

Mixed-solvothermal synthesis, structures, luminescent and surface photovoltage properties of four new transition metal diphosphonates with a 3D supramolecular structure

Hui Tian, Yan-Yu Zhu, Zhen-Gang Sun,* Fei Tong, Jiang Zhu, Wei Chu, Shou-Hui Sun, Ming-Jing Zheng

Supplementary Materials

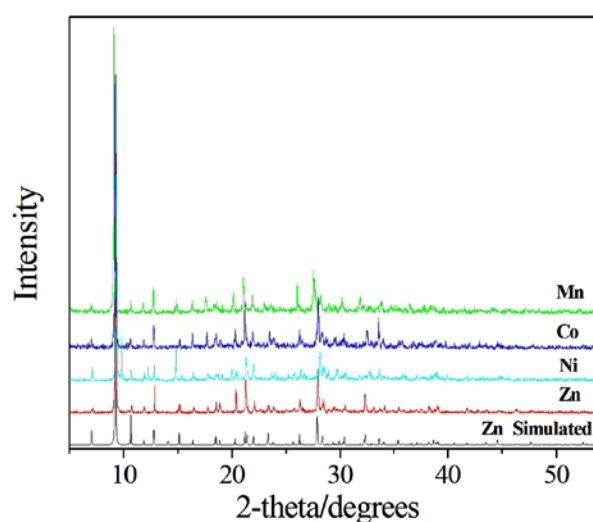


Fig. S1 The simulated XRD pattern of compound **4** (down) and experimental powder XRD patterns of compounds **1–4** (up).

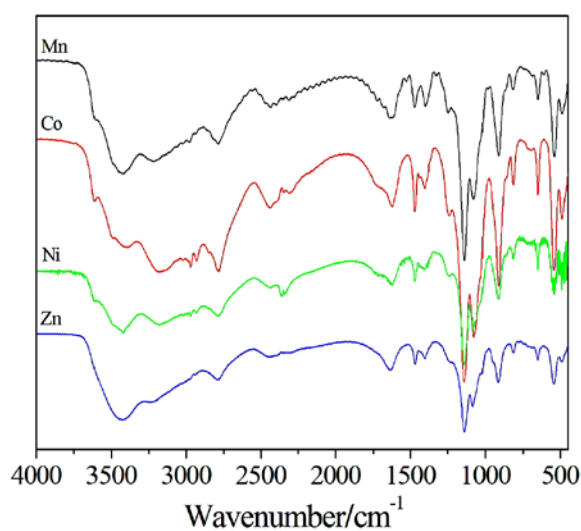


Fig. S2 IR spectra of compounds **1–4**.

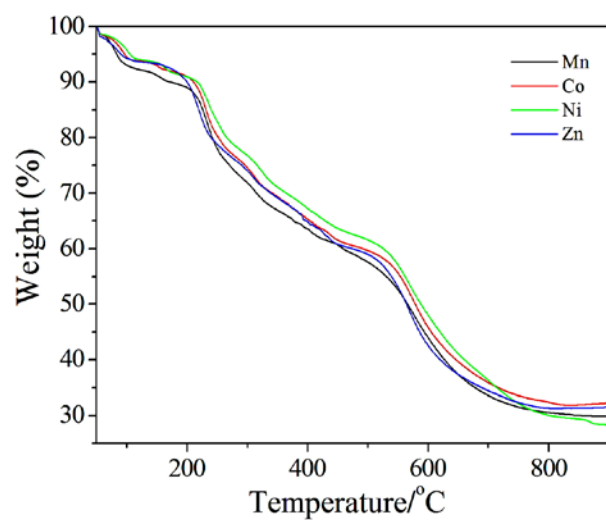


Fig. S3 TGA curves of compounds 1–4.

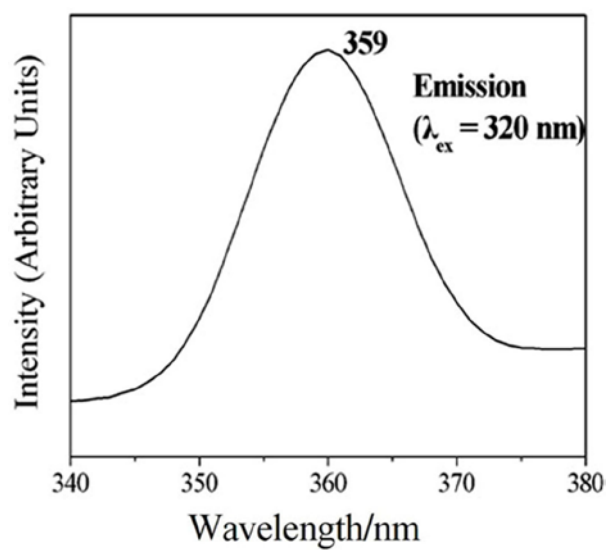


Fig. S4 Solid–state emission spectrum of hedpH₄ at room temperature.

Table S1. Selected bond lengths (Å) for compounds **1–4**

	1 (Mn)	2 (Co)	3 (Ni)	4 (Zn)
M(1)–O(1)#1	2.129(3)	2.074(3)	2.051(3)	2.057(4)
M(1)–O(1)#2	2.129(3)	2.074(3)	2.051(3)	2.057(4)
M(1)–O(1)	2.129(3)	2.074(3)	2.051(3)	2.057(4)
M(1)–O(7)#2	2.196(3)	2.126(2)	2.092(3)	2.137(4)
M(1)–O(7)#1	2.196(3)	2.126(2)	2.092(3)	2.137(4)
M(1)–O(7)	2.196(3)	2.126(2)	2.092(3)	2.137(4)

^a Symmetry transformations used to generate equivalent atoms: #1 $-x + y, -x + 1, z$; #2 $-y + 1, x - y + 1, z$.

Table S2 Selected angles (°) for compounds **1–4**

	1 (Mn)	2 (Co)	3 (Ni)	4 (Zn)
O(1)#1–M(1)–O(1)#2	94.35(13)	92.59(11)	91.37(12)	92.94(16)
O(1)#1–M(1)–O(1)	94.35(13)	92.59(11)	91.37(12)	92.94(16)
O(1)#2–M(1)–O(1)	94.35(13)	92.59(11)	91.37(12)	92.94(16)
O(1)#1–M(1)–O(7)#2	90.84(13)	90.51(11)	90.80(12)	92.12(15)
O(1)#2–M(1)–O(7)#2	89.27(12)	90.73(10)	91.56(11)	90.70(14)
O(1)–M(1)–O(7)#2	173.42(14)	175.34(11)	176.31(12)	174.40(16)
O(1)#1–M(1)–O(7)#1	89.27(12)	90.73(10)	91.56(11)	90.70(14)
O(1)#2–M(1)–O(7)#1	173.42(14)	175.34(11)	176.31(12)	174.40(16)
O(1)–M(1)–O(7)#1	90.84(13)	90.51(11)	90.80(12)	91.12(15)
O(7)#2–M(1)–O(7)#1	85.18(13)	85.98(11)	86.16(12)	84.97(15)
O(1)#1–M(1)–O(7)	173.42(14)	175.34(11)	176.31(12)	174.40(16)
O(1)#2–M(1)–O(7)	90.84(13)	90.51(11)	90.80(12)	91.12(15)
O(1)–M(1)–O(7)	89.27(12)	90.73(10)	91.56(11)	90.70(14)
O(7)#2–M(1)–O(7)	85.18(13)	85.98(11)	86.16(12)	84.97(15)
O(7)#1–M(1)–O(7)	85.18(13)	85.98(11)	86.16(12)	84.97(15)

^a Symmetry transformations used to generate equivalent atoms: #1 $-x + y, -x + 1, z$; #2 $-y + 1, x - y + 1, z$.