Electronic Supplementary Information (ESI)

Structural diversity and magnetic properties of three metal−organic frameworks assembled from a T-shaped linker

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Figure S1. a) the coordination mode of the Mn(II) in **JLU-Liu11**; b) a (3, 6)-connected framework.

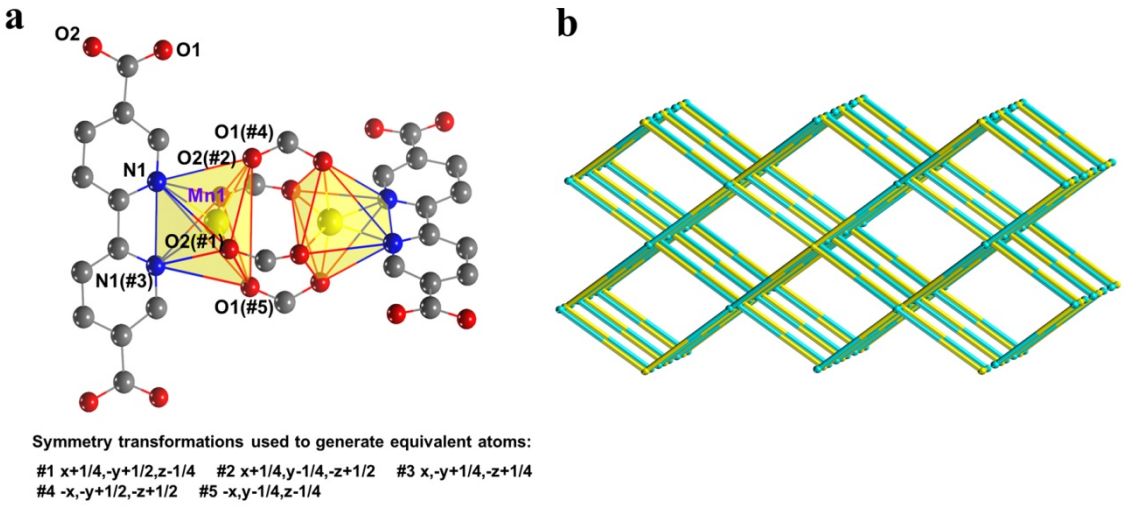


Figure S2. a) the coordination mode of the Co(II) in **JLU-Liu12**; b) a (3, 3)-connected framework; c) two types of helical chains; d) characteristics of helical chains along the [111] direction (green: left chains, pink: right chains).

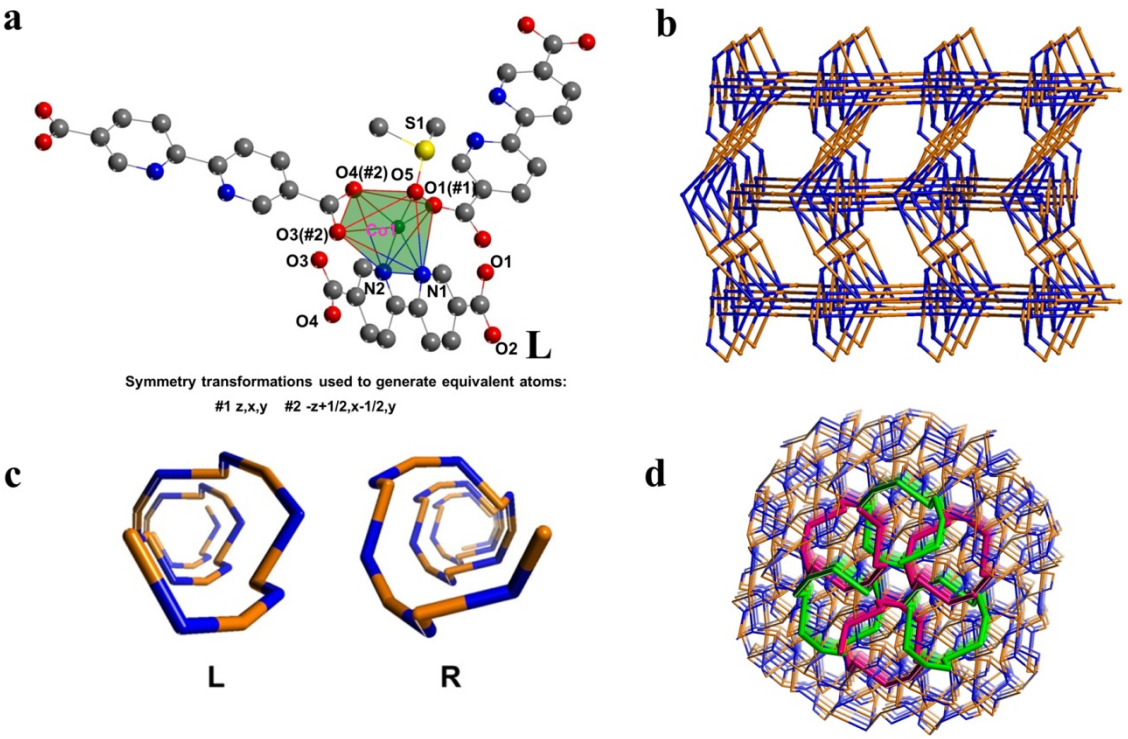


Figure S3. a) the coordination mode of the Co(II) in **JLU-Liu13**; b) a (3, 3)-connected framework; c) the hydrogen bonds on the terminal water are shown; d) the hydrogen bonding in **JLU-Liu13** structure.

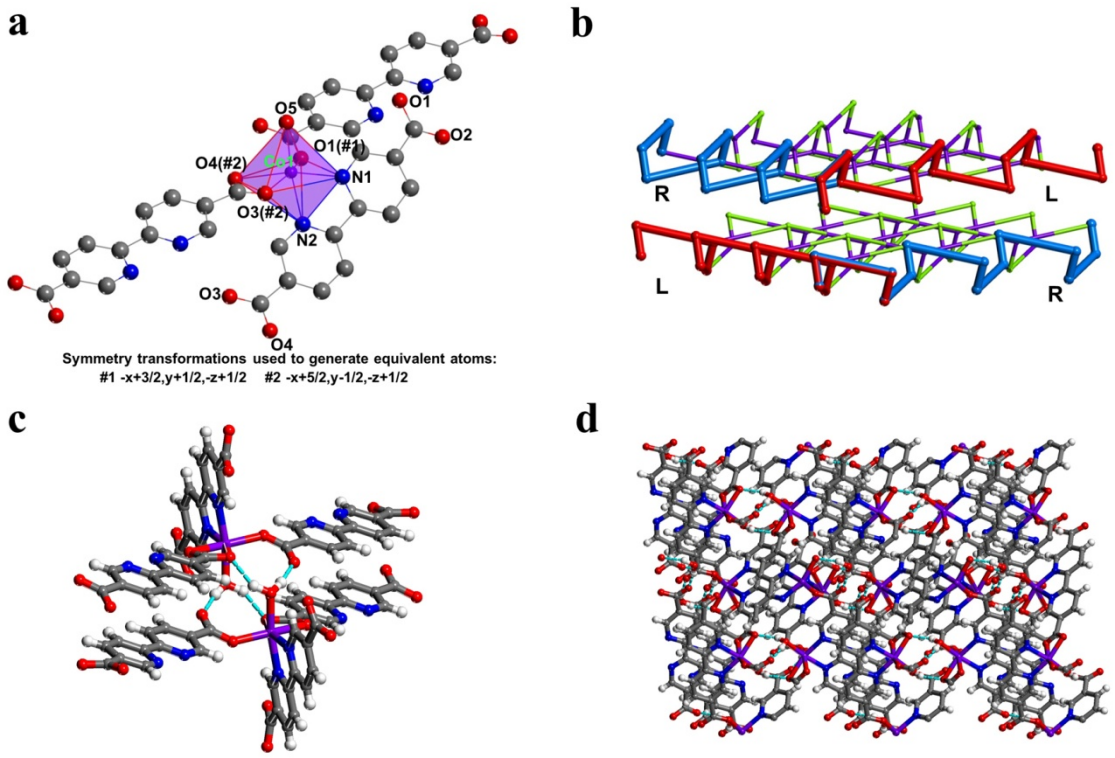


Figure S4. Topological features of **JLU-Liu11** and **JLU-Liu12**.

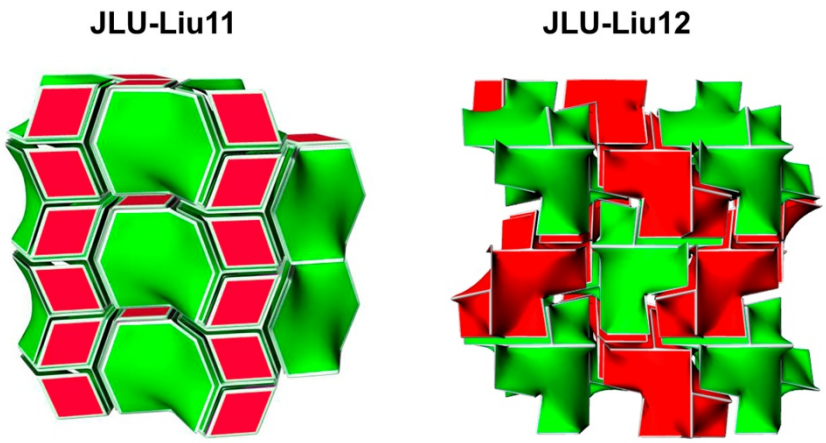


Figure S5. Angles for **JLU-Liu12** and **JLU-Liu13** in 3-connected simplified structures.

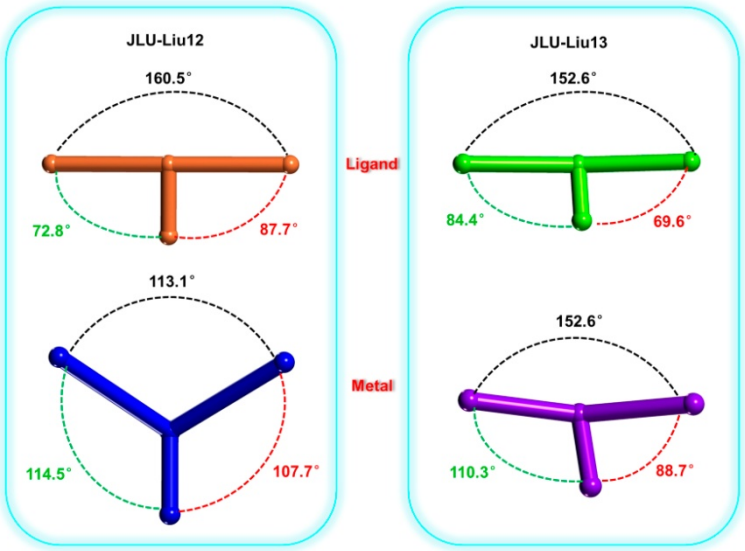


Figure S6. FT-IR spectra for compounds **JLU-Liu11**, **JLU-Liu12** and **JLU-Liu13**.

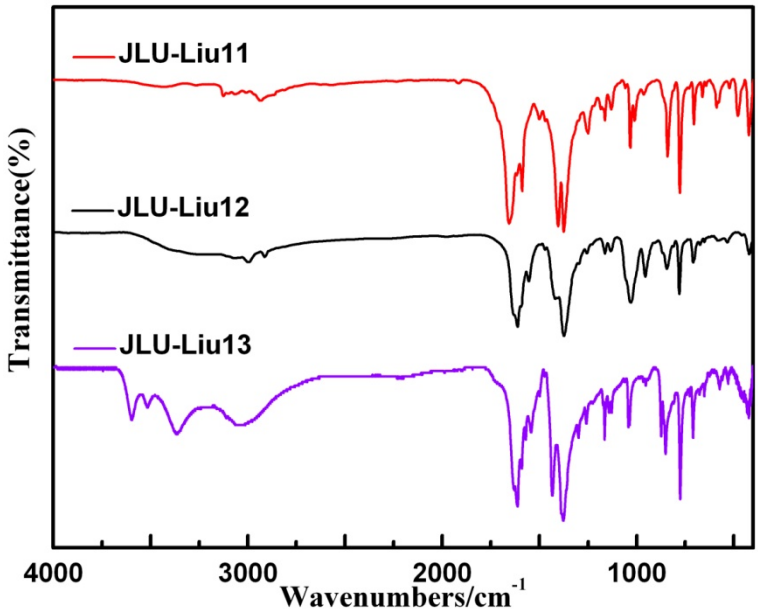


Figure S7. TGA curves for **JLU-Liu11**, **JLU-Liu12** and **JLU-Liu13**.

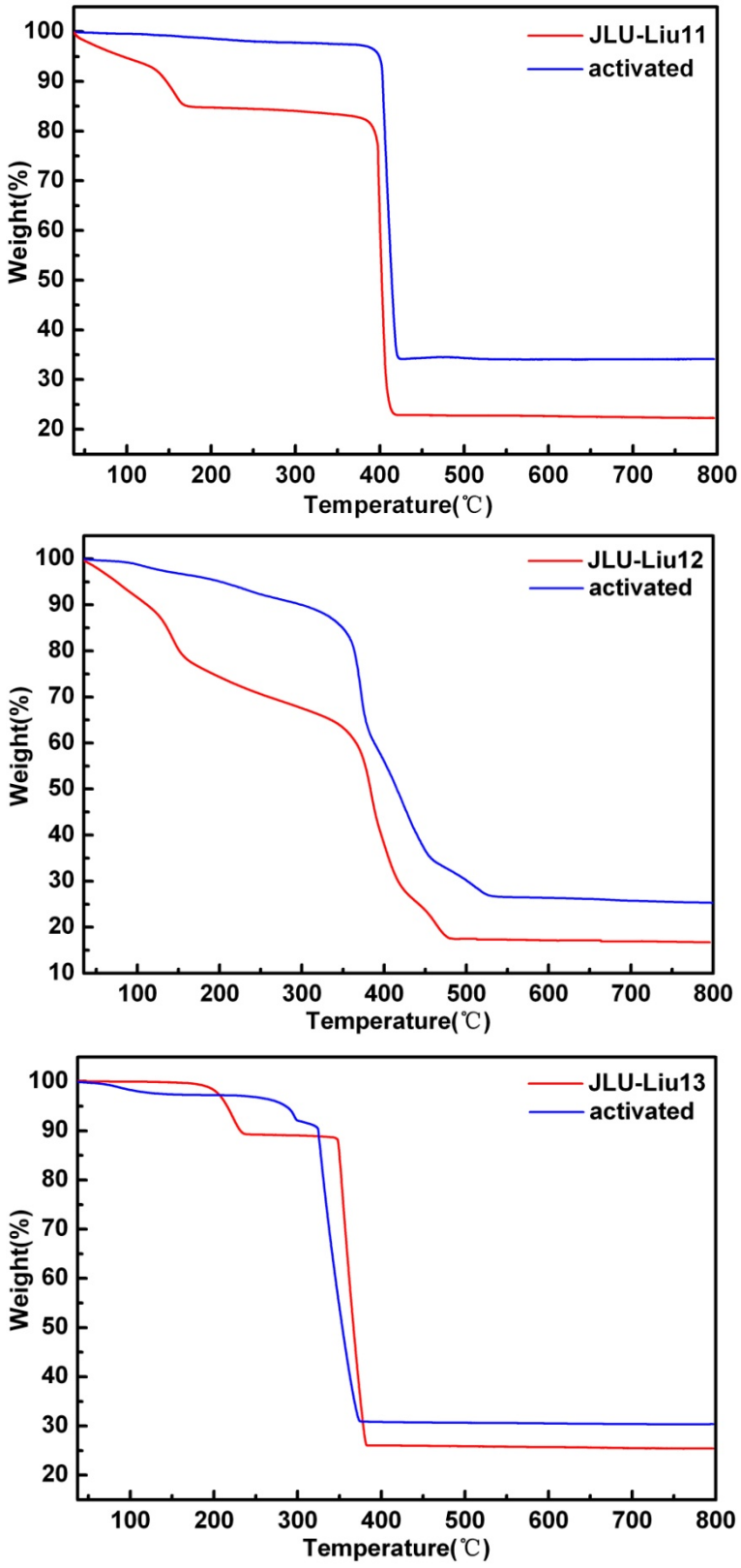


Figure S8. PXRD patterns of the activated, as-synthesized and simulated compounds: a) **JLU-Liu11**, b) **JLU-Liu12**.

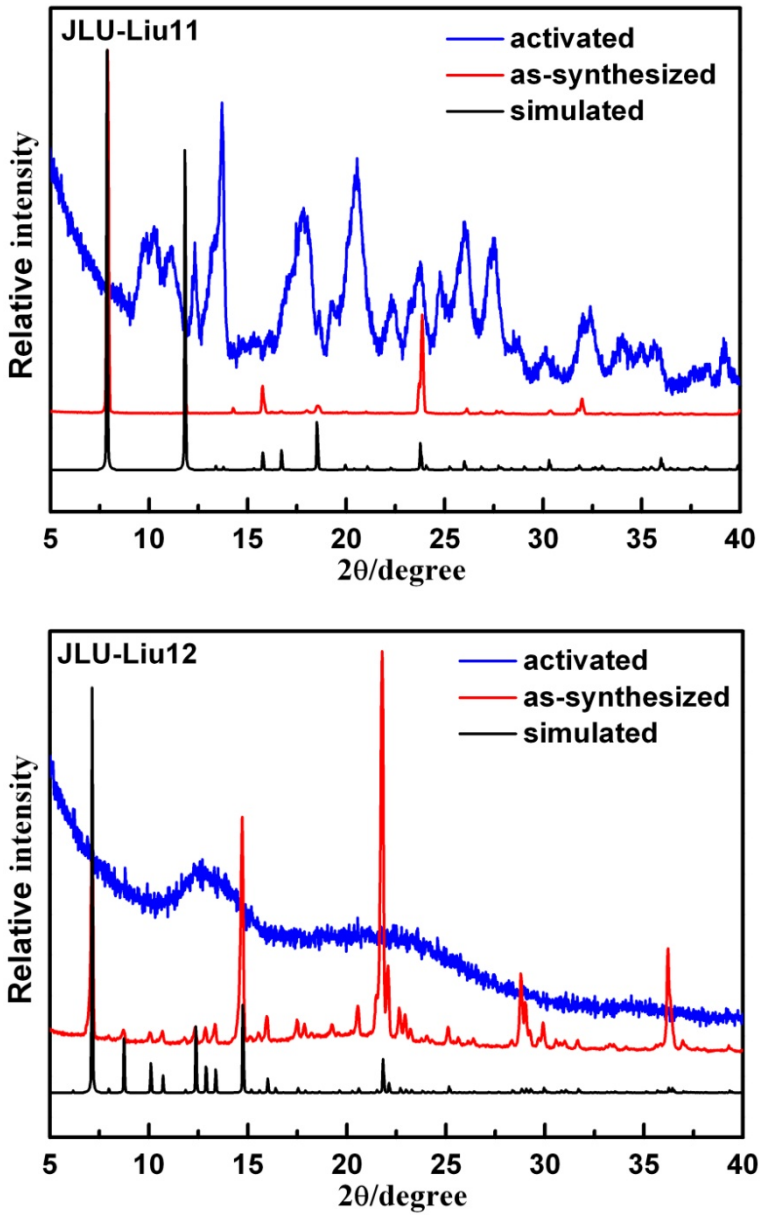


Figure S9. The PXRD patterns of **JLU-Liu13** after immersed in different solvents.

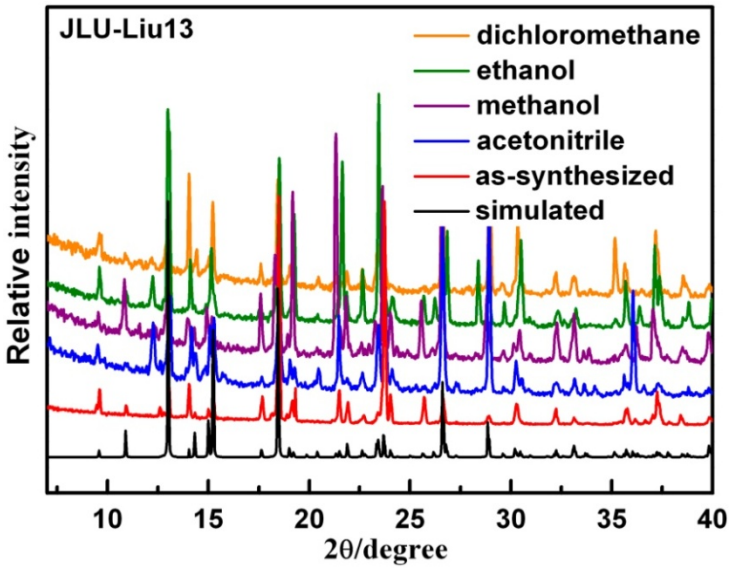
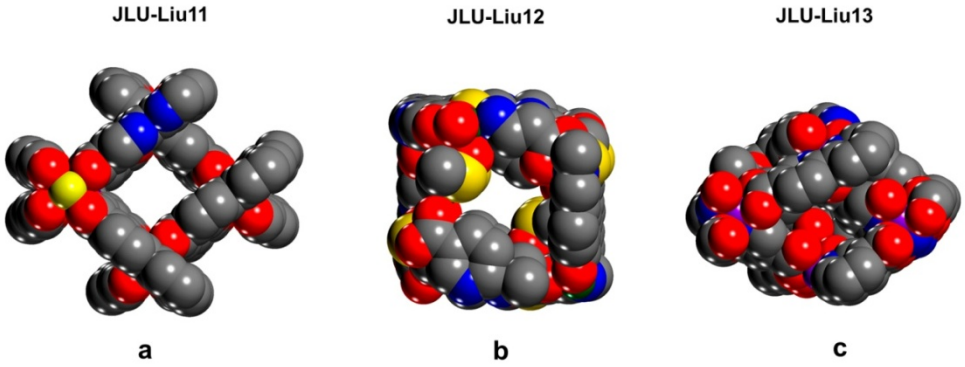


Figure S10. The pores of **JLU-Liu11**, **JLU-Liu12** and **JLU-Liu13**.



Scheme S1. The synthetic routes for MOFs based on H_2bpydc ligand in this work and reported by our group.

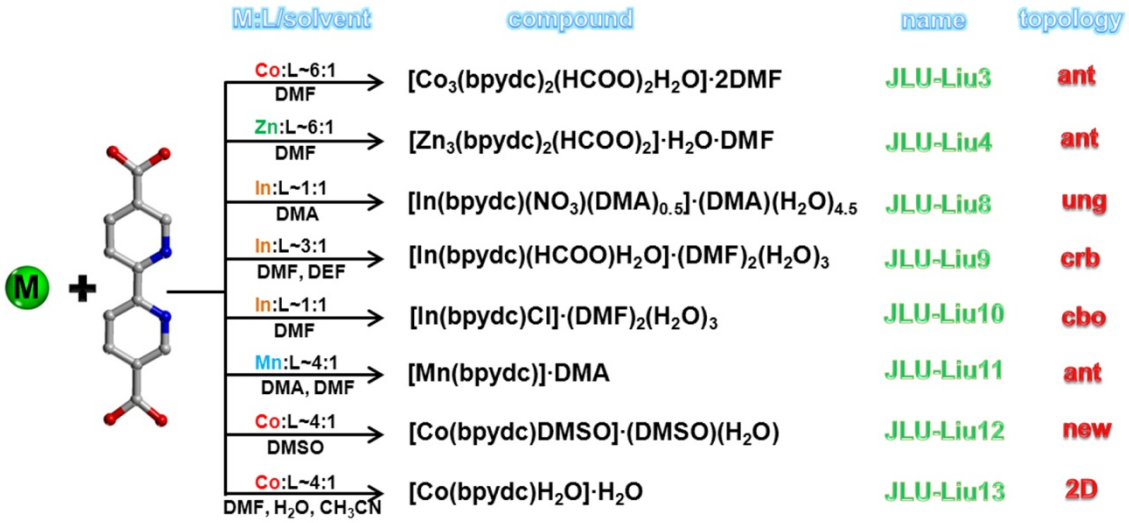


Table S1. Selected bond lengths (Å) and angles (°) for **JLU-Liu11**.

Mn(1)-O(2)#1	2.041(3)	C(1)-C(2)	1.46(3)
Mn(1)-O(2)#2	2.041(3)	C(1)-H(1)	0.9300
Mn(1)-N(1')#3	2.30(3)	C(1')-C(2)	1.33(3)
Mn(1)-N(1')	2.30(3)	C(1')-H(1')	0.9300
Mn(1)-O(1)#4	2.348(3)	C(2)-C(3')	1.352(18)
Mn(1)-O(1)#5	2.348(3)	C(2)-C(3)	1.473(17)
Mn(1)-N(1)#3	2.37(3)	C(2)-C(6)	1.493(7)
Mn(1)-N(1)	2.37(3)	C(3)-C(4)	1.43(2)
O(1)-C(6)	1.240(6)	C(3)-H(3)	0.9300
O(1)-Mn(1)#4	2.348(3)	C(3')-C(4')	1.37(2)
O(2)-C(6)	1.265(6)	C(3')-H(3')	0.9300
O(2)-Mn(1)#6	2.041(3)	C(4)-C(5)	1.385(15)
N(1)-C(1)	1.27(4)	C(4)-H(4)	0.9300
N(1)-C(5)	1.32(3)	C(4')-C(5)	1.428(14)
N(1')-C(5)	1.37(3)	C(4')-H(4')	0.9300
N(1')-C(1')	1.39(4)	C(5)-C(5)#3	1.520(9)
O(2)#1-Mn(1)-O(2)#2	165.0(2)	C(2)-C(1')-N(1')	128(2)
O(2)#1-Mn(1)-N(1')#3	99.5(4)	C(2)-C(1')-H(1')	116.0
O(2)#2-Mn(1)-N(1')#3	92.7(4)	N(1')-C(1')-H(1')	116.0
O(2)#1-Mn(1)-N(1')	92.7(4)	C(1')-C(2)-C(3')	117.7(13)
O(2)#2-Mn(1)-N(1')	99.5(4)	C(1')-C(2)-C(1)	16.9(14)
N(1')#3-Mn(1)-N(1')	71.0(14)	C(3')-C(2)-C(1)	112.5(12)
O(2)#1-Mn(1)-O(1)#4	87.10(17)	C(1')-C(2)-C(3)	113.1(15)
O(2)#2-Mn(1)-O(1)#4	85.95(16)	C(3')-C(2)-C(3)	30.8(12)
N(1')#3-Mn(1)-O(1)#4	152.8(7)	C(1)-C(2)-C(3)	117.7(13)
N(1')-Mn(1)-O(1)#4	82.5(7)	C(1')-C(2)-C(6)	121.3(12)
O(2)#1-Mn(1)-O(1)#5	85.95(16)	C(3')-C(2)-C(6)	120.7(8)
O(2)#2-Mn(1)-O(1)#5	87.10(17)	C(1)-C(2)-C(6)	122.4(11)
N(1')#3-Mn(1)-O(1)#5	82.5(7)	C(3)-C(2)-C(6)	119.0(8)
N(1')-Mn(1)-O(1)#5	152.8(7)	C(4)-C(3)-C(2)	116.5(13)
O(1)#4-Mn(1)-O(1)#5	124.48(17)	C(4)-C(3)-H(3)	121.7
O(2)#1-Mn(1)-N(1)#3	89.9(5)	C(2)-C(3)-H(3)	121.7
O(2)#2-Mn(1)-N(1)#3	102.4(5)	C(2)-C(3')-C(4')	120.4(13)
N(1')#3-Mn(1)-N(1)#3	9.7(8)	C(2)-C(3')-H(3')	119.8
N(1')-Mn(1)-N(1)#3	69.8(2)	C(4')-C(3')-H(3')	119.8
O(1)#4-Mn(1)-N(1)#3	151.9(6)	C(5)-C(4)-C(3)	117.5(12)
O(1)#5-Mn(1)-N(1)#3	83.1(7)	C(5)-C(4)-H(4)	121.3
O(2)#1-Mn(1)-N(1)	102.4(5)	C(3)-C(4)-H(4)	121.3
O(2)#2-Mn(1)-N(1)	89.9(5)	C(3')-C(4')-C(5)	118.1(11)
N(1')#3-Mn(1)-N(1)	69.8(2)	C(3')-C(4')-H(4')	120.9
N(1')-Mn(1)-N(1)	9.7(8)	C(5)-C(4')-H(4')	120.9
O(1)#4-Mn(1)-N(1)	83.1(7)	N(1)-C(5)-N(1')	16.9(13)
O(1)#5-Mn(1)-N(1)	151.9(6)	N(1)-C(5)-C(4)	123.8(14)

N(1)#3-Mn(1)-N(1)	70.3(13)	N(1')-C(5)-C(4)	121.4(14)
C(6)-O(1)-Mn(1)#4	143.4(3)	N(1)-C(5)-C(4')	114.8(12)
C(6)-O(2)-Mn(1)#6	125.2(3)	N(1')-C(5)-C(4')	123.0(12)
C(1)-N(1)-C(5)	123(3)	C(4)-C(5)-C(4')	32.3(7)
C(1)-N(1)-Mn(1)	119(2)	N(1)-C(5)-C(5)#3	117.2(12)
C(5)-N(1)-Mn(1)	117.2(15)	N(1')-C(5)-C(5)#3	113.5(11)
C(5)-N(1')-C(1')	111(2)	C(4)-C(5)-C(5)#3	118.2(6)
C(5)-N(1')-Mn(1)	118.6(15)	C(4')-C(5)-C(5)#3	122.8(6)
C(1')-N(1')-Mn(1)	127(2)	O(1)-C(6)-O(2)	126.0(4)
N(1)-C(1)-C(2)	120(2)	O(1)-C(6)-C(2)	119.5(4)
N(1)-C(1)-H(1)	120.0	O(2)-C(6)-C(2)	114.5(5)
C(2)-C(1)-H(1)	120.0		

Symmetry transformations used to generate equivalent atoms:

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

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

Table S2. Selected bond lengths (Å) and angles (°) for **JLU-Liu12**.

Co(1)-O(1)#1	1.974(11)	C(2)-C(3)	1.393(11)
Co(1)-O(1')#1	1.996(11)	C(2)-C(11)	1.490(9)
Co(1)-O(5)	2.071(5)	C(3)-C(4)	1.395(12)
Co(1)-N(2)	2.097(5)	C(3)-H(3)	0.9300
Co(1)-N(1)	2.112(5)	C(4)-C(5)	1.377(11)
Co(1)-O(4)#2	2.142(5)	C(4)-H(4)	0.9300
Co(1)-O(3)#2	2.311(5)	C(5)-C(6)	1.478(9)
S(1)-O(5)	1.508(5)	C(6)-C(7)	1.370(9)
S(1)-C(13')	1.54(3)	C(7)-C(8)	1.356(10)
S(1)-C(14')	1.62(3)	C(7)-H(7)	0.9300
S(1)-C(14)	1.72(3)	C(8)-C(9)	1.366(10)
S(1)-C(13)	1.87(3)	C(8)-H(8)	0.9300
O(1)-C(11)	1.207(13)	C(9)-C(10)	1.395(9)
O(1)-Co(1)#3	1.974(11)	C(9)-C(12)	1.508(9)
O(1')-C(11)	1.261(13)	C(10)-H(10)	0.9300
O(1')-Co(1)#3	1.996(11)	C(13)-H(13A)	0.9600
O(2)-C(11)	1.293(12)	C(13)-H(13B)	0.9600
O(2')-C(11)	1.274(13)	C(13)-H(13C)	0.9600
O(3)-C(12)	1.237(9)	C(14)-H(14A)	0.9600
O(3)-Co(1)#4	2.311(5)	C(14)-H(14B)	0.9600
O(4)-C(12)	1.242(8)	C(14)-H(14C)	0.9600
O(4)-Co(1)#4	2.142(5)	C(13')-H(13D)	0.9600
N(1)-C(1)	1.342(7)	C(13')-H(13E)	0.9600
N(1)-C(5)	1.351(8)	C(13')-H(13F)	0.9600
N(2)-C(10)	1.329(8)	C(14')-H(14D)	0.9600
N(2)-C(6)	1.331(8)	C(14')-H(14E)	0.9600
C(1)-C(2)	1.367(9)	C(14')-H(14F)	0.9600
C(1)-H(1)	0.9300		

O(1)#1-Co(1)-O(1')#1	11.6(5)	N(1)-C(5)-C(4)	120.4(7)
O(1)#1-Co(1)-O(5)	89.8(3)	N(1)-C(5)-C(6)	115.9(6)
O(1')#1-Co(1)-O(5)	101.1(3)	C(4)-C(5)-C(6)	123.7(7)
O(1)#1-Co(1)-N(2)	109.5(4)	N(2)-C(6)-C(7)	122.1(6)
O(1')#1-Co(1)-N(2)	111.3(3)	N(2)-C(6)-C(5)	114.4(5)
O(5)-Co(1)-N(2)	92.5(2)	C(7)-C(6)-C(5)	123.5(6)
O(1)#1-Co(1)-N(1)	96.4(3)	C(8)-C(7)-C(6)	119.2(7)
O(1')#1-Co(1)-N(1)	85.7(3)	C(6)-C(7)-H(7)	120.4
O(5)-Co(1)-N(1)	169.04(19)	C(7)-C(8)-C(9)	120.3(7)
N(2)-Co(1)-N(1)	76.92(18)	C(7)-C(8)-H(8)	119.9
O(1)#1-Co(1)-O(4)#2	92.7(3)	C(9)-C(8)-H(8)	119.9
O(1')#1-Co(1)-O(4)#2	89.2(3)	C(8)-C(9)-C(10)	117.4(6)
O(5)-Co(1)-O(4)#2	94.0(2)	C(8)-C(9)-C(12)	121.2(6)
N(2)-Co(1)-O(4)#2	156.87(19)	C(10)-C(9)-C(12)	121.4(6)
N(1)-Co(1)-O(4)#2	94.73(19)	N(2)-C(10)-C(9)	122.5(6)
O(1)#1-Co(1)-O(3)#2	151.2(4)	N(2)-C(10)-H(10)	118.7
O(1')#1-Co(1)-O(3)#2	146.3(3)	C(9)-C(10)-H(10)	118.7
O(5)-Co(1)-O(3)#2	91.3(2)	O(1)-C(11)-O(1')	18.5(7)
N(2)-Co(1)-O(3)#2	99.25(19)	O(1)-C(11)-O(2')	117.4(9)
N(1)-Co(1)-O(3)#2	87.59(19)	O(1')-C(11)-O(2')	128.2(9)
O(4)#2-Co(1)-O(3)#2	58.45(19)	O(1)-C(11)-O(2)	123.1(9)
O(5)-S(1)-C(13')	107.3(11)	O(1')-C(11)-O(2)	118.0(9)
O(5)-S(1)-C(14')	109.3(11)	O(2')-C(11)-O(2)	43.6(6)
C(13')-S(1)-C(14')	93.5(14)	O(1)-C(11)-C(2)	117.0(8)
O(5)-S(1)-C(14)	110.9(11)	O(1')-C(11)-C(2)	113.5(7)
C(13')-S(1)-C(14)	115.4(15)	O(2')-C(11)-C(2)	116.7(8)
C(14')-S(1)-C(14)	25.1(14)	O(2)-C(11)-C(2)	117.9(8)
O(5)-S(1)-C(13)	101.0(9)	O(3)-C(12)-O(4)	123.0(7)
C(13')-S(1)-C(13)	29.0(13)	O(3)-C(12)-C(9)	118.9(6)
C(14')-S(1)-C(13)	68.5(13)	O(4)-C(12)-C(9)	118.1(7)
C(14)-S(1)-C(13)	93.0(13)	S(1)-C(13)-H(13A)	109.5
C(11)-O(1)-Co(1)#3	133.3(8)	S(1)-C(13)-H(13B)	109.5
C(11)-O(1')-Co(1)#3	127.2(8)	H(13A)-C(13)-H(13B)	109.5
C(12)-O(3)-Co(1)#4	85.5(4)	S(1)-C(13)-H(13C)	109.5
C(12)-O(4)-Co(1)#4	93.1(5)	H(13A)-C(13)-H(13C)	109.5
S(1)-O(5)-Co(1)	137.7(3)	H(13B)-C(13)-H(13C)	109.5
C(1)-N(1)-C(5)	119.2(5)	S(1)-C(14)-H(14A)	109.5
C(1)-N(1)-Co(1)	125.5(4)	S(1)-C(14)-H(14B)	109.5
C(5)-N(1)-Co(1)	115.3(4)	H(14A)-C(14)-H(14B)	109.5
C(10)-N(2)-C(6)	118.4(5)	S(1)-C(14)-H(14C)	109.5
C(10)-N(2)-Co(1)	124.1(4)	H(14A)-C(14)-H(14C)	109.5
C(6)-N(2)-Co(1)	117.4(4)	H(14B)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	124.0(6)	S(1)-C(13')-H(13D)	109.5
N(1)-C(1)-H(1)	118.0	S(1)-C(13')-H(13E)	109.5

C(2)-C(1)-H(1)	118.0	H(13D)-C(13')-H(13E)	109.5
C(1)-C(2)-C(3)	117.1(6)	S(1)-C(13')-H(13F)	109.5
C(1)-C(2)-C(11)	121.6(6)	H(13D)-C(13')-H(13F)	109.5
C(3)-C(2)-C(11)	121.2(7)	H(13E)-C(13')-H(13F)	109.5
C(2)-C(3)-C(4)	119.4(9)	S(1)-C(14')-H(14D)	109.5
C(2)-C(3)-H(3)	120.3	S(1)-C(14')-H(14E)	109.5
C(4)-C(3)-H(3)	120.3	H(14D)-C(14')-H(14E)	109.5
C(5)-C(4)-C(3)	119.9(9)	S(1)-C(14')-H(14F)	109.5
C(5)-C(4)-H(4)	120.1	H(14D)-C(14')-H(14F)	109.5
C(3)-C(4)-H(4)	120.1	H(14E)-C(14')-H(14F)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table S3. Selected bond lengths (Å) and angles (°) for **JLU-Liu13**.

Co(1)-O(1)#1	2.0324(16)	N(2)-C(6)	1.347(3)
Co(1)-O(5)	2.0823(16)	C(1)-C(2)	1.385(3)
Co(1)-N(1)	2.0987(17)	C(1)-H(1)	0.9300
Co(1)-N(2)	2.1081(17)	C(2)-C(3)	1.382(3)
Co(1)-O(4)#2	2.1802(16)	C(2)-C(11)	1.515(3)
Co(1)-O(3)#2	2.2179(16)	C(3)-C(4)	1.379(3)
O(1)-C(11)	1.266(3)	C(3)-H(3)	0.9300
O(1)-Co(1)#3	2.0324(16)	C(4)-C(5)	1.385(3)
O(2)-C(11)	1.229(3)	C(4)-H(4)	0.9300
O(3)-C(12)	1.252(3)	C(5)-C(6)	1.490(3)
O(3)-Co(1)#4	2.2179(16)	C(6)-C(7)	1.388(3)
O(4)-C(12)	1.266(3)	C(7)-C(8)	1.386(3)
O(4)-Co(1)#4	2.1802(16)	C(7)-H(7)	0.9300
O(5)-H(5A)	0.931(18)	C(8)-C(9)	1.385(3)
O(5)-H(5B)	0.935(18)	C(8)-H(8)	0.9300
N(1)-C(1)	1.345(3)	C(9)-C(10)	1.388(3)
N(1)-C(5)	1.348(3)	C(9)-C(12)	1.494(3)
N(2)-C(10)	1.329(3)	C(10)-H(10)	0.9300
O(1)#1-Co(1)-O(5)	96.82(7)	C(1)-C(2)-C(11)	120.7(2)
O(1)#1-Co(1)-N(1)	95.92(7)	C(4)-C(3)-C(2)	119.6(2)
O(5)-Co(1)-N(1)	94.33(7)	C(4)-C(3)-H(3)	120.2
O(1)#1-Co(1)-N(2)	90.84(7)	C(2)-C(3)-H(3)	120.2
O(5)-Co(1)-N(2)	169.13(7)	C(3)-C(4)-C(5)	119.2(2)
N(1)-Co(1)-N(2)	77.15(7)	C(3)-C(4)-H(4)	120.4
O(1)#1-Co(1)-O(4)#2	103.61(6)	C(5)-C(4)-H(4)	120.4
O(5)-Co(1)-O(4)#2	91.36(6)	N(1)-C(5)-C(4)	121.90(19)
N(1)-Co(1)-O(4)#2	158.85(7)	N(1)-C(5)-C(6)	114.97(18)
N(2)-Co(1)-O(4)#2	94.33(6)	C(4)-C(5)-C(6)	123.10(19)
O(1)#1-Co(1)-O(3)#2	162.24(7)	N(2)-C(6)-C(7)	121.92(19)
O(5)-Co(1)-O(3)#2	90.51(6)	N(2)-C(6)-C(5)	114.77(18)
N(1)-Co(1)-O(3)#2	99.64(6)	C(7)-C(6)-C(5)	123.31(19)

N(2)-Co(1)-O(3)#2	84.37(7)	C(8)-C(7)-C(6)	118.8(2)
O(4)#2-Co(1)-O(3)#2	59.90(6)	C(8)-C(7)-H(7)	120.6
C(11)-O(1)-Co(1)#3	136.79(15)	C(6)-C(7)-H(7)	120.6
C(12)-O(3)-Co(1)#4	88.67(13)	C(9)-C(8)-C(7)	119.4(2)
C(12)-O(4)-Co(1)#4	90.02(13)	C(9)-C(8)-H(8)	120.3
Co(1)-O(5)-H(5A)	108(2)	C(7)-C(8)-H(8)	120.3
Co(1)-O(5)-H(5B)	113(3)	C(8)-C(9)-C(10)	118.0(2)
H(5A)-O(5)-H(5B)	114(3)	C(8)-C(9)-C(12)	122.9(2)
C(1)-N(1)-C(5)	118.19(18)	C(10)-C(9)-C(12)	119.07(19)
C(1)-N(1)-Co(1)	125.24(14)	N(2)-C(10)-C(9)	123.13(19)
C(5)-N(1)-Co(1)	116.57(14)	N(2)-C(10)-H(10)	118.4
C(10)-N(2)-C(6)	118.65(18)	C(9)-C(10)-H(10)	118.4
C(10)-N(2)-Co(1)	124.92(14)	O(2)-C(11)-O(1)	127.3(2)
C(6)-N(2)-Co(1)	116.41(13)	O(2)-C(11)-C(2)	117.2(2)
N(1)-C(1)-C(2)	123.0(2)	O(1)-C(11)-C(2)	115.48(19)
N(1)-C(1)-H(1)	118.5	O(3)-C(12)-O(4)	121.3(2)
C(2)-C(1)-H(1)	118.5	O(3)-C(12)-C(9)	120.0(2)
C(3)-C(2)-C(1)	118.1(2)	O(4)-C(12)-C(9)	118.6(2)
C(3)-C(2)-C(11)	121.1(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Hydrogen bonds for **JLU-Liu13** [lengths (Å) and angles (°)].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...O(2)#5	0.931(18)	1.73(2)	2.655(2)	168(4)
O(5)-H(5B)...O(4)#6	0.935(18)	1.90(3)	2.732(2)	147(4)

Symmetry transformations used to generate equivalent atoms:

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

#5 x+1/2,-y-1/2,z+1/2 #6 x-1/2,-y+1/2,z+1/2