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DFT Exploration on Molecular Characteristics of 6-Methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate

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ABSTRACT

Present investigation deals with the synthesis and density functional theory study (DFT) of a Biginelli adduct, 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MOPTHPC). The synthesis of a MOPTHPC has been carried out by the reaction of benzaldehyde, ethyl acetoacetate and urea in ethanol 70-80 °C under stirring condition in presence of catalytic amount of sulfamic acid. The structure of a synthesized chalcone is affirmed on the basis of ^{1}H NMR and ^{13}C NMR. The geometry of a MOPTHPC is optimized by using the density functional theory method at the B3LYP/6-311G(d,p) basis set. The optimized geometrical parameters like bond length and bond angles have been computed. Quantum chemical parameters have been determined and examined. Molecular electrostatic surface potential (MESP) surface plot analysis has been carried out at the same level of theory. Mulliken atomic charge study is also discussed in the present study.

1. Introduction

The Biginelli reaction is a multi-component reaction of aldehyde, urea, and acetoacetate involving Mannich reaction in the first step, which furnishes multifunctionalized 3,4-dihydropyrimidin-2-(1*H*)-ones (DHPMs) and related heterocyclic compounds. The Biginelli reaction is frequently used for the direct synthesis of 3,4-dihydropyrimidin-2(1*H*)-one "DHPM" derivatives which display interesting biological activities [1]. Notable examples are calcium channel modulators [3], antibacterials [4], antivirals [5], antifungals [6] and other biological activities have been discovered in DHPMs [7-14]. Calculations in theoretical chemistry are based on physicochemical calculations and quantum chemistry. Different molecular properties can be predicted using density functional theory (DFT) [15-20], UV-Vis spectra [21, 22], IR and Raman frequencies and intensities [23, 24], NMR chemical shifts [25], and spin-spin coupling constants [26] are the spectroscopic investigations that can be carried out. HOMO-LUMO energies [27-31], bond lengths and bond angles [32], and adsorption energies [33-35] can all be predicted using DFT calculations. DFT method with B3LYP functional has gained a lot of interest in the last two decades. B3LYP stands for "Becke, 3-parameter, Lee-Yang-Parr". The structural and chemical properties of organic molecules have been effectively explored using the density functional theory based on theoretical quantum calculations [38-42]. As theoretical calculations are compared to experimental findings, a lot of knowledge is gained. It is now possible to arrive at a reaction mechanistic pathway using computation tools. The current study looked at DFT analysis of molecular structure, bond length, bond angle, and Mulliken atomic charges. The DFT approach is also used to investigate important parameters such as total energy, HOMO-LUMO energies, and charge distribution. In last decades several green chemistry methods have been employed for the synthesis of variety of organic compounds [43-46]. In light of the above, I'd like to present a density functional theory investigation of previously synthesised 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MOPTHPC) compounds in this paper.

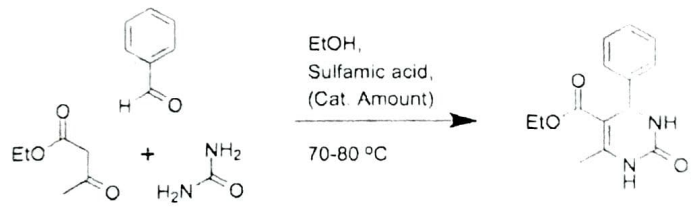
2. Experimental Methods

2.1 General Remarks

The chemicals with high purity were purchased from Virion Enterprises, India. 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 125 MHz using DMSO-d6 as a solvent. The reaction was monitored by thin-layer chromatography using aluminium sheets with silica gel 60 F254 (Merck).

2.2 Procedure for the Synthesis of Ethyl 6-Methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MOPTHPC)

As shown in Scheme 1, a mixture of benzaldehyde (0.01 mol), urea (0.01 mol), and ethyl acetoacetate, (0.01 mol) were mixed in 10 mL ethanol in the conical flask and catalytic amount of sulfamic acid were added to it. The resulting mixture was stirred on a magnetic stirrer at 70-80 °C for the required time which was monitored by TLC. The crude product was transferred into a beaker containing crushed ice, stirred, filtered, dried naturally, and recrystallized from ethanol to furnished pure white solid (m.p. 196 °C -198 °C).



Scheme 1 Synthesis of MOPTHPC

2.3 Computational Details

All of the calculations for this work have been performed at DFT (B3LYP) methods with 6-311G(d,p) basis sets using the Gaussian 03 W program [47]. The geometry optimization of the title compound and corresponding energy were calculated with a 6-311G(d,p) basis set by assuming C1 point group symmetry. Accordingly, the optimized geometrical parameters, energy, atomic charges, dipole moment, and other thermodynamic parameters were calculated theoretically

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