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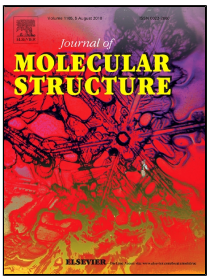

Structural features of 7-methoxy-5-methyl-2-(pyridin-3-yl)-11,12-dihydro-5,11-methano[1,2,4]triazolo[1,5-*c*][1,3,5]benzoxadiazocine: Experimental and theoretical (HF and DFT) studies, surface properties (MEP, Hirshfeld)

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Mustafa Kemal Gümüş[1], Sevgi Kansız[2,*], Ercan Aydemir[1,3], Nikolay Yu. Gorobets[4,5], Necmi Dege[2]

[1]*Artvin Coruh University, Science-Technology Research and Application Center, Artvin 08000, Turkey*

[*2]*Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139, Kurupelit, Samsun, Turkey*

[3]*T.R. Ministry of Forestry and Water Affairs, 11th Regional Directorate, 55030 Ilkadım-Samsun, Turkey*

[4]*SSI "Institute for Single Crystals" of National Academy of Sciences of Ukraine, 60 Nauky Ave., Kharkiv 61072, Ukraine*

[5]*V.N. Karazin Kharkiv National University, Svobody sq. 4, Kharkiv 61077, Ukraine*

[*]Corresponding author: e-mail: sevgi.koroglu@omu.edu.tr

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 ($C_{18}H_{17}N_5O_2$) 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) Å^3, 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,