

Synthesis, solar cell application, and biological study of vinyl substituted isophorone derivatives

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Abstract

In this study, isophorone derivatives, which are single step aldol products, were designed and synthesized. Our overview of the synthesis of solar cell application and biological applications of series vinyl substituted isophorone compounds is reported. All synthesized compounds were characterized both through experimental techniques and calculations with density functional theory. Additionally, we investigated the photophysical properties of small organic compounds for organic bulk heterojunction photovoltaic cells. The solar cell efficiency results were compared and compound 4 was found to be more efficient than the other compounds. It was found that the optical quantum yield values were very close. Isophorone derivatives showed better antioxidant activities, which were DPPH, metal chelating, reducing activity, and antimicrobial activities against Salmonella typhimurium, Klebsiella pneumonia, Candida albicans, Staphylococcus aureus, Bacillus subtilis, and Escherichia coli. Compound 7 (which is substituted quinoline) and compound 5 (which is substituted cyno) had the highest antioxidant effect. The 4-brom phenyl, 4-cyno phenyl were used against gram negative bacteria and the 4-ter-butyl phenyl group was indicated for gram positive bacteria and yeast.

Keywords Aldol · Isophorone · Organic photovoltaics

Introduction

Organic electronics plays important roles in economic and environmental systems. Organic bulk heterojunction photovoltaic (PV) cells have awoken interest as an alternative to crystalline silicon solar cells due to their low cost, flexibility, and

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light weights. To date, various organic compounds have been synthesized for suitable PV materials, such as carbazole [1–3], fullerene [4–6] and graphene derivatives [7–9]. Recently, owing to their diverse structure, flexibility, solubility, stability and different good fluorescence properties, PV cells have been developed and have shown potential for use as inorganic light emitting diodes (OLED), organic field effect transistors (OFET), and bioelectronics devices. Their highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO–LUMO) energy and also band gap properties make organic-based PV materials good candidates for use. When we changed the substituents, different HOMO–LUMO levels were observed, so we obtained suitable material for OPV device.

In this study, we investigated the photophysical properties of organic small compounds for organic solar cells. We synthesized single step aldol products, including a conjugated enone system. Aldol reaction generated with isophorone and (het)aromatic aldehyde compounds. We obtained a vinyl-substituted whole conjugate system. The choice of different electronic properties is crucial for substitute aromatic aldehyde because the targeting compounds should change the electronic properties and should therefore be attached to electron donating-withdrawing groups, and hydrogen bonding capability groups linkers. In particular, quinoline derivatives have photophysical potential as blue photoemitting fluorescence [10]. The oxidation and reduction potential determined using cyclic voltammetry, solvatochromic effect via ultraviole-visibly spectrophotometry, quantum yield calculation by fluorescence spectrophotometry, dipole moment, frontier molecular orbitals energy level, nonlinear optical properties (NLO) and optimization of compounds via density functional theory (DFT), can be members of photophysical properties, which is interesting in organic electronics. In this study, a series of vinyl-substituted isophorone derivatives were designed and synthesized. All synthesized compounds were characterized both by experimental techniques by ¹H-NMR, ¹³C NMR, MS, X-ray, and DFT calculations. Their optoelectronic activities were scrutinized using cyclic voltammetry, fluorescence quantum yield, and solvatochromic effect with the establishment of their structure-activity relationships. The continuation of our work is planned to examine the antimicrobial and antioxidant activities of synthesized compounds.

Experimental

Materials

All reagents and solvents were purchased from Merck and used following further purification of solvents. Melting points were recorded on a Thermo Scientific Barn-stead/Electrothermal Apparatus without correction.

Synthesis

Isophrone (2.1 mmol) was added into the solution of appropriate aldehyde (1 mmol) in ethanol. The methanolic 10 M NaOH solution was added drop-wise at room

temperature. After 12 h, the reaction mixture was evaporated and the resulting residue was then purified by column chromatography [11].

Computational

The theoretical analyses of compounds 1-8 were carried out using DFT/B3LYP/6-31G(*d*,*p*) with the Gaussian 09W software and Gauss View 5.0.9 graphical interface programs [12, 13]. The theoretical approaches were used for the calculations of some electronic properties related to structure, such as frontier molecular orbitals energy values, dipole moment, and NLO characterization. These are related to the photo-physical properties of compounds [14–16]. Furthermore, chemical properties of the compounds were analyzed through electronegativity, chemical potential, chemical softness-hardness and total dipole moment.

Determination of photophysical properties

Absorption: The molar absorptivity and maximum absorption wavelength, as well as the absorption spectra, were obtained from the different media. Solutions were prepared using different dielectric constants solvents: toluene (2.38), tetrahydrofuran (THF) (7.58), methyl alcohol (MeOH) (32.7) and *N*,*N*-dimethylformamide (DMF) (36.7) [17]. For compounds **1–8** the concentration of the solutions ranged from 1.0×10^{-1} M to 1×10^{-7} M in toluene, THF, MeOH, and DMF.

Fluorescence

The study was performed to determine the emission spectra, wavelength, and optical relative quantum yield in DMF and toluene solvents. Relative quantum yield was calculated using Eq. 1. Tryptophan was selected as a standard compound because its absorption wavelength is suitable for the comparing compounds 1-8 in 1×10^{-4} M toluene solvent [18–20].

$$\boldsymbol{\Phi}_{f} = \boldsymbol{\Phi}_{r} (I_{f}/I_{r}) \cdot (A_{r}/A_{f}) \cdot (n_{f}/n)^{2}, \qquad (1)$$

where I is Integrated fluorescence intensity, A absorbance at excitation wavelength, n refractive index of solvent, r standard, and f is the sample.

Electrochemical properties

Cyclic voltammograms were recorded on the Gammry-References 3000 series with reference, counter and working electrodes as Ag/AgCl, Pt, and glassy-carbon electrode, respectively. All compounds and standards were examined with 10^{-4} M solution in 1,2-dichlorobenzene/acetonitrile/0.1 M Bu₄NPF₆ solution as the supporting electrolyte [21, 22].

Fabrication of organic solar cell

Patterned ITO-coated glass substrates were cleaned ultrasonically in acetone, deionized water and ethanol, in turn. Glass substrates were dried with N₂ (99.999% purity). Ozone plasma treatment (50 W, plasma etch) was applied to all the substrates for 5 min for surface cleaning of the patterned ITO substrates. PEDOT:PSS was filtered through a 0.45 um membrane PVDF filter. The PEDOT: PSS (PH500) layer used as hole transport layer (HTL) (~60 nm), was spin-coated onto the ITO substrates at 2000 rpm for 60 s and then annealed at 120 °C for 20 min in the ambient atmosphere. N-type semiconductor acceptor material phenyl-C61-butyric acid methyl ester (PC₆₁BM, Sigma Aldrich with 99.995%) and donor material poly(3hexylthiophene) (P3HT, 96.6%, Ossila Ltd.) (Sigma Aldrich with 99.995%, were first dissolved in 1,2-dichloroenzene with 10 mg/ml concentration separately and stirred for 2 h at 50 °C. The two pristine solutions were then blended to make a solution and were left to mix overnight at 50 °C. The CX guest materials were also prepared in 1,2-dichloroenzene with 10 mg/ml concentration. They were then prepared with the concentration ratio of D:A:G (1:1:1) mixed for 1 day. The mixture of this D:A:G was used as an active layer of the solar cell, and it was filtered through a 0.45 µm PTFE membrane filter and spin-coated on HTL at 1200 rpm for 40 s. The films were annealed at 110 °C for 10 min to obtain the proper morphology. Finally, Ca (15 nm) and Al (~100 nm) were evaporated for the cathode electrode of the devices. The deposition rate of Ca and Al were maintained at 0.1 nm/s and 2.0 nm/s, respectively. During metal thin film depositions, the chamber pressure was kept under 3×10^{-6} mbar. Electrical characterizations of the devices were done in the glove-box system ($O_2 < 0.1$ ppm, $H_2O < 0.1$ ppm). The current density-voltage (J-V) characteristics of the devices were recorded under standard solar irradiation (AM 1.5, 100 mW/cm²) using a Xenon lamp as a light source and dark J-V characteristics computer-controlled voltage-current Keithley 2600 source meter at 25 °C.

Biological activity assay

Antioxidant assay

DPPH radical-scavenging assay

The antioxidant activity of compounds **1–8** were analyzed for scavenging properties to the 1,1-diphenyl-2-picryl-hydrazil (DPPH·). After 30 min of incubation at room temperature, samples and control were read spectrophotometrically at 515 nm using a microplate reader. The Blois method [23–25] assay mixture contained 3.0 ml of samples at 100 μ g/ml ethanol, and 1.0 ml of 0.1 mM DPPH ethanolic solution.

DPPH Radical Scavenging (%) = $(A_{\rm C} - A_{\rm S})/A_{\rm C} \times 100$,

where $A_{\rm C}$ is the absorbance of control and $A_{\rm S}$ the absorbance of the samples and standards.

Metal chelatting

The metal chelating activity was evaluated in accordance with the method of Dinis [26, 27]. Samples found in 100 μ g/ml in 0.4 ml were added to 0.05 ml FeCl₂ (2 mM in distilled water), and 0.2 ml ferrozine (5 mM in distilled water). After being shaken for 10 min at room temperature, the final volume was adjusted 4 ml via ethanol. Absorbance was measured as 562 nm spectrophotometrically with a plate reader.

Metal Chelating (%) = $(A_{\rm C} - A_{\rm S})/A_{\rm C} \times 100$,

where $A_{\rm C}$ is the absorbance of control and $A_{\rm S}$ the absorbance of the samples and standards.

Reducing power

To assess the reducing capacity of samples, Yen and Chen's [28, 29] methods were adapted to microvolumes using a microplate reader. The 70 μ l sample solution and 35 μ l of potassium ferricyanide were added before incubation was carried out for 20 min at 50 °C. 35 μ l distilled water, TCA (33 μ l, 10%), and 27 μ l 0.1% FeCl₃ were added to the sample mixture. After 10 min incubation, absorbance was read at 700 nm.

Antimicrobial assay

Antimicrobial activity studies were performed according to the Minimum Inhibitory Concentration (MIC) method [30, 31]. In this study, *Salmonella typhimurium* CCM 5445 (St.), *Klebsiella pneumoniae* ATCC 700603 (Kp.), *Candida albicans* ATCC 10231 (Ca.), *Staphylococcus aureus* ATCC 6538P (Sa.), *Bacillus subtilis* IMG 22 (Bs.), and *Escherichia coli* ATCC 25922 (Ec.) were used. All microorganisms were grown at 37 °C for one night and then suspended in 50 ml of nutrient broth. The resulting suspensions were adjusted to 0.5 McFarland turbidity standards [32]. The compounds **1–8** were dissolved in DMSO and added onto the microorganisms transferred to the tubes at appropriate concentrations. All the test cultures were grown at 37 °C in incubator. The last tube where no growth was seen was determined as the MIC value.

Results and discussion

Chemistry

We obtained attachment of an aromatic group containing molecules of interest through a conjugated system (Scheme 1). We synthesized eight aldol products for evaluation of their photo-physical properties. All vinylic groups geometry were (E), which were decided with NMR spectra and X-ray results [11].

UV–Vis absorbance spectra with maximum absorbance–wavelength were between 316 and 354 nm in toluene (Table 1). Moreover, we note that the maximum absorbance–wavelength of compounds 7 and 8 red-shifted compared to 1, 2 and 3:



Scheme 1 Synthesis route for compounds 1-8

354(8) < 344(7) < 322(2) < 318(1) < 316(3) respectively. Thiol and quinoline groups caused the extended effective conjugation [33–35]. In the literature, when hypocrellin A derivatives were analysed for synthesis and characterization, the UV–Vis spectra showed maximum absorption wavelength without substituted hypocrellin of approximately 499 nm, but the S-alkyl derivatives was 508 nm, similar to our compound **8** (Fig. 1) [36].

On the other hand, we changed the solvent system compounds, showing that the solvatochromic effect depended on the solvent polarity, dielectric constant and ability for hydrogen bonding to occur. Although the THF solvent indicated a hyp-sochromic shift, MeOH and DMF had a batochromic shift. Compounds 7 and 8 had hydrogen bonding ability so included OH groups, and SCH₃ unit thus showed more bathochromic shift than others. Molar absorptivities of the compounds in four different solvents, toluene, THF, MeOH, and DMF, were calculated using the Lambert–Beer law at controlled room temperature. Fluorosolvatochromic effect was analysed in quinoline derivatives, the results were that the moderated color

Com- pounds/ solvent	Toluen	THF	МеОН	DMF	Φ_{f}
1	7503.0 (318 nm)	7354.1 (315 nm)	5704.8 (324 nm)	4092.6 (321 nm)	0.243
2	6406.0 (322 nm)	6278.9 (324 nm)	5552.4 (329 nm)	3494.2 (327 nm)	0.239
3	6577.6 (316 nm)	5346.5 (315 nm)	6718.8 (319 nm)	6543.8(318 nm)	0.234
4	5762.4 (327 nm)	3786.1 (326 nm)	5354.7(334 nm)	5562.6(329 nm)	0.241
5	6027.8 (323 nm)	5724.0 (321 nm)	5029.9(323 nm)	5689.6(325 nm)	0.215
6	6240.2 (327 nm)	5932.8 (328 nm)	4062.4(332 nm)	4988.9(328 nm)	0.217
7	7511.6 (344 nm)	6364.9 (342 nm)	7255.1(341 nm)	6547.5(351 nm)	0.265
8	6668.3(354 nm)	3763.5 (352 nm)	6205.7(358 nm)	6870.7(348 nm)	0.250

Table 1 The compounds 1–8 molar absorption coefficients at the maximum wavelengths, ε (dm³ mol cm) (λ /nm), and quantum yields



Fig. 1 Emission, excitation, and UV-Vis absorption spectra of the compounds 5 and 8

shifted, especially in n-heptane and the DMSO solvent system [37]. We compared this result to our compounds: as a result of toluene and DMF solvents absorption wavelengths were different depending on the solvatochromic effect.

Molar absorptivity, which is a characteristic quantity of atomic or molecular systems, changes with the wavelength of the radiation [38–40]. The highest molar absorptivity value was 7511 (dm³ mol cm) (λ /nm) in toluene for compound **7**, and the lowest was 3494 (dm³ mol cm) (λ /nm) in DMF for compound **2**.

Electrochemical analyzes were made to calculate the HOMO–LUMO levels and gap energies (E_{gap}) from oxidation and reduction potentials [41] (Fig. 2). Not only the cyclic voltammetry calculations but also optical and theoretical results are summarized in Table 2. The band gap energy was decreased in compounds 7 and 8, and there was thus extra-conjugation.

Figure 3 displays the optimized molecular structure of compounds 1-8 via B3LYP/6-31G(*d*,*p*) levels. To understand the photophysical properties, the FMOs energy levels and gap, dipole moment, chemical properties and NLO properties were analyzed via DFT.



Fig. 2 Cylic voltammograms of compounds 5 and 8

	$E_{\rm OX}$	$E_{\rm RED}$	HOMO	LUMO	HOMO _T	LUMO _T	$E_{\rm gap}$	$E_{\rm opt}$	E_t
1	-0.892	2.183	-5.312	-2.137	-6.032	-2.262	3.175	3.251	3.769
2	-0.846	2.057	- 5.039	-2.014	-6.040	-2.300	3.025	3.225	3.740
3	-1.004	2.852	- 5.981	-2.792	-6.097	-2.172	3.189	3.244	3.925
4	-0.932	2.525	- 5.548	-2.472	- 5.560	-1.923	3.076	3.230	3.637
5	-0.998	2.487	- 5.955	-2.872	-6.378	-2.650	3.083	3.095	3.728
6	-0.763	1.571	-4.547	- 1.538	-5.800	- 1.990	3.009	3.338	3.810
7	-0.825	2.174	-4.914	-2.128	-5.782	-2.430	2.786	2.982	3.351
8	-0.985	2.708	- 5.869	-2.651	-5.541	-2.048	3.218	3.225	3.492

Table 2 Comparison of the optical band gap of the compounds **1–8** obtained from CV (E_{gap}), optical absorption (E_{opt}) measurements, and theoretical calculations (E_t) at eV unit



Fig. 3 The optimized molecular structure of title compounds (DFT/B3LYP/6-31G(d,p))

The organic photovoltaic system included two important energy parameters, which were used to decide which devices were applicable. The first energy gap was the donor materials between HOMO and LUMO; the second gap was between acceptor materials' LUMO energy level and donor materials' HOMO energy levels. We found that the energy level of HOMO was between -6.37 eV and -5.54 eV and LUMO between -2.65 eV and -1.92 eV, as seen in Table 2. The lowest LUMO

energy level was -2.65 in compound **5**; -2.43 for compound **7**, and -2.04 for compound **8**. When we compared these with the band gap, the lowest gap was 3.35 eV for compound **7**, and the highest was 3.92 eV for compound **3**. Electron transfer route was from PEDOT:PSS to P3HT:PCBM, but hole transfer was counter-way. The PEDOT:PSS polymer system LUMO energy level was -2.4 eV. Only **5** and **7** of synthesized compounds were suitable for electron transfer. We thus noted that compound **4** should be used in this solar cell device. Global descriptors for electronegativity, chemical potential, chemical softness-hardness and non-linear optical properties were calculated. Compound **5** showed the highest electronegativity value. The values of the first order hyperpolarizability were compared with urea, and compounds **6**, **7**, **8** exhibited the very highest NLO character (Table 3). First order hyperpolarizability of chalcone derivatives, which was included in the enone system, was calculated by Gopalakrishnan groups: 131×10^{-33} esu [41]. Otherwise, styrene was used as an NLO monomer for optoelectronic polymers [42].

Biological assay

Antioxidant activities

We tested the antioxidant activities of the compounds, with the aim of discovering the structure of the relationship between the activities. The compounds exhibited the highest DPPH activities and the results are compared with synthetic antioxidant standards of BHT and BHA in Fig. 4. The activity of compound 7 was the highest.

Metal chelating activity was related to transition metals via oxidative stress reaction. As seen in Fig. 5, the metal chelating activities of compounds 1-8 were compared to EDTA. The activity depended on the concentration of the compounds. The metal chelating activity values of Fe²⁺–ferrozine complex were as follows: 7 > 5 > 8 > 3 > 4 > 2 > 1, and compound 7 had a value of 43.76% in 250 µg/ml concentration.

The reducing activity method was used to identify the reduction of Fe^{3+} to Fe^{2+} . Figure 6 shows the reducing activity compared to Trolox and BHA. The

	-	-			-	-	
Compounds	χ (eV)	μ (eV)	$S(\mathrm{eV}^{-1})$	η (eV)	μ (D)	$\langle \alpha \rangle$ (×10 ⁻²⁴ esu)	$\begin{array}{c} \beta_{\rm tot} \\ (\times 10^{-33} {\rm esu}) \end{array}$
1	0.15242	-0.15242	14.43835	0.06926	3.59378	29.78537	2878.91
2	0.15324	-0.15324	14.55151	0.06872	3.51229	31.55476	28526.26
3	0.15196	-0.15196	13.86578	0.07212	5.77473	30.65374	13307.12
4	0.13751	-0.13751	14.96334	0.06683	6.51162	30.14855	20159.42
5	0.16591	-0.16591	14.59747	0.06850	3.49840	29.78537	2878.91
6	0.14314	-0.14314	14.28378	0.07001	5.06304	37.14634	33099.67
7	0.15091	-0.15091	16.23640	0.06159	2.57860	38.92706	40436.74
8	0.13947	-0.13947	15.58118	0.06418	4.05658	37.01766	74672.24

 Table 3
 The values of electronegativity, chemical potential, chemical softness-hardness, total dipole moment, mean polarizability, and first order hyperpolarizability for compounds



Fig. 4 DPPH activities of compounds 1-8 and BHA, BHT as standards



Fig. 5 Iron chelating activity of compounds compared to EDTA as standard



Fig. 6 Reducing capacity of compounds, Trolox, and BHA

highest was 0.375 in compound 7 and the activity related to concentrations was also important.

Antimicrobial

The antimicrobial work was performed using the MIC method and 3 g negative, 2 g positive and only one yeast were used as microorganisms. We conducted the MIC study due to determination of aryl and cyclohexanon substitute enone system behaviour against some bacteria and yeast. The bis-aromatic ring consisting of enone compounds was reactive against K. Pneumonia, B. Subtilis, and *E. Coli* [43, 44].

As shown in the Table 4, it was determined that compounds 1 and 5 had considerable effects, especially on gram negatives. When the MIC values for compound 1 were examined, they were 250, 375, 500 µg/ml for gram negative *S. typhimurium*, *K. pneumonia* and *E. coli* respectively. When compound 5 was investigated, the MIC values for the same gram-negative bacteria were 500, 500 and 1500 µg/ml, respectively. In addition, it appeared that compounds 7 and 8 were only effective on *S. typhimurium* from among the gram negative bacteria with MIC value of 375 µg/ml. However, compound 6 was found to have significant effects on gram-positive *S. aureus* and *B. subtilis* and yeast *C. albicans*. The MIC values for gram-positive *S. aureus* and *B. subtilis* were 250, while for *C. albicans* which was yeast, this value was found to be 375 µg/ml.

Organic solar cell application results

Figure 7a shows the structure of the solar cell fabricated, together with the band structure of its components. The charge-separation occurred in heterojunction composite of poly(3-hexylthiophene) (P3HT), [6]-phenyl-C71 butyric acid methyl ester (PC70BM) and compound layer. Poly(3,4ethylenedioxylenethiophene)-polystylene sulfonic acid (PEDOT:PSS)was a highly conductive hole transport layer (Table 5).

The energy-level diagram (Fig. 7b) indicates the HOMO energies and LUMO energies of the individual component materials. The current versus voltage (I–V) characteristics of bulk heterojunction solar cells with P3HT:PCBM:X under illumination from solar simulator with irradiation intensity of 300 W/cm² are shown in Figs. 8 and 9.

Figure 8 shows the non-ohmic electrical response of I–V characteristics curves P3HT:PCBM:X (a) X: 4-Br, (b) X:4-Cl, (c) X:4-OCH₃, (d) X:4-SCH₃ bulk heterojunction in dark and in light (300 W Xenon lamp) at room temperature. It was found that the dark current density of the devices was much smaller than that of the light current density, which indicated that the charge recombination was increased by illumination. It was presented our control device with plain P3HT:PCBM data in Fig. 9a. It can be seen solar cell parameters 4-SCH3 and control device with plain

Compounds	Gram-negative			Gram-positive		Yeast	
	St.	Kp.	Ec.	Sa.	Bs.	Ca.	
1	250	375	500	1500	3000	> 5000	
2	2000	> 5000	2000	> 5000	3000	> 5000	
3	4000	500	1000	>5000	3000	2000	
4	2000	1000	> 5000	> 5000	2000	> 5000	
5	500	500	1500	> 5000	4000	> 5000	
6	2000	> 5000	2000	250	250	375	
7	375	2000	2000	2000	2000	2000	
8	375	1000	4000	> 5000	> 5000	> 5000	
DMSO	>5000	> 5000	> 5000	> 5000	> 5000	> 5000	

Table 4 Antimicrobial activity of compounds 1–8 (MIC in µg/ ml)



Fig. 7 a Solar cell device architecture, b Energy diagrams of materials utilized in solar cell device

Table 5 Solar cell parameters of4-OCH3 and control device with	Device	I _{sc}	V _{oc}	FF	%n
plain P3HT:PCBM	Compound 4	$1.5 * 10^{-5} \text{ mA/cm}^2$	0.54	0.17	$1.47 * 10^{-8}$
	Control device	$0.68 * 10^{-3} \text{ mA/cm}^2$	0.6	0.49	$2 * 10^{-6}$

P3HT:PCBM from inset in Fig. 9a, b, the efficiency of the control device is relative high. The current values increased exponentially with an increase in the forward bias voltage. The turn-on voltage was around 0.7 V for the forward bias and there was a reverse bias breakdown voltage of 1.2 V as seen from the I–V curve in the dark (Fig. 9a).

The devices with compound **4** showed J_{sc} =5.17 mA/cm², V_{oc} =0.73 V, FF=0.42. A ternary organic solar cell is a promising device for improving the power conversion efficiency (PCE) of single-junction organic solar cells by broadening the light absorption spectrum with the incorporation of two electron donors and one acceptor or one donor and two acceptors. However, in most cases, the contribution of the third component to the absorption of light was reduced due to the fact that the third component was not morphologically compatible [45]. For this reason, although the ternary solar cell shows around ~2% efficiency, efficiency of our devices are low (Fig. 10).



Fig. 8 I–V characteristics curves P3HT:PCBM:CX **a** X: 4-Br, **b** X:4-Cl, **c** X:4-OCH₃, **d** X:4-SCH₃ bulk heterojunction in dark and in light (300 W Xenon lamp)



Fig. 9 a I–V characteristics curves of control device with plain P3HT:PCBM (The inset displayed the effect of control device with plain P3HT:PCBM on photovoltaic parameters of polymer solar cells). b I–V characteristics zoomed curves of compound **4** (The inset displayed the effect of blend P3HT: Compound **4** molecule on photovoltaic parameters of polymer solar cells)





Conclusion

We have reported the synthesis and characterization of isophrone vinyl derivatives. Upon application of these compounds, both the biological activity and solar cell efficiency were scrutinized. Theoretical calculations were used and the experimental results were correlated. Frontier molecular orbitals, band gap energy values and some chemical properties revealed the biological activity and photovoltaic properties. Another significant result was that enone-substituents influence not only physical parameters but also biological activity. Quinoline substituent, which had the lowest gap value but higher HOMO energy value, revealed a stunning level of antioxidant activity and antimicrobial activity, whereas solar cell efficiency was not higher than expected. It was shown that compound **4** had the lowest electronegativity and otherwise the highest chemical softness. So, compound **4** was characterized as hole transfer material. The lowest efficiency was seen in compounds **2** and **3**.

References

- 1. B. Nicolas, A. Michaud, M. Leclerc, Adv. Mater. 19(17), 2295 (2007)
- 2. B. Nicolas et al., J. Am. Chem. Soc. 130(2), 732 (2008)
- 3. S. Yamada et al., S Polym. 51(26), 6174 (2010)
- 4. C. Shuttle et al., Proc. Natl. Acad. Sci. 107(38), 16448 (2010)
- 5. R.B. Ross et al., Nat. Mater. 8(3), 208 (2009)
- 6. D. Gebeyehu et al., Synth. Metals 118(1-3), 1 (2001)
- 7. J. Shen et al., Chem. Commun. 48(31), 3686 (2012)
- 8. Y.Y. Choi et al., Sol. Energy Mater. Sol. Cells 96, 281 (2012)
- 9. F. Bonaccorso et al., Nat. Photon. 4(9), 611 (2010)
- 10. S. Pillai et al., J. Fluoresc. 22(4), 1021 (2012)
- 11. S. Eryilmaz et al., Acta Phys. Pol. A **132**(3), 738 (2017)
- 12. M. Frisch et al., Gaussian 09 Rev.C.01 (Gaussian Inc., Wallingford, 2009)
- 13. R. Dennington, T. Keith, J. Millam, *GaussView, version 5.0* (Semichem Inc., Shawnee Mission, 2009)
- 14. S. Di Bella et al., J. Am. Chem. Soc. 119(40), 9550 (1997)
- 15. S. Eryılmaz, Sak. Univ. J. Sci. 22(6), 1638 (2018)
- 16. S. Eryılmaz et al., J. Mol. Struct. 1108, 209 (2016)

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- M. Khimenko, A. VV, G. NN, Mezhdunarodnaya Kniga 39 Dimitrova ul., 113095, Moscow, Russia, p. 2914 (1973)
- 18. A.T.R. Williams, S.A. Winfield, J.N. Miller, Analyst 108(1290), 1067 (1983)
- 19. R.F. Chen, Anal. Lett. 1(1), 35 (1967)
- 20. H. Du et al., Photochem. Photobiol. 68(2), 141 (1998)
- 21. R. Antiochia et al., Electroanal. Int. J. Devot. Fundament. Pract. Asp Electroanal 16(17), 1451 (2004)
- 22. E. Portenkirchner et al., J. Organomet. Chem. 716, 19 (2012)
- 23. M.S. Blois, Nature 181(4617), 1199 (1958)
- 24. E. Pelit, J. Turk. Chem. Soc. Sect. A Chem. 4(2), 631 (2017)
- 25. M. Gul et al., J. Chem. 135, 8525 (2013)
- 26. T.C. Dinis, V.M. Madeira, L.M. Almeida, Arch. Biochem. Biophys. 315(1), 161 (1994)
- 27. T. Ak, İ. Gülçin, Chemico-biological interactions 174(1), 27 (2008)
- 28. G.C. Yen, H.-Y. Chen, J. Agric. Food Chem. 43(1), 27 (1995)
- 29. E.B. Ay et al., Indian journal of pharmaceutical education and research 52(4), 128 (2018)
- 30. R.A. Houghten et al., Nature **354**(6348), 84 (1991)
- 31. S. Eryılmaz et al., J. Mol. Struct. 1122, 219 (2016)
- 32. J.M. Andrew, J. Antimicrob. Chemother. 48(suppl_1), 5 (2001)
- 33. J.M. Tour, Chem. Rev. 96(1), 537 (1996)
- 34. J. Chen et al., J. Org Chem 65(10), 2900 (2000)
- 35. C. Wu et al., Dyes Pigm. 97(2), 273 (2013)
- 36. M. Weng et al., Dyes Pigm. **35**(4), 297 (1997)
- 37. M. Giardinetti et al., New J. Chem. 41(15), 7331 (2017)
- 38. G. Barrow, Physical Chemistry, Chap. 7 (MC Graw-Hill, New York, 1988)
- S.A. Grebenyuk, I.F. Perepichka, A.F. Popov, Spectrochim. Acta Part A Mol. Biomol. Spectrosc. 58(13), 2913 (2002)
- 40. M. Cipolloni et al., ARKIVOC: Online Journal of Organic Chemistry, (2011)
- 41. V. Ramkumar et al., CrystEngComm 15(13), 2438 (2013)
- 42. K.H. Park et al., React. Funct. Polym. 40(2), 169 (1999)
- 43. O.O. Ajani, O.C. Nwinyi, J. Heterocycl. Chem. 47(1), 179 (2010)
- 44. B.P. Bandgar et al., Bioorg. Med. Chem. 17(24), 8168 (2009)
- 45. J. Mai et al., J. Mater. Chem. A 5(23), 11739 (2017)

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