Indian Journal of Chemistry
Vol. 63, December 2024, pp. 1250-1262
DOI: 10.56042/ijc.v63i12.14051

Quantum chemical analysis of 3,5-dimethyl-2,6-diphenylpyridine and its *para* amino and nitro phenyl derivatives using density functional theory

Anan Haj Ichia Arisha[a,b]

[a] Department of Organic Chemistry, School of Chemistry, Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 6997801, Israel

[b] Department of Education, Beit Berl College, Beit Berl, Israel

E-mail: ananarisha@gmail.com

Received 29 September 2024; accepted (revised) 27 November 2024

In this study, density functional theory calculations at the wB97XD/Def2TZVPP level have been performed for 3,5-dimethyl-2,6-diphenylpyridine(**1**) compound and its *para* amino phenyl (**2**), *para* nitro phenyl(**3**), *para* amino nitro phenyl (**4**) derivatives. Global reactivity descriptors, namely, ionization potential, electron affinity, electronegativity, chemical potential, chemical hardness, softness, and electrophilicity index have been calculated using the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies. In addition, molecular electrostatic potential surfaces, Mulliken and natural charges, natural bond orbitals have been analyzed. Furthermore, ultraviolet–visible (UV–Vis) absorption characteristics and nonlinear optical parameters, *viz.* dipole moment, polarizability, and hyperpolarizability, have been calculated. The range of the energy-gap values (E_{LUMO}– E_{HOMO}) is 6.9470–8.8026 eV, indicating the chemical stability of **1**–**4**, with **4** exhibiting the smallest energy gap, lowest hardness, and most softness. According to the UV–Vis analysis, $\pi \rightarrow \pi^*$ transitions dominate, and in the HOMO–LUMO transition, the wavelength increases in the order of **4**>**3**>**2**>**1**. The hyperpolarizability values change drastically, with the $\beta_{total}/\beta_{urea}$ ratio for **1**, **2**, **3**, and **4** being 2.7, 28, 25, and 50, respectively. These materials, especially **4**, are promising for optoelectronics and industrial applications.

Keywords: 3,5-Dimethyl-2,6-diphenyl, Density functional theory, Natural bond orbital, Ultraviolet–visible, Nonlinear optical parameters