Electronic Supplementary Material (ESI) for RSC Advances.

Two novel oxovanadium–organophosphonate hybrids with a 3D supramolecular structure: synthesis, crystal structures, surface photovoltage and luminescent properties

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Supporting Information

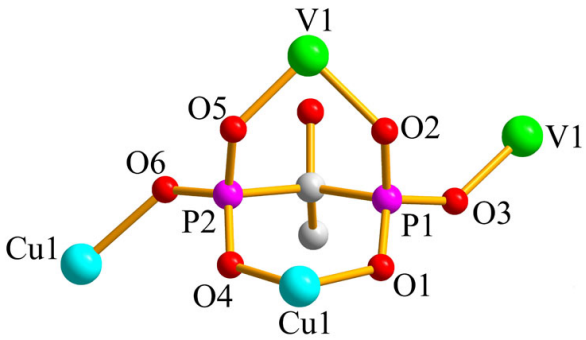

Fig. S1 The coordination mode of $hedpH_4$ in compound **1**.

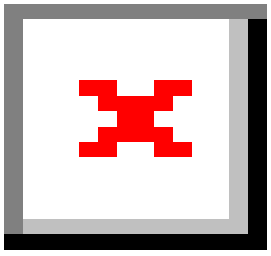

Fig. S2 The IR spectra of compounds **1** and **2**.

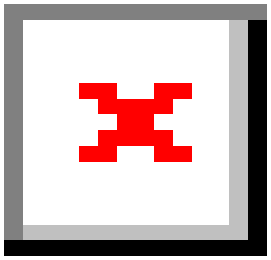

Fig. S3 The simulated XRD pattern of compound **1** (down) and experimental powder XRD patterns of compounds **1** and **2**.

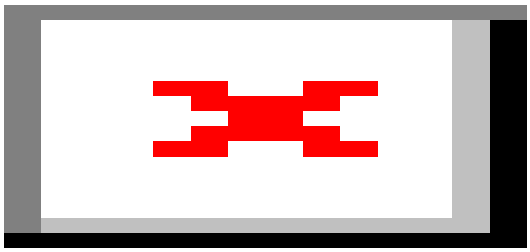

Fig. S4 The TG–DTG curves of compounds **1** (a), **2** (b).

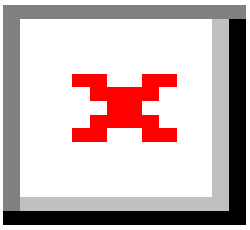

Fig. S5 Solid–state emission spectrum of hedpH_4 at room temperature.

Table S1 Selected bond lengths (Å) and angles (deg) for compounds **1** and **2**[a]

Compound **1**			
V(1)–O(9)	1.597(4)	Cu(1)–O(6)#1	2.152(3)
V(1)–O(5)	1.965(3)	P(1)–O(1)	1.507(3)
V(1)–O(3)#2	1.970(3)	P(1)–O(3)	1.523(4)
V(1)–O(2)	2.015(4)	P(1)–O(2)	1.549(4)
V(1)–O(8)	2.059(4)	P(1)–C(1)	1.830(6)
Cu(1)–O(4)	1.936(4)	P(2)–O(6)	1.511(4)
Cu(1)–O(1)	1.977(3)	P(2)–O(4)	1.519(4)
Cu(1)–N(1)	2.028(5)	P(2)–O(5)	1.529(4)
Cu(1)–N(2)	2.028(5)	P(2)–C(1)	1.837(5)
O(9)–V(1)–O(5)	102.68(18)	O(4)–Cu(1)–O(1)	92.45(15)
O(9)–V(1)–O(3)#2	102.54(18)	O(4)–Cu(1)–N(1)	91.47(18)
O(5)–V(1)–O(3)#2	154.31(16)	O(1)–Cu(1)–N(1)	160.92(17)
O(9)–V(1)–O(2)	98.07(18)	O(4)–Cu(1)–N(2)	170.41(19)
O(5)–V(1)–O(2)	90.95(14)	O(1)–Cu(1)–N(2)	92.71(17)
O(3)#2–V(1)–O(2)	90.32(15)	N(1)–Cu(1)–N(2)	81.1(2)
O(9)–V(1)–O(8)	101.69(18)	O(4)–Cu(1)–O(6)#1	92.77(14)
O(5)–V(1)–O(8)	86.39(15)	O(1)–Cu(1)–O(6)#1	109.05(14)
O(3)#2–V(1)–O(8)	83.80(15)	N(1)–Cu(1)–O(6)#1	89.39(16)
O(2)–V(1)–O(8)	160.17(15)	N(2)–Cu(1)–O(6)#1	93.18(17)
Compound **2**			
V(1)–O(9)	1.589(3)	Zn(1)–O(6)#1	1.961(3)
V(1)–O(5)	1.981(3)	P(1)–O(1)	1.510(3)
V(1)–O(3)#2	1.969(3)	P(1)–O(3)	1.522(3)
V(1)–O(2)	2.024(3)	P(1)–O(2)	1.543(3)
V(1)–O(8)	2.063(3)	P(1)–C(1)	1.842(4)
Zn(1)–O(4)	2.027(3)	P(2)–O(6)	1.522(3)
Zn(1)–O(1)	2.020(3)	P(2)–O(4)	1.508(3)
Zn(1)–N(1)	2.138(4)	P(2)–O(5)	1.537(3)
Zn(1)–N(2)	2.162(4)	P(2)–C(1)	1.842(4)
O(9)–V(1)–O(5)	102.47(15)	O(1)–Zn(1)–O(4)	92.21(11)
O(9)–V(1)–O(3)#2	102.94(15)	O(4)–Zn(1)–N(1)	90.06(14)
O(3)#2–V(1)–O(5)	154.04(13)	O(1)–Zn(1)–N(1)	146.60(14)
O(9)–V(1)–O(2)	98.86(14)	O(4)–Zn(1)–N(2)	160.65(14)
O(5)–V(1)–O(2)	91.30(12)	O(1)–Zn(1)–N(2)	91.10(13)
O(3)#2–V(1)–O(2)	89.95(11)	N(1)–Zn(1)–N(2)	76.87(15)
O(9)–V(1)–O(8)	100.71(15)	O(6)#1–Zn(1)–O(1)	115.48(12)
O(5)–V(1)–O(8)	86.24(12)	O(6)#1–Zn(1)–O(4)	96.35(12)
O(3)#2–V(1)–O(8)	83.95(12)	O(6)#1–Zn(1)–N(1)	97.34(14)
O(2)–V(1)–O(8)	160.35(12)	O(6)#1–Zn(1)–N(2)	99.41(14)

[a] Symmetry transformations used to generate equivalent atoms: #1 –x + 1/2, y + 1/2, –z + 1/2; #2 –x + 1/2, –y + 1/2, –z.

Table S2 The exploration of optimum experimental conditions of compounds **1** and **2**

Compound **1** ($NaVO_3 \cdot 2H_2O$/ $CuCl_2 \cdot 2H_2O$ /1,10−phen/$hedpH_4$)							
Molar ratio / Temperture (°C)	1:1:1:1	3:2:3:3	3:1:3:3	3:4:3:3	3:5:3:3	3:5:3:4	3:5:3:2
100	●	●	●	●	△	△	▲
120	●	△	△	■△	■	■△	▲
140	●	■△	■△	■△	■	■	▲
160	●	■△	■△	■△	▲	■	★
180	●	△	△	■△	■	●	▲
Compound **2** ($NaVO_3 \cdot 2H_2O/ZnSO_4 \cdot 7H_2O$/1,10−phen/$hedpH_4$)							
Molar ratio / Temperture (°C)	3:5:3:2	3:5:3:5	3:5:3:7	3:5:3:9	3:5:4:7	3:5:5:7	
100	●	●	●	●	●	▲	
120	●	●	●	▲	●	◆	
140	▲	▲	●	▲	▲	◆	
160	▲	▲	▲	▲	▲	★	
180	●	●	●	●	●	▲	

All the experiments were explored at reaction time of 72h

● Powders

△ Powders and red crystals

■ Powders and blue crystals

▲ Impure crystals or powders

◆ Green crystals but not good enough for X−ray diffraction study

★ Best green crystals