

Synthesis, structures, surface photovoltage and luminescent properties of two new nickel(II) carboxyphosphonates with a 3D framework structure

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Supplementary Materials

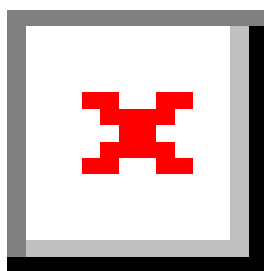


Fig. S1 The simulated XRD pattern of compound **1** (down) and experimental powder XRD pattern of compound **1** (up)

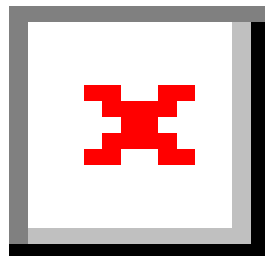


Fig. S2 The simulated XRD pattern of compound **2** (down) and experimental powder XRD pattern of compound **2** (up)

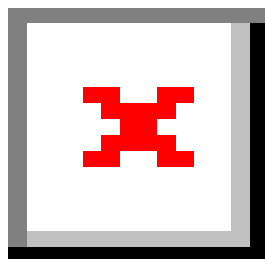
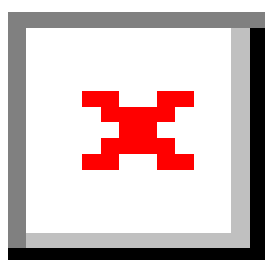


Fig. S3 The IR spectrum of compound 1.



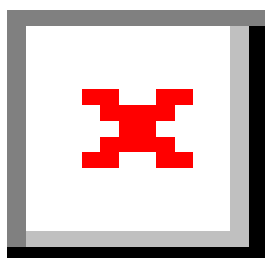


Fig. S4 The IR spectrum of compound **2**.

Fig. S5 The TG curve of compound **1**.

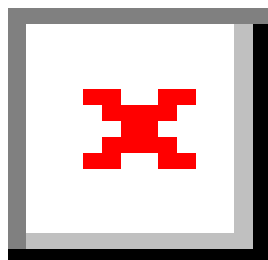


Fig. S6 The TG curve of compound **2**.

Fig. S7 The X-ray powder diffraction pattern of the final product in the thermal decomposition for compound **1**.

The final product is $\text{Ni}_2\text{P}_2\text{O}_7$ (JCPDS 01-074-1604).

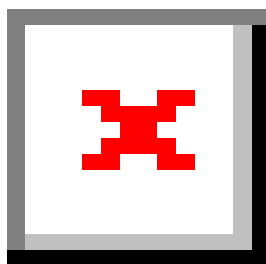


Fig. S8 The X-ray powder

final product in

for compound **2**.

$\text{Ni}_2\text{P}_2\text{O}_7$ (JCPDS 01-074-1604).

diffraction pattern of the

the thermal decomposition

The final product is

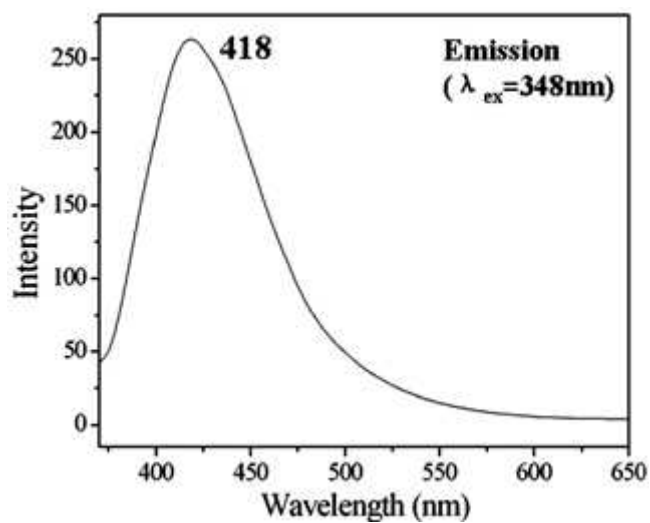


Fig. S9 Solid-state emission spectrum of 4,4'-bipy at room temperature.

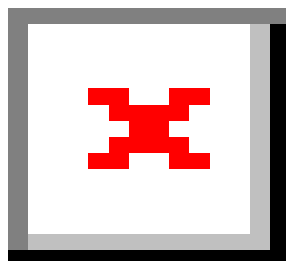


Fig. S10 Solid-state emission spectrum of H₃L at room temperature.

Table S1 Selected bond angles (°) for compounds **1** and **2**

Compound 1

O(4)–Ni(1)–O(1)	91.18(13)	O(9)–Ni(2)–O(10)#3	90.67(14)
O(4)–Ni(1)–O(3)#1	178.45(13)	O(2)–Ni(2)–O(10)	87.69(12)

O(8)#2–Ni(2)–N(3)	95.9	P(2)–O(4)–Ni(1)	114.5(3)
N(3)#2–Ni(2)–N(3)	179.75(10)		

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