



Influence of different electron acceptors in organic sensitizers on the performance of dye-sensitized solar cells



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ABSTRACT

Five kinds of triphenylamine-based organic dyes with different electron acceptors were designed and synthesized as sensitizers for dye-sensitized solar cells (DSSCs). The photophysical and electrochemical properties of these dyes were investigated and their performance as sensitizers in DSSCs was measured. The dye with cyanoacrylic acid electron acceptor exhibits the highest solar-to-electrical energy conversion efficiency of 4.93% (short-circuit photocurrent density $J_{sc} = 8.59 \text{ mA cm}^{-2}$, open-circuit photovoltage $V_{oc} = 0.77 \text{ V}$, and fill factor $ff = 0.75$) under 100 mW cm^{-2} -simulated AM 1.5 G solar irradiation.

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1. Introduction

Dye-sensitized solar cells (DSSCs) based on mesoporous nano-crystalline TiO_2 films have attracted significant attention because of their high efficiency, low cost, and facile fabrication [1–3]. The sensitizer is one of the key components in these cells for high power-conversion efficiency. DSSCs based on Ru(II) -polypyridyl complex photosensitizers, such as N3, N719, and black dye, have achieved remarkable conversion efficiencies of 10%–11% under AM 1.5 irradiation conditions [4,5]. However, the main drawbacks of Ru(II) complex sensitizers are the cost of the Ru metal, tedious purification processes, and environmentally related problems. Attention has recently focused on metal-free organic sensitizers because they present many advantages, such as high molar extinction coefficients, simple synthetic procedures, and environment friendliness [6–9].

A common organic dye for DSSCs contains an electron donor/acceptor (D–A) structure linked through a π -conjugated bridge, also called the D– π –A molecular structure [10]. Over the last decade, studies on D– π –A molecular structures have focused on donor groups, such as triphenylamine [6,11–14], coumarin [15–17], indoline [18–22], and carbazole [23–27], as well as on π -conjugated

bridges, including benzene [28–34], thiophene [35–39], thienothiophene [40–44], dithienothiophene [45–47], benzo [b]thiophene [48,49], and benzothiadiazole [50–53]. Despite the progress made in scholarly research, the influence of different electron acceptors on the D– π –A molecular structure is rarely reported [54]. In these organic dyes, cyanoacrylic acid is commonly introduced into the D– π –A system as an electron acceptor. Nevertheless, the rationale behind the frequent use of cyanoacrylic acid as an acceptor is unclear.

In the current study, five types of triphenylamine-based organic dyes **TPC**, **TPCC**, **TPEC**, **TPS**, and **TPNO** (molecular structures are shown in Fig. 1) with different electron acceptors were designed and synthesized as sensitizers for DSSCs. The electron acceptors used are 2-cyanoacrylic acid, malonic acid, 3-ethoxy-3-oxopropanoic acid, cyanomethanesulfonic acid, and 3-(hydroxylimino)propanenitrile. The photophysical, electrochemical, and photovoltaic properties of the dyes were also investigated.

2. Experimental section

2.1. General analytical measurements

All chemicals were used from commercial sources without further purification. Solvents for chemical synthesis such as dichloromethane (CH_2Cl_2), *N,N*-dimethylformamide (DMF), toluene, and tetrahydrofuran (THF) were purified by distillation. ^1H

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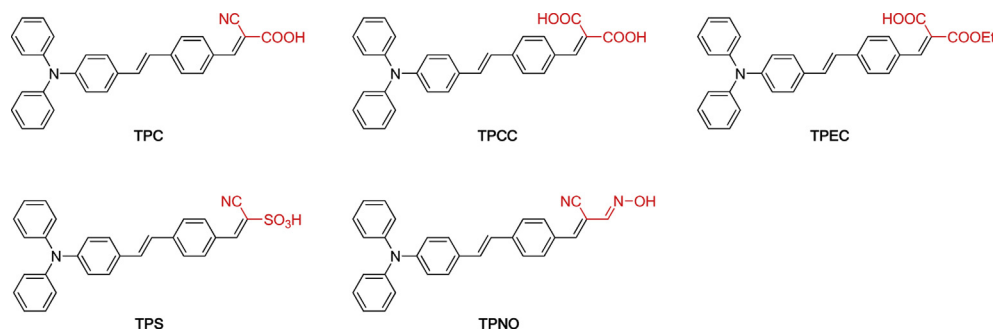


Fig. 1. Molecular structures of **TPC**, **TPCC**, **TPEC**, **TPS**, and **TPNO** dyes.

and ^{13}C NMR spectra were recorded on either a Varian Inova-400 spectrometer (400 MHz for ^1H , 100 MHz for ^{13}C) or a Bruker Avance II-400 spectrometer (400 MHz for ^1H , 100 MHz for ^{13}C); CDCl_3 and TMS were used as a solvent and an internal standard, respectively. High resolution mass spectra were recorded on either a Q-TOF mass spectrometry or a GC-TOF mass spectrometry.

2.2. Theoretical calculations

Gaussian 03 package was used for density functional theory (DFT) calculation [55]. The geometries and energies of dyes **TPC**, **TPCC**, **TPEC**, **TPS**, and **TPNO** were determined using the B3LYP method with the 6-31G (d) basis set.

2.3. Synthesis

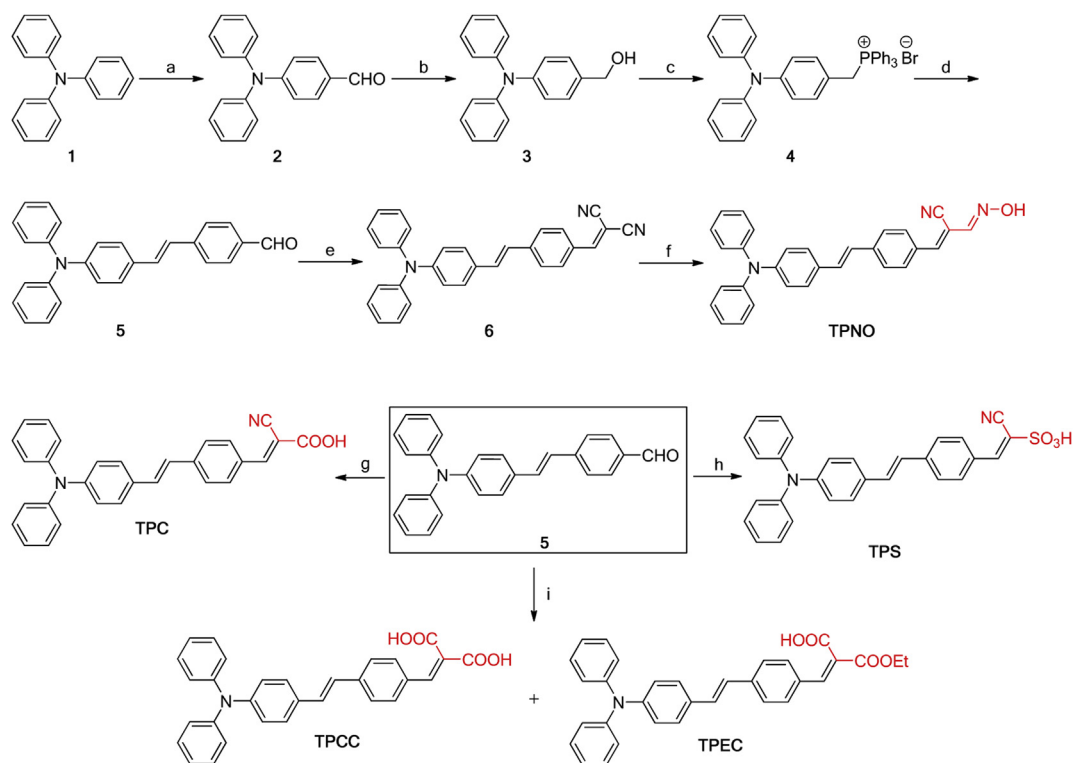
The synthetic routes of **TPC**, **TPCC**, **TPEC**, **TPS**, and **TPNO** dyes are shown in Scheme 1.

2.3.1. 4-(Diphenylamino)benzaldehyde (**2**) [46]

To a solution of triphenylamine (3.0 g, 12.2 mmol) in DMF (40 mL) was added POCl_3 (2.4 mL, 25.0 mmol) dropwise within 15 min. After stirring for 20 h at 95–100 °C under a nitrogen atmosphere, the mixture was then cooled to room temperature, poured into ice water, and neutralized with an aqueous NaOH. The solvent was removed by filtration, and the residue was purified via silica gel column chromatography (eluent: ethyl acetate/petroleum ether = 1:5) to afford the desired product **2** (3.0 g, 91%), mp 130–132 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.81 (s, 1H), 7.68 (d, $J = 8.8$ Hz, 2H), 7.36–7.32 (m, 4H), 7.19–7.15 (m, 6H), 7.02 (d, $J = 8.8$ Hz, 2H).

2.3.2. 4-(Diphenylamino)phenyl)methanol (**3**) [46]

To a solution of NaBH_4 (80 mg, 2.1 mmol) in CH_2Cl_2 (15 mL)/ethanol (5 mL) was added 4-(diphenylamino)benzaldehyde (0.546 g, 2.0 mmol), and the mixture was stirred at room temperature for 2 h. The reaction mixture was poured into water (25 mL) and vigorously stirred for 30 min. The solvent was removed under



Scheme 1. Synthesis of dyes **TPC**, **TPCC**, **TPEC**, **TPS**, and **TPNO**: a) phosphorus oxychloride, triethylamine, DMF, N_2 , 100 °C, 20 h b) sodium borohydride, CH_2Cl_2 , rt, 2 h c) triphenyl phosphorus hydrobromide, CHCl_3 , reflux, 2 h d) *p*-phthalaldehyde, potassium *tert*-butoxide, THF, N_2 , 0 °C, 8 h e) malononitrile, piperidine, EtOH, reflux, 2 h f) diisobutyl aluminum hydride, toluene, –7 °C, 50 min; hydroxylamine hydrochloride, triethylamine, EtOH, rt, 2 h g) 2-cyanoacetic acid, piperidine, CH_3CN , reflux, 2 h h) tetrabutylammonium bromide, sodium cyanomethanesulfonate, piperidine, CH_3CN , reflux, 20 h i) diethyl malonate, piperidine, benzene, reflux, 15 h; sodium hydroxide, THF, 50 °C, 15 h.

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