

# Synthesis and solar-cell applications of novel furanyl-substituted anthracene derivatives



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## ABSTRACT

At present, novel furanyl-substituted anthracene derivatives; namely 9,10-di(furan-2-yl)anthracene (DFA), 5,5'-(anthracene-9,10-diyl)bis(furan-2-carbaldehyde) (DAFA) and 2,2'-((5,5'-(anthracene-9,10-diyl)bis(furan-5,2-diyl))bis(methanylylidene))dimalononitrile (DCNFA) were designed and synthesized successfully by employing Stille Cross-Coupling, Vilsmeier-Haack and Knoevenagel condensation reactions, respectively. This methodology provides a practical new route for the synthesis of furanyl-substituted anthracene derivatives bearing strong electron-withdrawing groups. The electrochemical and electro-optical properties of these novel furanyl-substituted anthracene derivatives were also examined with strong acceptor- $\pi$ -donor- $\pi$ -acceptor interactions. Furthermore, Highest occupied molecular orbital (HOMO), Lowest Unoccupied molecular orbital (LUMO), and band gap (Eg) values were investigated by using spectroscopic methods. Electrochemical and electro-optical properties were calculated and compared to DFA, DAFA and DCNFA. Eg was found as **2.85**, **2.71**, and **2.33** eV, respectively. Consequently, Organic Solar Cells (OSC) were fabricated to investigate their solar cell performances. The strong electron withdrawing groups did not increase the solar cell performance of furanyl-anthracenes. Surprisingly, DFA was found to exhibit the best OSCs performance (Efficiency = 3.36). As a result, one could note that these novel furanyl-substituted anthracene derivatives are good candidate for the applications of the OSCs. Our results might help in the development of new materials with important electrochemical functions by giving the advantage of designing and further derivatization of new generation small organic molecules for photovoltaic device applications.

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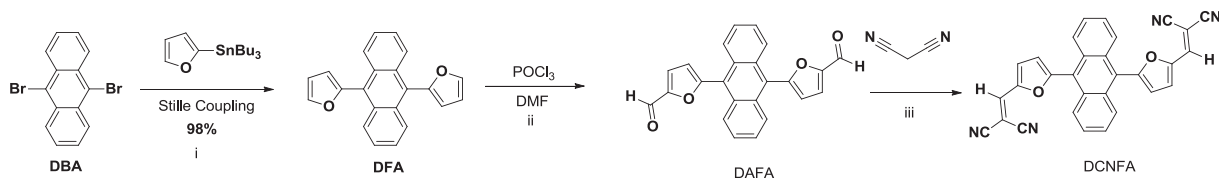
## 1. Introduction

Conjugated organic compounds have very important roles in material science due to their broad range applications [1], such as solar cells [2–4], transistors [5,6], LEDs [4], biosensors [7], sensors [8–10], and electrochromic devices [9,11–13]. Recently, considerable research effort has been focused on developing efficient small-molecule materials for improved device performance because the design and synthesis of efficient electron-transporting materials appear to be more attractive [14–17]. Until now, different structural design strategies have been improved for Organic Solar Cells

(OSC). The acceptor- $\pi$ -donor- $\pi$ -acceptor (A- $\pi$ -D- $\pi$ -A) type structures are the most popular in material science due to their advantages such as; light weight, quite thin (as thin as a paper), flexible, low cost, robust, electrochemically stable [18,19]. Lately, anthracene-based solar cells [20,21], dye sensitized solar cells [22], organic light emitting devices (OLEDs) [23], and organic thin film transistors were reported to have impressive charge carrier mobility and high energy conversion efficiency, ascribed to the crystalline, conjugated, and planar structure of anthracene structure [24–30]. Considering the recent studies, different kind of anthracene-based organic compounds were synthesized by applying various active groups and methodologies [26,31]. In contrast, the furanyl anthracene-based organic compounds have not been studied extensively except a small number of studies including their applications [32–34]. Ho et al. conduct a study to

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**Scheme 1.** (i) Synthesis of 9,10-di(thiophen-2-yl)anthracene **DFA** via Stille Coupling Reaction. (ii) Synthesis of 5,5'-(anthracene-9,10-diyl)bis(furan-2-carbaldehyde) (**DAFA**) via Vilsmeier–Haack Reaction. (iii) Synthesis of 2,2'-((5,5'-(anthracene-9,10-diyl)bis(furan-5,2-diyl))bis(methanylylidene))dimalononitrile (**DCNFA**) via the Knoevenagel condensation reaction.

synthesis 9,10-di(fur-2-yl) anthracene and examine its electro-optical properties by comparing other aromatics such as benzene and naphthalenes [34].

In the present study, novel acceptor-furan-anthracene-furan-acceptor type structures were designed and synthesized for OSCs. Their electrochemical and electro-optical properties were investigated. The HOMO–LUMO energy levels were calculated, and they were fabricated to find the best candidates for future photovoltaic cell applications.

## 2. Experimental

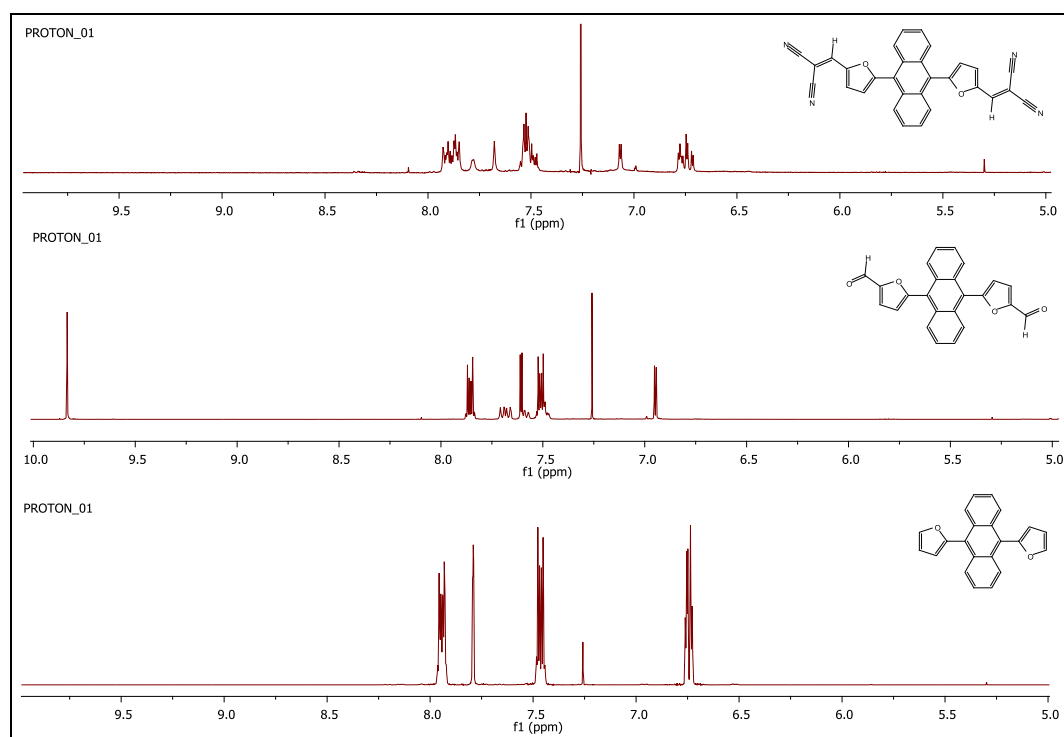
The design, synthesis, and photovoltaic characteristics of new A–D–A type anthracene derivatives containing strong electron withdrawing groups were studied. Synthesized molecules were determined by  $^1\text{H}$  and  $^{13}\text{C}$  NMR.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on an Agilent NMR (400 MHz) spectrometer. Chemical shifts are reported in parts per million (ppm) downfield from an internal TMS (trimethylsilane) reference. Coupling constants (J) are reported in hertz (Hz). In addition, spin multiplicities are presented by the following symbols: s (singlet), s (broad singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). DEPT  $^{13}\text{C}$  NMR information is given in parentheses as C, CH,  $\text{CH}_2$ , and  $\text{CH}_3$ . Flash chromatography was performed using thick-walled glass

columns and ‘flash grade’ silica (Merck 230–400 mesh). Thin layer chromatography (TLC) was performed by using commercially prepared 0.25 mm silica gel plates and visualization was effected with short wavelength UV lamp. The relative proportions of solvents in chromatography solvent mixtures was referred to the volume to volume ratio. Absorption spectra was measured on a Thermo Scientific Multiskan Go UV–VIS spectrophotometer. All commercially available reagents were used directly without purification unless otherwise stated. All the solvents used in reaction experiments were distilled for purity. The inert atmosphere was created by slight positive pressure (ca. 0.1 psi) of argon. All glassware was dried in an oven prior to use. The electrochemical properties were estimated depending on the cyclic voltammetry (CV) measurements, and compared with the ones obtained from UV–VIS measurements.

### 2.1. Synthesis of compounds

#### 2.1.1. Synthesis of 9,10-di(furan-2-yl)anthracene (**DFA**)

To a stirred solution of 9,10-dibromoanthracene (1.5 mmol, 0.5 g) and 2-(tributylstannyl)thiophene (3.7 mmol, 1.32 gr) in Toluene (40 mL) was added tetrakis(triphenylphosphine)palladium(0) ( $\text{Pd}(\text{PPh}_3)_4$ ) (0.058 mmol, 68 mg). Then, the solution was allowed to stir at 110 °C under Argon atmosphere for 24 h. After the



**Fig. 1.** Comparison of  $^1\text{H}$  NMR spectra of **DFA**, **DAFA** and **DCNFA**.

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