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Synthesis and DFT Insights on Molecular Structure, FMO's, MESP and Chemical Reactivity of the 2,4-Diphenylthiazole

A.R. Bukane[1,*] and B.S. Jagdale[2]

[1]PG Department of Chemistry, Mahatma Gandhi Vidyamandir's Arts, Science and Commerce College (Affiliated to Savitribai Phule Pune University, Pune), Manmad, Taluka-Nandgaon, District-Nashik-423104, India
[2]PG Department of Chemistry, Mahatma Gandhi Vidyamandir's Loknete Vyankatrao Hiray, Arts, Science and Commerce College (Affiliated to Savitribai Phule Pune University, Pune), Panchavati, District-Nashik-422003, India

ABSTRACT

The current study focuses on the synthesis and density functional theory (DFT) analysis of a 2,4-diphenylthiazole. The reaction of benzothioamide and 2-bromo-1-phenylethan-1-one in ethanol at 70-80°C under stirring resulted in the creation of a 2,4-diphenylthiazole (2,4-DPT). ^{1}H NMR and ^{13}C NMR spectrum techniques were used to confirm the structure of a synthetic thiazole. The geometry of the 2,4-diphenylthiazole was optimised using the DFT approach with the 6-311G++(d,p) basis set at the B3LYP functional. Geometrical characteristics such as bond length and bond angles were optimised, examined, and debated. The parameters of quantum chemistry have been determined and investigated. Surface plot analysis of the Molecular Electrostatic Potential (MEP) has been performed at the same theoretical level.The current study also discusses the Mulliken atomic charge investigation of the titled compound.

KEYWORDS: Thiazole, DFT, B3LYP, 6-311G++(d,p).

INTRODUCTION

The five-membered heterocyclic molecule thiazole is well-known. In recent decades, much research has focused on the thiazole ring in order to discover new compounds that act as antioxidants[1], analgesics[2], anti-inflammatory[3], antimicrobial[4], antifungal[5], antiviral[6], diuretic[7], anticonvulsant[8], neuroprotective[9], and antitumor[10] or cytotoxic drugs with fewer side effects. Thiazoles and their derivatives have been used in the creation of drugs for the treatment of allergies [11], Hypertension[12], schizophrenia[13], bacterial infections[14], HIV infections[15], hypnotics[16] and more recently for the treatment of pain[17], as fibrinogen receptor antagonists with antithrombotic activity[18] and as novel inhibitors of bacterial DNA gyrase B[19].Thiazole nucleus is also a component of all known penicillins, which have revolutionised bacterial disease treatment[20]. Several thiazole containing drugs are available such as; nizatidine is a histamine H_2-receptor antagonist that inhibits stomach acid production, and commonly used in the treatment of peptic ulcer disease (PUD) and gastroesophageal reflux disease (GERD), nirida- zole as schistosomicidal, sulfathiazole as antibiotic, fanetizole as anti-inflammatory, combendazole as fungicidal[21].Theoretical chemistry calculations are based on quantum chemistry and physicochemical calculations. Density functional theory (DFT) can be used to predict many molecular properties [22-27]. Spectroscopic experiments include UV/vis spectra [28-29], IR and Raman frequencies and intensities [30-31], NMR chemical shifts [32], and spin-spin coupling constants [33]. DFT computations can estimate HOMO-LUMO energies [34-38], bond lengths and angles [39], and absorption energies [40-42].A lot of knowledge is gained by comparing theoretical calculations to experimental data. Using computing data, it is now possible to arrive at a reaction mechanistic route. The current research looked at molecule structure, bond length, bond angle, and Mulliken atomic charges using DFT analysis. Important characteristics like as total energy, HOMO-LUMO energies, and charge distribution are also investigated using the DFT method. In light of the foregoing, I'd like to present in this paper a density functional theory analysis of previously synthesised 2,4-diphenylthiazole compounds.

Methodology

General remarks: The chemicals with high purity were purchased from Virion Enterprises. The chemicals were used as received without any further purification. The melting point was determined in open capillary and uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on a sophisticated multinuclear FT NMR Spectrometer model Advance-II (Bruker) with ^{1}H frequency 500 MHz and ^{13}C frequency 126 MHz using $CDCl_3$ as a solvent, the reaction was monitored by thin-layer chromatography using aluminium sheets with silica gel 60 F254 (Merck).