

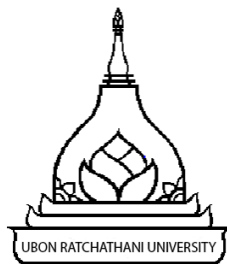


**A NOVEL OF NEW CHARGE IRIIDIUM COMPLEXES FOR
ORGANIC LIGHT-EMITTING DIODE
AND SENSOR APPLICATIONS**

KATTALIYA MOTHAJIT

**A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF MASTER OF SCIENCE
MAJOR IN CHEMISTRY
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MASTER OF SCIENCE
MAJOR IN CHEMISTRY FACULTY OF SCIENCE

TITLE A NOVEL OF NEW CHARGE IRIIDIUM COMPLEXES FOR ORGANIC
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Kattaliya Mothajit
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บทคัดย่อ

เรื่อง : สารเชิงซ้อนของโลหะอิริเดียมมีประจุชนิดใหม่เพื่อประยุกต์ใช้เป็นไดโอดเรืองอินทรีย์และตัวตรวจวัด

ผู้วิจัย : แคทลียา โนมทะจิตร

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คำสำคัญ : สารเชิงซ้อนของโลหะอิริเดียม (III), ไดโอดเรืองแสงอินทรีย์ (OLEDs), ตัวตรวจวัด

งานวิจัยนี้ได้รายงานการสังเคราะห์สารประกอบเชิงซ้อนของโลหะอิริเดียม (III) ที่มีประจุ 2 ชุด สารเชิงซ้อนเป้าหมายทั้งหมดได้พิสูจน์เอกลักษณ์ทางโครงสร้าง ศึกษาสมบัติทางแสงและสมบัติทางเคมีไฟฟ้า

ชุดที่ 1 ใช้เป็นไดโอดเรืองแสงอินทรีย์ (OLEDs) ได้แก่ $[\text{Ir}(\text{spiro})(\text{ppy})_2]\text{PF}_6$ (**KM01**), $[\text{Ir}(\text{spiro})(\text{thio})_2]\text{PF}_6$ (**KM02**), $[\text{Ir}(\text{spiro})(\text{difluoro})_2]\text{PF}_6$ (**KM03**) และ $[\text{Ir}(\text{spiro})(\text{ppz})_2]\text{PF}_6$ (**KM04**) โดยที่ spiro คือ 4,5-diaza-9,9'-spirobifluorene, ppy คือ 2-phenylpyridine, thio คือ 2-thiophenylpyridine, difluoro คือ 2',4'-difluorophenyl pyridine และ ppz คือ 2',4'-difluorophenyl 1H-pyrazole นำ **KM01-KM04** ไปขึ้นรูปเป็นอุปกรณ์ OLEDs โครงสร้างเป็น ITO/PEDOT:PSS/**KM01-KM04**:BMIMPF₆ (1:1 by mole)/TPBi/LiF/Al พบว่า **KM01** ให้ประสิทธิภาพทางไฟฟ้า (current efficiency) สูงสุดที่ 1.72 cd/A และความสว่างสูงสุด 2,027 cd/m²

ชุดที่ 2 ใช้เป็นตัวตรวจวัด n-butylamine ทางสี (colorimetric sensor) ได้แก่ $[\text{Ir}(\text{L1})(\text{ppy})_2]\text{PF}_6$ (**NU02**) และ $[\text{Ir}(\text{L2})(\text{ppy})_2]\text{PF}_6$ (**KM09**) โดยที่ **L1** คือ dimethyl-2,2'-bipyridine-3,3'-dicarboxylate และ **L2** คือ dimethyl-2,2'-bipyridine-4,4'-dicarboxylate จากศึกษาการเปลี่ยนแปลงสีของสารละลายเชิงซ้อนของโลหะอิริเดียม พบว่าเปลี่ยนจากสีแดง (528 นาโนเมตร) เป็นสีส้ม (450 นาโนเมตร) ในสภาวะกรด HCl (100 equiv.) และ n-butylamine (3 equiv.) หลังจากทำปฏิกิริยา 120 นาที

ABSTRACT

TITLE : A NOVEL OF NEW CHARGE Iridium COMPLEXES FOR ORGANIC LIGHT- EMITTING DIODE AND SENSOR APPLICATIONS

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DEGREE : MASTER OF SCIENCE

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KEYWORDS : Iridium (III) COMPLEX, LIGHT EMITTING DIODE (OLEDs) SENSOR

This study reported the synthesis of two charge iridium (III) complex series. All of the target complexes were characterized and studied their photophysical and electrochemical properties. In the first series, the complexes used for organic light-emitting diode (OLEDs) were [Ir(spiro)(ppy)₂]PF₆ (**KM01**), [Ir(spiro)(thio)₂]PF₆ (**KM02**), [Ir(spiro)(difluoro)₂]PF₆ (**KM03**), and [Ir(spiro)(ppz)₂]PF₆ (**KM04**) (spiro was 4,5-diaza-9,9'-spirobifluorene, ppy was 2-phenylpyridine, thio was 2-thiophenylpyridine, difluoro was 2',4'-difluorophenylpyridine, and ppz was 2',4'-difluorophenyl *1H*-pyrazole). Then, **KM01-KM04** were fabricated for OLED devices based on ITO/PEDOT:PSS/**KM01-KM04**:BMIMPF₆ (1:1 by mole)/TPBi/LiF/Al. It was found that **KM01** showed maximum current efficiency at 1.72 cd/A and brightness at 2,027 cd/m². In the second series, the complexes used for colorimetric n-butylamine sensor were [Ir(**L1**)(ppy)₂]PF₆ (**NU02**) and [Ir(**L2**)(ppy)₂]PF₆ (**KM09**) (**L1** was dimethyl-2,2'-bipyridine-3,3'-dicarboxylate and **L2** was dimethyl-2,2'-bipyridine-4,4'-dicarboxylate). It was found that the color of charge iridium(III) complex changed from red (528 nm) to orange (450 nm) in condition HCl (100 equiv.) and n-butylamine (3 equiv.) after 120 minutes of reaction.

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LIST OF ABBREVIATIONS

ABBREVIATION	FULL WORD
A	Absorbance
AR.	Analysis reagent
anh.	Anhydrous
Aq.	Aqueous
B	Brightness
^{13}C NMR	Carbon nuclear magnetic resonance
cm	Centimeter
cm^{-1}	Reciprocal centimeter (unit of wavenumber)
cm^3	Centimeter cubic unit
δ	Chemical shift in ppm relative to tetramethylsilane
CIE	Commission Internationale de L'Eclairage or International Commission on Illumination
conc.	Concentrated
<i>J</i>	Coupling constant (for NMR spectral data)
CE	Current efficiency (cd/A)
CV	Cyclic voltammetry
$^{\circ}\text{C}$	Degree Celsius
DI	Deionized Water
DFT	Density functional theory
DCM	Dichloromethane
DMSO	Dimethyl sulfoxide
d	Doublet (for NMR spectral data)
dd	Double of doublet (for NMR spectral data)
ETL	Electron transport layer
eV	Electron volt
ESI-MS	Electrospray ionization mass spectrometry
EML	Emitting layer

LIST OF ABBREVIATIONS (CONTINUED)

ABBREVIATION	FULL WORD
Eg	Energy gap
EtOAc	Ethyl acetate
EQE	External Quantum Efficiency
FTIR	Fourier transform infrared spectroscopy
Hz	Hertz
HOMO	Highest occupied molecular orbital
HTL	Hole transport layer
h	Hour
ITO	Indium-tin-oxide
LUMO	Lowest unoccupied molecular orbital
IR	Infrared
MS	Mass spectroscopy
MHz	Mega hertz
MLCT	Metal to ligand charge transfer
mmol	Milimole
mA	Milli ampere
ml	Milliliter
mmol	Milimole
mV	Millivolt
Min	Minutes
ϵ	Molar absorptivity
M	Molarity
Mw	Molecular weight
Mol	Moles
m	Multiplet (for NMR spectral data)
nm	Nanometers
NMR	Nuclear magnetic resonance

LIST OF ABBREVIATIONS (CONTINUED)

ABBREVIATION	FULL WORD
Ω	Ohm
OLED	Organic light-emitting diode
E_{ox}	Oxidation potential
ppm	Parts per million
ppy	Phenylpyridine
PL	Photoluminescence
PE	Power efficiency (lm/W)
E_{red}	Reduction potential
Rt	Room temperature
s	Singlet (for NMR spectral data)
m^2	Square meter
TMS	Tetra methylsilane
t	Triplet (for NMR spectral data)
UV-Vis	Ultra violet-visible
V	Voltage
v/v	Volume/volume