



# Design of Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 for Opto-nonlinear applications: Quantum Mechanical Study

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6 (5H) -dione-،3-c] pyrrole-4، Fullerene20-thieno [تصميم  
fullerene20 للتطبيقات البصرية غير الخطية: دراسة ميكانيكا الكم

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## ABSTRACT

### Background:

Many organic compounds are studied because of their nonlinear optical properties, which are crucial in photonics, optical switches, modulators, optical data storage, and other devices that use light to transport information. In experimental and theoretical researches, nonlinear optical phenomena, primarily resulting from interactions between matter and strong electric fields, have received considerable attention. Materials like these have numerous applications in science, engineering, and technology.

**Materials and Methods:** Fullerene 20 has been adopted as an electron donor, which was considered an NLO molecular material, while the thieno[2,3-c]pyrrole-4,6(5H)-dione has been adopted as an electron acceptor. Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF), as D-A-D, has been designed for nonlinear optical applications. Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF) was studied to determine its linear and nonlinear optical properties. For FTPDF, nonlinear optical properties were calculated with DFT/B3LYP using the basis set 6-31G(d,p). Various quantum calculations determine the structural and symmetry properties of Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20.

**Results:** The rotation increases the electric dipole moment  $\mu_{tot}$ , average linear polarizability  $\alpha_o$  and the first hyperpolarizability  $\beta_{tot}$ . And the anisotropic polarizability  $\Delta\alpha$  is smaller than the average polarizability, and the present structure has few deviations from spherical symmetry. FTPDF shows  $\mu_x$ -switch behavior. In particular, the rotation can raise the possibility for a new type of molecular  $\beta_x$ -switch.

**Conclusion:** The Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) energies estimated by DFT for the investigated molecules have been reported here. Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 has an increased first hyperpolarizability, making it a novel material suitable for the development of optoelectronic devices.

### Keywords:

Nonlinear optical properties, Intramolecular charge transfer, Rotation of angles, Optoelectronics, Molecular switching.



## 1. INTRODUCTION

Molecular hyperpolarization can be found in organic molecules with Non Linear Optics (NLO) activity for future applications in optoelectronic technologies for dynamic image nonlinear processing, optical computing, signal processing, optical switching, optical communication, information storage, high-resolution spectroscopy, and NLO sensors[1]. The reasons for focusing on organic molecules involve their facile synthesis, structural tailoring, and low cost, which allows synthesis tuning of their designs for preferred NLO characteristics. Accordingly, it will have a significant electric dipole moment difference between ground and excited states (charge asymmetry)[2]. Further functional groups can be substituted in the molecular structure to achieve this charge asymmetry[3]. NLO materials are characterized by intramolecular charge transfer (ICT), which mostly occurs between donor (D) and acceptor (A) moieties via  $\pi$ -conjugated spacers [3,4]. Electron-acceptor and electron-donor groups that are powerful enough to enhance polarizability can lead to large hyperpolarizabilities[3,4]. The expansive delocalization of the electrons with the electron donor and acceptor groups contributes to a more comfortable polarizability<sup>[5]</sup>. The co-planarity of a molecule plays an important role in improving the degree of conjugation, which in turn enhances molecular polarizability. Generally, the creation of high-performance NLO materials involves suitable donor- $\pi$ -conjugated bridge-acceptor (D- $\pi$ -A) procedures that can be tailored via structural conversion of the  $\pi$ -spacer, donor or acceptor groups[4,6,7]. Researchers have focused on enhancing nonlinear optical properties by substituting side groups); see Fig.1. Additionally, first static hyperpolarizabilities are inversely related to the energy gap [8,10]. In this regard, fullerene has been adopted in the present work as an electron donor, which was considered an NLO molecular material, while the thieno has been adopted as an electron acceptor. There are many allotropes of carbon, including fullerenes, which are relatively novel classifications compared to graphite and diamond, which are other carbon allotropes. In addition, it features a hollow carbon cage design and geometrical features[11,15]. Because the theoretical works can design and interpret the NLO property[16], fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF), as D-A-D, has been designed for nonlinear optical applications in present work.

In this work, density functional (DFT) calculation results on FTPDF structure have been reported. This study aims to provide the FTPDF's optimal molecular geometry, NLO, and optoelectronic properties. To further understand their performance improvement, the relationship between structure and property, as well as the origin of the NLO response, must be identified. For this purpose, the present work adopts two torsional angles ( $\Theta_1$  and  $\Theta_2$ ); see Fig.1.

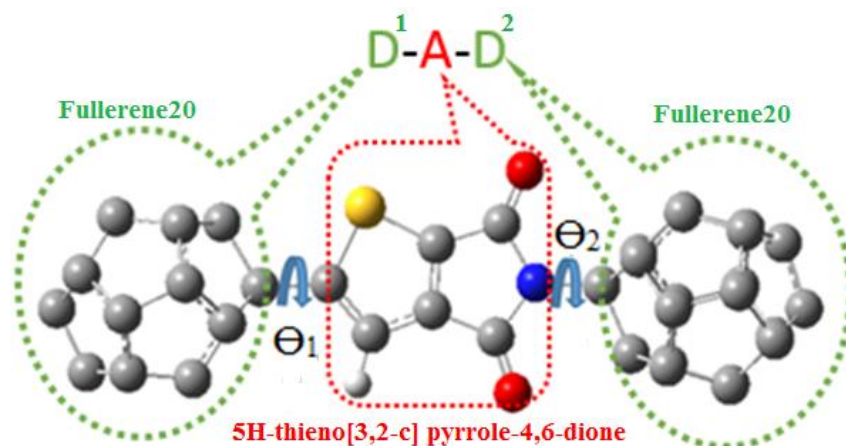


Figure 1. Shows the design of FTPDF as an NLO structure with positions of the two rotation angles ( $\Theta_1$  and  $\Theta_2$ ).

## 2.COMPUTATIONAL DETAILS

The charge density-based local and molecular reactivity descriptors can be obtained using a density functional approach [17,18]. The molecular geometric optimization of FTPDF, see Fig.1, has been evaluated using the B3LYP with the basis set 6-31+G(d,p) [19,20]. The calculations were performed with Gaussian 09 program[21], and the visualization was performed with Gauss View 05 package [22]. The torsion potentials were obtained for the FTPDF see Fig.1, for two dihedral angles ( $\Theta_1$  and  $\Theta_2$ ) between the 5H-thieno[3,2-c]pyrrole-4,6-dione group, which is as electron-acceptor, and the two fullerenes 20 respectively. The scan procedure involved simultaneous relaxation of the entire geometrical structure ranging between  $0^\circ$  and  $180^\circ$  degrees in  $10^\circ$  degree increments [3]. Under the static finite field ( $F$ ), the first hyperpolarizability( $\beta_{tot}$ ) is calculated by getting its components as follows:

$$E = E_o - \mu_i F_i - (1/2) \alpha_{ij} F_i F_j - (1/6) \beta_{ijk} F_i F_j F_k - (1/24) \gamma_{ijkl} F_i F_j F_k F_l \dots \quad (1)$$

where  $E_o$ ,  $\mu$ ,  $\alpha$ ,  $\beta$  and  $\gamma$  are the total energy ( $F=0$ ), dipole moment, linear polarizability, first-hyperpolarizability and second-hyperpolarizability, respectively. A molecule's dipole moment in an external electric field,  $F$ , can reset its charge density when the electric field is applied. Taking the derivative of a molecular energy ( $E$ ) and converting it into a component of the electrical field ( $F_i$ ) yields a component of the electric dipole moment ( $\mu_i$ ) in symbols [23]:

$$\mu_i = (\partial E / \partial F_i)_{(F=0)} \quad (2)$$

and the total dipole moment ( $\mu_{tot}$ ) is defined as:

$$\mu_{tot} = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \quad (3)$$

A gradient of the induced dipole can be used to describe polarizability:

$$\alpha_{ij} = (\partial^2 E / \partial F_i \partial F_j)_{(F=0)} \quad (4)$$

The isotropic polarizability ( $\alpha_o$ ) tensor is defined as:



$$\alpha_o = (1/3) (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (5)$$

where  $\alpha_{xx}$ ,  $\alpha_{yy}$ , and  $\alpha_{zz}$  are the polarizability matrix diagonal elements [23]. Anisotropic polarizability amplitudes are usually described as [23]:

$$\Delta\alpha = (1/2) [(\alpha_{xx}-\alpha_{yy})^2 + (\alpha_{yy}-\alpha_{zz})^2 + (\alpha_{zz}-\alpha_{xx})^2 + 6\alpha_{xz}^2]^{1/2} \quad (6)$$

In order to calculate molecular static first-hyperpolarizability components, we use the following equations:

$$\beta_{ijk} = (\partial^3 E / \partial F_i \partial F_j \partial F_k)_{(F=0)} \quad (7)$$

The static first-hyperpolarizability ( $\beta_{tot}$ ) can be calculated by:

$$\beta_{tot} = [\beta_x^2 + \beta_y^2 + \beta_z^2]^{1/2} \quad (8)$$

where  $\beta_x$ ,  $\beta_y$  and  $\beta_z$  are  $\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})$ ,  $\beta_y = (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})$ ,  $\beta_z = (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})$  respectively [24].

As the dipole moment moves along, the first component of hyperpolarizability is represented by  $\beta_\mu$ , which is usually expressed as:

$$\beta_\mu = (3/5) (\mu_x \beta_x + \mu_y \beta_y + \mu_z \beta_z) / \mu \quad (9)$$

The hyperpolarizability (XY-plane) is expressed as follows:

$$\beta_{xy-plane} = \beta_{xxx} + \beta_{xxy} + \beta_{xyy} + \beta_{yyy} \quad (10)$$

which is a measure of a molecule's hyperpolarizability in the XY plane. Static first-hyperpolarizability is a tensor of third rank described as a matrix of  $3 \times 3 \times 3$ . As a result of Kleinman's symmetry ( $\beta_{xyy} = \beta_{yxy} = \beta_{yyx} = \beta_{xyx} = \beta_{zyy} = \beta_{yzy}$ ), as well as these 27 components, can be reduced to 10 [25, 26].

### 3.RESULTS AND DISCUSSION

Molecular optimized geometry of the FTPDF is estimated using B3LYP/6-31+G(d,p), which is depicted in Fig.1. To describe the conformational flexibility of the FTPDF, the relative energy ( $\Delta E$ ) as a function of the torsion angle is shown in Fig.2, where the torsional angle was varied. Fig.2 shows the occurring probability of angle rotation for  $\Theta_1$  higher than the  $\Theta_2$ . Generally, the rotation energy for both angles is very little if we compare it with the available literature [3, 27, 28].

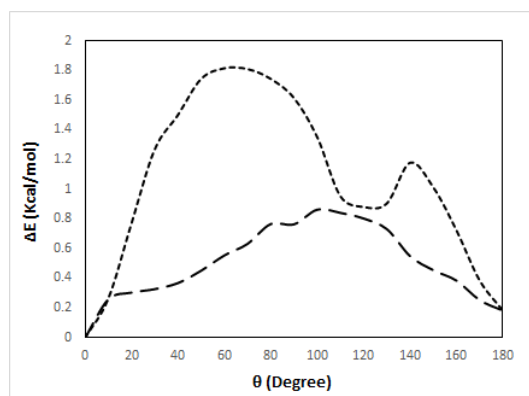


Figure 2. The relative stability  $\Delta E$  for the design NLO structure (FTPDF) along with the torsional angles (— — —  $\Theta_1$  and - - - - -  $\Theta_2$  respectively) employing the B3LYB/6-31+G(d,p) method.

The molecular charge distribution is represented as a vector in three dimensions by the dipole moment. In this case, it depends on where the positive and negative charges are located. The molecular dipole moment and the polarizability can be influenced by intramolecular charge transfer (ICT) from the electron-donor to electron-acceptor groups. Fig.3 shows that the  $\Theta_2$  rotation increases the total electric dipole moment  $\mu_{tot}$ , while the  $\Theta_1$  decreases it. The increasing  $\mu_{tot}$  value may be because of the distances decreasing among the oxygen atoms with fullerene ( $D^1$ )[3]. Fig. 3 shows that  $\mu_x$  has two switching behaviour with  $\Theta_1$  and  $\Theta_2$ , respectively[3]. Generally, the order of electric dipole components of the designed structure FTPDF was:  $\mu_x > \mu_y > \mu_z$ , respectively, where  $\mu_{tot}$  has a direct proportion with  $\mu_x$  so that  $\mu_{tot} \sim \mu_x$ .

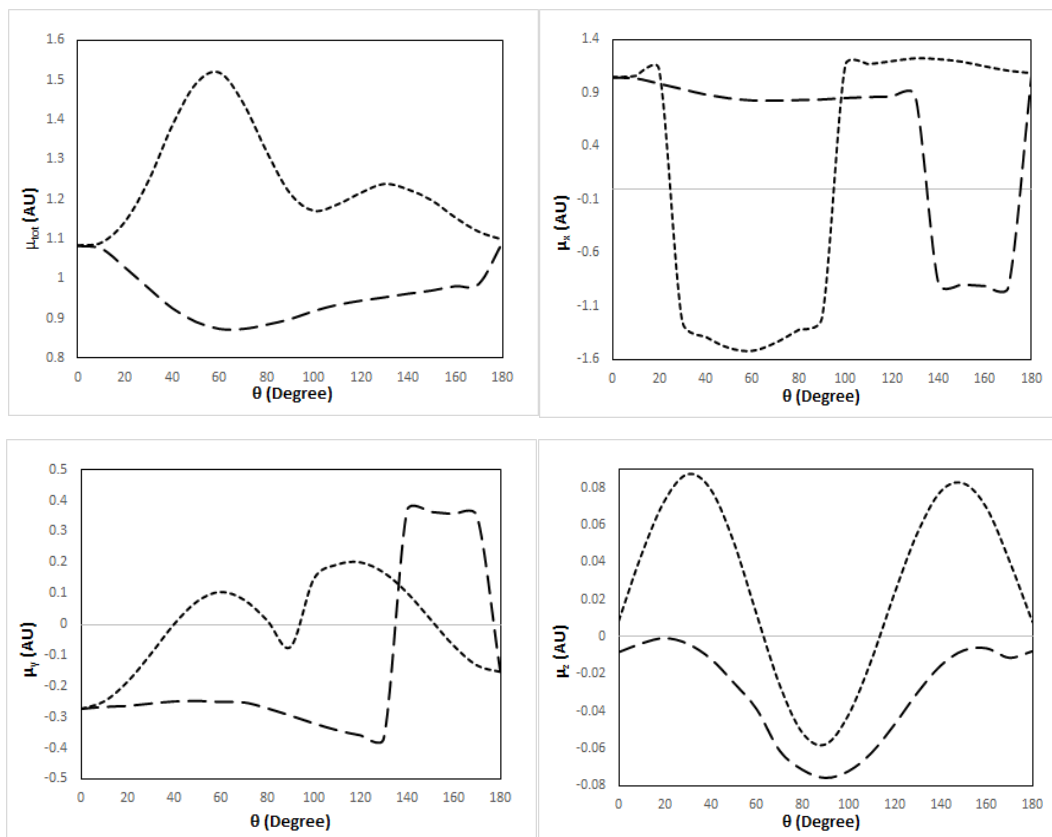


Figure 3. The total dipole moment and components ( $\mu_{tot}$ ,  $\mu_x$ ,  $\mu_y$  and  $\mu_z$ ) for the design NLO structure (FTPDF) along with the torsional angles ( $\text{---}$   $\Theta_1$  and  $\text{- - -}$   $\Theta_2$  respectively) using the B3LYB/6-31+G(d,p) method.

Isotropic polarizability and the first hyperpolarizability of molecular strategies are understood to be dependent upon the efficiency of electron transmission between electron-donor and electron-acceptor since that is what enables intramolecular charge transfer[29, 30]. A design structure's linear optical properties, such as polarizability, determine its response to an intense electric field. In the D-A-D molecule, the asymmetric polarization induced by electron acceptor and donor groups specifies intramolecular charge transfer (FTPDF). Due to Fig.4, the  $\Theta_1$  rotation gave higher isotropic polarizability  $\alpha_o$  and  $\alpha_{yy}$  than  $\Theta_2$ , while the inverse behavior with  $\alpha_{xx}$  and  $\alpha_{zz}$ . The anisotropy polarizability  $\Delta\alpha$ , which is the difference between the polarizability along the permanent dipole moment ( $\alpha_{||}$ ) and the average value perpendicular to it ( $\alpha_{\perp}$ ), was lower than isotropic polarizability  $\alpha_o$ , also the  $\Theta_1$  rotation angle lower  $\Delta\alpha$ . Generally, the three diagonal polarizability component values are near the isotropic polarization value.

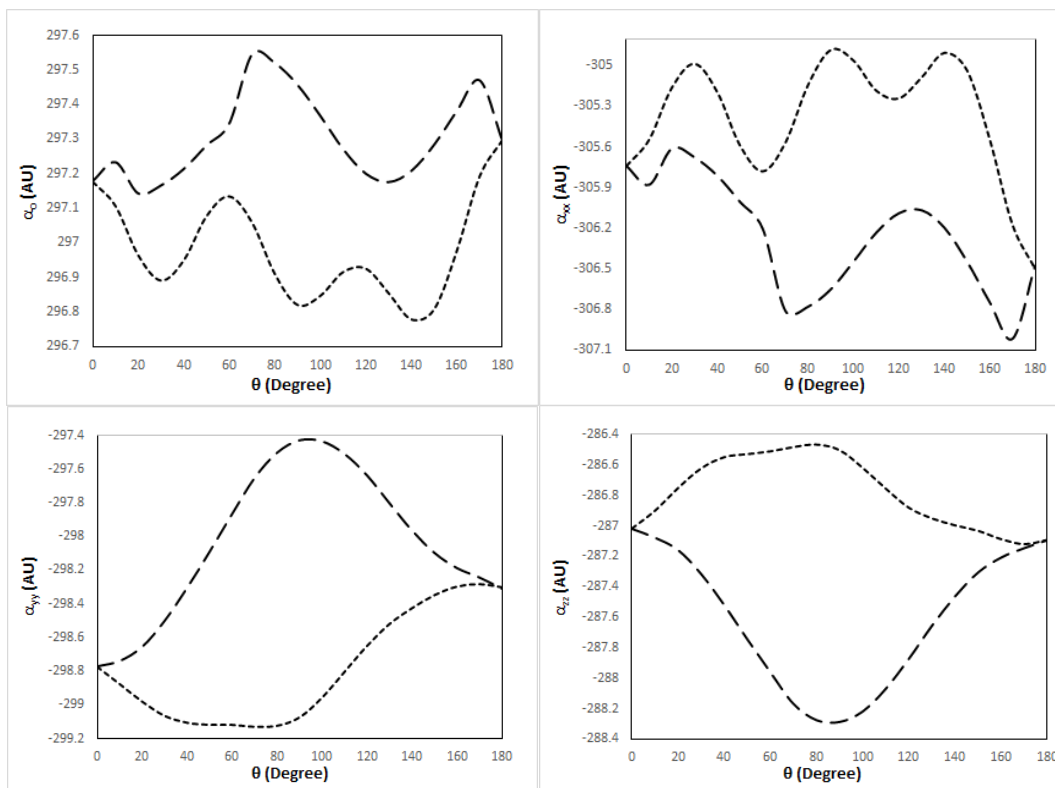


Figure 4. Shows the isotropic polarizability  $\alpha_0$  and its major components ( $\alpha_{xx}$ ,  $\alpha_{yy}$  and  $\alpha_{zz}$ ) for the design NLO structure (FTPDF) along with the torsional angles ( $\text{---}\text{---}\text{---}\theta_1$  and  $\text{-----}\theta_2$  respectively) using the B3LYB/6-31+G(d,p) method.

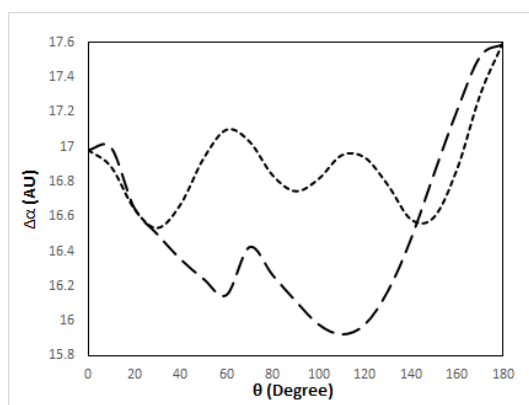


Figure 5. Shows the anisotropy polarizability  $\Delta\alpha$  for the design NLO structure (FTPDF) along with the torsional angles ( $\text{---}\text{---}\text{---}\theta_1$  and  $\text{-----}\theta_2$  respectively) using the B3LYB/6-31+G(d,p) method.

When designing the performance of a D-A-D molecule, NLO characteristics are important because they represent the molecule's tendency to experience intramolecular charge transfers. The electron correlations play an influential function in calculating the first hyperpolarizability. Therefore, the hyperpolarizability tensor components must be accurately calculated where it is

necessary to consider the effect of electron correlation. Fig.6 shows the results of the static hyperpolarizabilities of the present molecule. Rotation angle  $\Theta_2$  enhances hyperpolarizability, which indicates a more promising NLO response than rotation angle  $\Theta_1$ [3]. The same behaviour was for the  $\beta_{xy\text{-plane}}$  and  $\beta_\mu$ , which shows the measure of hyperpolarizability ( $\beta_{tot}$ ) in the XY-plane of the FTPDF and along the direction of the dipole moment  $\mu$ , respectively, but the  $\Theta_1$  dropped the  $\beta_\mu$  beyond  $\Theta_1 \sim 130^\circ$  rapidly.

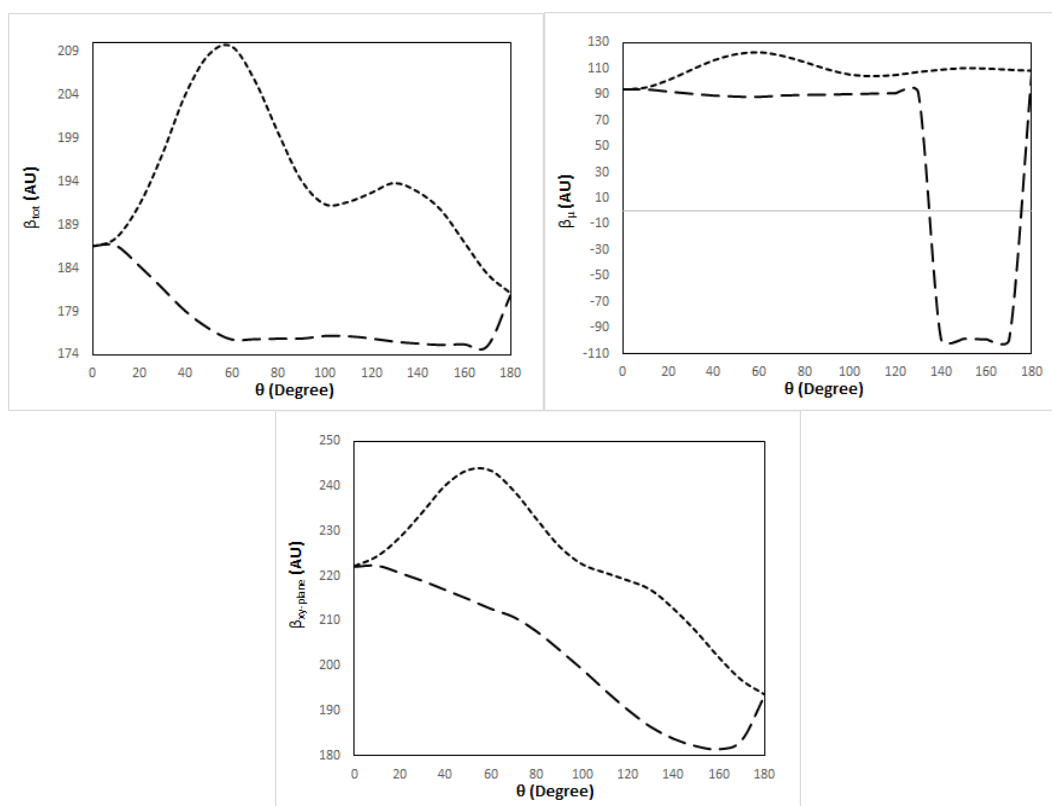


Figure 6. Shows the static hyperpolarizability  $\beta_{tot}$ ,  $\beta_\mu$  and  $\beta_{xy\text{-plane}}$  for the design NLO structure (FTPDF) along with the torsional angles ( $\text{---}\text{---}\text{---}\Theta_1$  and  $\text{-----}\Theta_2$  respectively) employing the B3LYB/6-31+G(d,p) method.

The hyperpolarizability components ( $\beta_x$ ,  $\beta_y$ , and  $\beta_z$ ) were examined with the variation of the dihedral angles ( $\Theta_1$  and  $\Theta_2$ ) for the FTPDF, as illustrated in Fig. 7, where only  $\beta_x$  has a high value with switching behaviour with  $\Theta_2$ , which may be suitable for optical sensor applications with a note that their behaviour is close to the previous results[3]. Generally, the hyperpolarizability  $\beta_{tot}$  majority depends on the component  $\beta_x$ , so that  $\beta_{tot} \sim \beta_x$ .



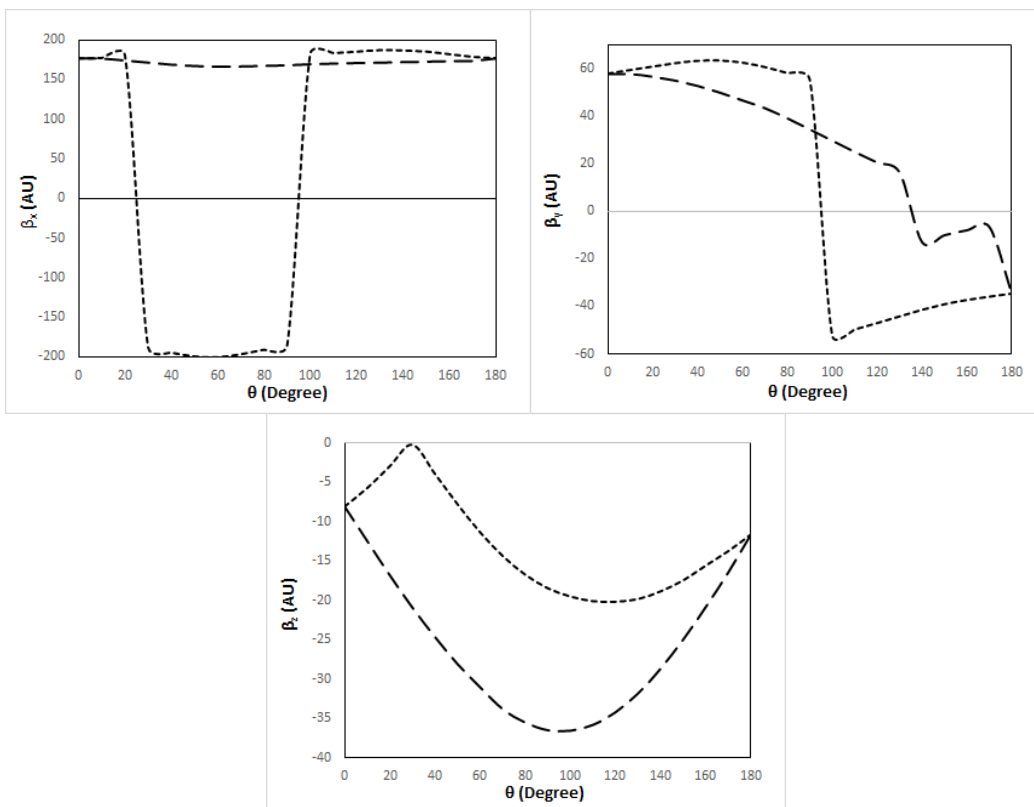


Figure 7. Shows the hyperpolarizability components ( $\beta_x$ ,  $\beta_y$  and  $\beta_z$ ) for the design NLO structure (FTPDPF) along with the dihedral angles (— — —  $\Theta_1$  and - - - - -  $\Theta_2$  respectively) using the B3LYB/6-31+G(d,p) method.

LUMO and HOMO orbitals provide a new way of presenting the molecular reactivity and kinetic stability associated with electron affinity [28]. This is also used in the frontier electron density to indicate the most reactive position in a conjugated structure as well as to illustrate several types of responses described by the frontier electron density [28, 30]. The present study predicts the LUMO and HOMO energies by using the B3LYP/6-31+G(d,p) process. As a result, the front molecular orbitals (FMOs) energy level distribution of FTPDPF was investigated and displayed in Fig. 8. Due to Fig. 8, the highest occupied molecular orbitals (HOMO) is localised over fullerene ( $D^1$ ), which is on the life of electron-acceptor, see Fig.1. In contrast, the lowest-lying unoccupied molecular orbitals (LUMO) are localized over fullerene ( $D^2$ ) on the right of the electron-acceptor, see Fig.1. As the fullerene ( $D^1$ ) rotates to  $\Theta_2=60^\circ$ , the  $\mu_{tot}$ ,  $\Delta\alpha$ ,  $\beta_{tot}$ ,  $\beta_{\mu}$  and  $\beta_{xy-plane}$  be at maximum. While, as the fullerene ( $D^2$ ) rotates to  $\Theta_1=60^\circ$ , they have been at a minimum. Generally, the shapes of HOMO and LUMO are not changing, but the rotations change their cemetery. However, the intramolecular charge transfer direction is from the fullerene ( $D^1$ ) through the 5H-thieno[3,2-c]pyrrole-4,6-dione (acceptor) towards the fullerene ( $D^2$ ). These results indicate an efficient intramolecular charge transfer (ICT).

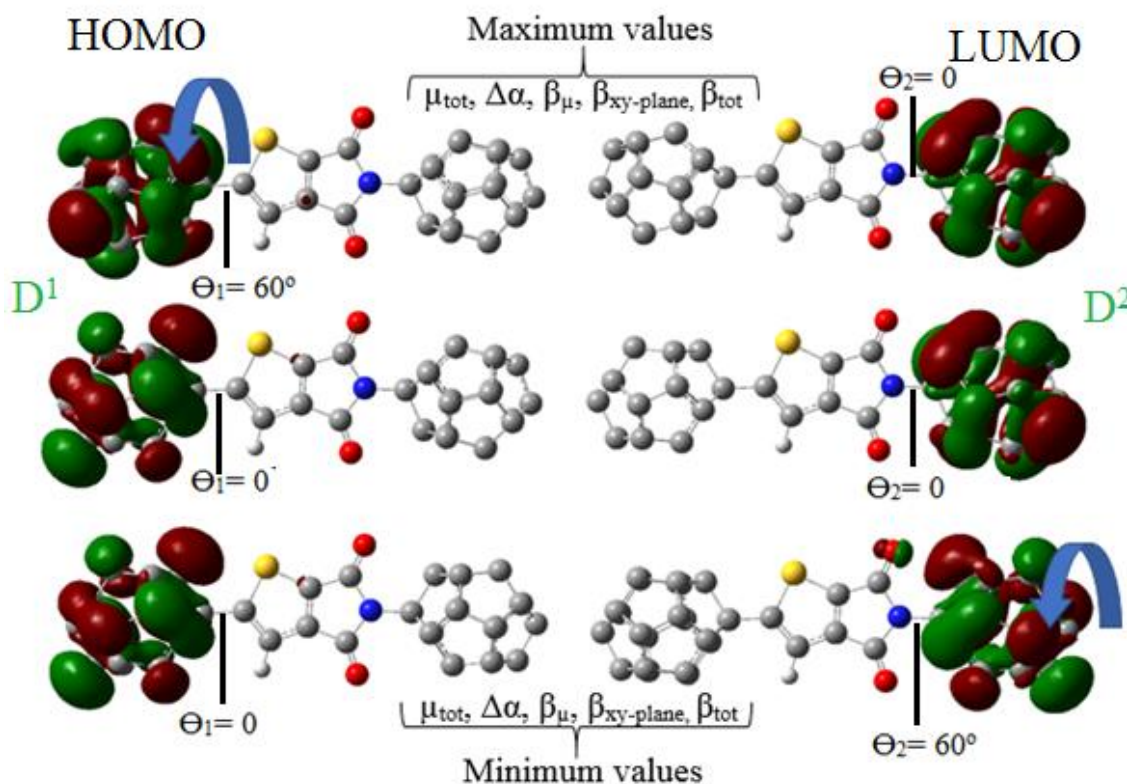


Figure 8: Frontier molecular orbitals of the design NLO structure (FTPDF) along with the two dihedral angles ( $\Theta_1=0:\Theta_2=60^\circ$ ,  $\Theta_1=\Theta_2=0$  and  $\Theta_1=60^\circ:\Theta_2=0$  respectively).

#### 4. CONCLUSIONS:

The optimized structural parameters (dihedral angles), the electronic energy, the dipole moment ( $\mu$ ), the HOMO energy, the lowest LUMO energy, the polarizability ( $\alpha$ ), and the hyperpolarizability ( $\beta$ ) values of the fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 has been calculated by B3LYP/6-31+G(d,p). Shows that the  $\Theta_2$  rotation increases the electric dipole moment  $\mu_{\text{tot}}$ , average linear polarizability  $\alpha_0$  and the first hyperpolarizability  $\beta_{\text{tot}}$  while the  $\Theta_1$  decreases them. In addition, the anisotropic polarizability  $\Delta\alpha$  is smaller than the average polarizability, and the present structure has few deviations from spherical symmetry. FTPDF shows  $\mu_x$ -switch behavior. In particular, when  $\Theta_2$  rotation, thus raises the possibility for a new type of molecular  $\beta_x$ -switch. Generally, it can be concluded that the rotation of the dihedral angle can affect the compound's electronic, linear and nonlinear properties. It is of great importance for the scientific community involved in investigating promising NLO structures to take note of our findings. It is a good candidate for designing NLO molecules that respond massively to NLO.

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### Conflict of interests.

There are non-conflicts of interest.

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## الخلاصة

**المقدمة:** تتم دراسة العديد من المركبات العضوية بسبب خصائصها الضوئية غير الخطية ، والتي تعتبر ضرورية في الضوئيات والمفاتيح الضوئية والمعدلات وتخزين البيانات الضوئية والأجهزة الأخرى التي تستخدم الضوء لنقل المعلومات. في البحوث التجريبية والنظرية، حظيت الظواهر البصرية غير الخطية، الناتجة أساساً عن التفاعلات بين المادة والمجالات الكهربائية القوية، باهتمام كبير. مواد مثل هذه لها العديد من التطبيقات في العلوم والهندسة والتكنولوجيا.

**المواد وطرق العمل:** تم اعتماد الفوليرين 20 كمانح للإلكترون ، والذي كان يعتبر مادة جزيئية غير خطية، بينما تم اعتماد thieno[2,3-c]pyrrole-4,6(5H)-dione-20، Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-20 كمتقبل للإلكترون. وتم تصميم Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-20 (FTPDF) ، لتطبيقات البصرية غير الخطية. تمت دراسة Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF) لتحديد خصائصه البصرية الخطية وغير الخطية. بالنسبة إلى FTPDF ، تم حساب الخصائص البصرية غير الخطية بالاعتماد على DFT/B3LYP وباستخدام مجموعة الدوال الأساسية 6-31G(d,p). تحدد حسابات الكم المختلفة الخصائص الهيكلية والتناظرية ل Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF).

**الاستنتاجات:** يزيد الدوران من عزم ثنائي القطب الكهربائي  $\mu_{tot}$  ، ومتوسط الاستقطاب الخطي  $\alpha_0$  وأول فرط استقطاب  $\beta_{tot}$ . وقابلية الاستقطاب متباينة الخواص  $\Delta\alpha$  أصغر من متوسط الاستقطاب ، والبنية الحالية بها انحرافات قليلة عن التناظر الكروي. يُظهر FTPDF سلوك التبديل  $\mu_x$ . على وجه الخصوص، يمكن للدوران أن يزيد من احتمال وجود نوع جديد من التبديل الجزيئي  $\beta_x$ .

**خاتمة:** تم الإشارة هنا عن طاقات أعلى المدارات الجزيئية المشغولة (HOMO) و طاقات اوطى المدارات الجزيئية غير المشغولة (LUMO) المحسوبة بواسطة DFT للجزيئات التي تم دراستها. يحتوي Fullerene20-thieno[2,3-c]pyrrole-4,6(5H)-dione-fullerene20 (FTPDF) على زيادة فرط الاستقطاب الأول، مما يجعله مادة جديدة مناسبة لتطوير الأجهزة الإلكترونية الضوئية.

## الكلمات المفتاحية:

الخصائص البصرية غير الخطية، نقل الشحنة داخل الجزيء، دوران الزوايا، الإلكترونيات الضوئية، المفاتيح الجزيئي.