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Self-assembly and Magnetic Properties of Ni(II)/Co(II) Coordination Polymers Based on 1,4-Bis(imidazol-1-yl)benzene and Varying Biphenyltetracarboxylates

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Table S1 Bond Lengths [Å] and Angles [°] for **1-5**

Compound **1**			
Ni(1)-N(5)	2.056(6)	Ni(1)-O(5)	2.063(5)
Ni(1)-N(1)	2.073(6)	Ni(1)-N(4)$^{\#1}$	2.084(6)
Ni(1)-O(1)	2.118(5)	Ni(1)-O(2)	2.179(5)
N(5)-Ni(1)-O(5)	96.5(2)	N(5)-Ni(1)-N(1)	90.5(2)
O(5)-Ni(1)-N(1)	91.9(2)	N(5)-Ni(1)-N(4)$^{\#1}$	90.2(2)
O(5)-Ni(1)-N(4)$^{\#1}$	88.8(2)	N(1)-Ni(1)-N(4)$^{\#1}$	178.9(3)
N(5)-Ni(1)-O(1)	107.4(2)	O(5)-Ni(1)-O(1)	155.7(2)
N(1)-Ni(1)-O(1)	92.4(2)	N(4)$^{\#1}$-Ni(1)-O(1)	86.6(2)
N(5)-Ni(1)-O(2)	168.8(2)	O(5)-Ni(1)-O(2)	94.6(2)
N(1)-Ni(1)-O(2)	90.5(2)	N(4)$^{\#1}$-Ni(1)-O(2)	88.6(2)
O(1)-Ni(1)-O(2)	61.4(2)		

Symmetry codes: #1 x − 1/2, y + 1/2, z

Compound **2**			
Ni(1)-O(1)	2.073(4)	Ni(1)-N(1)	2.074(4)
Ni(1)-O(3)	2.075(4)	Ni(1)-N(5)	2.086(4)
Ni(1)-N(4)	2.095(4)	Ni(1)-O(5)	2.102(4)
O(1)-Ni(1)-N(1)	90.82(16)	O(1)-Ni(1)-O(3)	179.84(14)
N(1)-Ni(1)-O(3)	89.33(15)	O(1)-Ni(1)-N(5)	85.57(17)
N(1)-Ni(1)-N(5)	90.35(16)	O(3)-Ni(1)-N(5)	94.47(16)
O(1)-Ni(1)-N(4)	89.28(16)	N(1)-Ni(1)-N(4)	177.61(16)
O(3)-Ni(1)-N(4)	90.56(16)	N(5)-Ni(1)-N(4)	92.03(16)
O(1)-Ni(1)-O(5)	91.84(17)	N(1)-Ni(1)-O(5)	93.14(16)
O(3)-Ni(1)-O(5)	88.12(15)	N(5)-Ni(1)-O(5)	175.68(15)
N(4)-Ni(1)-O(5)	84.47(15)		

Compound **3**			
Co(1)-O(2)$^{\#1}$	2.042(2)	Co(1)-O(1)	2.046(2)
Co(1)-N(1)	2.110(3)	Co(1)-N(4)	2.145(3)
Co(1)-O(5)	2.163(3)	Co(1)-O(6)	2.180(3)
O(2)$^{\#1}$-Co(1)-O(1)	102.20(10)	O(2)$^{\#1}$-Co(1)-N(1)	88.45(10)
O(1)-Co(1)-N(1)	85.90(10)	O(2)$^{\#1}$-Co(1)-N(4)	93.64(10)
O(1)-Co(1)-N(4)	93.13(10)	N(1)-Co(1)-N(4)	177.84(11)
O(2)$^{\#1}$-Co(1)-O(5)	169.27(10)	O(1)-Co(1)-O(5)	88.47(10)
N(1)-Co(1)-O(5)	91.24(11)	N(4)-Co(1)-O(5)	86.81(11)
O(2)$^{\#1}$-Co(1)-O(6)	84.75(10)	O(1)-Co(1)-O(6)	170.70(11)
N(1)-Co(1)-O(6)	88.15(12)	N(4)-Co(1)-O(6)	92.58(12)
O(5)-Co(1)-O(6)	84.72(11)		

Symmetry codes: #1 −x + 1, −y + 2, −z + 2

Compound **4**			
Ni(1)-O(3)	2.040(4)	Ni(1)-O(1)	2.066(4)
Ni(1)-O(5)	2.066(4)	Ni(1)-N(1)	2.087(4)
Ni(1)-N(3)	2.090(4)	Ni(1)-O(1)#1	2.141(4)
Ni(1)-Ni(1)A	3.229(1)		
O(3)-Ni(1)-O(1)	92.54(15)	O(3)-Ni(1)-O(5)	92.47(16)
O(1)-Ni(1)-O(5)	174.59(15)	O(3)-Ni(1)-N(1)	83.72(17)
O(1)-Ni(1)-N(1)	89.16(16)	O(5)-Ni(1)-N(1)	89.37(16)
O(3)-Ni(1)-N(3)	96.62(18)	O(1)-Ni(1)-N(3)	95.38(17)
O(5)-Ni(1)-N(3)	86.06(17)	N(1)-Ni(1)-N(3)	175.42(18)
O(3)-Ni(1)-O(1)#1	167.71(16)	O(1)-Ni(1)-O(1)#1	79.70(15)
O(5)-Ni(1)-O(1)#1	95.02(15)	N(1)-Ni(1)-O(1)#1	86.62(16)
N(3)-Ni(1)-O(1)#1	93.61(16)	Ni(1)-O(1)- Ni(1)#1	100.3(2)

Symmetry codes:#1 −x + 1, −y + 1, −z + 1; #2(A) 1 − x, 1 − y, 1 − z

Compound **5**			
Co(1)-O(3)	2.061(1)	Co(1)-O(5)	2.098(2)
Co(1)-O(1)	2.105(1)	Co(1)-N(4)	2.133(2)
Co(1)-N(1)	2.146(2)	Co(1)-O(1)$^{\#1}$	2.1146(2)
Co(1)-Co(1A)$^{\#2}$	3.268(1)		
O(3)-Co(1)-O(5)	96.02(9)	O(3)-Co(1)-O(1)	89.52(7)
O(5)-Co(1)-O(1)	174.01(8)	O(3)-Co(1)-N(4)	97.87(8)
O(5)-Co(1)-N(4)	86.16(9)	O(1)-Co(1)-N(4)	95.36(8)
O(3)-Co(1)-N(1)	82.68(8)	O(5)-Co(1)-N(1)	88.80(8)
O(1)-Co(1)-N(1)	89.65(8)	N(4)-Co(1)-N(1)	174.95(8)
O(3)-Co(1)-O(1)$^{\#1}$	164.92(7)	O(5)-Co(1)-O(1)$^{\#1}$	93.82(8)
O(1)-Co(1)-O(1)$^{\#1}$	80.31(7)	N(4)-Co(1)-O(1)$^{\#1}$	94.17(8)
N(1)-Co(1)-O(1)$^{\#1}$	86.13(8)	Co(1)-O(1)- Co(1)	99.7(1)

Symmetry codes: #1 −x + 1, −y + 1, −z + 1; #2(A) 1 − x, 1 − y, 1 − z

Table S2 Hydrogen Bonds for **1-5** [Å and deg.]

Compound **1**				
O(5)-H(5A)...O(2)#5	0.82	2.01	2.752(7)	149.7

Symmetry code: #5 −x + 1/2, −y + 3/2, −z

Compound **2**				
O(7)-H(7D)...O(6)$^{\#7}$	0.88	2.12	2.872(9)	143.5
O(7)-H(7C)...O(2)$^{\#8}$	0.84	2.03	2.778(10)	148.5
O(6)-H(6D)...O(7)	0.82	2.45	3.203(10)	153.7
O(6)-H(6C)...O(4)$^{\#4}$	0.82	2.03	2.786(7)	151.6
O(8)-H(8C)...O(2)$^{\#6}$	0.83	2.15	2.959(17)	164.0
O(5)-H(5D)...O(3)$^{\#6}$	0.82	2.07	2.764(5)	141.0
O(5)-H(5C)...O(2)	0.83	1.91	2.704(7)	160.2

Symmetry codes: #4 −x + 1/2, y + 1/2, −z + 1/2; #6 −x + 1/2, −y + 1/2, −z + 1; #7 −x + 1, y, −z + 1/2; #8 x, −y + 1, z − 1/2

Compound **3**				
O(5)-H(5A)...O(3)$^{\#5}$	0.94(5)	1.85(5)	2.786(4)	177(4)
O(5)-H(5B)...O(4)$^{\#6}$	0.79(4)	1.91(4)	2.695(3)	170(4)
O(6)-H(6A)...O(3)$^{\#6}$	0.77(4)	2.05(4)	2.820(4)	174(5)
O(6)-H(6B)...O(4)$^{\#5}$	0.89(4)	1.88(4)	2.765(4)	175(4)

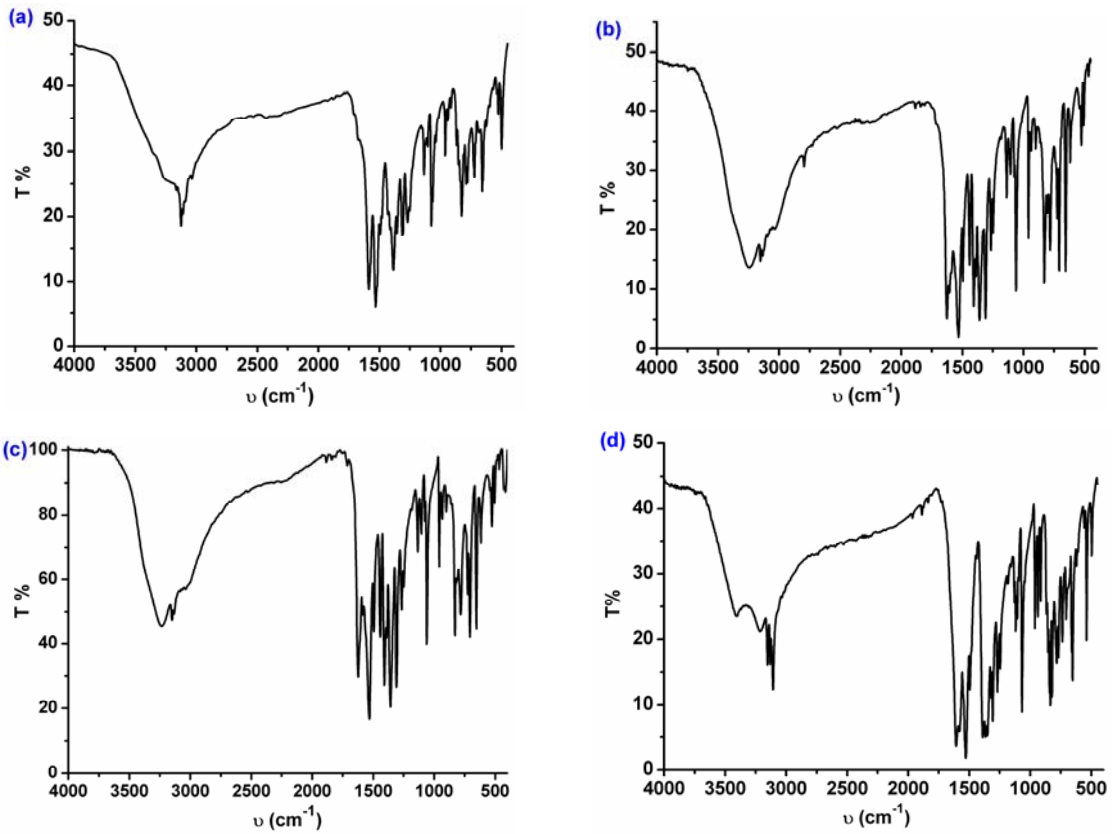
Symmetry codes: #5 x, −y + 3/2, z + 1/2; #6 −x, y + 1/2, −z + 3/2

Compound **4**				
O(5)-H(5A)...O(3)$^{\#5}$	0.82	1.97	2.792(5)	174.8
O(5)-H(5B)...O(2)$^{\#1}$	0.82	2.07	2.797(6)	148

Symmetry codes: #1 −x + 1, −y + 1, −z + 1; #5 −x + 1, −y + 1, −z + 1

Compound **5**				
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11)...O(4)$^{\#5}$	0.93	2.34	3.248(3)	165.4
C(2)-H(2)O(2)$^{\#6}$	0.93	2.47	3.256(3)	142.9
C(3)-H(3)...O(4)$^{\#7}$	0.93	2.43	3.269(3)	149.4
C(18)-H(18)...O(4)$^{\#8}$	0.93	2.52	3.376(3)	152.5
O(5)-H(5A)...O(2)$^{\#1}$	0.78(3)	2.13(3)	2.827(3)	148(3)
O(5)-H(5B)...O(3)$^{\#7}$	0.86(4)	1.93(4)	2.790(3)	178(3)

Symmetry code: #1 −x − 1, −y, −z + 1; #5 x, y − 1, z; #7 −x, −y, −z + 1; #8 −x, −y, −z;



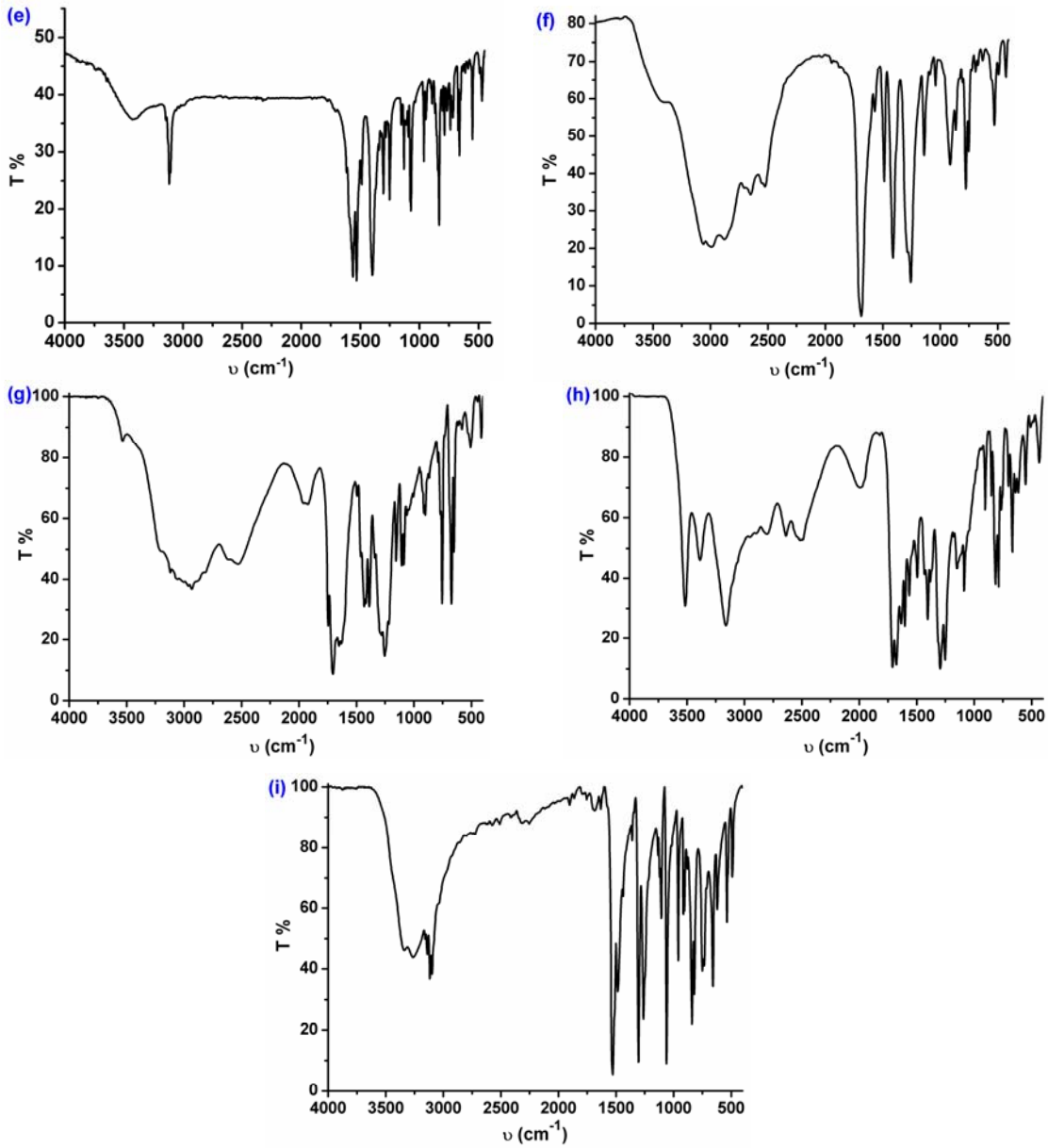


Figure S1 The FTIR spectra of of **1** (a), **2** (b), **3** (c) , **4** (d), **5** (e), H4(*o,m*-bpta) (f), H4(*m,m*-bpta) (g), H4(*m,p*-bpta) (h), and 1,4-bib.

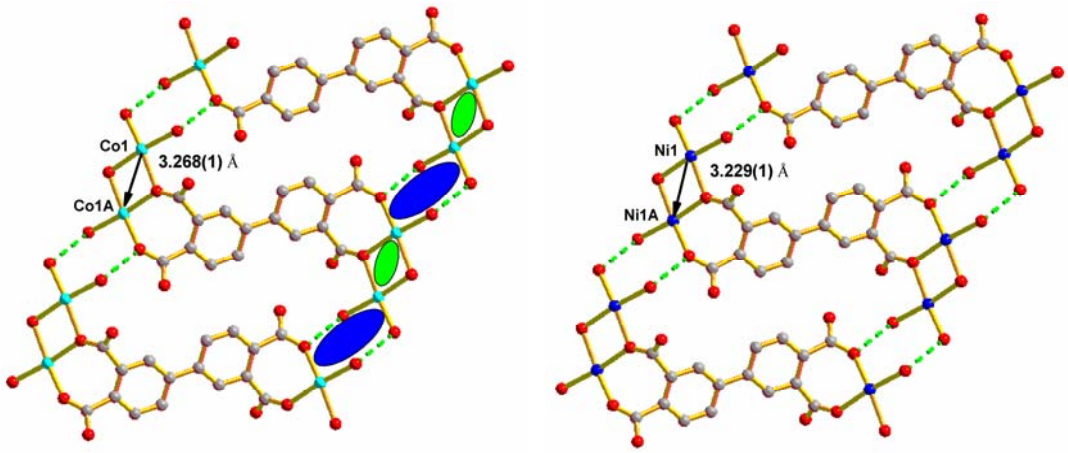


Figure S2 Compare the distance of Co1−Co1A with the distance of Ni1−Ni1A in compound **4**, and **5**

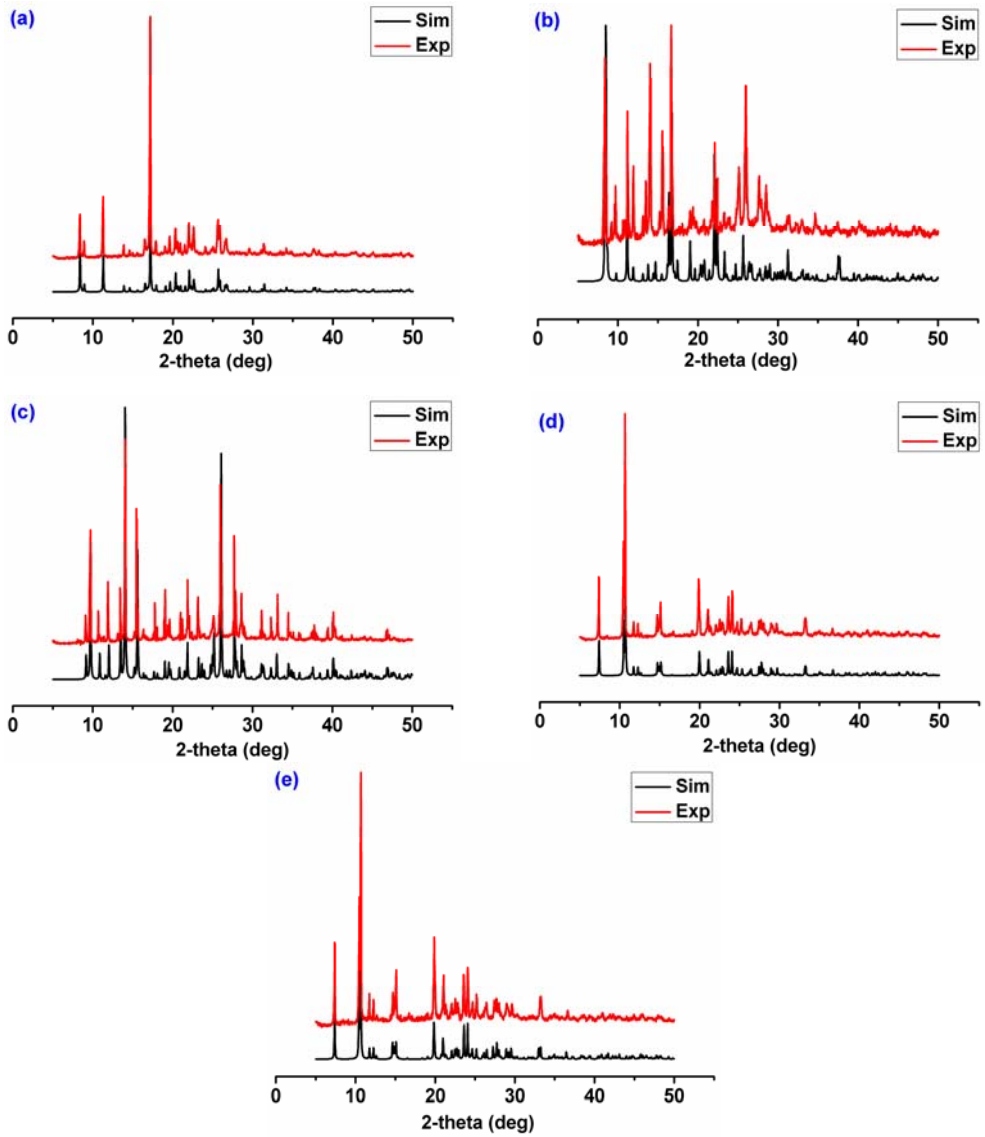


Figure S3 Comparison of the simulated and experimental XRPD patterns of **1** (a), **2** (b), **3** (c) , **4** (d), and **5** (e)

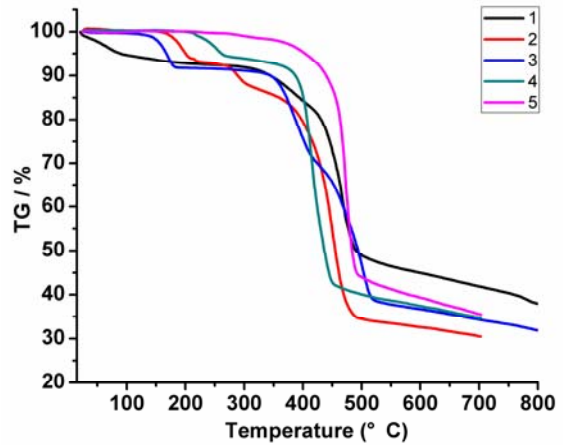


Figure S4 TGA curves of **1**-**5**

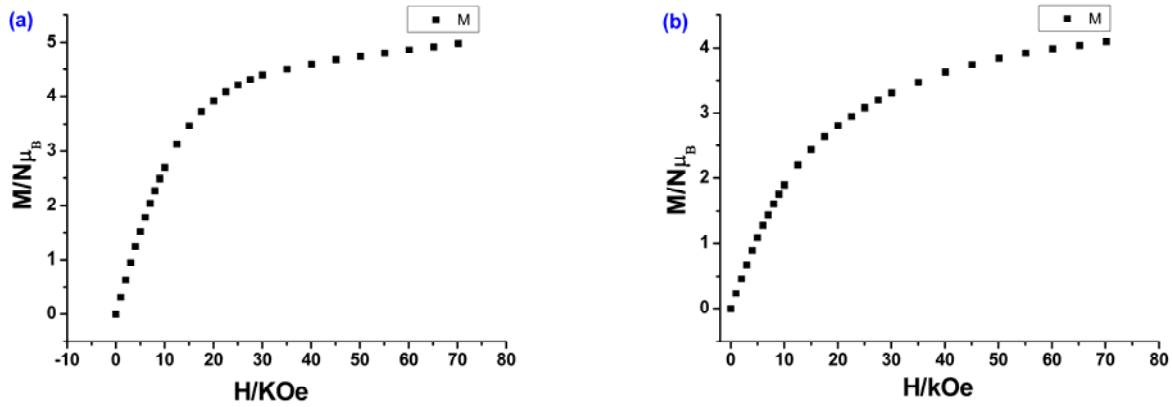


Figure S5 Plots of field dependence of the magnetization (M) of compounds **4** (a), and **5** (b) at 1.8 K.