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Genuine supramolecular isomers based on Y-shaped pyridinedicarboxylate ligand with distinct topologies: 2D 6^3 layer, *kgd* layer to 3D *rtl* Net

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Table S1. Selected bond lengths [Å] and angles [°] for **1a-1c**.

1a			
Co(1)-O(1)	1.989(5)	Co(1)-N(1b)	2.085(6)
Co(1)-O(4a)	2.010(5)	Co(1)-O(1W)	2.141(6)
Co(1)-O(2W)	2.075(6)		
O(1)-Co(1)-O(4a)	126.6(2)	O(2W)-Co(1)-N(1b)	94.8(3)
O(1)-Co(1)-O(2W)	96.5(3)	O(1)-Co(1)-O(1W)	85.7(2)
O(4a)-Co(1)-O(2W)	91.4(3)	O(4a)-Co(1)-O(1W)	86.2(2)
O(1)-Co(1)-N(1b)	133.5(2)	O(2W)-Co(1)-O(1W)	177.5(2)
O(4a)-Co(1)-N(1b)	97.9(2)	N(1b)-Co(1)-O(1W)	84.5(3)

Symmetry transformations used to generate equivalent atoms: a) x+1, y, z+1; b) -x+1, y-1/2, -z+3/2.

1b			
Co(1)-O(3c)	2.0394(16)	Co(1)-O(1)	2.1207(15)
Co(1)-O(1W)	2.090(2)	Co(1)-N(1a)	2.1511(18)
Co(1)-O(2W)	2.1115(19)	Co(1)-O(1b)	2.2050(15)
O(3c)-Co(1)-O(1W)	95.14(8)	O(2W)-Co(1)-N(1a)	177.18(8)
O(3c)-Co(1)-O(2W)	90.25(7)	O(1)-Co(1)-N(1a)	90.90(6)
O(1W)-Co(1)-O(2W)	90.36(8)	O(3c)-Co(1)-O(1b)	94.04(7)
O(3c)-Co(1)-O(1)	173.66(6)	O(1W)-Co(1)-O(1b)	170.82(7)
O(1W)-Co(1)-O(1)	90.89(8)	O(2W)-Co(1)-O(1b)	89.45(7)
O(2W)-Co(1)-O(1)	91.68(7)	O(1)-Co(1)-O(1b)	79.95(6)
O(3c)-Co(1)-N(1a)	87.06(7)	N(1a)-Co(1)-O(1b)	89.89(6)
O(1W)-Co(1)-N(1a)	90.72(8)		

Symmetry transformations used to generate equivalent atoms: a) -x+2, -y+1, -z+2; b) -x+1,-y+1,-z+2; c) x-1, y, z-1.

1c			
Co(1)-O(4)	2.069(2)	Co(3)-O(8)	2.063(2)
Co(1)-O(2W)	2.088(2)	Co(3)-O(5W)	2.091(2)
Co(1)-O(1W)	2.095(2)	Co(3)-O(6W)	2.100(2)
Co(1)-O(10a)	2.128(2)	Co(3)-O(1)	2.136(2)
Co(1)-N(3b)	2.152(3)	Co(3)-N(1e)	2.158(3)
Co(1)-O(3c)	2.195(2)	Co(3)-O(13)	2.192(2)
Co(2)-O(16d)	2.049(2)	Co(4)-O(11)	2.071(2)
Co(2)-O(4W)	2.080(3)	Co(4)-O(8W)	2.076(2)
Co(2)-O(3W)	2.111(2)	Co(4)-O(7W)	2.107(2)
Co(2)-O(5e)	2.128(2)	Co(4)-O(13)	2.130(2)
Co(2)-N(2)	2.162(3)	Co(4)-N(4g)	2.175(3)
Co(2)-O(10f)	2.179(2)	Co(4)-O(1)	2.204(2)
O(4)-Co(1)-O(2W)	95.03(10)	O(8)-Co(3)-O(5W)	93.96(10)
O(4)-Co(1)-O(1W)	99.90(10)	O(8)-Co(3)-O(6W)	99.92(10)
O(2W)-Co(1)-O(1W)	90.79(10)	O(5W)-Co(3)-O(6W)	90.30(10)
O(4)-Co(1)-O(10a)	94.41(9)	O(8)-Co(3)-O(1)	95.25(9)
O(2W)-Co(1)-O(10a)	169.75(9)	O(5W)-Co(3)-O(1)	170.29(9)
O(1W)-Co(1)-O(10a)	91.52(9)	O(6W)-Co(3)-O(1)	91.15(9)
O(4)-Co(1)-N(3b)	86.39(10)	O(8)-Co(3)-N(1e)	85.81(10)
O(2W)-Co(1)-N(3b)	86.02(10)	O(5W)-Co(3)-N(1e)	86.34(10)
O(1W)-Co(1)-N(3b)	173.19(10)	O(6W)-Co(3)-N(1e)	173.56(10)
O(10a)-Co(1)-N(3b)	90.60(9)	O(1)-Co(3)-N(1e)	91.26(9)
O(4)-Co(1)-O(3c)	173.70(9)	O(8)-Co(3)-O(13)	174.16(9)
O(2W)-Co(1)-O(3c)	90.24(9)	O(5W)-Co(3)-O(13)	90.46(9)
O(1W)-Co(1)-O(3c)	83.44(9)	O(6W)-Co(3)-O(13)	83.86(9)
O(10a)-Co(1)-O(3c)	80.11(8)	O(1)-Co(3)-O(13)	80.15(8)
N(3b)-Co(1)-O(3c)	90.55(9)	N(1e)-Co(3)-O(13)	90.67(9)
O(16d)-Co(2)-O(4W)	95.50(11)	O(11)-Co(4)-O(8W)	95.53(10)
O(16d)-Co(2)-O(3W)	97.39(10)	O(11)-Co(4)-O(7W)	98.81(9)
O(4W)-Co(2)-O(3W)	91.21(10)	O(8W)-Co(4)-O(7W)	89.56(10)
O(16d)-Co(2)-O(5e)	97.57(10)	O(11)-Co(4)-O(13)	94.34(9)
O(4W)-Co(2)-O(5e)	166.62(10)	O(8W)-Co(4)-O(13)	170.04(9)
O(3W)-Co(2)-O(5e)	89.92(9)	O(7W)-Co(4)-O(13)	90.29(9)
O(16d)-Co(2)-N(2)	85.37(10)	O(11)-Co(4)-N(4g)	86.61(10)
O(4W)-Co(2)-N(2)	86.42(10)	O(8W)-Co(4)-N(4g)	87.19(10)
O(3W)-Co(2)-N(2)	176.52(10)	O(7W)-Co(4)-N(4g)	173.93(10)
O(5e)-Co(2)-N(2)	91.81(9)	O(13)-Co(4)-N(4g)	92.03(9)
O(16d)-Co(2)-O(10f)	177.26(10)	O(11)-Co(4)-O(1)	173.97(9)

O(4W)-Co(2)-O(10f)	86.35(10)	O(8W)-Co(4)-O(1)	90.08(9)
O(3W)-Co(2)-O(10f)	84.57(9)	O(7W)-Co(4)-O(1)	83.42(9)
O(5e)-Co(2)-O(10f)	80.48(8)	O(13)-Co(4)-O(1)	80.01(8)
N(2)-Co(2)-O(10f)	92.73(9)	N(4g)-Co(4)-O(1)	91.46(9)

Symmetry transformations used to generate equivalent atoms: a) -x-3, -y, -z; b) -x-2, -y, -z; c) -x, -y, -z+1; d) -x-4, -y-1, -z; e) x-1, y, z; f) x+2, y, z+1; g) x+1, y, z.

Table S2. Ratio effects in the syntheses of **1a**, **1b** and **1c** under hydro(solvo)thermal conditions (R: the mole ratio of $CoCl_2$:H_2cpna; ▲: **1a**; ●: **1b**; ■: **1c**).

Isomers \ R	1:1	2:1	3:1	4:1	5:1	6:1
▲ **1a**	▲	▲				
● **1b**			●	●	●	●
■ **1c**			■	■	■	■
			●	●	●	●
			■	■	■	■

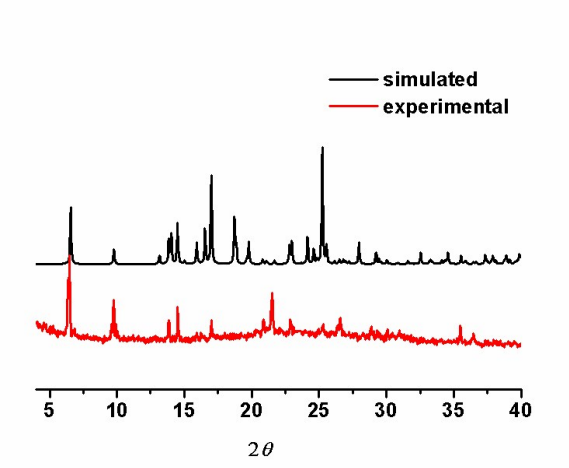


Figure S1. PXRD patterns of isomer **1a**. Black: Simulated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

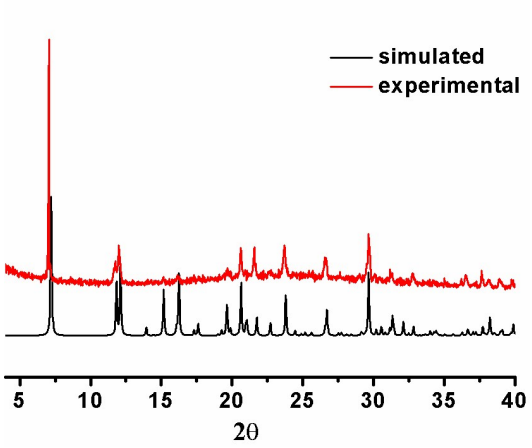


Figure S2. PXRD patterns of isomer **1b**. Black: Simulated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

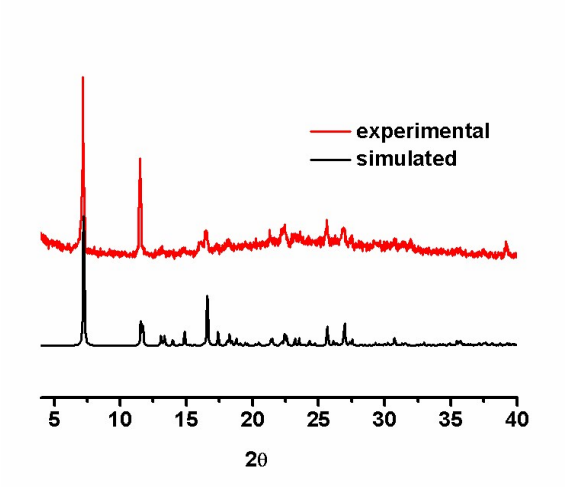


Figure S3. PXRD patterns of isomer **1c**. Black: Simulated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

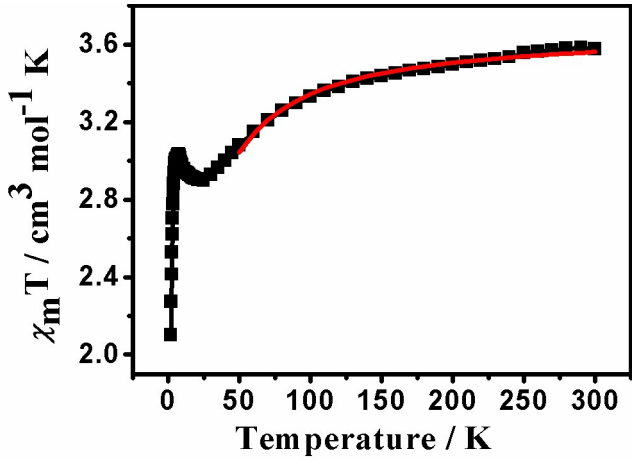


Figure S4. The best-fit (red line) of $\chi_m T$ versus T curve at 50-300 K for **1b** according

eqn (1).

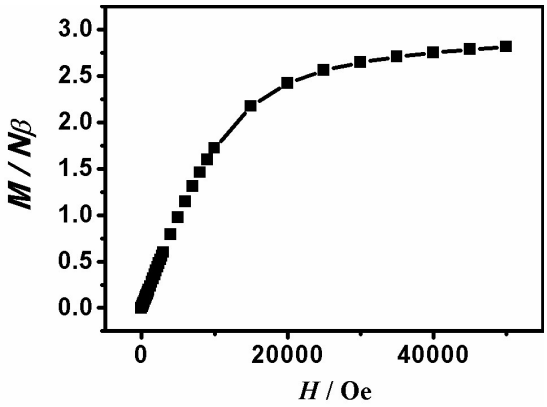


Figure S5. The *M* versus *H* plots for **1b** measured at 2 K.

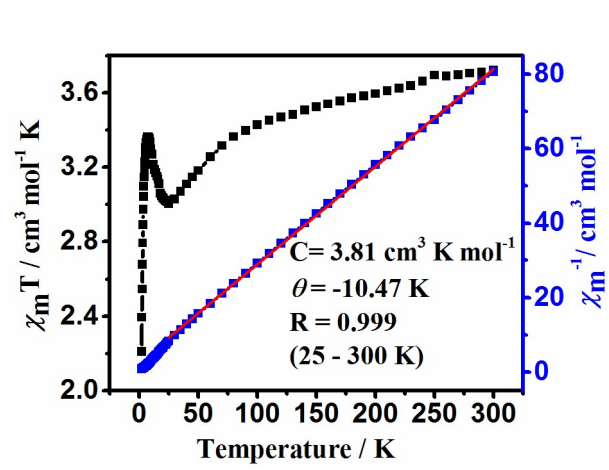


Figure S6. The $\chi_m T$ versus T and χ_m versus T curves measured under an applied field of 1000 Oe for **1c**. The solid lines represent the best linear fit results with the parameters.

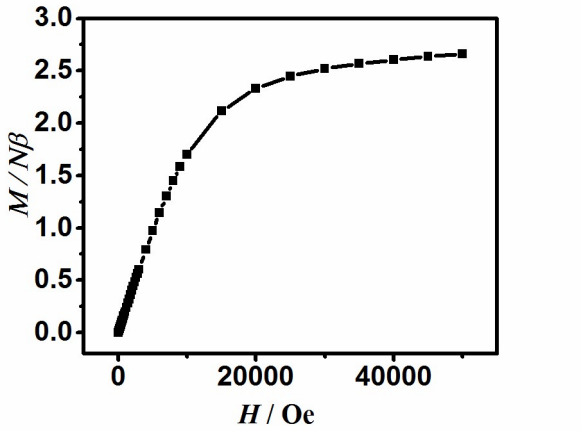


Figure S7. The *M* versus *H* plots for **1c** measured at 2 K.

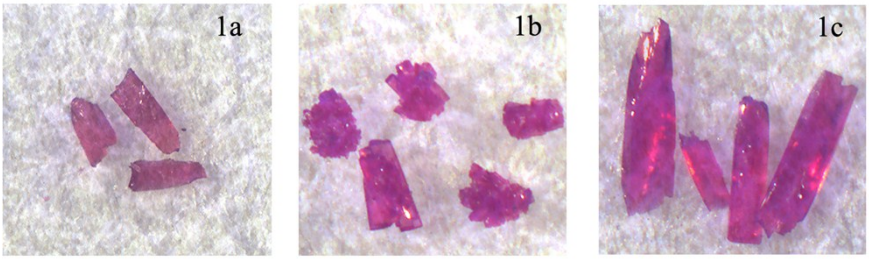
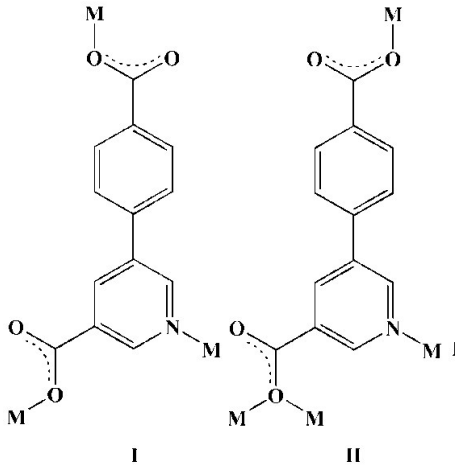


Figure S8. Crystal photos of 1a, 1b and 1c.



Scheme S1. Schematic views of the coordination modes seen in compounds **1a-1c** (mode I in **1a**, mode II in **1b** and **1c**).