Four new metal–organic frameworks based on a rigid linear ligand: Synthesis, optical property and structural investigation

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Dedicated to Professor Xinquan Xin on the occasion of his 80th birthday

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Table S1. Selected Bond Lengths (Å) and Angles (deg) for Complexes **1-4**.

Complex **1**

Cd(1)-N(1)	2.287(6)	Cd(1)-O(3)	2.301(5)
Cd(1)-O(4)#2	2.320(5)	Cd(1)-O(1)	2.377(5)
Cd(1)-O(2)	2.429(5)	Cd(1)-N(3)	2.279(5)
O(4)#2-Cd(1)-O(2)	91.77(19)	O(1)-Cd(1)-O(2)	54.32(19)
N(3)-Cd(1)-O(3)	90.1(2)	N(1)-Cd(1)-O(3)	97.6(2)
N(3)-Cd(1)-O(4)#2	85.1(2)	N(1)-Cd(1)-O(4)#2	84.4(2)
O(3)-Cd(1)-O(4)#2	125.77(18)	N(3)-Cd(1)-O(1)	90.7(2)
N(1)-Cd(1)-O(1)	96.8(2)	O(3)-Cd(1)-O(1)	88.46(18)
O(4)#2-Cd(1)-O(1)	145.42(18)	N(3)-Cd(1)-O(2)	94.6(2)
N(1)-Cd(1)-O(2)	83.7(2)	O(3)-Cd(1)-O(2)	142.45(19)

Complex **2**

Co(1)-N(4)	2.105(3)	Co(1)-O(14)	2.109(2)
Co(1)-O(15)	2.110(2)	Co(1)-N(5)	2.109(3)

Co(1)-O(17)	2.125(3)	Co(1)-O(16)	2.128(2)
Co(2)-O(6)	2.092(3)	Co(2)-O(7)	2.106(2)
Co(2)-O(5)	2.110(2)	Co(2)-N(3)	2.126(3)
Co(2)-N(1)	2.129(3)	Co(2)-O(8)	2.133(3)
O(17)-Co(1)-O(16)	89.84(10)	N(5)-Co(1)-O(16)	89.38(10)
N(4)-Co(1)-O(16)	89.44(10)	N(4)-Co(1)-O(14)	93.39(10)
O(15)-Co(1)-O(16)	92.36(9)	O(14)-Co(1)-O(16)	177.17(9)
N(5)-Co(1)-O(17)	89.95(11)	O(15)-Co(1)-O(17)	175.30(9)
O(14)-Co(1)-O(17)	90.14(10)	N(4)-Co(1)-O(17)	88.29(11)
O(15)-Co(1)-N(5)	94.22(11)	O(14)-Co(1)-N(5)	87.79(10)
N(4)-Co(1)-N(5)	177.88(12)	O(14)-Co(1)-O(15)	87.87(9)
N(4)-Co(1)-O(15)	87.59(10)	O(6)-Co(2)-O(7)	88.21(11)
N(1)-Co(2)-O(8)	88.02(11)	N(3)-Co(2)-O(8)	88.62(11)
O(5)-Co(2)-O(8)	91.34(11)	O(7)-Co(2)-O(8)	92.22(10)
O(6)-Co(2)-O(8)	177.62(11)	N(3)-Co(2)-N(1)	173.16(12)
O(5)-Co(2)-N(1)	86.11(10)	O(7)-Co(2)-N(1)	91.02(11)
O(6)-Co(2)-N(1)	89.64(11)	O(5)-Co(2)-N(3)	88.02(12)
O(7)-Co(2)-N(3)	95.06(12)	O(6)-Co(2)-N(3)	93.66(12)
O(7)-Co(2)-O(5)	175.34(10)	O(6)-Co(2)-O(5)	88.10(11)

Complex **3**

Ni(1)-O(5)	2.0631(12)	Ni(1)-O(5)#1	2.0631(12)
Ni(1)-N(3)	2.0780(14)	Ni(1)-N(3)#1	2.0780(14)
Ni(1)-O(3)#1	2.1085(12)	Ni(1)-O(3)	2.1085(12)
Ni(2)-O(6)	2.0786(12)	Ni(2)-O(6)#2	2.0786(12)
Ni(2)-N(1)	2.0903(14)	Ni(2)-N(1)#2	2.0903(14)
Ni(2)-O(2)#2	2.0955(12)	Ni(2)-O(2)	2.0955(12)
O(5)-Ni(1)-O(5)#1	180.0	O(5)-Ni(1)-N(3)	88.50(5)

O(2)#2-Ni(2)-O(2)	180.00(6)	N(1)#2-Ni(2)-O(2)	86.96(5)
N(1)-Ni(2)-O(2)	93.04(5)	O(6)#2-Ni(2)-O(2)	92.87(5)
O(6)-Ni(2)-O(2)	87.13(5)	N(1)#2-Ni(2)-O(2)#2	93.04(5)
N(1)-Ni(2)-O(2)#2	86.96(5)	O(6)#2-Ni(2)-O(2)#2	87.13(5)
O(6)-Ni(2)-O(2)#2	92.87(5)	N(1)-Ni(2)-N(1)#2	180.00(10)
O(6)#2-Ni(2)-N(1)#2	93.72(5)	O(6)-Ni(2)-N(1)#2	86.28(5)
O(6)#2-Ni(2)-N(1)	86.28(5)	O(6)-Ni(2)-N(1)	93.72(5)
O(6)-Ni(2)-O(6)#2	180.0	O(3)#1-Ni(1)-O(3)	180.000(1)
N(3)#1-Ni(1)-O(3)	93.00(5)	N(3)-Ni(1)-O(3)	87.00(5)
O(5)#1-Ni(1)-O(3)	92.01(5)	O(5)-Ni(1)-O(3)	87.99(5)
N(3)#1-Ni(1)-O(3)#1	87.00(5)	N(3)-Ni(1)-O(3)#1	93.00(5)
O(5)#1-Ni(1)-O(3)#1	87.99(5)	O(5)-Ni(1)-O(3)#1	92.01(5)
N(3)-Ni(1)-N(3)#1	180.000(1)	O(5)#1-Ni(1)-N(3)#1	88.50(5)
O(5)-Ni(1)-N(3)#1	91.50(5)	O(5)#1-Ni(1)-N(3)	91.50(5)

Complex **4**

Ni(1)-O(1)#1	2.0614(19)	Ni(1)-O(1)	2.0614(19)
Ni(1)-O(3)	2.105(3)	Ni(1)-O(4)	2.104(3)
Ni(1)-N(1)	2.066(2)	Ni(1)-N(1)#1	2.066(2)
O(1)#1-Ni(1)-O(1)	91.22(12)	O(1)#1-Ni(1)-N(1)	87.19(9)
O(4)-Ni(1)-O(3)	175.84(11)	N(1)#1-Ni(1)-O(3)	91.27(9)
N(1)-Ni(1)-O(3)	91.27(9)	O(1)-Ni(1)-O(3)	85.95(8)
O(1)#1-Ni(1)-O(3)	85.95(8)	N(1)#1-Ni(1)-O(4)	91.56(9)
N(1)-Ni(1)-O(4)	91.56(9)	O(1)-Ni(1)-O(4)	91.15(8)
O(1)#1-Ni(1)-O(4)	91.15(8)	N(1)-Ni(1)-N(1)#1	94.28(13)
O(1)-Ni(1)-N(1)#1	87.19(9)	O(1)#1-Ni(1)-N(1)#1	176.89(9)
O(1)-Ni(1)-N(1)	176.89(9)		

Symmetry codes: for **1**: #2 = $-x+1, -y+1, -z+1$; for **3**: #1 $-x+1, -y+1, -z+2$; #2 = $-x, -y-1, -z$; for **4**: #1 = $x, y, -z+1/2$

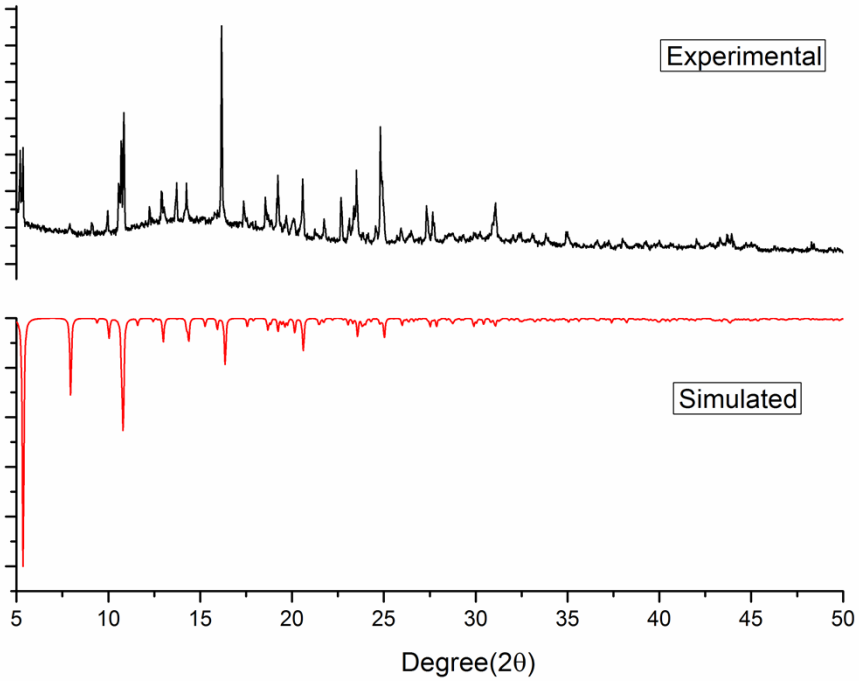

Figure S1. Powder X-ray diffraction patterns of complex **1**

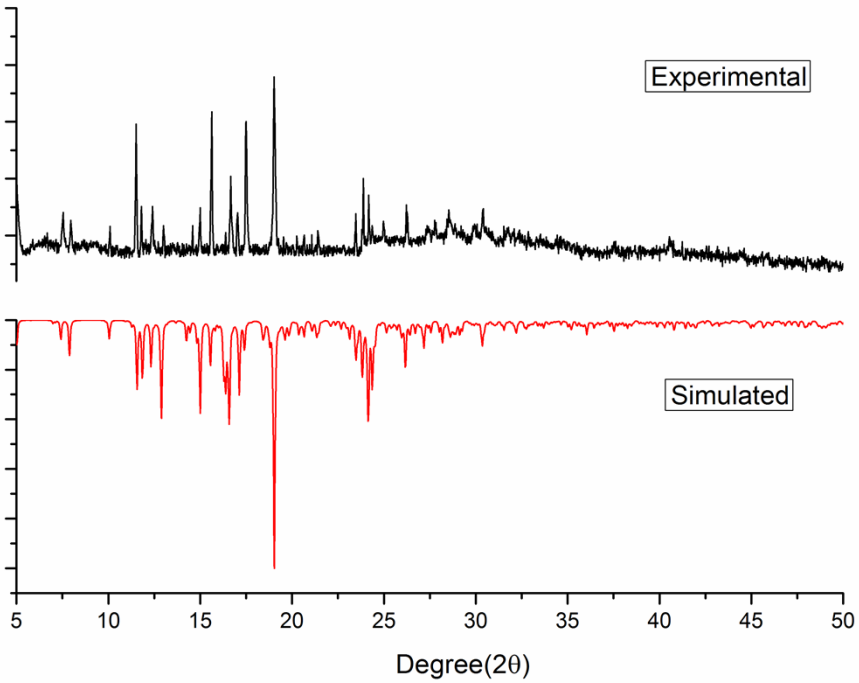

Figure S2. Powder X-ray diffraction patterns of complex **2**

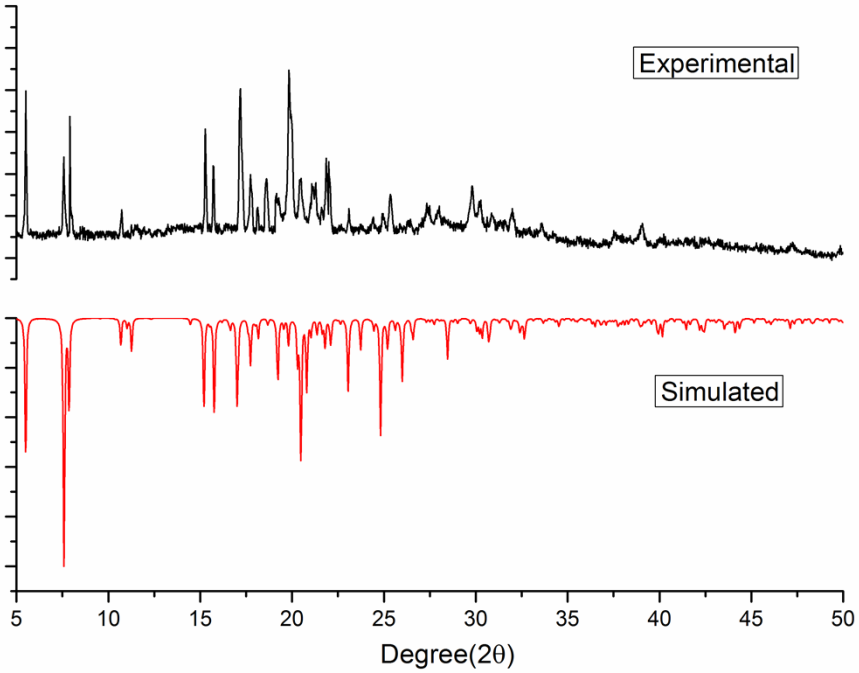

Figure S3. Powder X-ray diffraction patterns of complex **3**

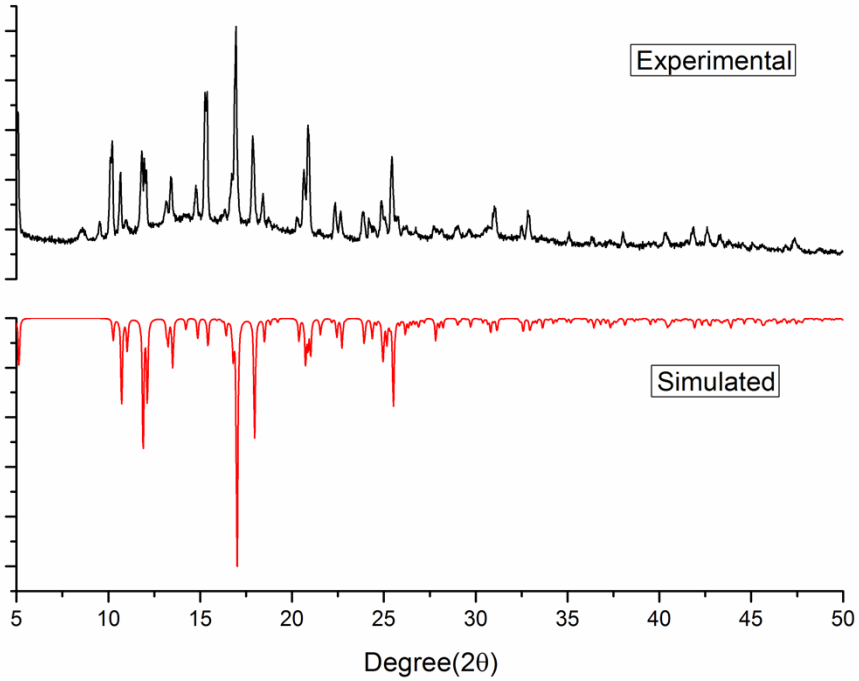

Figure S4. Powder X-ray diffraction patterns of complex **4**

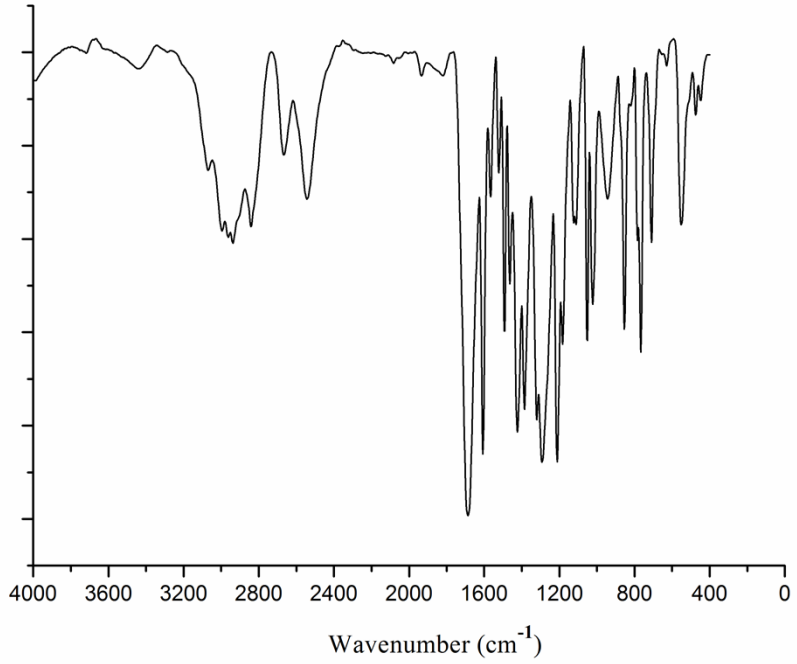

Figure S5. IR spectra of H_2L ligand

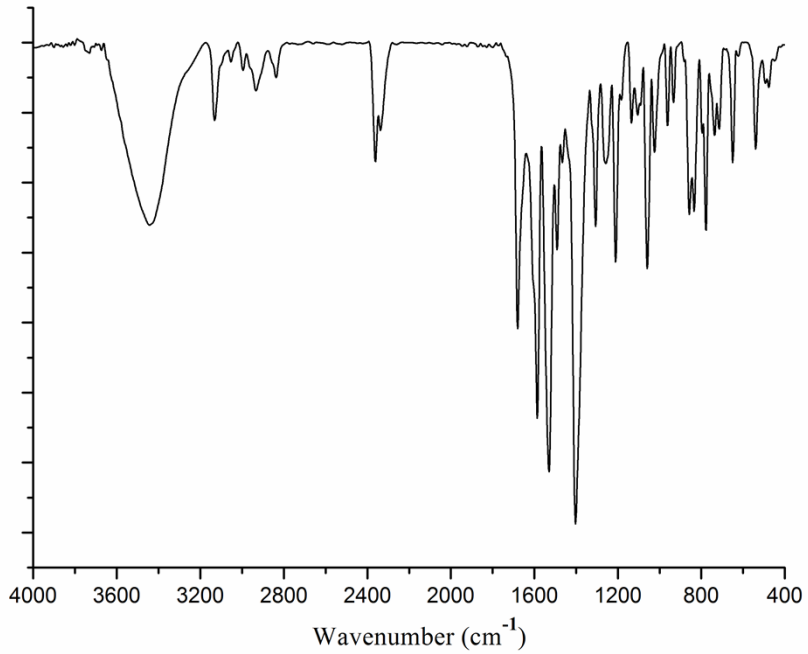

Figure S6. IR spectra of complex **1**

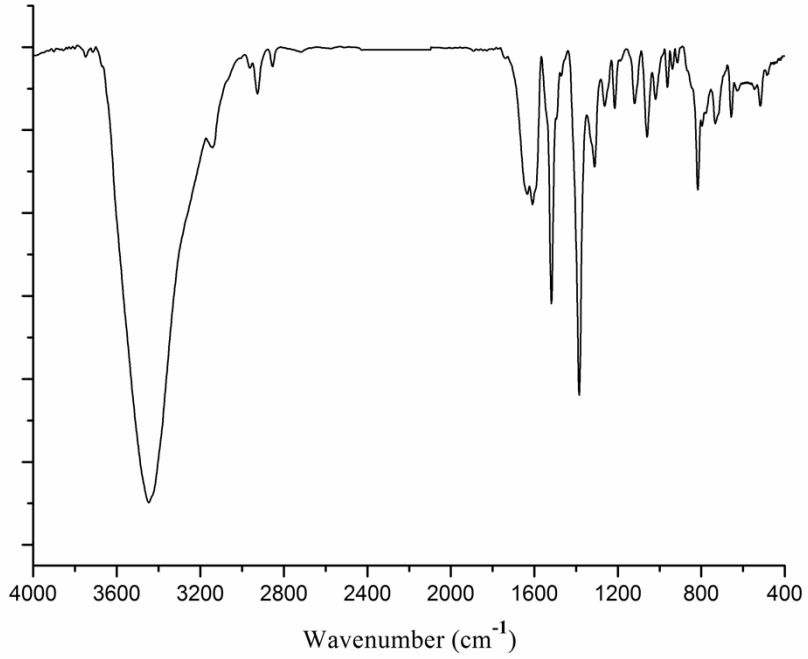

Figure S7. IR spectra of complex **2**

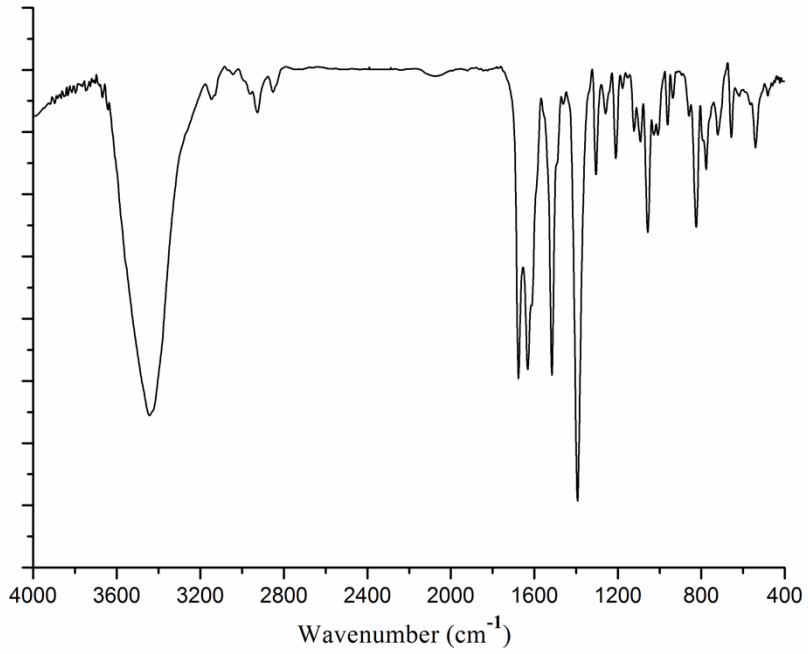

Figure S8. IR spectra of complex **3**

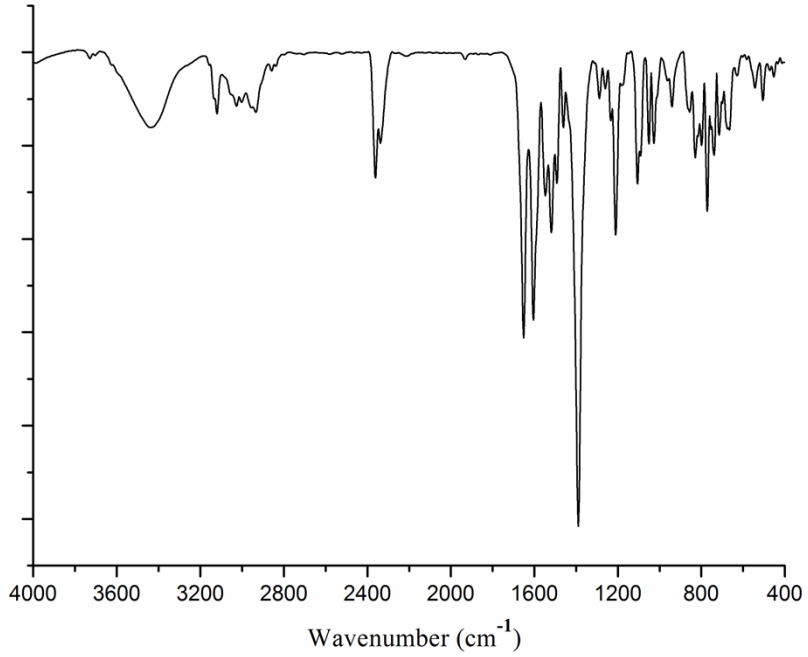

Figure S9. IR spectra of complex **4**

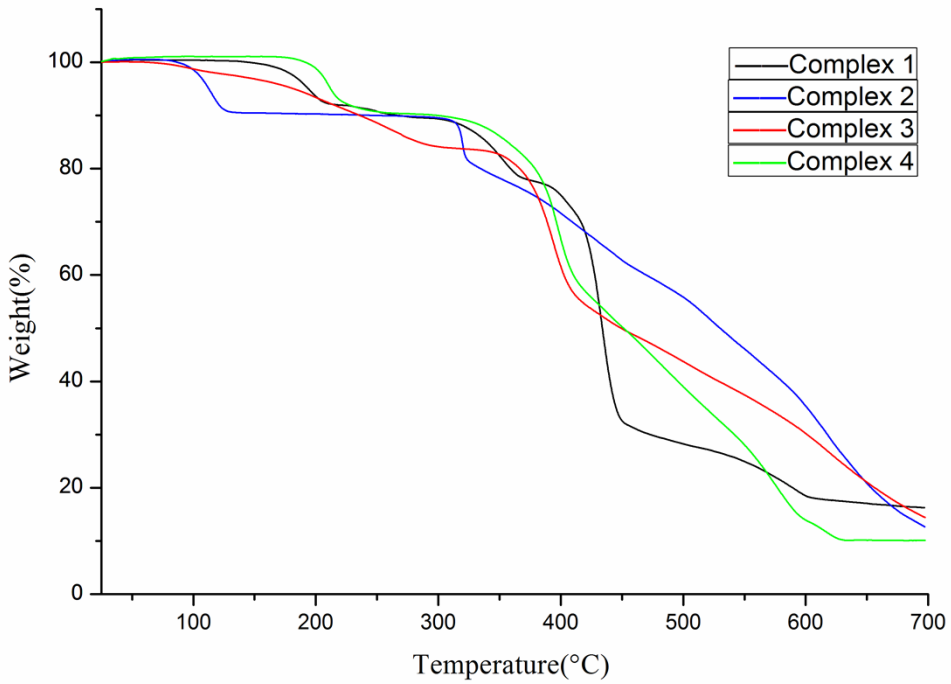

Figure S10. The TGA diagrams of complexes **1-4.**