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Four cobalt(II) complexes based on a new tricarboxylate with naphthalene ring and different N-containing ligands: synthesis, crystal structures and magnetic properties

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Table S1 The selected bond lengths (Å) and angles (°) for complexes **1** - **4**.

Complex **1** Symmetry code for #1 x, y, 1+z ; #2 -x, 1-y, 2-z; #3 -x, 2-y, 3-z; #4 -x, 1-y, 1-z; #5 x, 1+y, 2+z

Bond Distance					
Co1#1-O1#1	2.090(2)	Co1#1-O2#2	2.087(2)	Co1#1-O5	2.125(2)
Co1#1-O6	2.099(2)	Co1#1-N1#1	2.106(2)	Co1#1-N5#1	2.143(2)
Co2#5-O4	2.166(6)	Co2#5-O4#3	2.166(6)	Co2#5-O8#4	2.057(2)
Co2#5-O8#5	2.057(2)	Co2#5-N4#4	2.134(2)	Co2#5-N4#5	2.134(2)

Bond Angles			
O1#1-Co1#1-O2#2	105.62(9)	O1#1-Co1#1-O6	84.45(9)
O1#1-Co1#1-N1#1	90.47(9)	O1#1-Co1#1-N5#1	87.28(10)
O5-Co1#1-O2#2	85.98(9)	O5-Co1#1-O6	83.52(9)
O5-Co1#1-NI#1	94.27(8)	O5-Co1#1-N5#1	89.07(9)
N4#4-Co2#5-O4	88.94(8)	N4#4-Co2#5-O4#3	91.06(8)
N4#4-Co2#5-O8#4	91.28(9)	N4#4-Co2#5-O8#5	88.72(9)
N4#5-Co2#5-O4	91.06(8)	N4#5-Co2#5-O4#3	88.94(8)
N4#5-Co2#5-O8#4	88.72(10)	N4#5-Co2#5-O8#5	91.28(9)

Complex **2** Symmetry code for #1 0.5-x, y, 0.5-z

Bond Distance					
Co1-O1	2.198(3)	Co2-O9	2.083(3)	Co3-O1	2.168(3)
Co1-O1#1	2.198(3)	Co2-O9#1	2.083(3)	Co3-O1#1	2.168(3)
Co1-O2	2.243(3)	Co2-O10	2.240(3)	Co3-O5	2.072(3)
Co1-O2#1	2.243(3)	Co2-O10#1	2.240(3)	Co3-O5#1	2.072(3)
Co1-N5	2.004(3)	Co2-N3	2.107(3)	Co3-N1	2.077(3)
Co1-N5#1	2.004(3)	Co2-N3#1	2.107(3)	Co3-N1#1	2.077(3)

Bond Angles			
O2-Co1-O1	58.75(11)	N3#1-Co2-O9#1	92.39(12)
O2-Co1-O1#1	110.97(10)	N3#1-Co2-O10	94.45(12)

O2-Co1-N5	94.57(13)	N3#1-Co2-O10#1	87.63(12)
O2-Co1-N5#1	109.7(2)	N3#1-Co2-N3	91.73(19)
O2#1-Co1-O1	110.97(10)	O5-Co3-O1	84.25(11)
O2#1-Co1-O1#1	58.75(11)	O5-Co3-O1#1	85.00(11)
O2#1-Co1-N5	92.25(13)	O5-Co3-N1	95.40(13)
O2#1-Co1-N5#1	94.57(13)	O5-Co3-N1#1	93.77(12)
O9-Co2-O9#1	83.50(16)	O5#1-Co3-O1	84.99(11)
O9-Co2-O10	86.33(12)	O5#1-Co3-O1#1	84.25(11)
O9-Co2-O10#1	91.44(12)	O5#1-Co3-N1	93.77(12)
O9-Co2-N3	92.39(12)	O5#1-Co3-N1#1	95.40(13)

Complex **3** Symmetry code for #1 1-x, 1-y, 2-z

Bond Distance					
Co1-O4	2.009(2)	Co1-O7	2.062(2)	Co1-N2	2.041(3)
Co1-O6	2.341(3)	Co1-O7#1	2.389(2)	Co1-N4	2.067(3)

Bond Angles

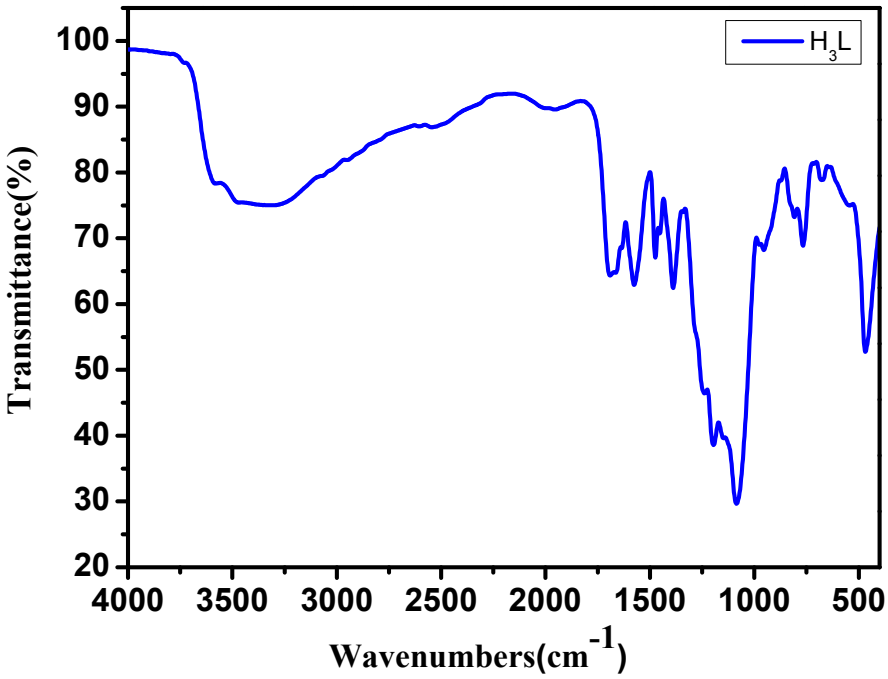
O6-Co1-O7	59.30(9)	O4-Co1-O7	98.92(10)
O6-Co1-O7#1	96.41(9)	O4-Co1-O7#1	85.52(9)
O6-Co1-N2	90.43(10)	O4-Co1-N2	113.08(10)
O6-Co1-N4	85.59(11)	O4-Co1-N4	89.87(11)

Complex **4** Symmetry code for #1 0.5+x, 0.5-y, -0.25+z ; #2 0.5-x, -0.5+y, 0.25+z

Bond Distance					
Co1-O1	2.134(3)	Co1-O4#1	2.042(3)	Co2-O5#2	2.059(3)
Co1-O2	2.137(3)	Co1-O5	2.261(2)	Co2-O6	2.019(3)
Co1-O3	2.074(3)	Co2-O2	2.263(3)	Co2-O8	2.084(3)
Co1-O4	2.031(3)	Co2-O4	2.114(2)	Co2-N1	2.105(3)

Bond Angles

O2-Co1-O1	96.56(10)	O4-Co2-O2	74.35(10)
O2-Co1-O4	78.83(10)	O4-Co2-O5#2	82.83(10)
O2-Co1-O4#1	96.92(10)	O4-Co2-O6	98.45(10)
O2-Co1-O5	84.09(10)	O4-Co2-O8	87.36(10)
O3-Co1-O1	95.97(11)	N1-Co2-O2	102.54(11)
O3-Co1-O4	89.81(11)	N1-Co2-O5#2	94.70(12)
O3-Co1-O4#1	92.98(10)	N1-Co2-O6	83.36(13)
O3-Co1-O5	85.19(10)	N1-Co2-O8	95.66(12)


H3L
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Wavenumbers(cm-1)
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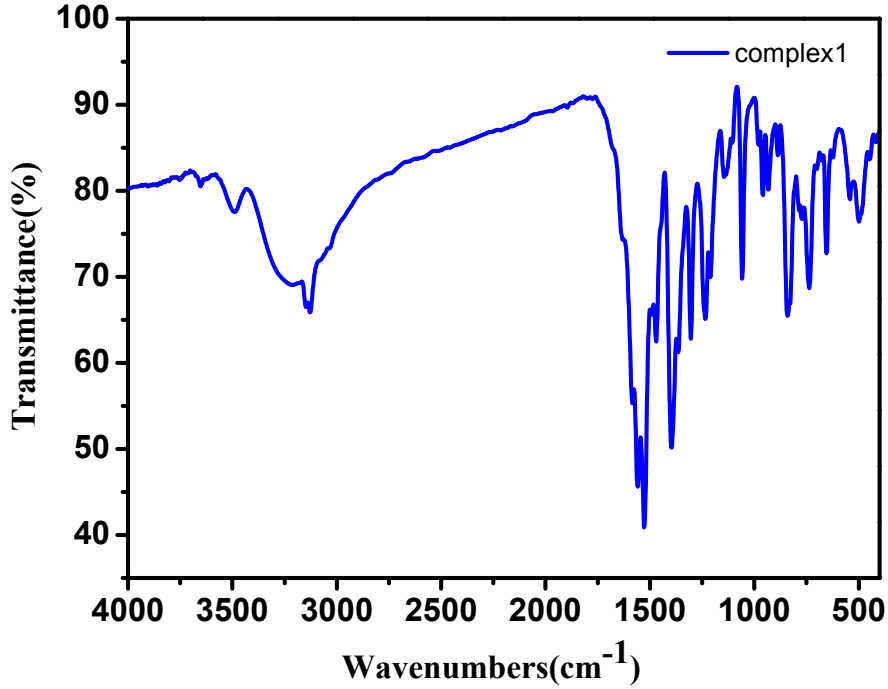
80
70
60
50
40
30
20
4000
3500
3000
2500
2000
1500
1000
500


complex1
Transmittance(%)
Wavenumbers(cm-1)
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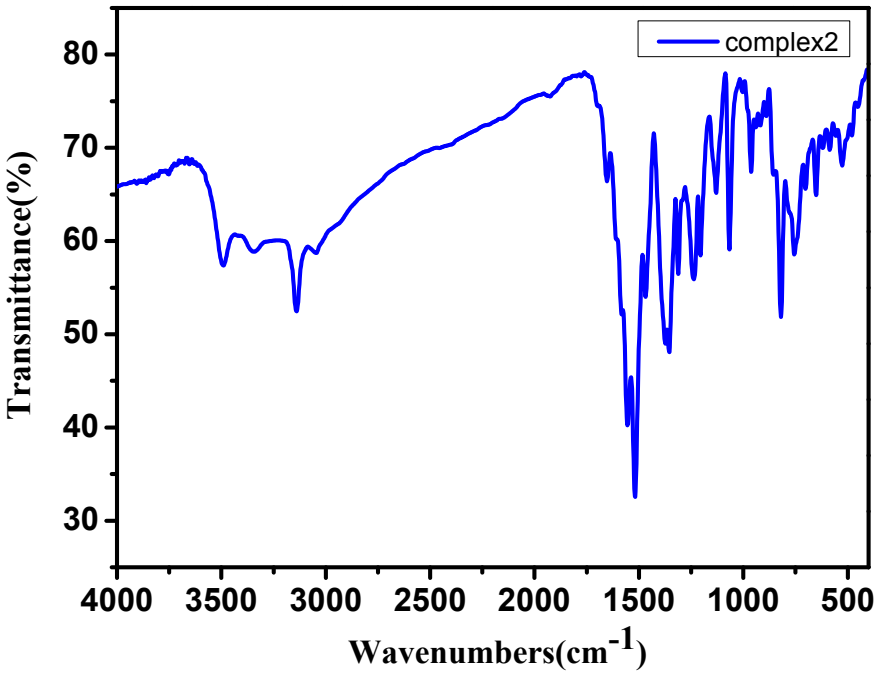
80
70
60
50
40
4000
3500
3000
2500
2000
1500
1000
500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Transmittance(%)
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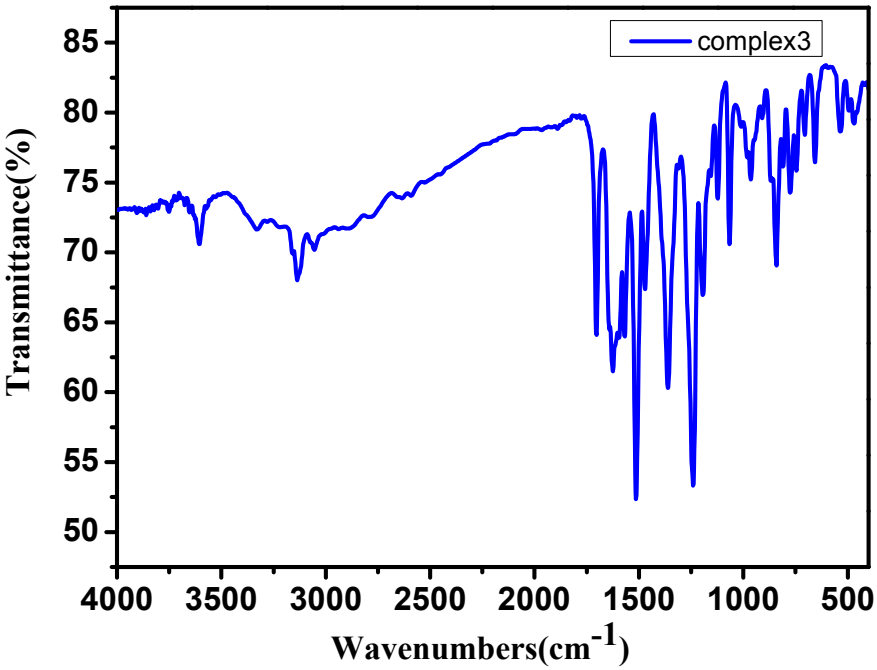
70
60
50
40
30
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers(cm-1)


complex3
Transmittance(%)
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60
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50
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers(cm-1)

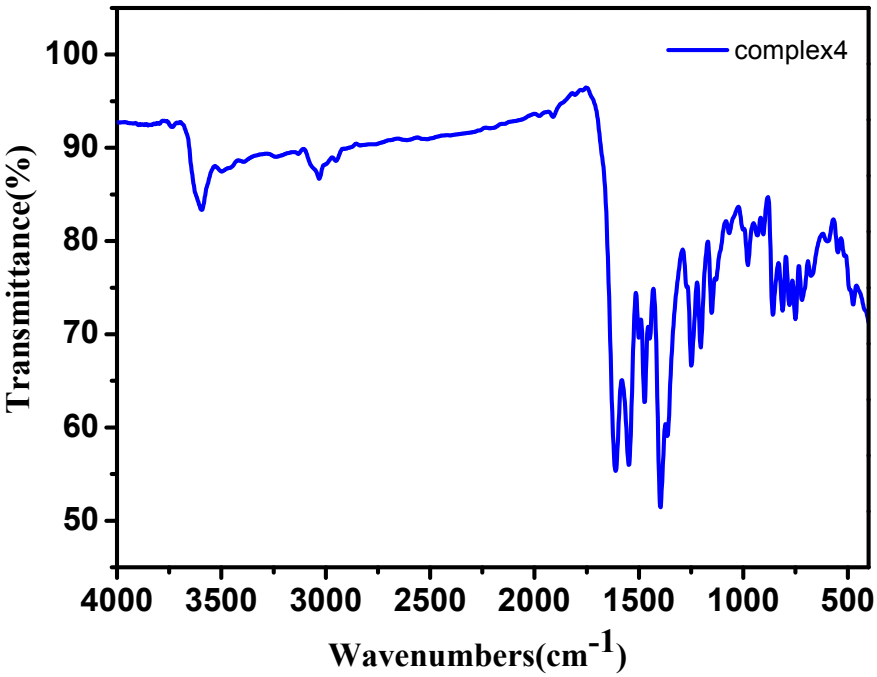
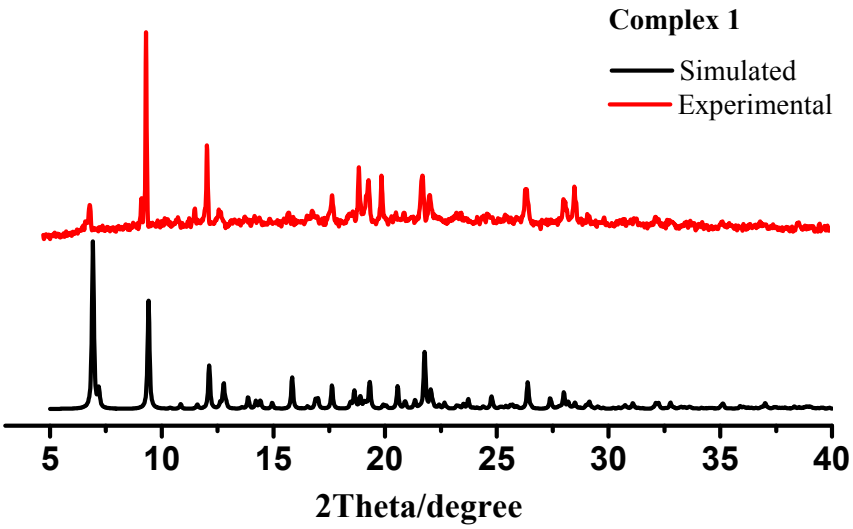
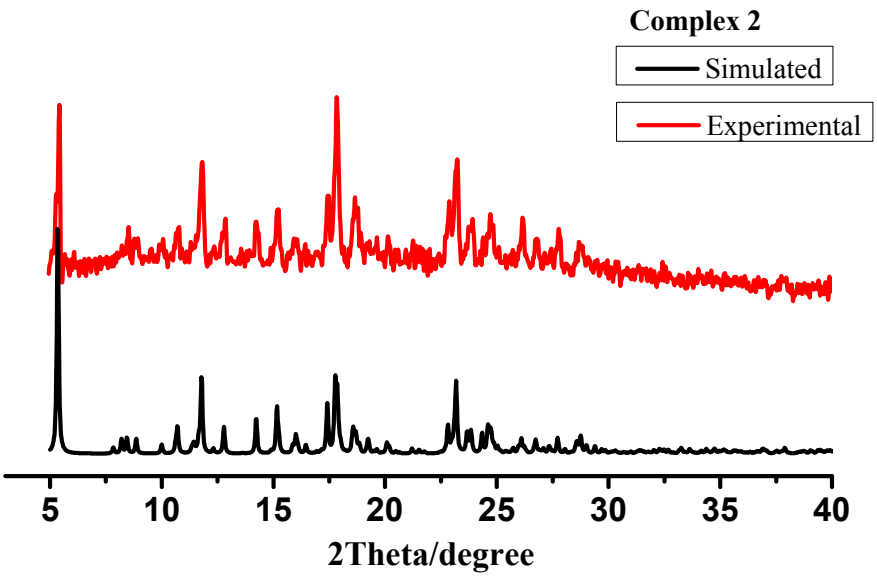
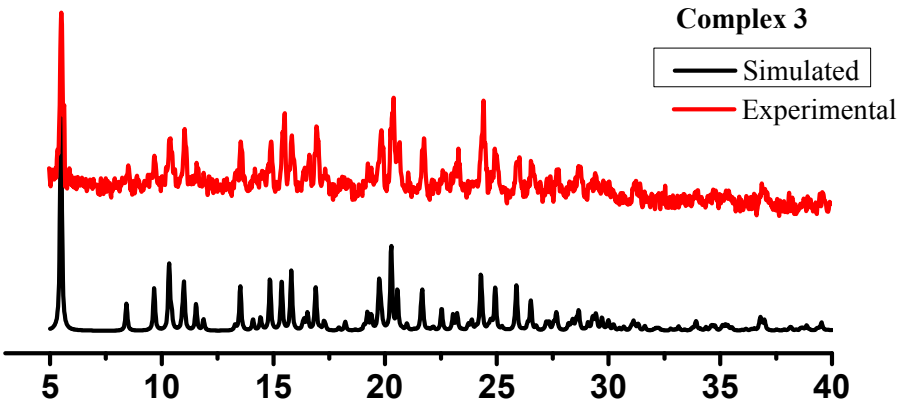


Figure. S1: IR of ligand H_3L and complexes **1** - **4**.




Complex 2
Simulated
Experimental
5
10
15
20
25
30
35
40
2Theta/degree


Complex 3
Simulated
Experimental
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15
20
25
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35
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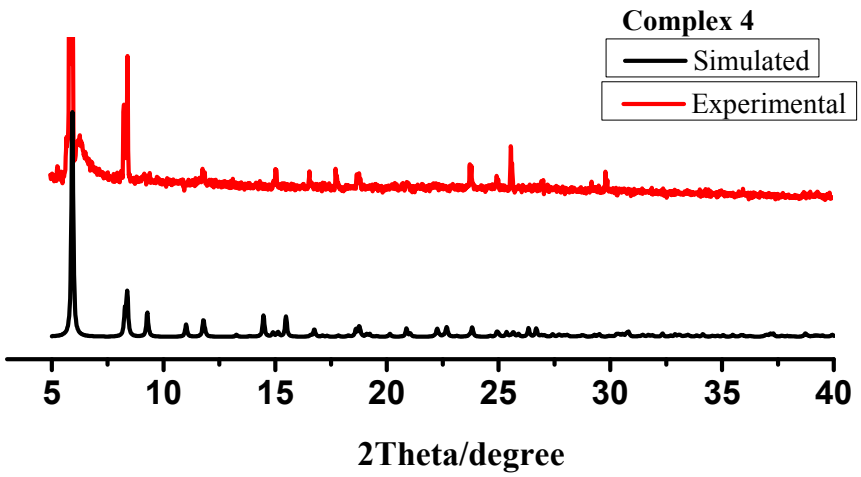

Figure S2. Simulated and observed PXRD patterns of complexes **1** - **4**.

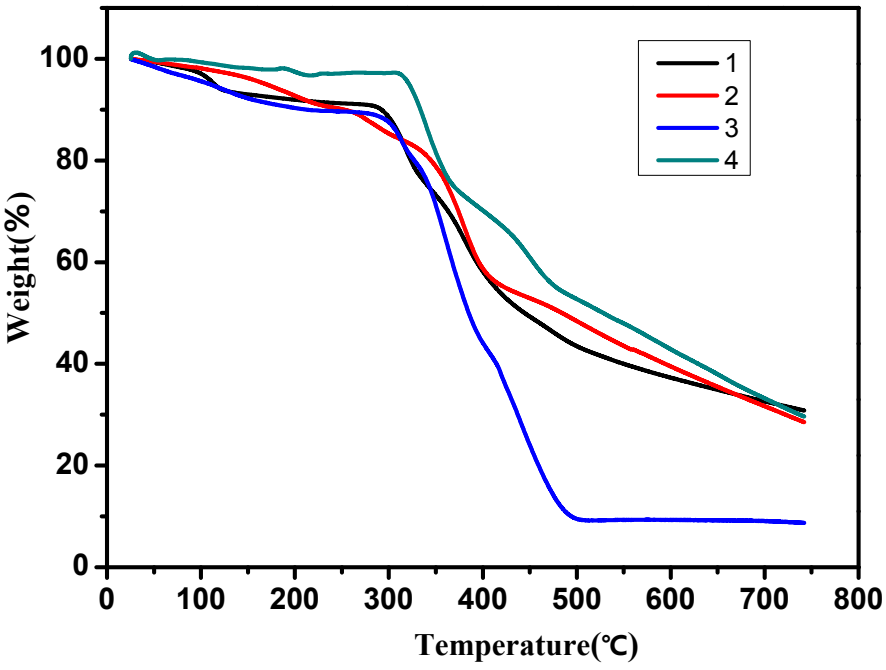

Figure S3. TGA of complexes **1** - **4**.