Accepted Manuscript

Combined spectroscopic, XRD crystal structure and DFT studies on 2-(ethylthio) pyrimidine-4,6-diamine

MOLE GULAR STRUCTURE

Ebru Aktan, Banu Babür, Nurgül Seferoğlu, Berna Çatikkaş, F. Betül Kaynak, Zeynel Seferoğlu

PII: S0022-2860(17)30669-5

DOI: 10.1016/j.molstruc.2017.05.058

Reference: MOLSTR 23799

To appear in: Journal of Molecular Structure

Received Date: 21 March 2017

Revised Date: 12 May 2017

Accepted Date: 13 May 2017

Please cite this article as: Ebru Aktan, Banu Babür, Nurgül Seferoğlu, Berna Çatikkaş, F. Betül Kaynak, Zeynel Seferoğlu, Combined spectroscopic, XRD crystal structure and DFT studies on 2-(ethylthio)pyrimidine-4,6-diamine, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc. 2017.05.058

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.

ACCEPTED MANUSCRIPT

Highlights

- ETPD has been resynthesized and obtaned in single crytal form.
- The structural geometry was obtained by XRD and quantum mechanical calculations.
- •The molecular, vibrational and some chemical properties have computed.

Download English Version:

https://daneshyari.com/en/article/5160196

Download Persian Version:

https://daneshyari.com/article/5160196

<u>Daneshyari.com</u>