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Investigation of Molecular Structure, Chemical Reactivity and Stability for Pyrrole Substitutes (Dual Anchoring System) Using Density Functional Theory.

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Abstract

The theoretical electron properties of Pyrrole Substitutes (R1, R2, R3 and R4) were carried out by using quantum chemical calculations. The optimized structures were obtained by the Density Functional Theory DFT/B3LYP level of theory using the basis set 6-31G. The optimized structures of compounds have the global minimum energy. It was found that the dipole moment of compound (R1) have high values compared with the Compounds (R2,R3,R4). Global descriptors such as the MO energies of HOMO, LUMO levels and ΔE, were determined and used to identify the differences in the stability and reactivity of compounds. In general, the calculated values lead to the conclusion that on the one hand the stability of the compounds are R3>R4>R1>R2. On the other hand, the theoretical study of novel acceptor-donor organic materials based on these compounds has been investigated. Different electron side groups were introduced to investigate their effects on the electronic structure; HOMO, LUMO and energy gap. The structural and electronic study as shown in this paper in hand for these compounds could help to design more efficient functional photovoltaic organic materials.

Keywords: Pyrrole Substitutes, structural and electronic properties, DFT/B3LYP, Band Gap.

1.Introduction

Organic compounds can have a variety of structures. These structures can be acyclic or cyclic. The cyclic systems containing only carbon atoms are called carbocyclic and the cyclic systems containing carbons and at least an other whatsoever element are called heterocyclic. Heterocyclic compounds are classified as aliphatic and aromatic heterocyclic. The heterocyclic which show aromatic behavior as in benzene are called the aromatic heterocyclic compounds such as pyrrole, furan, thiophene. Aromatic heterocyclic compounds based on pyrrole or pyrdinium core including carboxylate derivatives, Schiff-bases and their metal complexes, are materials of much interest to researcher due to their wide applications in medicine[1-2], catalysis, luminescence[3], optical devices[4] and clean energy[5-6]. The π-