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Theoretical Investigation of Structural and Electronic Properties of Donor-Acceptor Organic Molecules for Optoelectronic Applications

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***Abstract*— In this work, we have studied the structural, electronic and global reactivity of three donor-acceptor organic molecules PTFBH, TFPCBP and TFPTP as a density functional theory system using the B3LYP/6-311G(d,p) level of theory. The calculations were carried out in Gaussian 09 and the molecular geometry and the frontier molecular orbitals were plotted in GaussView 5. The optimized structures were used to examine the total electronic energies, dipole moments, HOMO-LUMO energies, energy gaps and the global reactivity of those molecules. In comparison to all the other molecules studied, TFPTP showed the highest dipole moment with a value of 5.1567 D and the lowest HOMO-LUMO energy gap with a value of 4.6136 eV, which represents a better electronic and charge transfer behavior. PTFBH exhibited an intermediate behavior with an energy gap of 5.1519 eV and the largest gap with 6.3294 eV of TFPCBP. The results suggest that TFPTP is the most electronically responsive molecule in the studied systems and is therefore the one to be studied further in optoelectronic and nonlinear optical applications.**

***Keywords*—Density Functional Theory (DFT); B3LYP/6-311G(d,p); Donor-Acceptor Molecules; Frontier Molecular Orbitals; Global Reactivity Descriptors.**

I. INTRODUCTION

The continuous development of molecular materials with controllable electronic and optical properties has been a driving force behind the development of modern organic electronics, photonics and nonlinear optical technologies. Organic molecular systems are particularly attractive because their electronic properties can be altered by rational changes in molecular structure (e.g., conjugated framework, strength of electron-donating and electron-withdrawing groups, etc.) and the electronic communication between different molecular fragments [1-4].

Organic molecules are very flexible compared to inorganic molecules and can be tuned for absorption and charge transfer, energy, polarization [1,2, 5-8].

Among the various methods for design of organic materials, the incorporation of electron-donor (D) and electron-acceptor (A) in a conjugated molecular framework can be an effective tool to adjust electronic properties. In such systems the electronic communication between donor and acceptor moieties can induce the ICT, especially when the two units are connected by an electronically communicating π-conjugated bridge [5-8].

The degree of ICT depends strongly on the electronic strength of the donor and acceptor groups, molecular geometry, conjugation length, and orbital overlap. Thus, small changes in structure can lead to significant changes in the charge distribution and electronic excitation. Donor-acceptor molecular architectures have attracted great interest due to their role in many optoelectronic systems. The formation and evolution of charge transfer states is particularly important in organic solar cells, photodetectors, organic light-emitting devices and other molecular electronic systems [1,2,9-12]. In organic photovoltaic materials, for example, the relative energies and spatial distributions of donor- and acceptor-derived electronic states strongly influence photoinduced charge separation and charge transport [9-11]. Recent progress in molecular design, particularly involving donor-acceptor and acceptor-donor-acceptor architectures, has demonstrated that careful control of molecular structure can provide effective tuning of optical absorption and frontier energy levels [10,11].

The push-pull character associated with donor-π-acceptor systems is also of considerable importance for nonlinear optical (NLO) applications. Organic chromophores containing electron-rich and electron-deficient termini connected through conjugated bridges can exhibit strong polarization changes upon electronic excitation [7,13-15]. The resulting redistribution of electron density may enhance molecular polarizability and hyperpolarizability, which are important quantities governing linear and nonlinear optical responses.

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Earlier experimental and theoretical studies established the importance of molecular asymmetry, extended conjugation, and donor-acceptor interactions in the design of efficient organic NLO chromophores [13-15]. More recent studies continue to emphasize the relationship between π-conjugation, electronic delocalization, and push-pull interactions in controlling the optical response of molecular systems [15,16].

A useful first approach for examining the electronic characteristics of such molecules is frontier molecular orbital analysis. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) provide valuable qualitative information about the distribution of electronically active regions within a molecule [17,18]. In general, the HOMO is associated with the region from which electron density can be most readily removed, whereas the LUMO represents a low-energy orbital available for electron-density acceptance. The energy separation between these orbitals, commonly expressed as the HOMO-LUMO gap, is widely employed as a comparative descriptor of electronic excitation, kinetic stability, and susceptibility to charge redistribution [17-20]. In donor-acceptor systems, the spatial localization of the HOMO and LUMO can be equally important because separation of these orbitals over different molecular segments may indicate a favorable pathway for intramolecular charge transfer.

The conceptual basis for relating frontier orbitals to chemical reactivity has been extensively developed within density functional theory and conceptual density functional theory [17-21]. Parr and Yang established an important connection between density functional concepts and frontier-electron theory, providing a theoretical framework for understanding chemical reactivity in terms of changes in electron density [17]. Furthermore, quantities such as electronegativity, chemical potential, chemical hardness, softness, and electrophilicity have been developed as useful descriptors of the global response of a molecular system toward electron transfer [18-21]. The concepts of absolute electronegativity and chemical hardness provide information regarding the tendency of a molecule to attract electron density and its resistance to charge redistribution, respectively [18]. The electrophilicity index subsequently introduced by Parr and co-workers provides an additional measure of the stabilization associated with electron acceptance [20]. Together, these descriptors have become widely used for comparative studies of molecular stability and reactivity [21].

Density functional theory (DFT) provides a suitable theoretical framework to study these structural and electronic properties at molecular level. With the development of the fundamental Hohenberg-Kohn theorems and Kohn-Sham formalism, DFT has emerged as one of the most prominent theoretical approaches for computational chemistry and materials research [22,23]. The development of the practical exchange-correlation functionals (the hybrid functionals) further extended the scope of the DFT approach to molecular systems [24,25].

The geometry optimization can be used to obtain equilibrium molecular structures, and the calculations based on the optimized geometry can be used to study the total electronic energies (and dipole moments, electron distributions, frontier molecular orbitals and reactivity descriptors). This type of theoretical studies can be particularly useful for comparison of molecules that are structurally related and for the correlation between molecular structure and electronic properties. In this work, we have compared three donor-acceptor organic molecules: PTFBH, TFPCBP and TFPTP by means of quantum chemical calculations.

We have studied these molecules in the best way possible with respect to their optimized molecular geometry, their total electronic energies, dipole moments, frontier molecular orbitals, HOMO-LUMO energy gaps and global reactivity descriptors. These parameters are selected to provide a comparison of the ways in which molecular structure influences the polarity, electron donating and electron accepting tendencies and the overall electronic response. The calculated results of these three molecules show significant differences.

The largest dipole moment of TFPTP is 5.1567 D, which is the largest overall polarization in the studied series. It also has the smallest HOMO-LUMO energy gap of 4.6136 eV compared with 5.1519 eV for PTFBH and 6.3294 eV for TFPCBP. For each molecule in this series, the smaller calculated frontier-orbital separation of TFPTP indicates that it is easier to transfer electrons and that it is potentially stronger in charge transfer. The more negative LUMO energy is calculated for TFPTP, also showing that it is stronger in accepting electrons. TFPCBP, on the other hand, has the largest HOMO-LUMO gap and tends to be more resistant to electronic excitation and charge redistribution whereas PTFBH is almost intermediate. These trends can help us to establish the structure and property relationships between the three molecules studied here.

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This study is therefore aimed at understanding the link between donor-acceptor molecular structure and electronic behavior through a detailed comparison of structural and frontier orbital properties. Instead of considering only one descriptor, the mixed interpretation of optimized geometry, molecular polarity and HOMO-LUMO energies, and conceptual-DFT based reactivity parameters gives a more complete picture of the electronic properties of the studied molecules. Based on the results, TFPTP is the most electronically responsive molecule of the present series and would be of interest for the next step in terms of spectroscopic calculations and experimental characterization, and therefore should be investigated further, by studying the excited-state calculations and solvent effects, optical absorption and linear and nonlinear optical properties, which may also be involved by means of the spectroscopic analyses.

II. Methodology

The quantum chemical calculations of PTFBH, TFPCBP, and TFPTP were carried out using density functional theory (DFT) with the B3LYP exchange-correlation functional and the 6-311G(d,p) basis set, as implemented in the Gaussian 09 program package [24-27]. All molecular structures were fully optimized without imposing any geometrical constraints, and frequency calculations were performed at the same level of theory to confirm the stability of the optimized structures.

The optimized geometries were subsequently used to calculate the total electronic energies, dipole moments, frontier molecular orbital energies, and global reactivity parameters. The HOMO and LUMO energies were analyzed to understand the electronic properties and charge-transfer characteristics of the studied molecules. In addition, global reactivity descriptors, including ionization potential, electron affinity, electronegativity, chemical potential, hardness, softness, and electrophilicity, were estimated using the calculated frontier orbital energies within the framework of conceptual DFT [18-20]. The optimized molecular structures and frontier molecular orbital distributions were visualized using the GaussView 5.0 molecular visualization program. The calculated parameters were comparatively analyzed to establish the relationship between molecular structure, electronic behavior, and reactivity.

III. Results And Discussion

3.1 Optimized Geometry

The optimized molecular geometries of PTFBH, TFPCBP, and TFPTP molecules are shown in Figure 1. These structures were obtained through quantum chemical calculations and serve as the basis for evaluating their electronic and reactivity properties. The geometry optimization helps ensure that each molecule is in its lowest energy configuration, which is essential for accurate determination of further properties.

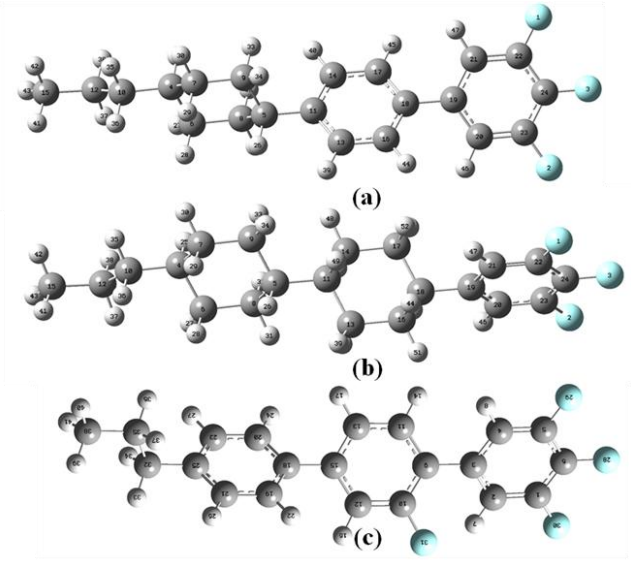

Figure 1: Optimized geometry of (a) PTFBH, (b) TFPCBP, and (c) TFPTP molecules.

The total electronic energies and dipole moments of the three molecules are presented in Table 1. Among them, TFPTP exhibits the most negative energy value (-1209.5444 Hartree), indicating it is the most thermodynamically stable structure. PTFBH (-1113.9074 Hartree) and TFPCBP (-1117.5318 Hartree) follow in increasing order of energy.

Table 1: Energy and dipole moment of (a) PTFBH, (b) TFPCBP, and (c) TFPTP molecules

Molecule	Energy (Hartree)	Dipole moment (debye)
PTFPBH	-1113.9074	4.1455
TFPCBP	-1117.5318	3.8139
TFPTP	-1209.5444	5.1567

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The dipole moments further reveal the polarity of the molecules. TFPTP shows the highest dipole moment (5.1567 Debye), suggesting stronger polarity and potential for interaction in polar solvents or alignment under electric fields. PTFBH (4.1455 D) and TFPCBP (3.8139 D) show moderate polarity. High dipole moments are often desirable in nonlinear optical (NLO) materials and for applications in electro-optic devices

3.2 Global Reactivity Parameters

Table 2 summarizes the global reactivity descriptors based on the HOMO and LUMO energies. These parameters reveal the chemical stability, reactivity and ability of the molecules to participate in charge-transfer processes. TFPCBP has the deepest HOMO (-6.9434 eV) and is thus less likely to donate electrons. TFPTP has a higher HOMO energy (-6.3224 eV) and is more likely to donate electrons. For LUMO, TFPTP has the most negative value (-1.7088 eV) and therefore can accept electrons more easily.

Energy gap (ΔE): The energy gap between HOMO and LUMO is very important in terms of molecular reactivity as a bigger gap indicates lower reactivity and more kinetic stability. TFPTP has the lowest energy gap (4.6136 eV) and is therefore the most chemically reactive of the three. PTFBH (5.1519 eV) and TFPCBP (6.3294 eV) follow.

Ionization potential (IP) and Electron Affinity (EA): IP and EA are related to the ease of electron removal and acceptance, respectively. TFPTP has the highest EA (1.7088 eV) indicating its strong electron acceptance. TFPCBP has the lowest EA (0.6139 eV). This is because of its poor electrophilic nature.

Electronegativity and Chemical Potential: Electronegativity is the tendency of a molecule to attract electrons. TFPTP has the highest electronegativity (4.0156 eV) and the most negative chemical potential (-4.0156 eV) so as to indicate its reactive, electron-accepting nature.

Hardness and Softness: Hardness measures resistance to charge transfer, while softness is its inverse. TFPCBP is the hardest molecule (-3.1647 eV) and is less reactive, while TFPTP is the softest (-0.4335 eV^{-1}) and thus more chemically responsive.

Electrophilicity Index (ω): This parameter estimates the electrophilic power of a molecule. TFPCBP has the highest electrophilicity index (-22.5934 eV) and is thus very electrophilic (the negative sign might be due to computational convention and should be interpreted accordingly).

Table 2: Global reactivity parameters of (a) PTFBH, (b) TFPCBP, and (c) TFPTP molecules

Global Reactivity Parameters	PTFBH	TFPCBP	TFPTP
HOMO (eV)	-6.4601	-6.9434	-6.3224
LUMO (eV)	-1.3082	-0.6139	-1.7088
Ionization Potential (eV)	6.4601	6.9434	6.3224
Electron Affinity (eV)	1.3082	0.6139	1.7088
Electronegativity (eV)	3.8841	3.7787	4.0156
Chemical potential (eV)	-3.8841	-3.7787	-4.0156
Hardness (eV)	-2.5759	-3.1647	-2.3068
Softness (eV^{-1})	-0.3882	-0.3160	-0.4335
Electrophilicity index (eV)	-19.4308	-22.5934	-18.5982
Energy gap (eV)	5.1519	6.3294	4.6136

3.3 Frontier Molecular Orbitals (FMOs)

FMOs, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are important to understand the chemical structure of organic molecules. HOMO is the outermost orbital that will be filled with electrons that will be donated to them in a chemical interaction whereas LUMO is the lowest energy orbital that can accept them. The energy difference between these two orbitals, called the HOMO-LUMO gap, is one of the most important indicators of the chemical reactivity, stability and optical properties of organic molecules. A smaller energy gap indicates higher reactivity and charge transfer capability of organic molecules and makes them more suitable for optoelectronic and nonlinear optical (NLO) applications.

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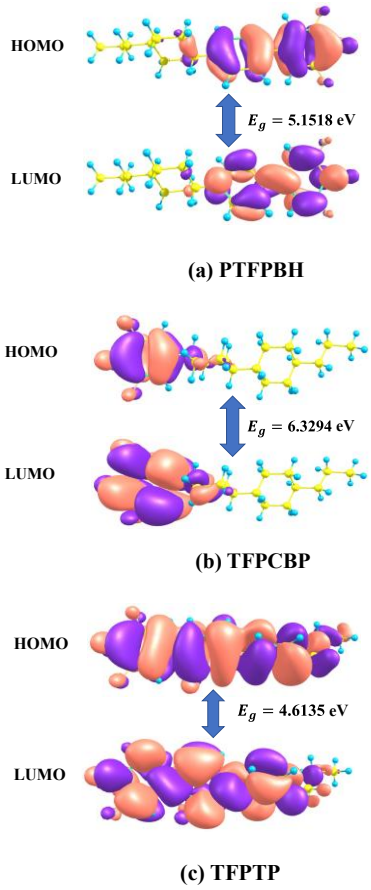

Figure 2: Frontier molecular orbital of (a) PTFBH, (b) TFPCBP, and (c) TFPTP molecules.

In this study, the HOMO and LUMO energies of PTFBH, TFPCBP and TFPTP molecules were determined and their energy gaps were studied. Of the three molecules, TFPTP has the lowest HOMO-LUMO energy gap of 4.6136 eV, PTFBH with 5.1519 eV and TFPCBP with the highest energy gap of 6.3294 eV. Its smaller energy gap indicates that TFPTP has the highest reactivity and higher charge transfer characteristics, which is a good candidate for organic electronics and photonic devices. TFPCBP has the largest energy gap and is the least reactive, which indicates that it would be more suitable for applications in chemical inert environments.

The visual representation of FMOs (as shown in Fig. 2) provides further insight into the nature of electron distribution in each molecule. In a push-pull or donor-acceptor system, the HOMO is localized over the electron-donating groups and the LUMO is distributed over the electron-accepting parts.

With this spatial separation between the HOMO and LUMO orbitals, charge transfer is facilitated in the ion-to-electron interactions. In TFPTP, the strong donor-acceptor interaction results in a well-separated HOMO and LUMO distribution which enables efficient electron flow and better polarizability. PTFBH also exhibits a moderate charge transfer but has more localized orbitals and less effective electron delocalization.

IV. Conclusion

In this paper, the structural, electronic and global reactivity properties of three organic molecules PTFBH, TFPCBP and TFPTP have been studied using quantum chemical methods. The optimized geometries have shown stable molecules, while the dipole moments and total energies of the molecules have been calculated to demonstrate their polarity and thermodynamic stability. As a result, TFPTP is the most promising molecule and has the largest dipole moment, the smallest HOMO-LUMO energy gap and the best electron affinity and electronegativity. These features indicate that the molecule is highly charge-transporting, more reactive and better at accepting electrons and thus is a good choice for optoelectronic and nonlinear optical applications. TFPCBP is considered the most chemically stable molecule as it has a large energy gap and lower reactivity, while PTFBH is a bit of the other end of the spectrum with balanced reactivity and stability. Based on these results, future work could be focused on the experimental synthesis and characterization of the TFPTP molecule to validate its predicted electronic behavior and NLO properties. Furthermore, further computational studies using solvent effects, time-dependent DFT (TD-DFT) simulations and third-order NLO property calculations can help us understand the photophysical behavior of these molecules. Structural variation of these molecules by adding different donor or acceptor groups could be a good option to fine-tune the electronic properties of these molecules. Finally, using these molecules in devices such as organic solar cells, field-effect transistors and electro-optic modulators would be an interesting next step to check their application in the real world.

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