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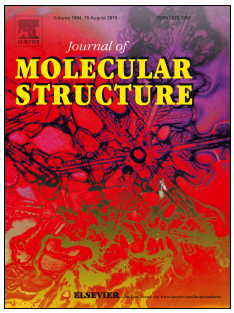

Synthesis, DFT calculations, electronic structure, electronic absorption spectra, natural bond orbital (NBO) and nonlinear optical (NLO) analysis of the novel 5-methyl-8*H*-benzo[*h*]chromeno[2,3-*b*][1,6] naphthyridine-6(5*H*),8-dione (MBCND)

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Synthesis, DFT calculations, electronic structure, electronic absorption spectra, Natural Bond Orbital (NBO) and nonlinear optical (NLO) analysis of the novel 5-methyl-8*H*-benzo[*h*]chromeno[2,3-*b*][1,6]naphthyridine-6(5*H*),8-dione (MBCND)

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Abstract

New derivative of heteroannulated chromone identified as 5-methyl-8*H*-benzo[*h*]chromeno[2,3-*b*][1,6]naphthyridine-6(5*H*),8-dione (**5**, **MBCND**) was easily and efficiently synthesized from DBU catalyzed condensation reaction of 2-aminochromone-3-carboxaldehyde (**1**) with 4-hydroxy-1-methylquinolin-2(1*H*)-one (**2**). The same product **5** was isolated from condensation reaction of aldeyde **1** with 3-(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-3-oxopropanoic acid (**3**) or ethyl 4-(4-hydroxy-1-methyl-2-oxo-1,2-dihydroquinolin-3-yl)-2,4-dioxobutanoate (**4**). Structure of compound (**5, MBCND**) was deduced based on their elemental analyses and spectral data (IR, ^{1}H NMR and mass spectra). Density Functional Theory (DFT) calculations at the B3LYP/6-311G (d,p) level of theory have been carried out to investigate the equilibrium geometry of the novel compound (**5**, **MBCND**). Moreover, total energy, energy of HOMO and LUMO and Mullikan atomic charges were calculated. In addition, the dipole moment, theoretical study of the electronic structure, nonlinear optical properties (NLO), and natural bonding orbital (NBO) analysis and orientation have been performed and discussed. Also the electronic absorption spectra were measured in polar (methanol) as well as non polar (dioxane) solvents and the assignment of the observed bands has been discussed by TD-DFT calculations. The correspondences between calculated and experimental transitions energies are satisfactory.

Keywords: TD-DFT, theoretical investigation, 2-aminochromone-3-carboxaldehyde, chromeno[2,3-*b*]pyridine, cyclocondensation, UV-spectra, MO-calculation, NBO and NLO analysis.

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