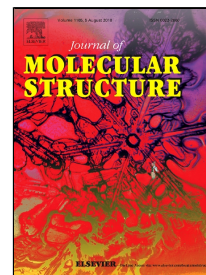


Accepted Manuscript



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PII: S0022-2860(18)30592-1
DOI: 10.1016/j.molstruc.2018.05.032
Reference: MOLSTR 25205
To appear in: *Journal of Molecular Structure*
Received Date: 29 January 2018
Revised Date: 08 May 2018
Accepted Date: 08 May 2018

Please cite this article as: Mustafa Kemal Gümüş, Sevgi Kansız, Ercan Aydemir, Nikolay Yu. Gorobets, Necmi Dege, Structural features of 7-methoxy-5-methyl-2-(pyridin-3-yl)-11,12-dihydro-5,11-methano[1,2,4]triazolo[1,5-c][1,3,5]benzoxadiazocine: Experimental and theoretical (HF and DFT) studies, surface properties (MEP, Hirshfeld), *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.05.032

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Structural features of 7-methoxy-5-methyl-2-(pyridin-3-yl)-11,12-dihydro-5,11-methano[1,2,4]triazolo[1,5-c][1,3,5]benzoxadiazocine: Experimental and theoretical (HF and DFT) studies, surface properties (MEP, Hirshfeld)

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Keywords: Biginelli condensation, benzoxadiazocine, Hartree-Fock (HF), Density functional theory (DFT), HOMO-LUMO, Hirshfeld surface.

Abstract

The molecular structure of 7-methoxy-5-methyl-2-(pyridin-3-yl)-11,12-dihydro-5,11-methano[1,2,4]triazolo[1,5-c][1,3,5]benzoxadiazocine that formulated as (C₁₈H₁₇N₅O₂) was determined by single-crystal X-ray diffraction and FT-IR spectroscopy. The crystal structure is triclinic, space group P-1 with parameters a=10.0175(7) Å, b=9.9702(6) Å, c=17.5941(10) Å, α=96.546(5)°, β=106.069(5)°, γ=97.178(5)°, V=1654.87(19) Å³, Z=4. Theoretical calculations have been carried out by using Hartree-Fock (HF) and Density Functional Theory (DFT) methods. The vibrational frequencies were calculated by using HF/6-31G(d,p) and DFT/B3LYP/6-31G(d,p) basis sets in ground state. The calculated structural parameters (bond lengths, bond angles, torsion angles) and vibrational assignments were compared with their experimental data. Molecular Electrostatic Potential (MEP) map of the compound was obtained by using the optimized structures. Furthermore,

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