2017.11.040

Application of terahertz spectroscopy and theoretical calculation in dimethylurea isomers investigation

Yonghong Zhao[a,b], Zhi Li[a,c,*], Jianjun Liu[b,e], Tao Chen[b], Huo Zhang[a], Binyi Qin[a], Yifang Wu[d]

[a] *School of Mechano-Electronic Engineering, Xidian University, Xi'an, Shanxi 710126, China*
[b] *Guangxi Key Laboratory of Automatic Detecting Technology and Instruments, School of Electronic Engineering and Automation, Guilin University of Electronic Technology, Guilin, Guangxi 541004, China*
[c] *Guilin University Of Aerospace Technology, Guilin, Guangxi 541004, China*
[d] *Department of Chemistry and Chemical Engineering, Heze University, Heze, Shandong 274015, China*
[e] *eSouthwest University, chongqing 400715,China*

Abstract

The characteristic absorption spectra of two structural isomers of dimethylurea(DMU) in 0.6∼1.8 THz region have been measured using terahertz time-domain spectroscopy (THZ-TDS) at room temperature. Significant differences have been found between their terahertz spectra and implied that the THZ-TDS is an effective means of identifying structural isomers. To simulate their spectra, calculations on single molecule and cluster of 1,1-DMU and 1,3-DMU were performed, and we found that the cluster calculations using DFT-D3 method are better to predict the experimental spectra. Using the normal mode as displacements in redundant internal coordinates and the GaussView program, most observed THz vibrational modes are assigned to bending and rocking modes related to the intermolecular hydrogen bonding interactions, and twisting mode of ethyl groups. The different spectral features of two isomers mainly arise from different intermolecular hydrogen bonds resulting from different atom arrangements in molecules and different molecule arrangements in crystals. Using the reduced-density-gradient (RDG) analysis, the positions and types of inter-

*Corresponding author
Email address: guet.lizhi@yahoo.com (Zhi Li)