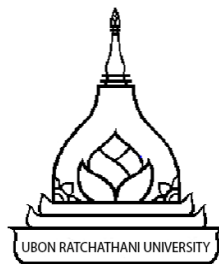


**DEVELOPMENT OF DYE SENSITIZED SOLAR CELLS  
FROM RUTHENIUM(II) COMPLEXES**

**PREEYAPAT PROMPAN**

**A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS  
FOR THE DEGREE OF MASTER OF SCIENCE  
MAJOR IN CHEMISTRY  
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Preeyapat Prompan  
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## บทคัดย่อ

เรื่อง : การพัฒนาเซลล์พลังงานแสงอาทิตย์ชนิดสีย้อมไวแสงจากสารประกอบเชิงซ้อนของโลหะรูทีเนียม(II)  
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 คำสำคัญ : เซลล์แสงอาทิตย์ชนิดสีย้อมไวแสง, สารประกอบเชิงซ้อนของโลหะรูทีเนียม(II), สีย้อมร่วม, สารประกอบเชิงซ้อนของโลหะรูทีเนียมชนิดไม่มีลิแกนด์ไทโอไซยาเนต

งานวิจัยนี้ได้รายงานการสังเคราะห์สารประกอบเชิงซ้อนของโลหะรูทีเนียม(II) 2 ชุด สารเป้าหมายทั้งหมดได้พิสูจน์เอกลักษณ์ทางโครงสร้าง ศึกษาสมบัติทางแสง สมบัติทางเคมีไฟฟ้า และการเป็นสีย้อมในเซลล์พลังงานแสงอาทิตย์ชนิดสีย้อมไวแสง ระบบอิเล็กทรอนิกส์ ไอโอดีน/ไตรไอโอดีน ภายใต้ความเข้มแสงมาตรฐานที่ AM 1.5 ความเข้มแสงเท่ากับ  $100 \text{ mW/cm}^2$

ชุดที่ 1 สีย้อมร่วม ได้แก่ **P2+N719** และ **YN07+N719** ซึ่ง **P2** คือ 2-phenyl-5-(trifluoromethyl)pyrido bis (2,2'-bipyridine-4,4'-dicarboxylic acid)ruthenium(II) hexafluorophosphate และ **YN07** คือ cis [bis(thiocyanato) bis (2,2'-biquinoline-4,4'-dicarboxylic acid (4-carboxy-2,2'-bipyridine-4'-caboxylate)ruthenium(II)] tetrabutylammonium พบว่าสีย้อมร่วมให้ประสิทธิภาพเป็น 2.37% และ 1.59% เมื่อเทียบกับ **P2** (1.42%), **YN07** (0.46%) และ **N719** (5.17%)

ชุดที่ 2 สีย้อมชนิดไม่มีลิแกนด์ไทโอไซยาเนต เป็น  $[\text{Ru}(\text{dcbpy})_2(\text{ppy})]\text{PF}_6$ : (**PP1**),  $[\text{Ru}(\text{dcbpy})_2(\text{PL1})]\text{PF}_6$ : (**PP2**),  $[\text{Ru}(\text{dcbpy})_2(\text{PL2})]\text{PF}_6$ : (**PP3**) และ  $[\text{Ru}(\text{dcbpy})_2(\text{PL3})]\text{PF}_6$ : (**PP5**) โดยที่ dcbpy คือ 2,2'-bipyridine-4,4'-dicarboxylic acid, **ppy** คือ 2-phenylpyridine, **PL1** คือ 2-phenylpyridine-3-(pyridin-2-yl)benzoate, **PL2** คือ methyl-2-phenylisonicotinate และ **PL3** คือ methyl-2-(3-(methoxycarbonyl)phenyl)isonicotinate จากการศึกษพบว่าให้ประสิทธิภาพเท่ากับ 3.10%, 0.69%, 1.54% และ 1.53% ตามลำดับ เทียบกับ **N719** (7.44%)

## ABSTRACT

TITLE : DEVELOPMENT OF DYE-SENSITIZED SOLAR CELLS FROM RUTHENIUM(II) COMPLEXES

AUTHOR : PREEYAPAT PROMPAN

DEGREE : MASTER OF SCIENCE

MAJOR : CHEMISTRY

ADVISOR : ASST. PROF. RUKKIAT JITCHATI, Ph.D

KEYWORDS : DYE-SENSITIZED SOLAR CELL (DSSC), RUTHENIUM(II) COMPLEX, CO-SENSITIZATION, THIOCYANATE FREE RUTHENIUM(II) COMPLEX

This thesis reported the synthesis of TWO series of ruthenium(II) complexes of which the physical, photophysical, and electrochemical properties of the target complexes were studied. The materials were studied by dye-sensitized solar cell (DSSCs) with iodide/tri-iodide electrolyte under standard AM 1.5 (100 mW/cm<sup>2</sup>). In the first part, the co-sensitized dyes, specifically **P2+N719** and **YN07+N719** (**P2** was 2-phenyl-5-(trifluoromethyl)pyrido) bis (2,2'-bipyridine-4,4'-dicarboxylic acid)ruthenium(II) hexafluorophosphate and **YN07** was cis [bis(thiocyanato) bis (2,2'-biquinoline-4,4'-dicarboxylic acid(4-carboxy-2,2'-bipyridine-4'-carboxylate)ruthenium(II)] tetrabutyl-ammonium). It was found that the co-dyes showed photovoltaic efficiencies of 2.37% and 1.59% compared with pure dyes **P2** (1.42%), **YN07** (0.46%), and **N719** (5.17%). In the second part, the thiocyanate free ruthenium(II) complexes were coded as [Ru(dcbpy)<sub>2</sub>(**ppy**)]PF<sub>6</sub>: (**PP1**), [Ru(dcbpy)<sub>2</sub>(**PL1**)]PF<sub>6</sub>: (**PP2**), [Ru(dcbpy)<sub>2</sub>(**PL2**)]PF<sub>6</sub>: (**PP3**), and [Ru(dcbpy)<sub>2</sub>(**PL3**)]PF<sub>6</sub>: (**PP5**) (dcbpy was 2,2'-bipyridine-4,4'-dicarboxylic acid, **ppy** was 2-phenylpyridine, **PL1** was 2-phenylpyridine-3-(pyridin-2-yl)benzoate, **PL2** was methyl-2-phenylisonicotinate, and **PL3** was methyl-2-(3-(methoxycarbonyl)-phenyl)isonicotinate. It was found that DSSCs showed photovoltaic efficiencies at 3.10%, 0.69%, 1.54%, and 1.53% respectively, compared with **N719** (7.44%).

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**LIST OF ABBREVIATIONS**

<b>ABBREVIATION</b>	<b>DEFINITION</b>
A	Ampere
Ag/AgCl	Silver/ Silver chloride (reference electrode)
AR.	Analysis reagent
Aq.	Aqueous
AM	Air mass
anh.	Anhydrous
ATR	Attenuated total reflectance
conc.	Concentrated
cm <sup>-1</sup>	Reciprocal centimeter (unit of wavenumber)
<sup>13</sup> C NMR	Carbon nuclear magnetic resonance
°C	Degree Celsius
CB	Conduction band
cm	Centimeter
cm <sup>3</sup>	Centimeter cubic unit
CV	Cyclic voltammetry
d	Doublet (for NMR spectral data)
dcbpy	2,2'-Bipyridine-4,4'-dicarboxylic acid
dFppyCF <sub>3</sub>	2-(2,4-Difluorophenyl)-5-trifluoromethylpyridine
dd	Double of doublet (for NMR spectral data)
DCM	Dichloromethane
dcbiq	4,4'-Dicarboxy-2,2' -biquinoline
DFT	Density functional theory
DI	Deionized Water
DMF	Dimethylformamide
DMSO	Dimethyl sulfoxide
DSSCs	Dye-Sensitized Solar Cells
E	Energy

**LIST OF ABBREVIATIONS (CONTINUED)**

<b>ABBREVIATION</b>	<b>DEFINITION</b>
$E_g$	Energy gap
$E_{ap}$	Anodic peak potentials
$E_{cp}$	Cathodic peak potentials
eV	Electron volt
$E_{ox}$	Oxidation potential
$E_{ox, onset}$	Onset oxidation potential
$E_{red}$	Reduction potential
$E_{red, onset}$	Onset reduction potential
ESI-MS	Electrospray ionization mass spectrometry
EtOAc	Ethyl acetate
Fc/Fc <sup>+</sup>	Ferrocene/Ferrocenium
FF	Fill factor
FTIR	Fourier transform infrared spectroscopy
FTO	Fluoride doped tin oxide
HOMO	Highest occupied molecular orbital
Hz	Hertz
$I_0$	The energy of incident sunlight (100 mW/cm <sup>2</sup> )
IPCE	Incident Photon to Current Conversion Efficiency
IR	Infrared
$J$	Coupling constant (for NMR spectral data)
$J_{max}$	Maximum current
$J_{sc}$	Short circuit current density
$J_{ph}$	The short circuit photocurrent density generated by mono chromatic light
L	Liter
LUMO	Lowest unoccupied molecular orbital
M	Molarity



**LIST OF ABBREVIATIONS (CONTINUED)**

<b>ABBREVIATION</b>	<b>DEFINITION</b>
m	Multiplet (for NMR spectral data)
m <sup>2</sup>	Square meter
MHz	Mega hertz
ml	Milliliter
MLCT	Metal to ligand charge transfer
mM	Millimolar
mmol	Millimol
mV	Millivolt
MW	Molecular weight
Red	Reduction
S	The ground state
S*	The excited state
S <sup>+</sup>	The oxidized dye
s	Singlet (for NMR spectral data)
s	Second
TBAOH	Tetra butyl ammonium hydroxide
TCO	Transparent conducting oxides
TDDFT	Time-dependent density functional theory
TLC	Thin layer chromatography
TMS	Tetra methylsilane
t	Triplet (for NMR spectral data)
UV-Vis	Ultra violet-visible
V	Voltage
v/v	Volume/volume
V <sub>max</sub>	Maximum voltage
V <sub>OC</sub>	Open circuit voltage
W	Watt

**LIST OF ABBREVIATIONS (CONTINUED)**

<b>ABBREVIATION</b>	<b>DEFINITION</b>
$\delta$	Chemical shift (for NMR spectral data)
$\eta$	The power conversion efficiency
$\mu\text{A}$	Microampere
$\mu\text{m}$	Micrometer
$\mu\text{W}$	Microwatt
$\alpha$	Alpha
$\Omega$	Ohm (Unit of electrical resistance)
$p$	Para-substitution
$\varepsilon$	Molar extinction coefficient
$\lambda$	Wavelength
$\pi$	Pi-orbital
$\Delta$	Delta
%	Percent