Electronic Supplementary Material (ESI) for New Journal of Chemistry

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Transition metal phosphonates with supramolecular structures: syntheses, structures, surface photovoltage and luminescent properties

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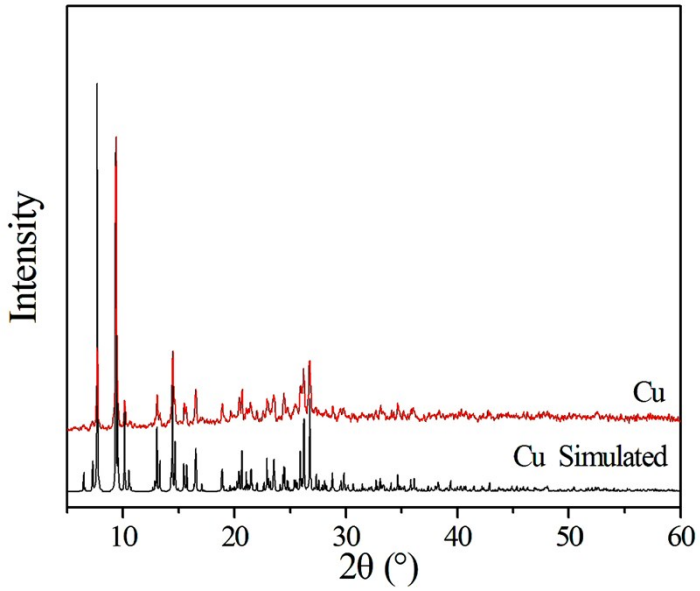

Fig S1. The experimental powder XRD pattern and the simulated XRD pattern of compound **1.**

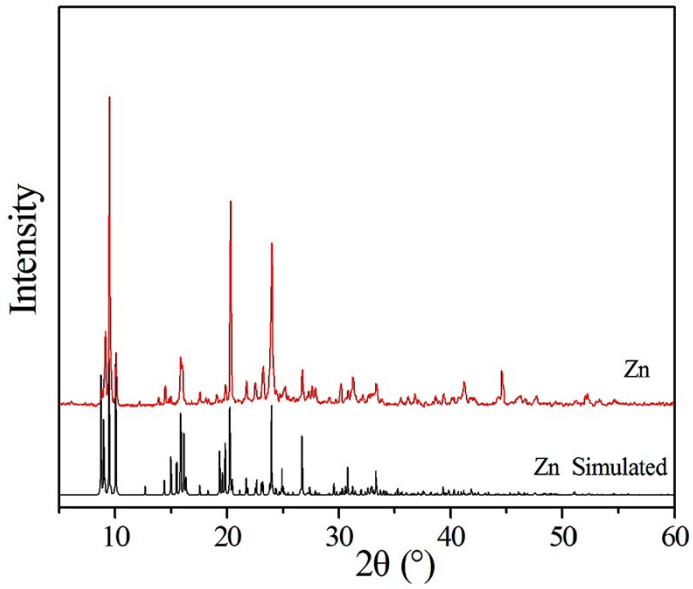

Fig S2. The experimental powder XRD pattern and the simulated XRD pattern of compound **2.**

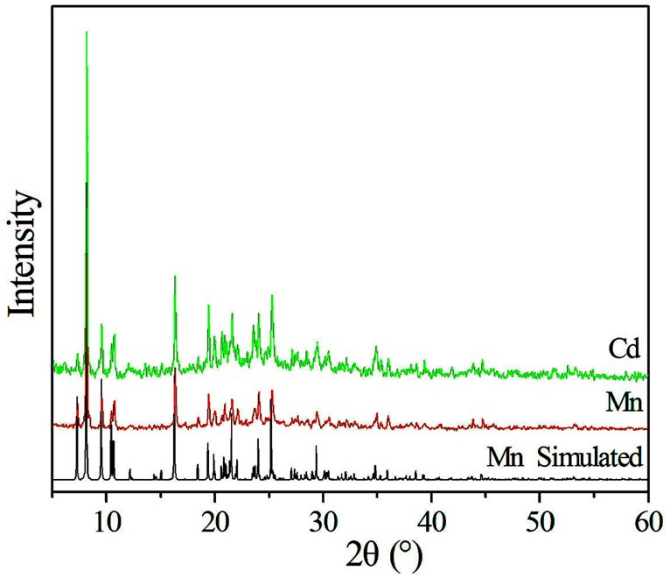

Fig S3. The simulated XRD pattern of compound **3** (down) and experimental powder XRD patterns of compounds **3** and **4.**

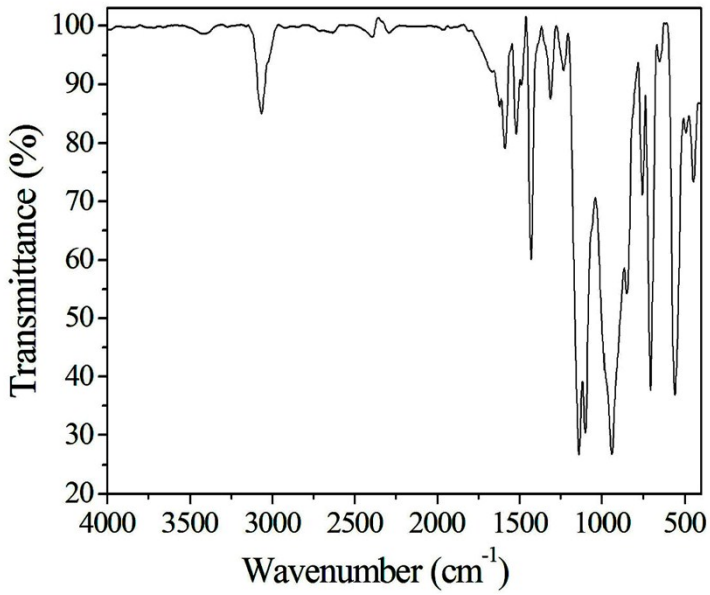

Fig S4. The IR spectrum of compound **1.**

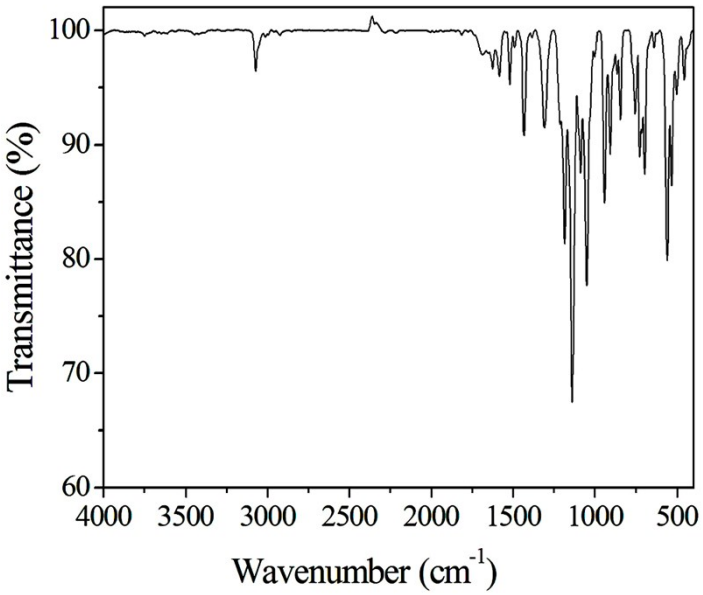

Fig S5. The IR spectrum of compound **2.**

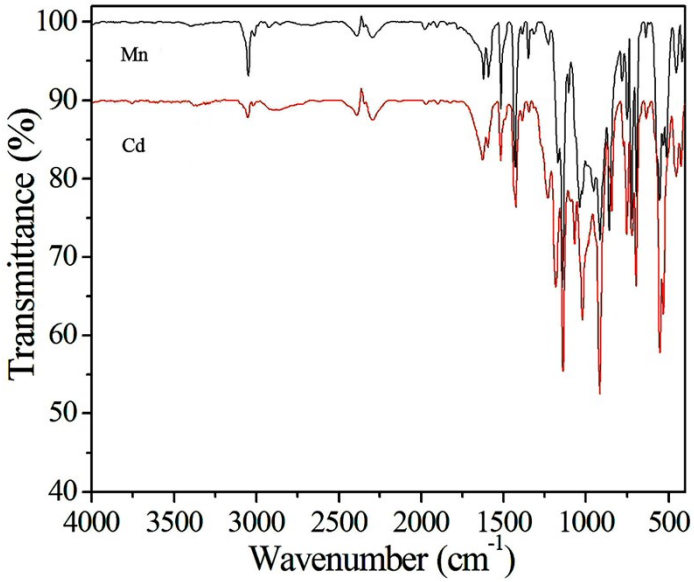

Fig S6. The IR spectra of compounds **3** and **4.**

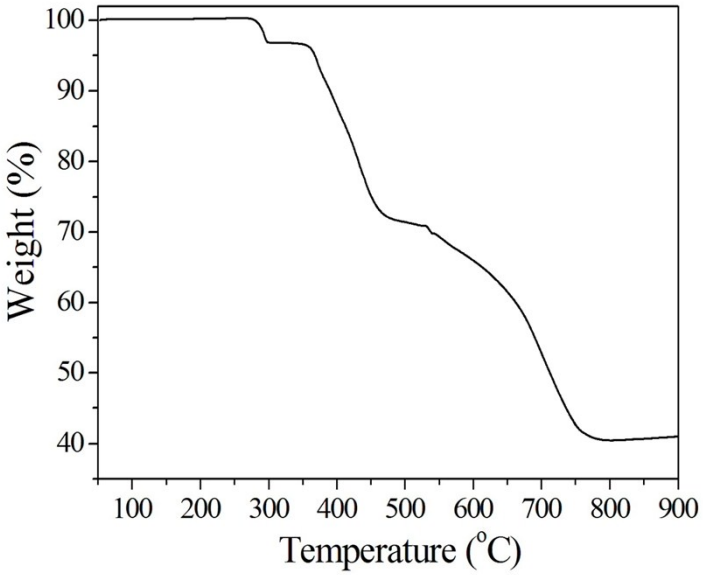

Fig S7. The TG curve of compound **1.**

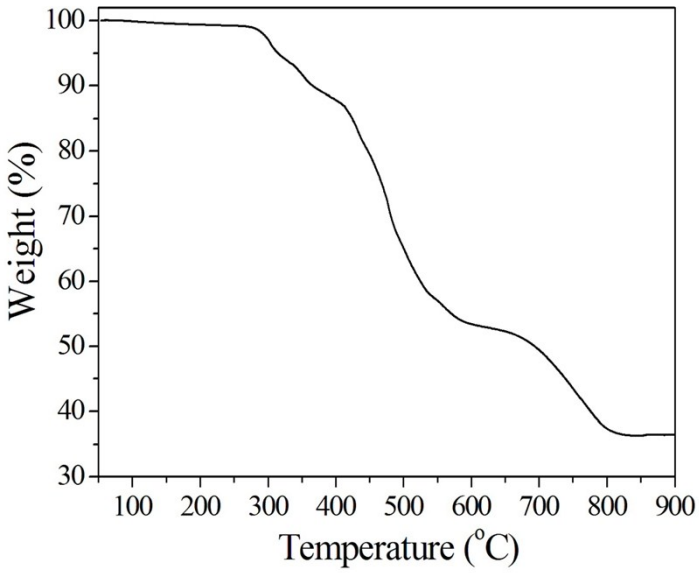

Fig. S8. The TG curve of compound **2.**

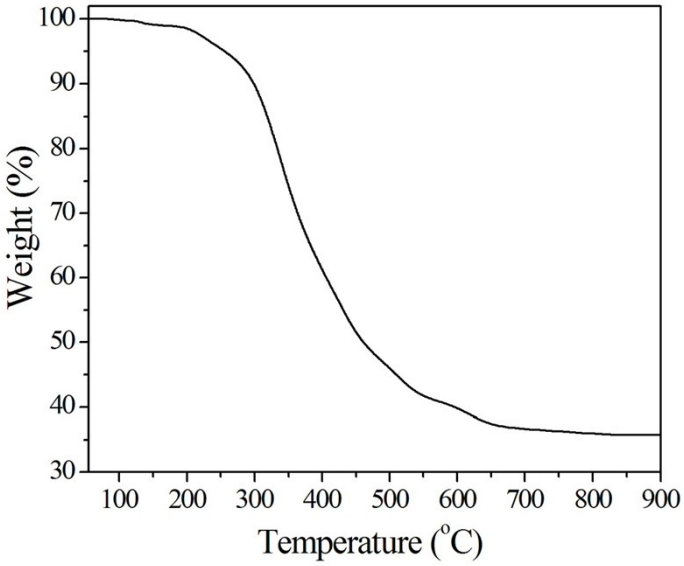

Fig. S9. The TG curve of compound **3.**

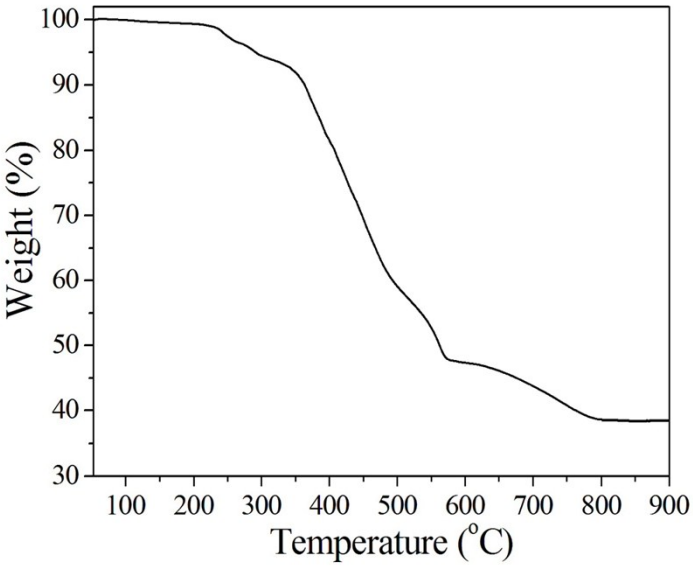

Fig. S10. The TG curve of compound **4.**

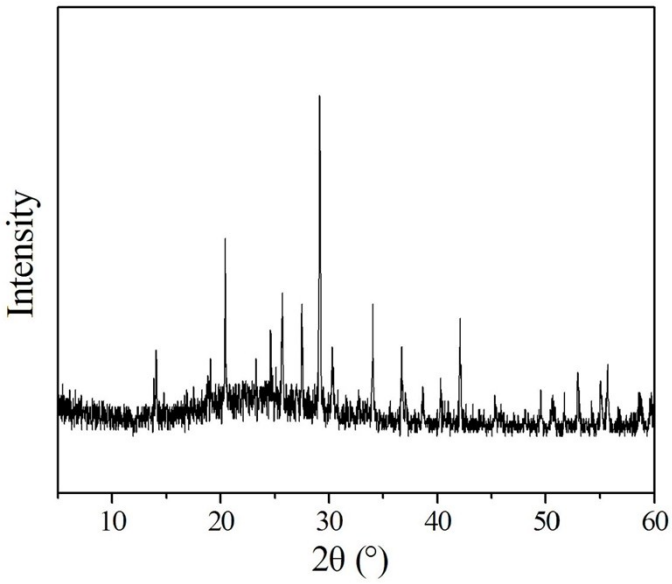

Fig. S11. The X–ray power diffraction pattern of the final product in the thermal decomposition for compound **3.** The final product is $Mn(PO_3)_2$ (JCPDS 00–029–0892).

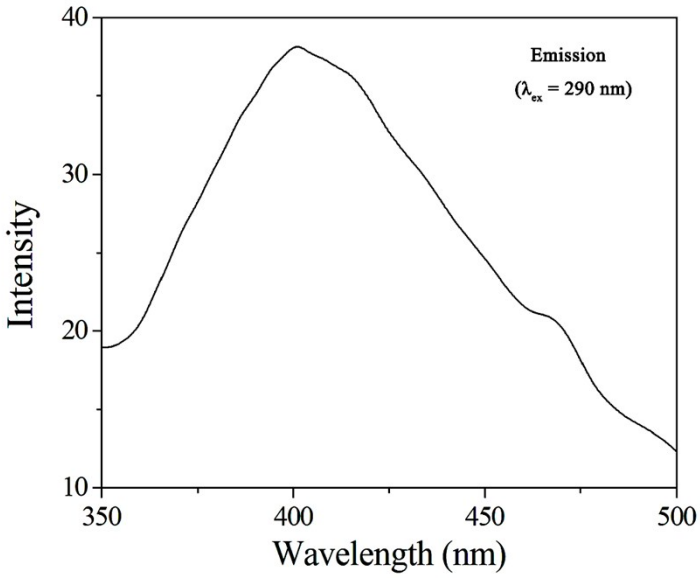

Fig. S12. Solid–state emission spectrum of phenylphosphonic acid (H_2L) at room

temperature.

Table S1 Selected bond lengths (Å) and angles (deg) for compound **1**

Cu(1)−O(4)	1.907(2)	P(2)−O(6)	1.512(3)
Cu(1)−O(7)	1.994(2)	P(2)−O(5)	1.552(3)
Cu(1)−N(2)	1.999(3)	P(2)−C(7)	1.794(4)
Cu(1)−N(1)	2.016(3)	P(3)−O(9)	1.519(3)
Cu(1)−O(1)	2.286(2)	P(3)−O(8)	1.517(3)
Cu(2)−O(6)	1.935(2)	P(3)−O(7)	1.529(3)
Cu(2)−O(1)	1.976(2)	P(3)−C(13)	1.804(4)
Cu(2)−N(3)	2.001(3)	P(4)−O(10)	1.496(10)
Cu(2)−N(4)	2.027(3)	P(4)−O(12)	1.494(8)
Cu(2)−O(7)	2.296(2)	P(4)−O(11)	1.559(11)
P(1)−O(2)	1.495(3)	P(4)−C(19)	1.814(6)
P(1)−O(1)	1.541(2)	P(4')−O(11')	1.513(14)
P(1)−O(3)	1.545(3)	P(4')−O(12')	1.513(11)
P(1)−C(1)	1.795(4)	P(4')−O(10')	1.540(15)
P(2)−O(4)	1.507(3)	P(4')−C(19)	1.834(8)
N(2)−Cu(1)−N(1)	81.15(13)	O(6)−Cu(2)−O(1)	95.13(10)
O(4)−Cu(1)−O(1)	91.51(10)	O(6)−Cu(2)−N(3)	90.11(11)
O(7)−Cu(1)−O(1)	80.50(9)	O(1)−Cu(2)−N(3)	169.69(11)
N(2)−Cu(1)−O(1)	95.07(11)	O(6)−Cu(2)−N(4)	169.66(11)
N(1)−Cu(1)−O(1)	114.93(10)	O(1)−Cu(2)−N(4)	92.27(11)
O(4)−Cu(1)−O(7)	94.86(11)	N(3)−Cu(2)−N(4)	81.50(12)
O(4)−Cu(1)−N(2)	169.93(12)	O(6)−Cu(2)−O(7)	93.21(10)
O(7)−Cu(1)−N(2)	93.74(12)	O(1)−Cu(2)−O(7)	80.64(9)
O(4)−Cu(1)−N(1)	89.17(12)	N(3)−Cu(2)−O(7)	107.98(10)
O(7)−Cu(1)−N(1)	164.00(11)	N(4)−Cu(2)−O(7)	95.11(10)

Table S2 Selected bond lengths (Å) and angles (deg) for compound **2**

Zn(1)−O(4)	1.9599(13)	P(1)−O(3)	1.5774(13)
Zn(1)−O(6)#1	1.9860(13)	P(1)−C(1)	1.802(2)
Zn(1)−O(1)	2.0326(13)	P(2)−O(6)	1.5009(13)
Zn(1)−N(1)	2.1241(16)	P(2)−O(4)	1.5070(14)
Zn(1)−N(2)	2.2143(16)	P(2)−O(5)	1.5625(13)
P(1)−O(1)	1.5014(13)	P(2)−C(7)	1.8015(19)
P(1)−O(2)	1.5076(14)		
O(4)−Zn(1)−O(6)#1	119.78(6)	O(1)−Zn(1)−N(1)	90.70(6)
O(4)−Zn(1)−O(1)	98.14(6)	O(4)−Zn(1)−N(2)	99.93(6)
O(6)#1−Zn(1)−O(1)	93.24(5)	O(6)#1−Zn(1)−N(2)	85.03(6)
O(4)−Zn(1)−N(1)	106.51(6)	O(1)−Zn(1)−N(2)	160.08(6)
O(6)#1−Zn(1)−N(1)	132.37(6)	N(1)−Zn(1)−N(2)	76.19(6)

Symmetry transformations used to generate equivalent atoms: #1 − x, − y, − z.

Table S3 Selected bond lengths (Å) and angles (deg) for compounds **3** and **4**

Compound **3**			
Mn(1)–O(7)	2.1163(13)	P(1)–C(1)	1.800(3)
Mn(1)–O(1)	2.1682(14)	P(2)–O(5)	1.4974(15)
Mn(1)–O(4)	2.2123(13)	P(2)–O(4)	1.5283(13)
Mn(1)–O(4)#1	2.2188(13)	P(2)–O(6)	1.5665(15)
Mn(1)–N(1)	2.2837(16)	P(2)–C(7)	1.793(2)
Mn(1)–N(2)	2.3551(17)	P(3)–O(7)	1.4869(14)
P(1)–O(2)	1.5065(15)	P(3)–O(8)	1.5356(17)
P(1)–O(1)	1.5112(14)	P(3)–O(9)	1.5623(16)
P(1)–O(3)	1.5682(16)	P(3)–C(13)	1.797(2)
O(7)–Mn(1)–O(1)	88.37(6)	O(4)–Mn(1)–N(1)	98.10(5)
O(7)–Mn(1)–O(4)	88.02(5)	O(4)#1–Mn(1)–N(1)	93.23(5)
O(1)–Mn(1)–O(4)	166.23(5)	O(7)–Mn(1)–N(2)	99.64(6)
O(7)–Mn(1)–O(4)#1	95.54(5)	O(1)–Mn(1)–N(2)	93.56(6)
O(1)–Mn(1)–O(4)#1	89.85(5)	O(4)–Mn(1)–N(2)	100.14(5)
O(4)–Mn(1)–O(4)#1	77.28(5)	O(4)#1–Mn(1)–N(2)	164.52(5)
O(7)–Mn(1)–N(1)	170.24(6)	N(1)–Mn(1)–N(2)	71.88(6)
O(1)–Mn(1)–N(1)	87.38(6)		
Compound **4**			
Cd(1)–O(7)	2.2265(19)	P(1)–C(1)	1.798(4)
Cd(1)–O(1)	2.291(2)	P(2)–O(5)	1.502(2)
Cd(1)–O(4)	2.3050(19)	P(2)–O(4)	1.5181(19)
Cd(1)–O(4)#1	2.3225(17)	P(2)–O(6)	1.566(2)
Cd(1)–N(1)	2.323(2)	P(2)–C(7)	1.792(3)
Cd(1)–N(2)	2.400(2)	P(3)–O(7)	1.485(2)
P(1)–O(2)	1.505(2)	P(3)–O(8)	1.522(3)
P(1)–O(1)	1.507(2)	P(3)–O(9)	1.555(2)
P(1)–O(3)	1.565(2)	P(3)–C(13)	1.805(4)
O(7)–Cd(1)–O(1)	87.86(8)	O(4)–Cd(1)–N(1)	99.16(7)
O(7)–Cd(1)–O(4)	85.11(7)	O(4)#1–Cd(1)– N(1)	92.92(7)
O(1)–Cd(1)–O(4)	160.27(7)	O(7)–Cd(1)–N(2)	102.73(8)
O(7)–Cd(1)–O(4)#1	93.25(7)	O(1)–Cd(1)–N(2)	96.02(8)
O(1)–Cd(1)–O(4)#1	85.96(7)	O(4)–Cd(1)–N(2)	103.50(7)
O(4)–Cd(1)–O(4)#1	76.07(7)	O(4)#1–Cd(1)–N(2)	163.95(7)
O(7)–Cd(1)–N(1)	173.19(8)	N(1)–Cd(1)–N(2)	71.20(8)

O(1)–Cd(1)–N(1)	89.72(8)

Symmetry transformations used to generate equivalent atoms: #1 – x, – y + 2, – z.