Supporting Information

Table S1 Hydrogen bond distances [Å] and angles [°].

(D, donor atom; A, acceptor atom).

D-H	d(D-H)	d(H···A)	<DHA	d(D···A)	A
1[I]					
O1-H1	0.820	1.677	160.79	2.466	O3[a]
O5-H5	0.820	1.763	149.99	2.506	O8[b]
O9-H9B	0.850	1.956	164.61	2.785	O6[c]
O9-H9C	0.850	1.923	153.84	2.712	O13[d]
O10-H10A	0.850	2.096	147.31	2.848	O15[e]
O10-H10B	0.850	2.121	133.97	2.780	O13[f]
O11-H11A	0.850	2.060	156.26	2.859	O6[g]
O11-H11B	0.850	1.862	154.24	2.653	O7[h]
O12-H12A	0.850	2.191	138.19	2.881	O15[i]
O12-H12B	0.850	2.093	145.35	2.834	O9[j]
O13-H13A	0.850	1.915	160.82	2.732	O8[g]
O13-H13C	0.850	1.965	158.03	2.772	O14[j]
O14-H14A	0.850	1.889	160.06	2.703	O7
O14-H14C	0.850	2.357	145.03	3.092	O1
O15-H15A	0.850	2.057	158.66	2.865	O3[g]
O15-H15C	0.850	2.028	155.89	2.825	O14[k]
2[II]					
O(9)-H(9A)	0.85	2.28	150.6	3.047(4)	O(17)[a]
O(12)-H(12C)	0.85	1.99	156.8	2.791(4)	O(13)[b]
O(12)-H(12B)	0.85	2.11	147.6	2.862(4)	O(16)
O(13)-H(13D)	0.85	1.97	139.8	2.680(4)	O(4)
O(13)-H(13B)	0.85	1.99	144.4	2.727(4)	O(14)[c]
O(14)-H(14A)	0.85	1.83	173.2	2.672(4)	O(5)[d]
O(15)-H(15A)	0.85	1.90	175.9	2.747(4)	O(8)[e]
O(16)-H(16C)	0.85	1.77	164.3	2.603(5)	O(16)[f]
O(17)-H(17B)	0.85	2.24	144.8	2.972(4)	O(15)[g]
3[III]					
O(9)-H(9B)	0.85	2.04	153.7	2.830(5)	O(16)
O(10)-H(10A)	0.85	2.03	165.2	2.861(5)	O(16)
O(14)-H(14A)	0.85	2.07	147.9	2.824(5)	O(4)
O(9)-H(9A)	0.85	1.95	166.1	2.781(5)	O(7)[a]
O(10)-H(10B)	0.85	1.95	158.8	2.761(5)	O(12)[b]
O(11)-H(11A)	0.85	1.96	140.7	2.676(5)	O(6)[c]
O(11)-H(11B)	0.85	2.55	161.7	3.365(5)	O(17)[d]
O(12)-H(12A)	0.85	1.88	170.0	2.721(5)	O(3)[e]
O(16)-H(16A)	0.85	2.39	132.2	3.031(5)	O(13)[e]
O(16)-H(16C)	0.85	2.42	136.4	3.095(5)	O(14)[e]
O(12)-H(12B)	0.85	1.91	150.5	2.687(5)	O(1)d

O(13)-H(13B)	0.85	2.39	168.8	3.230(5)	O(17)[f]
O(15)-H(15A)	0.85	1.96	162.3	2.783(5)	O(17)[f]
O(13)-H(13A)	0.82	2.04	163.9	2.841(5)	O(9)[g]
O(14)-H(14B)	0.85	2.24	140.9	2.946(5)	O(4)[h]
O(15)-H(15B)	0.85	2.18	155.7	2.979(5)	O(3)[h]
O(17)-H(17A)	0.85	2.00	171.8	2.843(4)	O(8)[i]
O(17)-H(17B)	0.85	2.28	136.9	2.961(5)	O(10)[j]
4[IV]					
O(8)-H(8E)	0.85	1.85	132.6	2.500(8)	O(10)
O(5)-H(5A)	0.85	2.45	129.0	3.054(6)	O(9)[a]
O(5)-H(5B)	0.85	2.07	168.7	2.904(7)	O(6)[b]
O(6)-H(6A)	0.96	1.74	168.5	2.691(6)	O(2)[c]
O(6)-H(6B)	0.96	1.97	134.7	2.730(6)	O(4)[d]
O(8)-H(8C)	0.96	2.00	150.3	2.877(6)	O(4)[d]
O(7)-H(7B)	0.85	1.94	162.2	2.759(6)	O(1)[e]
O(7)-H(7C)	0.85	2.01	154.0	2.799(7)	O(5)[f]
5[V]					
O(6)-H(6A)	0.91	1.75	164.0	2.635(3)	O(5)[a]
O(8)-H(8)	0.89	1.76	167.0	2.635(3)	O(1)[b]
O(9)-H(9B)	0.85	2.14	146.9	2.887(4)	O(1)[c]
O(9)-H(9C)	0.85	2.03	157.9	2.839(4)	O(4)[d]
O(10)-H(10C)	0.85	2.35	142.4	3.069(2)	O(8)
O(10)-H(10D)	0.85	2.52	123.4	3.069(2)	O(8)[b]
6[VI]					
O2-H2A	0.820	1.815	170.13	2.627	O5[a]
O3-H3	0.820	1.806	177.63	2.626	O4[b]
O9-H9A	0.850	2.355	125.74	2.934	O5[c]
O9-H9B	0.850	2.021	169.39	2.860	O8[d]
O10-H10C	0.850	2.459	128.86	3.065	O2
O10-H10B	0.850	2.432	131.85	3.065	O2[a]

[I] Symmetry codes: [a] -x+2, y-1/2, -z+3/2; [b] -x+2, y+1/2, -z+1/2; [c] x+1/2, -y+1/2, -z+1; [d] x+1, y, z; [e] x+1, y, z+1; [f] x+1/2, -y+1/2, -z+2; [g] x-1/2, -y+1/2, -z+1; [h] -x+3/2, -y, z+1/2; [I] x-1/2, -y+1/2, -z+2; [j] -x+1, y+1/2, -z+3/2; [k] -x+3/2, -y, z-1/2.

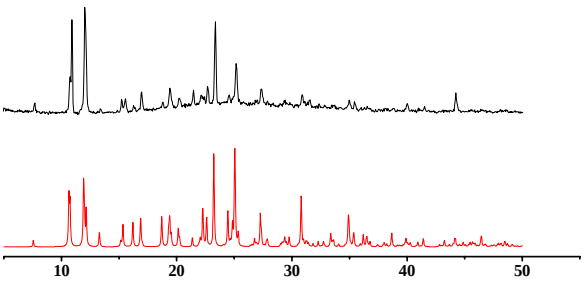
[II] Symmetry codes: [a]x, y-1, z-1; [b] x-1/2, y-1/2, z; [c] x, y, z-1; [d] x, y, z+1; [e] x, y+1, z; [f] -x, y, -z+1/2; [g] -x+1/2, -y+3/2, -z+1.

[III] Symmetry codes: [a] x-1, -y+1/2, z-1/2; [b] -x, y+1/2, -z+1/2; [c] -x, -y+1, -z+1; [d] -x, y-1/2, -z+1/2; [e] -y+1/2, z-1/2; [f] x-1, y-1, z; [g] -x-1, y-1/2, -z+1/2; [h] -x, -y, -z+1; [i] -x+1, y+1/2, -z+1/2; [j] x+1, y, z.

[IV] Symmetry codes: [a] x-1, y-1, z; [b] -y, z-1/2; [c] -x+1/2, -y+1/2, -z+1; [d] x+1/2, y-1/2, z+1; [e] -x, y, -z+1/2; [f] x, -y, z+1/2.

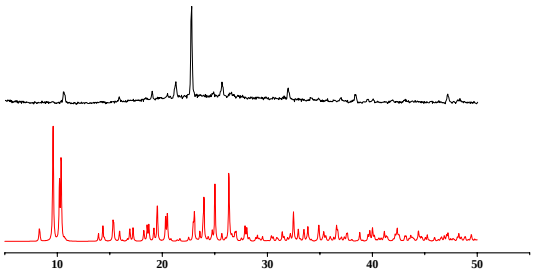
[V] Symmetry codes: [a] -x+2, -y+2, -z; [b] -x, -y+1, -z; [c] x, y+1, z-1; [d] x, y, z-1.

[VI] Symmetry codes: [a] -x+1,-y+1,-z; [b]-x+3,-y+2,-z; [c] -x+1,-y,-z+1; [d] -x+1,-y+1,-z+1.



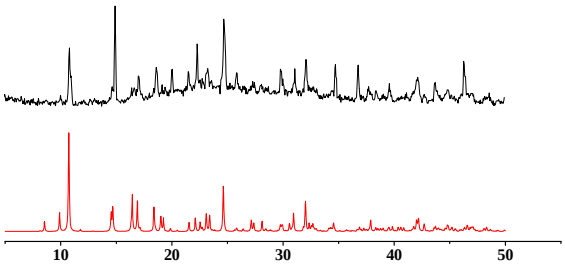
2 theta(deg.)

(a)



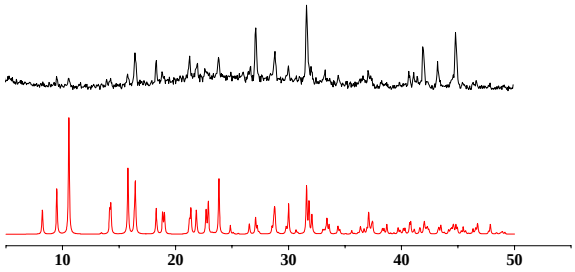
2 theta(deg.)

(b)



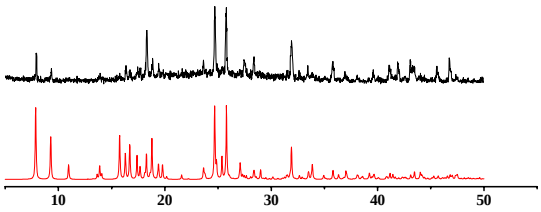
2 theta(deg.)

(c)



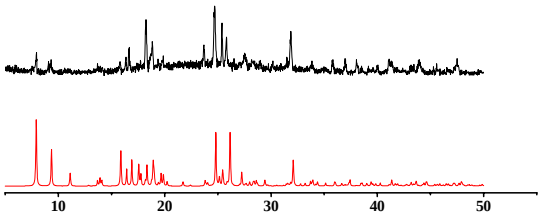
2 theta(deg.)

(d)



2 theta(deg.)

(e)



2 theta(deg.)

(f)

Figure S1 X-ray powder diffraction diagram of complexes **1**-**6** (a-f). Red: simulated figure; black: experimental data.

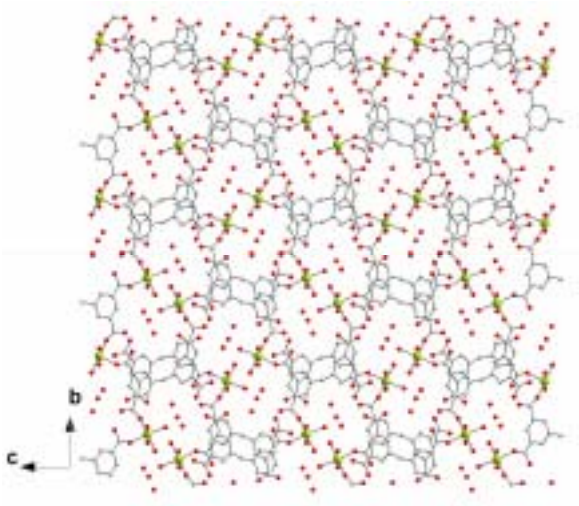
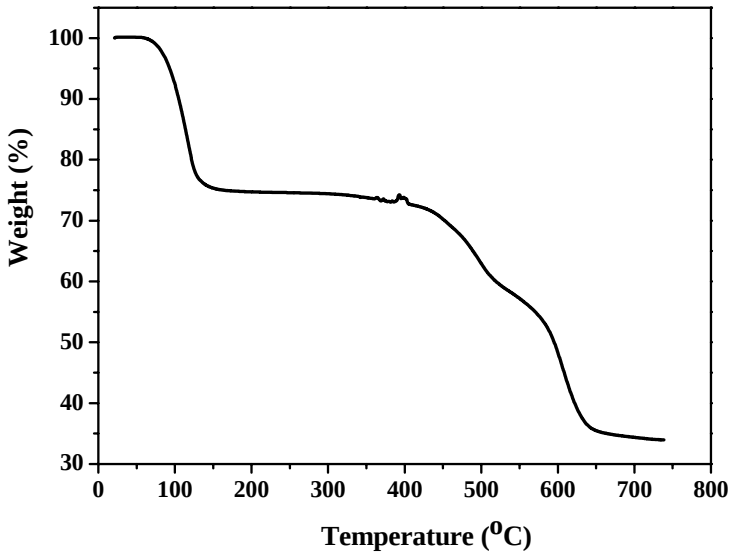
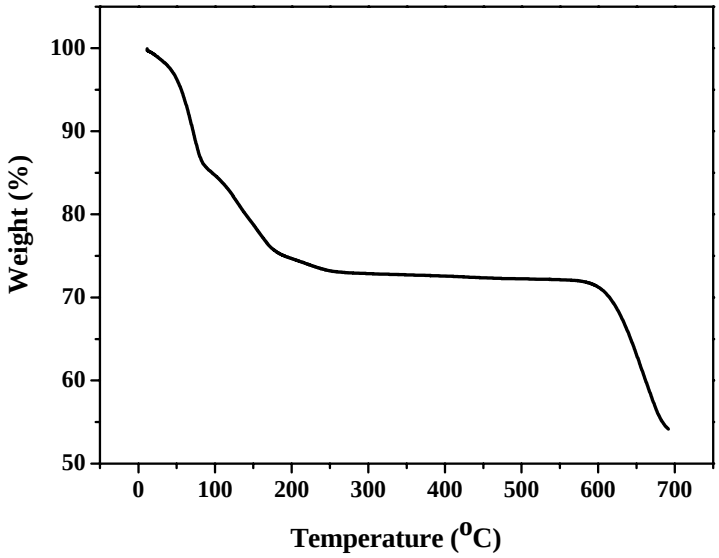


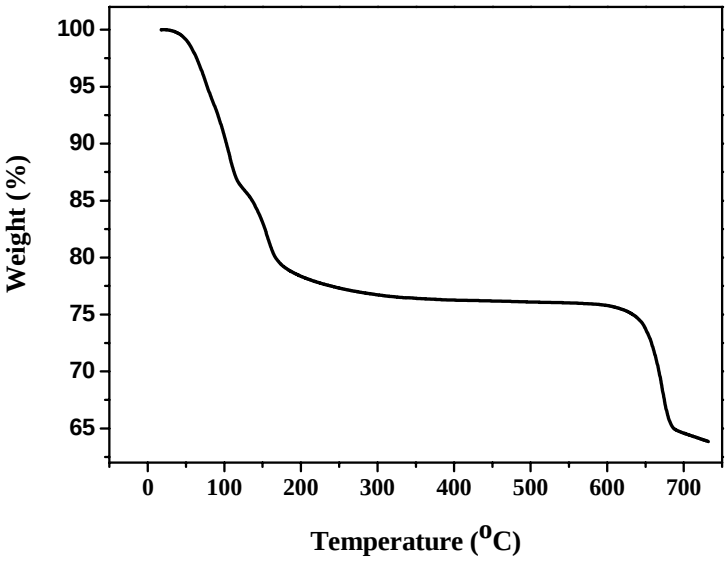
Figure S2 The adjacent layers stacking along *bc* plane of complex **1**.


Weight (%)
100
90
80
70
60
50
40
30
0
100
200
300
400
500
600
700
800
Temperature (°C)

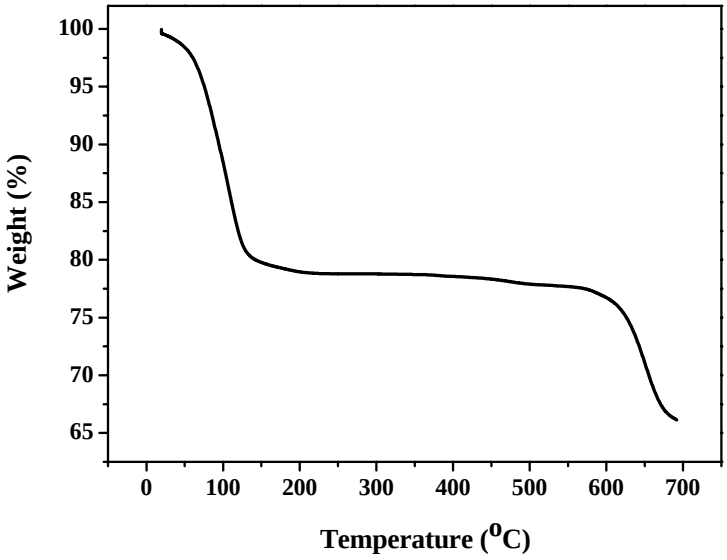
(a)


Weight (%)
100
90
80
70
60
50
0
100
200
300
400
500
600
700
Temperature (°C)

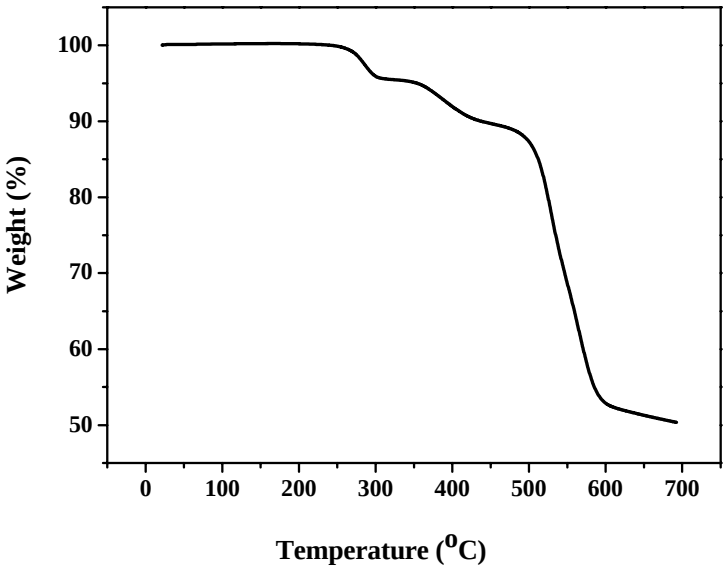
(b)


Weight (%)
100
95
90
85
80
75
70
65
0
100
200
300
400
500
600
700
Temperature (°C)

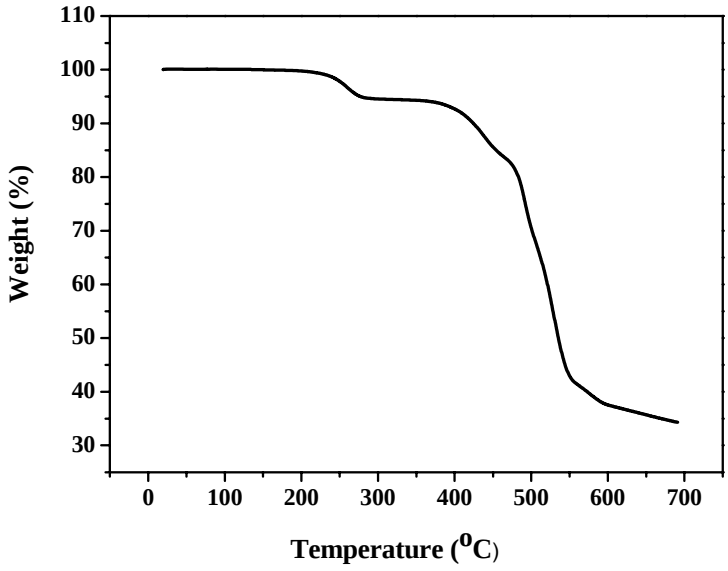
(c)


Weight (%)
100
95
90
85
80
75
70
65
0
100
200
300
400
500
600
700
Temperature (°C)

(d)



(e)



(f)

Figure S3 The TG curves of complexes **1-6** (a-f).