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Electrochemiluminescence properties, or luminescence sensing of four novel polymers derived from 3-(pyrazin-2-yl)-1*H*-Pyrazole-5-carboxylic acid

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Table S1 Crystal datas and refinement parameters for polymers **1–4.**

Polymer	**1**	**2**	**3**	**4**
Formula	$C_{16}H_8Cu_2N_8O_4$	$C_{16}H_{16}Cl_2N_8O_8Zn_3$	$C_8H_5ClN_4O_2Pb$	$C_8H_8N_4NiO_4$
Mr	503.4	715.44	431.80	282.87
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	*P2₁/c*	*P–1*	*P2₁/c*	*P2₁/c*
a(Å)	5.1833(4)	6.8724(4)	13.8772(7)	8.5821(10)
b(Å)	23.147(2)	8.5555(6)	9.5629(5)	13.5780(11)
c(Å)	6.8285(7)	10.8947(7)	7.5481(4)	9.2842(11)
α(°)	90	103.025(5)	90	90
β(°)	107.681(10)	102.889(5)	94.152(6)	116.067(15)
γ(°)	90	111.241(6)	90	90
V(Å^3)	780.57(13)	547.97(7)	999.05(9)	971.8(2)
F(000)	500	356	780	572
Z	4	2	4	4
Dc(g/cm^3)	2.142	2.168	2.864	1.926
μ(mm^{-1})	2.776	3.567	17.143	2.006
θ(°)	3.5–29.5	3.3–29.7	3.6–29.5	3.9–29.9
Ref.meas./indep	3682, 1864	7240, 2664	5157, 2408	4449, 2328
Obs.ref.[$I>2\sigma(I)$]	1480	2119	2021	1953
R_{int}	0.027	0.034	0.026	0.025
$R_1[I\geq2\sigma(I)]$[a]	0.0346	0.0340	0.0315	0.0322
wR_2(all data)[b]	0.0824	0.0809	0.0755	0.0761
GOF	1.04	1.062	1.08	1.03
Δρ(max.min)(e Å^{-3})	0.50, –0.45	0.65, –0.50	1.20, –1.79	0.39, –0.56

[a] $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ [b] $wR_2=[\Sigma w(|F^2_o|-|F^2_c|)^2/\Sigma w(|F^2_o|)^2]^{1/2}$

Table S2a Selected bond lengths (Å) and angles (◦) for polymer **1.**

Cu(1)–N(1)	1.919(2)	Cu(1)–N(2)^{i}	1.935(2)
Cu(1)–O(1)	1.973(2)	Cu(1)–N(3)^{i}	2.040(2)
N(1)–Cu(1)–N(2)^{i}	93.82(10)	N(1)–Cu(1)–O(1)	81.60(9)
N(2)^{i}–Cu(1)–O(1)	169.33(9)	N(1)–Cu(1)–N(3)^{i}	173.28(9)
N(2)^{i}–Cu(1)–N(3)^{i}	79.66(10)	O(1)–Cu(1)–N(3)^{i}	104.55(9)
Symmetry code: (i) –x+1, –y+1, –z+1			

Table S2b Selected bond lengths (Å) and angles (◦) for polymer **2.**

Zn(1)–O(4)	2.048(2)	Zn(1)–O(2)^{i}	2.0660(19)
Zn(1)–N(3)	2.101(2)	Zn(1)–N(1)	2.173(2)
Zn(1)–Cl(1)	2.2751(9)	Zn(2)–N(4)^{ii}	2.067(2)
Zn(2)–N(4)	2.067(2)	Zn(2)–O(1)^{ii}	2.171(2)
Zn(2)–O(1)	2.171(2)	Zn(2)–O(3)^{ii}	2.180(3)
Zn(2)–O(3)	2.180(3)		
O(4)–Zn(1)–O(2)^{i}	88.42(9)	O(4)–Zn(1)–N(3)	91.64(9)
O(2)^{i}–Zn(1)–N(3)	152.14(9)	O(4)–Zn(1)–N(1)	136.16(9)
O(2)^{i}–Zn(1)–N(1)	83.70(8)	N(3)–Zn(1)–N(1)	77.05(8)
O(4)–Zn(1)–Cl(1)	112.68(7)	O(2)^{i} –Zn(1)–Cl(1)	104.30(7)
N(3)–Zn(1)–Cl(1)	101.35(7)	N(1)–Zn(1)–Cl(1)	111.06(7)
N(4)^{ii}–Zn(2)–N(4)	180.0	N(4)^{ii} –Zn(2)–O(3)^{ii}	90.37(9)
N(4)^{ii}–Zn(2)–O(1)^{ii}	78.12(8)	N(4)–Zn(2)–O(3)^{ii}	89.63(9)
N(4)–Zn(2)–O(1)^{ii}	101.88(8)	O(1)^{ii}–Zn(2)–O(3)^{ii}	92.65(10)
N(4)^{ii}–Zn(2)–O(1)	101.88(8)	O(1)–Zn(2)–O(3)^{ii}	87.35(10)
N(4)–Zn(2)–O(1)	78.12(8)	N(4)^{ii}–Zn(2)–O(3)	89.63(9)
O(1)^{ii}–Zn(2)–O(1)	180.0	N(4)–Zn(2)–O(3)	90.37(9)
O(1)^{ii}–Zn(2)–O(3)	87.35(10)	O(3)^{ii}–Zn(2)–O(3)	180.0
O(1)–Zn(2)–O(3)	92.65(10)		

Symmetry code: (i) x, y–1, z; (ii) –x+1, –y+1, –z.

Table S2c Selected bond lengths (Å) and angles (◦) for polymer **3.**

Pb(1)–N(2)	2.466(5)	Pb(1)–N(3)	2.681(5)
Pb(1)–O(1)^{i}	2.538(4)	Pb(1)–Cl(1)	2.685(2)
N(2)–Pb(1)–O(1)^{i}	76.80(15)	N(2)–Pb(1)–N(3)	63.65(16)
O(1)^{i}–Pb(1)–N(3)	138.20(14)	N(2)–Pb(1)–Cl(1)	87.52(14)
O(1)^{i}–Pb(1)–Cl(1)	83.02(14)	N(3)–Pb(1)–Cl(1)	82.34(13)
Symmetry code: (i) –x, y–1/2, –z+1/2			

Table S2d Selected bond lengths (Å) and angles (◦) for polymer **1.**

Ni(1)–O(3)	2.129(2)	Ni(1)–N(2)	2.0035(19)
Ni(1)–N(3)	2.1596(19)	Ni(1)–O(1)^{i}	2.1199(18)
Ni(1)–N(1)^{i}	1.9903(18)	Ni(1)–N(4)^{iii}	2.1320(19)
O(3)–Ni(1)–N(2)	92.09(8)	O(3)–Ni(1)–N(3)	88.70(7)
O(1)^{ii}–Ni(1)–O(3)	87.64(8)	O(3)–Ni(1)–N(1)^{ii}	92.59(8)
O(3)–Ni(1)–N(4)^{iii}	170.76(10)	N(2)–Ni(1)–N(3)	77.36(7)
O(1)^{ii}–Ni(1)–N(2)	172.03(7)	N(1)^{ii}–Ni(1)–N(2)	93.86(8)
N(2)–Ni(1)–N(4)^{ii}	93.04(8)	O(1)^{ii}–Ni(1)–N(3)	110.60(7)
N(1)^{ii}–Ni(1)–N(3)	171.17(8)	N(3)–Ni(1)–N(4)^{iii}	84.92(7)
O(1)^{ii}–Ni(1)–N(1)^{ii}	78.19(7)	O(1)^{ii}–Ni(1)–N(4)^{iii}	88.34(8)
N(1)^{ii}–Ni(1)–N(4)^{iii}	94.73(8)		
Symmetry code: (i) x, 1/2–y, –1/2+z; (ii) 1–x, –y, 1–z; (iii) x, 1/2–y, 1/2+z			

Table S3 Putative hydrogen bond interactions (Å,◦) for the polymers **1–4.**

D–H···A	*D–H*	*H···A*	*D···A*	*D–H···A*
1				
C(3)–H(3)···O(2)^{i}	0.93	2.56	3.357(4)	144.2
C(8)–H(8)...N(4)^{ii}	0.93	2.43	3.347(4)	167.6
Symmetry code: i = –x+3, –y+1, –z+2; ii = x–1, –y+1/2, z–1/2.				
2				
O3–H3A···Cl1^{i}	0.70(6)	2.72(6)	3.376(3)	159(8)
C2–H2···Cl1^{ii}	0.93	2.75	3.613(3)	154
Symmetry code:i = –x, –y, –z, ii = 1–x, –y, 1–z				
3				
C7–H7···Cl^{i}	0.93	2.75	3.489(7)	138
Symmetry code: i = –x, 2–y, –z				
4				
O(3)–H3B···O(2)^{i}	0.76(4)	1.96(4)	2.718(3)	171(4)
Symmetry code: i = 2–x, –y, 1–z				

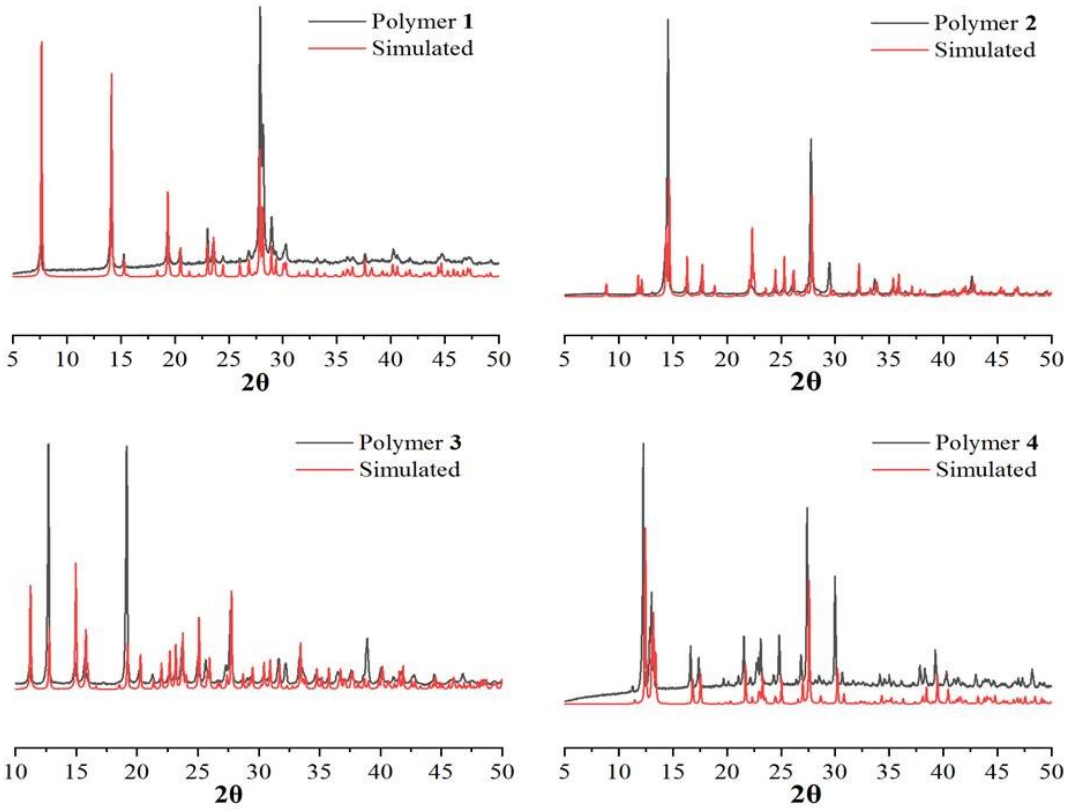

Figure S1 PXRD patterns of polymers polymers **1**–**4.**

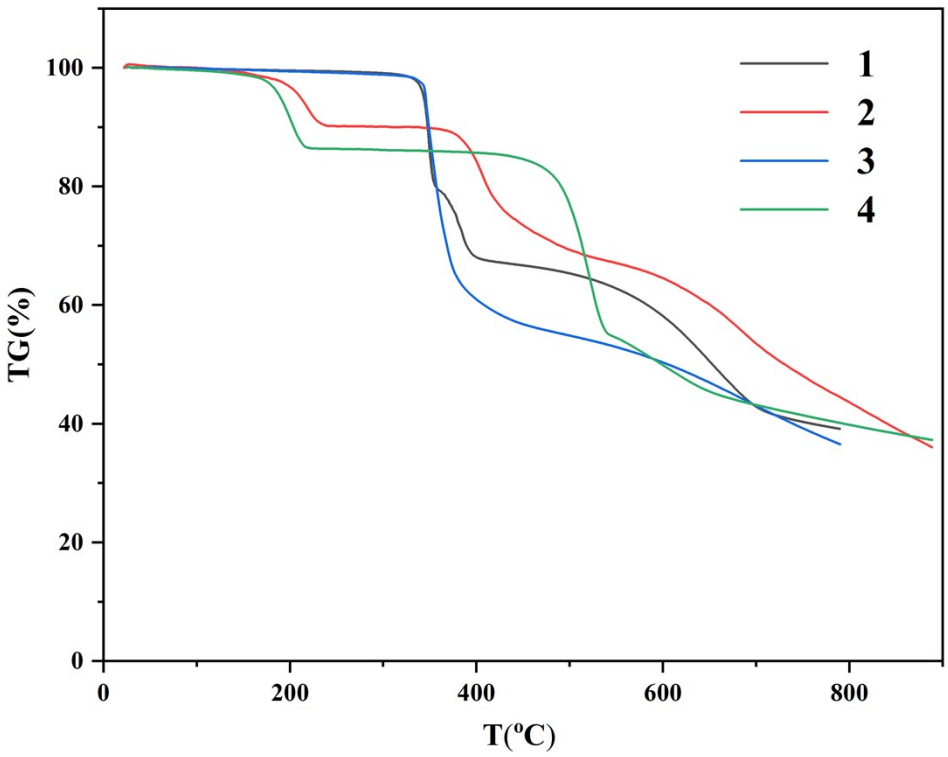

Figure S2 Thermogravimetric analysis of polymers **1-4.**

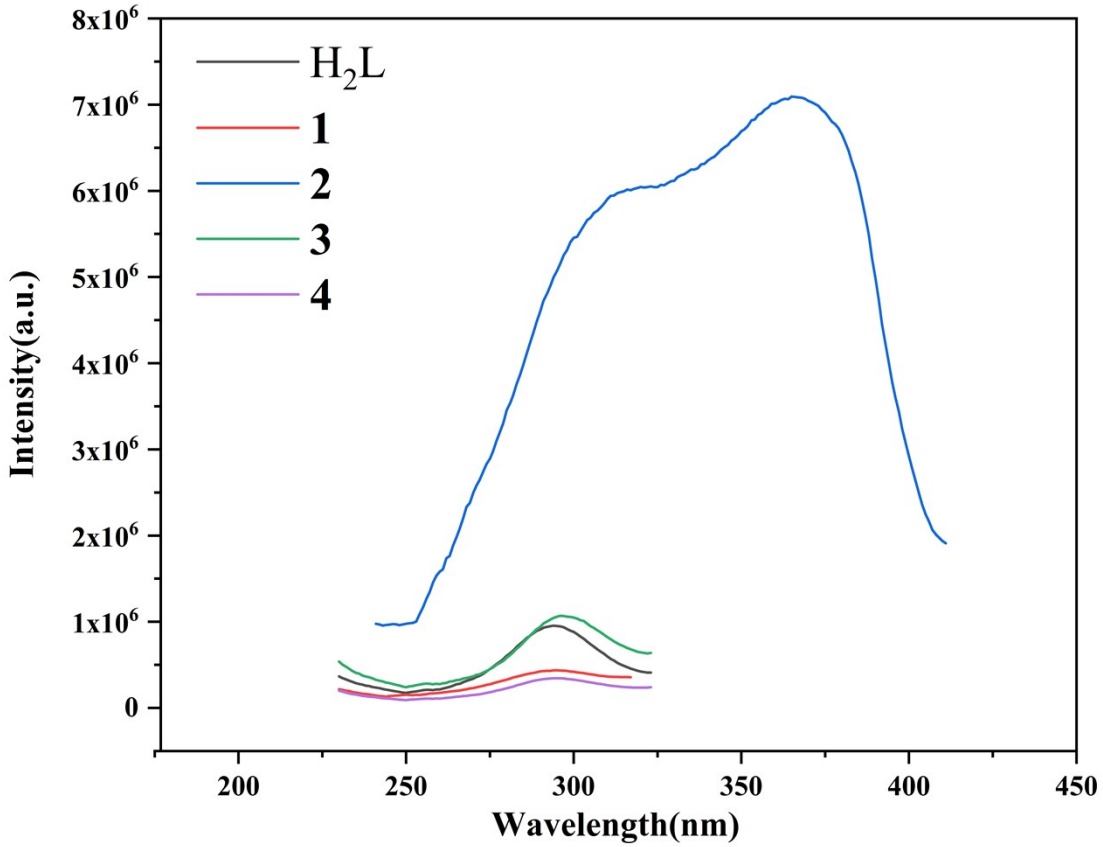

Fig.S3 The fluorescence excitation spectra of polymers **1-4** compared with the free H_2L ligand**.**

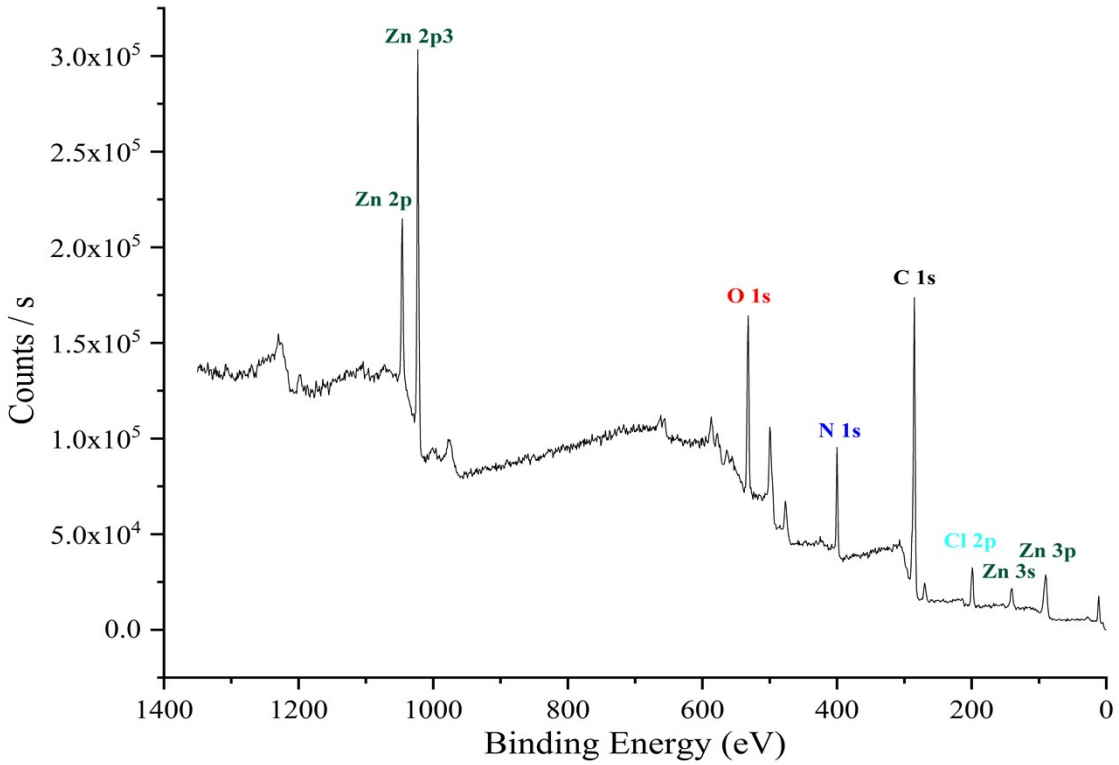

Figure S4 XPS of CP 2.

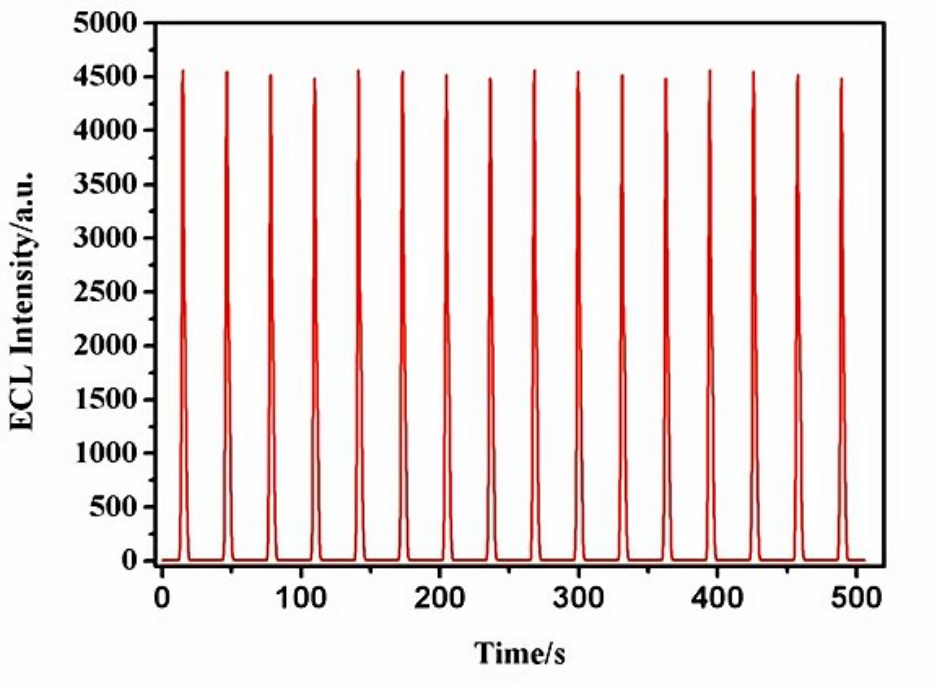

Figure. S5 Electrochemical luminescence for $Ru(bpy)_3^{2+}$