



Theoretical Study of the Properties of Isatin (1H-indole-2,3-dione) Based Alternating Donor-acceptor Type Conjugated Oligomers

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Authors' contributions

This work was carried out in collaboration between all authors. Author OGO designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Authors IAA and OOA managed the analyses of the study. Author FUA managed the literature searches. All authors read and approved the final manuscript.

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ABSTRACT

The potential of Isatin (1H-indole-2,3-dione) as a donor moiety in an alternating donor-acceptor conjugated oligomer models was studied. Eight different electron acceptor molecules investigated are: thiazole (Z),thiadiazole (D), thienopyrazine (TP), thienothiadiazole (TD), benzothiadiazole (BT), thiadiazolothienopyrazine (TPD), benzobisthiadiazole (BDD) and thienopyridine (TPY). The geometry and electronic properties of the oligomers were investigated using density functional theory (DFT) method at B3LYP/ 6-31G (d) level. Properties such as torsional angle, bond length and intramolecular charge transfer were analysed. The lowest excitation energies (E_{ex}) and the maximal absorption wavelength (λ_{abs}) were studied with time-dependent density functional theory (TD-DFT) method. The HOMO-LUMO level and band gap energies were calculated for all the model oligomers. The effect of addition of another isatin moiety to isatin-acceptor type oligomers give rise to D-A-D type structures and the band gap energies was investigated. It was discovered

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that (ISAT-TPD-ISAT) and (ISAT-BDD-ISAT) have lower band gaps (E_g) of 1.55 and 1.93 eV respectively. This result suggests that the two oligomers could be used as active layer materials in photovoltaic devices.

Keywords: Oligomer; Isatin; thiazole; HOMO-LUMO band gap.

1. INTRODUCTION

There has been a serious search for alternative source of energy to complement the inadequate supply of world energy currently sourced from fossil fuel and nuclear power plants. The world energy need is increasing on daily basis. However, these sources of energy are limited. Besides, carbon (IV) oxide, the final product of fossil fuel combustion has been identified as one of the major contributors to global warming. Also, nuclear energy has been a subject of public debate due to the security, health risks of nuclear power stations and problems in the management of radioactive wastes generated from nuclear power plants. Hence, there is a need to search for low cost and safer sources of renewable energy.

Solar energy is a better alternative source of energy. It is readily available, reliable, clean, and can be used all over the world. Sunlight can be converted directly to electricity by using photovoltaic cells. These are otherwise known as organic solar cells and are constructed by using conjugated polymers as photoactive layers.

Conjugated polymers are π -bonded macromolecules in which the fundamental monomer unit is repeated several times [1]. There has been a tremendous increase in research interest in conjugated polymers due to their wide applications such as polymer light-emitting diodes (PLED) [2-4], thin film transistors, all-polymer integrated circuits [1], chemical sensors [5], transparent conductors [6-8] and photovoltaic devices [9,10]. Donor-acceptor type conjugated polymers have been designed to induce minimum twisted arrangements between consecutive repeating units in the system. Interaction of the donor-acceptor moieties enhances the double bond character between the repeating units. As a result a conjugated polymer with an alternating sequence of the appropriate donor and acceptor units in the main chain can induce a reduction in its band gap energy [11].

Various polymers have been designed and synthesized for application in photovoltaic

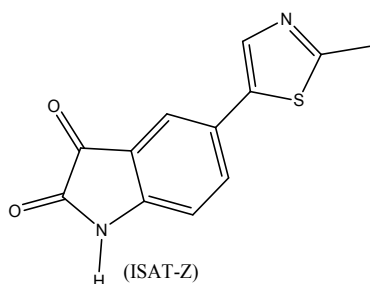
devices. They include poly (p-phenylenevinylene) (PPV) [12-14], polythiophene (PT) [15-17], poly (3,4-ethylenedioxythiophene) (PEDOT) [18-19], polyvinylcarbazole (PVK) [20]. Several solar cells have been constructed with various degree of efficiencies in the recent time. Smith et al. [21] developed bulk heterojunction solar cells using poly (3-dodecyl-2,5-thienylene vinylene) with maximum efficiency of 0.24%. Reynolds et al [22] blended cyanovinylene-dioxythiophene polymer with PCBM in ratio 1:4 to obtain a solar cell with 0.10% efficiency. A critical factor for further improving the efficiency of the solar cells is that polymer photovoltaic materials mismatch the photon flux spectrum from the sun whose maximum flux is around 700 nm. Also, the use of low band gap polymers ($E_g < 1.8$ eV) helps in better harvesting of the solar spectrum and increasing efficiency [23-25].

Conjugated polymers based on isatin have not been extensively studied. Isatin or 1H-indole-2,3-dione is an indole derivative. Schiff bases of isatin are investigated for their pharmaceutical properties [26]. Recently, Zhang et al synthesized a series of isoindigo-based low energy band gap polymers. The optical band gaps of the polymers are optimized for solar cell applications and are found to be about 1.5 eV [27]. Also, two conjugated polymers, IIDDT and IIDT based on an isoindigo core were developed for organic field-effect transistors by Lei et al. [28] Evaluation of their field-effect performance indicated that IIDDT exhibited air-stable mobility up to 0.79 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, which is quite high among polymer FET materials. Stalder et al. [29] synthesized six representatives of isoindigo-based donor-acceptor conjugated polymers whose band gaps are found to be between 1.77 and 1.99 eV.

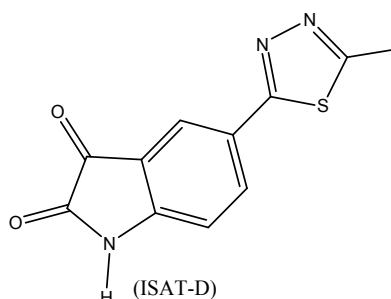
In this work, we describe a theoretical study of the electronic structure and optoelectronic properties of isatin-based alternating donor-acceptor and donor-acceptor-donor conjugated oligomers. The molecular structures of the eight studied compounds are shown in Fig. 1. These correspond to eight different electron acceptors namely; Thiazole (Z), Thiadiazole (D), Thienopyrazine (TP), Thienothiadiazole (TD),

Benzothiadiazole (BT), Thiadiazolothienopyrazine (TPD), Benzobisthiadiazole (BDD) and Thienopyridine (TPY) This study has used these widely reported electron accepting groups along with a less studied electron donating group to construct donor-acceptor oligomers for potential applications in organic photovoltaic devices. Benzothiadiazole (BT) [30-34] for example has been extensively used as electron accepting unit in combination with several electron donating units such as cyclopentadithiophene (CPDT). It is observed that compounds made up of this electron accepting unit have lower-energy levels and reduced band gap as compare with other D-A alternating copolymers [30-34].

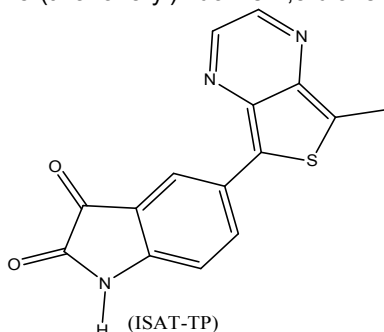
These series of acceptors allow a comprehensive understanding of the effects of the backbone ring, heteroatom and fused rings on the geometric and electronic properties of the studied compounds. The geometric structures and electronic properties of the compounds were investigated by the density functional theory (DFT) at the B3LYP/ 6-31G (d) level. The bond length of the isatin-acceptor bridge, torsional angle and intramolecular charge transfer of the studied compounds were analyzed and correlated with their corresponding chemical structures. The effects of the acceptor strength on the electronic properties, including the HOMO-LUMO level and energy gap were also studied.



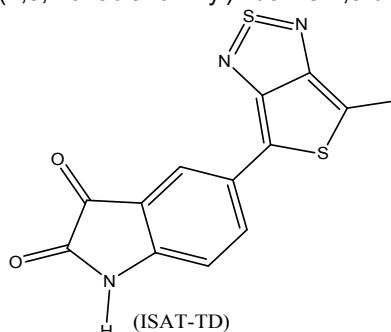
5-(thiazol-5-yl)indoline-2,3-dione



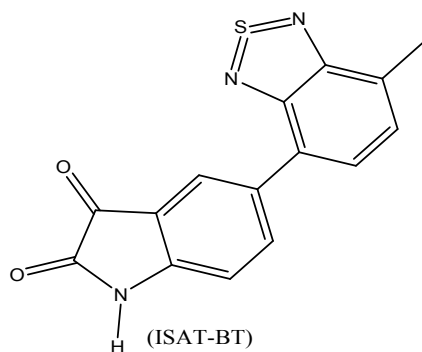
5-(1,3,4-thiadiazol-2-yl)indoline-2,3-dione



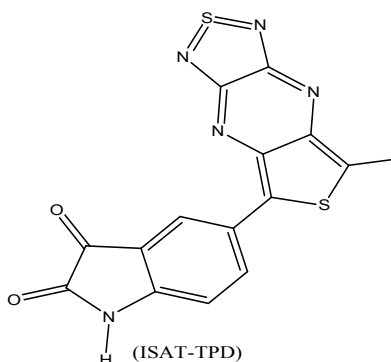
5-(thieno[3,4-b]pyrazin-5-yl)indoline-2,3-dione



5-(1H,3H-thieno[3,4-c][1,2,5]thiadiazol-4-yl)indoline-2,3-dione



5-(7-methylbenzo[c][1,2,5]thiadiazol-4-yl)indoline-2,3-dione



5-(1H,3H-[1,2,5]thiadiazolo[3,4-b]thieno[3,4-e]pyrazin-5-yl)indoline-2,3-dione

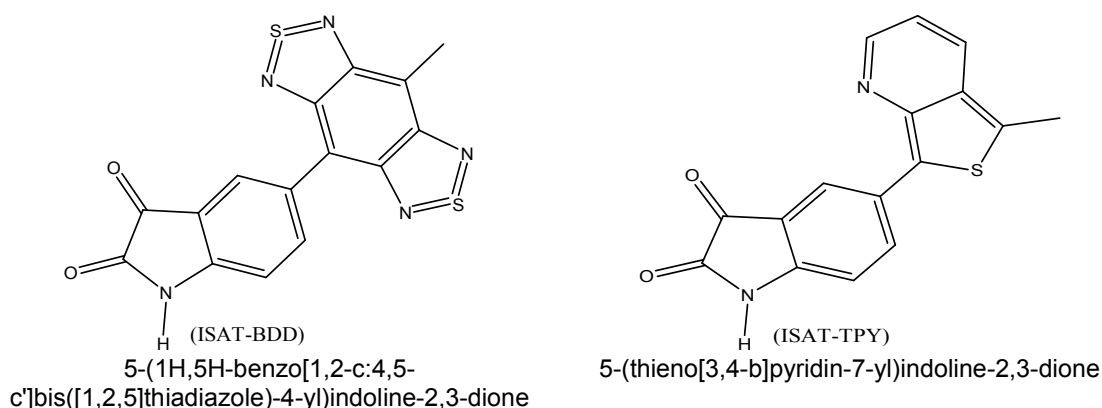


Fig. 1. Molecular structures of the studied compounds

2. COMPUTATIONAL METHOD

Quantum chemical calculations of the ground state molecular structures of thiazole (Z),thiadiazole (D),thienopyrazine (TP), thienothiadiazole (TD), benzothiadiazole (BT), thiadiazolothienopyrazine (TPD), benzobisthiadiazole (BDD) and thienopyridine (TPY) were performed using the Spartan'10 software package [30] on a 2.5GHz personal computer. Calculations on the ground state geometry, energy orbitals, dipole moments, and energy gaps of (ISAT)-acceptor oligomers were investigated with the Ab initio restricted HF-DFT self consistent field methods [31]. This has been found to be an accurate method for calculating the geometrical, electronic structures and optical properties of several organic molecules [32-38]. The HOMO-LUMO levels were obtained for the system. Also, the energy gap is obtained as the difference between the HOMO and LUMO energies. The electronic transition energies of the oligomers were also obtained using the time dependent density functional theory (TD-DFT) [39].

3. RESULTS AND DISCUSSION

3.1 Molecular Structure

Using compound ISAT-BDD as an example, the definitions of torsional angle (Θ), intramolecular charge transfer (ICT) and bridge length (dB) are illustrated in Fig. 2. The optimized structure, atomic charge distribution and the HOMO-LUMO surface diagram are also shown in Fig. 3.

Torsional angle is the deviation from coplanarity between the donor and acceptor. The large

torsional angle (Θ^0) of (ISAT-Z), (ISAT-BT) and (ISAT-TPY) studied compounds (Table 1) reveal that strong steric hindrance exist between the donor and acceptor moieties. The smallest dihedral angle values of (ISAT-TP) (-19.69°), (ISAT-TPD) (-21.17°) and (ISAT-BDD) (-35.71°) showed the coplanarity of the thienopyrazine, thiadiazolothienopyrazine and benzobisthiadiazole rings between ISAT unit [32,40]. The LUMO energy levels of the studied acceptors: Z, D, TP, TD, BT, TPD, BDD and TPY as obtained from the 6-31G (d) level are -0.75, -1.27, -2.26, -2.74, -2.34, -3.72, -3.56 and -1.76 eV respectively. It has been reported that the lower the LUMO energy level of the acceptor molecules, the higher the acceptor strength [32]. Hence, the order of the acceptor strength is as follows: TPD > BDD > TD > BT > TP > TPY > D > Z.

Table 1. The optimum geometry results (Θ , dB and ICT) for model compounds calculated by B3LYP/6-31G (d) level

Compound	Θ^0	dB(Å)	ICT(e)
(ISAT)2	0.00	1.448	-0.001
ISAT-Z	28.33	1.467	-0.001
ISAT-D	0.00	1.467	0.001
ISAT-TP	-19.69	1.464	-0.02
ISAT-TD	-5.11	1.457	-0.023
ISAT-BT	37.53	1.481	0.00
ISAT-TPD	-21.17	1.461	-0.002
ISAT-BDD	-35.71	1.475	-0.004
ISAT-TPY	19.32	1.465	0.00

NB: ISAT=Isatin, thiazole (Z),thiadiazole (D), thienopyrazine (TP), thienothiadiazole (TD), benzothiadiazole (BT), thiadiazolothienopyrazine (TPD), benzobisthiadiazole (BDD) and thienopyridine (TPY)

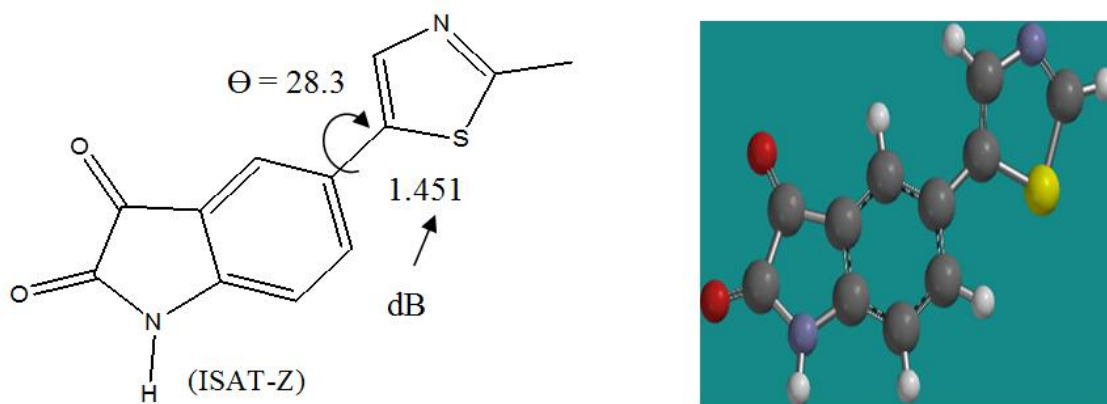
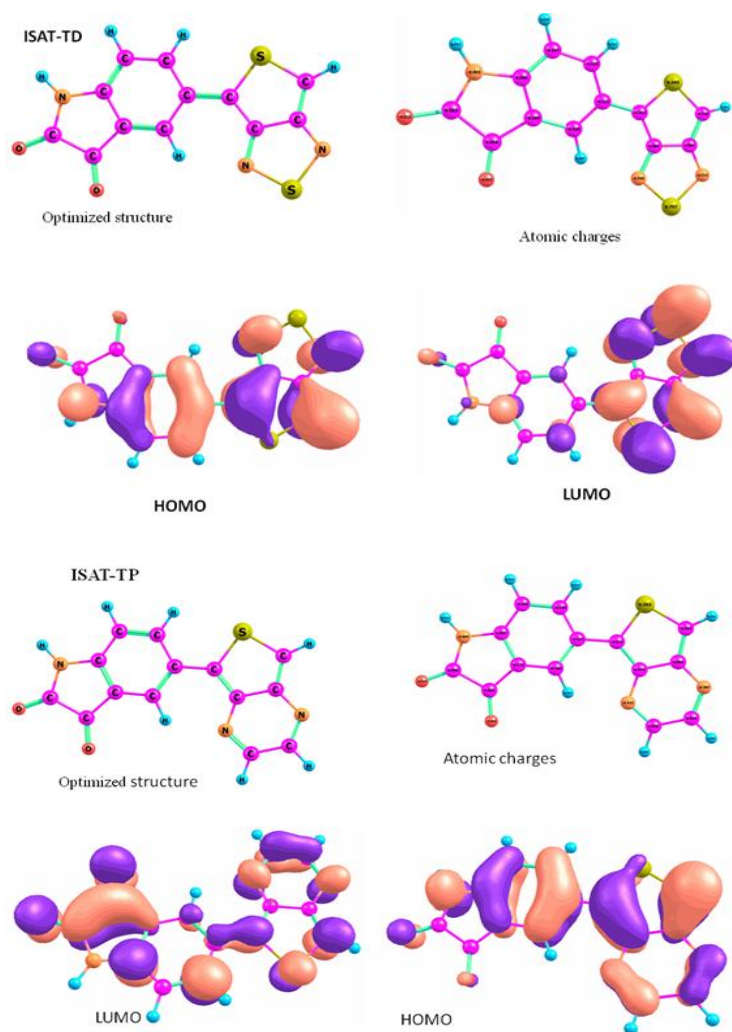
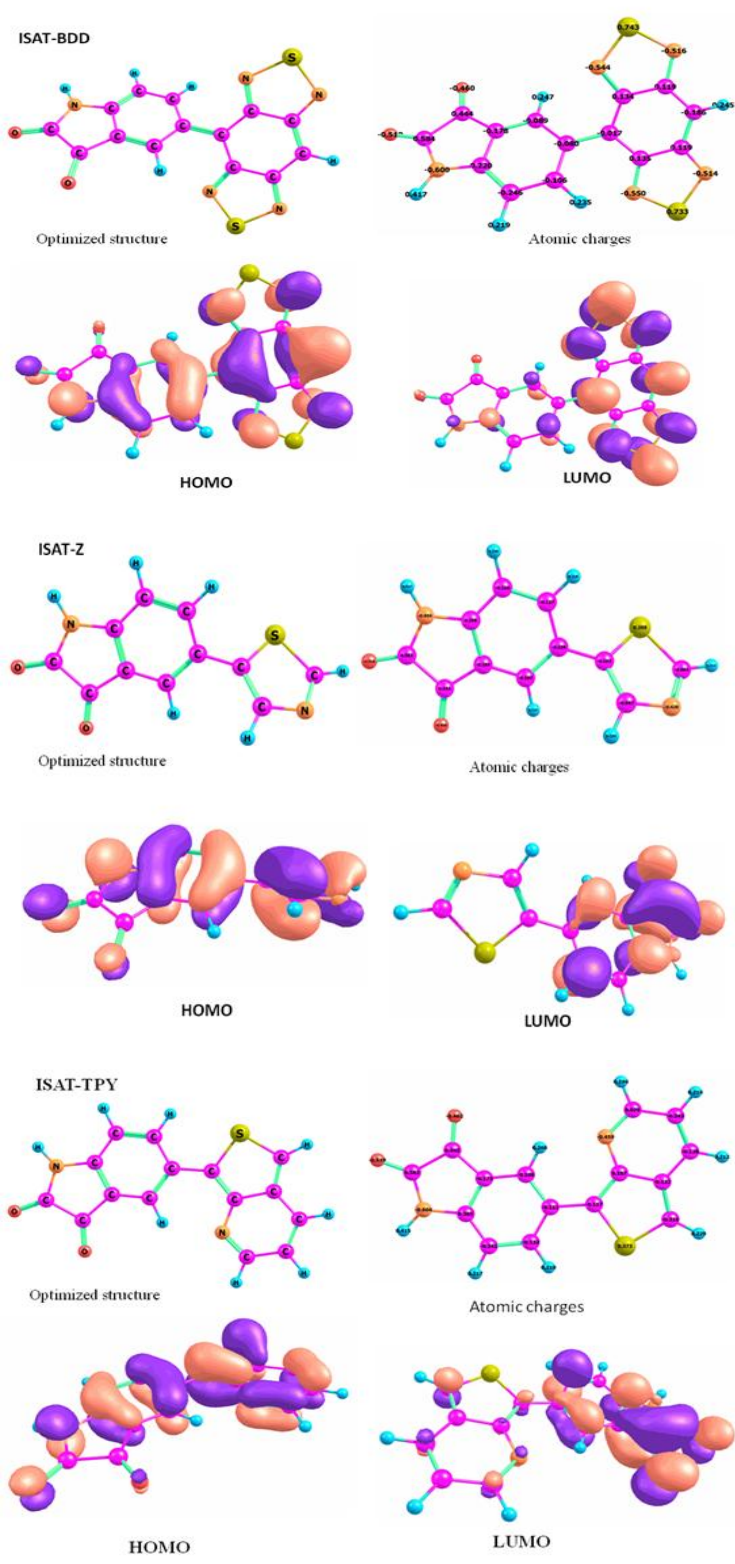
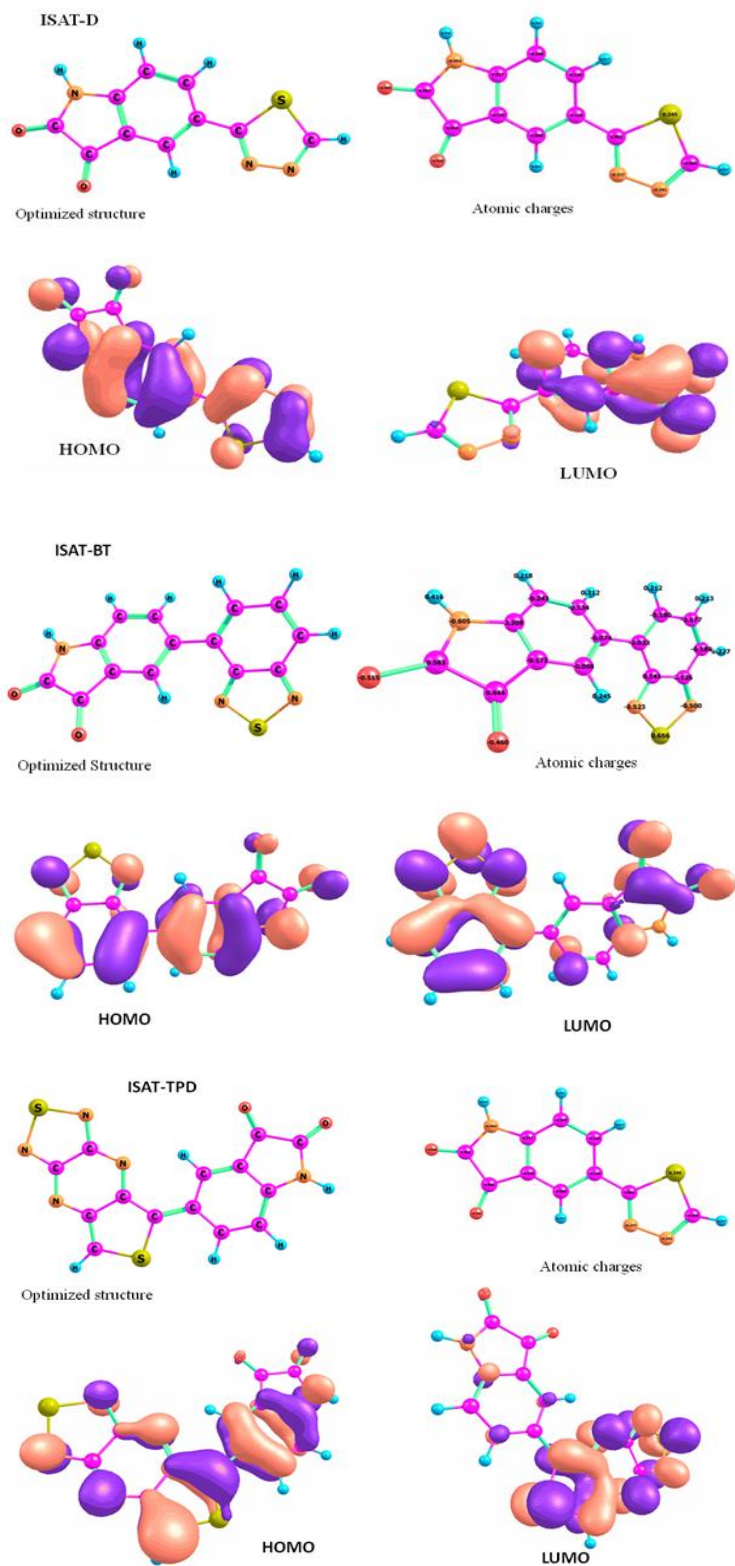
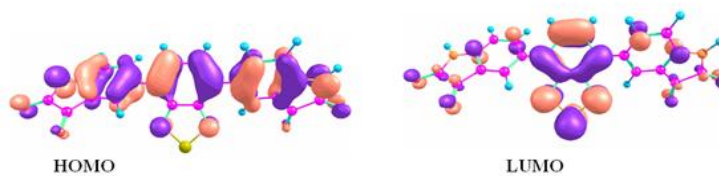
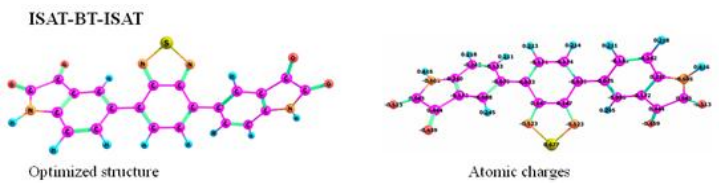
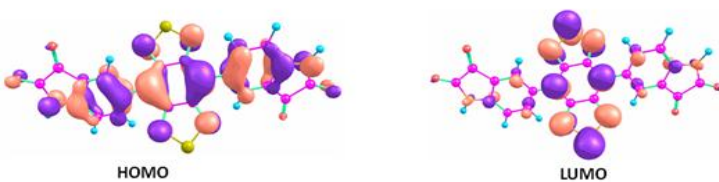
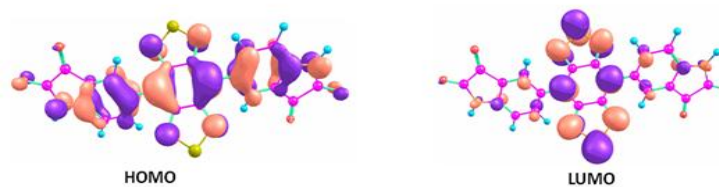
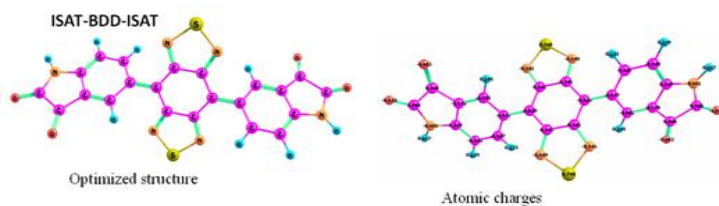


Fig. 2. Representative Plot of the optimized geometry of ISAT-Z showing torsional angle (Θ) in degree, Mulliken charge distribution (ICT) in e and bond length (dB) in Å.

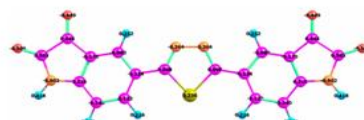




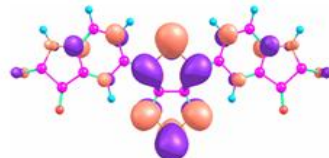
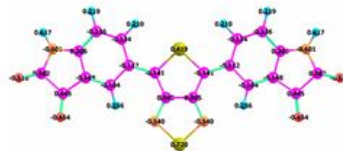
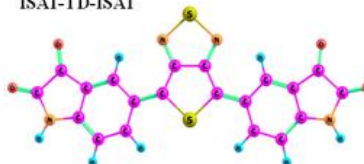




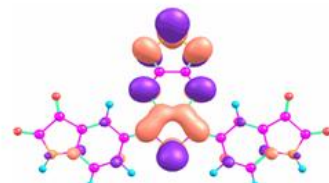
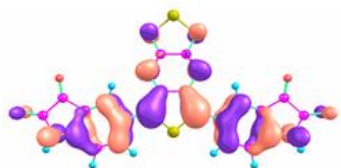
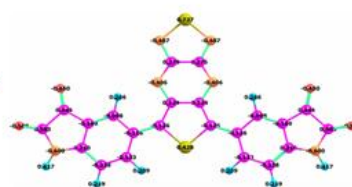
ISAT-D-ISAT



ISAT-TD-ISAT



ISAT-TPD-ISAT



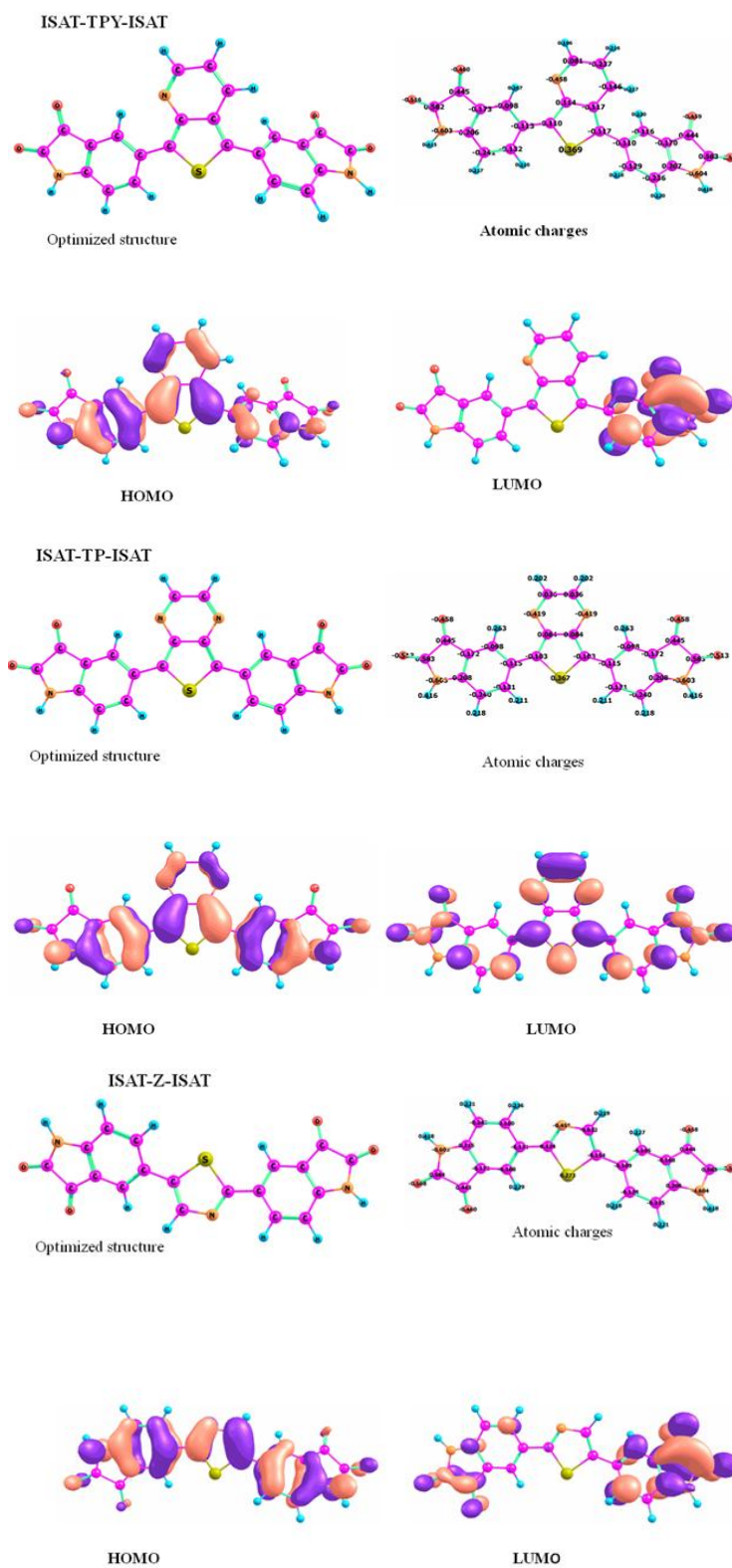


Fig. 3. Optimized structures, Atomic charge distribution and HOMO-LUMO surface diagram

Intramolecular charge transfer was calculated as the average of the summation of Mulliken charge distribution of the donor and acceptor. The order of the intramolecular charge transfer (ICT) obtained from the Mulliken charge distribution with the 6-31G(d) level is (ISAT-D) > (ISAT-BT), (ISAT-TPY) > (ISAT-Z), (ISAT)2 > (ISAT-TPD) > (ISAT-BDD) > (ISAT-TP) > (ISAT-TD) as shown in Table 1. The trend of the ICT is nearly similar to that of the acceptor strength except for (ISAT-D). Similar result was observed in the case of (EDOT-D) [32] and ((Cbz-Edot)-D) [40]. The unusually high value of ICT of (ISAT-D) is probably due to two adjacent imine nitrogen atoms with high electronegativity value in the thiadiazole ring, which could localize electrons while the adjacent ISAT moiety localize a hole.

Bond length is the bond distance between the donor and acceptor. The bond length between the donor and the acceptor dB (Table 1) decreases for the five-membered ring acceptor molecules with the acceptor strength: (ISAT-TD) < (ISAT-TPD) < (ISAT-TP) < (ISAT-D). Similar trend is observed for the six-membered ring acceptor moieties: (ISAT-TPY) < (ISAT-BDD) < (ISAT-BT).

Dipole moment is an important parameter that determines the polarity of system. From the result obtained, it can be seen that the dipole moment of (ISAT-Z), (ISAT-D), (ISAT-TP), (ISAT-TD), (ISAT-BT), (ISAT-TPD), (ISAT-BDD) and (ISAT-TPY) are 5.98, 7.71, 5.51, 6.50, 6.85, 6.60, 5.38 and 7.20 Debye respectively. This result indicates that the polarities of the studied molecules are enhanced by the introduction of thiadiazole and thienopyridine acceptors. Similar observation was made for (Cbz-Edot)-based molecules [40]. Quadrupole moment is determined for the studied compounds and the values are presented in Table 2. The average of the diagonal quadrupole moment tensor elements Q_{ii} and unique quadrupole moment Q are as defined below:

$$Q_{ii} = (Q_{xx} + Q_{yy} + Q_{zz}) / 3 \quad (3.1)$$

$$Q = Q_{xx} - Q_{yy} \quad (3.2)$$

As revealed in Table 2, all the diagonal elements of the quadrupole moment tensor for the model compounds are negative. This indicates that the negative charge distribution is farther removed from the molecular centre of the nuclear charges. The values of the off-diagonal elements Q_{xz} and

Q_{yz} of the molecules are relatively lower which can be attributed to its symmetric plane nearly perpendicular to the z-axis. It can be observed that the dipole and quadrupole moment values of (ISAT-D), (ISAT-TPD), (ISAT-BDD) and (ISAT-TPY) are relatively higher, indicating that the thiadiazole and thienopyridine are stronger electron donor. The [40] made the same observation for (Cbz-Edot)-TPD and (Cbz-Edot)-TD.

3.2 Molecular Energies and Related Properties

The electronic properties of all the studied compounds were obtained by DFT calculations at the B3LYP/6-31 G (d) level. Table 3 and Fig. 4 show the result of the analysis of HOMO-LUMO energy gap of studied compounds.

As shown in Table 3, the LUMO energy level of model compounds decreases in the order: (ISAT-TPY) > (ISAT-BT) > (ISAT-TP) > (ISAT-Z) > (ISAT-D) > (ISAT)2 > (ISAT-TD) > (ISAT-BDD) > (ISAT-TPD), which is the same order as the acceptor strength. The HOMO energy level of the model compounds is between -5.53 and -6.71 eV. The calculated band gap, E_g of the studied compounds increases in the order as follows: (ISAT-TPD) < (ISAT-BDD) < (ISAT-TD) < (ISAT-TPY) < (ISAT-TP) < (ISAT-BT) < (ISAT-Z) < (ISAT-D) < (ISAT)2 < (ISAT). The significant reduction in E_g value of (ISAT-TPD), (ISAT-BDD) and (ISAT-TD) compared to that of (ISAT) indicates the profound effect of intramolecular charge transfer. The frontier molecular orbital (MO) contribution is essential in determining the charge-separated states of the model oligomers. In order to create an efficient charge-separated state, the highest occupied MO (HOMO) must be localized on the extended donor moiety and the lowest unoccupied MO (LUMO) on the acceptor moiety.

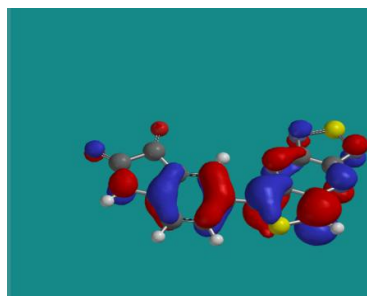
It is revealed in Fig. 3 that the HOMO state density is distributed entirely over the conjugated molecules, while the LUMO electron density is mainly on the acceptors' moieties. A significant contribution to the LUMO of the electron accepting groups was observed in (ISAT-BDD), (ISAT-TD) and (ISAT-TPD). The reduction in the band gap of these compounds compared with others is due to the introduction of the thiadiazole segment in their structures. Similar observation was made in (Cbz-Edot)-based counterparts [40].

Table 2. Quadrupole moments (in Debye Å) of the model compounds calculated by B3LYP/ 6-31G (d) method

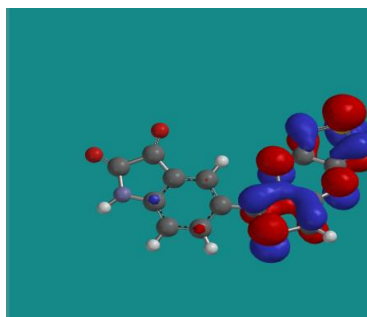
Compound	Qxx	Qyy	Qzz	Qxy	Qxz	Qyz	Qii	Q
(ISAT)2	-109.12	-100.25	-173.15	-0.00	0.00	0.00	-127.51	-8.88
(ISAT-Z)	-133.62	-94.13	-97.17	-8.97	4.63	-0.29	-101.64	-19.49
(ISAT-D)	-105.07	-97.56	-96	-6.33	0	0	-99.55	-7.51
(ISAT-TP)	-132.62	-109.61	-118.7	-23.45	-4.26	-0.1	-120.31	-23
(ISAT-TD)	-133.85	-114.75	-119.05	-18.2	-4.15	1.37	-122.55	-19.1
(ISAT-BT)	-134.17	-111.56	-117.41	-14.19	-10.13	-0.7	-121.04	-22.61
(ISAT-TPD)	-150.04	-139.16	-139.3	-29.99	-5.68	-0.86	-142.83	-10.88
(ISAT-BDD)	-170.54	-129.9	-138.78	-14.81	-11.04	1.35	-146.41	-40.64
(ISAT-TPY)	-115.67	-112.67	-120.73	-23.75	4.3	0.59	-116.36	-3.01

Table 3. Electronic properties (HOMO, LUMO and Eg) of model compounds as calculated by B3LYP/6-31G (d).

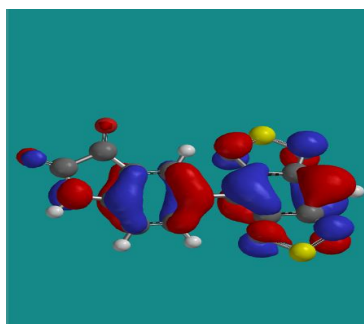
Model Compound	HOMO (eV)	LUMO (eV)	Eg (eV)
ISAT	-6.55	-2.65	3.9
(ISAT)2	-6.71	-3.06	3.65
(ISAT-Z)	-6.23	-2.85	3.48
(ISAT-D)	-6.56	-2.93	3.63
(ISAT-TP)	-5.78	-2.73	3.05
(ISAT-TD)	-5.63	-3.08	2.55
(ISAT-BT)	-6.15	-2.7	3.45
(ISAT-TPD)	-5.78	-3.87	1.91
(ISAT-BDD)	-5.91	-3.68	2.23
(ISAT-TPY)	-5.53	-2.25	2.98



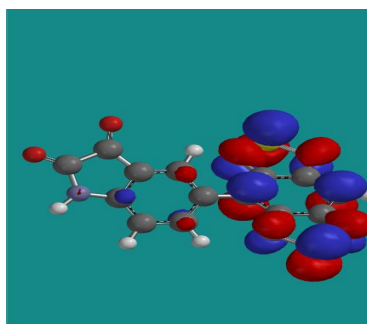
HOMO of ISAT-TPD



LUMO of ISAT-TPD



HOMO of ISAT-BDD



LUMO of ISAT-BDD

Fig. 4. Representative Plot of frontier orbital's of studied compounds by DFT/B3LYP/6-31 G (d) level

Table 4. Electronic transition data for the model compounds obtained by TD/DFT-B3LYP/6-31G (d) calculation

Electronic transition	$\lambda_{abs.}(nm)$	E _{ex.} (eV)	O.S	MO/Character	Coefficient
(ISAT-Z)					
S0→S1	464.49	2.6692	0.0004	HOMO → LUMO	0.9778
S0→S2	433	4.0266	0.0076	HOMO-1 → LUMO	0.976
S0→S3	307.91	4.3871	0.0719	HOMO-2 → LUMO	0.7034
(ISAT-D)					
S0→S1	465.5	2.6635	0.0001	HOMO → LUMO	0.9845
S0→S2	402.76	4.0145	0.0000	HOMO-1 → LUMO	0.9787
S0→S3	308.84	4.2843	0.0000	HOMO-6 → LUMO	0.6269
(ISAT-TP)					
S0→S1	472.89	2.6218	0.0479	HOMO → LUMO	0.8294
S0→S2	461.22	2.6882	0.0065	HOMO-1 → LUMO	0.8144
S0→S3	422.3	2.9359	0.2117	HOMO → LUMO+1	0.8538
(ISAT-TD)					
S0→S1	508.26	2.4394	0.097	HOMO → LUMO	0.5195
S0→S2	484.49	2.6708	0.0001	HOMO-1 → LUMO	0.3806
S0→S3	464.21	3.7905	0.0077	HOMO-2 → LUMO	0.8284
(ISAT-BT)					
S0→S1	462.42	2.6812	0.0004	HOMO → LUMO	0.8854
S0→S2	419.38	3.7222	0.0007	HOMO → LUMO+1	0.8988
S0→S3	385.15	3.9152	0.0014	HOMO-1 → LUMO+1	0.3553
(ISAT-TPD)					
S0→S1	709.93	1.7464	0.1379	HOMO → LUMO	0.9603
S0→S2	530.31	2.338	0.0006	HOMO-3 → LUMO	0.9639
S0→S3	490.61	2.5271	0.0281	HOMO-1 → LUMO+1	0.2344
(ISAT-BDD)					
S0→S1	558.73	2.219	0.2904	HOMO → LUMO	0.9407
S0→S2	467.74	2.6507	0.0054	HOMO-1 → LUMO	0.6819
S0→S3	457.99	2.7552	0.0161	HOMO → LUMO+1	0.6633
(ISAT-TPY)					
S0→S1	489.87	2.5309	0.0447	HOMO → LUMO	0.9595
S0→S2	460.53	2.6922	0.0011	HOMO-1 → LUMO	0.9579
S0→S3	385.93	3.2126	0.3331	HOMO → LUMO+1	0.9323

3.3 Absorption Properties

For a new material to be considered useful in photovoltaic devices its absorption spectrum must match with the solar emission spectrum which is located at approximately 700 nm which corresponds to a low energy of 1.77eV [41]. Also, a good photovoltaic material should have broad and strong visible absorption characteristics. Using the optimum ground-state structures of the studied compounds, the excitation energy, E_{ex.} (eV), absorption wavelength, $\lambda_{max.}(nm)$ and oscillator strength (O.S) are calculated and are as shown in Table 4. The values are calculated by TD-DFT method using the optimized geometry obtained by B3LYP/6-31G (d) level.

The calculated absorption wavelength of the model compounds decreases in this order:

(ISAT-TPD) > (ISAT-BDD) > (ISAT-TD) > (ISAT-TPY) > (ISAT-TP) > (ISAT-D) > (ISAT-Z) > (ISAT-BT). This order is the same as obtained for the acceptor strength. It is noteworthy that the largest oscillator strength originates from S0→S1 electronic transition. The band signals observed at 464.49, 465.50, 472.89, 508.26, 462.42, 709.93, 558.73 and 489.87 nm correspond to the HOMO-LUMO transition. There is a difference of about 351.20 nm between the maximum absorption wavelengths of (ISAT-TPD) and (ISAT-BDD).

3.4 Effect of the Conjugation Length on the Electronic Properties

It is an accepted technique to decrease the band gap of conjugated polymers by increasing their conjugation length. The effect of increasing the

Table 5. The HOMO, LUMO and band gap energies, Eg obtained by DFT-B3LYP/6-31G (d) calculation for the studied oligomers

Model compound	HOMO (eV)	LUMO (eV)	Eg (eV)
ISAT-Z-ISAT	-5.97	-2.93	3.04
(ISAT-D-ISAT)	-6.29	-3	3.29
(ISAT-TP-ISAT)	-5.59	-2.96	2.63
(ISAT-TD-ISAT)	-5.43	-3.36	2.07
(ISAT-BT-ISAT)	-6	-2.86	3.14
(ISAT-TPD-ISAT)	-5.57	-4.02	1.55
(ISAT-BDD-ISAT)	-5.73	-3.8	1.93
(ISAT-TPY-ISAT)	-5.49	-2.96	2.53

conjugation length of the donor-acceptor type oligomers by adding another donor molecule on the electronic properties was studied. The values of calculated HOMO, LUMO and energy gap (Eg) of the alternating donor-acceptor-donor oligomers as obtained by DFT-B3LYP/6-31G (d) are as shown in Table 5.

It can be seen from Table 5 that the increasing order of the calculated energy gap Eg (eV) is: (ISAT-TPD-ISAT) < (ISAT-BDD-ISAT) < (ISAT-TD-ISAT) < (ISAT-TPY-ISAT) < (ISAT-TP-ISAT) < (ISAT-Z-ISAT) < (ISAT-BT-ISAT) < (ISAT-D-ISAT). This order corresponds with the order of the acceptor strength. (ISAT-TPD-ISAT) and (ISAT-BDD-ISAT) have smaller energy gap values, compared to other studied oligomers. Chang *et al.*, [30] recently reported the synthesis and optoelectronic properties investigation of alternating conjugated polymers containing cyclopentadithiophene (CPDT) and benzothiadiazole (BT) as electron donor and acceptor units respectively. They observed an increase in the band gap energy value for a polymeric system with an additional CPDT unit (CPDT-BT-CPDT) which was attributed to a weaker charge transfer between the D-A units. However, in our studied oligomeric systems, we observed a reduction in the band gap energy value for ISAT-BT-ISAT which shows an excellent charge transfer between our donor and acceptor units

4. CONCLUSION

The structural, geometric and electronic properties of isatin-based alternating donor-acceptor type oligomers have been studied theoretically using density functional theory at B3LYP/6-31G (d) level. It was observed that the HOMO level, LUMO level and energy band gap of the studied compounds were controlled by the acceptor strength. From the study, it was discovered that (ISAT-TPD-ISAT) and (ISAT-

BDD-ISAT) have the least energy band gap of 1.55 and 1.93 eV, respectively. These values suggest that they could serve as active layers in photovoltaic devices which require that the absorption spectrum of the material matches with the emission spectrum of the sun whose maximum flux is around 700 nm.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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