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**Original Research Article**

# Synthesis and Theoretical Studies of [2-amino-3-(ethoxycarbonyl)-1,4-dihydro-1-phenyl-4-pyridinyl] Ferrocene Derivatives

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## ABSTRACT

In this study, syntheses of [2-amino-3-(ethoxycarbonyl)-1,4-dihydro-1-phenyl-4-pyridinyl]ferrocene derivatives from reaction of ferrocenecarboxaldehyde, ethyl cyanoacetate, aniline, and acetylenic esters in the presence of piperidine were reported in good yields. The reaction proceeded smoothly and cleanly under mild reaction conditions and no side reactions were observed. The structures of the products were confirmed by IR, $^{1}$H NMR, $^{13}$C NMR, mass spectroscopy, and elemental analysis. Then, structure, electronic and spectroscopic properties of the synthesized molecules were computed at the CAM-B3LYP/jorge-DZP (H,C,N,O) and Def2-TZVPPD (Fe) level of theory. First hyperpolarizability value were calculated to describe the nonlinear optical (NLO) properties of these molecules. The HOMO-LUMO study to find the band gap of the prepared molecules was extended to calculate global hardness, chemical potential and global electrophilicity for the investigation of the chemical behavior of the compounds. The energies of iron *d*-orbitals and formal electron configurations of iron atom were calculated by natural bond orbital (NBO) analysis.

**Keywords:** Frontier orbitals; hyperpolarizability; ferrocenecarboxaldehyde; NBO analysis.

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