

Hydrothermal synthesis, structures, and luminescent properties of four new zinc(II) diphosphonate hybrids with mixed ligands

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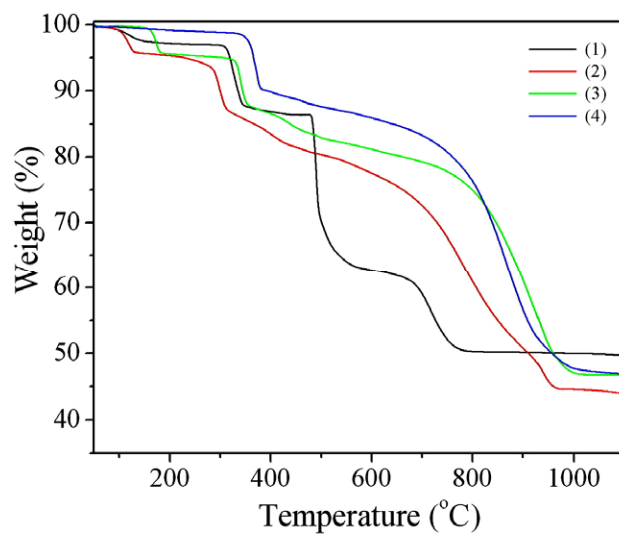


Fig. S1 The TGA curves of compounds 1– 4

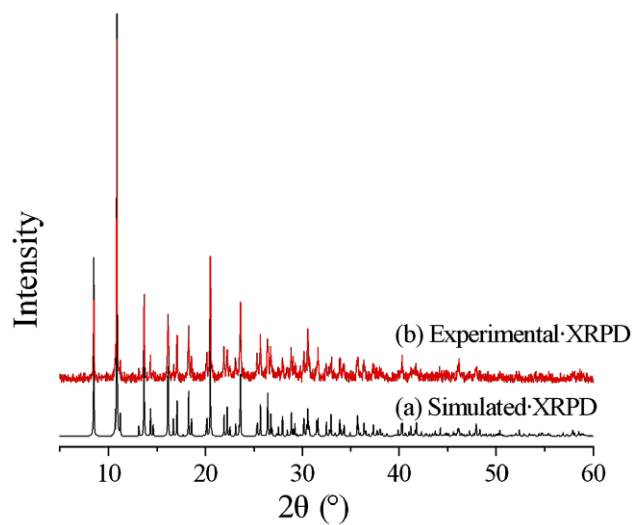


Fig. S2 The simulated and experimental XRD powder patterns for compound 1 (a) and (b)

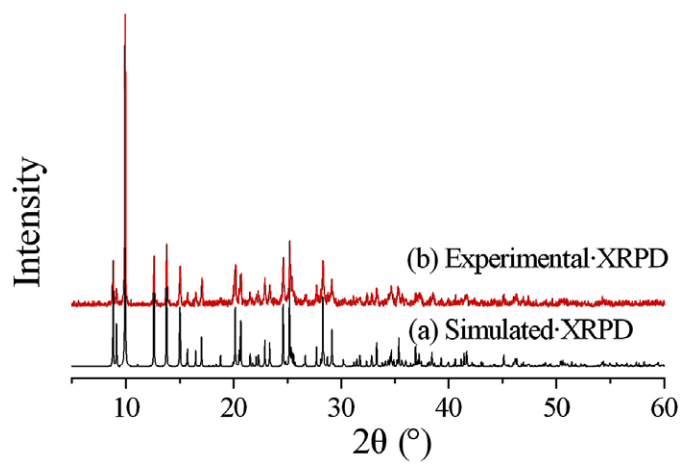


Fig. S3 The simulated and experimental XRD powder patterns for compound 2 (a) and (b)

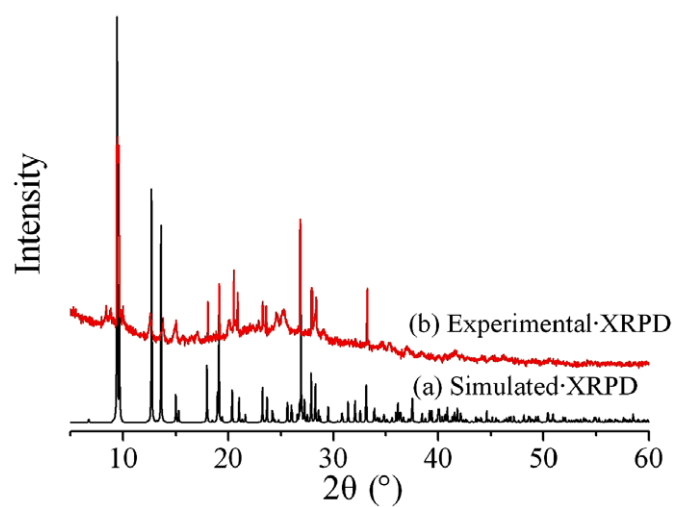


Fig. S4 The simulated and experimental XRD powder patterns for compound **3** (a) and (b)

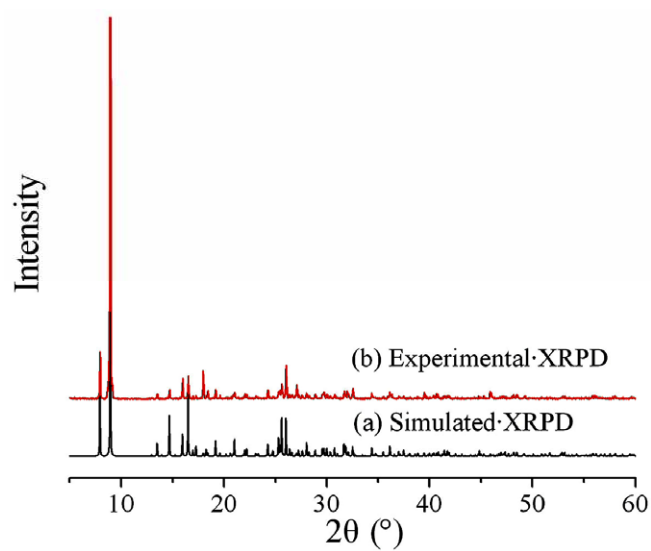


Fig. S5 The simulated and experimental XRD powder patterns for compound **4** (a) and (b)

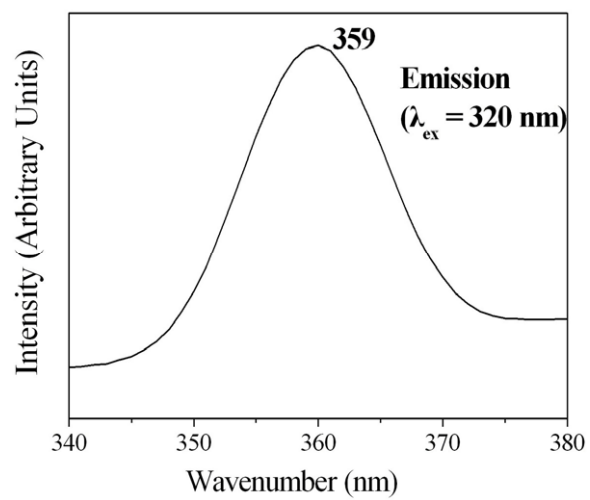


Fig. S6 The room-temperature luminescent emission spectrum of hedpH₄ solution.

Table S1 Selected bond lengths (Å) and angles (°) for compounds **1–4**

Compound 1			
Zn(1)–O(4)	1.958(2)	Zn(1)–O(2)A	1.972(2)
Zn(1)–N(2)	2.086(3)	Zn(1)–O(1)	2.114(2)
Zn(1)–N(1)	2.146(3)	P(1)–O(2)	1.502(2)
P(1)–O(1)	1.516(2)	P(1)–O(3)	1.557(2)
P(1)–C(1)	1.829(4)	P(2)–O(5)	1.491(3)
P(2)–O(4)	1.497(3)	P(2)–O(6)	1.575(3)
P(2)–C(1)	1.844(4)	O(2)–Zn(1)A	1.972(2)
O(4)–Zn(1)–O(2)A	108.75(11)	O(4)–Zn(1)–N(2)	127.53(12)
O(2)A–Zn(1)–N(2)	122.10(11)	O(4)–Zn(1)–O(1)	98.93(9)
O(2)A–Zn(1)–O(1)	90.65(9)	N(2)–Zn(1)–O(1)	92.92(10)
O(4)–Zn(1)–N(1)	89.51(11)	O(2)A–Zn(1)–N(1)	92.43(11)
N(2)–Zn(1)–N(1)	77.01(12)	O(1)–Zn(1)–N(1)	169.57(10)
Compound 2			
Zn(1)–O(2)A	1.986(2)	Zn(1)–O(4)	1.988(2)
Zn(1)–O(1)	2.068(2)	Zn(1)–N(1)	2.118(3)
Zn(1)–N(2)	2.145(3)	P(1)–O(2)	1.502(2)
P(1)–O(1)	1.515(2)	P(1)–O(3)	1.568(2)
P(1)–C(1)	1.843(3)	P(2)–O(6)	1.487(3)
P(2)–O(4)	1.525(2)	P(2)–O(5)	1.576(2)
P(2)–C(1)	1.838(3)	O(2)–Zn(1)A	1.986(2)
O(2)A–Zn(1)–O(4)	102.83(10)	O(2)A–Zn(1)–O(1)	95.76(9)
O(4)–Zn(1)–O(1)	95.28(9)	O(2)A–Zn(1)–N(1)	136.09(11)
O(4)–Zn(1)–N(1)	120.16(10)	O(1)–Zn(1)–N(1)	89.20(10)
O(2)A–Zn(1)–N(2)	87.21(10)	O(4)–Zn(1)–N(2)	99.80(10)
O(1)–Zn(1)–N(2)	163.59(10)	N(1)–Zn(1)–N(2)	77.67(11)
Compound 3			
Zn(1)–O(3)A	2.0946(18)	Zn(1)–O(3)	2.0946(18)
Zn(1)–N(1)	2.121(2)	Zn(1)–N(1)A	2.121(2)
Zn(1)–O(4)A	2.1451(17)	Zn(1)–O(4)	2.1451(17)
Zn(2)–O(1)	1.9305(18)	Zn(2)–O(1)B	1.9305(18)
Zn(2)–O(5)B	1.9391(18)	Zn(2)–O(5)	1.9391(18)
P(1)–O(3)	1.5016(18)	P(1)–O(1)	1.5053(18)
P(1)–O(2)	1.5683(19)	P(1)–C(1)	1.839(3)
P(2)–O(5)	1.5071(18)	P(2)–O(4)	1.5122(17)
P(2)–O(6)	1.5572(19)	P(2)–C(1)	1.838(3)
O(3)A–Zn(1)–O(3)	84.49(10)	O(3)A–Zn(1)–N(1)	177.31(8)
O(3)A–Zn(1)–N(1)	177.31(8)	O(3)–Zn(1)–N(1)	98.17(8)
O(3)A–Zn(1)–N(1)A	98.17(8)	O(3)–Zn(1)–N(1)A	177.31(8)
N(1)–Zn(1)–N(1)A	79.17(13)	O(3)A–Zn(1)–O(4)A	93.14(7)
O(3)–Zn(1)–O(4)A	84.72(7)	N(1)–Zn(1)–O(4)A	86.73(8)
N(1)A–Zn(1)–O(4)A	95.50(8)	O(3)A–Zn(1)–O(4)	84.72(7)
O(3)–Zn(1)–O(4)	93.14(7)	N(1)–Zn(1)–O(4)	95.50(8)

N(1)A–Zn(1)–O(4)	86.73(8)	O(4)A–Zn(1)–O(4)	177.12(9)
O(1)–Zn(2)–O(1)B	114.69(12)	O(1)–Zn(2)–O(5)B	112.69(8)
O(1)B–Zn(2)–O(5)B	102.22(8)	O(1)–Zn(2)–O(5)	102.22(8)
O(1)B–Zn(2)–O(5)	112.69(8)	O(5)B–Zn(2)–O(5)	112.77(12)
Compound 4			
Zn(1)–O(5)A	1.975(2)	Zn(1)–O(1)	2.011(2)
Zn(1)–O(4)	1.978(2)	Zn(1)–N(1)	2.174(3)
Zn(1)–N(2)	2.170(3)	P(1)–O(3)	1.512(2)
P(1)–O(1)	1.502(2)	P(1)–C(1)	1.832(3)
P(1)–O(2)	1.576(2)	P(2)–O(4)	1.517(2)
P(2)–O(5)	1.498(2)	P(2)–C(1)	1.845(4)
P(2)–O(6)	1.568(2)	O(5)A–Zn(1)–O(1)	98.02(9)
O(5)A–Zn(1)–O(4)	103.41(10)	O(5)A–Zn(1)–N(2)	85.50(10)
O(4)–Zn(1)–O(1)	96.73(9)	O(1)–Zn(1)–N(2)	158.02(10)
O(4)–Zn(1)–N(2)	103.58(10)	O(4)–Zn(1)–N(1)	116.26(10)
O(5)A–Zn(1)–N(1)	138.92(10)	N(2)–Zn(1)–N(1)	75.63(10)
O(1)–Zn(1)–N(1)	87.97(9)		

Symmetry transformations used to generate equivalent atoms for **1**: A $-x, -y+2, -z$; for **2**: A $-x+1, -y, -z$; for **3**: A $-x+3/2, -y, z$; B $x, -y+1/2, -z+1/2$; for **4**: A $-x+1/2, y+1/2, -z+1/2$.

Table S2 Hydrogen bonds for compounds **1–4**

D–H \cdots A	D(D–H)/ Å	d(H \cdots A)/ Å	D–H–A/ °	d(D \cdots A)/ Å
compound 1				
O3–H3A \cdots O5	0.85	1.71	160	2.530(3)
compound 2				
O5–H5D \cdots O4	0.85	1.93	164	2.755(3)
O1W–H1WC \cdots O6	0.85	2.16	160	2.977(4)
O3–H3A \cdots O1W	0.85	1.82	169	2.659(3)
compound 3				
O6–H3A \cdots O4	0.85	1.87	166	2.705(3)
compound 4				
O2–H2D \cdots O3	0.82	1.78	175	2.603(3)