



Iridium dimer complex for dye sensitized solar cells using electrolyte combinations with different ionic liquids

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ABSTRACT

In this paper, we report the synthesis and characterization of a new cyclometallated iridium complex, [tetrakis(2,2'-bipyridine-4,4'-dicarboxylic acid)(μ -dichloro)diiridium(III)] chloride complex, [(dcbpy)₂Ir(μ -Cl)]₂Cl₄. Four different ionic liquids are also synthesized and characterized for electrolyte combinations. Photovoltaic performance of dye sensitized solar cells have been studied by using four different ionic liquids. The dye sensitized nanocrystalline TiO₂ solar cell (DSSC) based on the iridium complex using triethyleneglycol-bis(3-methylimidazolium)diiodide [K36-TFSI] as ionic liquid in electrolyte showed the best photovoltaic performance with a maximum short-circuit photocurrent density (J_{sc}) of 4.45 mA cm⁻², an open circuit photovoltage (V_{oc}) of 550 mV, and a fill factor (FF) of 0.60, corresponding to an overall conversion efficiency of 1.47% under AM 1.5 sun light.

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1. Introduction

Dye sensitized solar cells (DSSCs) have attracted considerable attention because of their low costs and easy fabrication processes for the conversion of sunlight into electricity [1,2]. The most efficient devices have been achieved with Ruthenium(II) polypyridine complexes comprising carboxyl anchoring groups on nanocrystalline TiO₂ surfaces, whose lowest energy excited states are metal to ligand charge transfer (MLCT) states [3–5]. Heteroleptic ruthenium dyes are studied in the literature because of their high efficiencies [6–9]. Recently, the synthesis of other transition-metal dye complexes for DSSC sensitizers has received much attention. Iridium complexes have particular interest because of their higher thermal and chemical stability compared to ruthenium

complexes, longer excited state lifetimes, comparable quantum yields for conversion of absorbed photons to current [10], large color tunability so iridium complexes are potentially good candidates for application in DSSCs. Moreover, in DSSCs containing a Ru complex as sensitizer, the current production is based only on injection from metal to ligand charge transfer (MLCT) whereas it is possible to incorporate injection both from MLCT and ligand to ligand charge transfer (LLCT) for the iridium complexes [10,11]. The photophysical and photochemical properties of the iridium complexes have been widely investigated in last decades to understand the energy electron transfer processes. Despite the potential benefits, there are critical factors to limit the efficiency of the iridium complexes such as low molar extinction coefficient and a narrow absorption spectrum. However, there is an exciting challenge to increase the molar extinction coefficient of iridium complexes and to improve the light harvesting properties. Because, iridium complexes are just a newly developed dye family in dye sensitized solar cells. Large d-orbitals splitting to high MC states, likely to render

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the molecule more stable compared to ruthenium complexes, may be very advantageous for long term stability problem [12].

Here we report the synthesis and characterization of a new iridium complex, [tetrakis(2,2'-bipyridine-4,4'-dicarboxylic acid)(μ -dichloro)diiridium(III)] chloride complex, $[(dcbpy)_2Ir(\mu-Cl)]_2Cl_4$. In addition we report the absorption–emission spectra and cyclic voltammetry studies. We report the performances according to different electrolyte combinations using different ionic liquids. We try to improve the conversion efficiency of the iridium complex using different ionic liquids in electrolyte combinations. The best performance is obtained the dichloro-bridged iridium dimer complex based DSSC using K36-TFSI ionic liquid in electrolyte combination with the overall conversion efficiency (η) of 1.47, short circuit current density (J_{sc}) of 4.45 mA cm^{-2} , open circuit voltage (V_{oc}) of 550 mV and filling factor (FF) of 0.60. Fig. 1 shows the molecular structure of iridium complex and schematic representation of iridium sensitized TiO_2 electrode.

2. Experimental

All materials are reagent grade and are used as received unless otherwise noted.

2.1. Materials

All chemicals are purchased from commercial sources, and used as received. All organic solvents used are of high

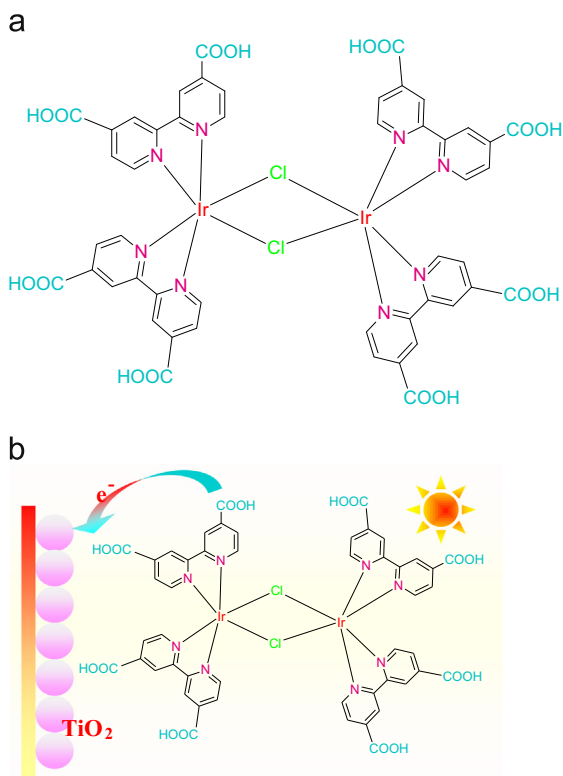
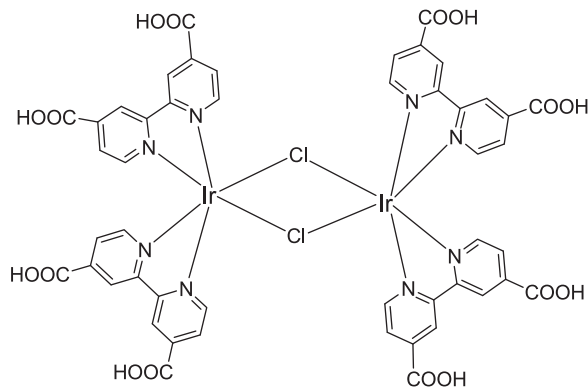


Fig. 1. Structure of iridium complex.

quality from Fluka and J.T. Baker. 1,2-Bis-(2-iodoethoxy) ethane, 1-methylimidazole, bis(trifluoromethane)sulfonamide lithium salt, iridium(III) chloride hydrate and 2,2'-Bipyridine-4,4'-dicarboxylic acid (dcbpy) are purchased from Aldrich. 1,8-Diiodooctane is purchased from Fluka. Ionic liquids were synthesized according to slightly modified procedure reported in the literature [13].

2.2. Characterization

The UV–vis absorption spectra of synthesized dyes are recorded in a 1 cm path length quartz cell by using Analytic JENA S 600. The infrared (IR) spectra are obtained by using Perkin-Elmer, FT-IR/MIR-FIR (ATR) spectrophotometer. 1H -NMR spectra are measured on a Bruker 400 MHz spectrometer. Cyclic voltammetry measurements of synthesized dye are taken by using CH-Instrument 660 B Model Potentiostat equipment. Dye sensitized solar cells are characterized by current–voltage (J – V) measurement. All current–voltage (J – V) are done under 100 mW cm^{-2} light intensity and AM 1.5 conditions. 450 W Xenon light source (Oriel) is used to give an irradiance of various intensities. J – V data collection is made by using Keithley 2400 Source-Meter and LabView data acquisition software.



2.3. Synthesis of the complex and ionic liquids

2.3.1. Synthesis of [tetrakis(2,2'-bipyridine-4,4'-dicarboxylic acid)(μ -dichloro)diiridium(III)] chloride complex, $[(dcbpy)_2Ir(\mu-Cl)]_2Cl_4$

2,2'-Bipyridine-4,4'-dicarboxylic acid (dcbpy) (0.9 mmol, 0.22 g) is added to a mixture of iridium chloride trihydrate (0.40 mmol, 0.14 g) in a DMF:ethylene glycol:water (2:1:2) solution. The reaction vessel is heated under reflux (120 °C) with constant stirring for 24 h. After cooling to room temperature, the reaction mixture is filtered, and the solvent is removed under vacuum. The remaining solid is dissolved in water and filtered again. The product is precipitated by adding acetone. It is collected by filtration and washed with diethyl ether, then dried under vacuum. 418 mg, 73% yield. Anal. Calc. For $C_{48}H_{32}N_8O_{16}Cl_6Ir_2$: C, 36.63; H, 2.05; N, 7.12. Found: C, 36.59; H, 2.01; N, 7.09%. FT-IR (ATR, cm^{-1}): 3382, 3067, 2780, 2454, 1716, 1635, 1544, 1467, 1361, 1232. 1H NMR (D_2O) δ ppm: 9.02–8.56

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