



## Synthesis of Series of Low Band Gap Small Organic Molecules and Evaluation of their Solar Cell Activity

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Organic solar cells have attracted much attention in the recent years but still in search of devices with efficiency comparable to that of silicon solar cells. In this view, a series of highly conjugated imidazolinone molecules were synthesized by a simple *in situ* coupling method, which resulted in high yield (85-95 %) of the products compared to the traditional method of synthesis. UV-visible studies performed in varying solvents differing in polarity, showing shift in their spectra with change in polarity. The band gap calculated thereafter ranged between 2.8-3.1 eV showing their potential for use in photovoltaic cell. Studies of the I-V characteristics of the photovoltaic devices fabricated with the newly synthesized molecules were performed. The devices with naphthalene substituent showed the highest power conversion efficiency of 0.1 % compared to others, thereby opening up room for use in organic solar cells.

**Keywords:** Organic solar cells, Imidazolinone, Band gap, Power conversion efficiency.

### INTRODUCTION

Solar energy has been identified round the globe as an area of significance in providing solutions to the problem of meeting future energy needs. Today the most promising tool to make use of solar energy is its direct conversion into electrical energy in photovoltaic cells. But until now the photovoltaic cell have been dominated by solid state junction devices, often made of silicon. Though the power conversion efficiency of inorganic solar cells has gone up to 44.7 % in lab [1], their high energy consumption at fabrication and cost intensiveness has created a snag to their use in research and development. The limitations of the inorganic solar cells has been challenged by a new generation of photovoltaics based on organic compounds. Organic solar cells with  $\pi$ -conjugated materials as active layer has attracted much attention as a renewable energy source owing to their low energy consumption at fabrication, compatibility with flexible substrates, environment friendly and unlimited variability [2-5].

The recent surge in organic/polymer solar cell research began with the pioneering work by Tang [6] who developed bilayer organic semiconductors with an efficiency of around 1 %. Subsequently, Spanggaard and Krebs devised the first polymer/C60 based cell [7]. But the power conversion efficiency of organic solar cells is only 8.4 % in lab and tandem organic solar cell, 11.5 % thereby opening up room for further research [8,9].

Literature reports reveal that small conjugated molecules like imidazolinones as active layer in device fabrication has proved to be promising. The reason for this positivity is its flexibility to molecular property alteration, bio-degradable ability and user friendliness [10].

We report here the synthesis of nine highly conjugated imidazolinone molecules by a novel method, which resulted in high yield of the products. UV-visible studies were performed in solvents varying in their polarity to find the band gap of the active layer. The devices showed photovoltaic effect when exposed to light and their current-voltage (I-V) characteristics studied. The results showed the potential of these compounds to be used in organic solar cells (OSCs).

### EXPERIMENTAL

**Detection method:** The purity of the compounds was checked by TLC (ethyl acetate/hexane, 1:9). IR spectra of samples (solid powders) were recorded on a Shimadzu IR spectrometer. <sup>1</sup>H and <sup>13</sup>C NMR spectra were obtained on JNM-ECS400 spectrometer with TMS as the internal standard and CDCl<sub>3</sub> as the solvent. Elemental analysis was carried on a EuroEA Elemental Analyser. Melting points were determined on melting point apparatus and are not corrected. UV-visible spectra were recorded on a Double Beam JASCO spectrophotometer in 2 × 10<sup>-5</sup> M methanolic solution.

**General procedure for the preparation of compounds**

**(a-h):** A mixture of oxazolone (1 g, 4.2 mmol), aromatic amine {naphthylamine (0.31 g, 2.2 mmol) or 4-aminoazobenzene (0.45 g, 2.3 mmol)} and ZnCl<sub>2</sub> (0.18 g, 1.3 mmol) in 10 mL THF was refluxed at 80-110 °C for 1 h. TLC (10 % acetone/hexane) check was performed for determining the progress of the reaction. After 1.5 h, anhydrous ZnCl<sub>2</sub> (0.38 g, 2.8 mmol) and aromatic aldehyde {1-naphthaldehyde (0.55 g, 3.5 mmol) and 9-anthraldehyde (0.23 g, 1.1 mmol)} and 10 mL THF was added to the reaction mixture and the reflux continued for another 3 h at 80-110 °C. TLC showed single spot confirming the formation of product. The products were recrystallized with ethyl acetate and hexane.

**5-Benzylidene-3-naphthalen-1-yl-2-(2-naphthalen-1-yl-vinyl)-3,5-dihydro-imidazol-4-one (a):** Yellow powder; Yield 80 %; m.p.: 143-144 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.60 (d, *J* = 16.2 Hz, 1H, =CHAr), 6.55 (d, *J* = 7.8 Hz, 1H, ArH), 6.61 (d, *J* = 16.2 Hz, 1H, =CHAr), 7.16 (d, *J* = 8.0 Hz, 2H, ArH), 7.21 (m, 3H, ArH), 7.28 (d, *J* = 8.4 Hz, 2H, ArH), 7.36 (d, *J* = 8.5 Hz, 1H, ArH), 7.55 (d, *J* = 8.6 Hz, 2H, ArH), 7.60 (s, 1H, =CHAr), 7.66 (m, 4H, ArH), 7.68 (m, 4H, ArH); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 168, 164, 142, 136, 135.5, 134.9, 134.5, 134, 133.4, 132.3, 130.9, 128.5, 128.4, 128, 127.7, 126.2, 126, 125.9, 125.6, 125.4, 124.6, 123.4, 120.7, 118, 112, 109; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3057, 1718, 1688, 1641, 1510, 1405, 771, 799, 691; Anal. calcd. (%) for C<sub>32</sub>H<sub>22</sub>N<sub>2</sub>O: C: 85.31; H, 4.92; N, 6.22; Found: C: 85.28; H, 4.90; N, 6.18.

**2-(2-Anthracen-9-yl-vinyl)-5-benzylidene-3-naphthalen-1-yl-3,5-dihydro-imidazol-4-one (b):** Dark Yellow powder; Yield 85 %; m.p.: 162-163 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.61 (d, *J* = 16.1 Hz, 1H, =CHAr), 6.58 (d, *J* = 8.0 Hz, 1H, ArH), 6.67 (d, *J* = 16.1 Hz, 1H, =CHAr), 7.20 (d, 8.3 Hz, 2H, ArH), 7.30 (d, *J* = 8.5 Hz, 2H, ArH), 7.25 (m, 3H, ArH), 7.65 (s, 1H, =CHAr), 7.66 (m, 4H, ArH), 7.90 (m, 9H, ArH); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 168, 164, 142, 136, 134.9, 134.2, 134, 133.7, 132.3, 131.4, 129.2, 128.4, 128.3, 127.7, 126.2, 125.9, 125.6, 125.3, 125.1, 124.6, 123.4, 120.7, 118.7, 112, 109.4; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3055, 2925, 2856, 1717, 1631, 1518, 1437, 923, 774, 691; Anal. calcd. (%) for C<sub>36</sub>H<sub>24</sub>N<sub>2</sub>O: C: 86.38; H, 4.83; N, 5.60; Found: C: 86.34; H, 4.80; N, 5.58.

**3-Naphthalen-1-yl-5-naphthalen-1-ylmethylene-2-(2-naphthalen-1-yl-vinyl)-3,5-dihydro-imidazol-4-one (c):** Orange crystals; Yield 90 %; m.p.: 154-155 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.65 (d, *J* = 16.4 Hz, 1H, =CHAr), 6.58 (d, *J* = 7.9 Hz, 1H, ArH), 6.68 (d, *J* = 16.4 Hz, 1H, =CHAr), 7.18 (d, 8.0 Hz, 2H, ArH), 7.27 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H, ArH), 7.28 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H, ArH), 7.36 (d, *J* = 8.5 Hz, 1H, ArH), 7.37 (d, *J* = 8.5 Hz, 1H, ArH), 7.55 (d, *J* = 8.6 Hz, 1H, ArH), 7.56 (d, *J* = 8.6 Hz, 1H, ArH), 7.64 (s, 1H, =CHAr), 7.66 (m, 4H, ArH), 7.67 (m, 4H, ArH), 7.69 (m, 4H, ArH); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 168, 164, 142, 136, 135.5, 134.5, 134.2, 133.4, 132.3, 128.5, 128.3, 128, 126.2, 125.9, 125.4, 125.6, 125.4, 124.6, 123.7, 123.4, 120.7, 118.7, 112, 109.4; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3242, 3001, 1699, 1652, 1507, 1437, 774, 694, 605; Anal. calcd. (%) for C<sub>36</sub>H<sub>24</sub>N<sub>2</sub>O: C: 86.38; H, 4.83; N, 5.60; Found: C: 86.35; H, 4.80; N, 5.55.

**2-(2-Anthracen-9-yl-vinyl)-3-naphthalen-1-yl-5-naphthalen-1-ylmethylene-3,5-dihydro-imidazol-4-one (d):**

Orange crystals; Yield 80 %; m.p.: 168-169 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.66 (d, *J* = 16.3 Hz, 1H, =CHAr), 6.58 (d, *J* = 8.0 Hz, 1H, ArH), 6.66 (d, *J* = 16.3 Hz, 1H, =CHAr), 7.19 (d, *J* = 8.2 Hz, 2H, ArH), 7.30 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H, ArH), 7.36 (d, *J* = 8.6 Hz, 1H, ArH), 7.58 (d, *J* = 8.8 Hz, 1H, ArH), 7.64 (s, 1H, =CHAr), 7.66 (m, 4H, ArH), 7.67 (m, 4H, ArH), 7.91 (m, 9H, ArH); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 168, 164, 142, 136, 135.5, 134.2, 134, 133.7, 133.4, 132.3, 131.4, 130.9, 129.2, 128.5, 128.3, 128, 126.2, 125.9, 125.6, 125.4, 125.3, 125.1, 124.6, 123.7, 123.4, 120.7, 118.7, 112, 109.4; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3053, 1716, 1627, 1578, 1405, 918, 776, 734; Anal. calcd. (%) for C<sub>40</sub>H<sub>26</sub>N<sub>2</sub>O: C: 87.25; H, 4.76; N, 5.09; Found: C: 87.21; H, 4.76; N, 5.05.

**4-[1-Naphthalen-1-yl-2-(2-naphthalen-1-yl-vinyl)-5-oxo-1,5-dihydro-imidazol-4-ylidenemethyl]-benzaldehyde (e):** Red Powder; Yield 90 %; m.p.: 160-161 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.65 (d, *J* = 16.4 Hz, 1H, =CHAr), 6.58 (d, *J* = 7.8 Hz, 1H, ArH), 6.68 (d, *J* = 16.4 Hz, 1H, =CHAr), 7.17 (d, *J* = 8.0 Hz, 2H, ArH), 7.27 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H, ArH), 7.36 (d, *J* = 8.5 Hz, 1H, ArH), 7.49 (d, *J* = 8.7 Hz, 2H, ArH), 7.56 (d, *J* = 8.8 Hz, 1H, ArH), 7.63 (s, 1H, =CHAr), 7.67 (m, 4H, ArH), 7.69 (m, 4H, ArH), 7.76 (d, *J* = 8.7 Hz, 2H, ArH), 9.87 (s, 1H, -CHO); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 190, 168, 164, 142, 140.7, 136, 135.9, 135.5, 134.5, 134.2, 133.4, 132.3, 130.9, 129.6, 128.5, 138.3, 128, 126.7, 126.2, 125.9, 125.6, 125.4, 124.6, 124.4, 123.7, 123.4, 120.7, 118.7, 112, 109.4; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3253, 3052, 2920, 1674, 1602, 1501, 1379, 825, 771, 540; Anal. calcd. (%) for C<sub>33</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>: C: 82.83; H, 4.63; N, 5.85; Found: C: 82.80; H, 4.62; N, 5.80.

**4-[2-(2-Anthracen-9-yl-vinyl)-1-naphthalen-1-yl-5-oxo-1,5-dihydro-imidazol-4-ylidenemethyl]-benzaldehyde (f):** Red powder; Yield 80 %; m.p.: 175-176 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.66 (d, *J* = 16.4 Hz, 1H, =CHAr), 6.58 (d, *J* = 8.1 Hz, 1H, ArH), 6.68 (d, *J* = 16.4 Hz, 1H, =CHAr), 7.20 (d, *J* = 8.3 Hz, 2H, ArH), 7.48 (d, *J* = 8.5 Hz, 2H, ArH), 7.64 (s, 1H, =CHAr), 7.67 (m, 4H, ArH), 7.78 (d, *J* = 8.5 Hz, 2H, ArH), 7.92 (m, 9H, ArH), 9.88 (s, 1H, -CHO); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 190, 168, 164, 142, 140.7, 136, 135.9, 134.5, 134.2, 133.7, 132.3, 131.4, 129.6, 129.2, 128.3, 126.7, 126.2, 125.9, 125.6, 125.3, 125.1, 124.6, 123.4, 120.7, 118.7, 109.4; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3255, 3050, 1713, 1674, 1627, 1597, 1501, 1377, 825, 771, 542; Anal. calcd. (%) for C<sub>37</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>: C: 84.07; H, 4.58; N, 5.30; Found: C: 84.05; H, 4.53; N, 5.27.

**4-[2-(2-Naphthalen-1-yl-vinyl)-5-oxo-1-(4-phenylazo-phenyl)-1,5-dihydro-imidazol-4-ylidenemethyl]-benzaldehyde (g):** Red powder; Yield 88 %; m.p.: 150-151 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 5.65 (d, *J* = 16.4 Hz, 1H, =CHAr), 6.68 (d, *J* = 16.4 Hz, 1H, =CHAr), 7.27 (dd, *J* = 8.2 Hz, 1.8 Hz, 1H, ArH), 7.36 (d, *J* = 8.5 Hz, 1H, ArH), 7.46 (m, 3H, ArH), 7.49 (d, *J* = 8.7 Hz, 2H, ArH), 7.55 (d, *J* = 8.6 Hz, 1H, ArH), 7.58 (d, *J* = 8.8 Hz, 1H, ArH), 7.64 (s, 1H, =CHAr), 7.67 (m, 4H, ArH), 7.76 (d, *J* = 9.0 Hz, 2H, ArH), 7.84 (d, *J* = 8.6 Hz, 2H, ArH), 7.91 (d, *J* = 8.6 Hz, 2H, ArH), 7.93 (d, *J* = 8.6 Hz, 2H, ArH), 9.87 (s, 1H, -CHO); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>): δ 190, 168, 164, 152.5, 148.1, 140.7, 136, 135.9, 135.5, 133.4, 132.3, 130.9, 130.7, 129.6, 128.8, 128.5, 128, 126.7, 125.9, 125.6, 125.4, 123.7, 123.4, 122.9, 122.7, 120.7, 112; IR (KBr, *v*<sub>max</sub>, cm<sup>-1</sup>): 3263, 3050, 1671, 1598, 1503, 1380, 828, 768,

694, 544; Anal. calcd. (%) for  $C_{35}H_{24}N_4O_2$ : C: 78.93; H, 4.54; N, 10.52; Found: C: 78.90; H, 4.50; N, 10.48.

**4-[2-(2-Anthracen-9-yl-vinyl)-5-oxo-1-(4-phenylazo-phenyl)-1,5-dihydro-imidazol-4-ylidene-methyl]benzaldehyde (h):** Red powder; Yield 82 %; m.p.: 170-171 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  5.66 (d,  $J = 16.3$  Hz, 1H, =CHAr), 6.66 (d,  $J = 16.3$  Hz, 1H, =CHAr), 7.45 (m, 3H, ArH), 7.47 (d,  $J = 8.6$  Hz, 2H, ArH), 7.65 (s, 1H, =CHAr), 7.76 (d,  $J = 8.8$  Hz, 2H, ArH), 7.83 (d,  $J = 8.5$  Hz, 2H, ArH), 7.90 (d,  $J = 8.5$  Hz, 2H, ArH), 7.92 (d,  $J = 8.4$  Hz, 2H, ArH), 7.94 (m, 9H, ArH), 9.88 (s, 1H, -CHO);  $^{13}C$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  190, 167, 163, 152.5, 148.1, 140.7, 140.4, 136, 135.9, 134.5, 133.7, 132.3, 131.4, 130.7, 129.6, 129.2, 128.8, 128.3, 126.7, 126.2, 125.9, 125.3, 125.1, 122.9, 122.7, 120.7, 112; IR (KBr,  $\nu_{max}$ ,  $cm^{-1}$ ): 3263, 3052, 1674, 1597, 1501, 1379, 976, 828, 767, 697; Anal. calcd. (%) for  $C_{39}H_{26}N_4O_2$ : C: 80.39; H, 4.50; N, 9.62; Found: C: 80.35; H, 4.48; N, 9.60.

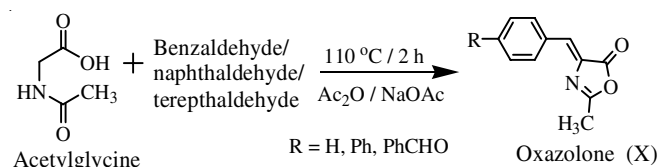
**Procedure for the preparation of compound (i):** 2 M NaOH (1 mL, 1.74 mmol) was added slowly under stirring condition to compound **e** (0.5 g, 1.05 mmol) in 10 mL ethanol. To the reaction mixture acetone (0.2 mL, 3.44 mmol) was added and stirring continued for 45 min. The reaction mixture was cooled in ice-cold water bath followed by filtration. The residue was washed with ice-cold solution of 5 % acetic acid and ethanol and then dried overnight in air. TLC (10 % acetone/hexane) showed single spot confirming the formation of product.

**3-Naphthalen-1-yl-2-(2-naphthalen-1-yl-vinyl)-5-[4-(3-oxo-but-1-enyl)-benzylidene]-3,5-dihydro-imidazol-4-one (i):** Dark yellow; Yield 80 %; m.p.: 190-191 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  2.0 (s, 1H, -OH), 3.03 (d,  $J = 7.5$  Hz, 1H, -CH), 5.04 (t,  $J = 7.1$  Hz, 2H, -CH<sub>2</sub>), 5.65 (d,  $J = 16.4$  Hz, 1H, =CHAr), 6.58 (d,  $J = 7.8$  Hz, 1H, ArH), 6.68 (d,  $J = 16.4$  Hz, 1H, =CHAr), 7.14 (d,  $J = 8.2$  Hz, 2H, ArH), 7.17 (d, 8.0 Hz, 2H, ArH), 7.23 (d,  $J = 8.2$  Hz, 2H, ArH), 7.23 (d,  $J = 8.2$  Hz, 2H, ArH); 7.27 (dd,  $J = 8.2$  Hz, 1.8 Hz, 1H, ArH), 7.36 (d,  $J = 8.5$  Hz, 1H, ArH), 7.44 (m, 3H, ArH), 7.56 (d,  $J = 8.7$  Hz, 1H, ArH), 7.63 (s, 1H, =CHAr), 7.67 (m, 4H, ArH), 7.69 (m, 4H, ArH), 7.89 (d,  $J = 8.4$  Hz, 2H, ArH)  $^{13}C$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  197.6, 169, 160, 142.5, 140.1, 137.4, 136, 135.5, 134.5, 134.2, 133.8, 133.4, 132.9, 132.3, 130.9, 128.6, 128.5, 128.4, 128.3, 128, 127.2, 126.4, 126.2, 125.9, 125.6, 125.4, 124.6, 123.7, 123.4, 120.7, 118.7, 112, 109.4, 69.2, 48.4; IR (KBr,  $\nu_{max}$ ,  $cm^{-1}$ ): 3300, 3229, 3050, 1674, 1597, 1500, 1375, 809, 770, 542; Anal. calcd. (%) for  $C_{41}H_{30}N_2O_3$ : C: 80.39; H, 4.50; N, 9.62; Found: C: 80.35; H, 4.48; N, 9.60.

## RESULTS AND DISCUSSION

**Synthesis:** Design and synthesis of nine highly conjugated molecules in three steps are reported. Firstly, acetyl glycine was prepared by the traditional method [11]. Next oxazolone with three different aldehydes, benzaldehyde, naphthaldehyde

and terephthaldehyde were synthesized in bulk (**Scheme-I**) [11].



**Scheme-I:** Preparation of substituted oxazolone

The third step includes the *in situ* synthesis of the highly conjugated imidazolin-5-one compounds in presence of an inert solvent THF by Lewis acid catalyzed vinylogous condensation [12] (**Scheme-II**).

After the synthesis of eight products by *in situ* method, a fourth step Aldol condensation reaction was performed with compound **e** and acetone as the starting materials in order to introduce further conjugation to **e** (**Scheme-III**). The reason for selecting **e** as the starting material was its high yield compared to the others. The results showed the formation of the aldol product.

UV-visible studies of all the compounds in solution state were performed in a double beam JASCO spectrophotometer. Compound **c** exhibited a  $\lambda_{max}$  value of 439 nm, which provided the lowest band gap value of 2.83 eV compared to all other compounds. The results of UV-visible studies for all the nine compounds in methanol are depicted in Table-1.

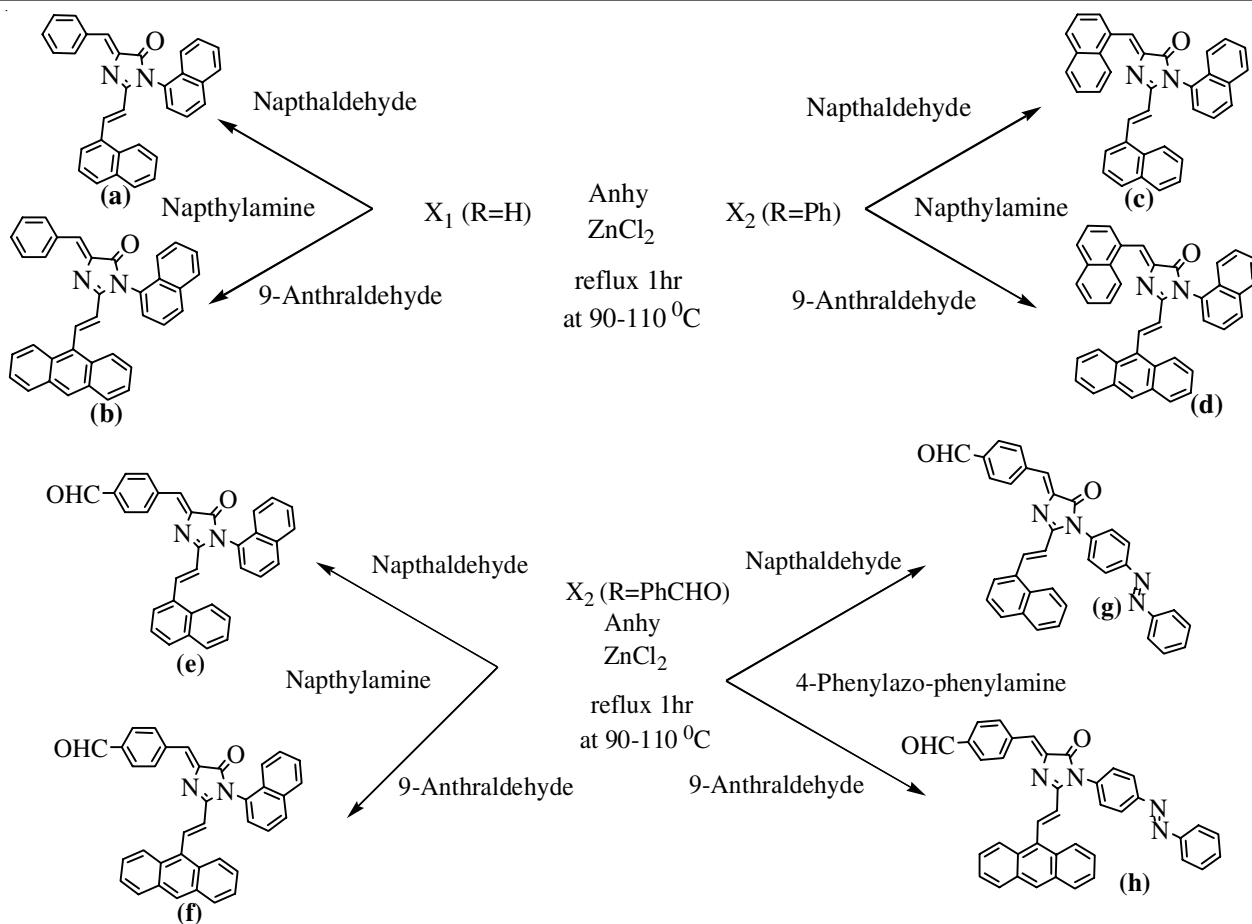
**Device fabrication and electrical characterization:** The photovoltaic devices were fabricated using the formula: ITO (130 nm) || WPTA (90 nm) || PEDOT:PSS (60 nm) || Organic layer (100 nm) || Al (100 nm). The current-voltage (I-V) characteristics of the photovoltaic solar cell were measured using a Keithley model 2420 source meter under day sunlight of 100 mW/cm<sup>2</sup> illumination. The solar illumination was measured by using a lux meter. In this study, the film thickness of the WPTA and PEDOT:PSS layer was controlled by varying the weight percent of their solutions during the spin-coating process while all other experimental conditions, such as rpm (3000 rpm) for 30 s and annealing temperature (115 °C), were fixed. The spin coating rpm of the organic layer was maintained at 1000 rpm for 60 s.

Table-2 shows a comparison of the I-V characteristics of the photovoltaic devices fabricated with nine different organic molecules.

Table-2 showed that the power conversion efficiency of the devices made with the nine molecules are in the order of  $D_c > D_b > D_d > D_h > D_g > D_a > D_e > D_i > D_f$ . The reason for device “Dc” showing the highest power conversion efficiency is because of the highest conjugation of compound “c” compared to all other imidazoline molecules used for devising the organic solar cell devices. The I-V characteristics of the device Dc is shown in Fig. 1.

TABLE-1  
UV-VISIBLE STUDIES OF ALL THE NINE COMPOUNDS SYNTHESIZED

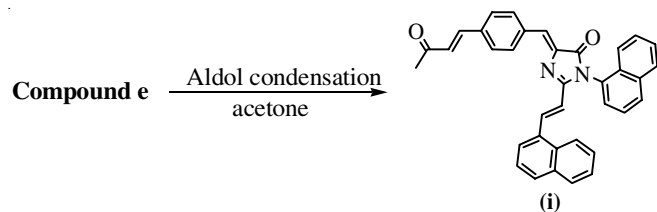
Compounds	a	b	c	d	e	f	g	h	i
$\lambda_{max}$ (nm)	355	430	439	405	330	278	333	344	279
Band gap	3.50	2.96	2.83	3.07	3.76	4.47	3.73	3.61	4.45



**Scheme-II:** Preparation of  $\pi$ -conjugated imidazolinone compounds

TABLE-2  
I-V CHARACTERISTICS OF THE NINE DEVICES

Organic solar cell device	$V_{oc}$ [V]	$J_{sc}$ [ $\text{mA cm}^{-2}$ ]	Fill factor	Power maximum ( $P_{max}$ )	Power conversion efficienc ( $\eta$ , %)
Da	0.25	1.00	0.27	0.07	0.007
Db	1.60	0.98	0.29	0.46	0.050
Dc	3.60	0.90	0.29	0.95	0.100
Dd	0.43	0.94	0.30	0.12	0.010
De	0.15	0.95	0.31	0.04	0.004
Df	0.09	0.95	0.31	0.03	0.003
Dg	0.07	0.92	0.31	0.02	0.002
Dh	0.28	1.00	0.30	0.08	0.008
Di	0.10	0.95	0.31	0.03	0.003



**Scheme-III:** Preparation of the aldol product of e

The bad gap values as observed from Table-1 also satisfies this justification as compound “c” shows the lowest band gap value of all. The WPTA layer in between the ITO and PEDOT: PSS layer could function as a stairway for hole transport in polymer solar cells.

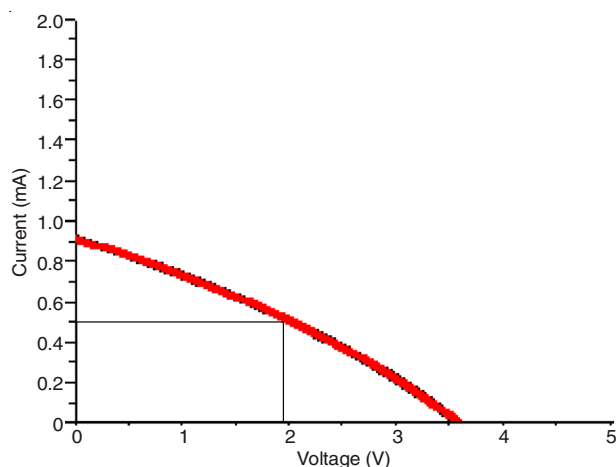


Fig. 1. I-V curve of the device Dc

## Conclusion

The paper describes the synthesis of nine small conjugated molecules with low band gaps by a novel synthetic methodology with high yields of 85-95 %. Photovoltaic devices were fabricated with the newly synthesized organic molecules as active layer and their I-V characterization was performed. The electrical studies showed that of all the nine devices, device Dc showed the highest power conversion efficiency of 0.1 %, thereby, showing potential for use as organic solar cells. The power conversion efficiency of the devices has scope of improvements through modification in the device fabrication techniques mainly the spin coating methods.

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