

Supporting Information

for

Cobalt coordination polymers regulated by *in situ* ligand transformation

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Table S1 Selected bond lengths (Å) for compounds **1-3**.

Compound 1			
Co1-O16 ¹	2.090(2)	Co1-O16	2.090(2)
Co1-O33	2.089(2)	Co1-O33 ¹	2.089(2)
Co1-N1 ²	2.182(3)	Co1-N1 ³	2.182(3)
Compound 2			
Co1-O3 ¹	2.109(1)	Co1-O3	2.109(4)
Co1-N4 ¹	2.157(2)	Co1-N4	2.157(2)
Co1-O1 ²	2.066(2)	Co1-O1 ³	2.066(2)
Compound 3			
Co1-O0AA	2.091(1)	Co1-O0AA ¹	2.091(1)
Co1-O1 ²	2.169(2)	Co1-O1 ³	2.169(2)
Co1-O2AA	2.093(1)	Co1-O2AA ¹	2.093(1)
Co2-N7	2.248(2)	Co2-O2 ⁴	2.051(2)
Co2-O1AA ⁵	2.062(2)	Co2-O2AA ⁵	2.127(1)
Co2 O2AA	2.097(2)	Co2-O3AA	2.108(2)

Symmetry codes for **1**: ¹1-X,1-Y,1-Z; ²1-X,1+Y,3/2-Z; ³+X,-Y,-1/2+Z; for **2**: ¹-X,-Y,-Z; ²-1+X,1+Y,+Z; ³1-X,-1-Y,-Z; for **3**: ¹2-X,1-Y,-Z; ²+X,+Y,-1+Z; ³2-X,1-Y,1-Z; ⁴1-X,1-Y,1-Z; ⁵1-X,1-Y,-Z.

Table S2. Selected hydrogen bond lengths (Å) in compounds **1** and **2**.

Compound 1			
O-H···O	2.663(1)	N-H···O O-H···N	2.789(2) 2.849(2)
	2.742(1)		
	2.788(2)		
	2.792(1)		
	2.845(2)		
Compound 2			
O-H···O	2.684(1)	O-H···N	3.825(2)
	2.721(1)		

Figure Captions

Fig. S1. ^1H NMR of **HL**_{1a}.

Fig. S2. View of the hydrogen-bonded structural motifs in compounds **1** (a) and **2** (b).

Fig. S3. A view of the 3D packing structure of compound **1**.

Fig. S4. A view of the 3D packing structure of compound **2**.

Fig. S5. Coordination modes for the organic ligand in compound **1-3**.

Fig. S6. Experimental and simulated PXRD patterns of compound **1**.

Fig. S7. Experimental and simulated PXRD patterns of compound **2**.

Fig. S8. CV curves for **HL**₁ in acetonitrile.

Fig. S9. Experimental and simulated PXRD patterns of compound **3**.

Fig. S10. TG curves of compounds **1-3**.

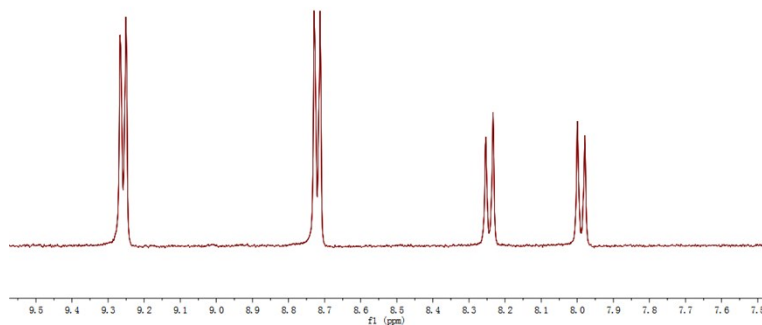


Fig. S1 ^1H NMR of **HL**_{1a} (dissolved in 20 μL of DCl (35 wt% in D_2O), $\text{DMSO-}d^6$): 9.26 (*d*, $J = 6.6$ Hz, 4H, Py-H), 8.72 (*d*, $J = 6.7$ Hz, 4H, Py-H), 8.24 (*d*, $J = 8.1$ Hz, 2H, Ar-H), 7.99 (*d*, $J = 8.2$ Hz, 2H, Ar-H)

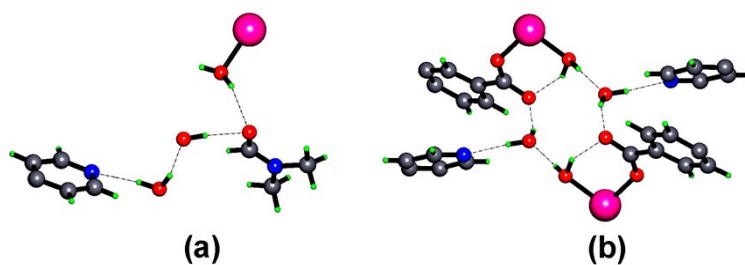


Fig. S2

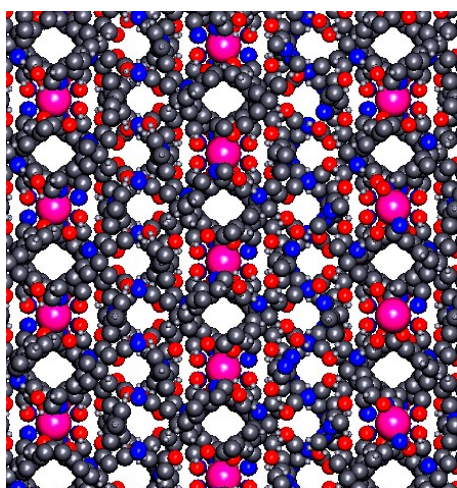


Fig. S3

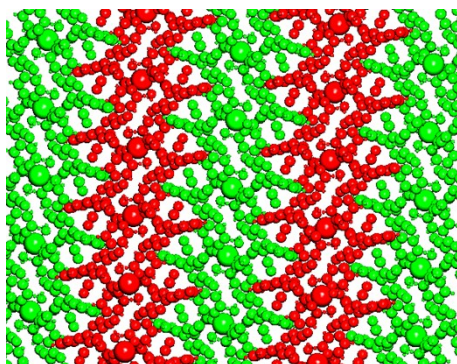


Fig. S4

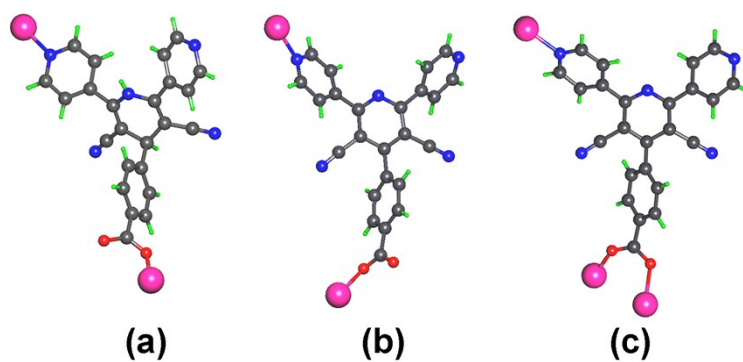


Fig. S5

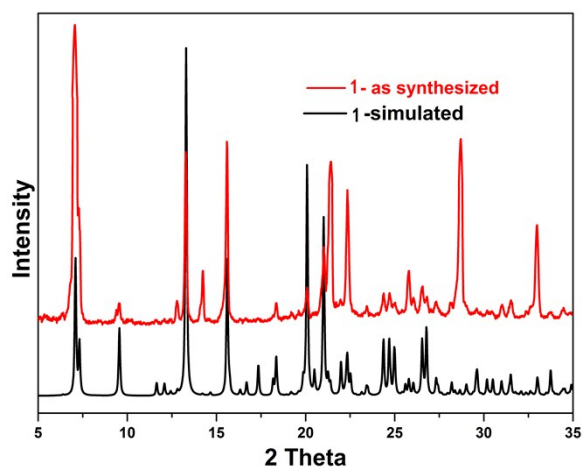


Fig. S6

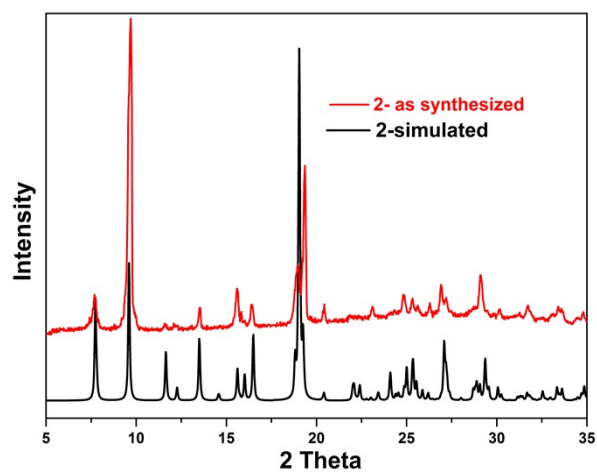


Fig. S7

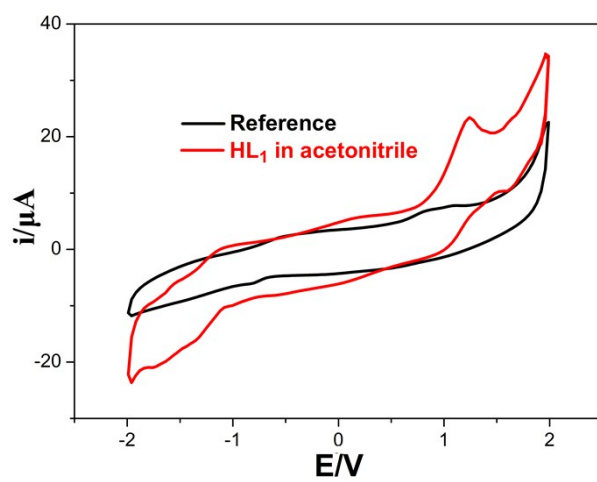


Fig. S8

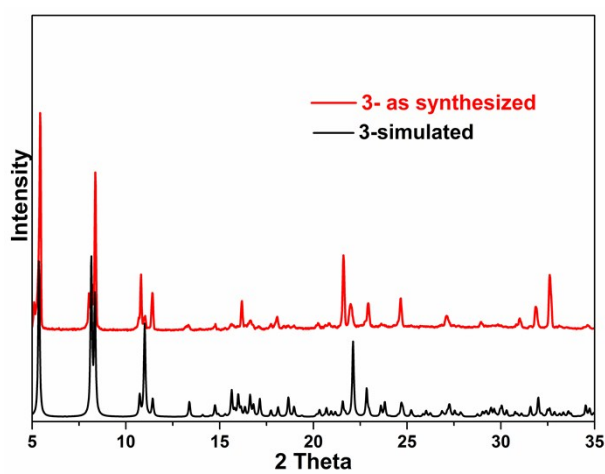


Fig. S9

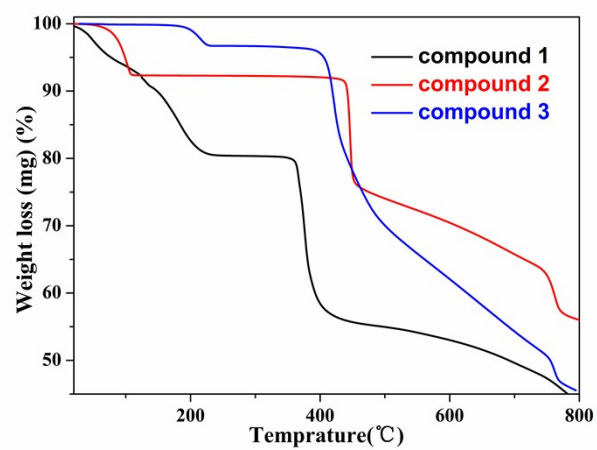


Fig. S10