Supplementary Information for

Toward white electroluminescence by ruthenium quinoxaline light emitting diodes

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Content:

S6c. The optimized structures of [Ru(dicnq)$(pyTz)_2$] and diagram of the three highest occupied and three lowest unoccupied molecular orbital levels of [Ru(dicnq)$(pyTz)_2$] by DFT calculation

S7. PL spectrum of PVK/Ru(dicnq) film (λ_{exc}=405 nm)

S1:

The wavelength of electroluminescence (EL) and photoluminescence (PL) emissions of ruthenium polypyridyl 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)

S2. Absorption and emission properties of Ru quinoxaline derivates.

compound	**Absorption: $\lambda_{max,}$nm(logε)**	**Emission: λ_{em}, nm ($ø_{em}$)**	**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
$[Ru(phen)(dicnq)]^{2+}$	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-*f*][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

S3.

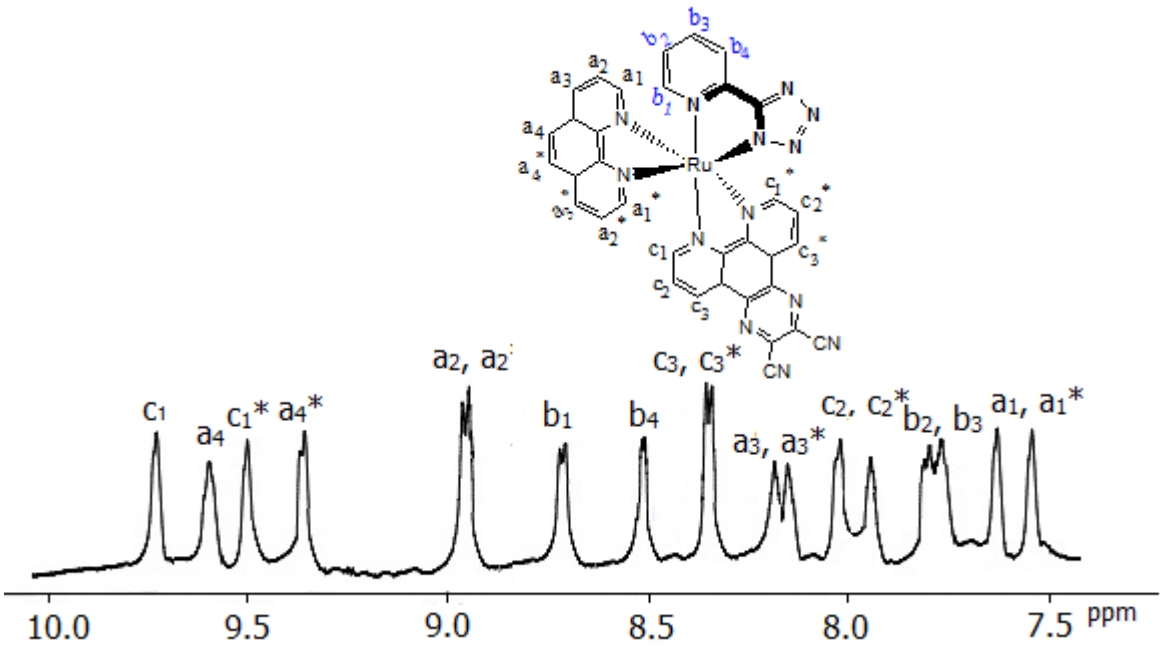

Figure S3a. ^{1}H-NMR spectrum of aromatic region of [Ru(dicnq)(pyTz)(phen)]BF_4 dissolved in DMSO solvent at room temperature.

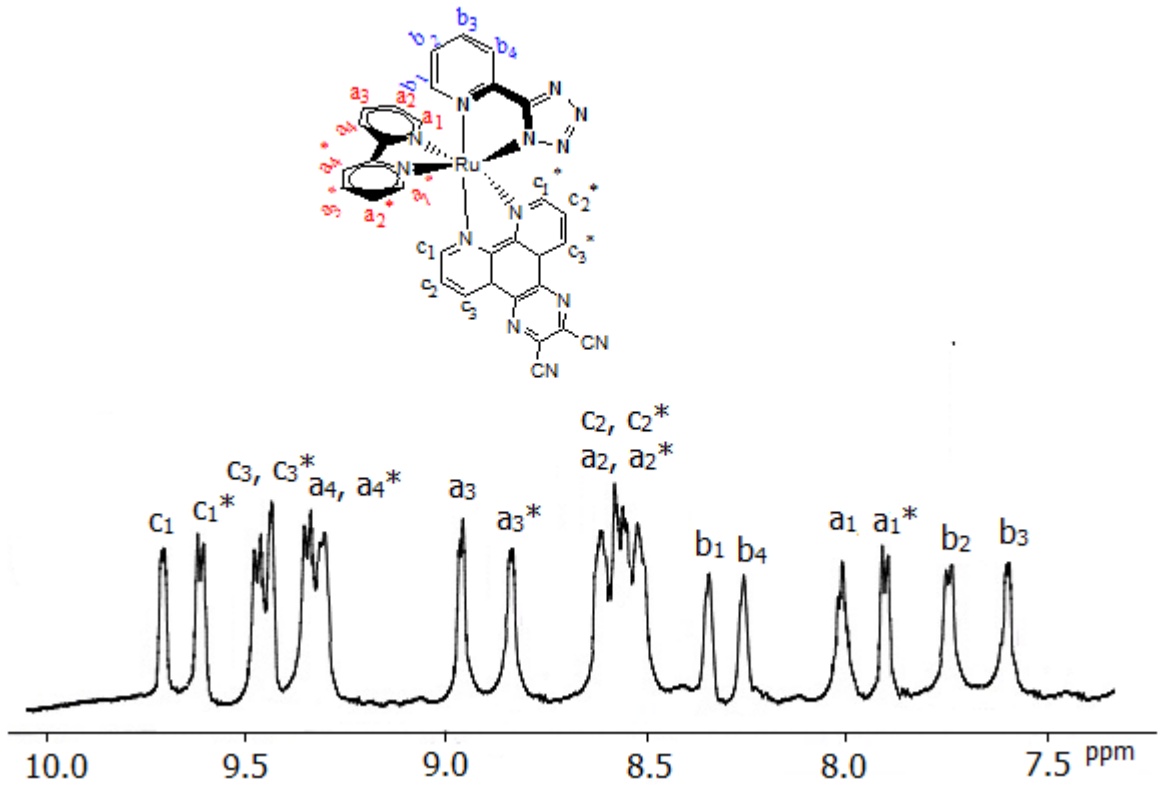

Figure S3b. ^{1}H-NMR spectrum of aromatic region of [Ru(dicnq)(pyTz)(bpy)]BF_4 dissolved in DMSO solvent at room temperature.

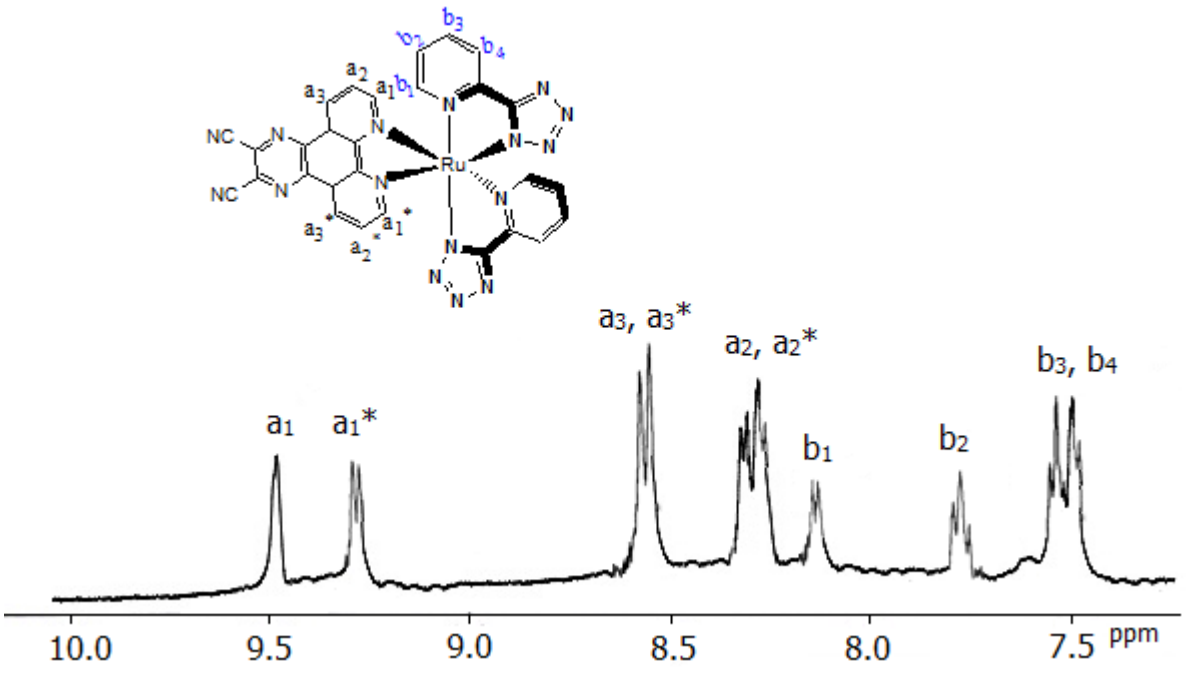

Figure S3c. ^{1}H-NMR spectrum of aromatic region of [Ru(dicnq)(pyTz)$_2$] dissolved in DMSO solvent at room temperature.

S4.

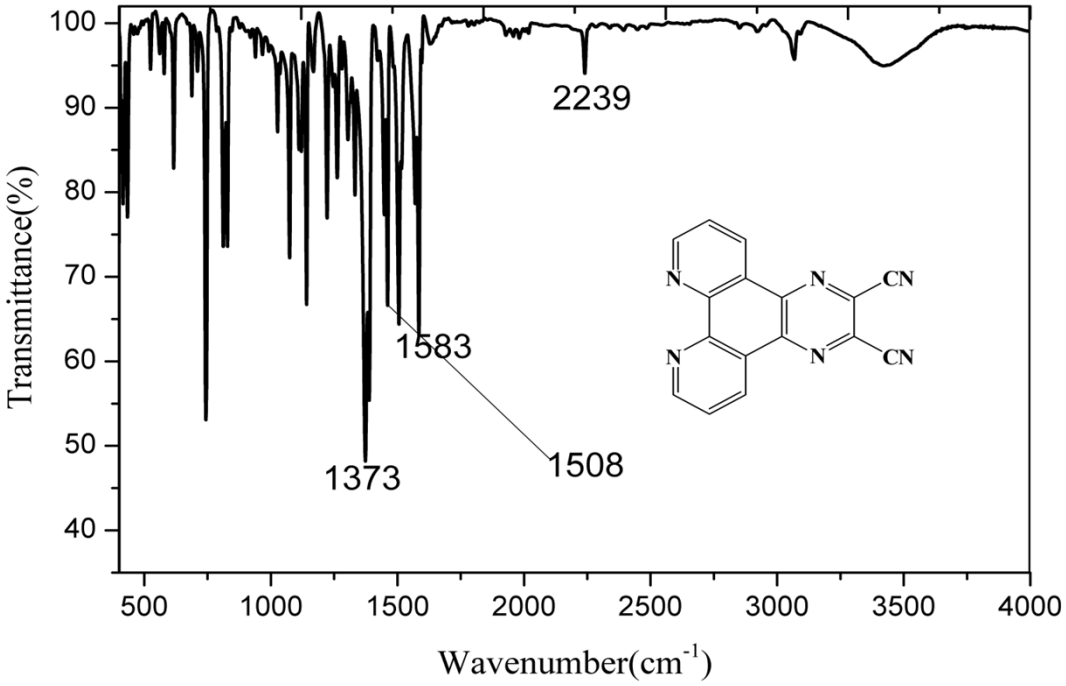

Figure S4a. FTIR spectrum of dicnq ligand with KBr disc.

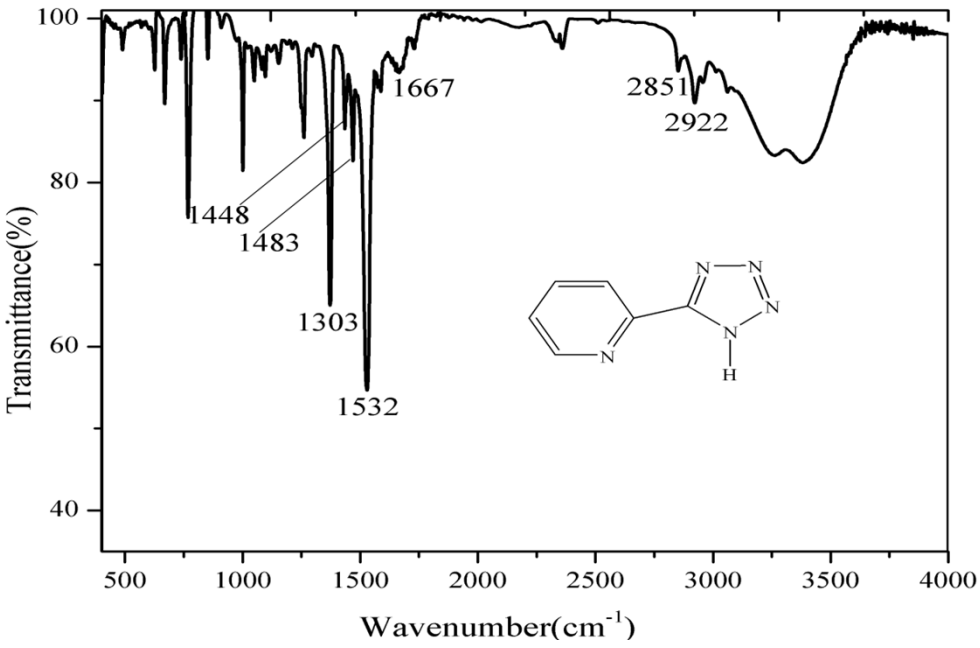

Figure S4b. FTIR spectrum of pyTz ligand with KBr disc.

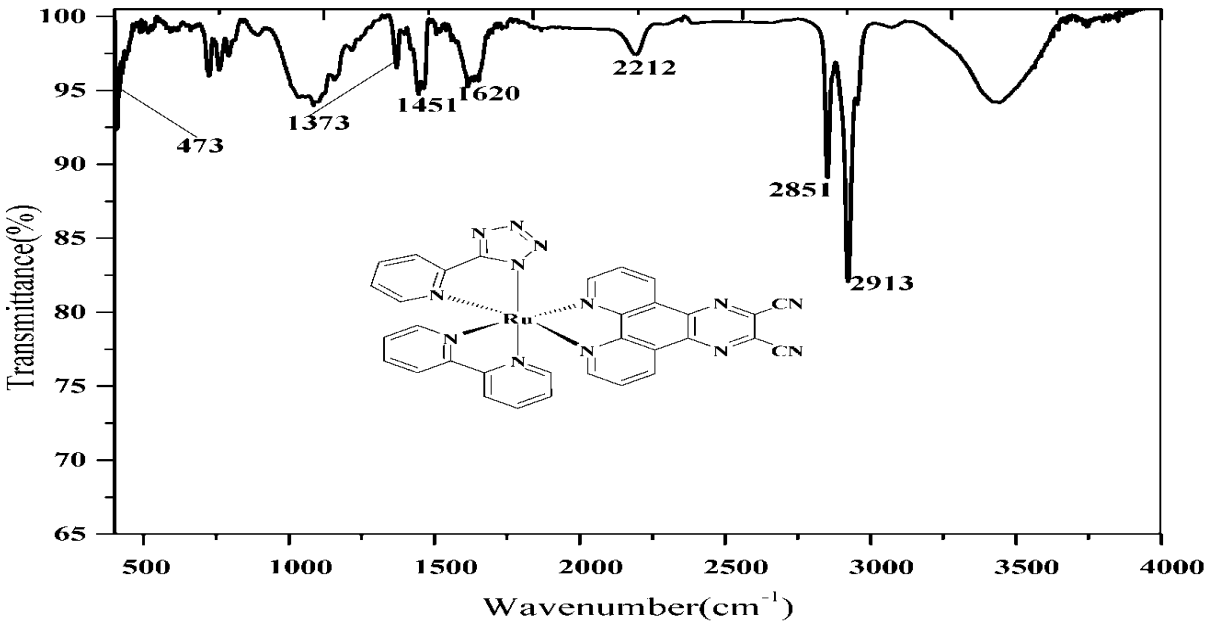

Figure S4c. FTIR spectrum of [Ru(dicnq)(pyTz)(bpy)]BF_4 with KBr disc.

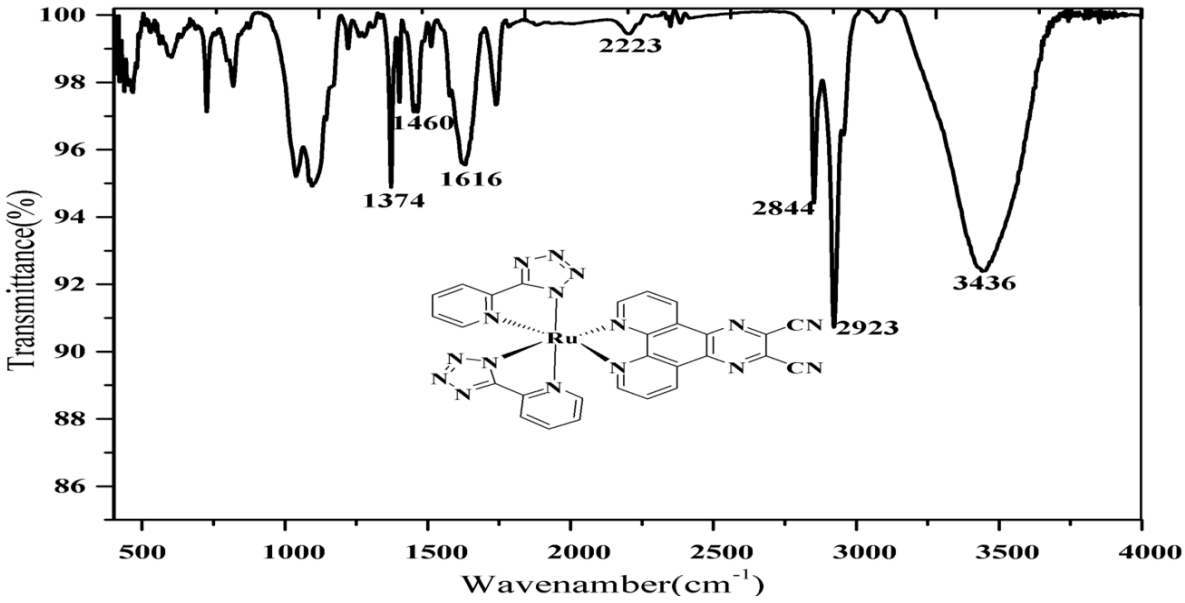

Figure S4d. FTIR spectrum of [Ru(dicnq)$(pyTz)_2$] with KBr disc.

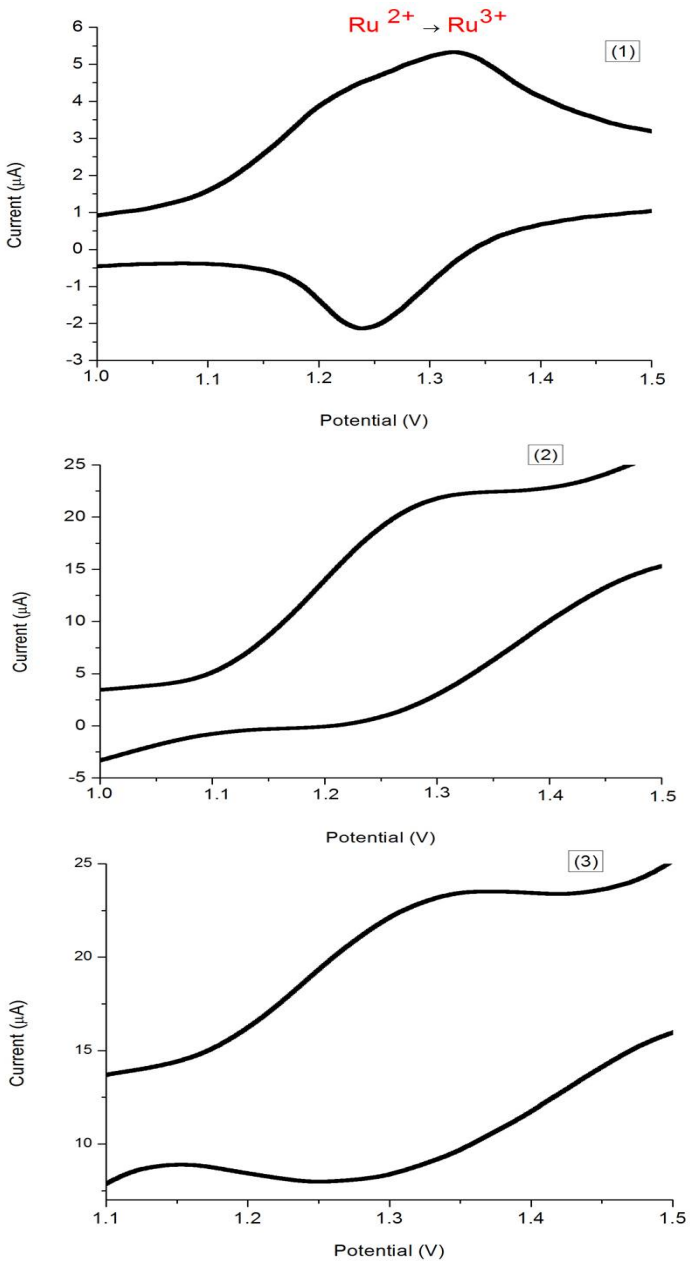

Figure S5. Cyclic voltammograms of Ru(dicnq) complexes (1-3) in MeCN solution containing 0.1 M tetra-n-butyl ammonium tetrafloroborate at room temperature.

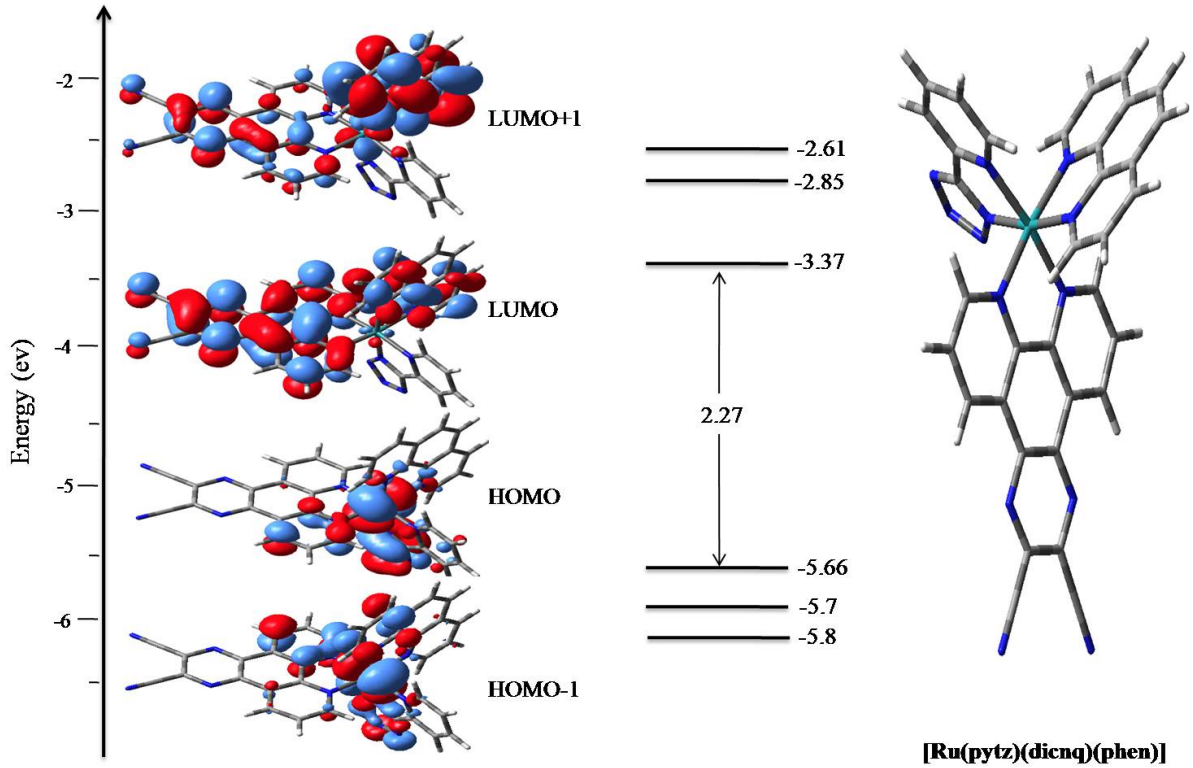

Figure S6a. Left: the optimized structures of [Ru(dicnq)(pyTz)(phen)]BF_4. Right: Diagram of the three highest occupied and three lowest unoccupied molecular orbital levels of [Ru(dicnq)(pyTz)(phen)]BF_4 by DFT calculation .

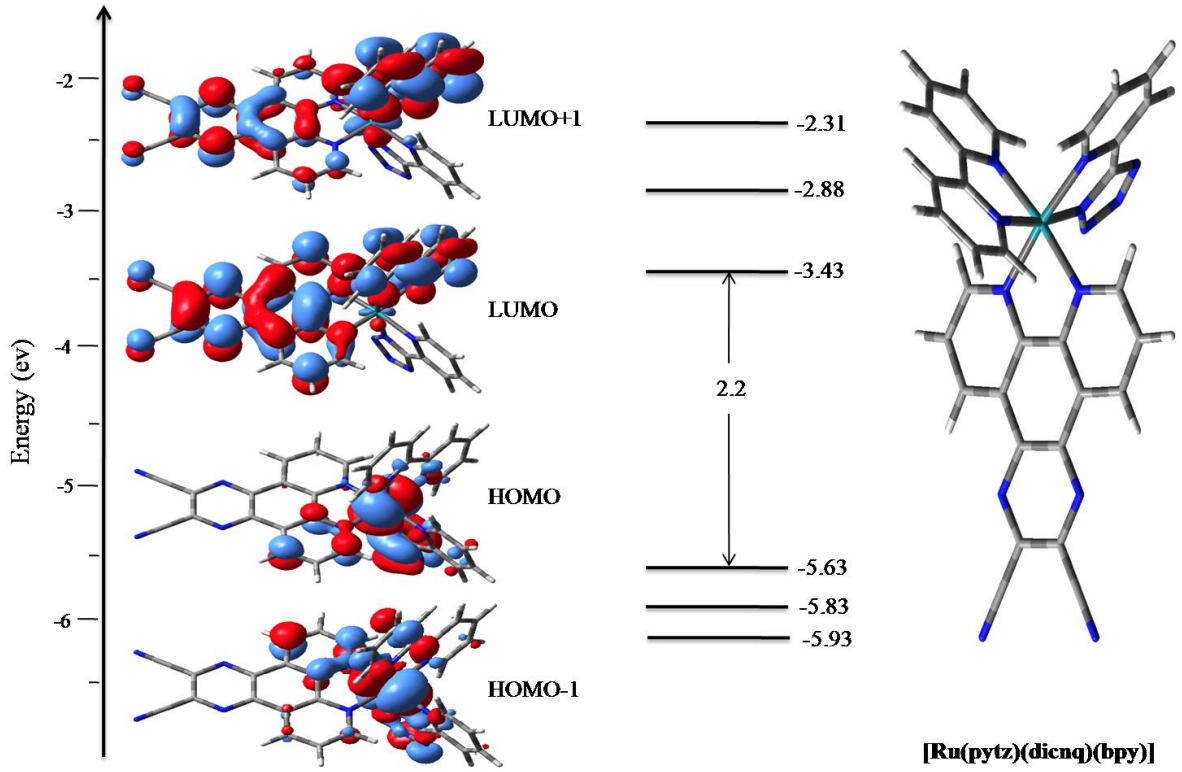

Figure S6b. Left: the optimized structures of [Ru(dicnq)(pyTz)(bpy)]BF_4. Right: Diagram of the three highest occupied and three lowest unoccupied molecular orbital levels of [Ru(dicnq)(pyTz)(bpy)]BF_4 DFT calculation .

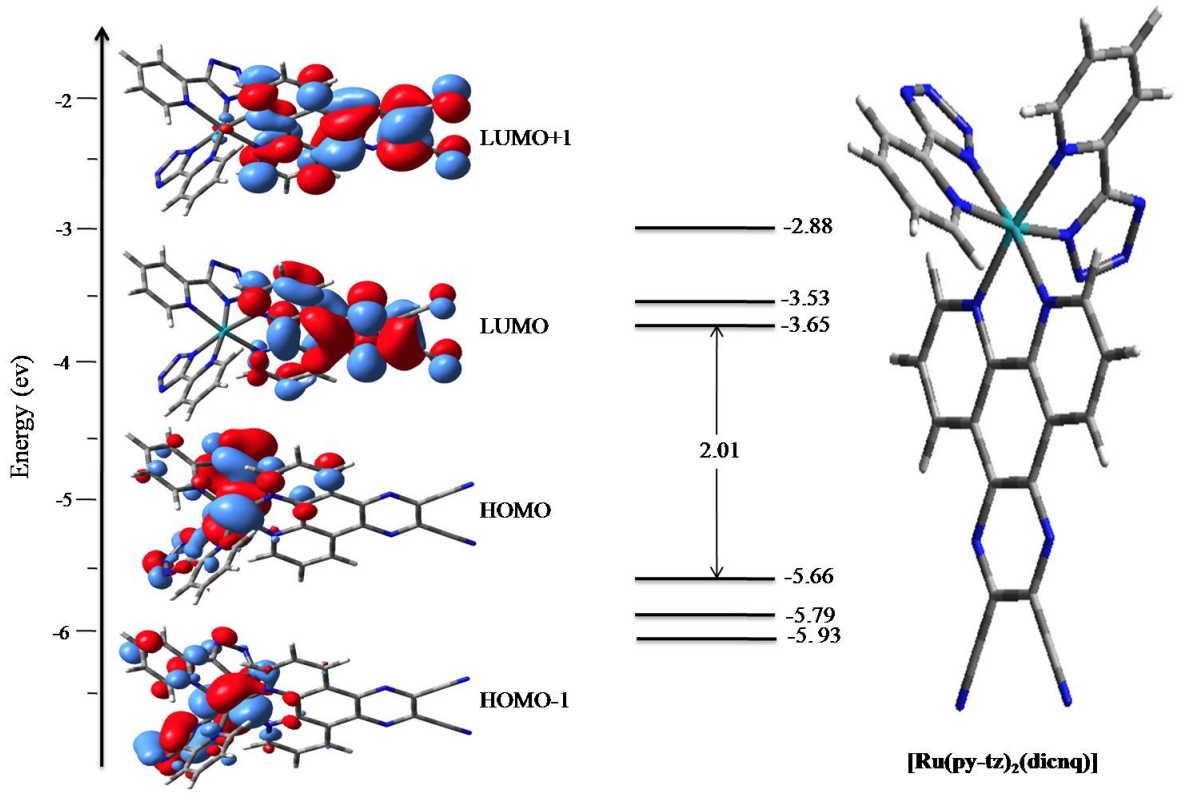

Figure S6c. Left: the optimized structures of [Ru(dicnq)(pyTz)$_2$]. Right: Diagram of the three highest occupied and three lowest unoccupied molecular orbital levels of [Ru(dicnq)(pyTz)$_2$] by DFT calculation .

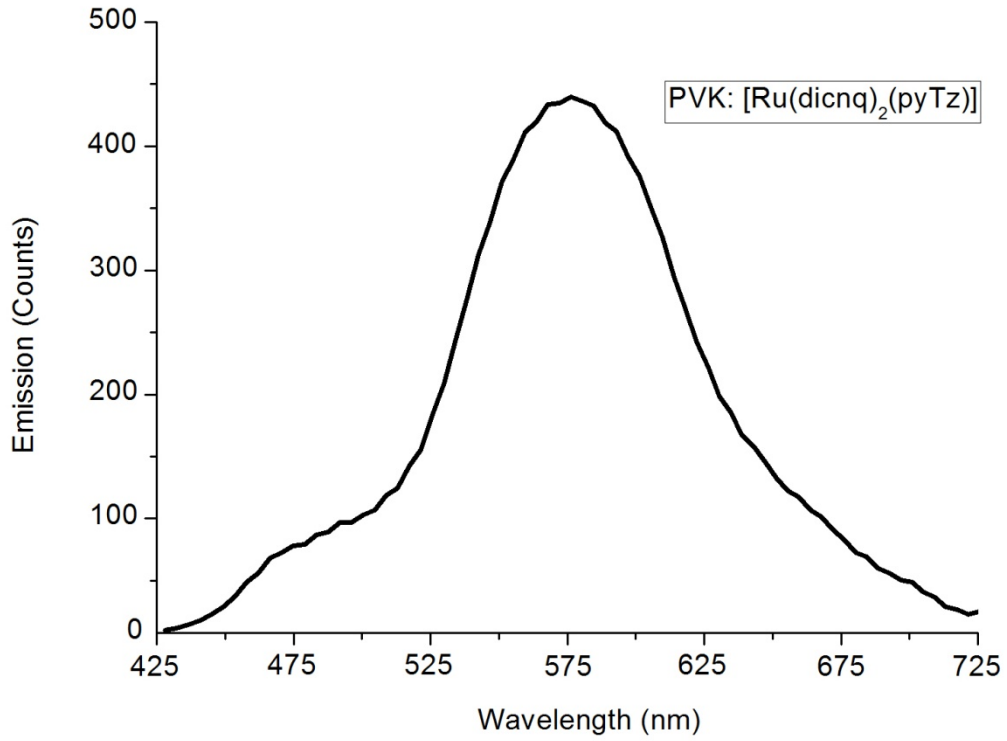

Figure S7. PL spectrum of PVK/Ru(dicnq) film (λ_{exc}=405 nm).

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