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DFT BASED ANALYSIS OF N-(3-METHYL-2, 6-DIPHENYL-PIPERIDIN-4-YLIDINE)-N'-PHENYL HYDRAZINE (3-MDPYP) MOLECULE

M. Dinesh Kumar[1*], P. Rajesh[2], M. Ezhil Inban[3] and P. Kumaradhas[4]
[1]Department of Chemistry, Karpagam Academy of Higher Education,
Coimbatore-641 021, (Tamilnadu) India
[2]Department of Chemistry, Government Arts College, Coimbatore-641 018, (Tamilnadu) India
[3]Department of Physics, Government Arts College, Coimbatore-641 018, (Tamilnadu) India
[4]Department of Physics, Periyar University, Coimbatore-641062 (Tamilnadu) India
*E-mail: dinemca@gmail.com

ABSTRACT

To analyze the geometrical and topological parameters of the3-MDPYP molecule, the quantum chemical calculations using Density Function Theory (DFT) is performed. This method along with the 6-311G** basis set, confirms the exact geometry of the selected molecule. The vital role of Piperidin-4-ones and its derivatives are found to have great potential in terms of becoming potent compounds in drug design. In this regard, characterizing such compounds to study theoretically and their structure becomes important and economical in performing the suitability test. This paper is a record of such research attempt on studying geometrical properties like the bond angle, bond lengths, torsion angles and bond topological properties of the 3-MDPYP molecule.

Keywords: 3-MDPYP, DFT, Bond topology, Deformation density, Laplacian electron density

INTRODUCTION

In today's drug discovery, it is a task challenging to understand the drug-receptor interaction[1]. Many methods have been proposed in the previous years to investigate the drug-receptor interactions[2]. However, *in silico* computer modeling techniques along with in vitro studies are playing an important role and helps confirm the drug-receptor mechanism. Always the drug and receptor molecules will have complementary charges, so that the drug molecule may be well inside the binding pocket of the receptor[3,4]. The drug-receptor plays an important role in three-dimensional structures and also in the atomic level interaction of the molecule[5]. It is based on the strength of electrostatic interaction and charge distribution of atoms in the binding of sites. Further, the same electrostatic interaction of molecule is used to verify the variable regions of the active drug molecule. This regard could be clarified through the accurate calculation of topological and electrostatic parameters determined from multipole analysis[6]of charge density distribution of the molecule, which includes the effects of lone pair and p-electron density. So the understanding of charge density distribution is important to determine the molecular properties and to predict the intermolecular interactions[7].

This work explains the theoretical analysis of charge density distribution and some topological parameters of the 3-MDPYP molecule through quantum chemical calculations. In today's scenario, Piperine-4-one compounds play a prime activity in all areas of drug discovery and form important drugs with an essential molecular structures[8-13]. These are reported to possess analgesic[8], anti-inflammatory[9], central nervous system[10], local analgesics[11], anticancer[12] and antibacterial activity[13]. To explore this kind of activity in 3-MDPYP molecule, some theoretical operations with the help of DFT are performed. A clear idea of charge density distribution and topological properties of this molecule has allowed realizing the strength of intermolecular interactions and electrostatic interactions between the drug candidate and receptor which facilitate to examine the interactions of drug-receptor.