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Synthesis of Small Organic Molecule Based on Malononitrile Group toward Green Energy Performance in Organic Photovoltaic Solar Cells †

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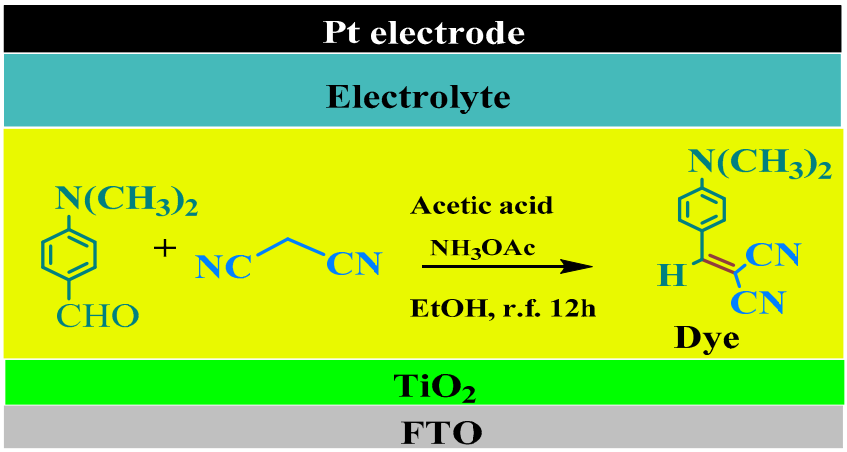
Abstract: In this study, a small organic compound containing cyano and *N*,*N*-dimethyl aniline as acceptor and donor groups, respectively linked through the conjugate system, were synthesized. Then, its structure was confirmed by FT-IR spectroscopy. Next, in order to investigate the photovoltaic properties of these organic molecules, it was tested in the fabrication of organic photovoltaic solar cells (OPVSCs). The organic solar cell with FTO/TiO_2/dye molecules/electrolyte/Pt electrode configuration was constructed.

Keywords: green energy; organic solar cell; cyano acceptor groups; green solar cell

1. Introduction

Energy from fossil fuels is recognized as a source of unrenewable energy [1]. Recently, due to the reduction of unrenewable resources, increased greenhouse gas emissions and environmental pollution, and endangered human health, people have been forced to replace non-renewable energy sources with renewable energy sources [2,3]. The most important devices for converting solar energy into electrical energy are solar cells. The organic photovoltaic solar cells (OPVSCs) are a green class of solar cells.

To attach onto a surface of metal oxide and electron injection from the light absorber to metal oxide layer as well as electrical circuit generation in organic solar cells, dye molecules require at least one or more acceptor groups [4]. Some of the acceptor groups of dye molecules, such as carboxylic acids, cyano acrylic acids, tetracyanate, perylene dicarboxylic acid anhydride, and 2-hydroxybenzonitrile, were reported in the literature [5]. In this study, in connection with our recent work on green protocols [6–10], an organic molecule from OPVSCs was synthesized via the Knoevenagel condensation of benzaldehyde with malononitrile in ethanol (Scheme 1).



Scheme 1. Schematic image of the fabricated organic solar cell and dye molecule.

2. Experimental

2.1. General

All raw materials and solvents required were purchased from Merck and Aldrich. The FT-IR spectrum of the product was taken by Shimadzu IR-470 spectrometer on KBr pellet.

2.2. Synthesis of 2-(4-(dimethylamino) benzylidene)malononitrile

First, 1.1 mmol of 4-(dimethylamino)benzaldehyde, 1 mmol of malononitrile, 0.171 mL of acetic acid and 0.0192 g of ammonium acetate were mixed in toluene. After that, the mixture was heated at 100 °C for 12 h. Finally, the precipitate was washed with water and ethyl acetate.

2.3. Fabrication of Organic Photovoltaic Solar Cell Devices

Initially, the FTO layer was washed separately with ethanol and water for 10 min in an ultrasonic bath. Secondly, the photoanode was coated with titanium dioxide of a specific thickness. Then, it was dried for 30 min at 450 °C. Thirdly, the photoanode electrode was placed in a solution of dye for 24 h to absorb the dye molecules by TiO_2 film. Finally, the cathode (counter electrode) was coated by the carbon layer and placed on the photoanode electrode, and the electrolyte was injected into the space of two electrodes.

3. Results and Discussion

The structure of the synthesized dye molecule was tested by FT-IR spectroscopy. The bands at 3097 and 2990 cm^{-1} were due to the presence of stretching vibrations =C-H and -C-H groups, respectively. Two sharp bands at 2216 and 2289 cm^{-1} were related to CN groups. Also,the C=C band was 1566 cm^{-1}. After fabrication of an organic solar cell, it was tested by simulated sunlight to confirm its efficiency. A summary of the results appears in Table 1.

Table 1. Result of device efficiency for the designed organic photovoltaic solar cells (OPVSCs).

Cell structure	Voc (V)	Jsc ($mA.cm^{-2}$)	FF	Efficiency (%)
FTO/TiO_2/dye/molecules/electrolyte/Pt electrode	0.233	0.029	0.3194	0.002

4. Conclusions

In summary, we have synthesized a small organic molecule based on malononitrile group with D- π -A structure and characterized by FT-IR spectroscopy. Finally, in order to evaluate its

photovoltaic properties, it was tested in OPVSCs. We are continuing to investigate further aspects of this work in our research laboratory.

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