

Structural library of coordination polymers based on flexible linkers exploiting the role of linker coordination angle; synthesis structural characterization and magnetic properties

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Section-1

Complete list of Bondlengths and Bond angles of the compounds presented in the study

Compound 1a

Co(1)-O(3)#1	2.009(2)	O(3)#1-Co(1)-N(3)	109.22(10)
Co(1)-N(3)	2.035(3)	O(3)#1-Co(1)-N(1)	114.22(10)
Co(1)-N(1)	2.035(3)	N(3)-Co(1)-N(1)	112.33(11)
Co(1)-O(1)	2.042(2)	O(3)#1-Co(1)-O(1)	122.71(9)
O(1)-C(1)	1.265(4)	N(3)-Co(1)-O(1)	92.59(10)
O(2)-C(1)	1.237(4)	N(1)-Co(1)-O(1)	103.87(10)
O(3)-C(10)	1.277(4)	C(1)-O(1)-Co(1)	102.5(2)
O(3)-Co(1)#2	2.009(2)	C(10)-O(3)-Co(1)#2	105.01(19)
O(4)-C(10)	1.232(4)	C(11)-N(2)-C(13)	106.3(3)
N(2)-C(11)	1.336(4)	C(11)-N(2)-C(14)	125.4(3)
N(2)-C(13)	1.374(4)	C(13)-N(2)-C(14)	128.2(3)
N(2)-C(14)	1.468(4)	C(11)-N(1)-C(12)	104.1(3)
N(1)-C(11)	1.316(4)	C(11)-N(1)-Co(1)	126.5(2)
N(1)-C(12)	1.376(4)	C(12)-N(1)-Co(1)	129.4(2)
N(4)-C(21)	1.345(4)	C(21)-N(4)-C(23)	106.4(3)
N(4)-C(23)	1.370(4)	C(21)-N(4)-C(24)	125.2(3)
N(4)-C(24)	1.467(4)	C(23)-N(4)-C(24)	128.1(3)
N(3)-C(21)	1.321(4)	C(21)-N(3)-C(22)	105.5(3)
N(3)-C(22)	1.382(4)	C(21)-N(3)-Co(1)	124.9(2)
C(3)-C(4)	1.394(4)	C(22)-N(3)-Co(1)	129.5(2)
C(3)-C(8)	1.398(5)	C(4)-C(3)-C(8)	118.8(3)
C(3)-C(2)	1.509(4)	C(4)-C(3)-C(2)	120.1(3)
C(20)-C(15)	1.389(4)	C(8)-C(3)-C(2)	121.0(3)
C(20)-C(19)	1.394(5)	C(15)-C(20)-C(19)	119.4(3)
C(20)-C(24)#3	1.513(4)	C(15)-C(20)-C(24)#3	121.9(3)
C(1)-C(2)	1.542(4)	C(19)-C(20)-C(24)#3	118.7(3)
C(10)-C(9)	1.533(4)	O(2)-C(1)-O(1)	122.4(3)
C(8)-C(7)	1.399(4)	O(2)-C(1)-C(2)	120.5(3)
C(8)-C(9)	1.494(4)	O(1)-C(1)-C(2)	117.1(3)
C(19)-C(18)	1.379(4)	O(4)-C(10)-O(3)	123.0(3)
C(15)-C(16)	1.395(4)	O(4)-C(10)-C(9)	118.6(3)
C(15)-C(14)	1.515(5)	O(3)-C(10)-C(9)	118.5(3)
C(13)-C(12)	1.344(5)	C(7)-C(8)-C(3)	118.5(3)
C(16)-C(17)	1.376(5)	C(7)-C(8)-C(9)	119.1(3)
C(7)-C(6)	1.370(5)	C(3)-C(8)-C(9)	122.4(3)
C(23)-C(22)	1.345(5)	C(18)-C(19)-C(20)	120.8(3)
C(17)-C(18)	1.373(5)	C(20)-C(15)-C(16)	118.9(3)
C(4)-C(5)	1.375(5)	C(20)-C(15)-C(14)	122.7(3)
C(6)-C(5)	1.370(5)	C(16)-C(15)-C(14)	118.4(3)
C(6)-H(31)	0.9300	C(12)-C(13)-N(2)	106.2(3)
C(24)-C(20)#4	1.513(4)	C(17)-C(16)-C(15)	121.1(3)
		N(1)-C(11)-N(2)	112.8(3)
		C(13)-C(12)-N(1)	110.5(3)

C(6)-C(7)-C(8)	121.5(4)	N(2)-C(14)-C(15)	111.7(3)
C(22)-C(23)-N(4)	107.4(3)	N(2)-C(14)-H(32A)	109.3
C(18)-C(17)-C(16)	120.0(3)	N(4)-C(24)-C(20)#4	112.3(3)
C(5)-C(4)-C(3)	121.4(4)	C(8)-C(9)-C(10)	117.5(3)
C(3)-C(2)-C(1)	113.6(3)		
C(23)-C(22)-N(3)	109.1(3)	C(6)-C(5)-C(4)	119.8(4)
C(23)-C(22)-H(30)	125.5	C(17)-C(18)-C(19)	119.9(3)
N(3)-C(22)-H(30)	125.5		
C(5)-C(6)-C(7)	119.9(4)		

Symmetry transformations used to generate equivalent atoms:

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

Compound 2a

Co(1)-O(1)	1.957(2)	C(10)-N(1)-Co(1)	126.2(2)
Co(1)-O(1)#1	1.957(2)	C(1)-O(1)-Co(1)	115.8(2)
Co(1)-N(1)#1	2.023(3)	C(9)-C(8)-C(9)#2	106.8(4)
Co(1)-N(1)	2.023(3)	C(9)-C(8)-C(5)#2	113.51(19)
F(2)-C(9)	1.344(5)	C(9)#2-C(8)-C(5)#2	106.50(18)
F(3)-C(9)	1.331(4)	C(9)-C(8)-C(5)	106.51(18)
F(1)-C(9)	1.338(4)	C(9)#2-C(8)-C(5)	113.51(19)
O(2)-C(1)	1.243(4)	C(5)#2-C(8)-C(5)	110.1(4)
N(1)-C(12)	1.323(4)	C(3)-C(2)-C(7)	119.0(3)
N(1)-C(10)	1.377(5)	C(3)-C(2)-C(1)	120.4(3)
O(1)-C(1)	1.287(4)	C(7)-C(2)-C(1)	120.6(3)
C(8)-C(9)	1.544(5)	F(3)-C(9)-F(1)	107.3(3)
C(8)-C(9)#2	1.545(5)	F(3)-C(9)-F(2)	106.6(3)
C(8)-C(5)#2	1.550(4)	F(1)-C(9)-F(2)	106.7(3)
C(8)-C(5)	1.550(4)	F(3)-C(9)-C(8)	113.7(3)
C(2)-C(3)	1.386(5)	F(1)-C(9)-C(8)	111.0(3)
C(2)-C(7)	1.390(5)	F(2)-C(9)-C(8)	111.1(3)
C(2)-C(1)	1.511(5)	C(6)-C(7)-C(2)	120.2(3)
C(7)-C(6)	1.384(5)	C(12)-N(2)-C(11)	107.0(3)
N(2)-C(12)	1.342(4)	C(12)-N(2)-C(13)	127.1(3)
N(2)-C(11)	1.371(4)	C(11)-N(2)-C(13)	125.9(3)
N(2)-C(13)	1.481(4)	O(2)-C(1)-O(1)	124.9(3)
C(15)-C(16)	1.385(5)	O(2)-C(1)-C(2)	119.9(3)
C(15)-C(14)	1.389(5)	O(1)-C(1)-C(2)	115.1(3)
C(5)-C(6)	1.388(5)	N(1)-C(12)-N(2)	111.6(3)
C(5)-C(4)	1.392(5)	C(16)-C(15)-C(14)	120.8(3)
C(3)-C(4)	1.391(5)	C(6)-C(5)-C(4)	118.8(3)
C(14)-C(14)#3	1.402(7)	C(6)-C(5)-C(8)	117.0(3)
C(14)-C(13)	1.511(5)	C(4)-C(5)-C(8)	124.2(3)
C(16)-C(16)#3	1.386(7)	C(2)-C(3)-C(4)	120.8(3)
C(11)-C(10)	1.352(5)	C(7)-C(6)-C(5)	121.0(3)
		C(15)-C(14)-C(14)#3	119.3(2)
O(1)-Co(1)-O(1)#1	115.92(16)	C(15)-C(14)-C(13)	117.2(3)
O(1)-Co(1)-N(1)#1	112.32(10)	C(14)#3-C(14)-C(13)	123.5(2)
O(1)#1-Co(1)-N(1)#1	107.52(10)	C(3)-C(4)-C(5)	120.1(3)
O(1)-Co(1)-N(1)	107.52(10)	C(15)-C(16)-C(16)#3	119.8(2)
O(1)#1-Co(1)-N(1)	112.32(10)	N(2)-C(13)-C(14)	110.9(3)
N(1)#1-Co(1)-N(1)	100.17(16)	C(11)-C(10)-N(1)	109.6(3)
C(12)-N(1)-C(10)	105.3(3)		
C(12)-N(1)-Co(1)	128.5(2)		

Compound 3a

C(17)-C(16)	1.349(4)	C(16)-C(17)-N(2)	107.1(3)
C(17)-N(2)	1.355(4)	C(8)-C(7)-C(6)	109.0(2)
C(7)-C(8)	1.516(4)	N(2)-C(18)-C(28)#1	114.0(3)
C(7)-C(6)	1.519(4)	C(7)-C(6)-C(11)	110.1(3)
C(18)-N(2)	1.458(4)	C(7)-C(6)-C(4)	110.9(3)
C(18)-C(28)#1	1.507(4)	C(11)-C(6)-C(4)	108.6(2)
C(6)-C(11)	1.524(4)	N(4)-C(22)-C(23)	115.0(2)
C(6)-C(4)	1.527(4)	C(17)-C(16)-N(1)	108.9(3)
C(22)-N(4)	1.451(3)	C(26)-C(27)-C(28)	121.1(3)
C(22)-C(23)	1.510(4)	C(25)-C(24)-C(23)	121.2(3)
C(16)-N(1)	1.370(3)	C(25)-C(26)-C(27)	120.2(3)
C(27)-C(26)	1.373(4)	C(6)-C(4)-C(3)	110.2(2)
C(27)-C(28)	1.386(4)	C(7)-C(8)-C(12)	109.4(3)
C(24)-C(25)	1.375(4)	C(7)-C(8)-C(9)	109.5(3)
C(24)-C(23)	1.383(4)	C(12)-C(8)-C(9)	108.5(2)
C(26)-C(25)	1.370(4)	C(8)-C(12)-C(3)	111.4(2)
C(4)-C(3)	1.528(3)	C(20)-C(21)-N(4)	106.6(2)
C(8)-C(12)	1.518(4)	C(26)-C(25)-C(24)	119.5(3)
C(8)-C(9)	1.524(4)	N(1)-C(15)-N(2)	111.3(3)
C(12)-C(3)	1.544(4)	C(21)-C(20)-N(3)	109.6(3)
C(21)-C(20)	1.339(4)	C(10)-C(11)-C(6)	110.4(2)
C(21)-N(4)	1.372(4)	O(3)-C(13)-O(4)	119.7(3)
C(15)-N(1)	1.315(3)	O(3)-C(13)-C(14)	118.6(3)
C(15)-N(2)	1.340(3)	O(4)-C(13)-C(14)	121.7(3)
O(3)-C(13)	1.243(4)	C(27)-C(28)-C(23)	118.7(3)
C(20)-N(3)	1.375(3)	C(27)-C(28)-C(18)#2	121.9(3)
C(11)-C(10)	1.524(4)	C(23)-C(28)-C(18)#2	119.3(3)
C(13)-O(4)	1.257(4)	C(8)-C(9)-C(10)	111.3(2)
C(13)-C(14)	1.511(4)	C(1)-C(2)-C(3)	119.1(2)
C(28)-C(23)	1.396(4)	N(3)-C(19)-N(4)	111.6(2)
C(28)-C(18)#2	1.507(4)	C(4)-C(3)-C(5)	108.3(2)
C(9)-C(10)	1.539(4)	C(4)-C(3)-C(2)	114.1(2)
C(2)-C(1)	1.511(4)	C(5)-C(3)-C(2)	110.7(2)
C(2)-C(3)	1.537(4)	C(4)-C(3)-C(12)	108.2(2)
C(19)-N(3)	1.306(3)	C(5)-C(3)-C(12)	108.2(2)
C(19)-N(4)	1.344(3)	C(2)-C(3)-C(12)	107.0(2)
C(3)-C(5)	1.534(3)	C(11)-C(10)-C(5)	109.1(2)
C(10)-C(5)	1.533(4)	C(11)-C(10)-C(9)	107.9(2)
C(10)-C(14)#3	1.543(4)	C(5)-C(10)-C(9)	108.0(2)
O(2)-C(1)	1.228(3)	C(11)-C(10)-C(14)#3	112.6(2)
C(1)-O(1)	1.263(3)	C(5)-C(10)-C(14)#3	112.5(2)
N(1)-Co(1)	2.053(2)	C(9)-C(10)-C(14)#3	106.5(2)
N(3)-Co(1)	2.056(2)	C(24)-C(23)-C(28)	119.2(3)
O(1)-Co(1)	1.9638(19)	C(24)-C(23)-C(22)	121.8(3)
O(4)-Co(1)	2.015(2)	C(28)-C(23)-C(22)	119.0(2)
C(14)-C(10)#4	1.543(4)	C(15)-N(2)-C(17)	106.9(3)
		C(15)-N(2)-C(18)	126.4(3)

C(17)-N(2)-C(18)	126.7(3)	C(20)-N(3)-Co(1)	119.03(18)
C(19)-N(4)-C(21)	106.5(2)	C(10)-C(5)-C(3)	111.2(2)
C(19)-N(4)-C(22)	125.8(3)	C(1)-O(1)-Co(1)	109.29(17)
C(21)-N(4)-C(22)	127.7(2)	C(13)-O(4)-Co(1)	100.83(19)
O(2)-C(1)-O(1)	122.0(3)	O(1)-Co(1)-O(4)	141.21(9)
O(2)-C(1)-C(2)	120.5(3)	O(1)-Co(1)-N(1)	106.33(9)
O(1)-C(1)-C(2)	117.3(2)	O(4)-Co(1)-N(1)	96.59(9)
C(15)-N(1)-C(16)	105.8(2)	O(1)-Co(1)-N(3)	95.75(9)
C(15)-N(1)-Co(1)	127.4(2)	O(4)-Co(1)-N(3)	106.29(9)
C(16)-N(1)-Co(1)	126.0(2)	N(1)-Co(1)-N(3)	108.43(9)
C(19)-N(3)-C(20)	105.6(2)	C(13)-C(14)-C(10)#4	116.8(2)
C(19)-N(3)-Co(1)	134.77(19)		

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y - 1/2, z - 1/2$ #2 $x, -y - 1/2, z + 1/2$

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

Compound 3b

Co(1)-O(3)	2.0515(17)	C(7)-C(14)#1	1.515(4)
Co(1)-N(3)	2.062(2)	C(10)-C(9)	1.391(4)
Co(1)-N(1)	2.082(2)	C(15)-C(16)	1.507(3)
Co(1)-O(1)	2.1582(18)	C(28)-C(27)#2	1.508(3)
Co(1)-O(2)	2.1674(18)	C(18)-C(19)	1.533(4)
Co(1)-O(4)	2.2718(16)	C(25)-C(20)	1.517(5)
Co(1)-C(28)	2.496(2)	C(25)-C(24)	1.519(4)
Co(1)-C(15)	2.502(2)	C(25)-C(26)	1.521(4)
O(4)-C(28)	1.256(3)	C(21)-C(19)	1.523(4)
N(2)-C(1)	1.342(3)	C(2)-C(3)	1.337(4)
N(2)-C(3)	1.374(3)	C(8)-C(9)	1.364(5)
N(2)-C(4)	1.457(3)	C(13)-C(12)	1.339(4)
O(3)-C(28)	1.261(3)	C(19)-C(20)	1.525(5)
O(2)-C(15)	1.260(3)	C(27)-C(28)#3	1.508(3)
O(1)-C(15)	1.245(3)	C(14)-C(7)#4	1.515(4)
C(17)-C(22)	1.526(3)		
C(17)-C(18)	1.529(3)	O(3)-Co(1)-N(3)	98.87(8)
C(17)-C(26)	1.529(3)	O(3)-Co(1)-N(1)	103.44(8)
C(17)-C(16)	1.545(3)	N(3)-Co(1)-N(1)	91.01(8)
N(1)-C(1)	1.308(3)	O(3)-Co(1)-O(1)	101.65(7)
N(1)-C(2)	1.378(3)	N(3)-Co(1)-O(1)	94.30(8)
N(4)-C(11)	1.343(3)	N(1)-Co(1)-O(1)	153.20(8)
N(4)-C(13)	1.356(3)	O(3)-Co(1)-O(2)	158.96(8)
N(4)-C(14)	1.465(3)	N(3)-Co(1)-O(2)	92.92(7)
C(5)-C(10)	1.375(3)	N(1)-Co(1)-O(2)	93.65(7)
C(5)-C(6)	1.390(3)	O(1)-Co(1)-O(2)	59.89(7)
C(5)-C(4)	1.499(3)	O(3)-Co(1)-O(4)	60.21(6)
N(3)-C(11)	1.313(3)	N(3)-Co(1)-O(4)	158.23(8)
N(3)-C(12)	1.367(3)	N(1)-Co(1)-O(4)	88.53(7)
C(23)-C(21)	1.520(3)	O(1)-Co(1)-O(4)	95.87(7)
C(23)-C(24)	1.524(3)	O(2)-Co(1)-O(4)	108.83(7)
C(23)-C(27)	1.533(3)	O(3)-Co(1)-C(28)	30.23(7)
C(23)-C(22)	1.539(3)	N(3)-Co(1)-C(28)	128.52(9)
C(7)-C(8)	1.360(4)	N(1)-Co(1)-C(28)	94.97(8)
C(7)-C(6)	1.382(4)	O(1)-Co(1)-C(28)	102.05(7)

O(2)-Co(1)-C(28)	137.36(8)	C(8)-C(7)-C(6)	118.7(3)
O(4)-Co(1)-C(28)	30.09(7)	C(8)-C(7)-C(14)#1	120.7(3)
O(3)-Co(1)-C(15)	131.32(8)	C(6)-C(7)-C(14)#1	120.6(3)
N(3)-Co(1)-C(15)	91.56(8)	N(1)-C(1)-N(2)	112.6(2)
N(1)-Co(1)-C(15)	123.90(8)	C(5)-C(10)-C(9)	120.5(3)
O(1)-Co(1)-C(15)	29.84(7)	O(1)-C(15)-O(2)	119.0(2)
O(2)-Co(1)-C(15)	30.25(7)	O(1)-C(15)-C(16)	121.0(2)
O(4)-Co(1)-C(15)	106.70(7)	O(2)-C(15)-C(16)	119.9(2)
C(28)-Co(1)-C(15)	124.91(8)	O(1)-C(15)-Co(1)	59.62(13)
C(28)-O(4)-Co(1)	84.89(14)	O(2)-C(15)-Co(1)	60.04(13)
C(1)-N(2)-C(3)	106.3(2)	C(16)-C(15)-Co(1)	171.61(16)
C(1)-N(2)-C(4)	126.4(2)	O(4)-C(28)-O(3)	119.7(2)
C(3)-N(2)-C(4)	126.7(2)	O(4)-C(28)-C(27)#2	120.8(2)
C(28)-O(3)-Co(1)	94.79(15)	O(3)-C(28)-C(27)#2	119.5(2)
C(15)-O(2)-Co(1)	89.70(15)	O(4)-C(28)-Co(1)	65.02(12)
C(15)-O(1)-Co(1)	90.54(15)	O(3)-C(28)-Co(1)	54.98(12)
C(22)-C(17)-C(18)	108.26(19)	C(27)#2-C(28)-Co(1)	170.89(18)
C(22)-C(17)-C(26)	107.8(2)	C(17)-C(18)-C(19)	109.7(2)
C(18)-C(17)-C(26)	109.1(2)	N(2)-C(4)-C(5)	112.5(2)
C(22)-C(17)-C(16)	111.62(19)	C(15)-C(16)-C(17)	114.37(19)
C(18)-C(17)-C(16)	112.33(19)	C(20)-C(25)-C(24)	109.6(2)
C(26)-C(17)-C(16)	107.67(19)	C(20)-C(25)-C(26)	108.9(3)
C(1)-N(1)-C(2)	104.3(2)	C(24)-C(25)-C(26)	109.9(2)
C(1)-N(1)-Co(1)	130.95(17)	C(7)-C(6)-C(5)	121.4(3)
C(2)-N(1)-Co(1)	122.43(18)	C(23)-C(21)-C(19)	110.3(2)
C(11)-N(4)-C(13)	107.2(2)	C(3)-C(2)-N(1)	110.7(2)
C(11)-N(4)-C(14)	126.5(3)	N(3)-C(11)-N(4)	111.2(2)
C(13)-N(4)-C(14)	126.4(2)	C(7)-C(8)-C(9)	121.5(3)
C(10)-C(5)-C(6)	118.2(2)	C(12)-C(13)-N(4)	106.3(2)
C(10)-C(5)-C(4)	121.2(2)	C(13)-C(12)-N(3)	110.2(3)
C(6)-C(5)-C(4)	120.5(2)	C(25)-C(26)-C(17)	110.7(2)
C(11)-N(3)-C(12)	105.1(2)	C(8)-C(9)-C(10)	119.5(3)
C(11)-N(3)-Co(1)	128.82(17)	C(21)-C(19)-C(20)	109.4(3)
C(12)-N(3)-Co(1)	125.82(19)	C(21)-C(19)-C(18)	109.6(2)
C(21)-C(23)-C(24)	108.8(2)	C(20)-C(19)-C(18)	109.9(2)
C(21)-C(23)-C(27)	111.6(2)	C(28)#3-C(27)-C(23)	116.2(2)
C(24)-C(23)-C(27)	112.4(2)	N(4)-C(14)-C(7)#4	112.2(2)
C(21)-C(23)-C(22)	108.63(19)	C(25)-C(24)-C(23)	110.5(2)
C(24)-C(23)-C(22)	107.61(19)	C(2)-C(3)-N(2)	106.1(2)
C(27)-C(23)-C(22)	107.65(18)	C(25)-C(20)-C(19)	109.3(2)
C(17)-C(22)-C(23)	112.21(18)		

Compound 4a

Co(1)-O(3)	2.0515(17)	O(4)-C(28)	1.256(3)
Co(1)-N(3)	2.062(2)	N(2)-C(1)	1.342(3)
Co(1)-N(1)	2.082(2)	N(2)-C(3)	1.374(3)
Co(1)-O(1)	2.1582(18)	N(2)-C(4)	1.457(3)
Co(1)-O(2)	2.1674(18)	O(3)-C(28)	1.261(3)
Co(1)-O(4)	2.2718(16)	O(2)-C(15)	1.260(3)
Co(1)-C(28)	2.496(2)	O(1)-C(15)	1.245(3)
Co(1)-C(15)	2.502(2)	C(17)-C(22)	1.526(3)

C(17)-C(18)	1.529(3)	O(3)-Co(1)-C(15)	131.32(8)
C(17)-C(26)	1.529(3)	N(3)-Co(1)-C(15)	91.56(8)
C(17)-C(16)	1.545(3)	N(1)-Co(1)-C(15)	123.90(8)
N(1)-C(1)	1.308(3)	O(1)-Co(1)-C(15)	29.84(7)
N(1)-C(2)	1.378(3)	O(2)-Co(1)-C(15)	30.25(7)
N(4)-C(11)	1.343(3)	O(4)-Co(1)-C(15)	106.70(7)
N(4)-C(13)	1.356(3)	C(28)-Co(1)-C(15)	124.91(8)
N(4)-C(14)	1.465(3)	C(28)-O(4)-Co(1)	84.89(14)
C(5)-C(10)	1.375(3)	C(1)-N(2)-C(3)	106.3(2)
C(5)-C(6)	1.390(3)	C(1)-N(2)-C(4)	126.4(2)
C(5)-C(4)	1.499(3)	C(3)-N(2)-C(4)	126.7(2)
N(3)-C(11)	1.313(3)	C(28)-O(3)-Co(1)	94.79(15)
N(3)-C(12)	1.367(3)	C(15)-O(2)-Co(1)	89.70(15)
C(23)-C(21)	1.520(3)	C(15)-O(1)-Co(1)	90.54(15)
C(23)-C(24)	1.524(3)	C(22)-C(17)-C(18)	108.26(19)
C(23)-C(27)	1.533(3)	C(22)-C(17)-C(26)	107.8(2)
C(23)-C(22)	1.539(3)	C(18)-C(17)-C(26)	109.1(2)
C(7)-C(8)	1.360(4)	C(22)-C(17)-C(16)	111.62(19)
C(7)-C(6)	1.382(4)	C(18)-C(17)-C(16)	112.33(19)
C(7)-C(14)#1	1.515(4)	C(26)-C(17)-C(16)	107.67(19)
C(10)-C(9)	1.391(4)	C(1)-N(1)-C(2)	104.3(2)
C(15)-C(16)	1.507(3)	C(1)-N(1)-Co(1)	130.95(17)
C(28)-C(27)#2	1.508(3)	C(2)-N(1)-Co(1)	122.43(18)
C(18)-C(19)	1.533(4)	C(11)-N(4)-C(13)	107.2(2)
C(25)-C(20)	1.517(5)	C(11)-N(4)-C(14)	126.5(3)
C(25)-C(24)	1.519(4)	C(13)-N(4)-C(14)	126.4(2)
C(25)-C(26)	1.521(4)	C(10)-C(5)-C(6)	118.2(2)
C(21)-C(19)	1.523(4)	C(10)-C(5)-C(4)	121.2(2)
C(2)-C(3)	1.337(4)	C(6)-C(5)-C(4)	120.5(2)
C(8)-C(9)	1.364(5)	C(11)-N(3)-C(12)	105.1(2)
C(13)-C(12)	1.339(4)	C(11)-N(3)-Co(1)	128.82(17)
C(19)-C(20)	1.525(5)	C(12)-N(3)-Co(1)	125.82(19)
C(27)-C(28)#3	1.508(3)	C(21)-C(23)-C(24)	108.8(2)
C(14)-C(7)#4	1.515(4)	C(21)-C(23)-C(27)	111.6(2)
		C(24)-C(23)-C(27)	112.4(2)
O(3)-Co(1)-N(3)	98.87(8)	C(21)-C(23)-C(22)	108.63(19)
O(3)-Co(1)-N(1)	103.44(8)	C(24)-C(23)-C(22)	107.61(19)
N(3)-Co(1)-N(1)	91.01(8)	C(27)-C(23)-C(22)	107.65(18)
O(3)-Co(1)-O(1)	101.65(7)	C(17)-C(22)-C(23)	112.21(18)
N(3)-Co(1)-O(1)	94.30(8)	C(8)-C(7)-C(6)	118.7(3)
N(1)-Co(1)-O(1)	153.20(8)	C(8)-C(7)-C(14)#1	120.7(3)
O(3)-Co(1)-O(2)	158.96(8)	C(6)-C(7)-C(14)#1	120.6(3)
N(3)-Co(1)-O(2)	92.92(7)	N(1)-C(1)-N(2)	112.6(2)
N(1)-Co(1)-O(2)	93.65(7)	C(5)-C(10)-C(9)	120.5(3)
O(1)-Co(1)-O(2)	59.89(7)	O(1)-C(15)-O(2)	119.0(2)
O(3)-Co(1)-O(4)	60.21(6)	O(1)-C(15)-C(16)	121.0(2)
N(3)-Co(1)-O(4)	158.23(8)	O(2)-C(15)-C(16)	119.9(2)
N(1)-Co(1)-O(4)	88.53(7)	O(1)-C(15)-Co(1)	59.62(13)
O(1)-Co(1)-O(4)	95.87(7)	O(2)-C(15)-Co(1)	60.04(13)
O(2)-Co(1)-O(4)	108.83(7)	C(16)-C(15)-Co(1)	171.61(16)
O(3)-Co(1)-C(28)	30.23(7)	O(4)-C(28)-O(3)	119.7(2)
N(3)-Co(1)-C(28)	128.52(9)	O(4)-C(28)-C(27)#2	120.8(2)
N(1)-Co(1)-C(28)	94.97(8)	O(3)-C(28)-C(27)#2	119.5(2)
O(1)-Co(1)-C(28)	102.05(7)	O(4)-C(28)-Co(1)	65.02(12)
O(2)-Co(1)-C(28)	137.36(8)	O(3)-C(28)-Co(1)	54.98(12)
O(4)-Co(1)-C(28)	30.09(7)	C(27)#2-C(28)-Co(1)	170.89(18)

C(17)-C(18)-C(19)	109.7(2)	C(13)-C(12)-N(3)	110.2(3)
N(2)-C(4)-C(5)	112.5(2)	C(25)-C(26)-C(17)	110.7(2)
C(15)-C(16)-C(17)	114.37(19)	C(8)-C(9)-C(10)	119.5(3)
C(20)-C(25)-C(24)	109.6(2)	C(21)-C(19)-C(20)	109.4(3)
C(20)-C(25)-C(26)	108.9(3)	C(21)-C(19)-C(18)	109.6(2)
C(24)-C(25)-C(26)	109.9(2)	C(20)-C(19)-C(18)	109.9(2)
C(7)-C(6)-C(5)	121.4(3)	C(28)#3-C(27)-C(23)	116.2(2)
C(23)-C(21)-C(19)	110.3(2)	N(4)-C(14)-C(7)#4	112.2(2)
C(3)-C(2)-N(1)	110.7(2)	C(25)-C(24)-C(23)	110.5(2)
N(3)-C(11)-N(4)	111.2(2)	C(2)-C(3)-N(2)	106.1(2)
C(7)-C(8)-C(9)	121.5(3)	C(25)-C(20)-C(19)	109.3(2)
C(12)-C(13)-N(4)	106.3(2)		

Symmetry transformations used to generate equivalent atoms:

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

Compound 4b

Co(1)-O(3)	1.939(3)	O(5)-Co(1)#1	1.989(4)
Co(1)-O(5)#1	1.989(4)	C(14)-C(15)	1.379(5)
Co(1)-O(1)	2.000(3)	C(14)-C(13)	1.395(5)
Co(1)-N(2)	2.116(3)	C(14)-C(17)#5	1.462(5)
Co(1)-N(1)	2.145(3)		
Co(2)-O(3)	1.951(3)	O(3)-Co(1)-O(5)#1	127.56(17)
Co(2)-O(2)#2	1.989(3)	O(3)-Co(1)-O(1)	121.80(15)
Co(2)-O(4)#3	2.004(3)	O(5)#1-Co(1)-O(1)	110.63(16)
Co(2)-N(5)	2.140(3)	O(3)-Co(1)-N(2)	82.58(12)
Co(2)-N(3)	2.177(3)	O(5)#1-Co(1)-N(2)	90.88(14)
O(1)-C(8)	1.239(5)	O(1)-Co(1)-N(2)	98.76(13)
C(5)-C(6)	1.381(6)	O(3)-Co(1)-N(1)	91.60(12)
C(5)-C(4)	1.405(6)	O(5)#1-Co(1)-N(1)	88.55(14)
C(3)-C(1)	1.386(7)	O(1)-Co(1)-N(1)	88.71(13)
C(3)-C(4)	1.392(6)	N(2)-Co(1)-N(1)	172.20(12)
C(6)-C(2)	1.396(7)	O(3)-Co(2)-O(2)#2	120.29(15)
C(6)-C(7)	1.514(6)	O(3)-Co(2)-O(4)#3	123.95(15)
C(1)-C(2)	1.378(7)	O(2)#2-Co(2)-O(4)#3	115.64(15)
C(8)-O(2)	1.251(5)	O(3)-Co(2)-N(5)	85.60(12)
C(8)-C(7)	1.511(6)	O(2)#2-Co(2)-N(5)	98.17(14)
C(4)-C(9)	1.509(6)	O(4)#3-Co(2)-N(5)	90.25(13)
N(1)-C(11)	1.336(5)	O(3)-Co(2)-N(3)	85.22(12)
N(1)-C(12)	1.347(5)	O(2)#2-Co(2)-N(3)	86.70(13)
O(2)-Co(2)#4	1.989(3)	O(4)#3-Co(2)-N(3)	94.66(13)
C(12)-C(15)	1.369(5)	N(5)-Co(2)-N(3)	170.82(12)
C(11)-C(13)	1.382(6)	C(8)-O(1)-Co(1)	142.4(3)
C(9)-C(10)	1.522(6)	C(6)-C(5)-C(4)	122.2(4)
C(10)-O(5)	1.238(6)	C(1)-C(3)-C(4)	120.7(5)
C(10)-O(4)	1.254(5)	C(5)-C(6)-C(2)	118.6(4)
N(2)-N(5)#4	1.315(4)	C(5)-C(6)-C(7)	120.9(4)
N(2)-N(3)	1.339(4)	C(2)-C(6)-C(7)	120.4(5)
N(5)-N(2)#2	1.315(4)	C(2)-C(1)-C(3)	120.6(4)
N(5)-N(6)	1.332(4)	C(1)-C(2)-C(6)	120.3(5)
N(3)-C(17)	1.339(5)	O(1)-C(8)-O(2)	126.1(4)

O(1)-C(8)-C(7)	118.9(4)	O(4)-C(10)-C(9)	117.6(4)
O(2)-C(8)-C(7)	115.0(4)	N(5)#4-N(2)-N(3)	109.3(3)
C(8)-C(7)-C(6)	116.4(4)	N(5)#4-N(2)-Co(1)	124.8(2)
C(3)-C(4)-C(5)	117.6(4)	N(3)-N(2)-Co(1)	125.9(2)
C(3)-C(4)-C(9)	120.6(4)	N(2)#2-N(5)-N(6)	110.0(3)
C(5)-C(4)-C(9)	121.8(4)	N(2)#2-N(5)-Co(2)	126.4(2)
Co(1)-O(3)-Co(2)	129.07(15)	N(6)-N(5)-Co(2)	122.9(2)
C(11)-N(1)-C(12)	116.6(3)	C(17)-N(3)-N(2)	104.9(3)
C(11)-N(1)-Co(1)	123.4(3)	C(17)-N(3)-Co(2)	139.7(3)
C(12)-N(1)-Co(1)	120.0(3)		
C(8)-O(2)-Co(2)#4	138.0(3)	C(10)-O(5)-Co(1)#1	140.3(3)
N(1)-C(12)-C(15)	123.7(4)	C(15)-C(14)-C(13)	117.8(4)
N(1)-C(11)-C(13)	123.5(4)	C(15)-C(14)-C(17)#5	119.6(3)
C(4)-C(9)-C(10)	110.5(4)	C(13)-C(14)-C(17)#5	122.6(4)
O(5)-C(10)-O(4)	126.8(5)	C(12)-C(15)-C(14)	119.5(4)
O(5)-C(10)-C(9)	115.5(4)	C(11)-C(13)-C(14)	118.9(4)

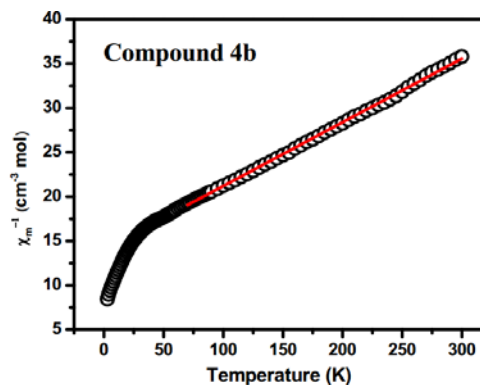
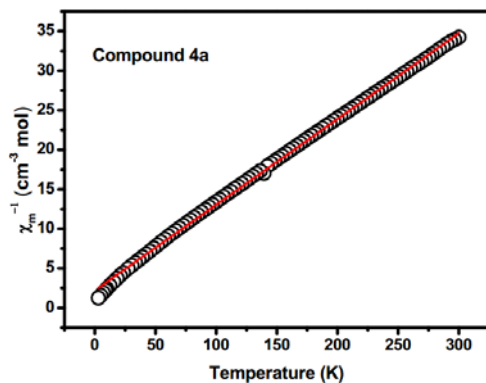
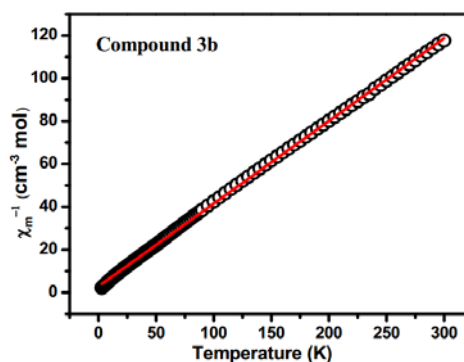
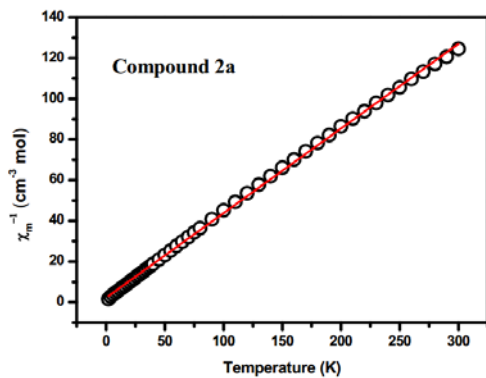
Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1 #2 x-1/2,-y+1/2,z-1/2

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#5 -x-1/2,y-1/2,-z+1/2

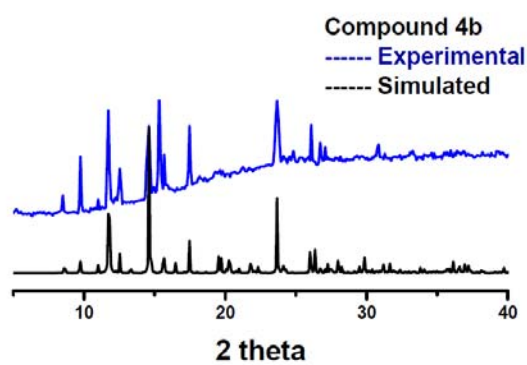
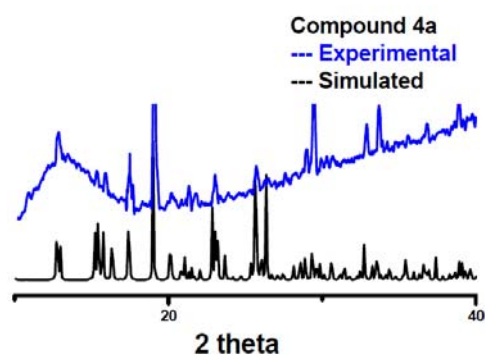
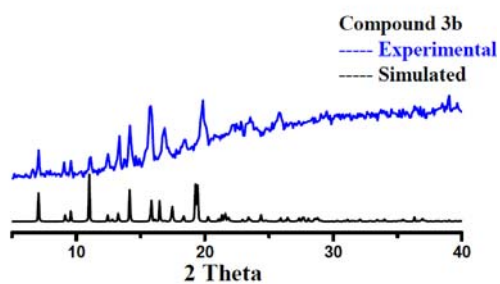
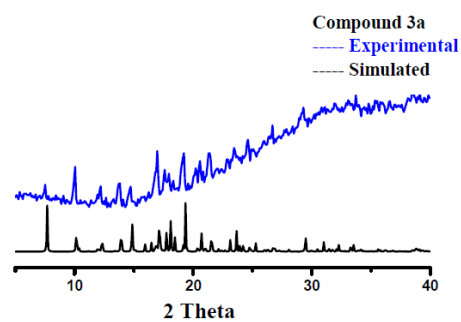
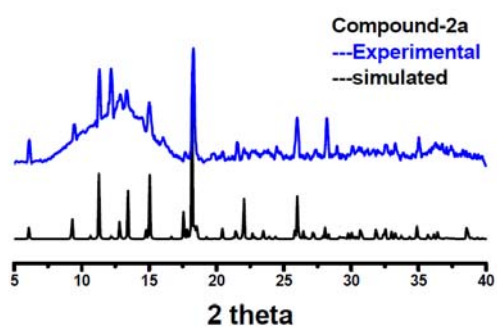
Section-2

1/ χ_M vs T plots of the compounds 2a, 3b, 4a and 4b



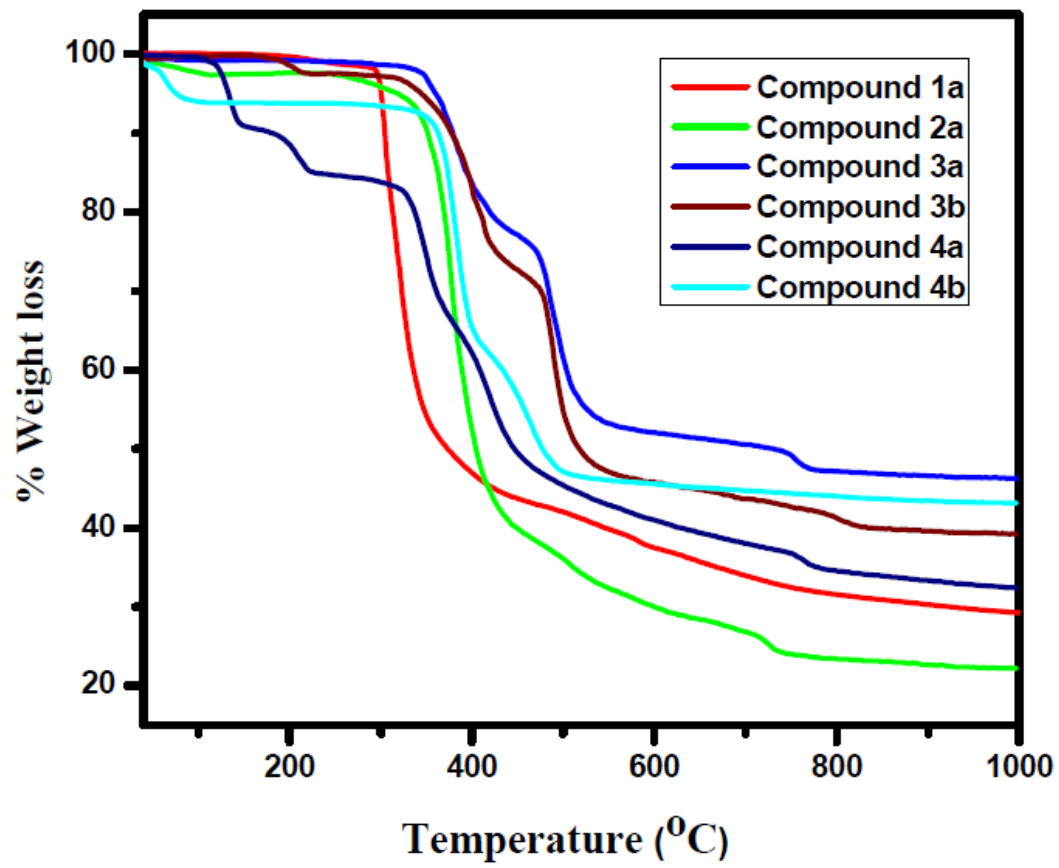
Section-3

Powder X-ray diffraction patterns



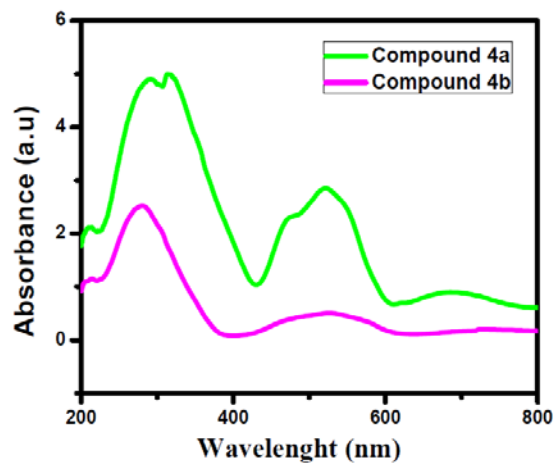
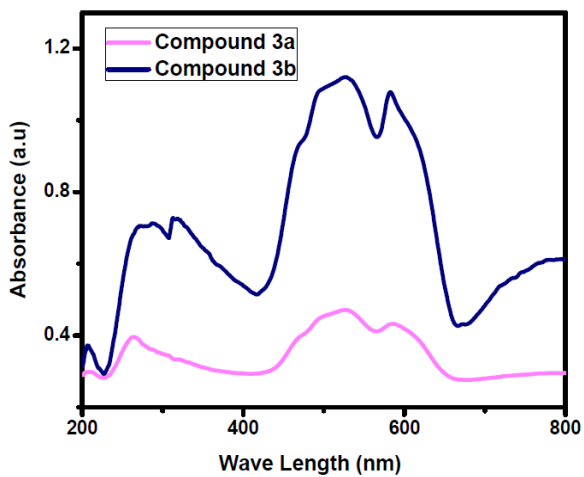
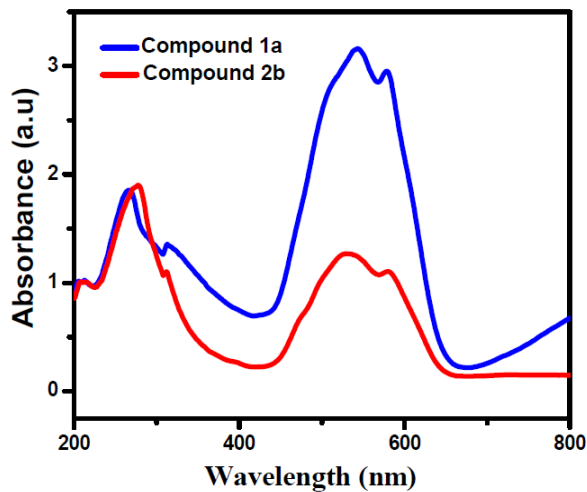
Section-4

TGA Curves



Section-5

Diffused Reflectanc Spectra



***** End of Supporting Information*****