



The effects of second electron acceptor group on the performance of tetrazole-based nanocrystalline TiO₂ sensitizers in DSSCs



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ABSTRACT

Three new organic sensitizers with two electron acceptor groups were synthesized and applied to nanocrystalline TiO₂ solar cells. The ethyl 2-(1*H*-tetrazol-5-yl) acetate, (2*H*-tetrazol-5-yl) acrylonitrile and 1*H*-tetrazole-5-acetic acid moieties were introduced to the triphenylamine as electron acceptor groups. The photophysical, electrochemical and photovoltaic properties of the solar cells based on the synthesized sensitizers were studied and compared with their counterparts of single electron acceptor type. Quantum chemical calculations were also carried out to consideration of the electronic and optical properties of these dyes. The dye with the (2*H*-tetrazol-5-yl) acrylonitrile electron acceptors showed the absorption maxima in the longer wavelength, compared to the dyes with ethyl 2-(1*H*-tetrazol-5-yl) acetate and 1*H*-tetrazole-5-acetic acid. The solar cell based on the dye with 1*H*-tetrazole-5-acetic acid showed the highest conversion efficiency of 3.53% (open circuit voltage = 569 mV, short circuit photocurrent density = 11.50 mA cm⁻², and fill factor of 54% under AM 1.5G conditions). The results also showed that the dyes with two electron acceptor groups gave the higher performance than the dyes with single electron acceptor.

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1. Introduction

Dye sensitized solar cells (DSSCs) discovered by Grätzel in 1991 [1] have attracted considerable attention as a low-cost and high-efficiency alternative to inorganic semiconductor-based photovoltaic devices for the conversion of sunlight into electricity [2]. Anode, cathode, electrolyte, and photosensitive dyes are four main factors that influence the performance of the DSSCs [3]. Upon light absorption by the dye anchored on the TiO₂ surface, the excited electrons are injected into the conduction band of TiO₂, generating an electric current. At the same time, the oxidized dye is regenerated by the electrolyte [4]. Therefore, the sensitizer (dye) is a crucial element, which significantly influences on the power conversion efficiency as well as the stability of the devices [5]. Conventional Ru-based sensitizers such as N3, N719 and the black dyes are investigated widely for DSSCs [6]. However, the scarcity of the Ru(II) metal, lack of good absorption in the red region of the visible spectrum and the difficulty of obtaining purified dyes have limited the practical application of these complexes for DSSCs [7]. Organic dyes, due to their many advantages including lower cost, easier modification and purification, environmental friendliness and high molar extinction coefficient are suitable as sensitizers for DSSCs [8]. Most organic sensitizers contain a dipolar structure with an electron donor (D) and an electron acceptor (A) separated by a π -conjugated bridge (B) [9].

Among the metal-free organic dyes, triphenylamine (TPA) and its derivatives have been investigated widely due to the prominent electron-donating ability and the hole-transport properties of triphenylamine [10–14]. The non-planar configuration of TPA also reduces the aggregation of sensitizer and suppresses charge recombination process of redox couple-TiO₂ system in DSSCs, which can lead to the higher overall conversion efficiencies [15].

Recently, the first triphenylamine-based dye for DSSC with the tetrazole anchoring group has been synthesized by Massin et al. The optoelectronic and photovoltaic properties of the tetrazole-based dye demonstrated the effectiveness of the tetrazole group as a serious alternative anchoring group for organic dyes in DSSCs [16].

We have also reported the triphenylamine-based dyes for DSSCs with the electron acceptor groups based on tetrazole [17] and investigated the modification of these sensitizers by introducing electron donor groups into the TPA moiety. In addition to the electron-donating groups, the introduction of withdrawing groups into the dye structure expands the π -conjugated system of the sensitizing molecules and gives charge-transfer character of absorption and broad and high absorptivity [18]. According to these strategies in molecular design of sensitizers, in this article, the modification of these triphenylamine dyes is reported with the electron acceptor groups based on tetrazole by introducing additional electron acceptors on the phenyl groups of TPA moiety (Fig. 1). The photovoltaic properties of these dyes were measured to identify the effects of additional electron acceptor group on the performance of DSSCs. Density functional theory (DFT) calculations were

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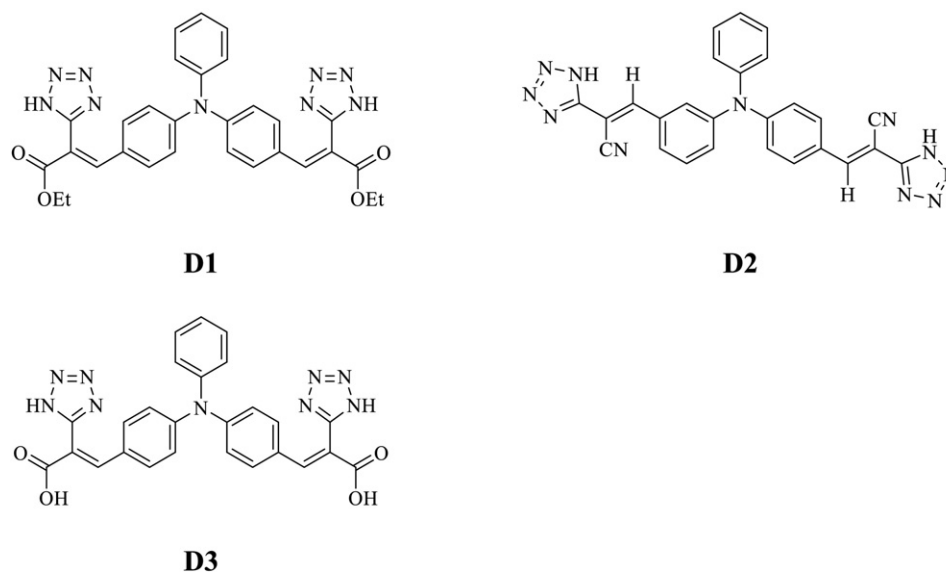


Fig. 1. Structure of the synthesized dyes with two electron acceptors.

also performed for consideration of the electronic structures and the optical properties of the dyes.

2. Materials and Methods

2.1. Materials and Reagents

All used solvents were obtained from Sigma-Aldrich and applied as received. All reagents were commercially available and used without new purification. Ethyl cyanoacetate and triphenylamine were purchased from Merck and used as received without further purification.

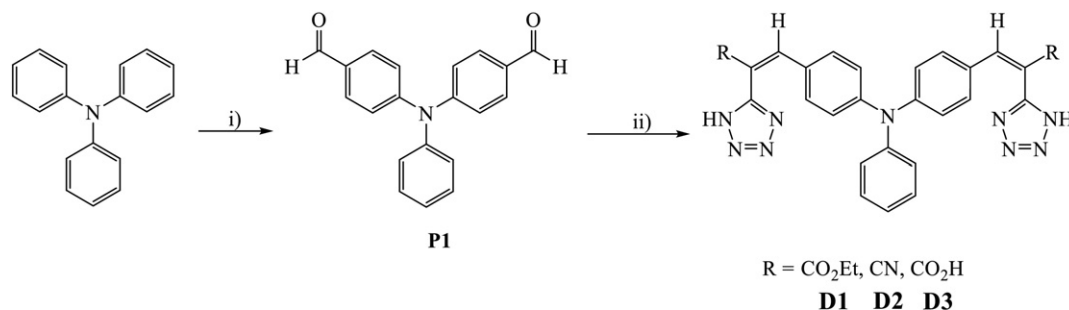
2.2. Analytical Instruments and Measurements

The ^1H and ^{13}C NMR spectra were recorded by means of Bruker 400 MHz spectrometers. FT-IR absorption spectra were taken in KBr pellets using a FT-IR Jasco 680 plus spectrometer. FT-IR spectrum of TiO_2 nanoparticles was subtracted from the spectra of TiO_2 -adsorbed dyes. Mass analysis was performed on a 5973 Network Mass Selective Detector (Agilent Technology (HP)) apparatus. UV-Vis spectra in solution and adsorbed on TiO_2 films were measured with a Jasco-570 UV/Vis spectrophotometer. Cyclic voltammetry data were gained using a SAMA 500 electroanalyser system, SAMA research center, Iran. The three-electrode system (Pt working electrode, Pt counter electrode and an Ag/AgCl reference electrode calibrated with ferrocenium/ferrocene as an internal reference) with 0.1 M tetrabutylammonium hexafluorophosphate as the salt support at a scan rate of 0.1 V/s at room temperature was

used. The precursor compound **P1** and the acceptor groups (Scheme 1) were synthesized according to the literature procedures [19,20].

2.3. Fabrication of Dye-sensitized Solar Cells

Fluorine-doped tin oxide (FTO) coated glass substrates were treated with 40 mM TiCl_4 aqueous solution at 70 °C for 30 min to form a blocking layer. The photoanodes were prepared by doctor blade and titania pastes (Sharif Solar Co.). They are composed of two layers of nanocrystalline TiO_2 particles including a transparent layer, composed of 20 nm TiO_2 particles with thickness of 7 μm and a scattering layer composed of 150–300 nm with thickness of 5 μm . The role of second layer is to enhance the light harvesting and improve the device performance. The TiO_2 -coated FTO films were sintered at 375 °C (10 min), 450 °C (15 min), and 500 °C (30 min). After reaching to environment temperature, the obtained films were again treated with 40 mM TiCl_4 aqueous solution at 70 °C for 30 min, washed with distilled water and heated at 500 °C for 30 min. Then, the TiO_2 electrodes were immersed into the dye solutions (0.4 mM in $\text{C}_2\text{H}_5\text{OH}$) for 20 h in the dark before washing. The counter electrode was prepared using FTO glass coated with a drop of solution of H_2PtCl_6 and then allowed to stand at 500 °C for 30 min. Two electrodes were assembled into a sandwich type cell with an iodine-based liquid electrolyte. The active area of each prepared DSSC was 0.25 cm^2 . Solar cells were illuminated by AM 1.5G solar simulator (Sharif Solar, SIM-1000) to give 100 mW/cm^2 at the surface of the cell. The photocurrent-voltage (I-V) measurements were performed using a Bio-Logic SAS model SP-300. The action spectra of monochromatic incident photon-to-current conversion efficiencies (IPCEs) for the solar



Scheme 1. Synthesis paths for the dyes **D1-D3**: (i) POCl_3 , DMF, 80 °C, 48 h, (ii) Ethyl 2-(1H-tetrazol-5-yl) acetate, (2H-tetrazol-5-yl) acrylonitrile, or 1H-tetrazole-5-acetic acid, $\text{NH}(\text{Et})_2$, CH_3CN , reflux, 48 h.

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