



Structural engineering of dipolar organic dyes with an electron-deficient diphenylquinoxaline moiety for efficient dye-sensitized solar cells



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ARTICLE INFO

Article history:

Received 7 February 2014

Accepted 27 February 2014

Available online 6 March 2014

Keywords:

Dye-sensitized solar cells

Organic dyes

Diphenylquinoxaline

ABSTRACT

A series of new organic dyes containing an electron-deficient diphenylquinoxaline moiety was synthesized and employed as the photosensitizers in dye-sensitized solar cells (DSSCs). The multiple phenyl rings in the peripheral positions of the dye structure provide a hydrophobic barrier to slow down the charge recombination. The photophysical and electrochemical properties of these dyes were investigated in detail. The cell performance and the associated photophysical and electrochemical properties can be easily tuned by the modification of the aromatic fragments within the π spacer. Dye **CR204**-based DSSC reached the best energy conversion efficiency of 6.49% with an open-circuit voltage of 666 mV, a short-circuit photocurrent density of 14.9 mA cm⁻², and a fill factor of 0.66. The IPCE of **CR204**-based DSSC covers the light-harvesting to NIR region.

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1. Introduction

A dye-sensitized solar cell (DSSC) is a thin film device, which can take the solar energy from the nature, usually comprising a platinum film on the transparent conductive oxide glass (TCO), an electrolyte layer, and a light-harvesting dye anchored onto titanium dioxide on a conductive glass.¹ Each of the parts in the DSSC is important and plays a key role toward a high power conversion ability. In the last decade, the design of organic dyes for DSSCs especially attracts great attentions from chemists aiming to provide an alternative energy source other than fossil fuel.² The dyes for the DSSCs were usually divided into two kinds due to the difference of dye species. The DSSCs based on metal-containing dyes, like ruthenium dyes and porphyrin dyes, often reached a higher efficiency than those based on metal-free dyes.³ However, the high cost of precious metal and the tedious and low-yield synthesis of porphyrin dyes have been a big obstacle for mass production of DSSCs based on these two classes of dyes. On the other hand, metal-free organic dyes have a great capacity for structural engineering to achieve light-harvesting from 500 to 800 nm and strong light absorption ability compared to metal-containing dyes and relatively straightforward synthetic procedures than porphyrin dyes.⁴

Indeed, the development of DSSCs based on metal-free dyes has witnessed a rapid advance in recent years with power conversion efficiencies reaching 10% or higher.⁵

In general, the organic dye is made of a D- π -A system containing an electron donor (D), a π -conjugated spacer (π) with various length, and an electron acceptor (A) behaving as the anchoring group as well.⁶ Another similar design of organic dyes in a D-A₁- π -A system usually possesses the light absorption in a wide range due to the decrease of the band gap and is capable of facilitating strong intramolecular charge transfer (ICT).⁷ Many electron-deficient moiety have been used as the A₁ fragment including quinoxaline,⁸ benzothiadiazole,⁹ diketopyrrolopyrrole,¹⁰ benzotriazole,¹¹ rhodanylidene,¹² boradiazaindacene,¹³ and squaraine.¹⁴ Previously, we have reported the DSSC studies based on a dipolar organic dye **CR147** containing an electron-deficient diphenylquinoxaline moiety in the structure.¹⁵ Not only did the DSSC with dye **CR147** as the photosensitizer yielded cell efficiency more than 7% under conventional liquid electrolyte condition, it was further optimized in conjunction with an ionic liquid electrolyte to produce a high open-circuit voltage over 0.8 V and an excellent conversion efficiency of 8.12%.¹⁶ In order to further improve the photovoltaic performance and meaningful structure-performance correlations based on the prototype structure of dye **CR147**, we structurally engineered dye **CR147** and prepared four new organic dyes in a D-A₁- π -A architecture

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to rationalize their structure–performance relationships (Fig. 1). The four new organic sensitizers are all imparted with an electron-deficient diphenylquinoxaline moiety in the π -conjugated framework along with various aromatic fragments in the π spacer to link the diarylamine donor and the cyanoacrylic acid acceptor.

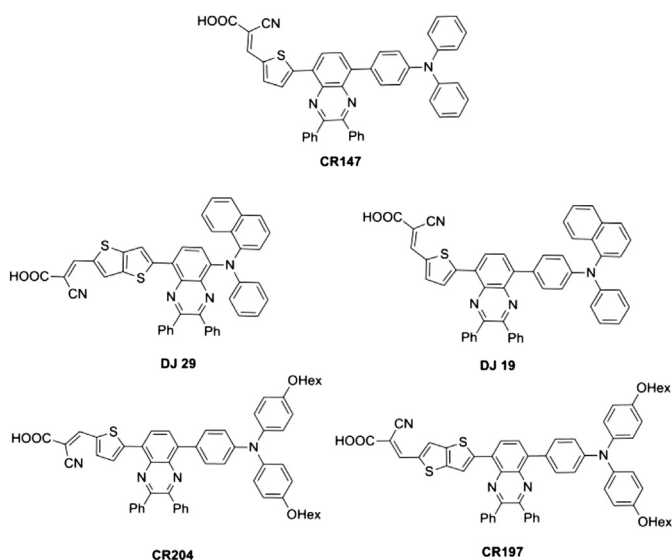


Fig. 1. Dyes with an electron-deficient diphenylquinoxaline moiety for DSSCs.

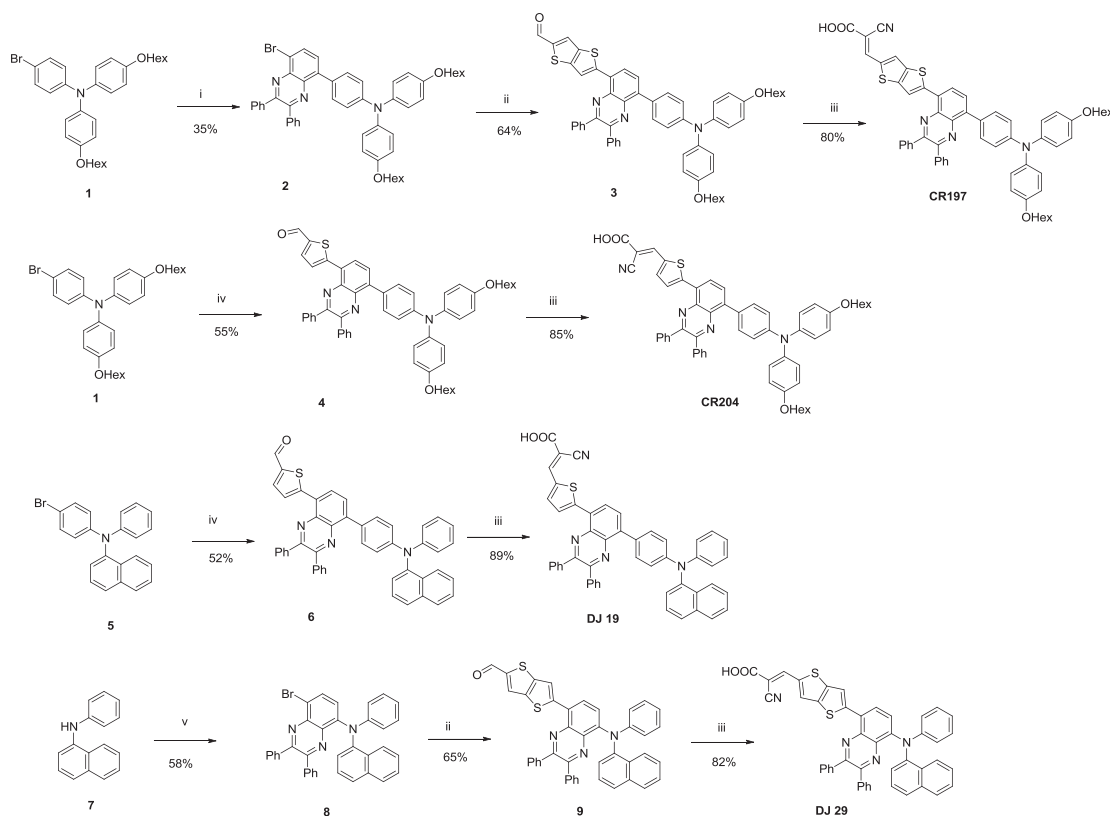
2. Results and discussion

2.1. Synthesis

The synthetic strategies of the new organic dyes were depicted in Scheme 1. Dye DJ29 was synthesized from compound 7 through a series of palladium(II) catalyzed Buchwald–Hartwig amination and Suzuki–Miyaura coupling reaction with arylboronic acid to compound 9 followed by the Knoevenagel condensation reaction. The sensitizer CR197 was prepared from compound 1 via a borylation using *n*-butyllithium and excess B(OMe)₃ in tetrahydrofuran (THF), the successive Suzuki–Miyaura coupling reactions with 5,8-dibromo-2,3-diphenylquinoxaline and then 5-formylthiophene [3,2-*b*]thiophen-2-ylboronic acid, and a final condensation reaction. CR204 and DJ19 were obtained from 1 and 5, respectively, by borylation, Suzuki–Miyaura coupling, and condensation reaction. All new organic dyes have been fully characterized by NMR spectroscopy, UV–vis, cyclic voltammetry, and high-resolution mass spectrometry.

2.2. Photophysical and electrochemical properties

The UV–vis absorption spectra measured in dimethylformamide (DMF) are shown in Fig. 2(a) and the photophysical data are summarized in Table 1. The absorption spectra are generally constituted of two bands. The absorption band in the near UV region is assigned to the π – π^* transition while the other band between 425 and 600 nm is due to the ICT transition. The ICT bands of the dyes reach the region from 550 to 600 nm and the λ_{max} fall in a range from 457 to 503 nm. The absorption spectral coverage follows the



Scheme 1. Synthetic procedures for organic dyes. Reagents and conditions: (i) (a) *n*-BuLi, B(OMe)₃, –78 °C–rt, 5 h; (b) 5,8-dibromo-2,3-diphenylquinoxaline, PdCl₂(PPh₃)₂, Na₂CO₃, H₂O/THF (2:1), rt, 12 h, (ii) arylboronic acid, PdCl₂(PPh₃)₂, Na₂CO₃, H₂O/THF (2:1), rt, 12 h, (iii) 2-cyanoacetic acid, CH₃COOH, NH₄OAc, toluene, reflux, 4 h, (iv) (a) *n*-BuLi, THF, B(OMe)₃, –78 °C–rt, 5 h; (b) Pd(PPh₃)₂Cl₂, Na₂CO₃, 5-(5-bromo-2,3-diphenylquinoxalin-8-yl)thiophene-2-carbaldehyde, THF/H₂O (2:1), rt, 12 h, (v) Pd(OAc)₂, NaO^tBu, dppf, toluene, reflux, 24 h.

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