Accepted Manuscript

Synthesis, structural characterization and quantum chemical calculations on 1-(isomeric methylbenzoyl)-3-(4-trifluoromethylphenyl)thioureas

Lei Qiao, Yu Zhang, Wei Hu, Jiajia Guo, Wenli Cao, Zimei Ding, Zhiwei Guo, An Fan, Jirong Song, Jie Huang

PII: S0022-2860(17)30418-0

DOI: 10.1016/j.molstruc.2017.03.113

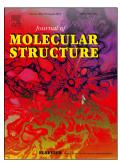
Reference: MOLSTR 23609

To appear in: Journal of Molecular Structure

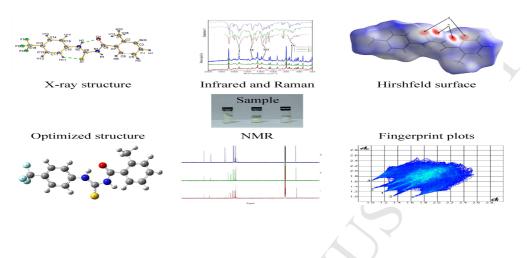
Received Date: 10 March 2017 Revised Date: 30 March 2017 Accepted Date: 30 March 2017

Please cite this article as: L. Qiao, Y. Zhang, W. Hu, J. Guo, W. Cao, Z. Ding, Z. Guo, A. Fan, J. Song, J. Huang, Synthesis, structural characterization and quantum chemical calculations on 1-(isomeric methylbenzoyl)-3-(4-trifluoromethylphenyl)thioureas, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.03.113.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Graphical abstract: The three novel isomeric acyl thiourea compounds were firstly prepared and characterized by some spectroscopic techniques. The molecular structure of compounds 1 and 3 was determined by X-ray diffraction analysis. A detailed analysis of the intermolecular contacts in the compounds 1 and 3 have been performed based on the Hirshfeld surfaces, their 2D fingerprint plots and the enrichment ratios. Conformational aspects are also discussed in terms of the vibrational spectra.



Download English Version:

https://daneshyari.com/en/article/5161116

Download Persian Version:

https://daneshyari.com/article/5161116

<u>Daneshyari.com</u>