Electronic Supplementary Material (ESI) for CrystEngComm
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Synthesis, crystal structures, and surface photovoltage properties of four new metal diphosphonates based on the mixed ligands

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Supporting Information

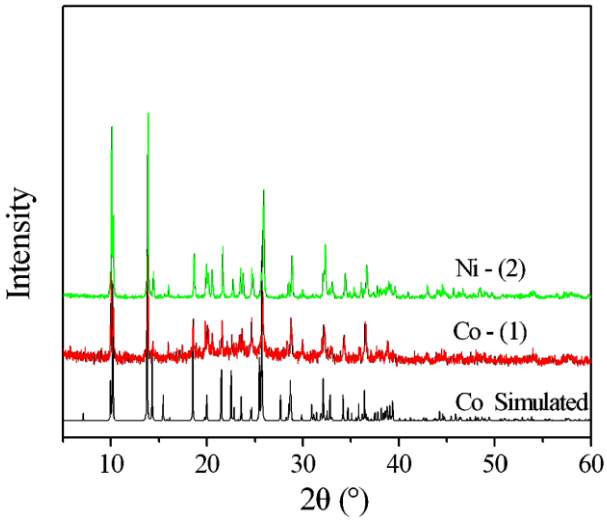

Fig. S1 The experimental powder XRD patterns of compounds **1** and **2** and the simulated XRD pattern of compound **1**.

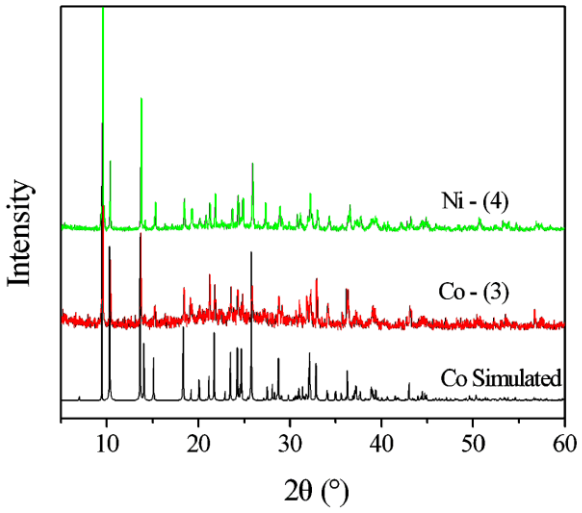

Fig. S2 The experimental powder XRD patterns of compounds **3** and **4** and the simulated XRD pattern of compound **3**.

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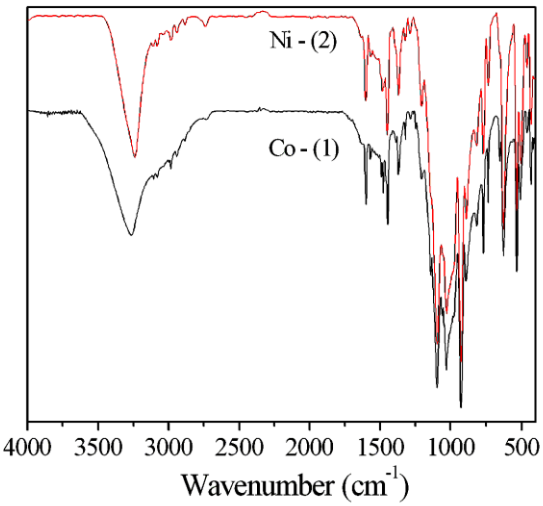

Fig. S3 The IR spectra of compounds **1** and **2**.

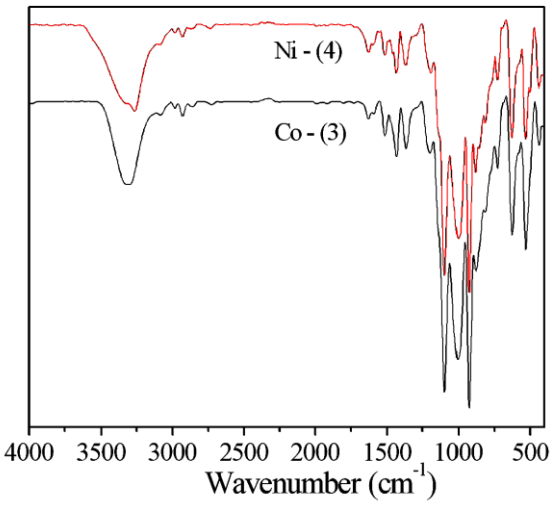

Fig. S4 The IR spectra of compounds **3** and **4**.

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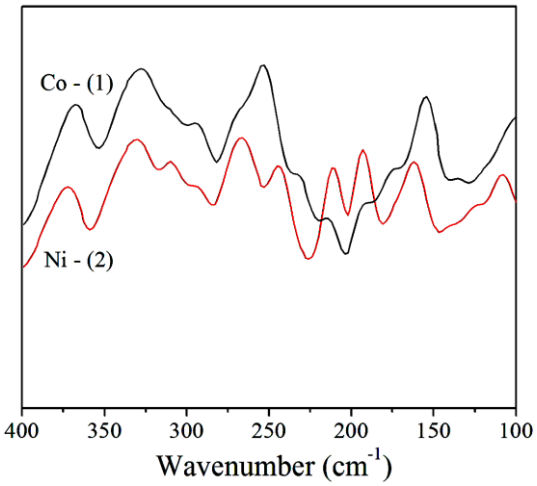

Fig. S5 The FIR spectra of compounds **1** and **2**.

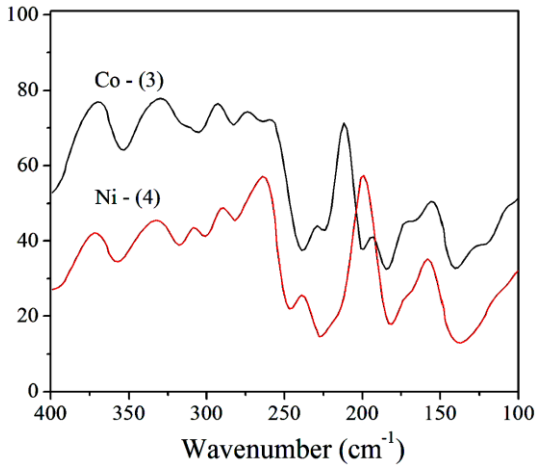

Fig. S6 The FIR spectra of compounds **3** and **4**.

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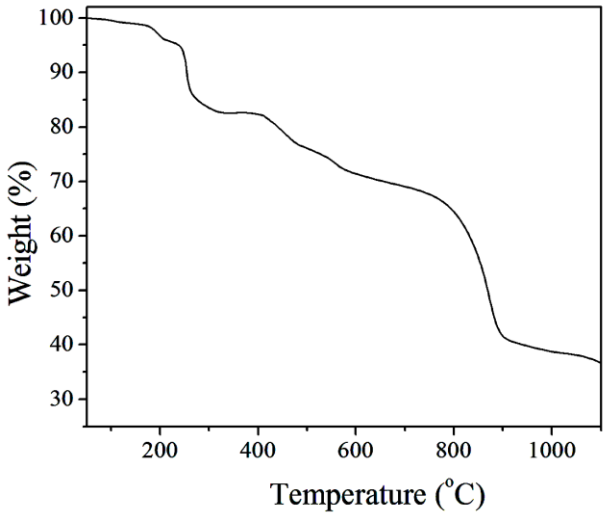

Fig. S7 The TG curve (5 K/min) of compound **2**.

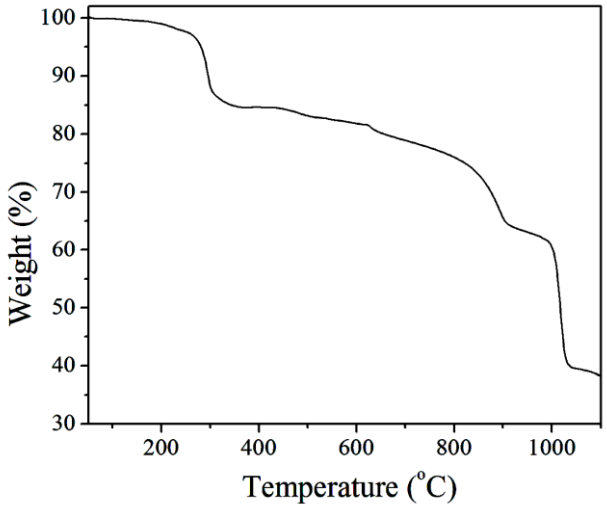

Fig. S8 The TG curve (5 K/min) of compound **4**.

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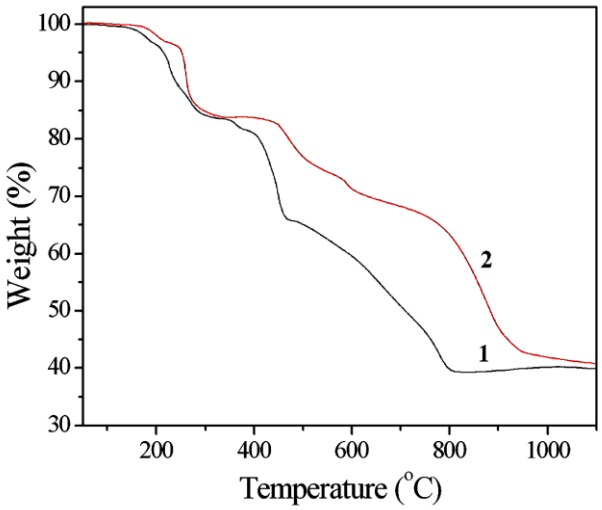

Fig. S9 The TG curves (10 K/min) of compounds **1** and **2**.

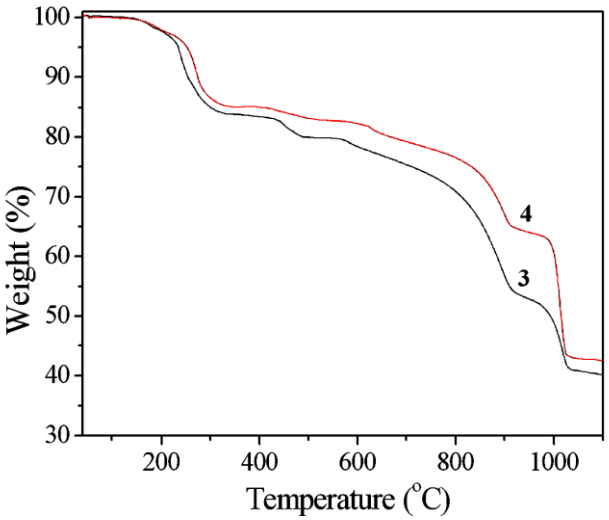

Fig. S10 The TG curves (10 K/min) of compounds **3** and **4**.

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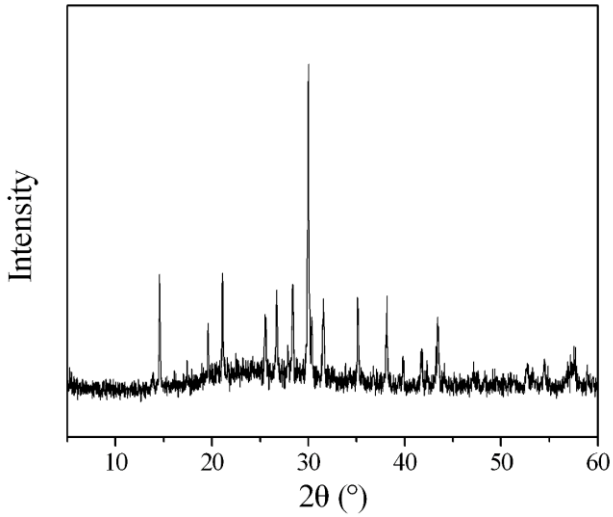

Fig. S11 The X–ray power diffraction patterns of the final product in the thermal decomposition for compound **2**. The final product is $Ni(PO_3)_2$ (JCPDS 00-028-0708).

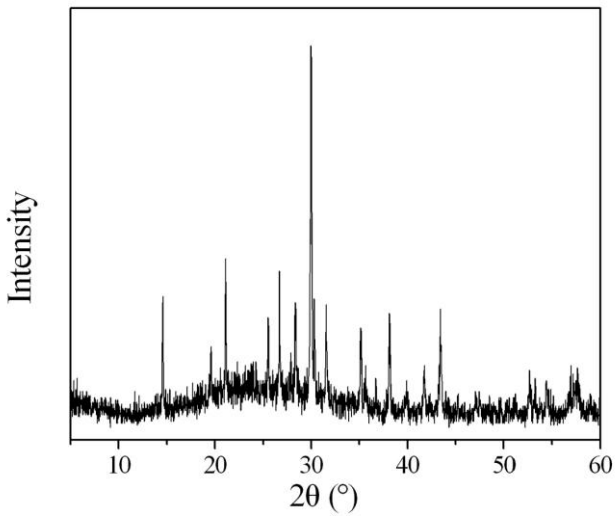

Fig. S12 The X–ray power diffraction patterns of the final product in the thermal decomposition for compound **4**. The final product is $Ni(PO_3)_2$ (JCPDS 00-028-0708).

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

Compound **1**			
Co(1)–N(1)#1	2.095(5)	P(1)–O(3)	1.514(4)
Co(1)–N(1)	2.095(5)	P(1)–O(1)	1.556(4)
Co(1)–O(6)#1	2.100(4)	P(1)–C(1)	1.834(5)
Co(1)–O(6)	2.100(4)	P(2)–O(6)	1.497(4)
Co(1)–O(3)#1	2.147(4)	P(2)–O(4)	1.544(4)
Co(1)–O(3)	2.147(4)	P(2)–O(5)	1.569(4)
P(1)–O(2)	1.508(4)	P(2)–C(1)	1.835(5)
N(1)#1–Co(1)–N(1)	78.5(3)	O(6)#1–Co(1)–O(3)#1	93.62(14)
N(1)#1–Co(1)–O(6)#1	98.39(17)	O(6)–Co(1)–O(3)#1	84.75(14)
N(1)–Co(1)–O(6)#1	176.84(17)	N(1)#1–Co(1)–O(3)	87.09(15)
N(1)#1–Co(1)–O(6)	176.84(17)	N(1)–Co(1)–O(3)	94.61(16)
N(1)–Co(1)–O(6)	98.39(17)	O(6)#1–Co(1)–O(3)	84.75(14)
O(6)#1–Co(1)–O(6)	84.8(2)	O(6)–Co(1)–O(3)	93.62(14)
N(1)#1–Co(1)–O(3)#1	94.61(16)	O(3)#1–Co(1)–O(3)	177.81(19)
N(1)–Co(1)–O(3)#1	87.09(15)		
Compound **2**			
Ni(1)–N(1)#1	2.046(5)	P(1)–O(3)	1.517(4)
Ni(1)–N(1)	2.046(5)	P(1)–O(1)	1.556(4)
Ni(1)–O(6)	2.076(4)	P(1)–C(1)	1.835(6)
Ni(1)–O(6)#1	2.076(4)	P(2)–O(6)	1.499(4)
Ni(1)–O(3)	2.116(4)	P(2)–O(5)	1.551(4)
Ni(1)–O(3)#1	2.116(4)	P(2)–O(4)	1.567(5)
P(1)–O(2)	1.508(4)	P(2)–C(1)	1.835(6)
N(1)#1–Ni(1)–N(1)	80.5(3)	O(6)–Ni(1)–O(3)	94.53(16)
N(1)#1–Ni(1)–O(6)	177.59(19)	O(6)#1–Ni(1)–O(3)	84.63(16)
N(1)–Ni(1)–O(6)	97.40(19)	N(1)#1–Ni(1)–O(3)#1	94.07(18)
N(1)#1–Ni(1)–O(6)#1	97.40(19)	N(1)–Ni(1)–O(3)#1	86.80(18)
N(1)–Ni(1)–O(6)#1	177.59(19)	O(6)–Ni(1)–O(3)#1	84.63(16)
O(6)–Ni(1)–O(6)#1	84.7(2)	O(6)#1–Ni(1)–O(3)#1	94.53(16)
N(1)#1–Ni(1)–O(3)	86.80(18)	O(3)–Ni(1)–O(3)#1	178.9(2)
N(1)–Ni(1)–O(3)	94.07(18)		

[a] Symmetry transformations used to generate equivalent atoms: #1 –x, y, –z + 3/2

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Table S2 Selected bond lengths (Å) and angles (deg) for compounds **3** and **4**[a]

Compound **3**			
Co(1)–O(1)#1	2.087(4)	P(1)–O(2)	1.509(4)
Co(1)–O(1)	2.087(4)	P(1)–O(3)	1.570(4)
Co(1)–N(1)	2.110(5)	P(1)–C(1)	1.835(6)
Co(1)–N(1)#1	2.110(5)	P(2)–O(6)	1.511(4)
Co(1)–O(6)	2.144(4)	P(2)–O(5)	1.541(4)
Co(1)–O(6)#1	2.144(4)	P(2)–O(4)	1.551(4)
P(1)–O(1)	1.499(4)	P(2)–C(1)	1.836(6)
O(1)#1–Co(1)–O(1)	85.9(2)	N(1)–Co(1)–O(6)	85.80(16)
O(1)#1–Co(1)–N(1)	97.27(18)	N(1)#1–Co(1)–O(6)	96.91(16)
O(1)–Co(1)–N(1)	176.68(18)	O(1)#1–Co(1)–O(6)#1	93.66(15)
O(1)#1–Co(1)–N(1)#1	176.68(18)	O(1)–Co(1)–O(6)#1	83.76(15)
O(1)–Co(1)–N(1)#1	97.27(18)	N(1)–Co(1)–O(6)#1	96.91(16)
N(1)–Co(1)–N(1)#1	79.6(3)	N(1)#1–Co(1)–O(6)#1	85.80(16)
O(1)#1–Co(1)–O(6)	83.76(15)	O(6)–Co(1)–O(6)#1	176.5(2)
O(1)–Co(1)–O(6)	93.66(15)		
Compound **4**			
Ni(1)–N(1)	2.062(5)	P(1)–O(2)	1.514(5)
Ni(1)–N(1)#1	2.062(5)	P(1)–O(3)	1.574(5)
Ni(1)–O(1)#1	2.063(4)	P(1)–C(1)	1.830(6)
Ni(1)–O(1)	2.063(4)	P(2)–O(6)	1.512(4)
Ni(1)–O(6)#1	2.115(4)	P(2)–O(5)	1.554(4)
Ni(1)–O(6)	2.115(4)	P(2)–O(4)	1.564(4)
P(1)–O(1)	1.503(4)	P(2)–C(1)	1.836(6)
N(1)–Ni(1)–N(1)#1	81.6(3)	O(1)#1–Ni(1)–O(6)#1	94.66(16)
N(1)–Ni(1)–O(1)#1	178.00(19)	O(1)–Ni(1)–O(6)#1	83.68(16)
N(1)#1–Ni(1)–O(1)#1	96.4(2)	N(1)–Ni(1)–O(6)	95.98(18)
N(1)–Ni(1)–O(1)	96.4(2)	N(1)#1–Ni(1)–O(6)	85.74(18)
N(1)#1–Ni(1)–O(1)	178.00(19)	O(1)#1–Ni(1)–O(6)	83.68(16)
O(1)#1–Ni(1)–O(1)	85.6(3)	O(1)–Ni(1)–O(6)	94.66(16)
N(1)–Ni(1)–O(6)#1	85.74(18)	O(6)#1–Ni(1)–O(6)	177.7(2)
N(1)#1–Ni(1)–O(6)#1	95.98(18)		

[a] Symmetry transformations used to generate equivalent atoms. For **3**: #1 –x, y, –z + 3/2; For **4**: #1 –x, y, –z + 1/2

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Table S3 Hydrogen bonds for compounds **1** and **3**

D–H···A	D(D–H)/ Å	*d*(H···A)/ Å	D–H–A/deg	*d*(D···A)/ Å
		compound **1**		
O1W–H1WA···O7	0.85	2.40	166.8	3.237(8)
		compound **3**		
O4–H4A···O6	0.85	1.82	164.9	2.644(6)