



Original Research Article

Substituent Effect on Bithiophene-Bipyridine Organic Conjugated Systems: Theoretical Investigation

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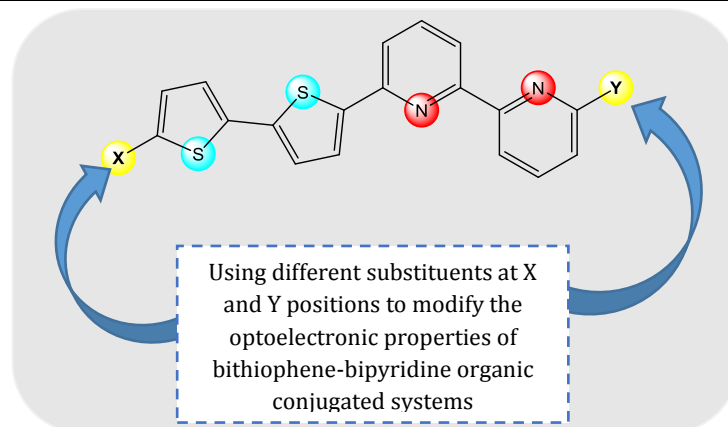
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ABSTRACT

Organic pi-conjugated compounds have attracted the interest of many researchers world wide due to their stability, high conductivity and intriguing optoelectrical properties. In this study, theoretical calculations were carried out to investigate the effect of electron-withdrawing and electron-donating groups at a different position on electronic properties, geometry and photophysical parameters of bithiophene and bipyridine ring linked by a single bond using density functional theory (DFT) and time dependent DFT (TD-DFT). The calculated energy gap (E_g) of the studied co-oligomers with substituents decreased with substituent strength. The reduction in the value of η (1.54eV to 1.8eV) of the substituted co-oligomers compared with 1.95eV of unsubstituted co-oligomer implies lower resistance to distortion which enhances electron-withdrawing. The theoretical maximum absorption (λ_{max}) values for substituted compounds range between 335.4nm to 404.2nm compared with 318.2nm of an unsubstituted compound. Hence, the study results show that the substitute groups' nature, species, and position affect both the electronic and absorption properties without any significant difference in the geometry of the bithiophene-bipyridine co-oligomer. The mutual comparison of substituted and unsubstituted compounds shows a decrease in energy gap (E_g) and significantly reflected bathochromic shift for all substituted compounds, especially compound with NO₂ substituent, indicating that the HOMO and LUMO level of the studied compounds were well controlled by the attached substituents groups. Hence, it is expected to be useful for opto electronic material design.

GRAPHICAL ABSTRACT



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Introduction

Organic pi-conjugated oligomers and polymers are used as active materials in electronic devices such as organic field effect transistors (OFETs) [1, 2], organic thin film transistor (OTFT) [3, 4], organic light emitting diodes (OLEDs) [5, 6], photovoltaic cells [7-10] and sensor materials [11]. Some of these organic materials exhibit either metalloid or semiconducting properties. A suitable modification of their organic nature allows low-cost deposition processes. The processing of these materials in solution with low temperature enlarges the scope of tolerant substrates and allows the fabrication of flexible, lightweight, and low-cost electronic devices [12]. However, the quality of organic electronic devices (OED) relies on the high performance of organic materials. The current performance and lifetimes of OE devices are significantly lower than those of traditional [13]. However, the chances of improving this device is quite large. A profound knowledge of the complex physical and chemical properties is required [13]. To reach such a solid understanding and therefore achieve optimization, a lot of work still has to be done by experimentalists and theoreticians in deep complementary. This work presents recent results on the structural details and electronic properties of bithiophen-bipyridin prototype organic semiconductors using density functional theory (DFT). Although, Photophysical properties of polythiophenes, polypyridine, polypyrroles, polyanilines, polyphenylenes, and some other pi-conjugated derivatives have been extensively studied. Both experimental and theoretical investigations on biphenyl, 2,2'-bipyridine [14], 2-phenylpyridine [15], and 2,2-bithiopene [16], have been reported. However, the study of this co-oligomers and their derivatives will constitute an essential class among pi-conjugated polymeric materials with promising electronic and optical technology because two aromatic pi-conjugated units are connected by a single bond to produce

new composite molecules, this constituting molecule can rotate around the single bond linking them together. Therefore, evaluating the substituted -donating group and electron-withdrawing group on bithiophen-bipyridine copolymers is critical for understanding their structure, relative energetic, and quantum chemical parameters.

Computational Methods

Quantum mechanical calculations of the ground state molecular structure of bithiophene-bipyridin co-oligomer and its derivatives were carried out using 1.2 version of the Spartan 14 software package [17]. Studied co-oligomers were subjected to a rigorous conformation analysis around the free rotation bonds before structural optimization. Structural optimization was done without constraints using the density functional Theory level of Becke's three parameters with the Lee-Yang-Parr (B3LYP) [18]. It has been shown that B3LYP/6-31G* gives an adequate description of carbon-based materials and decent ground state structures of conjugated polymers. Molecular orbital energies (HOMO and LUMO), band gap and quantum chemical descriptors such as electronegativity, chemical hardness and electropositivity index were estimated using DFT/B3LYP/6-31G(d,p) method [19-20]. The stationary points were checked through the vibrational frequency. This analysis ensures that only real vibrational frequencies (not imaginary frequencies) were obtained for the entire geometries. The description of CT states is enhanced by using LC functionals, Coulomb Attenuated Method (CAM-B3LYP), where the fraction of the HF exchange increases as the electron-electron separation increases and since Hybrid functionals combine a fraction of non-local Hartree-Fock (HF) exchange (B3LYP), they still do not offer a perfect representation of CT excited states [21]. The electron affinity (EA) and ionization potential

(IP) of the studied compounds were related to the E_{HOMO} and E_{LUMO} using Koopman's theorem [22]. These are clearly shown in equation 1 and 2:

$$IP = -E_{HOMO} \quad (1)$$

$$EA = -E_{LUMO} \quad (2)$$

$$\eta = \left(\frac{\delta^2 \varepsilon}{\delta N^2} \right)_{v(r)} = \frac{E_{LUMO} + E_{HOMO}}{2} = \frac{IP - EA}{2} \quad (3)$$

$$\chi = -\mu = \left(\frac{\delta \varepsilon}{\delta N} \right)_{v(r)} = -\frac{E_{LUMO} + E_{HOMO}}{2} = \frac{IP + EA}{2} \quad (4)$$

$$S = \frac{1}{\eta} \quad (5)$$

The three quantum parameters of organic inhibitors: softness, electronegativity, and hardness are beneficial in examining their chemical reactivity.

The electrophilicity index parameter of each molecule was estimated using equation 6 [20, 23]. This property measures the stabilization energy when charges are transferred to a system from the environment. It also measures the tendency of chemical species to accept electrons.

The electronegativity (χ) and absolute hardness values of the organic inhibitors were calculated using equation 3 and 4 respectively [23]. Meanwhile, softness, which is the inverse of hardness, is also a quantum parameter calculated using 5.

$$\omega = \frac{\mu^2}{2\eta} \quad (6)$$

When the values of μ and ω are low, the studied compounds are more reactive nucleophile while high values depict a more reactive electrophile.

All calculations were performed using Intel_Core™ i3-G42-247SB CPU, 2.30 GHz computer.

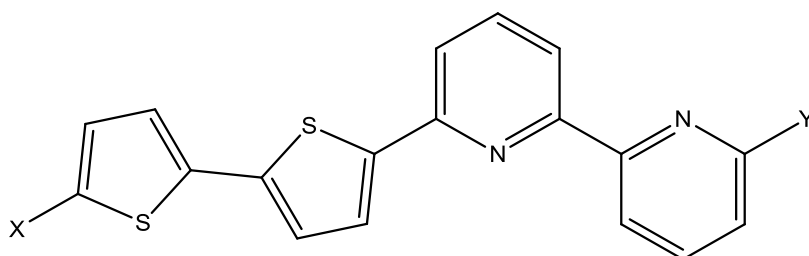


Figure 1. Structure of the Bithiophen-bipyridine co-oligomers

Table 1. list of substituents attached to bithiophen-bipyridine co-oligomers

Compounds	X	Y	Compounds	X	Y	Compounds	X	Y
BTBP ₁	H	H	BTBP _{4B}	NO ₂	H	BTBP _{7B}	CH ₃	H
BTBP _{2A}	H	F	BTBP _{5A}	H	C ₆ H ₅	BTBP _{8A}	H	OH
BTBP _{2B}	F	H	BTBP _{5B}	C ₆ H ₅	H	BTBP _{8B}	OH	H
BTBP _{3A}	H	I	BTBP _{6A}	H	C ₆ H ₅	BTBP _{9A}	H	OCH ₃
BTBP _{3B}	I	H	BTBP _{6B}	C ₆ H ₅	H	BTBP _{9B}	OCH ₃	H
BTBP _{4A}	H	NO ₂	BTBP _{7A}	H	CH ₃			

Results and Discussion

Geometries of optimized studied compounds

The structure of 2-(pyridine-2-yl)-6-(5-(thiophene-2-yl)thiophen-2-yl)pyridine (Bithiophene-bipyridine co-oligomers) (BTBP₁) and its fourteen derivatives were optimized and presented in Figure 2.

The results obtained in Table 2 shows the effects of fluorine (F), bromine (Br), Iodine (I), nitro (NO₂), phenyl (C₆H₅), methyl (CH₃), hydroxyl (-OH), and methoxy (-OCH₃) substituents on geometrical properties: bond lengths, bond angles and dihedral angles of bithiophene-bipyrimidin co-oligomer compound. When halogen group (F and I) were singly and separately attached to Thiophene, the bond lengths d1 (X-C₁) increased progressively from 1.082Å to 1.333Å, and 2.084Å respectively, following the order of electron-withdrawing nature of halogen. This is in tune with the conventional order of decrease in atomic radii (bond lengths) of halogen (0.072 nm < 0.133 nm) in the periodic table as electronegativity increases (F > I). When other substituents: -NO₂ - C₆H₅, -CH₃, -OH, and -OCH₃ were added, the bond lengths d1 (X-C₁) also increased progressively from 1.082Å to 1.427Å, 1.466 Å, 1.449 Å, 1.355 Å,

and 1.347Å respectively. However, bond lengths d5 (C₁₄-Y) remain unchanged when compared with the unsubstituted parent compound (1.082Å) as a result of the neutral chemical behavior of hydrogen at point Y(Pyridine). The reversed arrangement of the substituents (when -F, -I, -NO₂ -C₆H₅, -CH₃, -OH, and -OCH₃ were bonded to Pyridine) shows that the bond lengths d5 (C₁₄-Y) increased progressively from 1.089Å to 1.345Å, 2.144 Å, 1.498Å 1.488 Å, 1.509 Å, 1.355 Å & 1.354Å respectively. However, there is no significant difference between other intermolecular distances (i.e, distance between the thiophene and thiophene or thiophene and pyridine or pyridine-pyridine bonds) of the substituted and unsubstituted molecules. The bond angles of substituted (either at point X or Y position) and unsubstituted compounds are insignificantly different. This shows no structural change when substituents were grafted on either side of the parent compound. However, there is an improvement on the dihedral angles when substituted bithiophene-bipyridine compared with the unsubstituted bithiophene-bipyridine. The results showed that compounds with substituents are more planar; therefore, the mobility of pi-electrons is enhanced, which improves the electron transfer process offers a suitable electronic property.

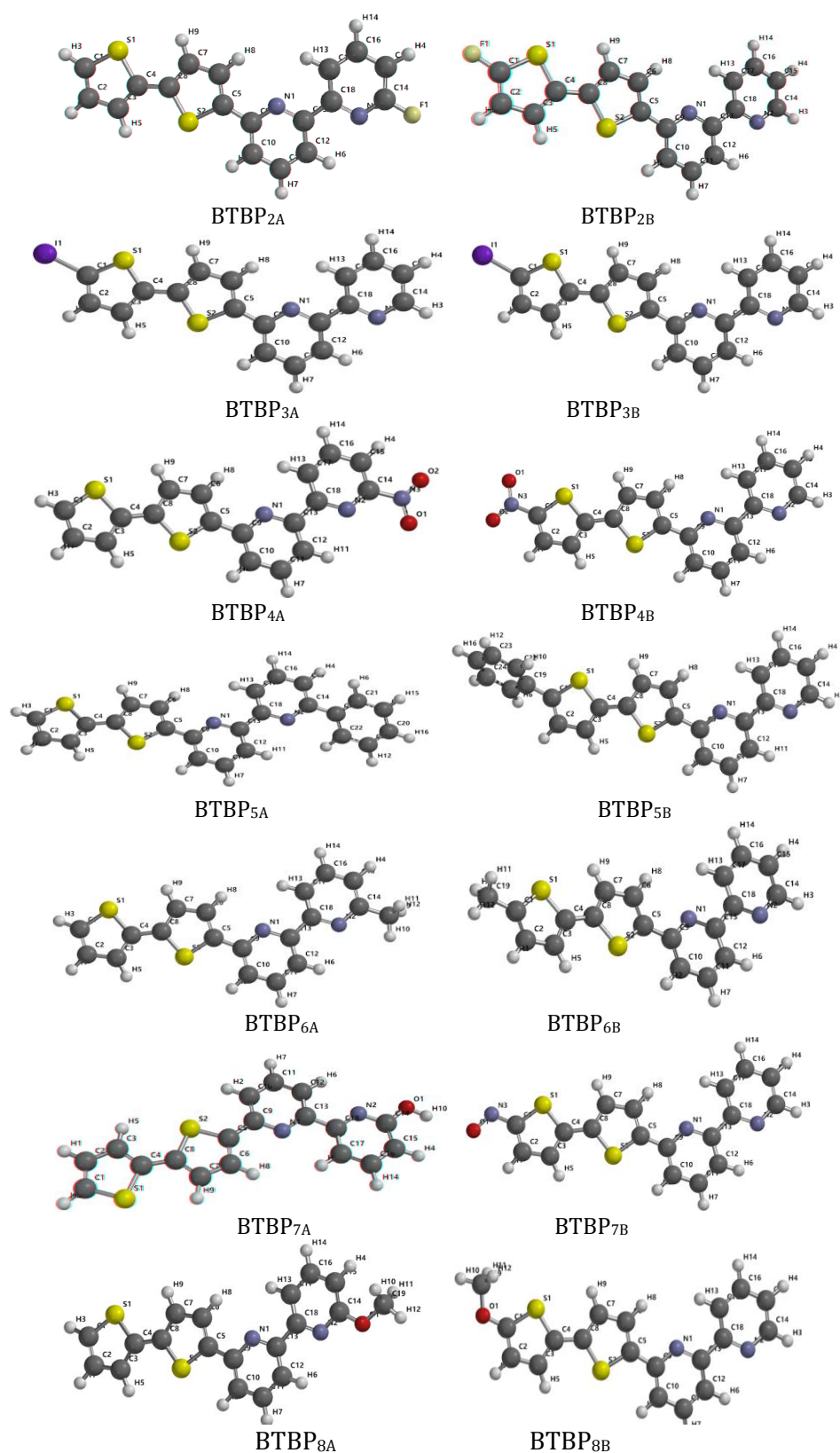


Figure 2. Optimized of Bithiophen-bipyridine co-oligomers

Table 2. Geometrical properties: bond lengths, bond angles and dihedral angles, of bithiophene-bipyrimidin co-oligomers

compounds	X	Y	d1(Å)	d2(Å)	d3(Å)	d4(Å)	d5(Å)	$\beta 1(^{\circ})$	$\beta 2(^{\circ})$	$\beta 3(^{\circ})$	$\beta 4(^{\circ})$	$\Phi 1 (^{\circ})$	$\Phi 2 (^{\circ})$	$\Phi 3 (^{\circ})$	$\Phi 4 (^{\circ})$
BTBP₁	H	H	1.082	1.448	1.460	1.486	1.089	91.76	92.26	118.58	118.08	165.48	179.29	179.74	179.23
BTBP_{2A}	H	F	1.082	1.450	1.463	1.489	1.345	91.76	92.28	117.16	117.63	161.15	178.98	179.81	179.11
BTBP_{2B}	F	H	1.333	1.447	1.460	1.486	1.089	90.09	92.22	118.58	118.08	164.46	179.10	179.76	179.31
BTBP_{3A}	H	I	1.082	1.450	1.462	1.489	2.144	91.76	92.24	117.12	118.56	162.3	175.1	179.12	178.8
BTBP_{3B}	I	H	2.084	1.448	1.464	1.491	1.089	91.40	92.16	118.57	118.08	167.2	174.8	179.9	179.2
BTBP_{4A}	H	NO ₂	1.082	1.447	1.459	1.483	1.498	91.74	92.27	118.43	117.73	175.84	179.92	179.89	179.66
BTBP_{4B}	NO ₂	H	1.427	1.444	1.461	1.486	1.089	90.11	92.10	118.56	118.05	175.84	179.73	179.82	179.11
BTBP_{5A}	H	C ₆ H ₅	1.082	1.447	1.460	1.487	1.488	91.73	92.24	118.72	118.82	174.93	179.86	179.88	178.32
BTBP_{5B}	C ₆ H ₅	H	1.466	1.445	1.460	1.486	1.089	92.29	92.24	117.34	118.05	162.58	179.33	179.97	179.88
BTBP_{6A}	H	CH ₃	1.082	1.448	1.463	1.491	1.509	91.75	92.24	117.30	119.16	161.54	178.99	179.79	179.54
BTBP_{6B}	CH ₃	H	1.449	1.447	1.462	1.491	1.089	92.23	92.24	118.56	118.10	179.85	179.38	179.71	179.11
BTBP_{7A}	H	OH	1.082	1.448	1.460	1.485	1.355	91.75	92.26	118.62	118.38	176.64	179.88	179.77	179.03
BTBP_{7B}	OH	H	1.355	1.444	1.459	1.486	1.089	91.10	92.26	117.24	118.08	174.79	179.68	179.96	179.17
BTBP_{8A}	H	OCH ₃	1.082	1.447	1.460	1.485	1.354	91.76	92.29	118.63	118.30	177.77	179.90	179.94	179.00
BTBP_{8B}	OCH ₃	H	1.347	1.448	1.460	1.486	1.089	90.32	92.23	118.59	118.09	160.44	179.22	179.56	179.59
BTBP_{8B}	OCH₃	H	1.347	1.448	1.460	1.486	1.089	90.32	92.23	118.59	118.09	160.44	179.22	179.56	179.59

Electronic and Absorption Properties of Studied Compounds

The observed results in Table 3 revealed that there was a reduction in bandgap from 3.90 eV of the unsubstituted compound (BTBP) to 3.70 eV (BTBP_{2A}) and 3.63 eV (BTBP_{3A}), where fluorine and Iodine atoms were substituents at pyridine (position Y), respectively. Further, reduction in band gaps (3.47 eV and 3.63 eV) were recorded when these halogens were attached to thiophene as shown in BTBP_{2B} and BTBP_{3B}. Fluorine possessed a strong electron-withdrawing affinity due to its high electronegativity. Similarly, -NO₂, -OH, -OCH₃, -C₆H₅, and -CH₃ substituents at either

X or Y position also reduced the band gap. However, a very low band gap of 3.12 eV recorded for BTBP_{4A} when NO₂ was attached to pyridine and further reduction to 3.07 eV in BTBP_{4B} when the substituent position of attachment changed to thiophene (position X) could be as a result of the destabilization of the highest unoccupied molecular orbital (LUMO) to lower energy level. The presence of a positive charge on Nitrogen atom in NO₂ deactivates the aromatic system and "suck" electron density from the aromatic system by positive inductive effect and influences the resonance stabilization of the system.

Table 3. Calculated HOMO, LUMO and band gap of the optimized oligomers

compounds	HOMO (eV)	LUMO (eV)	E _g (eV)
BTBP ₁	-5.61	-1.71	3.90
BTBP _{2A}	-5.61	-1.91	3.70
BTBP _{2B}	-5.40	-1.93	3.47
BTBP _{3A}	-5.63	-1.95	3.68
BTBP _{3B}	-5.61	-1.98	3.63
BTBP _{4A}	-5.57	-2.45	3.12
BTBP _{4B}	-5.93	-2.86	3.07
BTBP _{5A}	-5.35	-1.90	3.45
BTBP _{5B}	-5.21	-1.96	3.25
BTBP _{6A}	-5.41	-1.82	3.59
BTBP _{6B}	-5.35	-1.87	3.48
BTBP _{7A}	-5.37	-1.94	3.43
BTBP _{7B}	-5.09	-1.80	3.29
BTBP _{8A}	-5.32	-1.90	3.42
BTBP _{8B}	-5.11	-1.73	3.38

Table 4 s the electronic transition parameters, including the maximum absorption wavelength, oscillator strength energies, and orbital configuration. The maximum absorption wavelength (λ_{\max}) in an absorption spectrum is a single quantitative parameter that compares the absorption range of different molecules. When -F, -I, -NO₂, -C₆H₅, -CH₃, -OH and -OCH₃ were separately bonded to Pyridine (position Y), the calculated λ_{\max} are 335.4 nm, 368.2 nm 370.4 nm, 337.2 nm, 372.6 nm, 379.7 nm, 365.0 nm, 359.7 nm, 345.6 nm, 361.8 nm, and 361.8 nm respectively. When the order of arrangement was

reversed in such that -F, -I, -NO₂ -C₆H₅, -CH₃, -OH and -OCH₃ were separately and singly grafted on Thiophene (position X), the following results were obtained: 357.6 nm, 361.8 nm 366.0 nm 341.8 nm 370.4 nm, 404.2 nm, 355.5nm, 381.8 nm, 356.6 nm, 377.2 nm, and 367.1 nm, compared with 318.2 nm of an unsubstituted compound.

The obtained results indicate that oligomer NO₂ has the highest λ_{\max} among the donor/acceptor substituted oligomers. The higher the λ_{\max} , the higher the delocalization of electrons. This enhances their chemical stability, increases

absorption behavior, and makes them more conductive systems. The compounds also experienced a bathochromic (red) shift. All the values obtained for the calculated λ_{\max} are found to occur in the visible region.

Molecular reactivity descriptors of the studied compounds

Molecular global reactivity descriptors of the studied compounds give information on the reactivity and selectivity of the compounds. Such information was useful for comparing reactivity trends in different compounds. Table 5 reveals the analysis of the results obtained for Ionization

potential (IP) and Electron Affinity (EA) Molecular hardness (η eV) electrophilicity (μ eV), and chemical potentials (w eV).

The electron affinity for the above compounds varied between 1.91 eV to 2.45 eV, when -F, -I, -CN, and -NO₂ were separately attached to electron-deficient pyridine at position Y. When the substituents were attached to point Y, the values of electron affinity vary between 1.87 eV to 2.86 eV compared with 1.71 eV of electron affinity for the unsubstituted parent compound. Hence energy required to gain electrons was higher when the substituents were grafted on points X and Y.

Table 4. Electronic Transition parameters: orbital configuration, Wavelengths (nm), Oscillator Strength (*f*) and Energies (eV) Calculated with TD-DFT/ CAM-B3YP/6-31G(d,p).

Dyes	λ_{\max}	E_{opt} (eV)	<i>f</i>	MOs involved in the transition
BTBP ₁	318.2	3.8911	0.8701	H → L (97%)
BTBP _{2A}	335.4	3.6885	0.7045	H → L +1(98%)
BTBP _{2B}	357.6	3.5100	0.7710	H-2→L(33%) H → L (97%)
BTBP _{3A}	337.2	3.6874	0.6821	H→L+1(28%)
BTBP _{3B}	341.8	3.7174	0.7414	H→ L+1(34%)
BTBP _{4A}	379.7	3.1961	0.7118	H→L+2 (22%)
BTBP _{4B}	404.2	3.1421	0.8573	H → L (97%)
BTBP _{5A}	359.7	3.2974	0.6522	H → L (92%)
BTBP _{5B}	381.8	3.0996	0.5391	H→L+1(28%)
BTBP _{6A}	345.6	3.5820	0.8092	H-1 →L (86%) H→L+1(28%)
BTBP _{6B}	356.6	3.3884	0.7846	H→ L-1(38%)
BTBP _{7A}	361.8	3.4117	0.6147	H→L+2 (22%)
BTBP _{7B}	377.2	3.3105	0.5942	H → L (97%)
BTBP _{8A}	361.8	3.4167	0.5381	H → L (98%)
BTBP _{8B}	367.1	3.3674	0.5944	H-2→L(31%)

In a molecular system, molecular reactivity and stability are usually measured by calculating their absolute softness and hardness properties. Fundamentally, chemical hardness means resistance towards the polarization of the electron cloud in molecules or atoms under small perturbation of chemical reaction.

Molecules with small and large band gaps are usually termed soft and hard molecules, respectively. The calculated values of chemical hardness for substituted compounds show a remarkable reduction compared to unsubstituted

compound. Furthermore, substituent attachment to thiophene makes such substituted molecules softer than molecules in which substitution took place in the pyridine position.

When each substituent was interchanged, the chemical hardness varies from 1.56 eV to 1.84 eV, compared with 1.95 eV of chemical hardness for the unsubstituted parent compound. The decrease in the value of chemical hardness when substituents were grafted to the parent compound implies higher resistance to distortion. Also, the global electrophilicity index,

which measures the propensity of species to accept electrons was found within the range of 3.46 eV to 3.92 eV and later ranged between 3.62 eV and 3.88 eV when interchanged the substituents at position X and Y respectively, compared with 3.44 eV of the parent compound.

The electrophilicity and chemical hardness are inversely proportional to each other, which suggests that the substituents not hinder the delocalization of pi-electrons in the attached compounds.

Table 5. Calculated IP, EA, η , S, μ and ω

Compounds	IP(eV)	EA(eV)	η (eV)	s (eV)	μ^2 (eV)	ω (eV)
BTBP ₁	5.61	1.71	1.95	0.51	13.40	3.44
BTBP _{2A}	5.61	1.91	1.85	0.54	14.14	3.82
BTBP _{2B}	5.40	1.93	1.74	0.58	13.43	3.86
BTBP _{3A}	5.63	1.95	1.84	0.54	14.36	3.90
BTBP _{3B}	5.79	2.44	1.68	0.60	16.93	5.04
BTBP _{4A}	5.57	2.45	1.56	0.64	16.08	5.15
BTBP _{4B}	5.93	2.86	1.54	0.65	19.32	6.27
BTBP _{5A}	5.35	1.90	1.73	0.58	13.14	3.80
BTBP _{5B}	5.21	1.96	1.63	0.62	12.85	3.92
BTBP _{6A}	5.41	1.82	1.78	0.56	13.07	3.67
BTBP _{6B}	5.35	1.87	1.79	0.57	13.03	3.25
BTBP _{7A}	5.37	1.94	1.72	0.58	13.36	3.88
BTBP _{7B}	5.09	1.80	1.65	0.56	11.87	3.60
BTBP _{8A}	5.32	1.90	1.71	0.58	13.03	3.83
BTBP _{8B}	5.11	1.73	1.69	0.59	11.70	3.46

X= Substituent X, Y= Substituent Y, μ = Electrophilicity, IP=Ionization Potential, EA= Electron Affinity, ω = Chemical potential, η = Chemical hardness, S = Chemical softness

Conclusion

The theoretical investigation of geometric, electronic, and photophysical properties of modeled Bithiophene-bipyridine co-oligomers and their derivatives were successfully performed using DFT/B3LYP/6-3/G(d) and TD-DFT to elucidate their electronic structures molecular reactivity descriptors and predict their applicability in optoelectronic devices. The results obtained by mutual comparison of substituted and unsubstituted compounds revealed that Bithiophene-bipyridine co-oligomers with substituents are more planar, indicating that the mobility of pi-electrons will be enhanced. This will improve the electron transfer process and offer substituted Bithiophene-bipyridine co-oligomers a good electronic property. Also, there is a decrease in energy gap (E_g) and significantly bathochromic shift

(redshift to higher wavelength) for all substituted compounds, especially when substituents are attached to thiophene. This indicates that the HOMO and LUMO level of the Bithiophene-bipyridine co-oligomers can be controlled to desirable values by attaching substituents groups. More importantly, Bithiophene-bipyridine co-oligomers with substituent attachment to thiophene improve the optoelectronic properties than Bithiophene-bipyridine co-oligomers with substituents attached to pyridine.

Disclosure statement

No potential conflict of interest was reported by the authors.

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