Electronic Supplementary Information for

A series of divalent metal coordination polymers based on isomeric tetracarboxylic acid: Syntheses, structures and magnetic properties

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Table S1. Selected Bond Lengths (Å) and Angles (º) for **1–5**[a].

1			
Mn(1)-O(1)	2.1047(18)	Mn(1)-O(5)#1	2.1206(17)
Mn(1)-O(10)	2.204(2)	Mn(1)-O(9)	2.2120(17)
Mn(1)-N(2)	2.283(2)	Mn(1)-N(1)	2.292(2)
O(1)-Mn(1)-O(5)#1	100.22(8)	O(1)-Mn(1)-O(10)	90.52(9)
O(5)#1-Mn(1)-O(10)	89.69(7)	O(1)-Mn(1)-O(9)	91.43(8)
O(5)#1-Mn(1)-O(9)	87.28(7)	O(10)-Mn(1)-O(9)	176.64(7)
O(1)-Mn(1)-N(2)	164.85(8)	O(5)#1-Mn(1)-N(2)	94.92(8)
O(10)-Mn(1)-N(2)	89.49(10)	O(9)-Mn(1)-N(2)	89.33(8)
O(1)-Mn(1)-N(1)	92.59(8)	O(5)#1-Mn(1)-N(1)	166.77(7)
O(10)-Mn(1)-N(1)	93.49(8)	O(9)-Mn(1)-N(1)	89.15(7)
N(2)-Mn(1)-N(1)	72.29(9)		
2			
Co(1)-O(5)#1	2.059(3)	Co(1)-O(1)	2.059(2)
Co(1)-N(1)	2.094(3)	Co(1)-O(9)	2.109(3)
Co(1)-O(10)	2.127(3)	Co(1)-O(4)#1	2.205(3)
O(5)#1-Co(1)-O(1)	95.21(11)	O(5)#1-Co(1)-N(1)	172.07(13)
O(1)-Co(1)-N(1)	91.05(12)	O(5)#1-Co(1)-O(9)	83.01(13)
O(1)-Co(1)-O(9)	175.98(11)	N(1)-Co(1)-O(9)	91.04(14)
O(5)#1-Co(1)-O(10)	91.62(11)	O(1)-Co(1)-O(10)	89.55(11)
N(1)-Co(1)-O(10)	93.30(12)	O(9)-Co(1)-O(10)	86.90(12)
O(5)#1-Co(1)-O(4)#1	85.97(11)	O(1)-Co(1)-O(4)#1	91.10(11)
N(1)-Co(1)-O(4)#1	89.05(12)	O(9)-Co(1)-O(4)#1	92.38(12)
O(10)-Co(1)-O(4)#1	177.56(11)		
3			
Co(1)-O(1)	2.0605(19)	Co(1)-O(6)#1	2.077(2)
Co(1)-O(10)	2.087(2)	Co(1)-N(1)	2.089(3)
Co(1)-O(9)	2.143(2)	Co(1)-O(7)#1	2.2034(19)
O(1)-Co(1)-O(6)#1	94.19(8)	O(1)-Co(1)-O(10)	177.68(8)
O(6)#1-Co(1)-O(10)	84.64(9)	O(1)-Co(1)-N(1)	91.47(9)
O(6)#1-Co(1)-N(1)	173.60(9)	O(10)-Co(1)-N(1)	89.81(10)
O(1)-Co(1)-O(9)	88.06(8)	O(6)#1-Co(1)-O(9)	88.82(8)
O(10)-Co(1)-O(9)	89.91(8)	N(1)-Co(1)-O(9)	94.36(9)
O(1)-Co(1)-O(7)#1	89.17(8)	O(6)#1-Co(1)-O(7)#1	85.64(8)
O(10)-Co(1)-O(7)#1	92.73(8)	N(1)-Co(1)-O(7)#1	91.47(9)
O(9)-Co(1)-O(7)#1	173.61(8)		
4			
Ni(1)-O(1)#1	2.041(2)	Ni(1)-O(1)	2.041(2)
Ni(1)-N(3)#2	2.094(2)	Ni(1)-N(3)#3	2.094(2)
Ni(1)-O(9)#1	2.110(2)	Ni(1)-O(9)	2.110(2)
Ni(2)-O(2)	2.032(2)	Ni(2)-O(3)	2.043(2)
Ni(2)-N(1)	2.063(2)	Ni(2)-O(7)#2	2.075(2)
Ni(2)-O(10)	2.137(2)	Ni(2)-O(8)#2	2.185(2)

Ni(3)-O(11)#4	2.041(2)	Ni(3)-O(11)	2.041(2)
Ni(3)-O(6)#5	2.059(2)	Ni(3)-O(6)#6	2.059(2)
Ni(3)-O(4)#4	2.090(2)	Ni(3)-O(4)	2.090(2)
O(1)#1-Ni(1)-O(1)	180.0	O(1)#1-Ni(1)-N(3)#2	87.46(9)
O(1)-Ni(1)-N(3)#2	92.54(9)	O(1)#1-Ni(1)-N(3)#3	92.54(10)
O(1)-Ni(1)-N(3)#3	87.46(9)	N(3)#2-Ni(1)-N(3)#3	180.000(1)
O(1)#1-Ni(1)-O(9)#1	85.56(8)	O(1)-Ni(1)-O(9)#1	94.44(8)
N(3)#2-Ni(1)-O(9)#1	84.90(8)	N(3)#3-Ni(1)-O(9)#1	95.10(8)
O(1)#1-Ni(1)-O(9)	94.44(8)	O(1)-Ni(1)-O(9)	85.56(8)
N(3)#2-Ni(1)-O(9)	95.10(8)	N(3)#3-Ni(1)-O(9)	84.90(8)
O(9)#1-Ni(1)-O(9)	180.000(1)	O(2)-Ni(2)-O(3)	91.04(10)
O(2)-Ni(2)-N(1)	92.51(9)	O(3)-Ni(2)-N(1)	99.69(9)
O(2)-Ni(2)-O(7)#2	90.31(9)	O(3)-Ni(2)-O(7)#2	89.16(8)
N(1)-Ni(2)-O(7)#2	170.66(9)	O(2)-Ni(2)-O(10)	176.68(9)
N(1)-Ni(2)-O(10)	89.99(10)	O(7)#2-Ni(2)-O(10)	86.89(9)
O(2)-Ni(2)-O(8)#2	82.36(9)	O(3)-Ni(2)-O(8)#2	150.18(8)
N(1)-Ni(2)-O(8)#2	109.60(9)	O(7)#2-Ni(2)-O(8)#2	61.97(8)
O(10)-Ni(2)-O(8)#2	94.73(10)	O(3)-Ni(2)-O(10)	90.70(10)
O(11)#4-Ni(3)-O(6)#5	92.86(9)	O(11)#4-Ni(3)-O(11)	180.00(9)
O(11)#4-Ni(3)-O(6)#6	87.14(9)	O(11)-Ni(3)-O(6)#5	87.14(9)
O(6)#5-Ni(3)-O(6)#6	180.0	O(11)-Ni(3)-O(6)#6	92.86(9)
O(11)-Ni(3)-O(4)#4	91.73(8)	O(11)#4-Ni(3)-O(4)#4	88.27(8)
O(6)#6-Ni(3)-O(4)#4	90.94(9)	O(6)#5-Ni(3)-O(4)#4	89.06(9)
O(11)-Ni(3)-O(4)	88.27(8)	O(11)#4-Ni(3)-O(4)	91.73(8)
O(6)#6-Ni(3)-O(4)	89.06(9)	O(6)#5-Ni(3)-O(4)	90.94(9)
O(4)#4-Ni(3)-O(4)	180.00(9)		
5			
Co(1)-O(9)#1	2.069(2)	Co(1)-O(9)	2.069(2)
Co(1)-O(2)#1	2.108(2)	Co(1)-O(2)	2.108(2)
Co(1)-O(6)#2	2.120(2)	Co(1)-O(6)#3	2.120(2)
Co(2)-O(10)#4	2.0853(18)	Co(2)-O(10)	2.0853(18)
Co(2)-O(4)#4	2.0958(19)	Co(2)-O(4)	2.0958(19)
Co(2)-O(8)#5	2.110(2)	Co(2)-O(8)#6	2.110(2)
Co(3)-O(10)#7	2.0761(17)	Co(3)-O(10)	2.0873(18)
Co(3)-O(7)#8	2.0821(19)	Co(3)-O(3)#4	2.0974(18)
Co(3)-O(12)	2.160(2)	Co(3)-O(11)	2.1678(19)
O(9)#1-Co(1)-O(9)	180.00(5)	O(9)#1-Co(1)-O(2)#1	89.24(8)
O(9)-Co(1)-O(2)#1	90.76(8)	O(9)#1-Co(1)-O(2)	90.76(8)
O(9)-Co(1)-O(2)	89.24(8)	O(2)#1-Co(1)-O(2)	180.00(9)
O(9)#1-Co(1)-O(6)#2	91.89(8)	O(9)-Co(1)-O(6)#2	88.11(8)
O(2)#1-Co(1)-O(6)#2	90.13(9)	O(2)-Co(1)-O(6)#2	89.87(9)
O(9)#1-Co(1)-O(6)#3	88.11(8)	O(9)-Co(1)-O(6)#3	91.89(8)
O(2)#1-Co(1)-O(6)#3	89.87(9)	O(2)-Co(1)-O(6)#3	90.13(9)

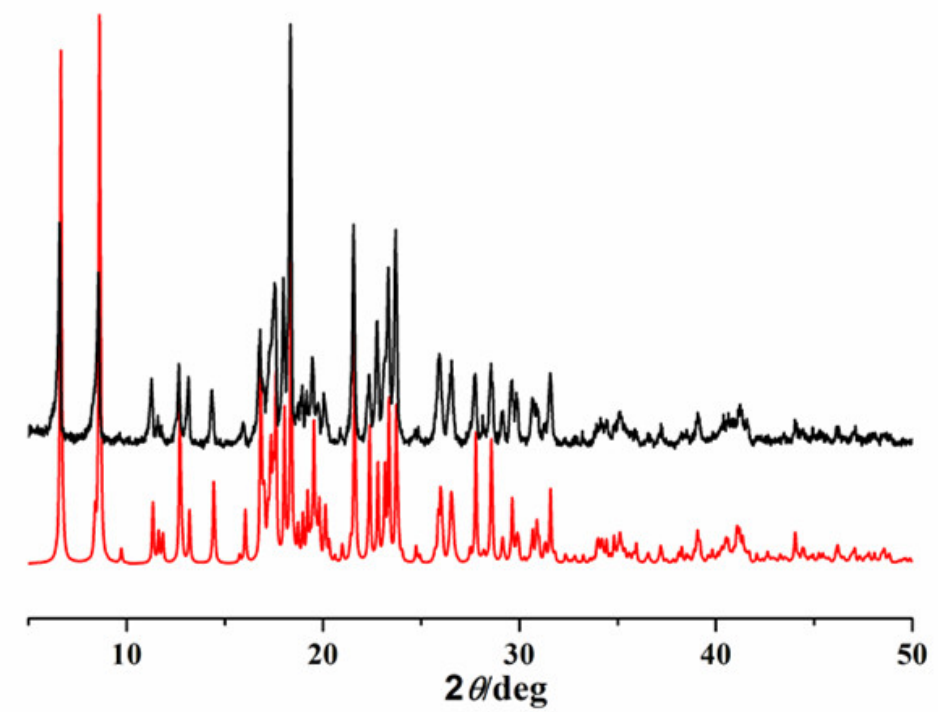
O(6)#2-Co(1)-O(6)#3	180.000(1)	O(10)-Co(2)-O(10)#4	180.00(2)
O(10)-Co(2)-O(4)	86.21(6)	O(10)#4-Co(2)-O(4)	93.79(6)
O(10)-Co(2)-O(4)#4	93.79(6)	O(10)#4-Co(2)-O(4)#4	86.21(6)
O(4)-Co(2)-O(4)#4	180.00(9)	O(10)-Co(2)-O(8)#5	84.58(6)
O(10)#4-Co(2)-O(8)#5	95.42(6)	O(4)-Co(2)-O(8)#5	89.85(8)
O(4)#4-Co(2)-O(8)#5	90.15(8)	O(10)-Co(2)-O(8)#6	95.42(6)
O(10)#4-Co(2)-O(8)#6	84.58(6)	O(4)-Co(2)-O(8)#6	90.15(8)
O(4)#4-Co(2)-O(8)#6	89.85(8)	O(8)#5-Co(2)-O(8)#6	180.0
O(10)#7-Co(3)-O(7)#8	95.53(7)	O(10)#7-Co(3)-O(10)	84.87(7)
O(7)#8-Co(3)-O(10)	93.12(7)	O(10)#7-Co(3)-O(3)#4	92.08(7)
O(7)#8-Co(3)-O(3)#4	168.77(7)	O(10)-Co(3)-O(3)#4	95.78(7)
O(10)#7-Co(3)-O(12)	92.09(8)	O(7)#8-Co(3)-O(12)	90.97(8)
O(10)-Co(3)-O(12)	175.12(7)	O(3)#4-Co(3)-O(12)	80.49(8)
O(10)#7-Co(3)-O(11)	175.04(7)	O(7)#8-Co(3)-O(11)	82.26(8)
O(10)-Co(3)-O(11)	90.80(7)	O(12)-Co(3)-O(11)	92.39(9)
O(3)#4-Co(3)-O(11)	90.76(8)		

[a] Symmetry codes: **1**: #1: *x* + 1, *y* + 1, *z*; **2**: #1: - *x*, - *y* + 1, - *z* + 1; **3**: #1: - *x*, - *y* + 1, - *z* + 1; **4**: #1: - *x* + 1, - *y* + 2, - *z* + 1; #2: *x*, - *y* + 3/2, *z* + 1/2; #3: - *x* + 1, *y* + 1/2, - *z* + 1/2; #4: - *x*, - *y* + 2, - *z* + 1; #5: *x*, - *y* + 5/2, *z* + 1/2; #6: - *x*, *y* - 1/2, - *z* + 1/2; **5**: #1: - *x* + 2, - *y* - 1, - *z* + 1; #2: *x*, - *y* - 1/2, *z* + 1/2; #3: - *x* + 2, *y* - 1/2, - *z* + 1/2; #4: - *x* + 1, - *y*, - *z* + 1; #5: *x*, - *y* + 1/2, *z* + 1/2; #6: - *x* + 1, *y* - 1/2, - *z* + 1/2; #7: - *x* + 1, - *y* + 1, - *z* + 1; #8: - x + 1, y + 1/2, - z + 1/2.

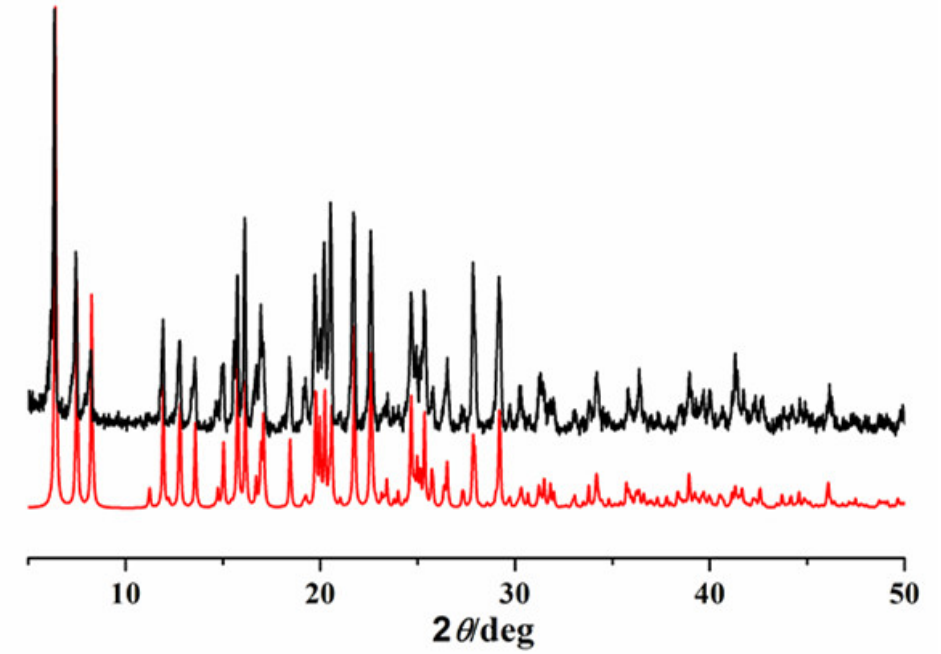
Table S2. Distance (Å) and angles (°) of hydrogen bonding for **1–3**[a].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
1				
O(3)-H(3A)···O(2)	0.881(18)	1.530(19)	2.410(3)	177(4)
O(7)-H(7A)···O(4)#3	0.851(18)	1.74(2)	2.580(3)	169(4)
O(9)-H(9A)···O(2)#4	0.833(16)	1.985(18)	2.813(3)	173(3)
O(9)-H(9B)···O(5)#5	0.860(16)	1.98(2)	2.811(3)	161(3)
O(10)-H(10B)···O(8)#6	0.89	1.99	2.876(3)	168.6
O(10)-H(10A)···O(6)#1	0.90	1.78	2.660(3)	164.3
2				
O(11)-H(11B)···O(1)#3	0.85	2.35	3.126(8)	152.9
O(11)-H(11A)···N(3)	0.85	2.15	3.003(8)	176.0
O(10)-H(10B)···O(2)	0.85	2.16	2.823(4)	134.1
O(10)-H(10A)···O(8)#3	0.85	2.03	2.855(5)	163.6
O(9)-H(9B)···O(8)#3	0.85	2.34	3.128(5)	155.4
O(9)-H(9A)···O(5)#4	0.85	1.80	2.651(5)	179.2
O(7)-H(7A)···O(6)#5	0.85	1.72	2.571(4)	175.9
O(3)-H(3A)···O(2)#6	0.85	1.68	2.501(4)	162.2
3				
O(10)-H(10A)···O(3)#3	0.85	2.06	2.869(3)	158.8
O(10)-H(10B)···O(6)#4	0.85	1.90	2.701(3)	157.2
O(9)-H(9B)···O(3)#3	0.85	2.57	2.996(3)	112.0
O(9)-H(9B)···O(5)#5	0.85	2.36	3.056(3)	139.6
O(9)-H(9A)···O(2)	0.85	1.97	2.739(3)	149.2
O(8)-H(8A)···O(2)#6	0.82	1.71	2.519(3)	167.9
O(4)-H(4A)···O(5)#7	0.82	1.76	2.573(3)	173.0

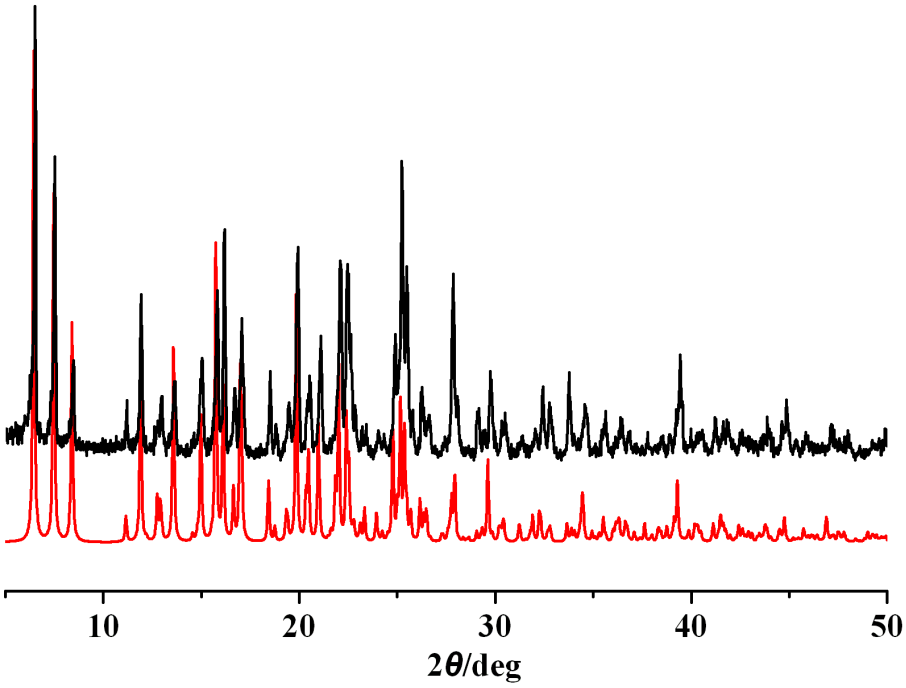
[a] Symmetry codes: **1**: *x* + 1, *y* + 1, *z*; #3: *x*, *y*, *z* + 1; #4: - *x* + 1, - *y* + 1, - *z*; #5: - *x*, - *y*, - *z*; #6: - *x* + 1, - *y*, - *z* + 1; **2**: #3: - *x* + 1/2, - *y* + 3/2, - *z* + 1; #4: *x* + 1/2, - *y* + 3/2, *z* + 1/2; #5: - *x*, *y* + 1, - *z* + 1/2; #6: - *x*, - *y*, - *z* + 1; **3**: #3: - *x* + 1/2, - *y* + 1/2, - *z* + 1; #4: *x* + 1/2, - *y* + 1/2, *z* + 1/2; #5: *x* + 1/2, - *y* + 3/2, *z* + 1/2; #6: - *x*, - *y* + 2, - *z* + 1; #7: - *x*, *y* - 1, - *z* + 1/2.



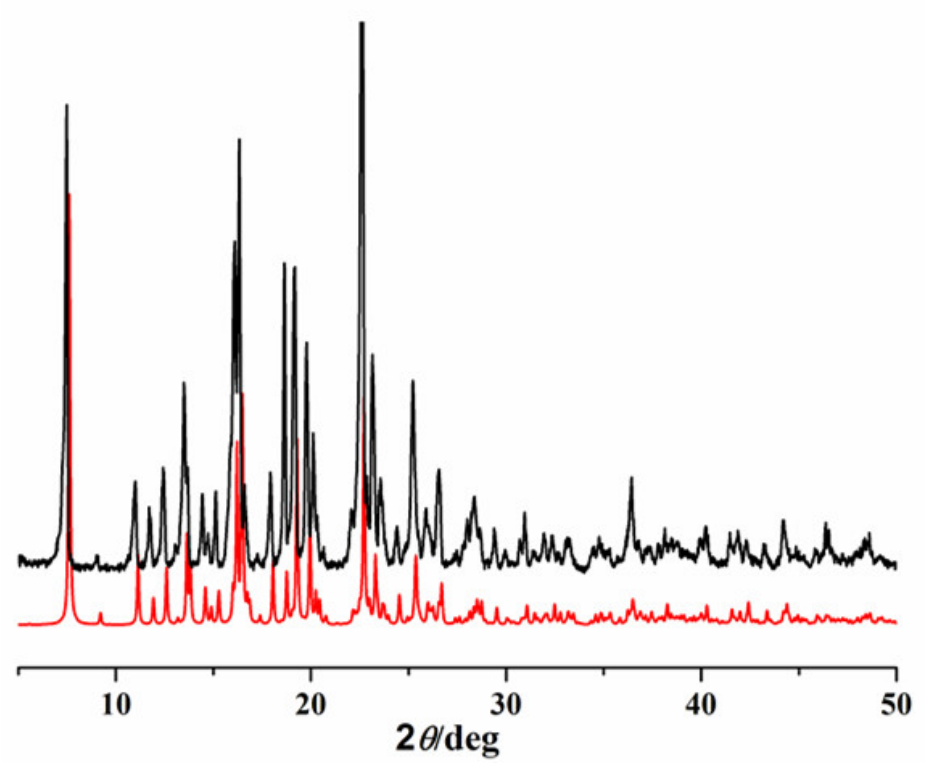
1



2



3



4

Figure S1. Comparison of the experimental and simulated PXRD patterns. In each case, the top is the experimental pattern and the bottom is the simulated one.

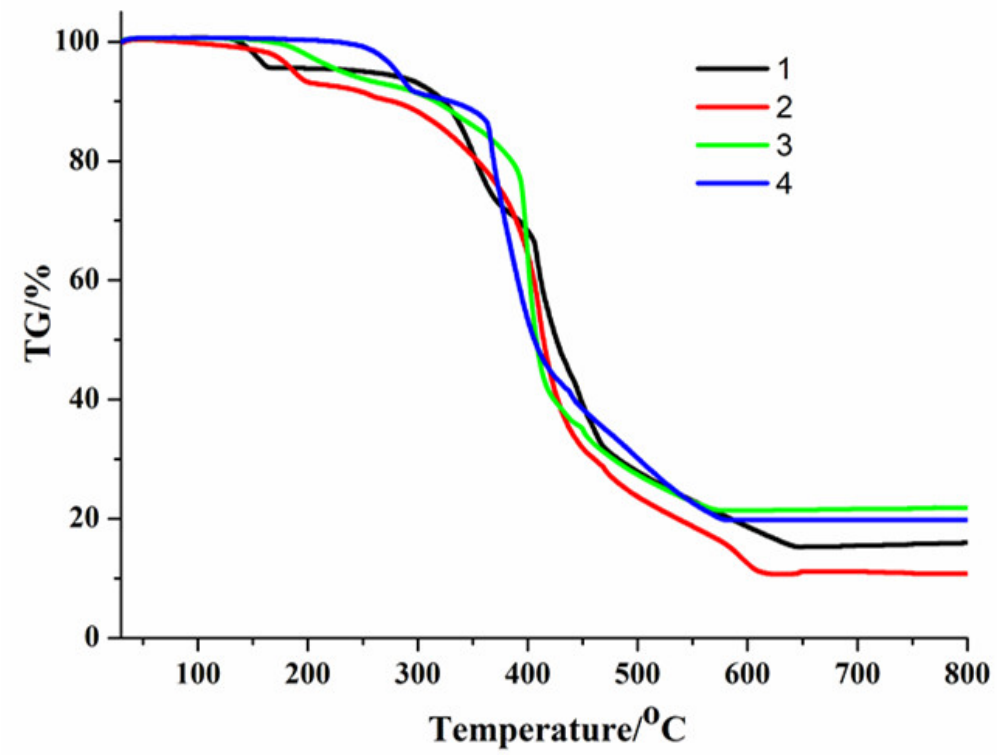


Figure S2. TGA plots of complexes **1**−**4**.