

Supporting Information for

Structural Diversity of Four Metal-Organic Frameworks Based

on Linear Homo/Heterotrimeric Nodes with

Furan-2,5-dicarboxylic Acid: Crystal Structures, Luminescent

and Magnetic Properties

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Table S1. Selected Bond Lengths (Å) and angles for the Nine Compounds.

1			
Co(1)-O(10)#1	2.038(2)	Co(2)-O(1)	2.041(2)
Co(1)-O(10)	2.038(2)	Co(2)-O(7)	2.052(2)
Co(1)-O(9)	2.133(2)	Co(2)-O(6)	2.074(2)
Co(1)-O(9)#1	2.133(2)	Co(2)-O(11)	2.093(2)
Co(1)-O(5)#1	2.139(2)	Co(2)-O(5)	2.108(2)
Co(1)-O(5)	2.139(2)	Co(2)-O(4)	2.309(2)
O(10)#1-Co(1)-O(10)	180.0	O(5)-Co(2)-O(4)	59.39(8)
O(10)#1-Co(1)-O(9)	88.59(9)	O(1)-Co(2)-O(7)	95.98(9)
O(10)-Co(1)-O(9)	91.42(9)	O(1)-Co(2)-O(6)	86.89(9)
O(10)#1-Co(1)-O(9)#1	91.41(9)	O(7)-Co(2)-O(6)	89.63(9)
O(10)-Co(1)-O(9)#1	88.58(9)	O(1)-Co(2)-O(11)	89.55(9)
O(9)-Co(1)-O(9)#1	180.0	O(7)-Co(2)-O(11)	91.57(10)
O(10)#1-Co(1)-O(5)#1	90.95(9)	O(6)-Co(2)-O(11)	176.34(10)
O(10)-Co(1)-O(5)#1	89.05(9)	O(1)-Co(2)-O(5)	161.87(9)
O(9)-Co(1)-O(5)#1	90.02(8)	O(7)-Co(2)-O(5)	102.15(9)
O(9)#1-Co(1)-O(5)#1	89.98(8)	O(6)-Co(2)-O(5)	93.37(9)

O(10)#1-Co(1)-O(5)	89.05(9)	O(11)-Co(2)-O(5)	89.76(9))
O(10)-Co(1)-O(5)	90.95(9)	O(1)-Co(2)-O(4)	102.50(9)
O(9)-Co(1)-O(5)	89.98(8)	O(7)-Co(2)-O(4)	161.27(9)
O(9)#1-Co(1)-O(5)	90.02(8)	O(6)-Co(2)-O(4)	94.33(9)
O(5)#1-Co(1)-O(5)	180.00(10)	O(11)-Co(2)-O(4)	85.63(10)
Co(2)-O(5)-Co(1)	112.00(10)		

2

Co(1)-O(5)#1	2.064(5)	Co(1)-O(3)#3	2.206(4)
Co(1)-O(5)	2.064(5)	Co(2)-O(8)#1	1.984(5)
Co(1)-O(7)#1	2.174(5)	Co(2)-O(4)	2.005(5)
Co(1)-O(7)	2.175(5)	Co(2)-O(9)#4	2.025(5)
Co(1)-O(3)#2	2.206(4)	Co(2)-O(3)#3	2.057(5)
O(5)#1-Co(1)-O(5)	180.0	O(5)-Co(1)-O(3)#3	86.58(18)
O(5)#1-Co(1)-O(7)#1	86.2(2)	O(7)#1-Co(1)-O(3)#3	91.91(17)
O(5)-Co(1)-O(7)#1	93.8(2)	O(7)-Co(1)-O(3)#3	88.09(17)
O(5)#1-Co(1)-O(7)	93.8(2)	O(3)#2-Co(1)-O(3)#3	179.998(1)
O(5)-Co(1)-O(7)	86.2(2)	O(8)#1-Co(2)-O(4)	98.2(2)
O(7)#1-Co(1)-O(7)	180.0(2)	O(8)#1-Co(2)-O(9)#4	97.8(2)
O(5)#1-Co(1)-O(3)#2	86.58(18)	O(4)-Co(2)-O(9)#4	108.30(19)
O(5)-Co(1)-O(3)#2	93.42(18)	O(8)#1-Co(2)-O(3)#3	107.1(2)
O(7)#1-Co(1)-O(3)#2	88.09(17)	O(4)-Co(2)-O(3)#3	104.29(19)
O(7)-Co(1)-O(3)#2	91.91(17)	O(9)#4-Co(2)-O(3)#3	135.2(2)
O(5)#1-Co(1)-O(3)#3	93.42(18)	Co(2)#5-O(3)-Co(1)#5	104.47(18)

3

Gd(1)-O(4)#1	2.288(8)	Gd(1)-O(7)#2	2.614(6)
Gd(1)-O(5)	2.300(7)	Co(1)-O(11)#3	2.029(6)
Gd(1)-O(10)	2.354(6)	Co(1)-O(11)	2.029(6)
Gd(1)-O(13)	2.436(8)	Co(1)-O(7)#4	2.086(6)
Gd(1)-O(3)	2.469(6)	Co(1)-O(7)#2	2.086(6)
Gd(1)-O(12)	2.484(7)	Co(1)-O(3)#3	2.110(6)

Gd(1)-O(8)#2	2.485(7)	Co(1)-O(3)	2.110(6)
Gd(1)-O(2)	2.538(6)	O(4)#1-Gd(1)-O(10)	150.0(3)
O(4)#1-Gd(1)-O(5)	100.3(3)	O(5)-Gd(1)-O(10)	76.4(2)
O(4)#1-Gd(1)-O(13)	80.4(3)	O(5)-Gd(1)-O(13)	138.7(3)
O(10)-Gd(1)-O(13)	83.0(3)	O(4)#1-Gd(1)-O(3)	126.5(3)
O(5)-Gd(1)-O(3)	73.8(2)	O(10)-Gd(1)-O(3)	81.8(2)
O(13)-Gd(1)-O(3)	138.2(3)	O(4)#1-Gd(1)-O(12)	72.4(3)
O(5)-Gd(1)-O(12)	72.3(3)	O(10)-Gd(1)-O(12)	78.3(2)
O(13)-Gd(1)-O(12)	68.6(3)	O(3)-Gd(1)-O(12)	143.8(3)
O(4)#1-Gd(1)-O(8)#2	75.3(3)	O(5)-Gd(1)-O(8)#2	147.1(3)
O(10)-Gd(1)-O(8)#2	123.2(2)	O(13)-Gd(1)-O(8)#2	73.6(3)
O(3)-Gd(1)-O(8)#2	82.7(2)	O(12)-Gd(1)-O(8)#2	133.4(3)
O(4)#1-Gd(1)-O(2)	75.4(3)	O(5)-Gd(1)-O(2)	71.9(2)
O(10)-Gd(1)-O(2)	129.2(2)	O(13)-Gd(1)-O(2)	144.6(3)
O(3)-Gd(1)-O(2)	51.9(2)	O(12)-Gd(1)-O(2)	125.7(2)
O(8)#2-Gd(1)-O(2)	75.5(2)	O(4)#1-Gd(1)-O(7)#2	124.7(2)
O(5)-Gd(1)-O(7)#2	131.3(2)	O(10)-Gd(1)-O(7)#2	72.8(2)
O(13)-Gd(1)-O(7)#2	73.0(2)	O(3)-Gd(1)-O(7)#2	65.3(2)
O(12)-Gd(1)-O(7)#2	134.1(2)	O(8)#2-Gd(1)-O(7)#2	51.1(2)
O(2)-Gd(1)-O(7)#2	100.2(2)	O(11)#3-Co(1)-O(11)	179.998(1)
O(11)#3-Co(1)-O(7)#4	91.4(2)	O(11)-Co(1)-O(7)#4	88.6(2)
O(11)#3-Co(1)-O(7)#2	88.6(2)	O(11)-Co(1)-O(7)#2	91.4(2)
O(7)#4-Co(1)-O(7)#2	179.998(1)	O(11)#3-Co(1)-O(3)#3	91.7(2)
O(11)-Co(1)-O(3)#3	88.3(2)	O(7)#4-Co(1)-O(3)#3	81.7(2)
O(7)#2-Co(1)-O(3)#3	98.3(2)	O(11)#3-Co(1)-O(3)	88.3(2)
O(11)-Co(1)-O(3)	91.7(2)	O(7)#4-Co(1)-O(3)	98.3(2)
O(7)#2-Co(1)-O(3)	81.7(2)	O(3)#3-Co(1)-O(3)	179.999(1)
Co(1)-O(3)-Gd(1)	105.3(3)	Co(1)#6-O(7)-Gd(1)#6	101.1(2)

Dy(1)-O(8)	2.251(6)	Dy(1)-O(7)#1	2.288(6)
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Dy(1)-O(4)	2.306(6)	Dy(1)-O(9)#2	2.318(6)
Dy(1)-O(11)	2.419(6)	Dy(1)-O(12)	2.427(6)
Dy(1)-O(1)#3	2.452(6)	Dy(1)-O(2)#3	2.506(6)
Co(1)-O(5)#4	2.015(6)	Co(1)-O(5)	2.015(6)
Co(1)-O(6)#5	2.127(5)	Co(1)-O(6)#1	2.127(5)
Co(1)-O(2)#3	2.169(5)	Co(1)-O(2)#6	2.169(5)
O(8)-Dy(1)-O(7)#1	149.2(2)	O(8)-Dy(1)-O(4)	91.7(2)
O(7)#1-Dy(1)-O(4)	93.1(2)	O(8)-Dy(1)-O(9)#2	107.2(2)
O(7)#1-Dy(1)-O(9)#2	83.7(2)	O(4)-Dy(1)-O(9)#2	148.2(2)
O(8)-Dy(1)-O(11)	70.0(2)	O(7)#1-Dy(1)-O(11)	140.8(2)
O(4)-Dy(1)-O(11)	83.3(2)	O(9)#2-Dy(1)-O(11)	79.7(2)
O(8)-Dy(1)-O(12)	136.4(2)	O(7)#1-Dy(1)-O(12)	73.9(2)
O(4)-Dy(1)-O(12)	73.9(2)	O(9)#2-Dy(1)-O(12)	74.9(2)
O(11)-Dy(1)-O(12)	67.6(2)	O(8)-Dy(1)-O(1)#3	75.3(2)
O(7)#1-Dy(1)-O(1)#3	79.3(2)	O(4)-Dy(1)-O(1)#3	133.2(2)
O(9)#2-Dy(1)-O(1)#3	77.4(2)	O(11)-Dy(1)-O(1)#3	129.99(18)
O(12)-Dy(1)-O(1)#3	143.1(2)	O(8)-Dy(1)-O(2)#3	76.4(2)
O(7)#1-Dy(1)-O(2)#3	74.44(19)	O(4)-Dy(1)-O(2)#3	80.3(2)
O(9)#2-Dy(1)-O(2)#3	128.3(2)	O(11)-Dy(1)-O(2)#3	142.0(2)
O(12)-Dy(1)-O(2)#3	137.5(2)	O(1)#3-Dy(1)-O(2)#3	53.00(19)
O(8)-Dy(1)-C(1)#3	73.45(18)	O(7)#1-Dy(1)-C(1)#3	75.98(16)
O(5)#4-Co(1)-O(5)	180.0	O(5)#4-Co(1)-O(6)#5	93.7(2)
O(5)-Co(1)-O(6)#5	86.3(2)	O(5)#4-Co(1)-O(6)#1	86.3(2)
O(5)-Co(1)-O(6)#1	93.7(2)	O(6)#5-Co(1)-O(6)#1	180.0
O(5)#4-Co(1)-O(2)#3	91.9(2)	O(5)-Co(1)-O(2)#3	88.1(2)
O(6)#5-Co(1)-O(2)#3	88.1(2)	O(6)#1-Co(1)-O(2)#3	91.9(2)
O(5)#4-Co(1)-O(2)#6	88.1(2)	O(5)-Co(1)-O(2)#6	91.9(2)
O(6)#5-Co(1)-O(2)#6	91.9(2)	O(6)#1-Co(1)-O(2)#6	88.1(2)
O(2)#3-Co(1)-O(2)#6	180.0	Co(1)#7-O(2)-Dy(1)#7	117.6(2)

Symmetry transformations used to generate equivalent atoms:

1, #1 $x, y-1, z$

2, #1 $-x+1, -y, -z+1$ #2 $-x+2, -y, -z+1$ #3 $x-1, y, z$

#4 $-x+1, y-1/2, -z+3/2$ #5 $x+1, y, z$

3, #1 $-x+2, -y, -z$ #2 $x+1, y, z$ #3 $-x+5/2, -y+1/2, -z$

#4 $-x+3/2, -y+1/2, -z$ #6 $x-1, y, z$

4, #1 $x, y-1, z$ #2 $-x+2, -y, -z+1$ #3 $x+1, y, z$

#4 $-x+2, -y, -z$ #5 $-x+2, -y+1, -z$ #6 $-x+1, -y, -z$ #7 $x-1, y, z$

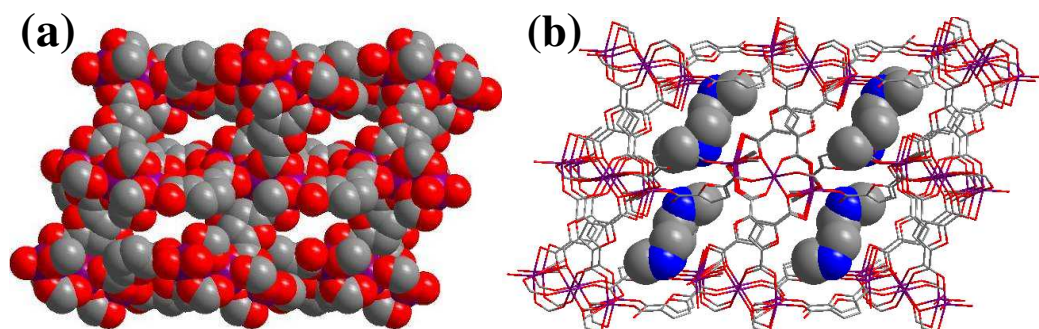


Figure S1 (a) Open channels of **1** along the [010] directions. (b) DMA cations are located in the channels along [010] direction in **1**. Color code: carbon, grey; nitrogen, blue; oxygen, red; cobalt, purple.

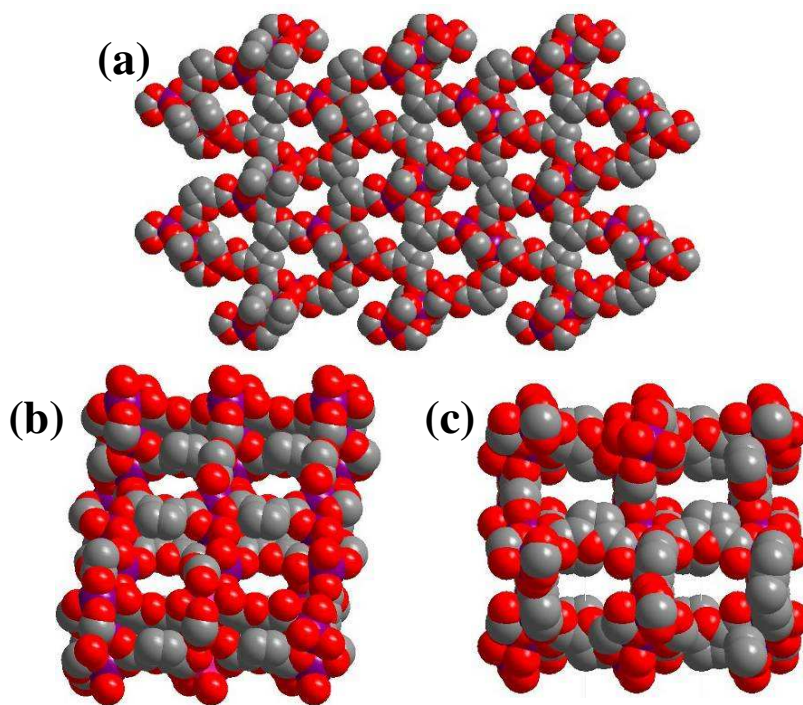


Figure S2 Open channels of **2** along the (a) [100] (b) [010] (c) [001] directions. Color code: carbon, grey; nitrogen, blue; oxygen, red; cobalt, purple.

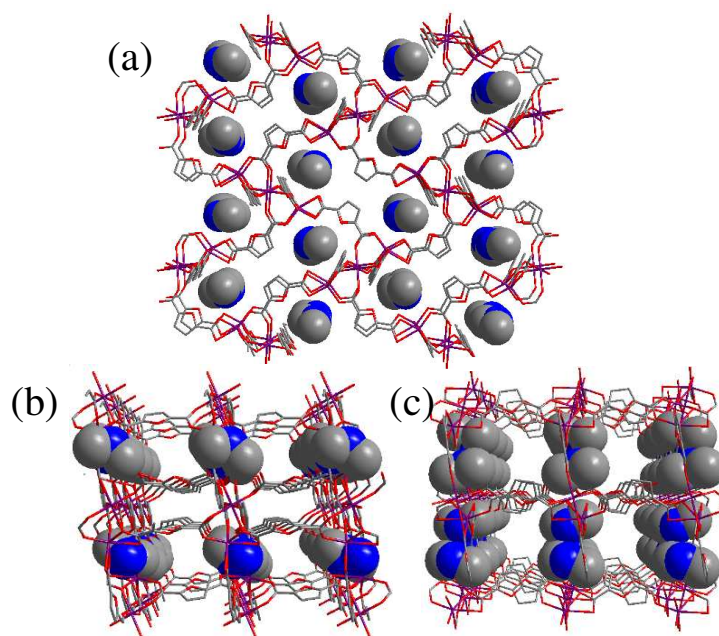


Figure S3 $\text{NH}_2(\text{CH}_3)_2$ cations are located in the channels along the (a) [100] (b) [010] (c) [001] directions in **2**. Color code: carbon, grey; nitrogen, blue; oxygen, red; cobalt, purple.

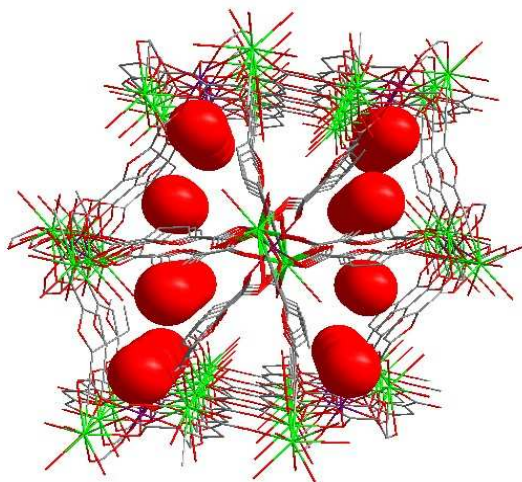


Figure S4 Free guest H_2O molecules are located in the channels along [110] direction in **3**. Color code: carbon, grey; nitrogen, blue; oxygen, red; cobalt, purple; gadolinium, green.

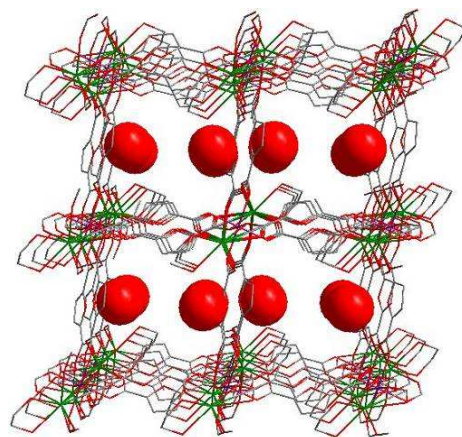


Figure S5 Free guest H₂O molecules are located in the channels along [001] direction in **4**. Color code: carbon, grey; nitrogen, blue; oxygen, red; cobalt, purple; dysprosium, green.

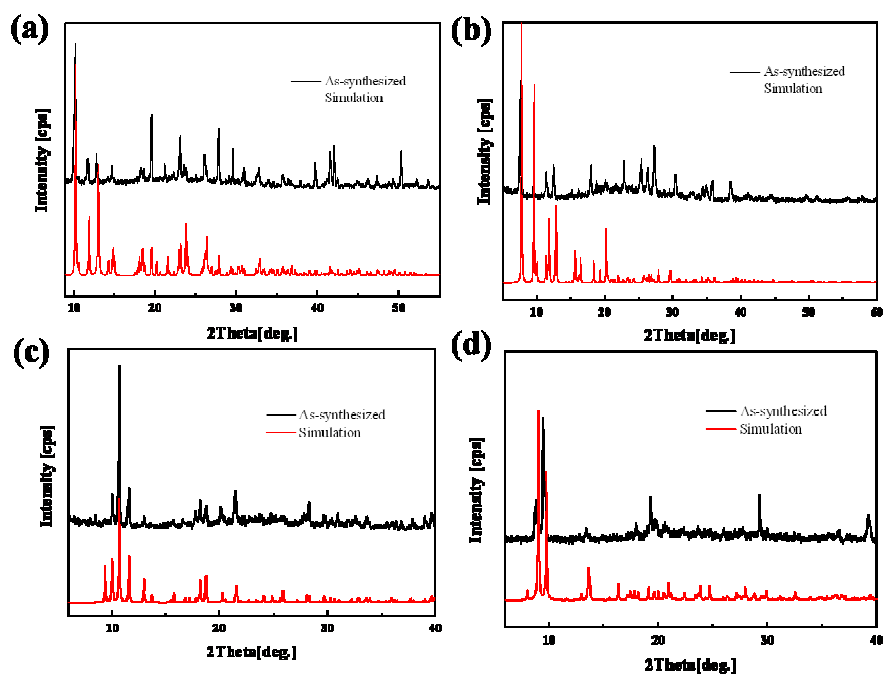


Figure S6 PXRD patterns of the compound simulated from the X-ray single-crystal structure and as-synthesized.