Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Key Role of Ancillary Ligand in Imparting Blue Shift in Electroluminescence Wavelength in Ruthenium Polypyridyl Light-Emitting Diodes

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Table S1.

The wavelength of electroluminescence (EL) and photoluminescence (PL) emissions of reported ruthenium complexes.

Complex/reactant	λ_{em} (nm)	λ_{EL} (nm)	ref
$Ru(bpy)_3^{2+}$	608	608	1,2,3
$Ru(bpy)_3^{2+}/C_2O_4^{2-}$	610	610	4
$Ru(bpy)_3^{2+}/C_2O_4^{2-}$		591	5
$Ru(bpy)_3^{2+}/S_2O_8^{2-}$	625	625	4,6
$Ru(bpy)_3^{2+}$ /TPrA	610	610	7
$Ru(dmbp)_3^{2+}$ /$C_2O_4^{2-}$		594	5
$Ru(phen)_3^{2+}$	590	590	8
$Ru(phen)_3^{2+}/C_2O_4^{2-}$		585	5
$Ru(dmphen)_3^{2+}/C_2O_4^{2-}$		591	5
$Ru(terpy)_3^{2+}$		660	8
$Ru(bpz)_3^{2+}$	585	585	9,10
$Ru(bpz)_3^{2+}/S_2O_8^{2-}$	585	590	11
$Ru(dp\text{-}bpy)_3^{2+}$	635	635	12

$Ru(dp\text{-}phen)_3^{2+}$	615	615	12
$(bpy)_2Ru(bphb)^{2+}$	624	624	13
$(bpy)_2Ru(bphb)^{2+}$ /TPrA	624	624	13
$(bpy)_2Ru(bphb)^{2+}/S_2O_8^{2-}$	624	624	13
$[(bpy)_2Ru]_2(bphb)^{4+}$	624	624	13
$[(bpy)_2Ru]_2(bphb)^{4+}$/TPrA	624	624	13
$[(bpy)_2Ru]_2(bphb)^{4+}/S_2O_8^{2-}$	624	624	13
$(bpy)_2Ru(AZA\text{-}bpy)^{2+}$/TPrA	603	603	14
$(bpy)_2Ru(AZA\text{-}bpy)^{2+}$/TPrA	613	613	14
$(bpy)_2Ru(CE\text{-}bpy)^{2+}$/TPrA		650	15
$(bpy)_2Ru(CE\text{-}bpy)^{2+}$/TPrA		655	15
$Ru(v\text{-}bpy)_3^{2+}$	630	650	16
$(bpy)_2Ru(DC\text{-}bpy)^{2+}$	629	629	17
$(bpy)_2Ru(DM\text{-}bpy)^{2+}$	605	605	17
$(bpy)_2Ru(dpen\text{-}bpy)^{2+}$ /PF_6^-	612	612	18

$Ru(m\text{-}bpy)_3^{2+}/PF_6^-$	609	612	18
$Ru(dtb\text{-}bpy)_3^{2+}/PF_6^-$	610	611	18
$(bpy)_2Ru(DIM)^{2+}$	600	600	19
$(bpy)_2Ru(PBIm\text{-}H)^{2+}/PF_6^-$		680	20
$[Ru(tpy)(tpy\text{-}COOEt)]/PF_6^-$	706	706	21
$Ru(DM\text{-}bpy)_3^{2+}$	604	615	22
$(bpy)_2Ru(dbeb)^{2+}/PF_6^-$	642	640	23
$(bpy)_2Ru(pbq)^{2+}$	900	900	24
$(PBIm\text{-}H)_2Ru(pbq)^{2+}$	945	945	24
$(PBIm\text{-}H)_2Ru(acac)^{2+}$	850	880	24
$[Ru(PBIM\text{-}H)_2]_2(pbq)^{+2}$	1040	1040	24
$Ru(tpy)(trz)^{2+}/PF_6^-$	723	717	25
$Ru(tpy\text{-}COOEt)(trz)^{2+}/PF_6^-$	717	725	25
$(bpy)_2Ru(Mt\text{-}bpy)^{2+}/PF_6^-$	625	557	26

RuTRu	625	598	26
$(bpy)_2Ru(aa\text{-}bpy)^{2+}$ /PF_6^-	649	699	27
Ru_2 $(bpy)_4$ (im-phen) / ClO_4^-	638	655	28
$(bpy)_2Ru(Eh\text{-}bpy)^{2+}$ /PF_6^-	427	600	29
$(bpy)_2Ru(Hmh\text{-}bpy)^{2+}$ /PF_6^-	427	600	29
(H2MPy3,4DMPP)Ru(bpy)2Cl /PF_6^-	655	656	30
$Ru_2(bpy)_2(tpy)_2(BTB)^{2+}$	680	710	31
$Ru_2(bpy)_2(tpy)_2(4\text{-}TBN)^{3+}$	676	680	31
$[Ru(bpy)_2]_2(bmpa\text{-}bpy)^{+2}$/ PF_6^-	642	596	32
$[Ru(bpy)_2]_2(bmdpa\text{-}bpy)^{+2}$/ PF_6^-	638	570	32
$[Ru(bpy)_2]_2(bmna\text{-}bpy)^{+2}$/ PF_6^-	636	570	32

m-bpy = 4-methyl-2,2′-bipyridine

dtb-bpy = 4,4′-di-tert-butyl-2,2′-bipyridine

dpen-bpy = 4,4′-di-n-pentyl-2,2′-bipyridine

DIM = 4,7-dimethyl-1,10-phenanthroline

PBIm-H =2-(2-pyridyl)-1H-benzoimidazole

tpy= 2,2′,6′,2″-terpyridine

tpy-COOEt = 2,2′,6′,2″, terpyridine-4′-carboxylic acid ethyl ester

DM-bpy = 4,4′-dimethyl-2,2′- bipyridine

dbeb= 4,4′-dibutyl ester-2,2′-bipyridine

pbq=2,3-bis(2-pyridyl)benzoquinoxaline

acac=acetylacetone

trz= 2-phenyl-4,6-dipyridin-2-yl-1,3,5-triazine

RuTRu = bis-2,2′-bipyridyl-ruthenium-bis-[2-((E)-4′-methyl-2,2′-bipyridinyl-4)-ethenyl]-thienyl-bis-2,2′-bipyridyl-ruthenium tetra hexafluorophosphate

Mt-bpy =4-methyl-4′-(2-thienylethenyl)-2,2′-bipyridine

aa-bpy= Acrylic acid 4′-acryloyloxymethyl-2,2′-bipyridinyl-4-ylmethyl ester

im-phen =1,2-bis(4-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenoxy)ethane

Eh-bpy =4,4′-bis(3-ethylheptyl)-2,2′-bipyridine

Hmh-bpy =4-dihexylmethyl-4′-heptyl-2,2′-bipyridine

H2MPy3,4DMPP = meso-tris-3,4-dimethoxyphenyl-mono-(4-pyridyl)porphyrin

4-TBN = 4-(1H-tetrazol-5-yl)benzonitrile

BTB = bis(1H-tetrazol-5-yl)benzene

bpy = 2,2′-bipyridine

$C_2\ O_4^{2-}$ = oxalate ion

$S_2\ O_8^{2-}$ = persulfate or peroxydisulfate

TPrA = tri-n-propylamine

dmbp = 4,4′-Me2bpy and DM-bpy = 4,4′-dimethyl-2,2′-bipyridine

phen = 1,10-phenanthroline

terpy = 2,2′,2″-terpyridine

bpz =2,2′-bipyrazine

dp-bpy = 4,4′-biphenyl-2,2′-bipyridyl

dp-phen =4,7-diphenyl-1,10-phenanthroline

dmphen = 4,7-dimethyl-1,10-phenanthroline

bphb = 1,4-bis(4′-methyl-2,2′-bipyridin-4-yl)benzene

AZA-bpy = 4-(N-aza-18-crown-6-methyl-2,2′-bipyridine

CE-bpy= bipyridine ligand where a crown ether (15-crown 5) is bound to the bpy ligand in the 3- and 3′-positions

v-bpy =4-vinyl-4′-methyl-2,2′-bipyridine

DC-bpy = 4,4′-dicarboxy-2,2′-bipyridine

PF_6^- =hexafluorophosphate

bmpa-bpy =bis(4′-methyl-2,2′-bipyridinyl-4-carbonyl)-(1,4-phenylediamine)

bmdpa-bpy =bis(4′-methyl-2,2′-bipyridinyl-4-carbonyl)-(1,4-diphenylediamine)

bmna-bpy =bis(4′-methyl-2,2′-bipyridinyl-4-carbonyl)-(1,4-naphthalenediamine)

Table S2. Absorption and emission properties of Ru(dpq) derivates.

Compound	**Absorption: λ_{max},nm(logε)**	**Emission: λ_{em}, nm (ϕ_{em})**	**Reference**
$[Ru(dpp)_3]^{2+}$	455 (1.54)		33
$[Ru(dpq)_3]^{2+}$	500 (1.51)	716	33
$[Ru(phen)_2(dpp)]^{2+}$	465 (1.06)	652	33
$[Ru(bpy)_2(dpp)]^{2+}$	464 (1.15)	660	33
$[Ru(phen)_2(dpq)]^{2+}$	516 (1.10)	756	33
$[Ru(bpy)_2(dpq)]^{2+}$	517 (0.84)	760	33
$[Ru(bpy)_2(tpphz)]^{2+}$	449 (1.72)	628 (0.100)	34
$[Ru(bpy)_2(dppx)]^{2+}$	446 (2.27)	623 (0.088)	34
$[Ru(bpy)_2(dppm2)]^{2+}$	447 (2.28)	630 (0.090)	34
$[Ru(bpy)_2(dppp2)]^{2+}$	441 (2.28)	745 (<0.005)	34
$[Ru(bpy)_2(dppz)]^{2+}$	445 (1.63)	631 (0.083)	35
$[Ru(bpy)_2(dpqp)]^{2+}$	457	618 (0.76)	35
$[Ru(phen)_2(dicnq)]^{2+}$	445 (4.33)	613 (0.012)	36
$[Ru(phen)(dicnq)_2]^{2+}$	441 (4.31)	610 (0.004)	36
$[Ru(bpy)_2(dicnq)]^{2+}$	439 (1.75)	640 (0.0055)	37
$[Ru(bpy)_2(dppzc)]^{2+}$	448 (1.95)	630 (0.009)	37

$[Ru(bpy)(dppzc)_2]^{2+}$	431 (2.51)		37
$[Ru(phen)_2(dppzc)]^{2+}$	431 (2.43)		37
$[Ru(bpy)_2(dpqOHCOOH)]^{2+}$	455 (1.78)	620 (0.068)	37
$[Ru(bpy)_2(dpq(OH)_2)]^{2+}$	453 (1.56)	627 (0.087)	37
$[Ru(phen)_2(dppz)]^{2+}$	439(2.23)	618	38
$[Ru(phen)_2(dppx)]^{2+}$	440(2.1)	610	38
$[Ru(phen)_2(dppm2)]^{2+}$	441(2.25)	615	38
$[Ru(phen)_2(dppa)]^{2+}$	438(2.34)	612	38
$[Ru(phen)_2(dppb)]^{2+}$	439(2.14)	660	38
$[Ru(phen)_2(dppp2)]^{2+}$	439(2.12)	620	38
$[Ru(phen)_2(dppp3)]^{2+}$	439(2.11)	616	38
$[Ru(phen)_2(dppn)]^{2+}$	443(2.56)	606	38

Dpp 2,3-bis(2'-pyridyl)pyrazine)

dpq Dipyrido[3,2-*f*:2',3-h]quinoxaline

tpphzTetrapyrido[3,2-a:2',3'-c:3",2"-h:2,3"'-j]phenazine

dppx 11,12-Dimethyl-dipyrido[3,2-a:2',3'-c]phenazine

dppm 10-Dimethyl-dipyrido[3,2-a:2',3'-c]phenazine

dppp Pyrido[2',3':5,6]pyrazino[2,3-*ff*][1,10]phenanthroline

dppz Dipyrido[3,2-a:2',3'-c]phenazine

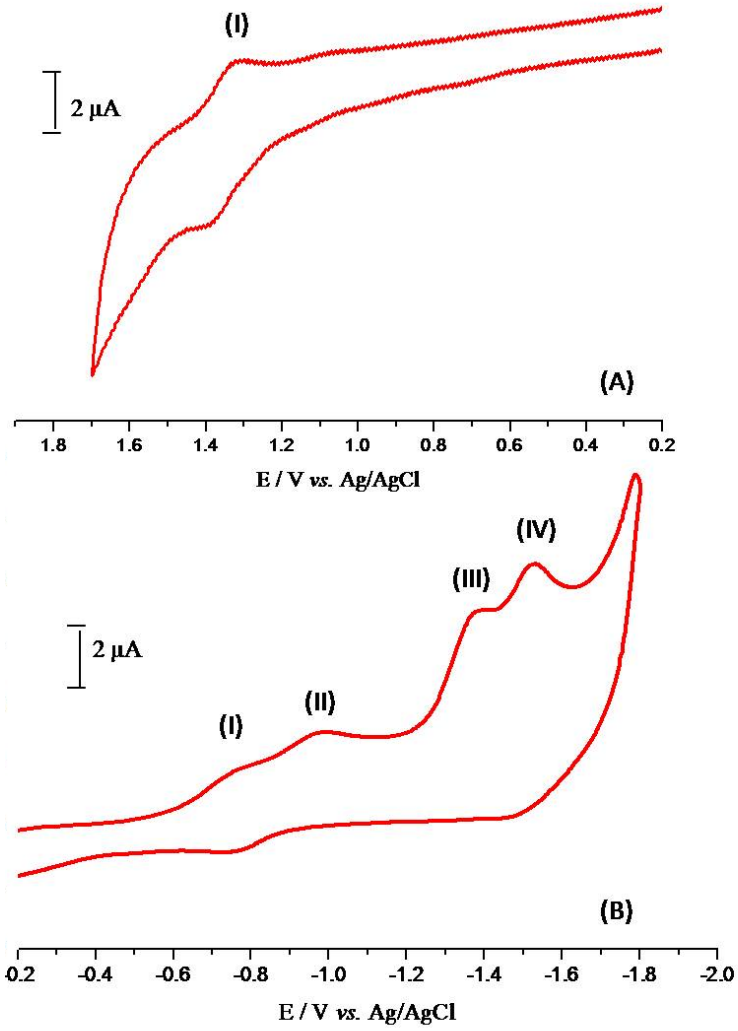
dpqp Dipyrido[2,3-a:3',2'-c]quinolino[3,2-*j*]phenazine

dicnq 6,7-dicyanodipyrido[2,2-*d*:2′,3′-*f*]quinoxaline

dppzc dipyrido[3,2-*a*:2′,3′-*c*]- phenazine-2-carboxylic acid

dppn 4,5,9,16-Tetraaza-dibenzo[a,c]naphthacene

Figure S2. Cyclic voltammogram of S104 in 0.1 M TBAP/MeCN solution at a Pt disk electrode (2 mm diameter), *T* = *25* °C, scan rate 100 mVs^{-1}: (A) Scan from -0.2 to -1.7 V; (B) scan from 0.2 to 1.7 V.



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