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OPTO-ELECTRONICS AND NONLINEAR OPTICAL PROPERTIES OF ISOINDOLINE-1,3-DIONE-FULLERENE20-ISOINDOLINE-1,3-DIONE USING DENSITY FUNCTIONAL THEORY [a]

OPTO-ELECTRÓNICA Y PROPIEDADES ÓPTICAS NO LINEALES DE ISOINDOLINA-1,3-DIONA-FULLERENO20-ISOINDOLINA-1,3-DIONA UTILIZANDO LA TEORÍA FUNCIONAL DE LA DENSIDAD

MOHANNED Al-ANBER[b *], SAMIRA RESAN[b]

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Research Paper

ABSTRACT: Linear and nonlinear properties of isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione with the five phases were studied. The geometries of the isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione combination were attained using density functional theory DFT/B3LYP/6-31G+(d,p). The calculated properties are static polarizability, anisotropy of polarizability and first static hyperpolarizability at equilibrium geometry. In this article, the theoretical design of NLO molecules is discussed. The results show that there is a good electronic transfer within this molecule, and have a reasonably good propensity for nonlinear optical activity.

KEYWORDS: NLO properties; A-D-A; Fullerene; Intramolecular charge transfer; Torsional angles.

RESUMEN: Se estudiaron las propiedades lineales y no lineales de isoindolina-1,3-diona-fullereno-isoindolina-1,3-diona con las cinco fases. Las geometrías de la combinación de isoindolina-1,3-diona-fullereno-isoindolina-1,3-diona se obtuvieron utilizando la teoría funcional de la densidad DFT/B3LYP/6-31G+(d,p). Las propieda- des calculadas son la polarizabilidad estática, la anisotropía de la polarizabilidad y la primera hiperpolarizabilidad estática en la geometría de equilibrio. En este artículo, se discuten los resultados del diseño teórico de moléculas NLO. Los resultados muestran que existe una buena transferencia electrónica dentro de esta molécula y tienen una propensión razonablemente buena a la actividad óptica no lineal.

PALABRAS CLAVE: Propiedades NLO; A-D-A; Fullereno; transferencia de carga intramolecular; ángulos de torsión.

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1. INTRODUCTION

The electro-optical and nonlinear optical (NLO) materials have received considerable attention due to their wide range of potential applications Kiven *et al.* (2023). When the donor and acceptor groups are present at opposite ends, it leads to significant change and plays an essential role in materials D-A systems; introducing potent electron-donor groups raises the HOMO levels. At the same time, introducing potent electron-withdrawing groups lowers the LUMO levels, resulting in the narrow HOMO-LUMO energy gap (Hashemi *et al.*, 2019). Thus, the fundamental design criterion is the selection of proper electron-donor and acceptor units to achieve desired HOMO and LUMO levels beneficial for developing organic-optoelectronic materials. Additionally, potent electron donors and acceptors increase the delocalization of π-electrons, making the material highly polarizable, which causes remarkable optical nonlinearities in such systems. Since A-D-A materials possess distinct advantages like lightweight, good film-forming properties, relatively low manufacturing cost, biocompatibility, moderate to high conductivity, and easy tunability of desired properties, they are broadly used as active components in optoelectronic/photonic devices such as OPVs, OLEDs, OFETs, and NLO (Khalid *et al.*, 2023).

The objective of the present paper is to design new organic compounds. Where in nonlinear optics, organic materials on delocalized π-electron systems have attracted significant research interest in carbon compounds; for this reason, the fullerene (C20) was adopted as an electron-donor group. At the same time, two molecules (isoindoline-1,3-dione), which were adopted as two terminal acceptor groups Janjua *et al.* (2017), are linked on the surface of fullerene, as shown in Figure 1.

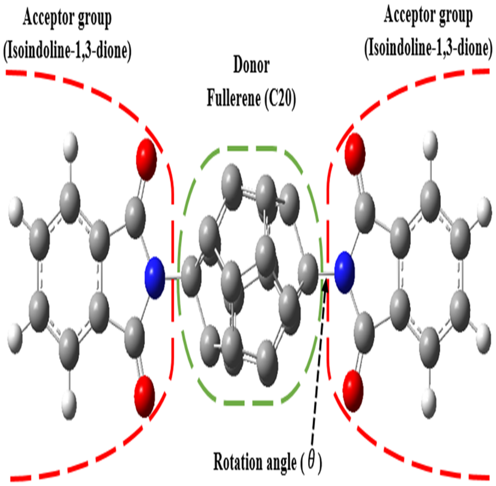


Figure 1: Shows the general molecular design of the NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) and the rotation angle. Source: Elaborated by the authors.

Therefore, isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione (IDF) was designed as an A-D-A type of conjugated system. In addition, two terminal acceptor groups were linked with different sites on the surface of fullerene, see Figure 2, so that they make a semi-angle (φ) between these two terminal acceptor groups around the fullerene, so five phases have appeared (IDF^1, IDF^2, IDF^3, IDF^4 and IDF^5, respectively). The theoretical calculations in this study are focused on the detailed analysis of the effects of various rotations (θ) of one isoindoline-1,3-dione group with the fullerene, see Figure 1, for the five phases.

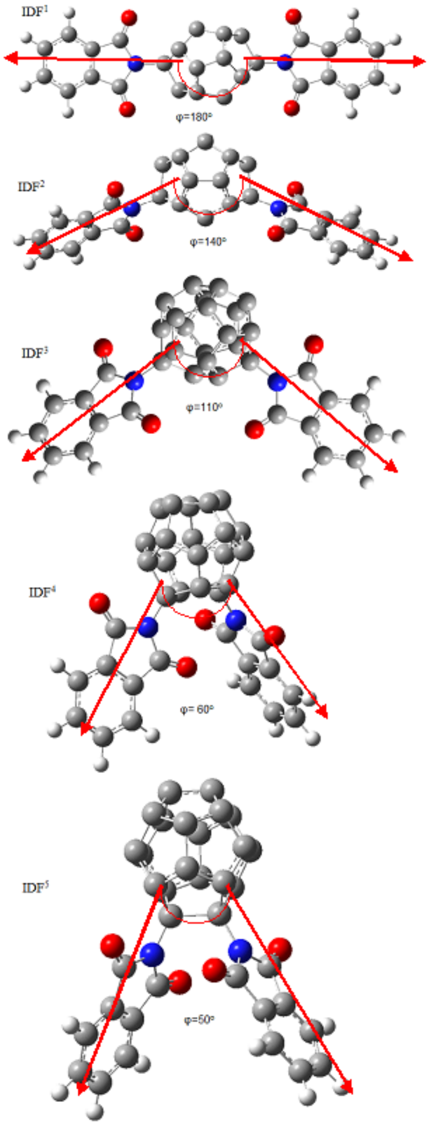


Figure 2: Shows the optimized geometry of the design NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) of the five phases (IDF^1, IDF^2, IDF^3, IDF^4 and IDF^5, respectively) using the B3LYB/6-31+G(d,p) method. Source: Elaborated by the authors.

2. METHOD AND COMPUTATIONAL PROCEDURE

The ground-state geometry optimizations for isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione of the five molecular phases, see Figure 2, have been explored by performing the density functional theory (DFT), which is one of the best computation methods of study for various types of molecules (Wazzan *et al.*, 2016; Kadadevarmath *et al.*, 2013). The torsion potentials were obtained for the isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) (IDF) as a function of the dihedral angle between the isoindoline-1,3-dione group and fullerene. During the scan process, the whole geometrical parameters were simultaneously relaxed so that they varied between 0°and 180°in 10°steps Resan *et al.* (2020). The electric dipole moment μ of molecules is a fundamental interest quantity in a structural molecule. While a molecule is subject to an external electric field ε, the molecular charge density may reset so that the dipole moment may change (Resan *et al.*, 2020). This change can be described as the first derivative of the molecular energy E to a component of the electric field (ε_i) that gives a component of the electric dipole moment in symbols (Shkir *et al.*, 2022):

$$\mu_i = (\partial E/\partial \varepsilon_i)_{(\varepsilon=0)} \tag{1}$$

where the total dipole moment (μ):

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{\frac{1}{2}} \tag{2}$$

The polarizability can be understood as the gradient of the induced dipole:

$$\alpha_{ij} = (\partial^2 E/\partial \varepsilon_i \partial \varepsilon_j)_{(\varepsilon=0)} \tag{3}$$

The average static polarizability <α> tensor is defined as:

$$< \alpha >= 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \tag{4}$$

where α_{xx}, α_{yy} and α_{zz} are the polarizability matrix diagonal elements Shkir *et al.* (2022). The anisotropic polarizability $\Delta\alpha$ amplitudes usually defined as (Shkir *et al.*, 2022):

$$\Delta\alpha = (1/2)[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xy}^2 + \alpha_{xz}^2 + \alpha_{yz}^2)]^{\frac{1}{2}} \tag{5}$$

The equations for the calculation of molecular static first-hyperpolarizability are given as follows:

$$\beta_{ijk} = (\partial^2 E/\partial \varepsilon_i \partial \varepsilon_j \partial \varepsilon_k)_{(\varepsilon=0)} \tag{6}$$

The static first-hyperpolarizability (β) is the third-rank tensor and is expressed as a $3 \times 3 \times 3$ matrix. Conferring to Kleinman symmetry ($\beta_{xyy} = \beta_{yxy} = \beta_{yyx} = \beta_{yyz} = \beta_{yzy} = \beta_{zyy}, \ldots$) likewise and these 27 components can be reduced to 10 Wagnière (1986). The complete equation for calculating the magnitudes of β from Gaussian 09 output provides ten components of this matrix as β_{xxx}; β_{xxy}; β_{xyy}; β_{yyy}; β_{xxz}; β_{xyz}; β_{yyz}; β_{xzz}; β_{yzz}; β_{zzz}, respectively, are reported in atomic units (AU), so that;

$$\beta_{tot} = [\beta_x^2 + \beta_y^2 + \beta_z^2]^{\frac{1}{2}} \tag{7}$$

where $\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz}), \beta_y = (\beta_{yyy} + \beta_{yzz} + \beta_{yxx}), \beta_z = (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})$ (G*ü*nay *et al.*, 2020). The first hyperpolarizability component along the direction of the dipole moment is represented by β_μ which is usually defined as:

$$\beta_\mu = (\mu_x\beta_x + \mu_y\beta_y + \mu_z\beta_z)/\mu \tag{8}$$

The XY-plane hyperpolarizability ($\beta_{xy-plane}$), which reflects the amount of β_{tot} in the XY-plane of the molecule, is given as (Khalid *et al.*, 2019):

$$\beta_{xy-plane} = \beta_{xxx} + \beta_{xxy} + \beta_{xyy} + \beta_{yyy} \tag{9}$$

The geometrical ground state, the electric dipole moment (μ), the mean polarizability <α>, and the first-order static hyperpolarizability (β) were calculated using the Gaussian 09W program Frisch *et al.* (2009). Output files were visualized via Gauss View 5 software Dennington *et al.* (2009). The isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione phases were determined by performing B3LYP (Becke′s three-parameter hybrid functional using the LYP correlation functional) (Soscún *et al.*, 2002; Mbala *et al.*, 2021). With the basis set 6-31+G(d,p) Soscún *et al.* (2002) where it is a split-valence basis set, which includes both diffuse (*s* and *p*-functions) for non-hydrogen atoms and added *d*-polarization functions on non-hydrogen atoms and *p*-polarization functions for hydrogen (Dikomang, 2019). Generally, many researchers have extensively used DFT/ B3LYP/6-31G+(d,p) for the first principle screening of nonlinear optical molecules (Yang *et al.*, 2016; Parol *et al.*, 2020; Resan *et al.*, 2020).

3. RESULTS AND DISCUSSION

In this article, we present the theoretical design results for NLO molecules. Because of the unique ability of intramolecular charge transfer between D and A, where A-D-A systems require consideration of non-linear optical (NLO) features Khalid *et al.* (2022). The design NLO structure (IDF), which contains five phases (IDF^1, IDF^2, IDF^3, IDF^4, and IDF^5, respectively), must be identified to conduct our inquiry. At first, it was necessary to find the most stable form of the design NLO structures (IDF^1, IDF^2, IDF^3, IDF^4 and IDF^5, respectively) before rotation, where the relative stability (ΔE) among them are very little and the five phases have same stability approximately. To add resilience to the NLO response of (IDF) throughout its design, the geometrical effect for the five phases was tested as a function of the torsional angles (Shettigar *et al.*, 2006). Figure 3 shows the fluctuation of relative stability ΔE with torsion angles for the five phases of IDF^1, IDF^2, IDF^3, IDF^4, and IDF^5, respectively. The fifth phase's stability (IDF^5) shows more instability

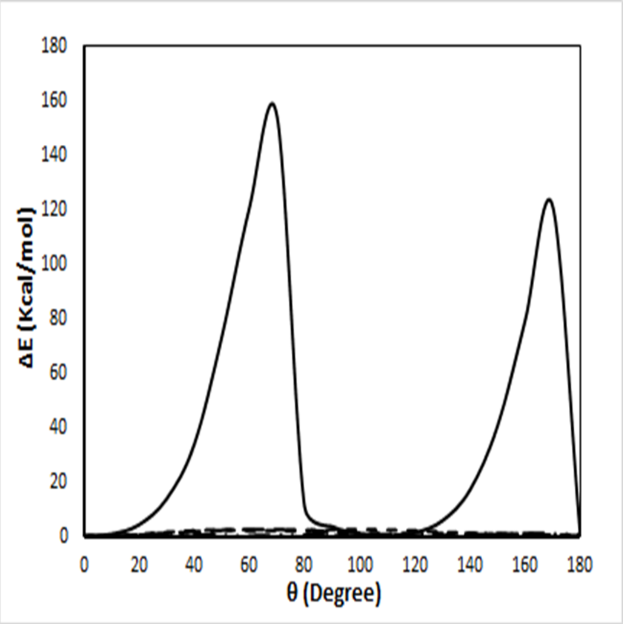
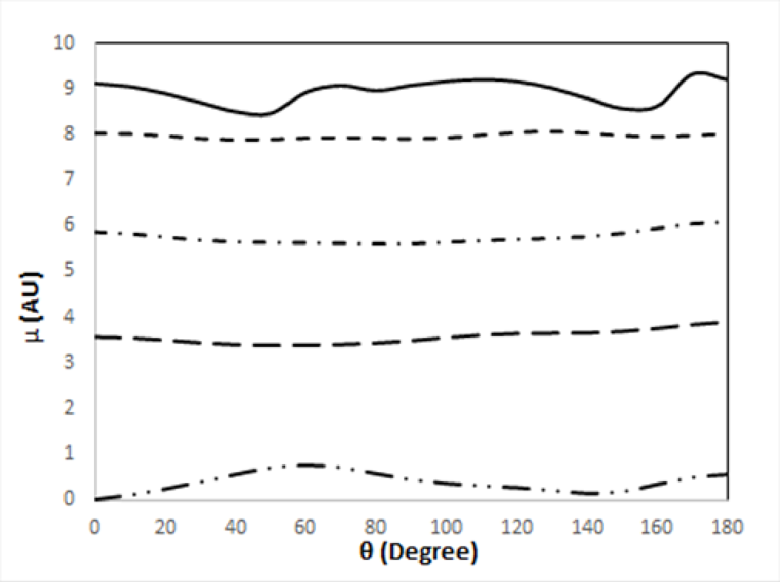


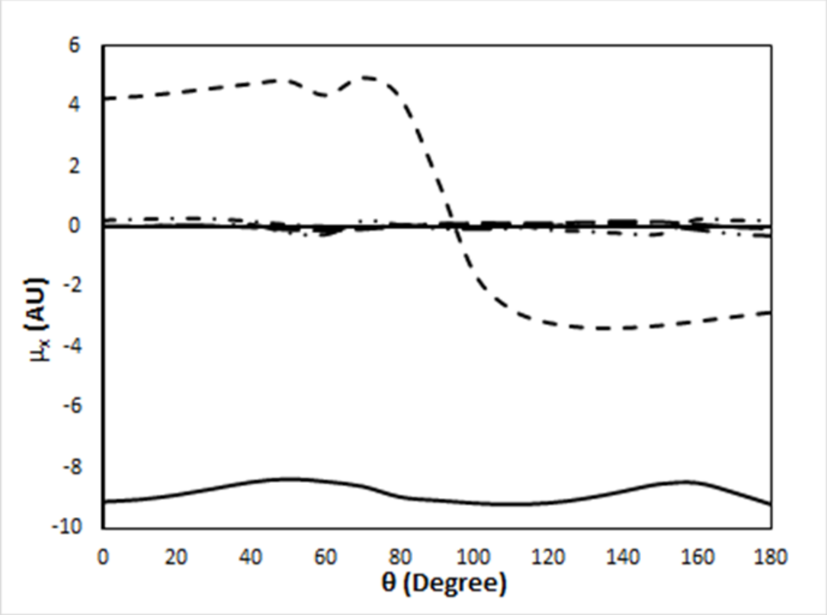
Figure 3: Shows the relative stability ΔE with the torsional angles for the design NLO (−.. − ..− IDF^1, − − −− IDF^2, −. − . − .− IDF^3, − − − − − IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 − 31+G(d,p) method. Source: Elaborated by the authors.

as the torsional angles increase forward to θ = 70° and 170°. However, the other phases showed very low instabilities compared to the results of Bahat *et al.* (2009) and Resan *et al.* (2020). Any results for IDF^5 at a high torsion angle will be ignored in favour of the other four phases due to requiring high energy for rotating, which is maybe because of the steric obstacle between the acceptor group (isoindoline-1,3-dione) and fullerene (Bahat *et al.*, 2009; Resan *et al.*, 2020; Bahrani *et al.*, 2022).

The dipole moment reflects the molecular charge distribution and is given as a vector in three dimensions. Therefore, it can be used as a descriptor to depict the charge movement across the molecule. The direction of the dipole moment vector in a molecule depends on the centers of positive and negative charges. For charged systems, its value depends on the choice of origin and molecular orientation. It is well known that the higher values of dipole moment, molecular polarizability, and hyperpolarizability are important for more active NLO properties. With the dihedral angle rotation, Figure 4 depicts the dipole moment (μ) and its three primary components. As the phases change from 1 to 5, the dipole moment values fluctuate due to angle rotates. Generally, the order of μ of designed structures was: IDF^5> IDF^4> IDF^3> IDF^2> IDF^1, but they have been little fluctuation with rotation compared with the results by Resan *et al.* (2020). As for the μ_x component, phases IDF^5 and IDF^4 are higher than the others and IDF^4 showed a switch behavior at 100°, see Figure 4. In addition, μ_y has high values (IDF^4> IDF^3> IDF^2 respectively) and contributes significantly to total dipole moment values. Also, IDF^3 showed good switch behavior for μ_y at 50°and 150°, with the caveat that this rotation does not need much energy, as seen in Figure 2. The total dipole moment (μ) value has been high because the component μ_y, so the designed molecule may be optically active in the y-direction.

The average polarizability and its components are another important molecule feature in the electronic characteristics. Therefore, calculating these properties is very important to assess the nonlinear optical potential of molecules. Values of average polarizability $<\alpha>$, anisotropic polarizability $\Delta\alpha$ and major contributing tensors (α_{xx}, α_{yy} and α_{zz}) of the five phases are shown in Figure 5.





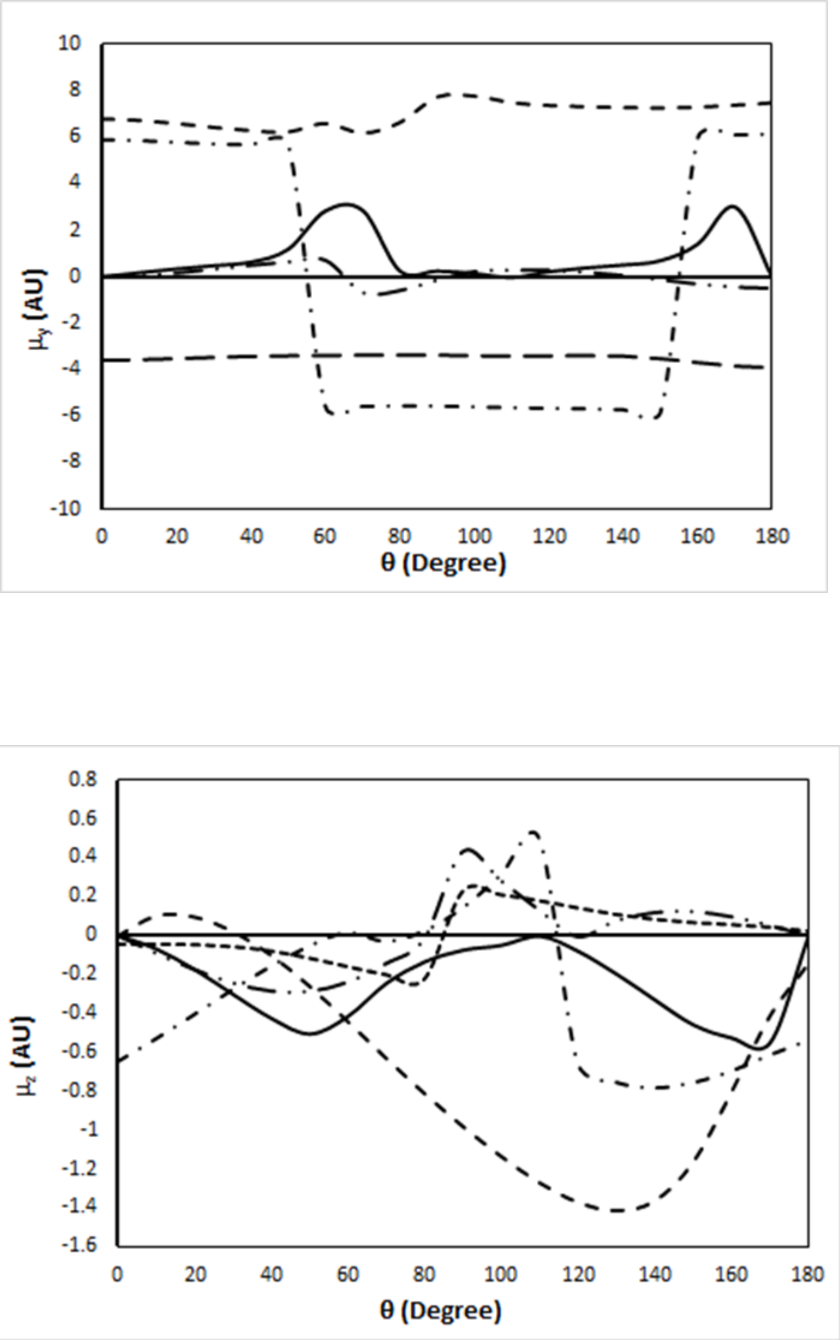
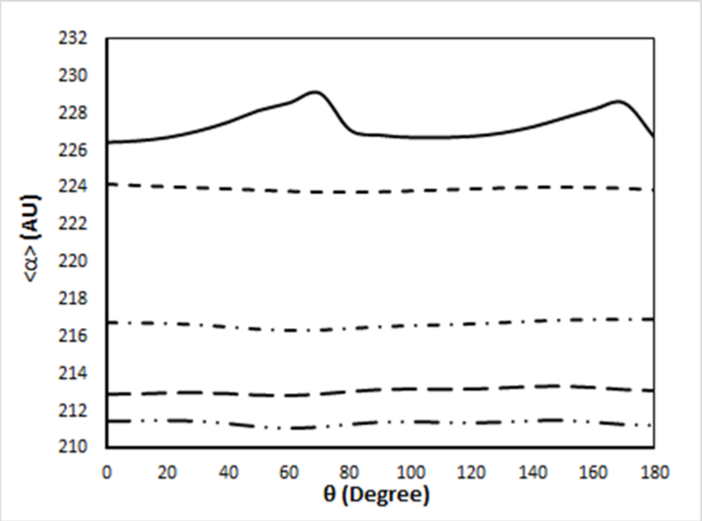
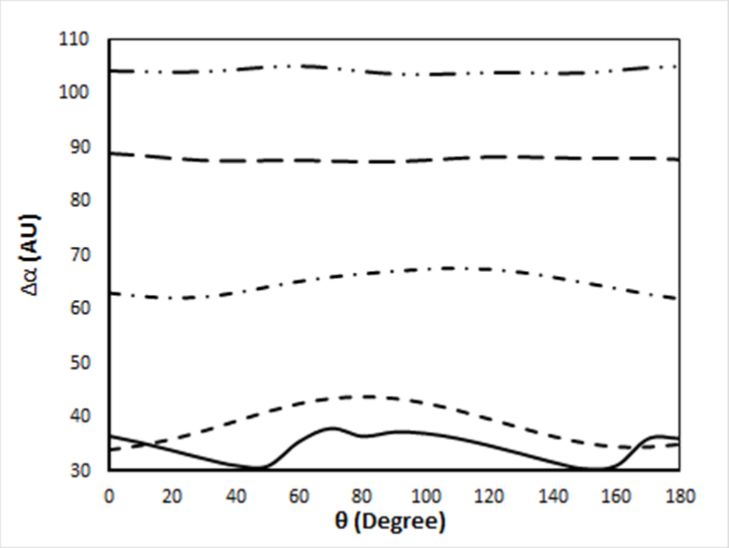
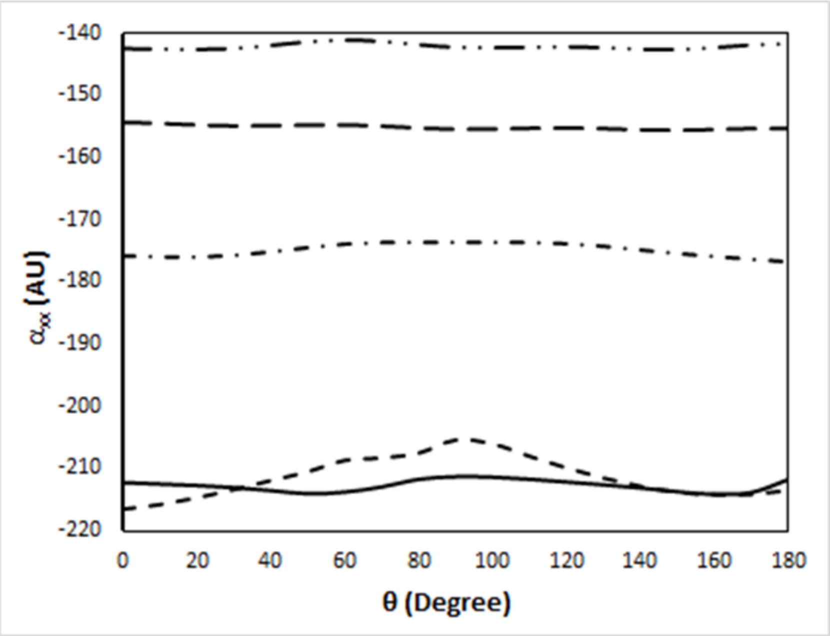


Figure 4: Shows the electric dipole moment (μ_{tot}) and dipole components (μ_x, μ_y and μ_z) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene- isoindoline-1,3-dione) with five phases (– ‥ – ‥ – IDF^1, – – – – IDF^2, – . – . – . – IDF^3, – – – – – IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 – 31+G(d,p) method. Source: Elaborated by the authors.

Order of average polarizability of designed structures was: IDF^5> IDF^4> IDF^3> IDF^2> IDF^1, but its values are still high compared with the results by Resan *et al.* (2020). Likewise, this will also increase the molecule′s refractive index Resan *et al.* (2020), and increases the π-electron deficiency and polarizability (Migalska-Zalas *et al.*, 2018). Generally, sizeable linear polarizability is required to obtain large hyperpolarizabilities (Ye *et al.*, 2022). Anisotropic polarizability Δα, which is dependent on the direction of the electric field, is one of the other NLO qualities for this design NLO structures showed inverse behaviour with average polarizability results. Where the five phases show values were lower than the average polarizability. When compared to perpendicular polarizability, it can be seen that torsional angles have no effect on polarizability parallel to the symmetry axes of the molecule. The values of the two compounds α_{zz} and α_{yy} are higher than the α_{xx} and showed more sensitivity to rotation dihedral angles.



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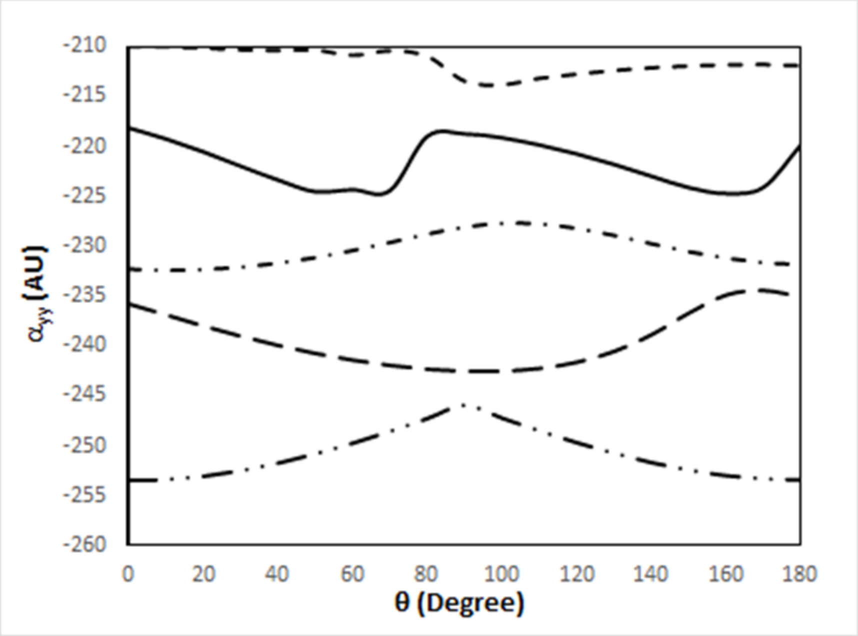
θ (Degree)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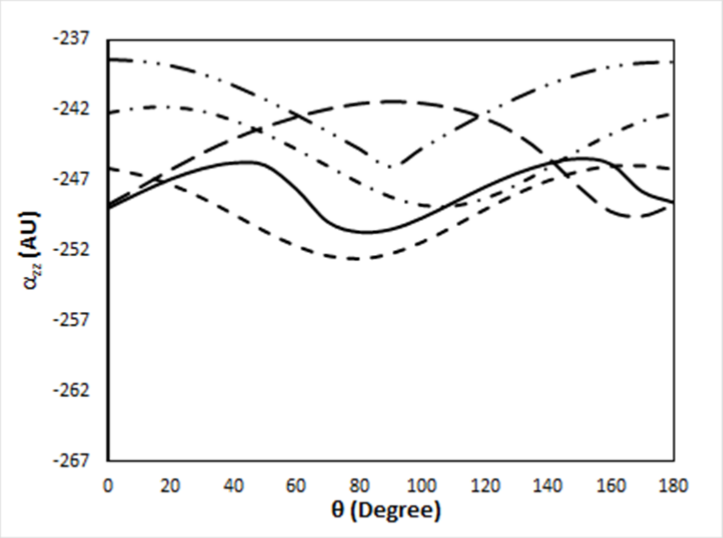


Figure 5: Shows the average polarizability <α>, the anisotropic polarizability Δα, and its major components (α_{xx}, α_{yy} and α_{zz}) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene- isoindoline-1,3-dione) with five phases (– .. – .. – IDF^1, – – – – IDF^2, – . – . – . – IDF^3, – – – – – – IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 – 31+G(d,p) method. Source: Elaborated by the authors.

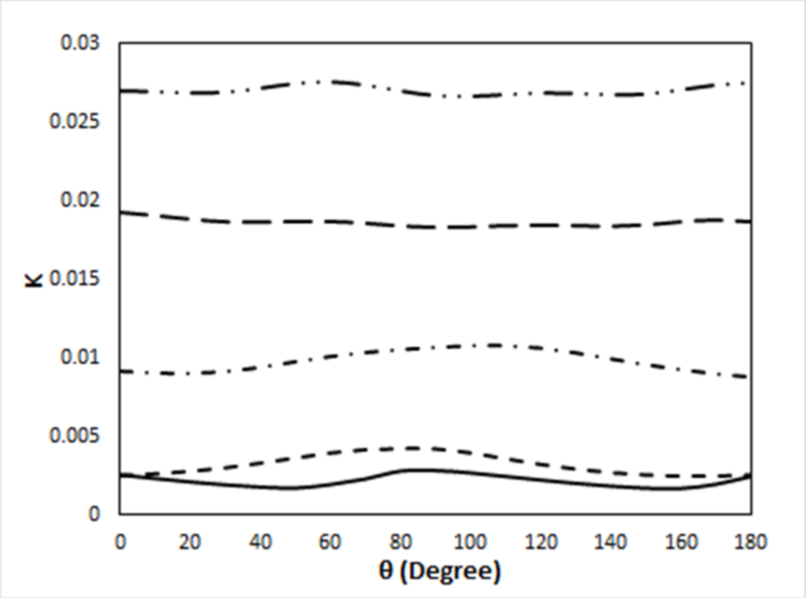
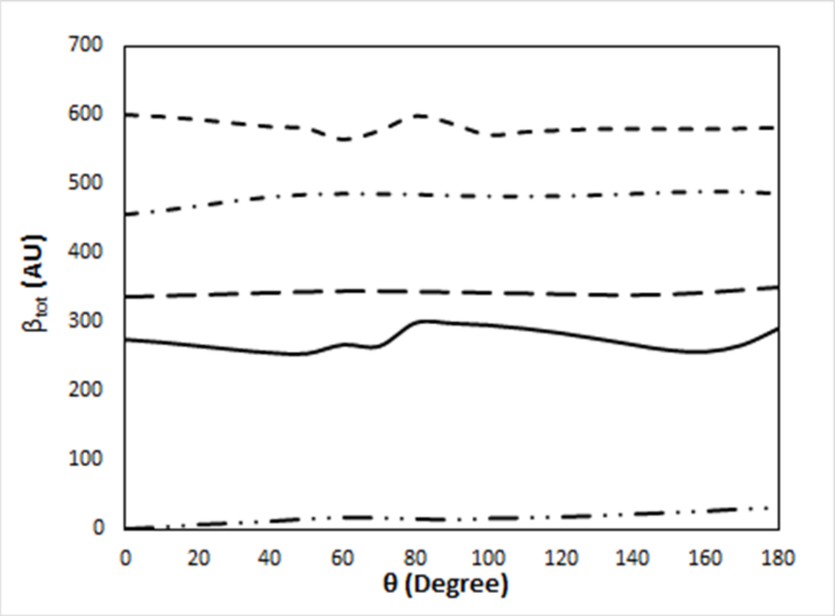


Figure 6: Shows the anisotropy (κ) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) with five phases (– .. – .. – IDF^1, – – – – IDF^2, – . – . – . – IDF^3, – – – – – – IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 – 31+G(d,p) method. Source: Elaborated by the authors.

Figure 6 shows the results of the anisotropy (κ), which gives a measure of deviations from spherical symmetry, with rotational angles for five phases, and order due to high spherical symmetry as IDF^4> IDF^5> IDF^1> IDF^2> IDF^3 respectively. In other words, the spherically symmetric charge distribution hasn′t been an interesting response to the rotation angles as the phases change from one to five. Generally, IDF^4 and IDF^5 have the highest spherical symmetric charge distribution (Labidi, 2016; Resan *et al.*, 2020).
A molecule′s hyperpolarizability and intramolecular charge transfer are the key factors for determining its nonlinear optical characteristics. Hyperpolarizability is a measurement of the nonlinear optical response of materials. The theoretical resolution of molecular hyperpolarizability (β_{tot}) is useful in explaining the link between molecular manufacturing and nonlinear optical properties. Figure 7 shows the order β_{tot} of five phases: IDF^4> IDF^3> IDF^2> IDF^5> IDF^1, respectively. The dihedral angle rotation has little influence on IDF^4> IDF^5 only. Figure 7 shows the results of hyperpolarizability along the dipole moment (β_μ), where the relationship between hyperpolarizability and dipole moment does not change with dihedral angle rotation. Moreover, the order β_μ of five phases is similar to β_{tot}. The variation of XY-plane hyperpolarizability ($\beta_{xy-plane}$) illustrates the amount of β_{tot} in the XY-plane of the isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione, as shown in Figure 7. Where IDF^4 and IDF^5 have been the highest $\beta_{xy-plane}$ value with little fluctuation along the rotation angle.

According to the results of the hyperpolarizability components (β_x, β_y, β_z) were examined the variation with the dihedral angles for the five phases of the NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione), as illustrated in Figure 8, where only β_x for two phases, IDF^4 and IDF^5 respectively, have high value with significant switching behaviour for IDF^4 by the rotation angle, which is the same as for μ_x component in Figure 4.



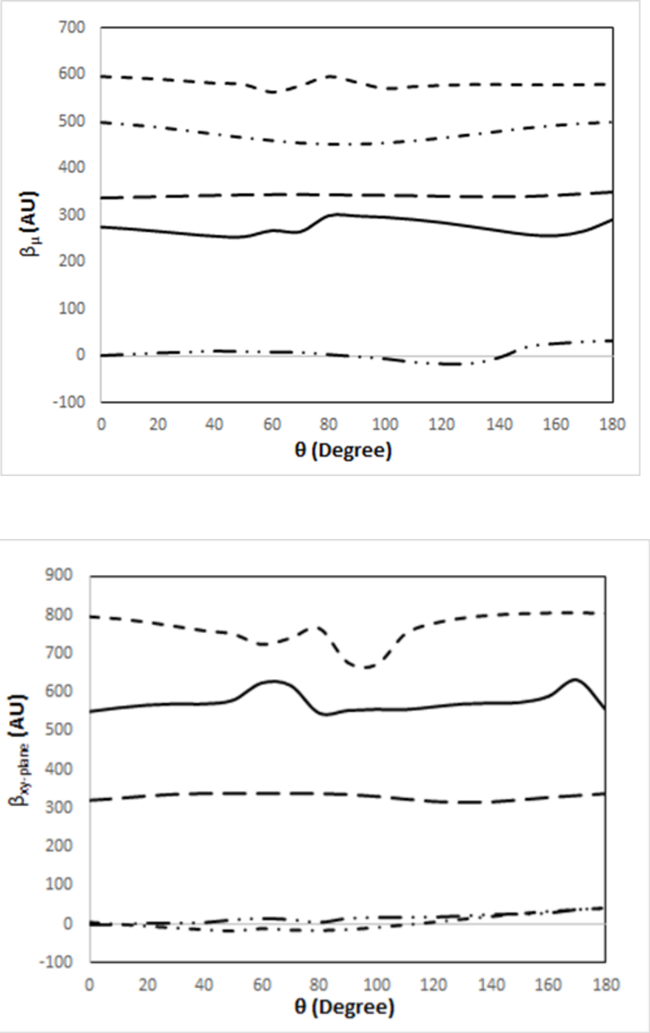
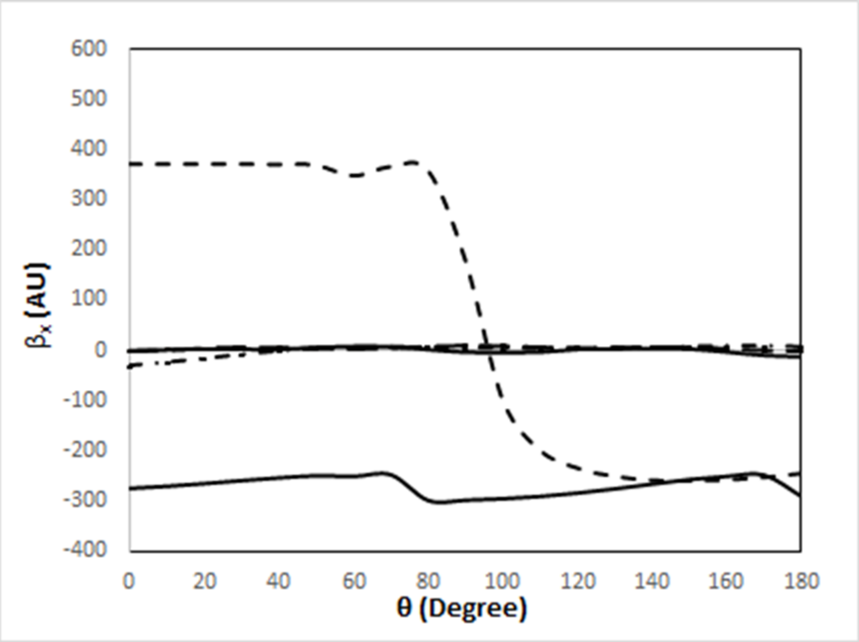


Figure 7: Shows the hyperpolarizability (β_{tot}), the hyperpolarizability along the direction of the dipole moment (β_μ) and the XY-plane hyperpolarizability ($\beta_{xy-plane}$) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione(C20)) with five phases (— ‥ — ‥ — IDF^1, — — — — IDF^2, — . — . — . — IDF^3, — — — — — IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 − 31+G(d,p) method. Source: Elaborated by the authors.

In addition, IDF^3 and IDF^4 have the highest values along the component β_y and more than the values of β_x. From the results of β_y, it is expected that the third phase will improve the charge transfer along the plane of the central molecule axis that is between the x and y-axis. Generally, the hyperpolarizability maybe depends on the component β_y, so that $\beta_{tot} \sim \beta_y$. Moreover, the biggest value of hyperpolarizability is seen in the β_y direction, which suggests that the significant delocalization of the electron cloud is greater in that direction. In addition, this is attributed to the strong electron-donating ability of the fullerene molecule, which creates an efficient push-pull system, owing to a greater degree of charge transfer from the donor to the acceptor. Higher NLO response may be due to enhancing charge transfer from donor to acceptor, but not along the x-axis, as reported (Khalid *et al.*, 2023).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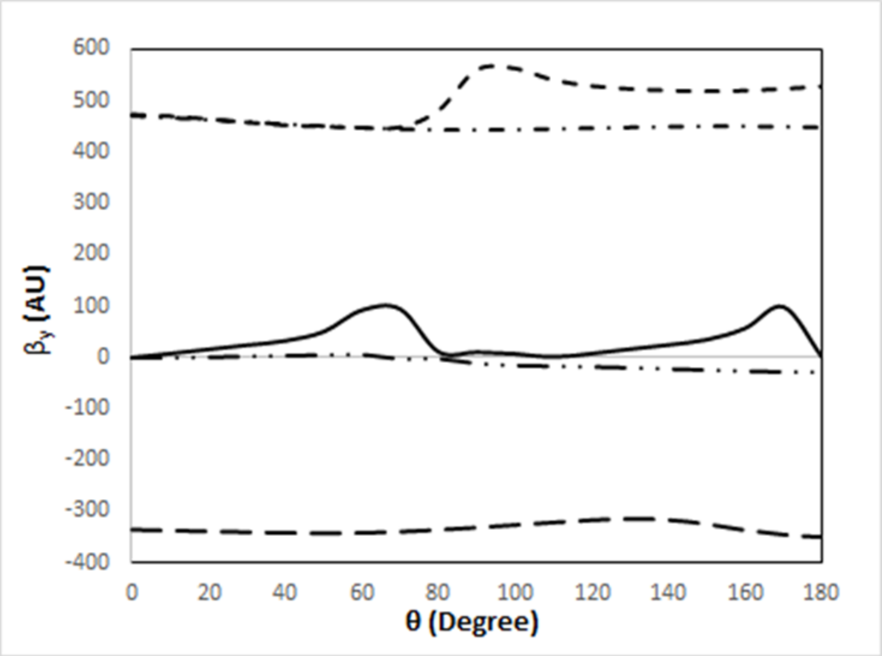
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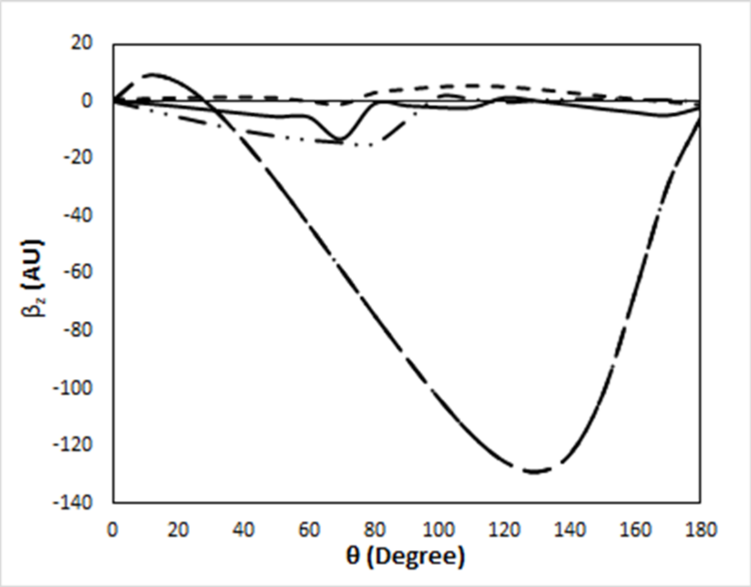
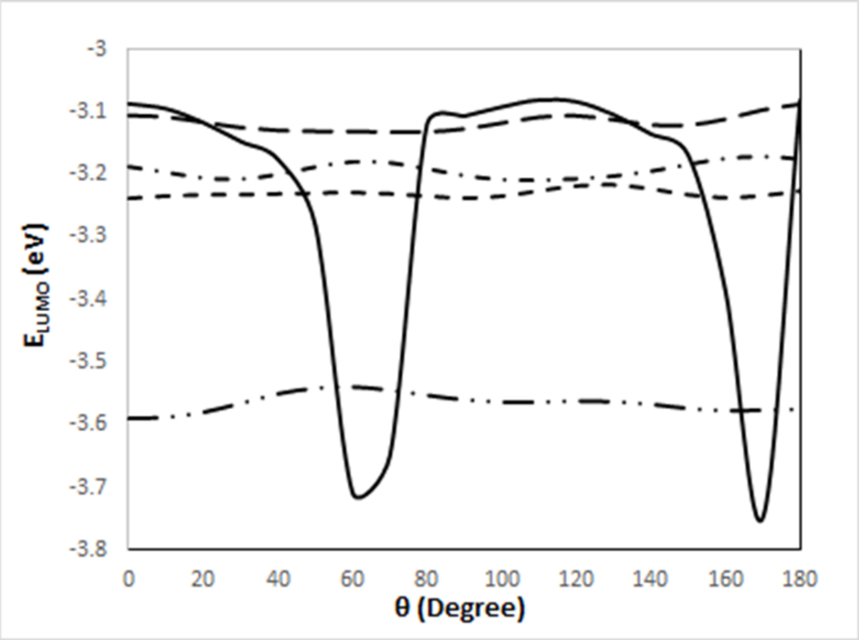
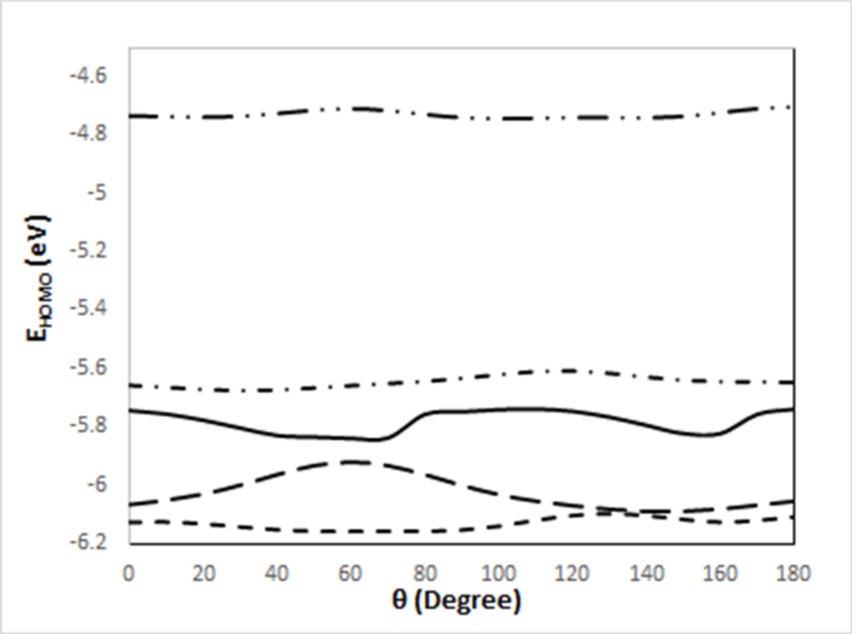


Figure 8: Shows the hyperpolarizability components (β_x, β_y, β_z) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene- isoindoline-1,3-dione) with five phases (– .. – .. – IDF^1, – – – – IDF^2, – . – . – . – IDF^3, – – – – – IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 − 31+G(d,p) method. Source: Elaborated by the authors.

Figure 9 shows that the energy levels of designed molecules are susceptible to the change from IDF^5 to IDF^1. Where all these phases have little sensitivity to rotation angles except IDF^5 and IDF^2. NLO design IDF^1, which is an A-D-A structure at the same straight line (φ1 =180°), is an excellent group for building low band gap dyes because it significantly the lower E_{LUMO} level, see Figure 9; (Kadhim *et al.*, 2022). While the E_{HOMO} level of IDF^1 is highest than the other phases. The variation of the HOMO-LUMO energy gap with the dihedral angles for the NLO structures (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) is shown in Figure 9. As a result, maybe a red-shifted absorption spectrum can be obtained. The HOMO-LUMO energy gap value is found to be 1.148 eV is the lowest one for IDF^1, while the energy gap of 2.887eV corresponds to the IDF^4, which has the highest hyperpolarizability. Maybe the inverse relationship between the energy gaps and the hyperpolarizability depends on the structure kind of the donor-acceptor group than their linking position effects. Generally, the change in energy gap with the dihedral angles was slightly compared to the value reported by Alyar *et al.* (2006), Resan *et al.* (2020).


-3
-3.1
-3.2
-3.3
-3.4
-3.5
-3.6
-3.7
-3.8
E_LUMO (eV)
0
20
40
60
80
100
120
140
160
180
θ (Degree)


-4.6
-4.8
-5
-5.2
-5.4
-5.6
-5.8
-6
-6.2
E_HOMO (eV)
0
20
40
60
80
100
120
140
160
180
θ (Degree)

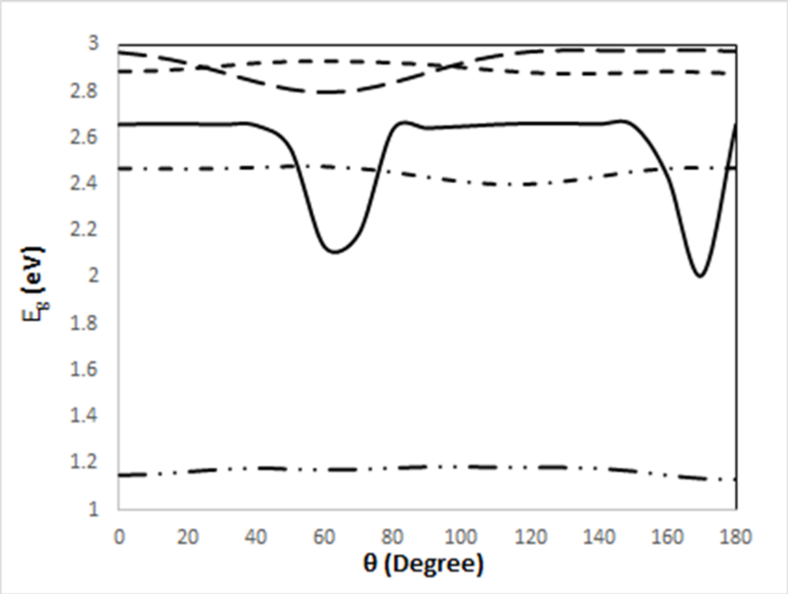


Figure 9: Shows the E$_{LUMO}$, E$_{HOMO}$ and energy gap (Eg) with the dihedral angles for the design NLO structure (isoindoline-1,3-dione-fullerene- isoindoline-1,3-dione) with five phases (− .. − .. − IDF^1, − − −− IDF^2, − . − . − . − IDF^3, − − − − − IDF^4 and _______ IDF^5, respectively) using the B3LYB/6 − 31+G(d,p) method. Source: Elaborated by the authors.

Frontier molecular orbital diagrams have been shown in Figure 10 for phases IDF^1, IDF^2, IDF^3, IDF^4 and IDF^5 respectively. Where the highest-occupancy molecular orbitals (HOMOs) and the lowest-occupancy molecular orbitals (LUMOs) are distributed over the whole fullerene and are extended to the isoindoline-1,3-dione group for all phases. Hyperpolarizability is associated with molecular electronic distribution under the influence of the electrical field depending on loosely or tightly bound electrons. Therefore, there is no clear approximate inverse relationship between the hyperpolarizability and HOMO-LUMO energy gaps.

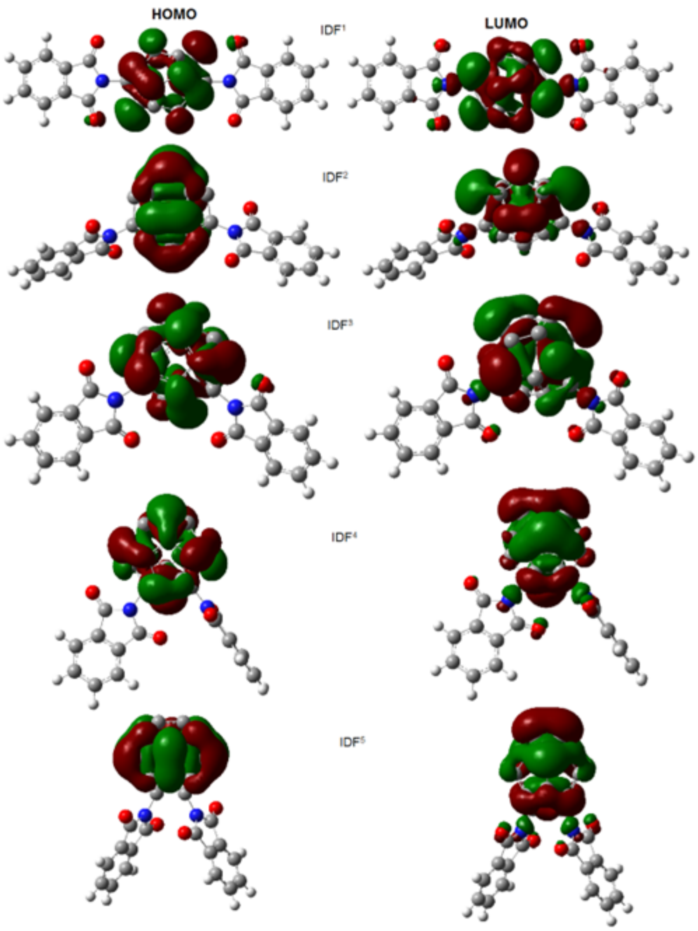


Figure 10: Frontier Molecular Orbitals of the design NLO structure (isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione) with five phases (IDF^1, IDF^2, IDF^3, IDF^4 and IDF^5, respectively) using the B3LYB/6-31+G(d,p) method. Source: Elaborated by the authors.

4. CONCLUSIONS

The study of isoindoline-1,3-dione-fullerene-isoindoline-1,3-dione, with five phases, were carried out. The equilibrium geometry, of the compound, has been investigated with the help of B3LYP density functional theory (DFT) using 6-31+G(d,p) as the basis set. The calculated HOMO and LUMO energies show that charge transfer occur within the molecule. From the results obtained, we observed that the rotation phase does have any effect on the optoelectronic properties of the molecule (title compound). At the B3LYP/6-31+G(d,p) level, there is some effect on the dipole moment, average polarizability, find first molecular hyperpolarizability for((isoindoline-1,3-dione-fullerene- isoindoline-1,3-dione).t can be concluded that A-D-A materials through investigation have high nonlinearity properties. The large value of β_{tot} of the donor-acceptor molecules is associated with intermolecular charge transfer resulting from an electron cloud movement from an electron donor to electron acceptor groups, which is a measure of the NLO activity of the molecules.

These properties of the organic compounds have made them propitious materials for electronics and optoelectronic devices with a high nonlinear optical (NLO) effect. Due to the fact that there are no corresponding experimental data in the existing literature, neither are there any other ab initio and DFT calculations on the optoelectronics properties of these molecules, we are optimistic that these results will serve as a benchmark for other studies.

Author's Contribution

S. Resan and M. Al-Anber conceived and designed the study. Calculations, data collection and analysis, were performed by S. Resan. The second author (M. Al-Anber) wrote the initial draft of the manuscript, and R. Resan commented and added some discussions on the initial version. Both authors read and approved the final manuscript.

Authors' declaration

Conflicts of Interest: None. We hereby confirm that all the Figures in the manuscript are ours. Ethical Clearance: The authors declare that the theoretical calculations were done according to ethical committee permission from the University of Basrah.

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