

Six new coordination compounds based on rigid 5-(3-carboxyphenoxy)-pyridine-2-carboxylic acid: synthesis, structural variations and properties

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Figure caption:

Table S1 Bond lengths (Å) and Angles (deg) for compounds **1-6**

Fig. S1 Ni₂(H₂O)₈ dimer in compound **1**

Fig. S2 The 2D supramolecular layer in compound **1**

Fig. S3 the experimental and simulated X-ray diffraction patterns (a) for compound **1**, (b) for compound **2**, (c) for compound **3**, (d) for compound **4**, (e) for compound **5**, (f) For compound **6**.

Fig. S4 (a) Emission spectra of compound **4** in different solvents when excited at 280 nm, (b) Fluorescence titration of compound **4** dispersed in ethanol by gradual addition of acetone in ethanol, (c) The emission intensities of compound **4** in ethanol as a function of acetone content.

Fig. S5 UV-Vis absorption spectra of the solvents

Fig.S6 The field dependence of magnetization of compound **5** at 2 K.

Table S1 Bond lengths (Å) and angles (deg) for compounds 1-6**Table S1** Bond lengths (Å) and angles (deg) for compounds 1-6

1			
Ni(1)-O(3W)	2.0375(18)	O(3W)-Ni(1)-O(1W)	88.55(8)
Ni(1)-O(3)	2.0487(17)	O(3)-Ni(1)-O(1W)	90.78(7)
Ni(1)-O(4W)	2.0525(18)	O(4W)-Ni(1)-O(1W)	86.64(8)
Ni(1)-N(1)	2.0618(19)	N(1)-Ni(1)-O(1W)	170.22(7)
Ni(1)-O(1W)	2.0656(18)	O(3W)-Ni(1)-O(2W)	85.97(8)
Ni(1)-O(2W)	2.0946(18)	O(3)-Ni(1)-O(2W)	91.30(7)
O(3W)-Ni(1)-O(3)	177.16(8)	O(4W)-Ni(1)-O(2W)	177.75(7)
O(3W)-Ni(1)-O(4W)	91.86(8)	N(1)-Ni(1)-O(2W)	91.42(7)
O(3)-Ni(1)-O(4W)	90.86(7)	O(1W)-Ni(1)-O(2W)	92.72(7)
O(3W)-Ni(1)-N(1)	100.58(8)	C(13)-O(3)-Ni(1)	115.74(14)
O(3)-Ni(1)-N(1)	80.27(7)	C(12)-N(1)-Ni(1)	128.27(16)
O(4W)-Ni(1)-N(1)	89.56(8)	C(11)-N(1)-Ni(1)	112.77(14)
2			
Co(1)-O(3W)	2.062(2)	O(3W)-Co(1)-N(1)	101.14(9)
Co(1)-O(1W)	2.083(2)	O(1W)-Co(1)-N(1)	88.38(9)
Co(1)-O(1)	2.0853(18)	O(1)-Co(1)-N(1)	78.14(8)
Co(1)-O(4W)	2.096(2)	O(4W)-Co(1)-N(1)	168.83(9)
Co(1)-N(1)	2.105(2)	O(3W)-Co(1)-O(2W)	86.06(10)
Co(1)-O(2W)	2.119(2)	O(1W)-Co(1)-O(2W)	177.83(10)
O(3W)-Co(1)-O(1W)	91.79(10)	O(1)-Co(1)-O(2W)	90.16(8)
O(3W)-Co(1)-O(1)	176.13(9)	O(4W)-Co(1)-O(2W)	92.52(9)
O(1W)-Co(1)-O(1)	91.99(9)	N(1)-Co(1)-O(2W)	92.36(9)
O(3W)-Co(1)-O(4W)	89.22(9)	C(1)-O(1)-Co(1)	116.73(16)
O(1W)-Co(1)-O(4W)	87.11(9)	C(6)-N(1)-Co(1)	127.82(18)
O(1)-Co(1)-O(4W)	91.81(8)	C(2)-N(1)-Co(1)	113.65(16)
3			
Cd(1)-O(2)	2.275(3)	N(1)-Cd(1)-O(3)#1	136.61(9)
Cd(1)-O(1W)	2.289(3)	O(4)#1-Cd(1)-O(3)#1	54.18(9)
Cd(1)-O(2W)	2.307(3)	O(5)-Cd(1)-O(3)#1	80.20(9)
Cd(1)-N(1)	2.389(3)	O(3W)-Cd(2)-O(6)	92.43(12)
Cd(1)-O(4)#1	2.409(3)	O(3W)-Cd(2)-N(2)	95.38(12)
Cd(1)-O(5)	2.414(3)	O(6)-Cd(2)-N(2)	70.81(9)
Cd(1)-O(3)#1	2.434(3)	O(3W)-Cd(2)-O(5W)	166.52(14)
Cd(2)-O(3W)	2.303(3)	O(6)-Cd(2)-O(5W)	82.61(13)
Cd(2)-O(6)	2.331(3)	N(2)-Cd(2)-O(5W)	94.81(12)
Cd(2)-N(2)	2.354(3)	O(3W)-Cd(2)-O(4W)	89.95(14)

Cd(2)-O(5W)	2.362(3)	O(6)-Cd(2)-O(4W)	73.70(10)
Cd(2)-O(4W)	2.369(3)	N(2)-Cd(2)-O(4W)	144.28(10)
Cd(2)-O(7)#2	2.412(3)	O(5W)-Cd(2)-O(4W)	76.64(13)
Cd(2)-O(8)#2	2.419(3)	O(3W)-Cd(2)-O(7)#2	85.36(12)
O(3)-Cd(1)#1	2.434(3)	O(6)-Cd(2)-O(7)#2	154.28(9)
O(4)-Cd(1)#1	2.409(3)	N(2)-Cd(2)-O(7)#2	134.90(9)
O(7)-Cd(2)#2	2.412(3)	O(5W)-Cd(2)-O(7)#2	93.67(13)
O(8)-Cd(2)#2	2.419(3)	O(4W)-Cd(2)-O(7)#2	80.67(10)
O(2)-Cd(1)-O(1W)	106.65(13)	O(3W)-Cd(2)-O(8)#2	98.23(11)
O(2)-Cd(1)-O(2W)	81.10(13)	O(6)-Cd(2)-O(8)#2	151.35(10)
O(1W)-Cd(1)-O(2W)	172.25(13)	N(2)-Cd(2)-O(8)#2	81.72(10)
O(2)-Cd(1)-N(1)	70.21(10)	O(5W)-Cd(2)-O(8)#2	91.96(13)
O(1W)-Cd(1)-N(1)	85.38(11)	O(4W)-Cd(2)-O(8)#2	132.45(10)
O(2W)-Cd(1)-N(1)	97.66(11)	O(7)#2-Cd(2)-O(8)#2	53.77(9)
O(2)-Cd(1)-O(4)#1	147.57(10)	C(6)-N(1)-Cd(1)	126.9(2)
O(1W)-Cd(1)-O(4)#1	87.57(12)	C(2)-N(1)-Cd(1)	114.6(2)
O(2W)-Cd(1)-O(4)#1	85.78(11)	C(19)-N(2)-Cd(2)	127.0(2)
N(1)-Cd(1)-O(4)#1	82.44(9)	C(15)-N(2)-Cd(2)	114.8(2)
O(2)-Cd(1)-O(5)	78.72(10)	C(1)-O(2)-Cd(1)	121.1(2)
O(1W)-Cd(1)-O(5)	82.85(11)	C(13)-O(3)-Cd(1)#1	91.1(2)
O(2W)-Cd(1)-O(5)	98.81(11)	C(13)-O(4)-Cd(1)#1	92.8(2)
N(1)-Cd(1)-O(5)	141.87(10)	C(14)-O(5)-Cd(1)	147.1(3)
O(4)#1-Cd(1)-O(5)	132.84(9)	C(14)-O(6)-Cd(2)	116.8(2)
O(2)-Cd(1)-O(3)#1	149.20(10)	C(26)-O(7)-Cd(2)#2	92.2(2)
O(1W)-Cd(1)-O(3)#1	92.65(11)	C(26)-O(8)-Cd(2)#2	92.6(2)
O(2W)-Cd(1)-O(3)#1	80.23(11)		

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O(3)-Cd(2)#1	2.428(6)	O(1)#2-Cd(1)-O(1)	89.4(3)
O(4)-Cd(2)#1	2.423(6)	O(5)-Cd(1)-O(2)	80.95(15)
O(5)-Cd(1)	2.255(9)	O(1W)#2-Cd(1)-O(2)	89.3(3)
O(7)-Cd(2)	2.341(6)	O(1W)-Cd(1)-O(2)	90.9(3)
O(2)-Cd(2)	2.386(6)	O(1)#2-Cd(1)-O(2)	143.8(2)
O(2)-Cd(1)	2.458(6)	O(1)-Cd(1)-O(2)	54.3(2)
O(2W)-Cd(2)	2.311(7)	O(5)-Cd(1)-O(2)#2	80.95(15)
O(3W)-Cd(2)	2.299(7)	O(1W)#2-Cd(1)-O(2)#2	90.9(3)
N(1)-Cd(2)	2.367(6)	O(1W)-Cd(1)-O(2)#2	89.3(3)
O(1W)-Cd(1)	2.296(8)	O(1)#2-Cd(1)-O(2)#2	54.3(2)
Cd(1)-O(1W)#2	2.296(8)	O(1)-Cd(1)-O(2)#2	143.8(2)
Cd(1)-O(1)#2	2.365(6)	O(2)-Cd(1)-O(2)#2	161.9(3)
Cd(1)-O(1)	2.365(6)	O(3W)-Cd(2)-O(2W)	171.5(3)

Cd(1)-O(2)#2	2.458(6)	O(3W)-Cd(2)-O(7)	88.4(3)
Cd(2)-O(4)#1	2.423(6)	O(2W)-Cd(2)-O(7)	85.4(2)
Cd(2)-O(3)#1	2.428(6)	O(3W)-Cd(2)-N(1)	91.0(3)
C(13)-O(3)-Cd(2)#1	91.5(5)	O(2W)-Cd(2)-N(1)	97.4(2)
C(13)-O(4)-Cd(2)#1	92.0(5)	O(7)-Cd(2)-N(1)	141.6(2)
P(1)-O(5)-Cd(1)	124.0(3)	O(3W)-Cd(2)-O(2)	100.8(3)
P(1)#2-O(5)-Cd(1)	124.0(3)	O(2W)-Cd(2)-O(2)	82.9(3)
P(1)-O(7)-Cd(2)	129.3(4)	O(7)-Cd(2)-O(2)	73.3(2)
C(1)-O(2)-Cd(2)	118.3(5)	N(1)-Cd(2)-O(2)	69.1(2)
C(1)-O(2)-Cd(1)	90.1(5)	O(3W)-Cd(2)-O(4)#1	93.7(3)
Cd(2)-O(2)-Cd(1)	151.6(3)	O(2W)-Cd(2)-O(4)#1	86.7(2)
C(6)-N(1)-Cd(2)	124.7(5)	O(7)-Cd(2)-O(4)#1	134.9(2)
C(2)-N(1)-Cd(2)	116.4(5)	N(1)-Cd(2)-O(4)#1	83.4(2)
O(5)-Cd(1)-O(1W)#2	90.5(2)	O(2)-Cd(2)-O(4)#1	148.9(2)
O(5)-Cd(1)-O(1W)	90.5(2)	O(3W)-Cd(2)-O(3)#1	88.7(2)
O(1W)#2-Cd(1)-O(1W)	178.9(4)	O(2W)-Cd(2)-O(3)#1	84.7(2)
O(5)-Cd(1)-O(1)#2	135.29(14)	O(7)-Cd(2)-O(3)#1	80.8(2)
O(1W)#2-Cd(1)-O(1)#2	90.0(3)	N(1)-Cd(2)-O(3)#1	137.5(2)
O(1W)-Cd(1)-O(1)#2	89.2(3)	O(2)-Cd(2)-O(3)#1	152.1(2)
O(5)-Cd(1)-O(1)	135.29(14)	O(4)#1-Cd(2)-O(3)#1	54.22(19)
O(1W)#2-Cd(1)-O(1)	89.2(3)	C(1)-O(1)-Cd(1)	94.4(5)
O(1W)-Cd(1)-O(1)	90.0(3)		

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O(4)-Cu(1)	1.930(2)	O(4)#1-Cu(1)-N(1)#1	83.62(8)
Cu(1)-O(4)#1	1.930(2)	O(4)-Cu(1)-N(1)	83.62(8)
Cu(1)-N(1)#1	1.965(2)	O(4)#1-Cu(1)-N(1)	96.38(8)
Cu(1)-N(1)	1.965(2)	N(1)#1-Cu(1)-N(1)	180.000(1)
C(13)-O(4)-Cu(1)	115.42(17)	C(8)-N(1)-Cu(1)	127.46(18)
O(4)-Cu(1)-O(4)#1	180.000(1)	C(12)-N(1)-Cu(1)	112.03(16)
O(4)-Cu(1)-N(1)#1	96.38(8)		

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O(16)-Mn(1)#1	2.134(2)	O(5W)-Mn(4)-O(9)	87.50(11)
O(2)-Mn(2)#2	2.119(2)	O(15)#3-Mn(4)-O(9)	143.21(9)
O(15)-Mn(4)#3	2.192(2)	O(13)-Mn(4)-O(9)	126.70(8)
N(4)-Mn(4)#3	2.276(2)	O(5W)-Mn(4)-N(3)	144.91(10)
O(12)-Mn(3)#4	2.119(2)	O(15)#3-Mn(4)-N(3)	92.65(9)
O(5W)-Mn(4)	2.175(3)	O(13)-Mn(4)-N(3)	86.07(9)
O(1W)-Mn(1)	2.189(2)	O(9)-Mn(4)-N(3)	73.77(9)
Mn(1)-O(16)#5	2.134(2)	O(5W)-Mn(4)-N(4)#3	84.12(9)
Mn(1)-O(16)#6	2.134(2)	O(15)#3-Mn(4)-N(4)#3	72.86(8)

Mn(1)-O(1W)#7	2.189(2)	O(13)-Mn(4)-N(4)#3	143.56(9)
Mn(1)-O(1)	2.202(2)	O(9)-Mn(4)-N(4)#3	85.80(8)
Mn(1)-O(1)#7	2.202(2)	N(3)-Mn(4)-N(4)#3	122.62(10)
Mn(4)-O(15)#3	2.192(3)	O(12)#4-Mn(3)-O(14)	91.03(10)
Mn(4)-O(13)	2.198(2)	O(12)#4-Mn(3)-O(3W)	92.42(9)
Mn(4)-O(9)	2.208(2)	O(14)-Mn(3)-O(3W)	130.48(9)
Mn(4)-N(3)	2.228(3)	O(12)#4-Mn(3)-O(4)	89.08(9)
Mn(4)-N(4)#3	2.276(2)	O(14)-Mn(3)-O(4)	129.71(8)
Mn(3)-O(12)#4	2.119(2)	O(3W)-Mn(3)-O(4)	99.73(10)
Mn(3)-O(14)	2.144(2)	O(12)#4-Mn(3)-O(4W)	177.25(9)
Mn(3)-O(3W)	2.150(2)	O(14)-Mn(3)-O(4W)	90.35(10)
Mn(3)-O(4)	2.199(2)	O(3W)-Mn(3)-O(4W)	84.87(10)
Mn(3)-O(4W)	2.203(3)	O(4)-Mn(3)-O(4W)	91.85(10)
Mn(2)-O(2)#2	2.119(2)	O(2)#2-Mn(2)-O(5)	115.84(9)
Mn(2)-O(5)	2.122(3)	O(2)#2-Mn(2)-O(2W)	82.69(11)
Mn(2)-O(2W)	2.186(3)	O(5)-Mn(2)-O(2W)	96.19(12)
Mn(2)-O(4)	2.195(3)	O(2)#2-Mn(2)-O(4)	90.34(9)
Mn(2)-N(1)	2.273(2)	O(5)-Mn(2)-O(4)	146.66(10)
Mn(2)-N(2)	2.284(3)	O(2W)-Mn(2)-O(4)	107.91(11)
C(41)-O(16)-Mn(1)#1	139.55(18)	O(2)#2-Mn(2)-N(1)	154.57(10)
C(1)-O(2)-Mn(2)#2	146.9(2)	O(5)-Mn(2)-N(1)	87.42(9)
C(41)-O(15)-Mn(4)#3	119.71(17)	O(2W)-Mn(2)-N(1)	84.77(11)
C(46)-N(4)-Mn(4)#3	126.3(2)	O(4)-Mn(2)-N(1)	72.64(8)
C(42)-N(4)-Mn(4)#3	114.97(17)	O(2)#2-Mn(2)-N(2)	83.12(10)
C(40)-O(12)-Mn(3)#4	128.7(2)	O(5)-Mn(2)-N(2)	74.71(10)
O(16)#5-Mn(1)-O(16)#6	180.00(14)	O(2W)-Mn(2)-N(2)	157.62(11)
O(16)#5-Mn(1)-O(1W)#7	88.44(10)	O(4)-Mn(2)-N(2)	89.38(10)
O(16)#6-Mn(1)-O(1W)#7	91.56(10)	N(1)-Mn(2)-N(2)	114.61(10)
O(16)#5-Mn(1)-O(1W)	91.56(10)	C(53)-O(14)-Mn(3)	107.67(18)
O(16)#6-Mn(1)-O(1W)	88.44(10)	C(53)-O(13)-Mn(4)	134.78(19)
O(1W)#7-Mn(1)-O(1W)	180.0(3)	C(27)-O(9)-Mn(4)	118.72(18)
O(16)#5-Mn(1)-O(1)	88.60(8)	C(14)-O(5)-Mn(2)	120.42(19)
O(16)#6-Mn(1)-O(1)	91.40(8)	C(29)-N(3)-Mn(4)	115.27(19)
O(1W)#7-Mn(1)-O(1)	90.79(10)	C(33)-N(3)-Mn(4)	126.3(2)
O(1W)-Mn(1)-O(1)	89.22(10)	C(1)-O(1)-Mn(1)	120.48(19)
O(16)#5-Mn(1)-O(1)#7	91.40(8)	C(13)-O(4)-Mn(2)	119.61(18)
O(16)#6-Mn(1)-O(1)#7	88.60(8)	C(13)-O(4)-Mn(3)	101.01(18)
O(1W)#7-Mn(1)-O(1)#7	89.22(10)	Mn(2)-O(4)-Mn(3)	138.27(10)
O(1W)-Mn(1)-O(1)#7	90.78(10)	C(11)-N(1)-Mn(2)	115.66(18)
O(1)-Mn(1)-O(1)#7	180.00(11)	C(12)-N(1)-Mn(2)	124.5(2)
O(5W)-Mn(4)-O(15)#3	118.67(11)	C(28)-N(2)-Mn(2)	128.1(2)

O(5W)-Mn(4)-O(13)	81.75(9)	C(15)-N(2)-Mn(2)	111.8(2)
O(15)#3-Mn(4)-O(13)	84.89(8)		

Symmetry transformations: compound 3: #1 $-x+1, -y+1, -z-1$, #2 $-x, -y, -z+1$. compound 4: #1 $-x+3/2, -y+1/2, -z+1$, #2 $-x+1, y, -z+1/2$. compound 5: #1 $-x+1, -y+2, -z+1$. compound 6: #1 $x+1, y+1, z+2$, #2 $-x+1, -y, -z+1$, #3 $-x+2, -y+1, -z+3$, #4 $-x+1, -y+1, -z+2$, #5 $-x+2, -y+1, -z+2$, #6 $x-1, y-1, z-2$, #7 $-x+1, -y, -z$.

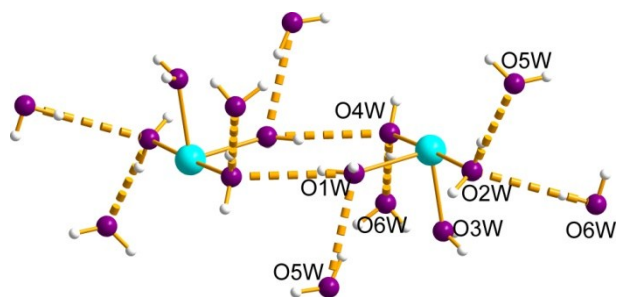


Fig. S1 $\text{Ni}_2(\text{H}_2\text{O})_8$ dimer in compound **1**

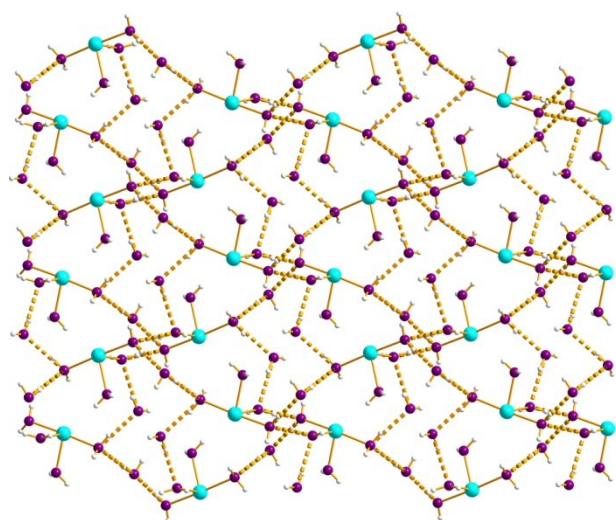


Fig. S2 The 2D supramolecular layer in compound **1**

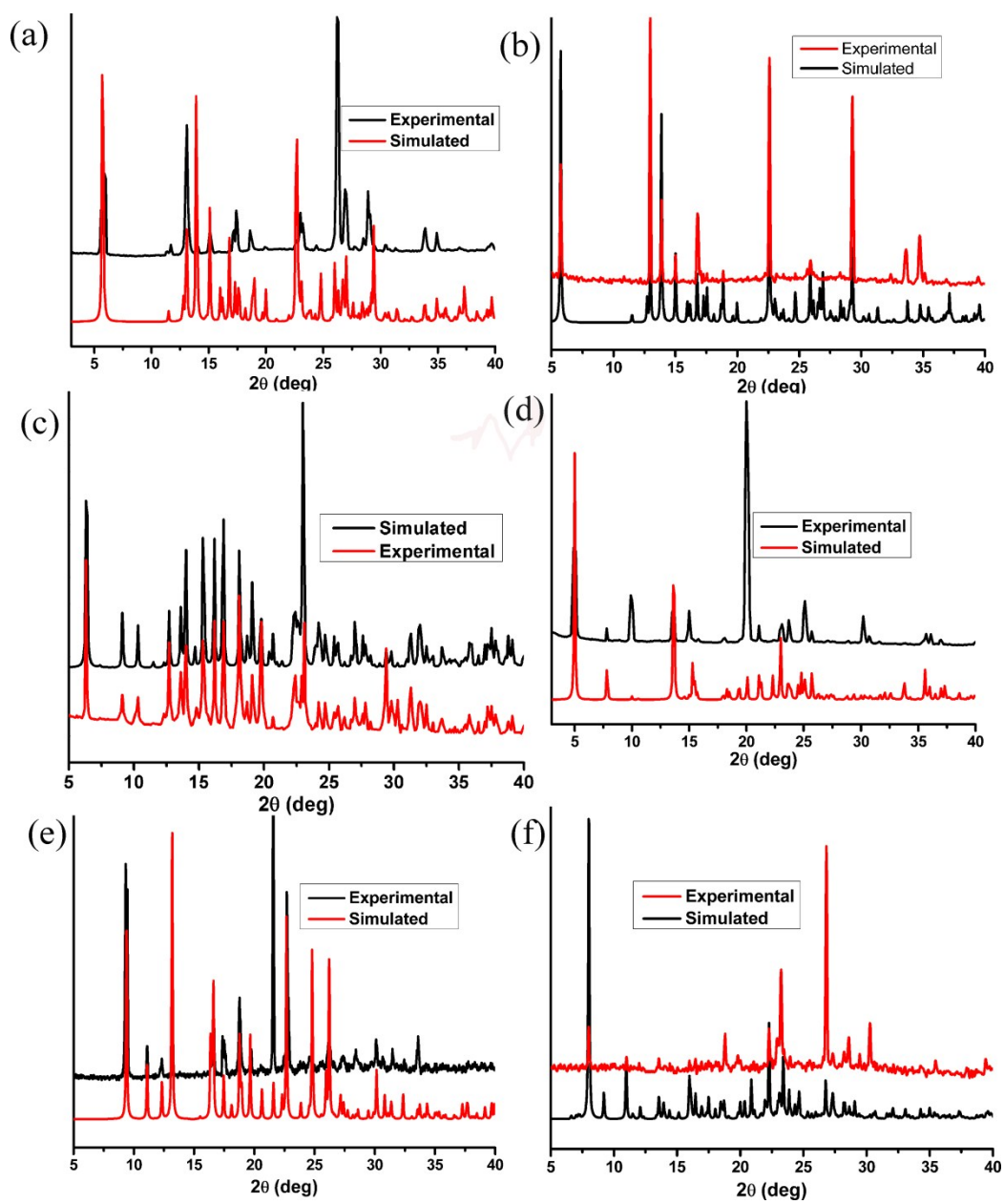


Fig. S3 the experimental and simulated X-ray diffraction patterns (a) for compound 1, (b) for compound 2, (c) for compound 3, (d) for compound 4, (e) for compound 5, (f) For compound 6.

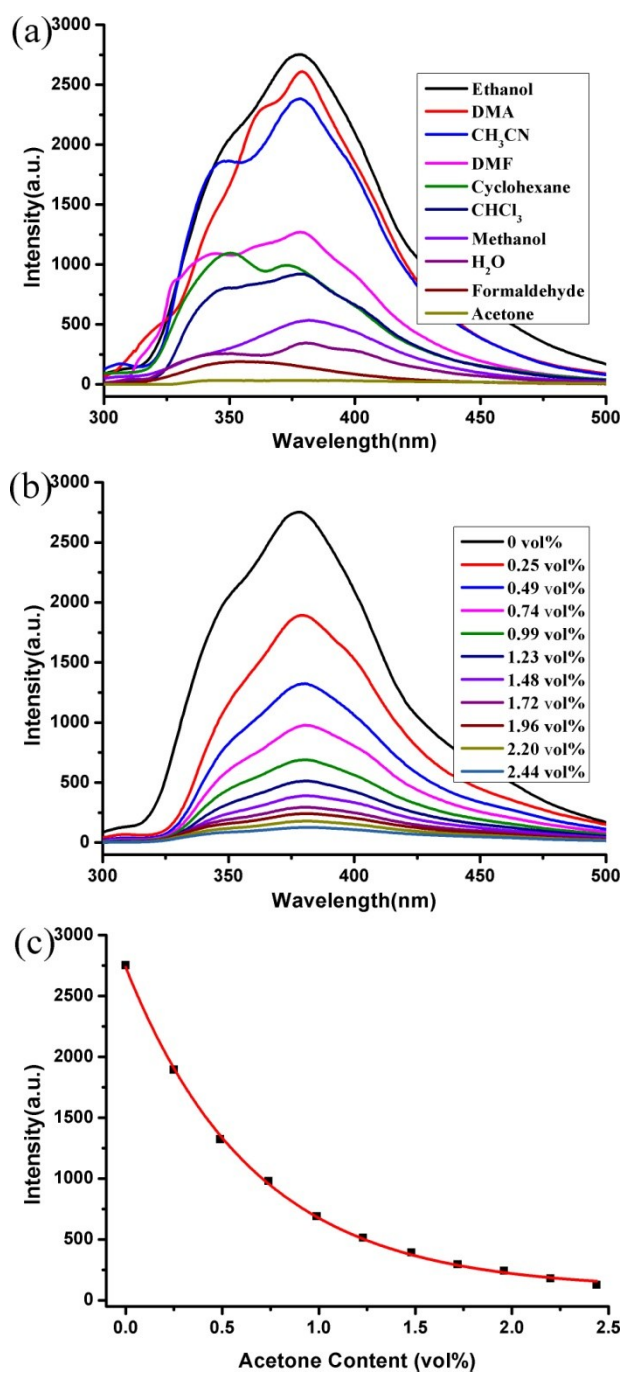


Fig. S4 (a) Emission spectra of compound **4** in different solvents when excited at 280 nm, (b) Fluorescence titration of compound **4** dispersed in ethanol by gradual addition of acetone in ethanol, (c) The emission intensities of compound **4** in ethanol as a function of acetone content.

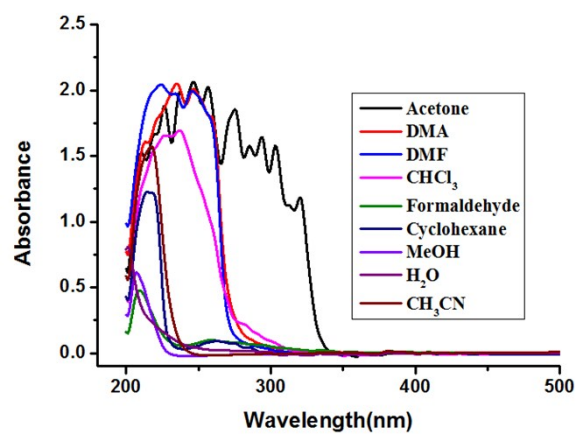


Fig. S5 UV-Vis absorption spectra of the solvents

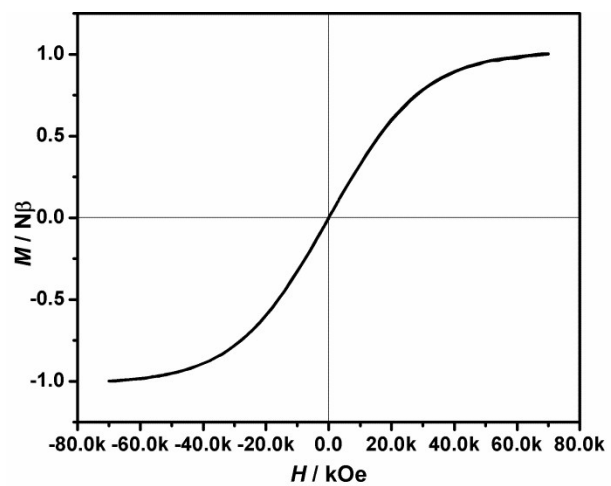


Fig.S6 The field dependence of magnetization of compound **5** at 2 K.