Electronic supplementary information (ESI)

Two-dimensional magnetic materials of cobalt(II) triangular lattices constructed by the mixed benzimidazole-dicarboxylate strategy

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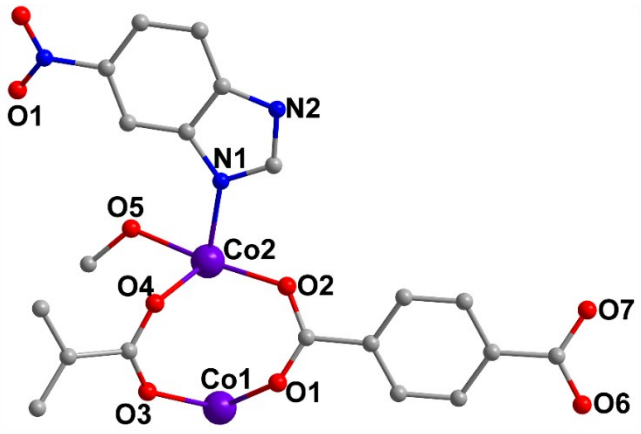

Figure S1. The asymmetric unit of **1**. Hydrogen atoms were omitted for clarity.

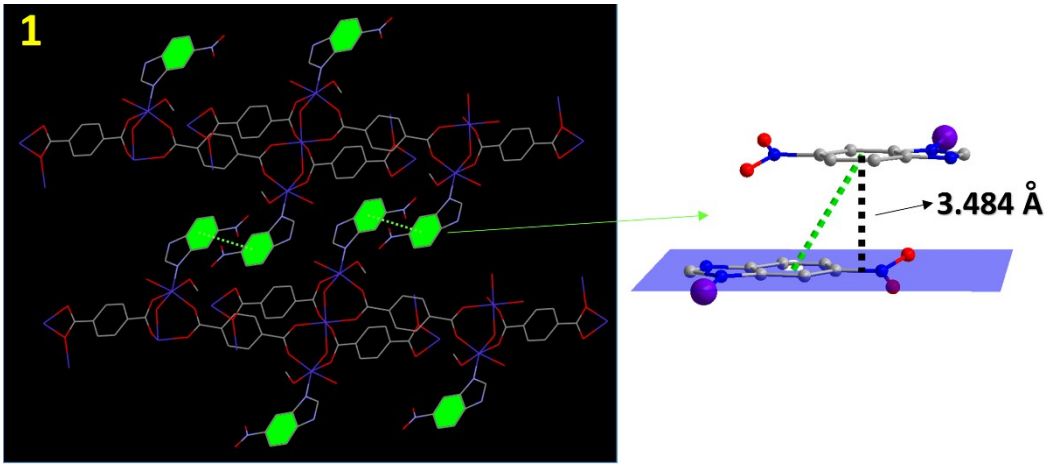

Figure S2. The packing structure of **1**.

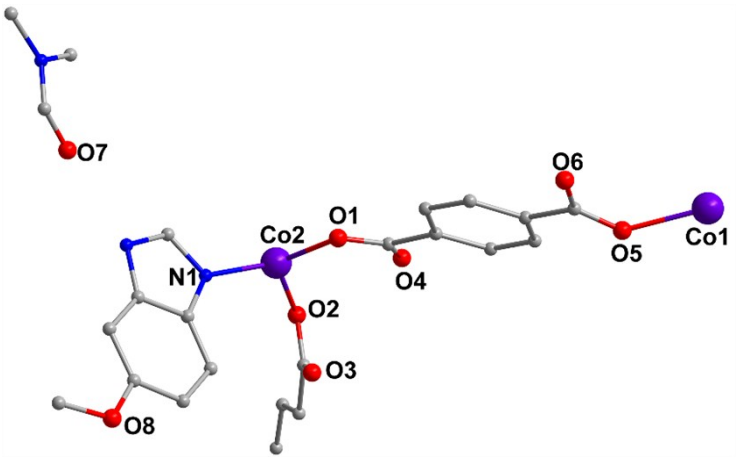

Figure S3. The asymmetric unit of **2**. Hydrogen atoms were omitted for clarity.

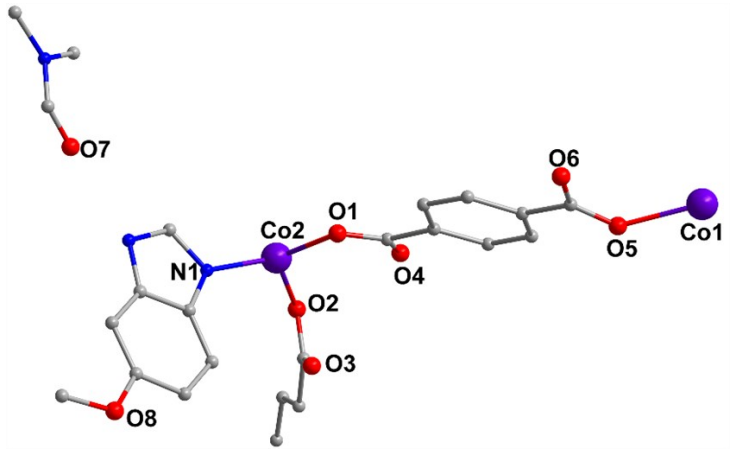

Figure S4. The asymmetric unit of **3**. Hydrogen atoms were omitted for clarity.

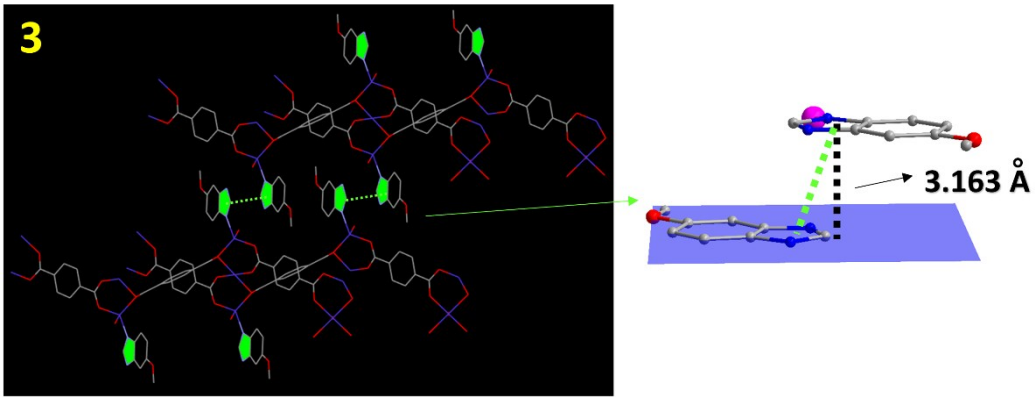

Figure S5. Packing structure of **2**.

Table S1. Selected bond lengths (Å), angles [°], and structural parameters for **1**.

1			
Co(1)-O(1)	2.0430(13)	Co(2)-O(2)	2.0365(13)
Co(1)-O(1)#1	2.0430(13)	Co(2)-O(4)	1.9779(13)
Co(1)-O(3)	2.0728(12)	Co(2)-N(1)	2.1023(15)
Co(1)-O(3)#1	2.0728(12)	Co(2)-O(6)#2	2.1769(12)
Co(1)-O(6)#2	2.1553(12)	Co(2)-O(5)	2.1825(14)
Co(1)-O(6)#3	2.1553(12)	Co(2)-O(7)#2	2.2317(13)
Co1-O_{aver}	2.0904	Co2-X_{aver}(X = N, O)	2.1179
O(1)-Co(1)-O(1)#1	180.00(3)	O(4)-Co(2)-O(2)	101.63(6)
O(1)-Co(1)-O(3)	94.80(5)	O(4)-Co(2)-N(1)	103.55(6)
O(1)#1-Co(1)-O(3)	85.20(5)	O(2)-Co(2)-N(1)	88.02(6)
O(1)-Co(1)-O(3)#1	85.20(5)	O(4)-Co(2)-O(6)#2	100.26(5)
O(1)#1-Co(1)-O(3)#1	94.80(5)	O(2)-Co(2)-O(6)#2	89.72(5)
O(3)-Co(1)-O(3)#1	180.0	N(1)-Co(2)-O(6)#2	156.05(5)
O(1)-Co(1)-O(6)#2	90.35(5)	O(4)-Co(2)-O(5)	86.41(6)
O(1)#1-Co(1)-O(6)#2	89.65(5)	O(2)-Co(2)-O(5)	171.94(6)
O(3)-Co(1)-O(6)#2	88.50(5)	N(1)-Co(2)-O(5)	90.61(6)
O(3)#1-Co(1)-O(6)#2	91.50(5)	O(6)#2-Co(2)-O(5)	88.31(5)
O(1)-Co(1)-O(6)#3	89.65(5)	O(4)-Co(2)-O(7)#2	157.93(5)
O(1)#1-Co(1)-O(6)#3	90.35(5)	O(2)-Co(2)-O(7)#2	87.65(6)
O(3)-Co(1)-O(6)#3	91.50(5)	N(1)-Co(2)-O(7)#2	96.68(5)
O(3)#1-Co(1)-O(6)#3	88.50(5)	O(6)#2-Co(2)-O(7)#2	59.40(5)
O(6)#2-Co(1)-O(6)#3	180.0	O(5)-Co(2)-O(7)#2	84.62(5)
Symmetry transformations used to generate equivalent atoms:			
#1 -x,-y+1,-z+1; #2 x,-y+3/2,z+1/2			
#3 -x,y-1/2,-z+1/2; #4 -x,y+1/2,-z+1/2			
#5 x,-y+3/2,z-1/2; #6 -x,-y,-z+1			

Table S2. Selected bond lengths (Å), angles [°], and structural parameters for **2**.

2			
Co(1)-O(6)	2.0267(13)	Co(2)-O(2)	1.9455(13)
Co(1)-O(6)#2	2.0267(13)	Co(2)-O(5)#1	1.9699(13)
Co(1)-O(3)#3	2.0551(13)	Co(2)-O(1)	1.9991(13)
Co(1)-O(3)#4	2.0551(13)	Co(2)-N(1)	2.0092(16)
Co(1)-O(1)#4	2.2041(13)		
Co(1)-O(1)#3	2.2041(13)		
Co1-O_{aver}	2.0953	Co2-X_{aver}(X = N, O)	1.9809
O(2)-Co(2)-O(5)#1	116.29(7)	O(3)#3-Co(1)-O(3)#4	180.000(1)
O(2)-Co(2)-O(1)	111.43(6)	O(6)-Co(1)-O(1)#4	92.25(5)
O(5)#1-Co(2)-O(1)	100.11(6)	O(6)#2-Co(1)-O(1)#4	87.75(5)
O(2)-Co(2)-N(1)	104.95(7)	O(3)#3-Co(1)-O(1)#4	88.21(5)
O(5)#1-Co(2)-N(1)	102.13(6)	O(3)#4-Co(1)-O(1)#4	91.79(5)
O(1)-Co(2)-N(1)	122.16(6)	O(6)-Co(1)-O(1)#3	87.75(5)
O(6)-Co(1)-O(6)#2	180.00(6)	O(6)#2-Co(1)-O(1)#3	92.25(5)
O(6)-Co(1)-O(3)#3	84.48(6)	O(3)#3-Co(1)-O(1)#3	91.79(5)
O(6)#2-Co(1)-O(3)#3	95.52(6)	O(3)#4-Co(1)-O(1)#3	88.21(5)
O(6)-Co(1)-O(3)#4	95.52(6)	O(1)#4-Co(1)-O(1)#3	180.0(1)
O(6)#2-Co(1)-O(3)#4	84.48(6)		
Symmetry transformations used to generate equivalent atoms:			
#1 x,-y,z-1/2; #2 -x+1/2,-y-1/2,-z+2			
#3 x,-y,z+1/2; #4 -x+1/2,y-1/2,-z+3/2			
#5 -x+1/2,y+1/2,-z+3/2; #6 -x+1/2,-y+3/2,-z+1			

Table S3. Selected bond lengths (Å), angles [°], and structural parameters for **3**.

3			
Co(1)-O(5)	2.040(3)	Co(2)-O(1)	1.959(3)
Co(1)-O(5)#2	2.040(3)	Co(2)-O(2)	1.975(3)
Co(1)-O(4)#3	2.067(3)	Co(2)-O(6)#1	1.984(3)
Co(1)-O(4)#4	2.067(3)	Co(2)-N(1)	2.002(4)
Co(1)-O(2)#4	2.174(3)		
Co(1)-O(2)#3	2.174(3)		
Co1-O_{aver}	2.0936	Co2-X_{aver}(X = N, O)	1.98
O(1)-Co(2)-O(2)	116.11(12)	O(5)-Co(1)-O(5)#2	180.000(1)
O(1)-Co(2)-O(6)#1	111.11(14)	O(5)-Co(1)-O(4)#3	85.81(13)
O(2)-Co(2)-O(6)#1	99.31(13)	O(5)#2-Co(1)-O(4)#3	94.19(13)
O(1)-Co(2)-N(1)	109.97(14)	O(5)-Co(1)-O(4)#4	94.19(13)
O(2)-Co(2)-N(1)	120.69(14)	O(5)#2-Co(1)-O(4)#4	85.81(13)
O(5)-Co(1)-O(2)#3	88.80(12)	O(4)#3-Co(1)-O(4)#4	180.000(1)
O(5)#2-Co(1)-O(2)#3	91.20(12)	O(5)-Co(1)-O(2)#4	91.20(12)
O(4)#3-Co(1)-O(2)#3	91.60(12)	O(5)#2-Co(1)-O(2)#4	88.80(12)
O(4)#4-Co(1)-O(2)#3	88.40(12)	O(4)#3-Co(1)-O(2)#4	88.40(12)
O(2)#4-Co(1)-O(2)#3	180.0(1)	O(4)#4-Co(1)-O(2)#4	91.60(12)

Symmetry transformations used to generate equivalent atoms:

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

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

#5 -x+2,y-1/2,-z+3/2; #6 -x+2,-y,-z+1

Table S4. The Co^{II} center of geometry analysis for **1** by SHAPE software

	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-5
Co1	31.090	29.066	**0.179**	16.114	32.267
Co2	29.541	24.065	**2.065**	13.423	28.196

Table S5. The Co^{II} center of geometry analysis for 2 by SHAPE software

	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-5
Co1	29.712	28.295	**0.334**	16.329	31.278
	SP-4	**T-4**	SS-4	vTBPY-4	
Co2	25.549	**0.945**	6.131	3.091	

Table S6. The Co^{II} center of geometry analysis for **3** by SHAPE software

	HP-6	PPY-6	**OC-6**	TPR-6	JPPY-5
Co1	30.669	28.818	**0.184**	16.360	31.961
	SP-4	**T-4**	SS-4	vTBPY-4	
Co2	27.760	**0.950**	6.677	1.829	

HP-6: Hexagon
PPY-6: Pentagonal pyramid
OC-6: Octahedron
TPR-6: Trigonal prism
JPPY-5: Johnson pentagonal pyramid
SP-4: Square
T-4: Tetrahedron
SS-4: Seesaw or sawhorse
vTBPY-4: Axially vacant trigonal bipyramid

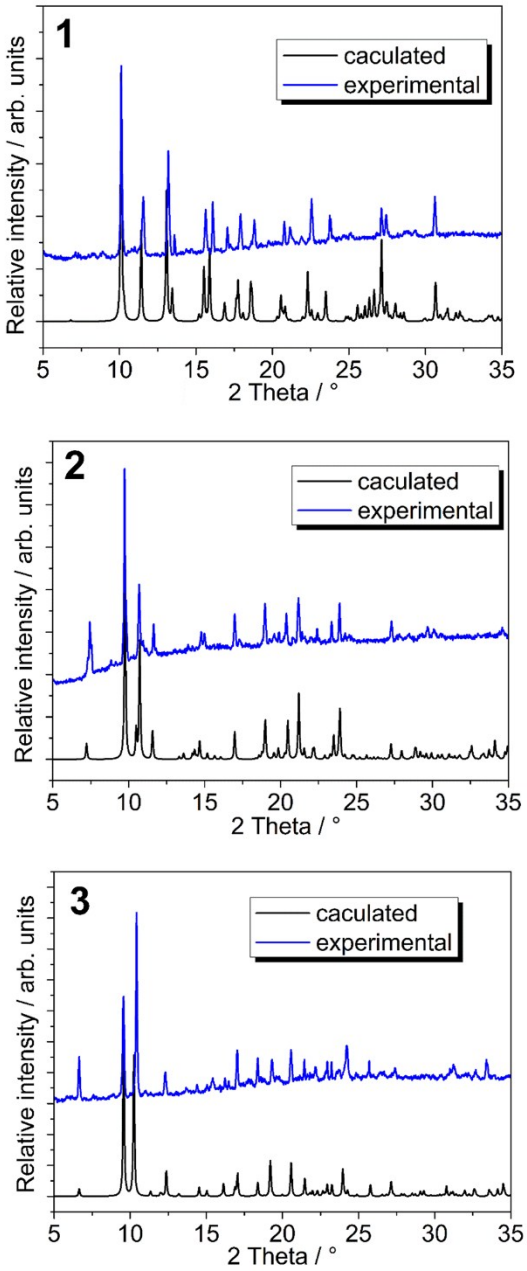

Figure S6. PXRD patterns for **1-3**.

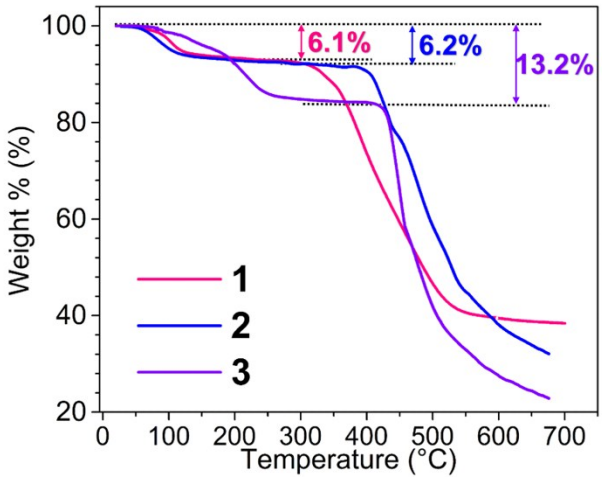

Figure S7. TGA curves for **1-3**.

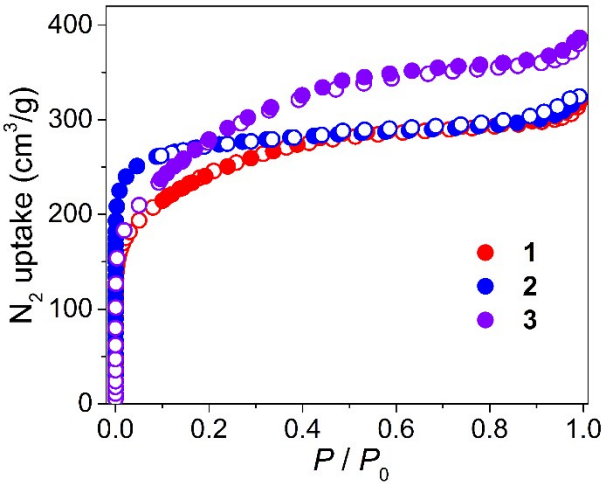

Figure S8. N_2 adsorption-desorption isotherms of **1-3** measured at 77 K

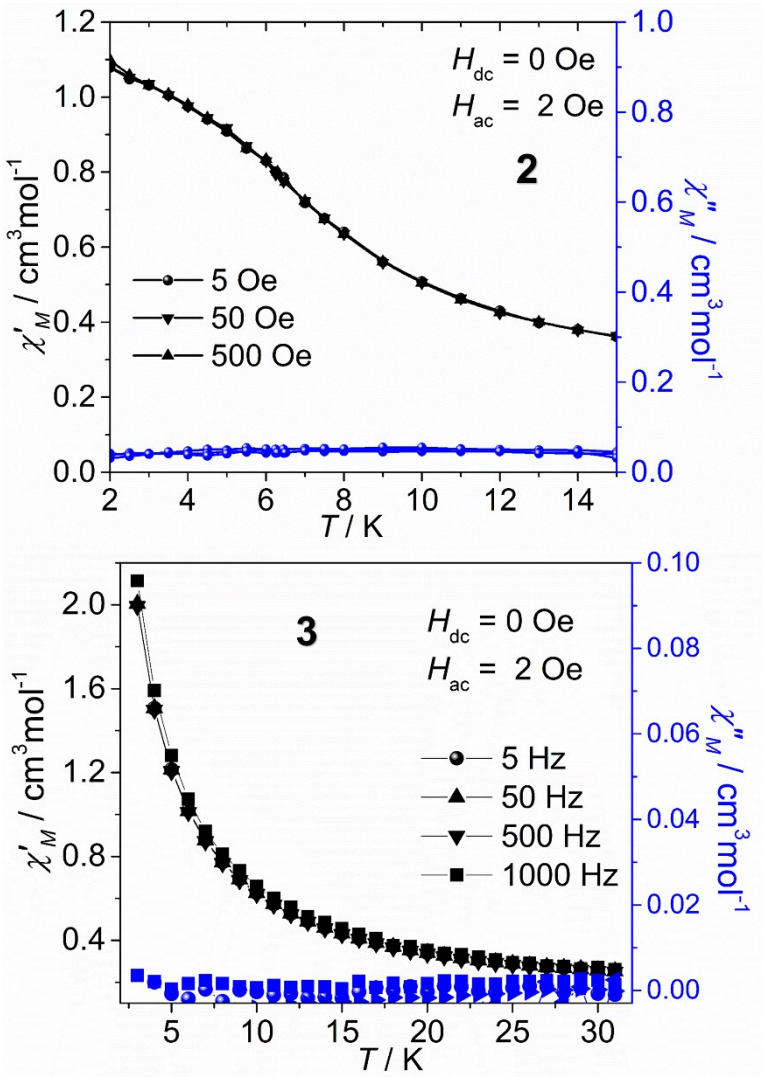

Figure S9. Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibilities measured under zero dc field at 1.8 K for **2** and **3**.