Electronic Supplementary Material (ESI) for CrystEngComm

Synthesis, characterization and observation of structural diversities in a series of transition metal based furan dicarboxylic acid system

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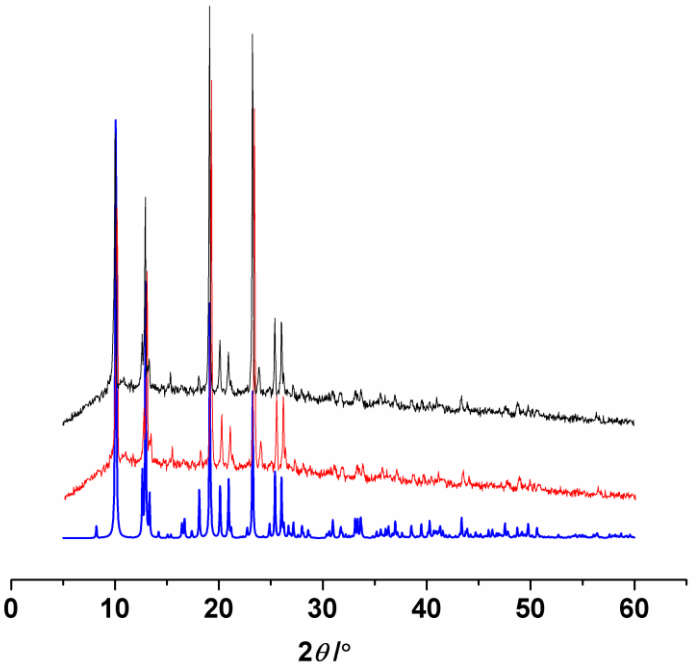

Figure S1. PXRD pattern of compound **1**, simulated from single crystal (blue), virgin compound before activation(red), after activation at 80°C (black).

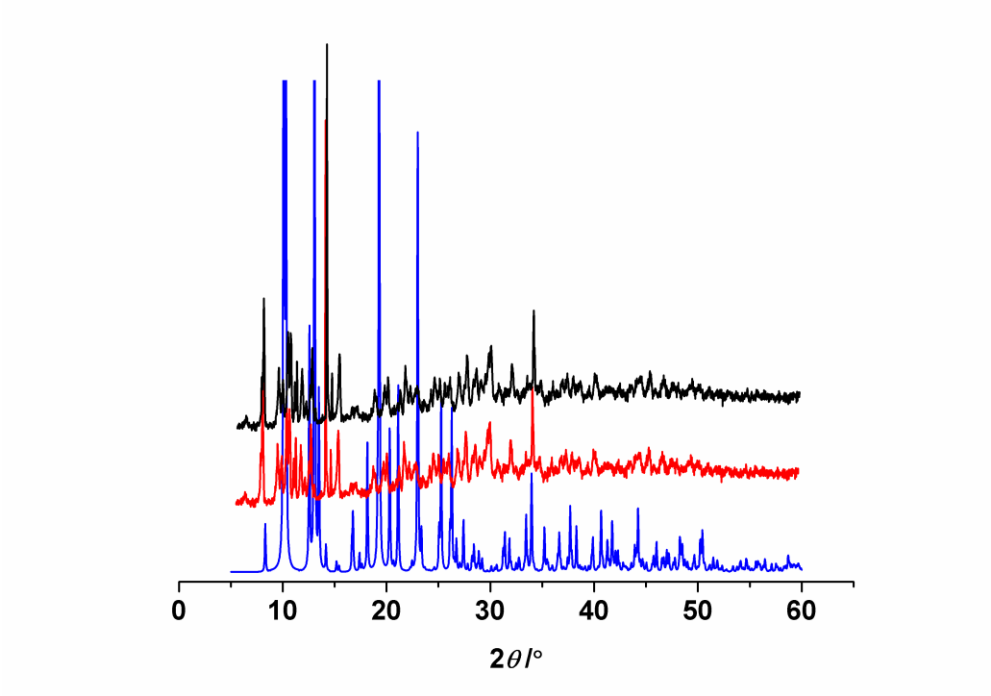

Figure S2. PXRD pattern of compound **2**, simulated from single crystal (blue), virgin compound before activation(red), after activation at 80°C (black).

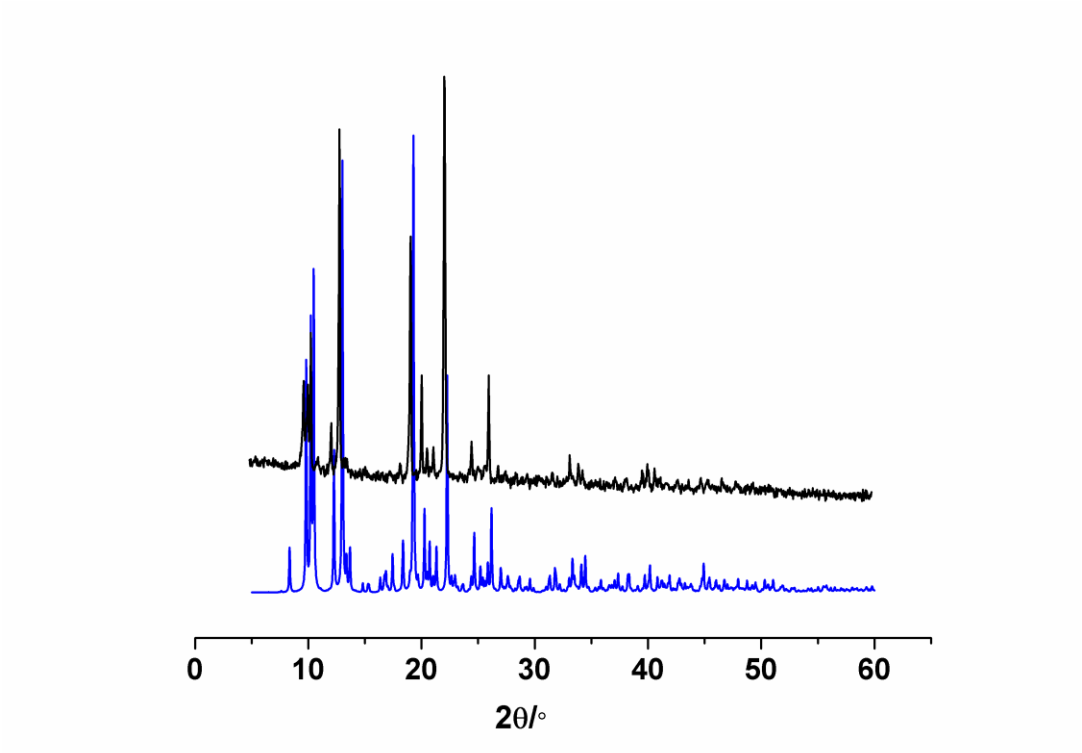

Figure S3. PXRD patterns of compound **3**, simulated from single crystal (blue) and pure compound (black).

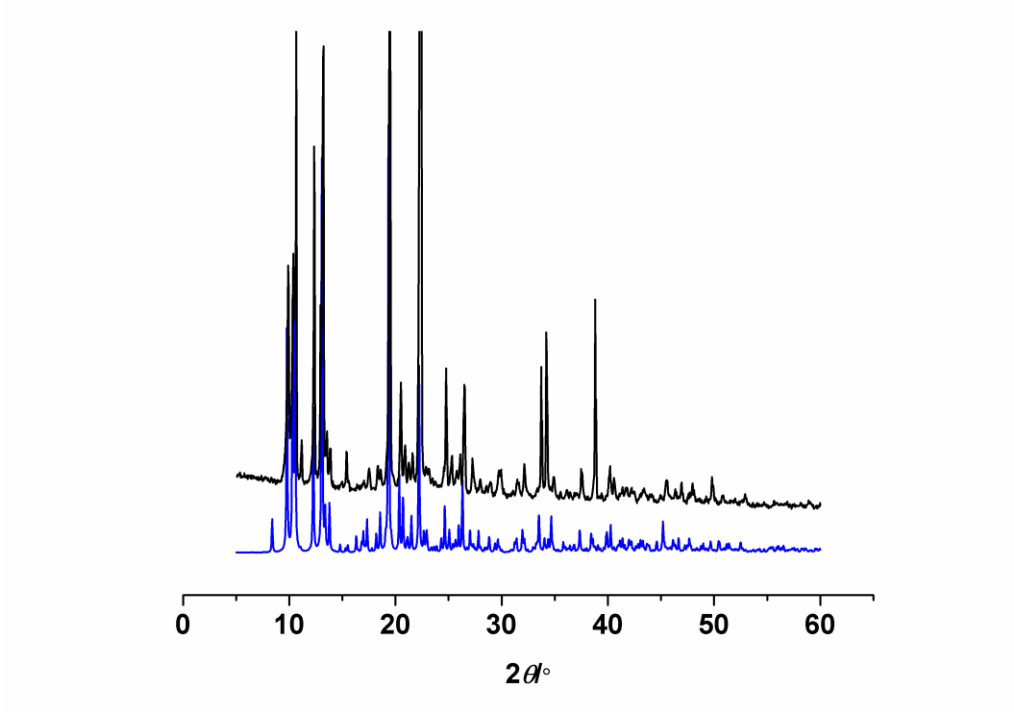

Figure S4. PXRD patterns of compound **4**, simulated from single crystal (blue) and pure compound (black).

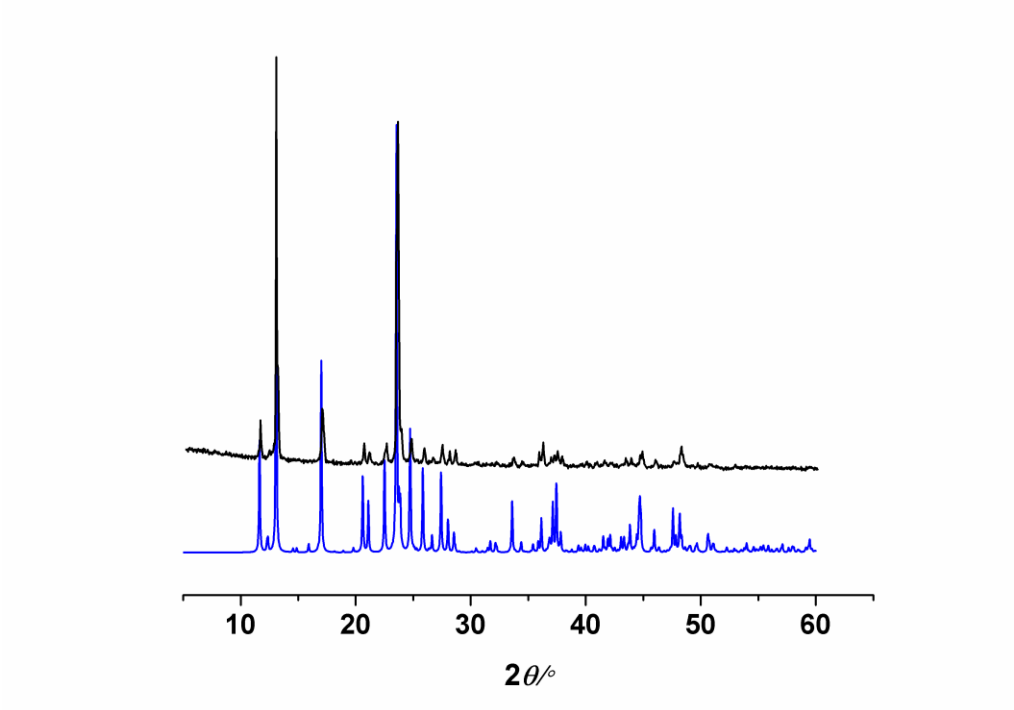

Figure S5. PXRD patterns of compound **5**, simulated from single crystal (blue) and pure compound (black).

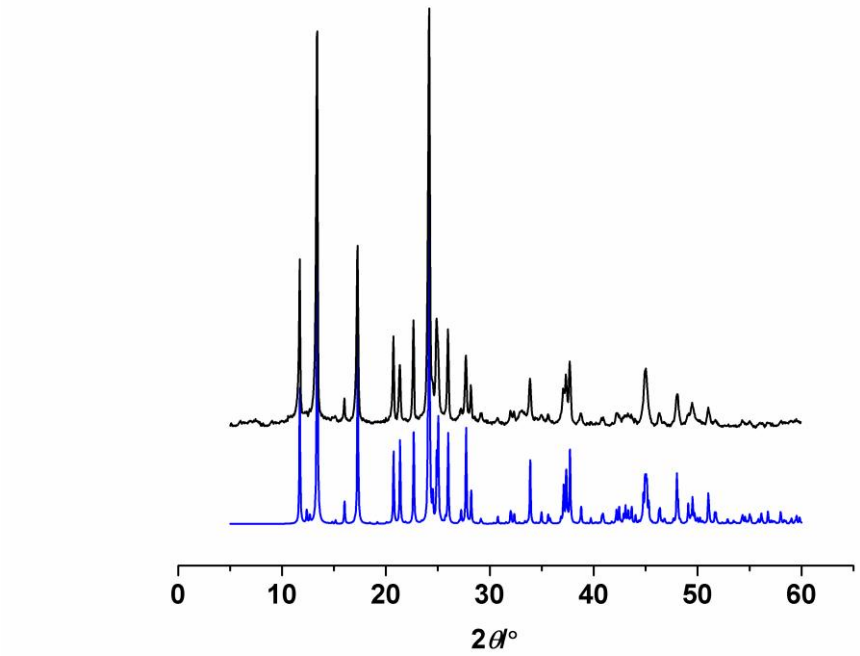

Figure S6. PXRD patterns of compound **6**, simulated from single crystal (blue) and pure compound (black).

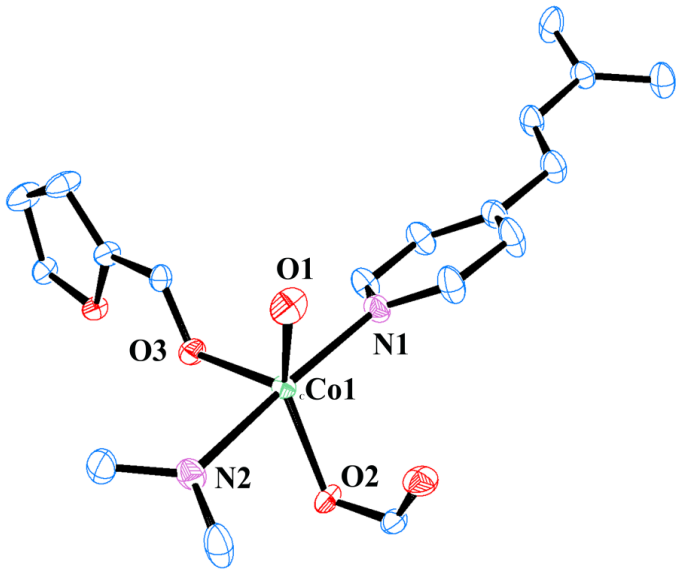

Figure S7 ORTEP diagram of compound **1** with 40% ellipsoid probability

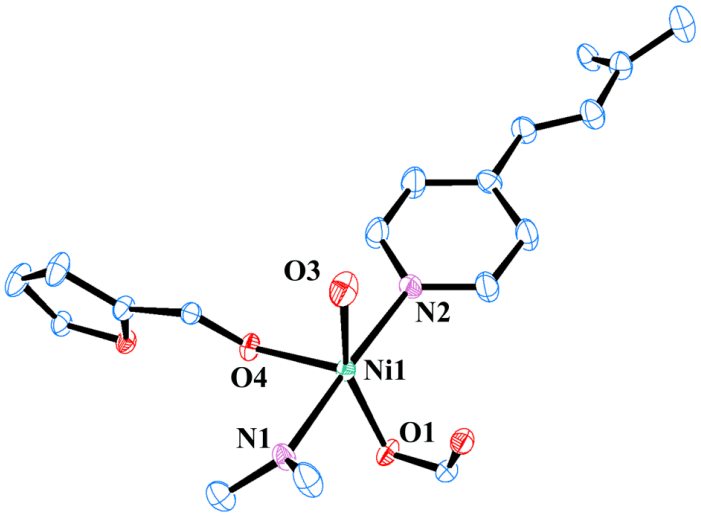

Figure S8 ORTEP diagram of compound **2** with 40% ellipsoid probability

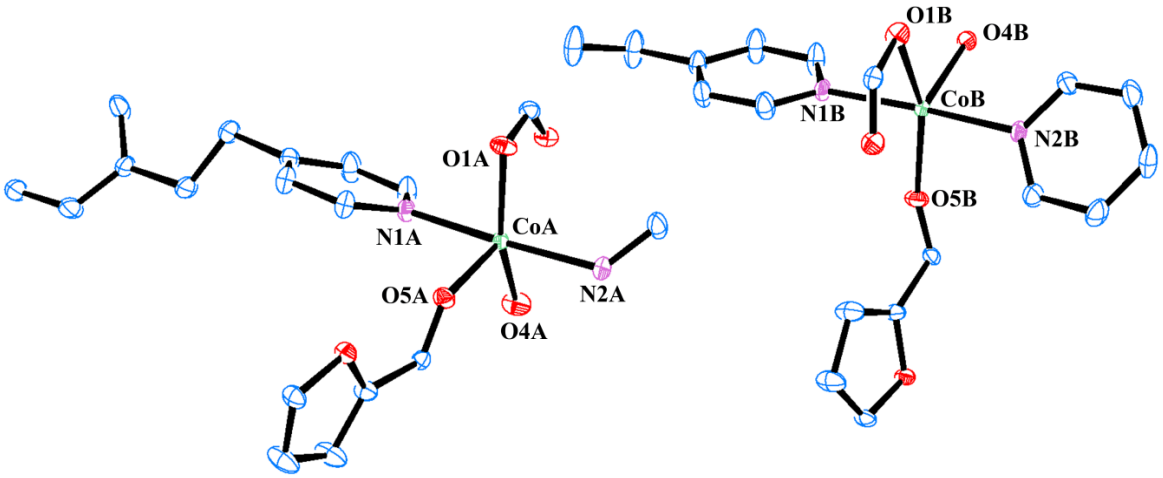

Figure S9 ORTEP diagram of compound **3** with 40% ellipsoid probability

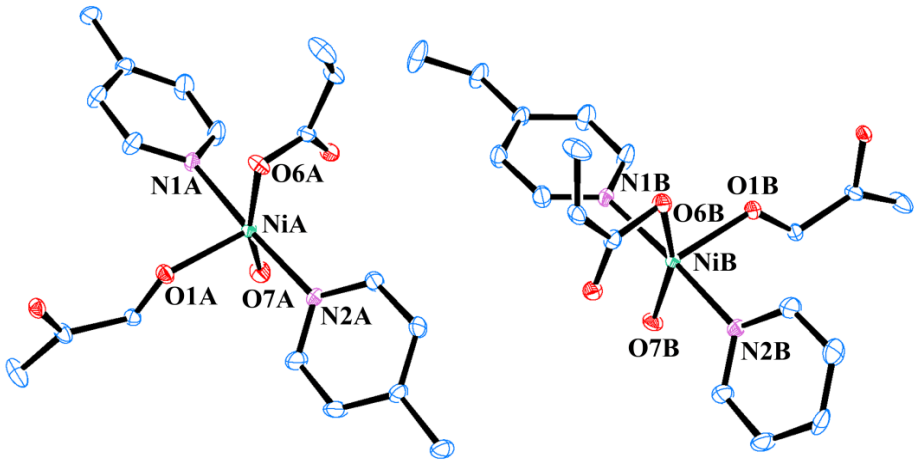

Figure S10 ORTEP diagram of compound **4** with 40% ellipsoid probability

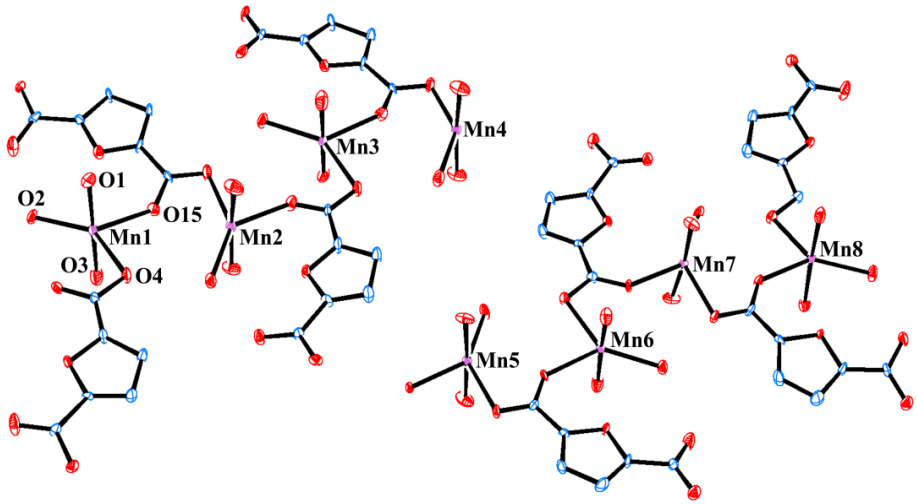

Figure S11 ORTEP diagram of compound **5** with 40% ellipsoid probability

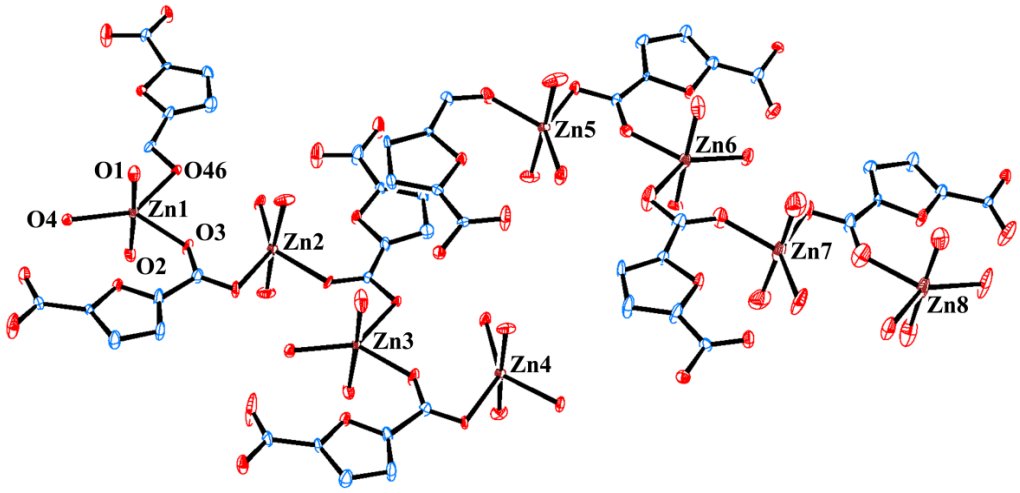

Figure S12 ORTEP diagram of compound **6** with 40% ellipsoid probability

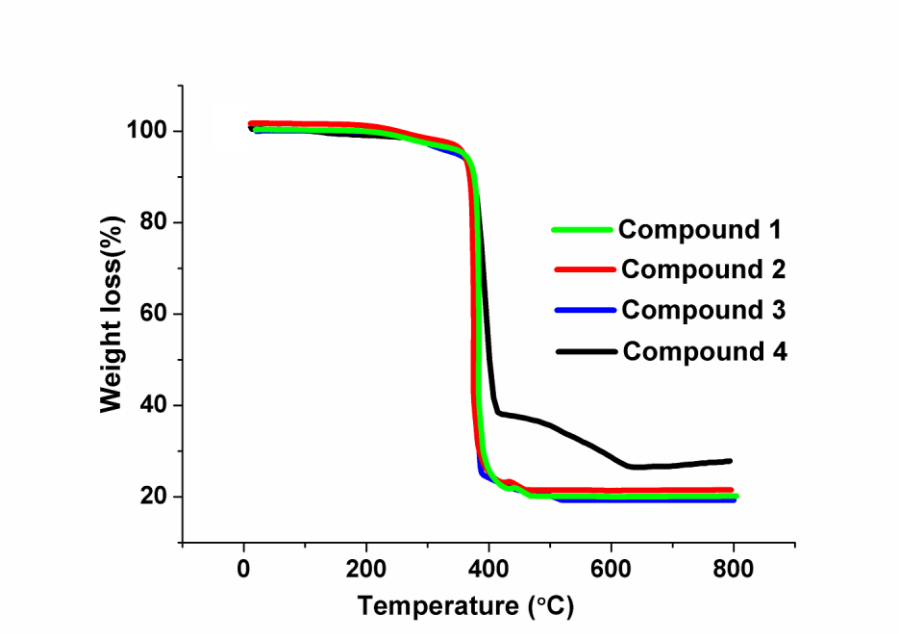

Figure S13. Thermogravimetric profile of compounds **1** to **4**.

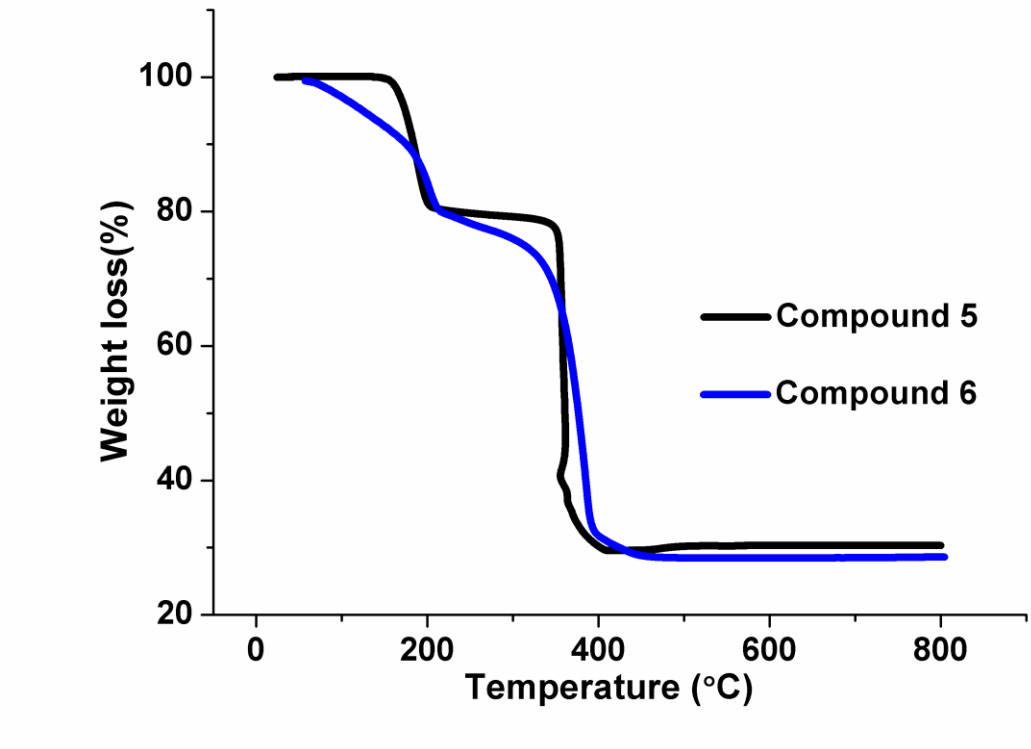

Figure S14. Thermogravimetric profile of compounds **5** and **6**.

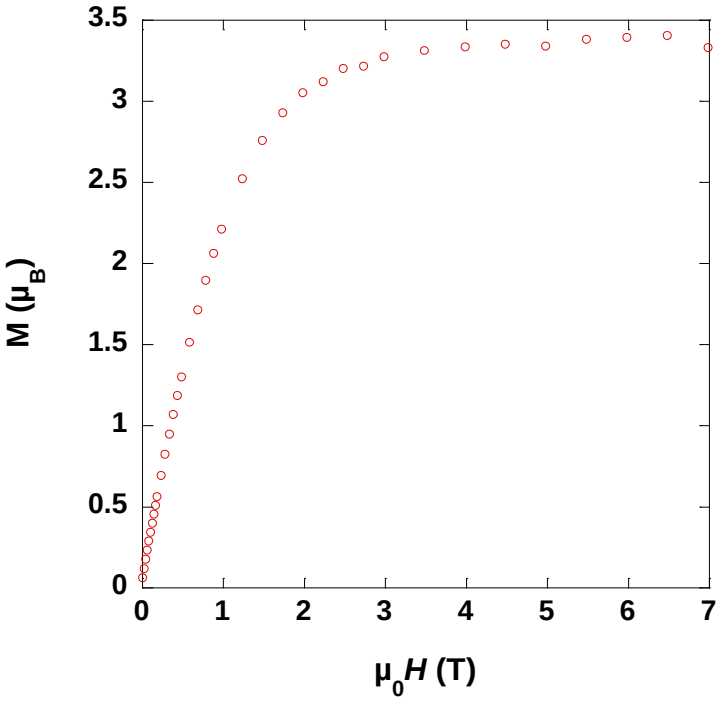

Figure S15. M *vs.* H at 1.8 K of compound **1**.

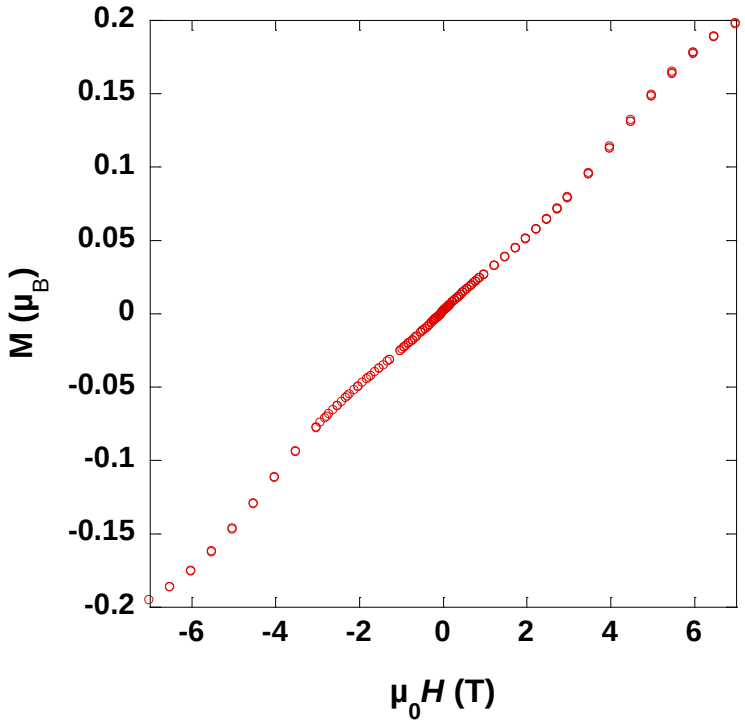

Figure S16. M *vs. H* at 1.8 K of compound **2**.

Table S1. Selected bond lengths [Å] and angles [º] for complexes **1** to **6**

Compound **1**			
Bond distances		Bond angles	
Co1-O1	1.982(3)	O1-Co1-O3	113.59(14)
Co1-O2	2.055(3)	O1-Co1-O2	146.01(14)
Co1-O3	2.051(3)	O2-Co1-O3	100.09(13)
Co1-N1	2.167(4)	O1-Co1-N1	86.35(15)
Co1-N2	2.143(4)	O2-Co1-N1	87.71(13)
C18-C19	1.316(7)	O3-Co1-N1	92.71(13)
O1-C2	1.240(5)	O1-Co1-N2	90.97(15)
O2-C11	1.270(5)	O2-Co1-N2	92.21(13)
C13-C14	1.382(6)	O3-Co1-N2	92.19(13)
C14-C15	1.385(6)	N1-Co1-N2	175.04(14)
Compound **2**			
Ni1-O1	2.067(4)	O1-Ni1-O2	59.59(12)
Ni1-O2	2.350(3)	O1-Ni1-N1	91.38(15)
Ni1-O3	2.014(4)	O1-Ni1-N2	89.79(15)
Ni1-O4	2.040(3)	O2-Ni1-O3	99.32(14)
Ni1-N1	2.077(4)	O2-Ni1-O4	154.96(13)
Ni1-N2	2.099(4)	O1-Ni1-O3	158.38(15)
C2-C3	1.484(6)	O1-Ni1-O4	95.71(14)
O1-C11	1.271(6)	O3-Ni1-O4	105.62(15)
O2-C11	1.244(6)	O3-Ni1-N2	85.64(17)
O3-C2	1.232(6)	O4-Ni1-N2	93.12(14)
Compound **3**			
	A	B	A	B
Co-O1	2.090(3)	2.110(3)	O4-Co-O5	107.47(12)	108.79(12)
Co-O2	2.403(3)	2.428(3)	O4-Co-O1	156.82(13)	96.59(11)
Co-O4	1.990(3)	2.068(3)	O5-Co-O1	95.70(11)	154.05(12)
Co-O5	2.061(3)	2.006(3)	O1-Co-N1	88.89(13)	91.89(12)
Co-N1	2.157(3)	2.159(3)	O1-Co-N2	90.79(13)	91.89(12)
Co-N2	2.135(3)	2.123(3)	O4-Co-N1	89.96(15)	91.69(12)
O1-C3	1.252(5)	1.266(5)	O5-Co-N1	94.24(13)	92.64(13)
O2-C3	1.253(5)	1.249(5)	O1-C3-O2	123.1(4)	122.9(4)
C3-C9	1.487(5)	1.483(5)	C3-O1-Co	96.6(2)	96.5(2)
Compound **4**			
	A	B	A	B
Ni-O1	2.053(5)	2.051(5)	O1-Ni-O7	95.30(13)	154.43(14)
Ni-O6	2.043(5)	2.024(5)	O1-Ni-O8	154.65(14)	94.22(13)
Ni-O7	2.108(5)	2.296(5)	O1-Ni-N20	90.77(15)	90.36(14)
Ni-O8	2.324(5)	2.086(5)	O6-Ni-O1	103.51(14)	102.57(14)
Ni-N12	2.119(5)	2.109(5)	O6-Ni-O7	160.60(14)	102.41(15)
Ni-N20	2.090(5)	2.099(5)	O6-Ni-N20	93.42(15)	86.56(17)
C2-C3	1.500(6)	1.489(6)	O1-Ni-N12	93.19(14)	94.29(15)
O1-C2	1.263(6)	1.265(6)	O6-Ni-N12	86.12(15)	90.99(17)
C2-O6	1.245(6)	1.245(6)	O7-Ni-N12	88.17(15)	90.61(14)
Compound **5**			
Mn1-O1	2.128(4)	O1-Mn1-O3	176.7(2)
Mn1-O2	2.089(5)	O2-Mn1-O3	86.7(2)
Mn1-O3	2.139(4)	O3-Mn1-O4	91.23(18)
Mn1-O4	2.211(5)	O2-Mn1-O1	91.00(2)
Mn1-O15	2.130(4)	O4-Mn1-O1	92.03(19)
Mn2-O16	2.211(5)	O4-Mn1-O2	140.77(18)
Mn2-O26	2.135(4)	O27-Mn2-O26	173.2(2)
Mn2-O27	2.138(4)	O28-Mn2-O27	86.20(2)
Mn3-O30	2.195(4)	O30-Mn3-O40	94.1(2)
Mn3-O40	2.118(4)	O30-Mn3-O42	140.38(18)
Mn4-O44	2.215(5)	O55-Mn4-O54	173.40(3)
Mn4-O54	2.125(5)	O54-Mn4-O56	86.30(2)
Compound **6**			
Zn1-O1	2.028(7)	O1-Zn1-O2	174.1(3)
Zn1-O2	2.064(6)	O1-Zn1-O3	89.2(2)
Zn1-O3	2.028(8)	O1-Zn1-O4	93.5(2)
Zn1-O4	2.109(6)	O1-Zn1-O46	90.6(3)
Zn1-O46	2.057(7)	O3-Zn1-O2	87.3(3)
Zn2-O5	2.034(6)	O3-Zn1-O4	137.5(3)
Zn3-O19	2.031(6)	O2-Zn1-O4	92.2(3)
Zn4-O33	2.029(6)	O5-Zn2-O17	88.4(3)
Zn5-O57	2.044(13)	O5-Zn2-O15	90.7(3)
Zn6-O61	2.043(10)	O5-Zn2-O18	87.7(2)
Zn7-O75	2.071(10)	O17-Zn2-O18	94.4(3)
Zn8-O89	2.056(9)	O15-Zn2-O18	91.4(3)

Table S2. Intermolecular and intramolecular hydrogen bonds in compounds **5** [Å, °]

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O1-H1A	0.829	2.043	169.39	2.862	O84 [x+1/2,-y+1, z-1/2]
O1-H1B	0.833	1.997	154.89	2.775	O69 [x+1, y-1,z]
O2-H2A	0.830	1.804	171.20	2.627	O25
O2-H2B	0.829	1.980	145.67	2.705	O44 [x+1/2, -y+1, z-1/2]
O3-H3A	0.824	1.878	166.48	2.686	O84 [x+1/2, -y+2, z-1/2]
O3-H3B	0.824	2.094	173.78	2.914	O70 [x+1, y, z]
O26-H26A	0.827	2.200	131.20	2.814	O98 [x+1, y-1,z]
O26-H26B	0.830	1.962	163.65	2.768	O83 [x+1/2, -y+1, z-1/2]
O27-H27A	0.831	1.966	156.54	2.748	O98 [x+1, y, z]
O27-H27B	0.830	2.262	137.18	2.926	O84 [x+1/2, -y+2, z-1/2]
O27-H27B	0.830	2.358	166.32	3.171	O83 [x+1/2, -y+2, z-1/2]
O28-H28A	0.831	1.885	163.73	2.693	O4
O28-H28B	0.832	1.804	173.73	2.632	O39
O40-H40A	0.832	2.044	160.52	2.841	O97 [x+1, y, z]
O40-H40B	0.829	2.036	157.36	2.819	O112 [x+1/2, -y+2, z-1/2]
O41-H41A	0.831	1.880	171.16	2.705	O112 [x+1/2, -y+1, z-1/2]
O41-H41B	0.827	2.141	175.34	2.965	O98 [x+1, y-1,z]
O41-H41B	0.827	2.532	128.35	3.113	O97 [x+1, -1, z]
O42-H42A	0.836	1.940	142.82	2.654	O52
O42-H42B	0.830	1.884	162.06	2.686	O16
O54-H54A	0.834	1.928	154.79	2.706	O70 [x+1/2, -y+1, z+1/2]
O54-H54B	0.833	2.322	171.58	3.148	O111 [x+1/2, -y+1, z-1/2]
O54-H54B	0.833	2.516	119.51	3.014	O112 [x+1/2, -y+1, z-1/2]

O55-H55A	0.834	2.151	141.97	2.854	O70 [x+1/2, -y+2, z+1/2]
O55-H55B	0.828	1.973	166.30	2.785	O111 [x+1/2, -y+2, z-1/2]
O56-H56A	0.828	1.930	153.27	2.695	O30
O56-H56B	0.825	1.811	167.53	2.623	O14 [x-1/2, -y+1, z+1/2]
O57-H57A	0.832	1.924	173.01	2.752	O53 [x-1/2, -y+2, z-1/2]
O57-H57B	0.831	2.391	169.05	3.211	O13 [x-1/2, -y+2, z+1/2]
O57-H57B	0.831	2.487	120.62	2.997	O14 [x-1/2, -y+2, z+1/2]
O58-H58A	0.828	1.976	137.63	2.647	O74
O58-H58B	0.827	1.901	152.53	2.662	O111 [x+1/2, -y+2, z-1/2]
O59-H59A	0.837	1.930	168.10	2.754	O53 [x-1/2, -y+1, z-1/2]
O59-H59B	0.832	2.239	140.76	2.931	O14 [x-1/2, -y+1, z+1/2]
O59-H59B	0.832	2.410	160.89	3.208	O13 [x-1/2, -y+1, z+1/2]
O71-H71A	0.828	1.959	168.73	2.775	O13 [x-1/2, -y+1, z+1/2]
O71-H71B	0.828	1.991	163.18	2.794	O25 [x-1, y, z]
O72-H72A	0.831	1.956	160.28	2.753	O13 [x-1/2, -y+2, z+1/2]
O72-H72B	0.831	2.237	143.18	2.944	O24 [x-1, y+1,z]
O72-H72B	0.831	2.362	154.52	3.132	O25 [x-1, y+1,z]
O73-H73A	0.829	1.987	140.45	2.678	O88
O73-H73B	0.829	1.870	160.49	2.665	O69
O85-H85A	0.834	1.904	169.72	2.729	O24 [x-1, y, z]
O85-H85B	0.827	2.216	169.14	3.033	O38 [x-1/2, -y+1, z+1/2]
O86-H86A	0.830	2.086	146.23	2.813	O39 [x-1/2, -y+2, z+1/2]
O86-H86A	0.830	2.589	155.33	3.360	O38 [x-1/2, -y+2, z+1/2]
O86-H86B	0.835	1.998	169.45	2.823	O24 [x-1, y+1, z]
O87-H87A	0.834	2.185	118.22	2.682	O102

O87-H87B	0.834	1.890	157.25	2.679	O83
O87-H87B	0.834	2.536	124.30	3.084	O78
O99-H99A	0.830	2.016	150.78	2.770	O38 [x-1/2, -y+1, z+1/2]
O99-H99B	0.831	2.351	172.25	3.176	O52 [x-1, y, z]
O99-H99B	0.831	2.394	132.57	3.019	O53 [x-1, y, z]
O100-H100	0.825	2.117	138.22	2.787	O38 [x-1/2, -y+2, z+1/2]
O100-H101	0.830	2.062	149.80	2.811	O52 [x-1, y+1,z]
O101-H102	0.829	1.888	156.86	2.670	O60 [x-1/2, -y+2, z+1/2]