Supporting Information

Title: Identification of a Robust and Reproducible Noncluster-type SBU: Effect of Coexistent Groups on Network Topologies, Helicity and Properties

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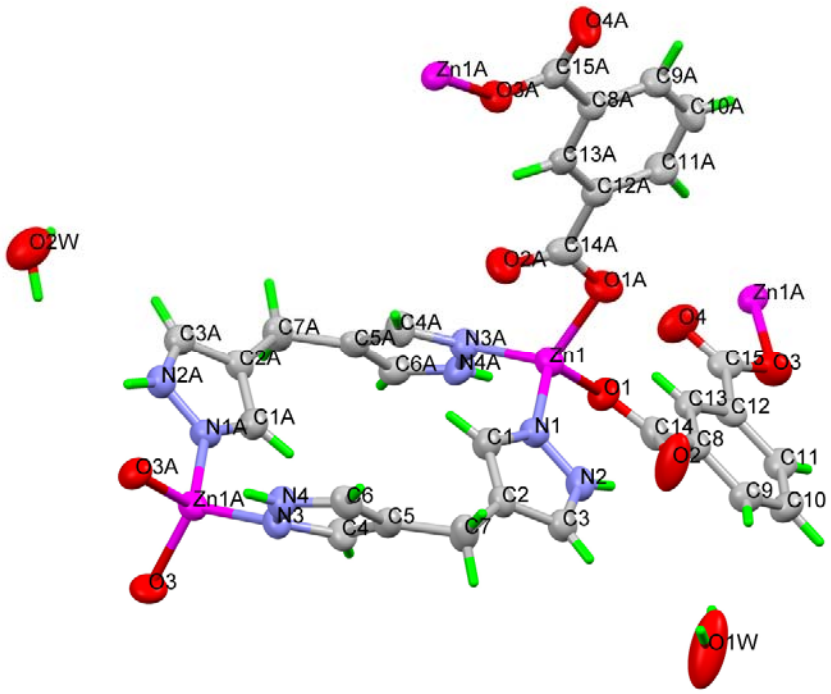


Figure SI-1. The coordination environment around the Zn(II) ion of compound **1.**

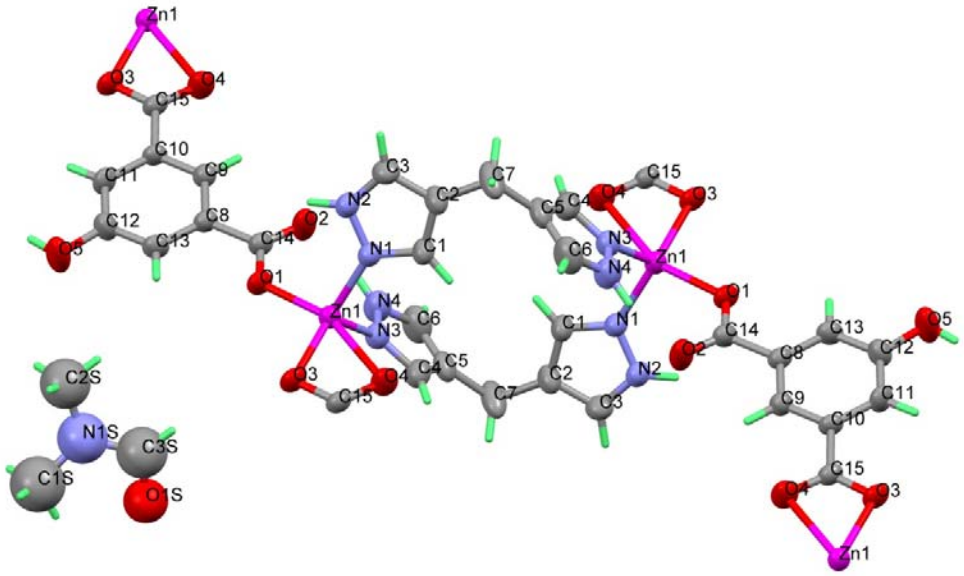


Figure SI-2. The coordination environment around the Zn(II) ion of compound **2.**

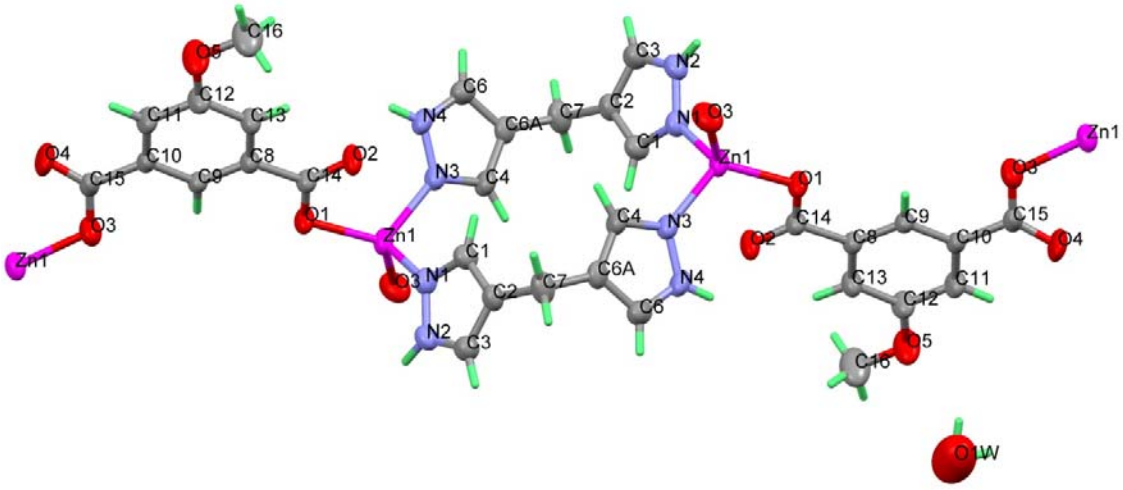


Figure SI-3. The coordination environment around the Zn(II) ion of compound **3.**

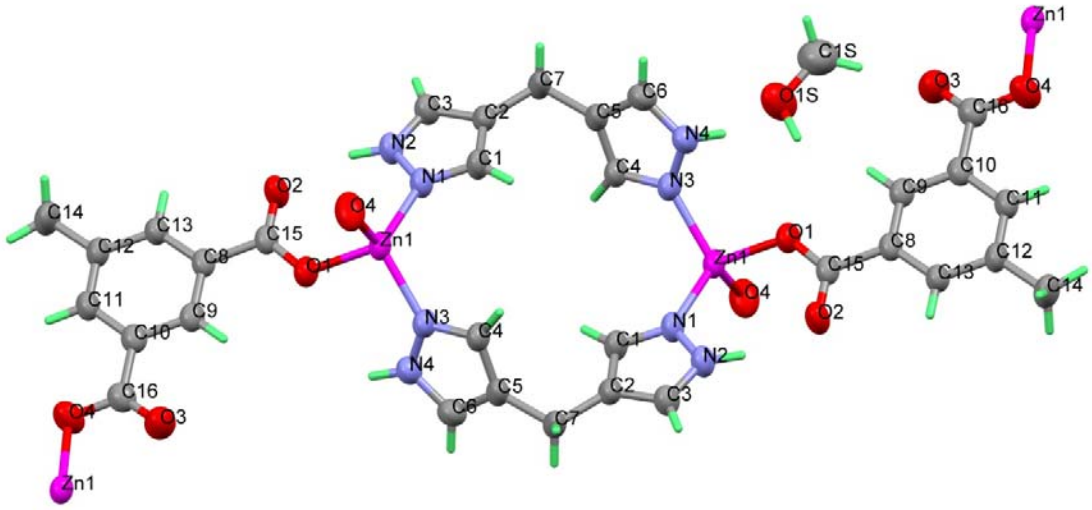


Figure SI-4. The coordination environment around the Zn(II) ion of compound **4.**

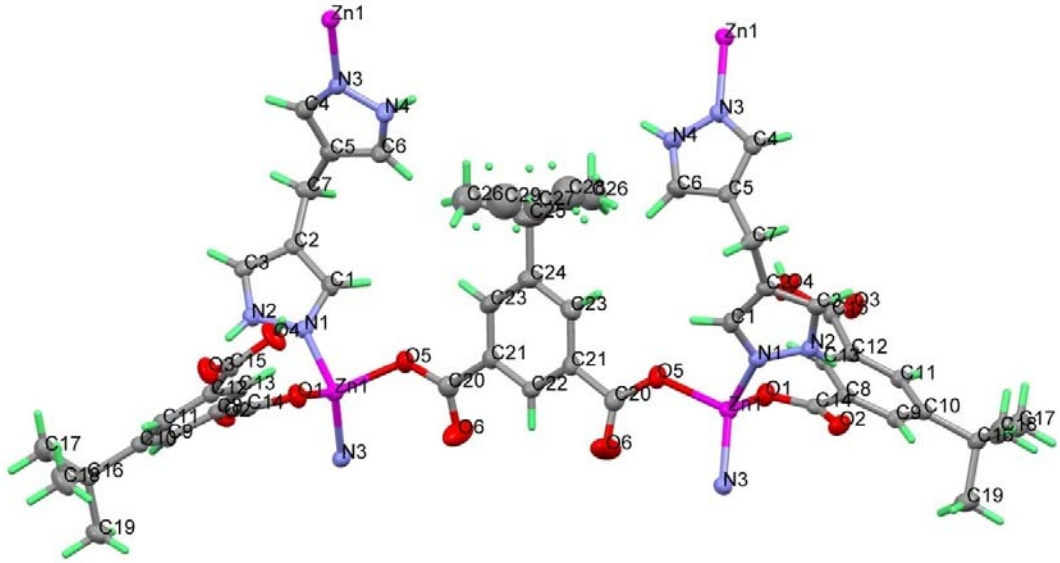


Figure SI-5. The coordination environment around the Zn(II) ion of compound **5.**

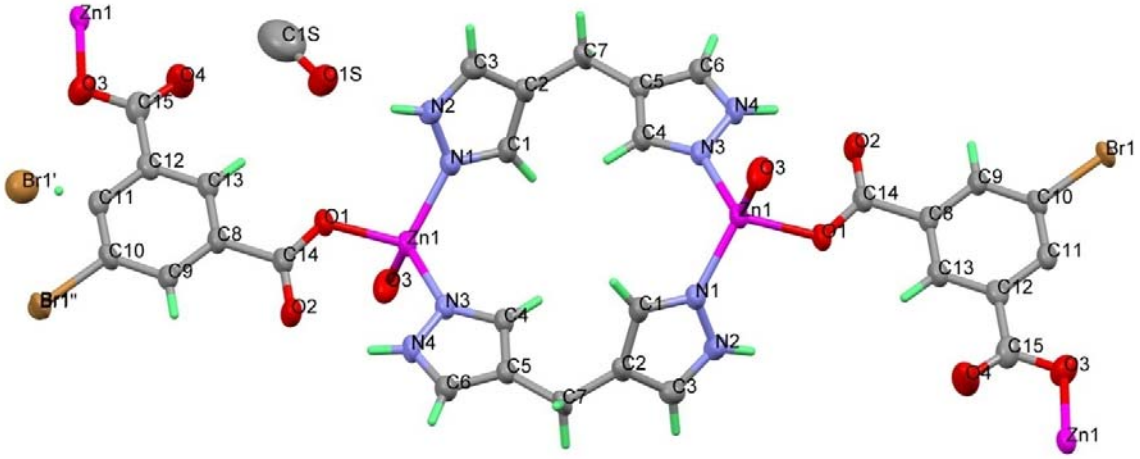


Figure SI-6. The coordination environment around the Zn(II) ion of compound **6.**

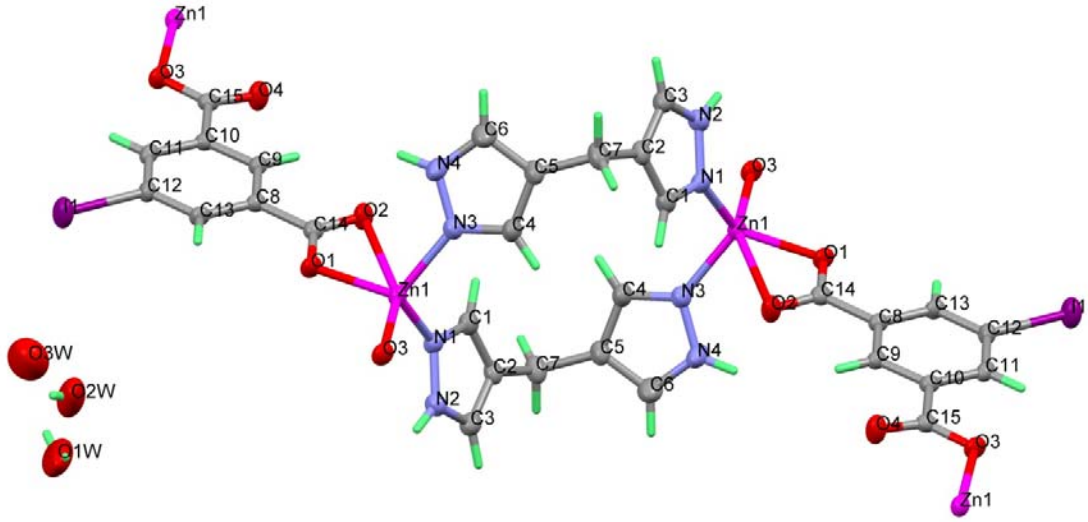


Figure SI-7. The coordination environment around the Zn(II) ion of compound **7.**

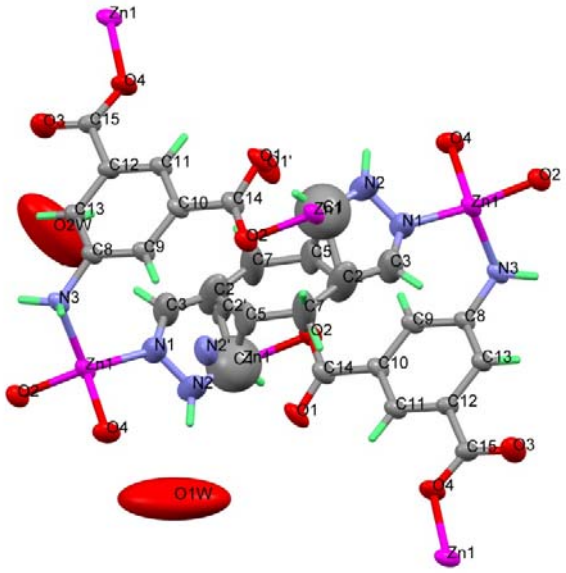


Figure SI-8. The coordination environment around the Zn(II) ion of compound **8.**

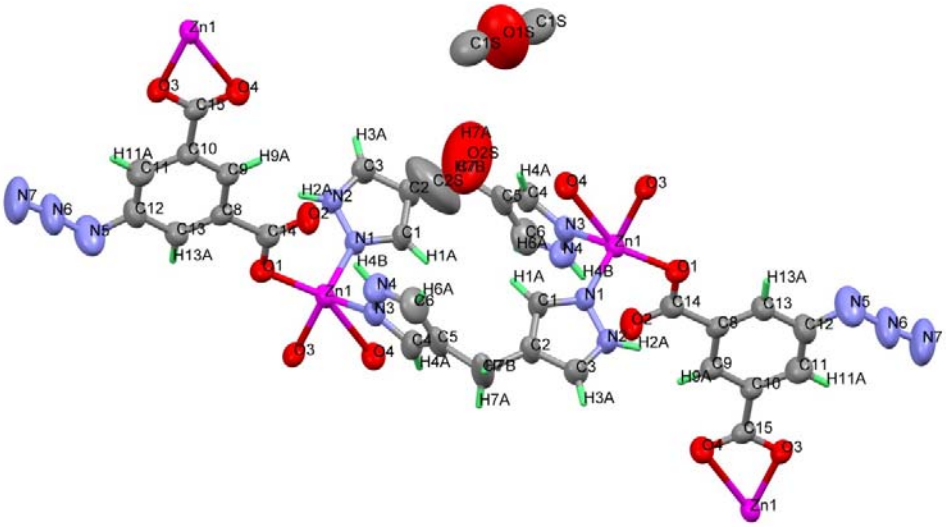


Figure SI-9. The coordination environment around the Zn(II) ion of compound **9.**

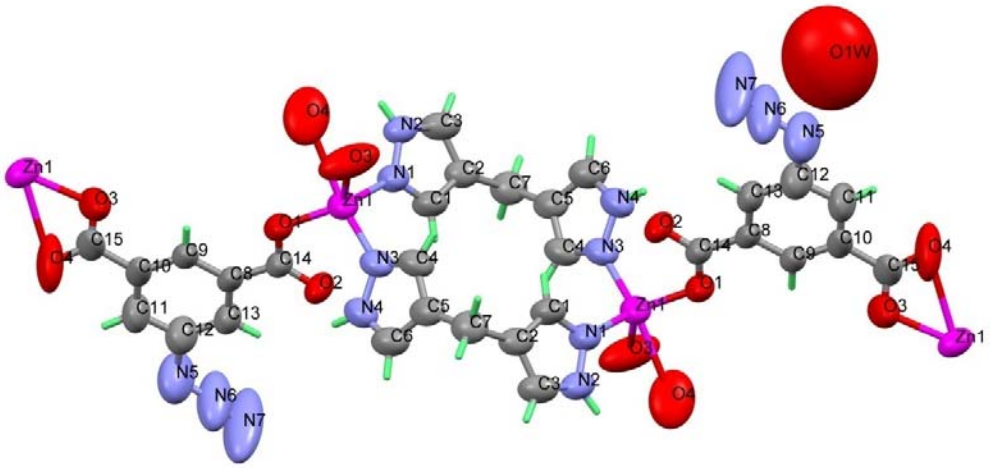


Figure SI-10. The coordination environment around the Zn(II) ion of compound **10.**

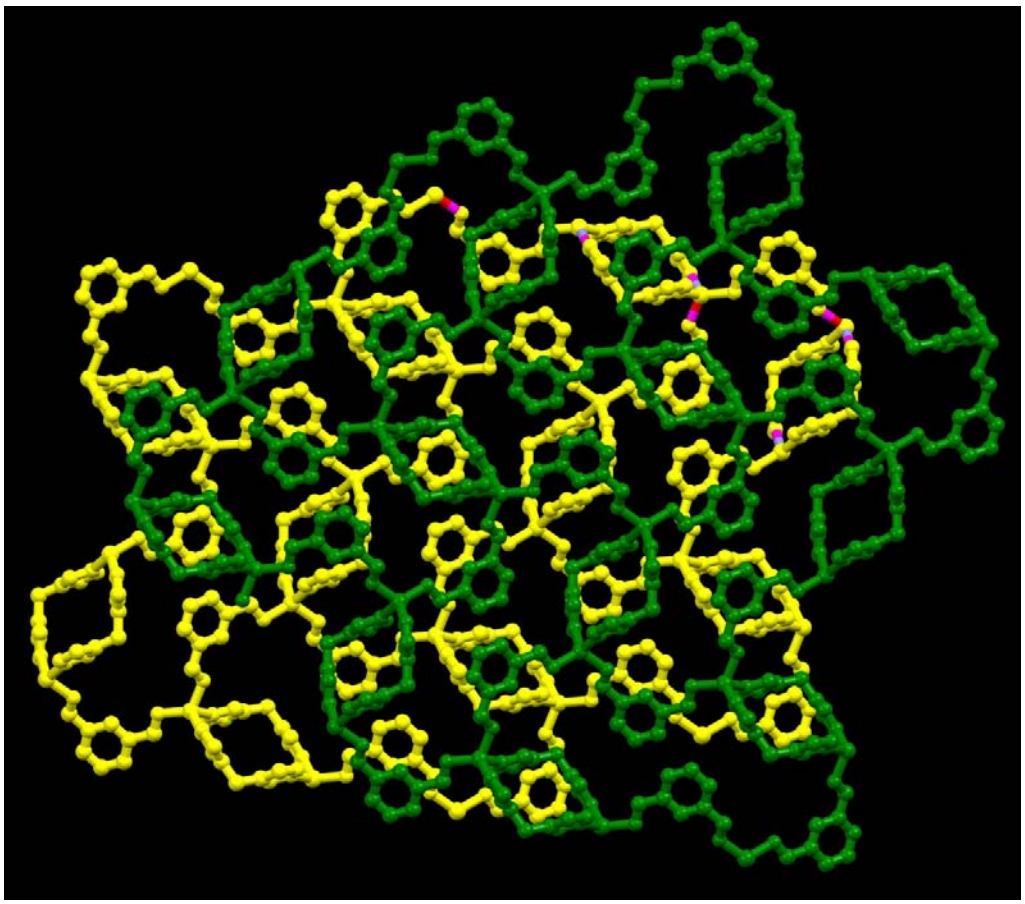


Figure SI-11. Crystal structure of **3** showing off-set stacking 2D grid networks.

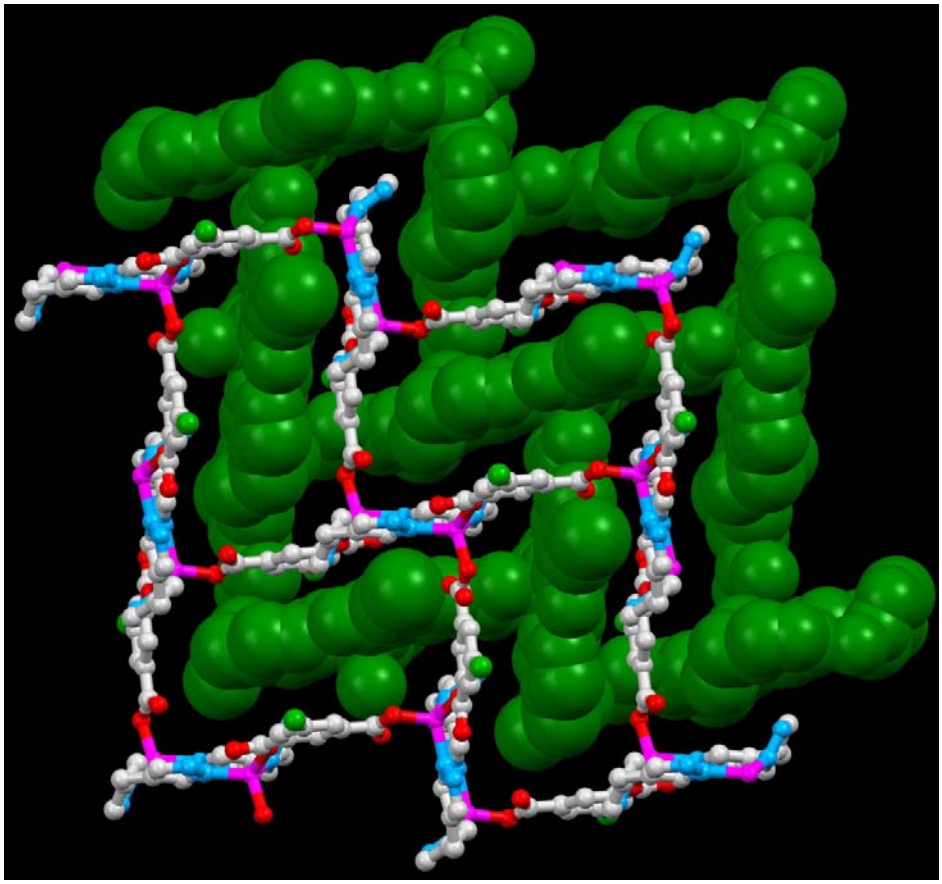
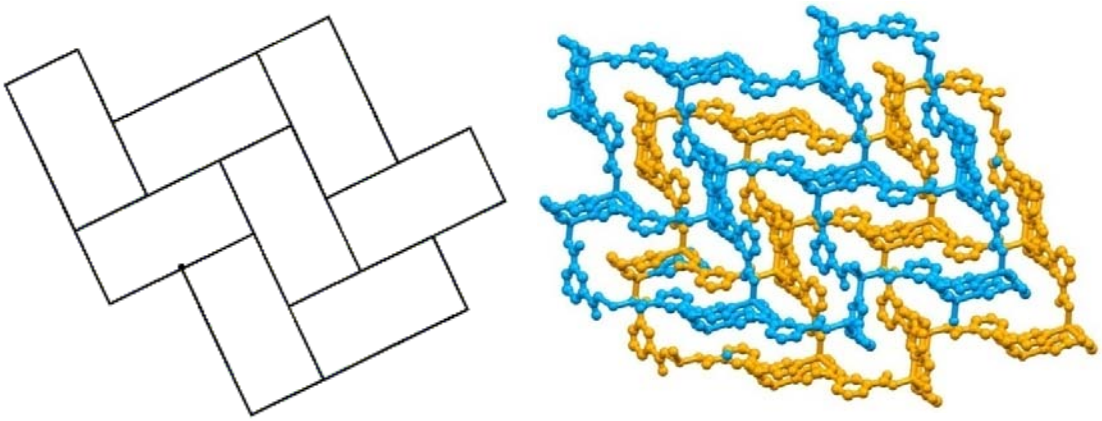


Figure SI-12. Crystal structure of **6** showing off-set stacking 2D grid networks.



a **b**

Figure SI-13. (a) Schematic diagram of 2D grid network and (b) off-set stacking of 2D grid networks of **1**.

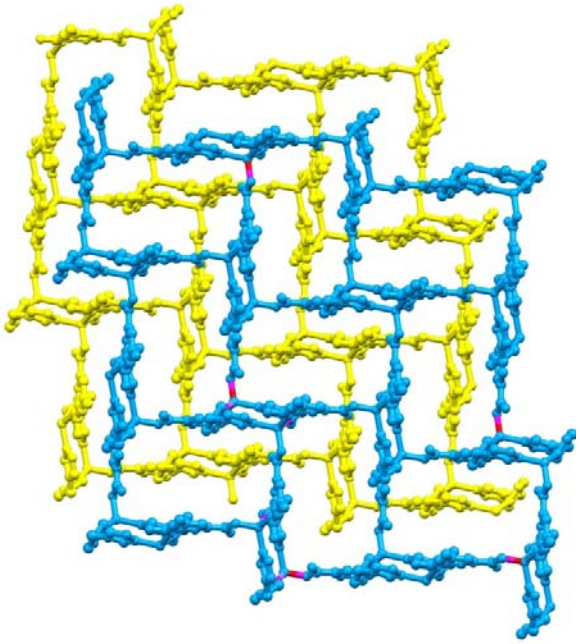


Figure SI-14.Off-set stackings of 2D networks of **4**.

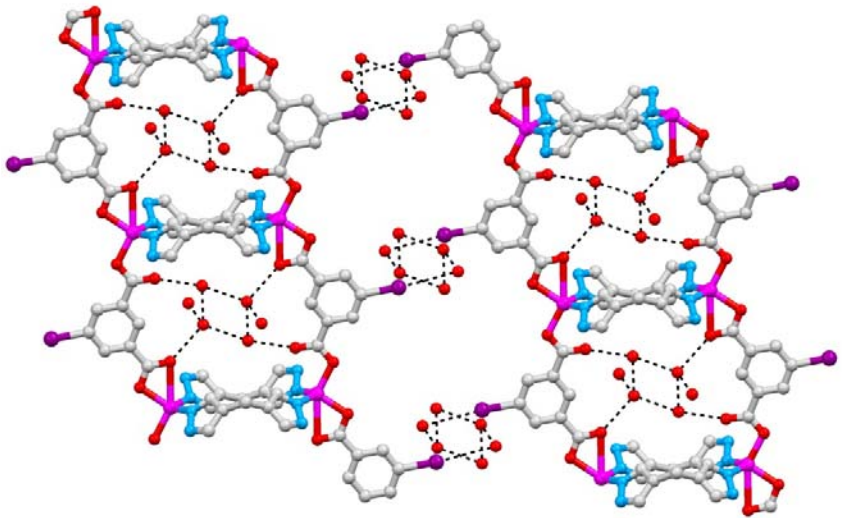
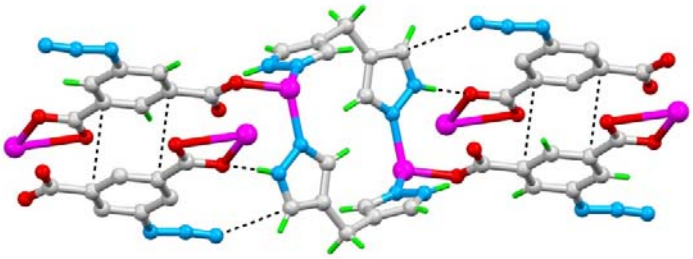
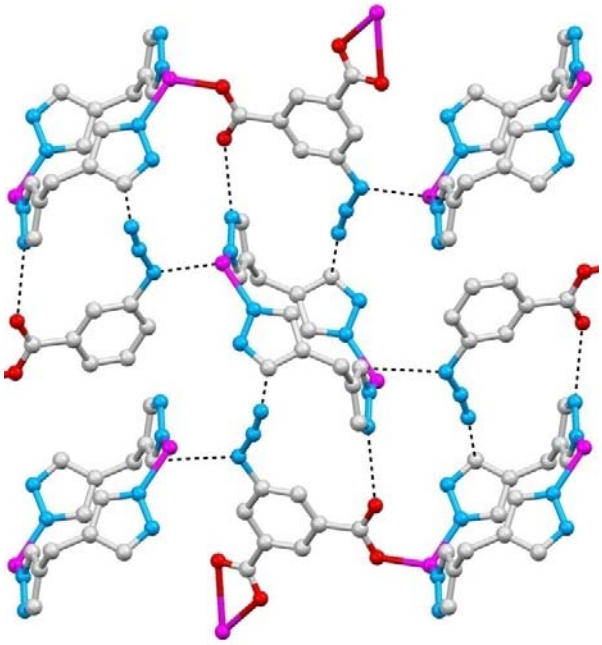


Figure SI-15. Crystal structure of 7 illustrating the role of water cluster in linking the adjacent 1D networks.



a



b

Figure SI-16. a) Crystal structure of **9** showing π-π stacked self-assembly of SBU-I based 1D networks. (b) Crystal structure of **10** showing novel azide-π interactions.

Powder X-ray diffraction pattern

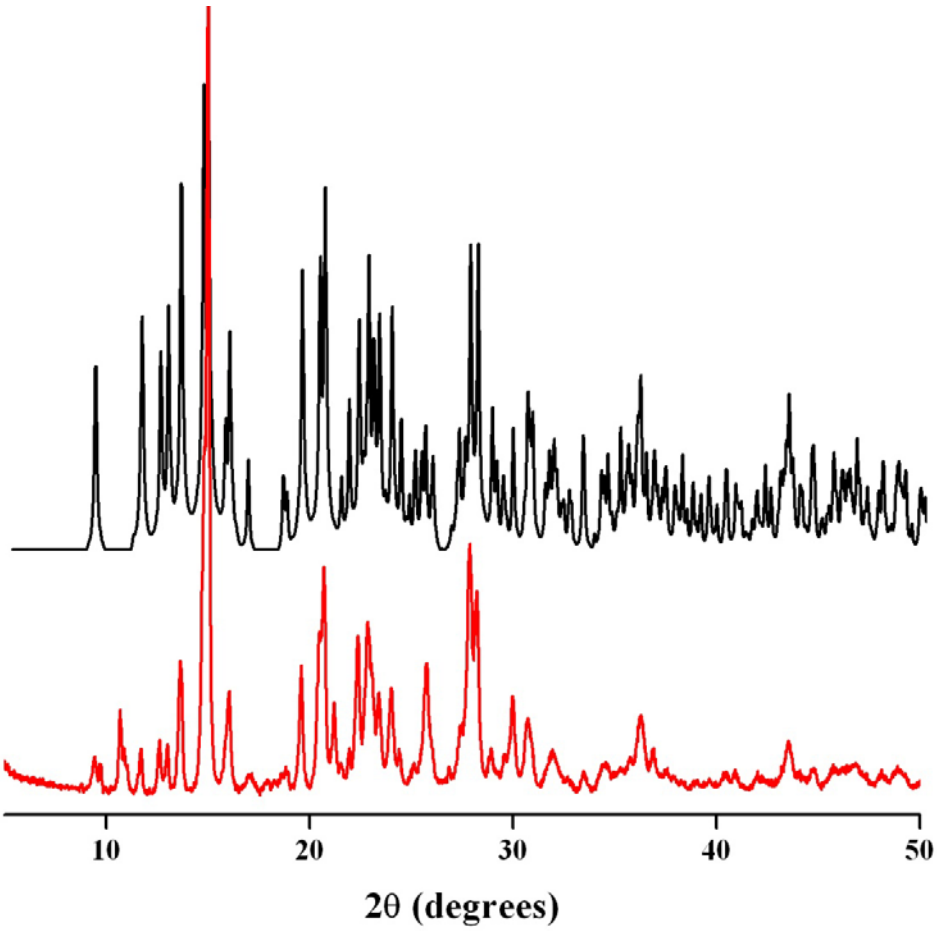


Figure SI-17. Powder XRD pattern of compound **1**, simulated (black), experimental (red).

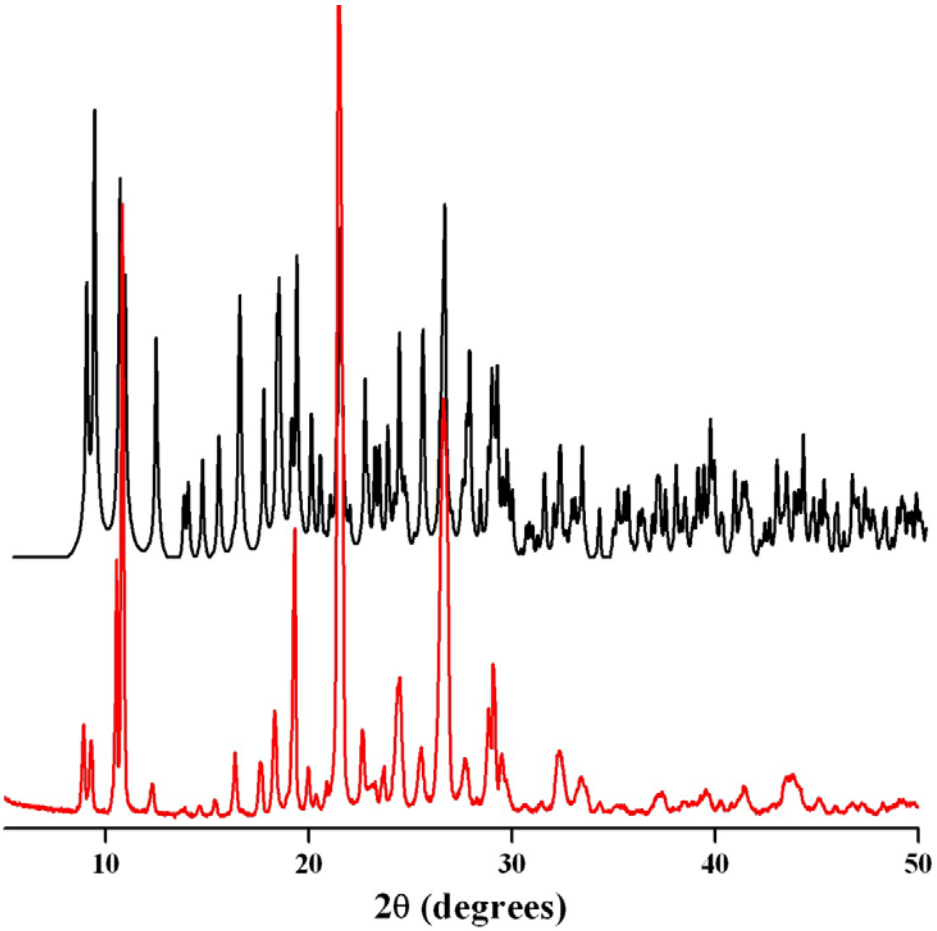


Figure SI-18. Powder XRD pattern of compound **2**, simulated (black), experimental (red).

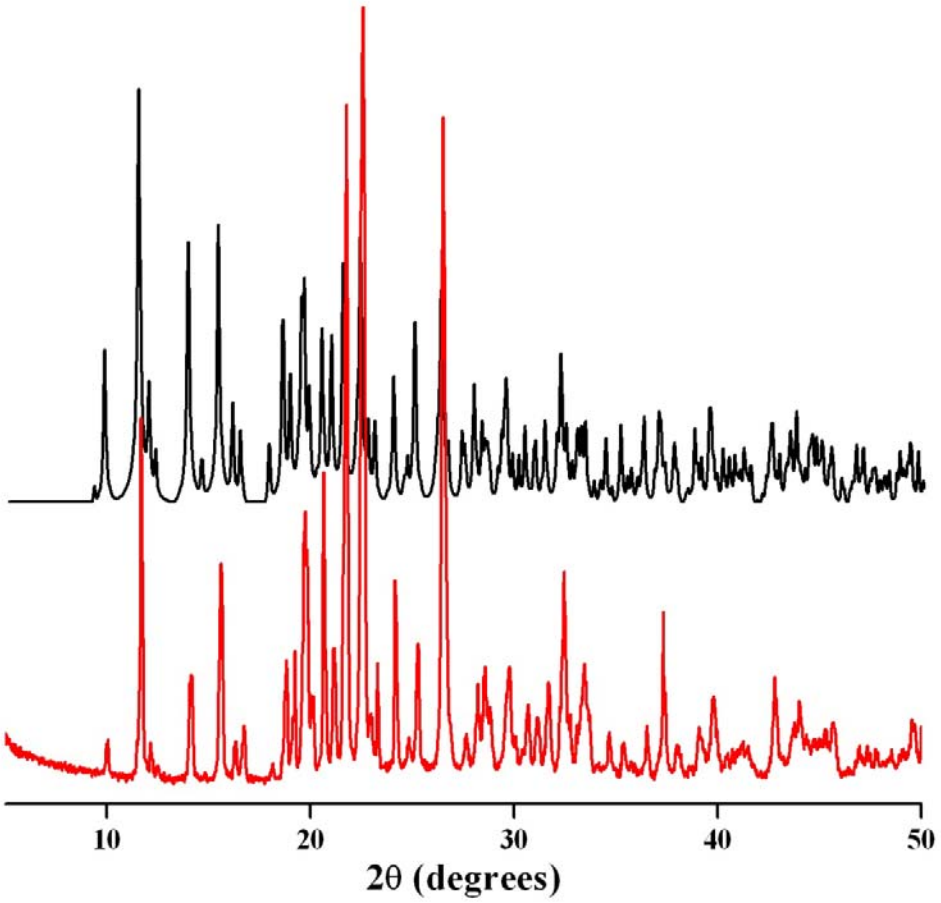


Figure SI-19. Powder XRD pattern of compound **3**, simulated (black), experimental (red)**.**

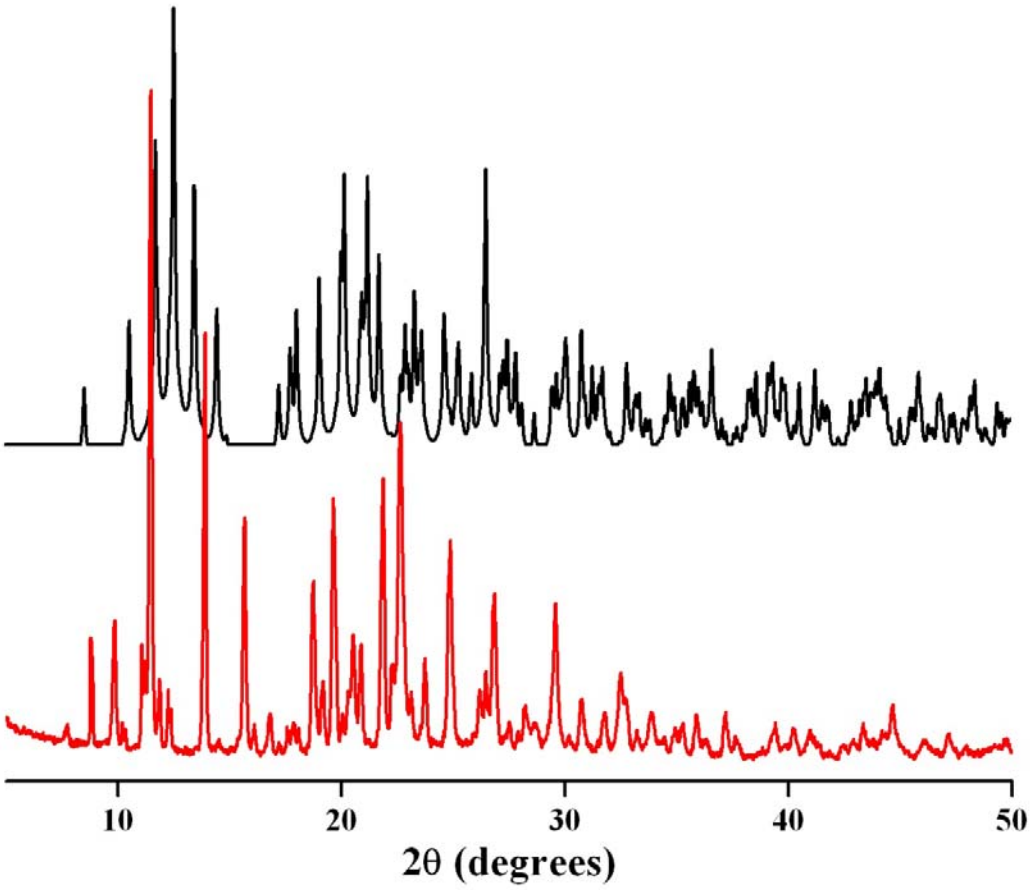


Figure SI-20. Powder XRD pattern of compound **4**, simulated (black), experimental (red)**.**

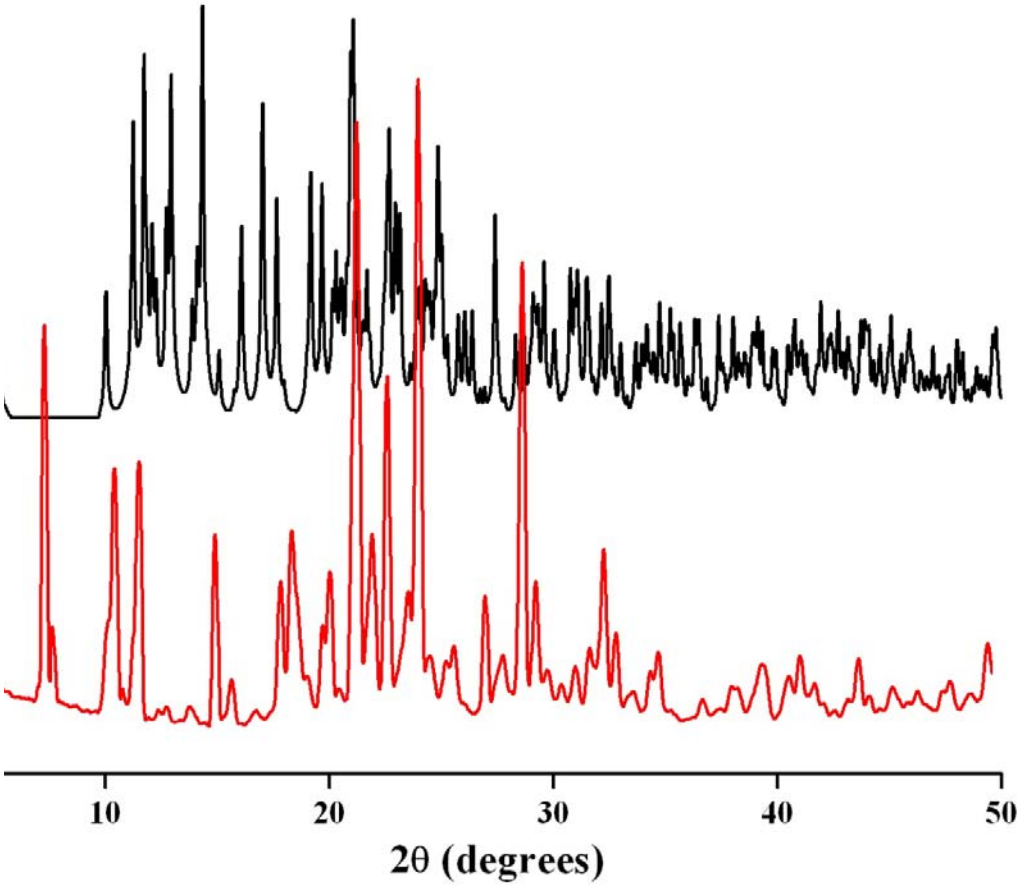


Figure SI-21. Powder XRD pattern of compound **5**, simulated (black), experimental (red)**.**

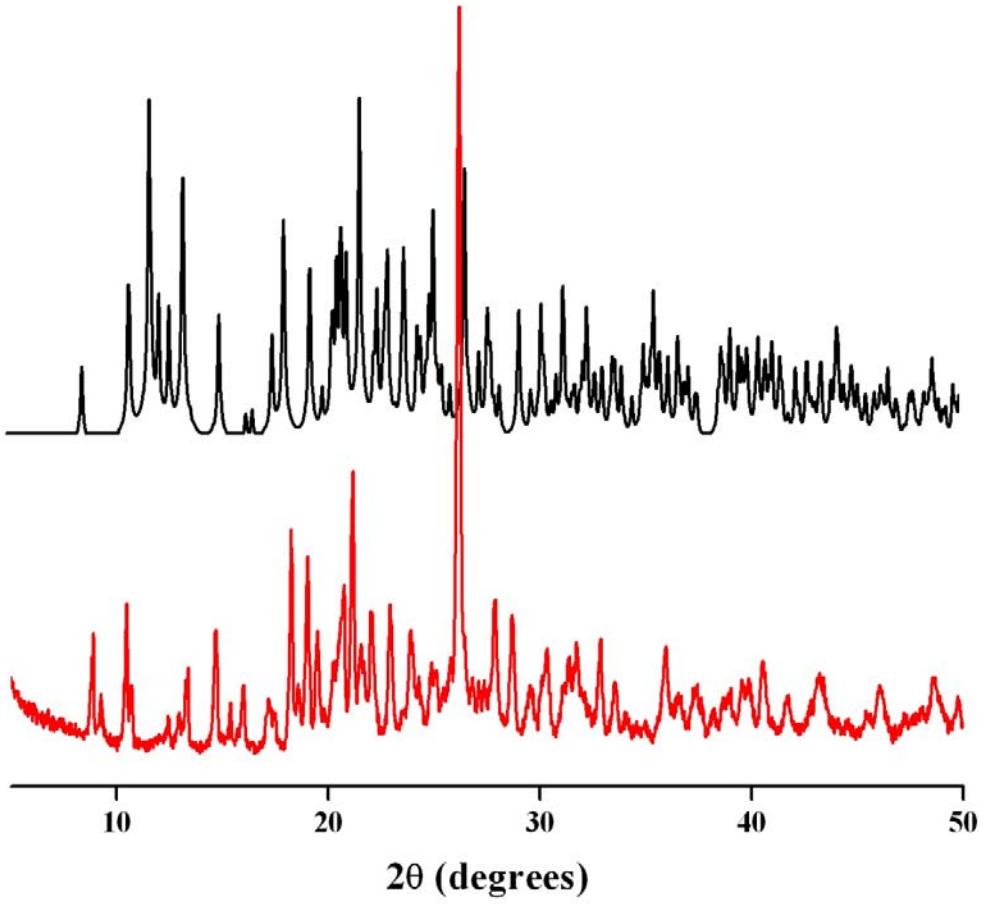


Figure SI-22. Powder XRD pattern of compound **6,** simulated (black), experimental (red)**.**

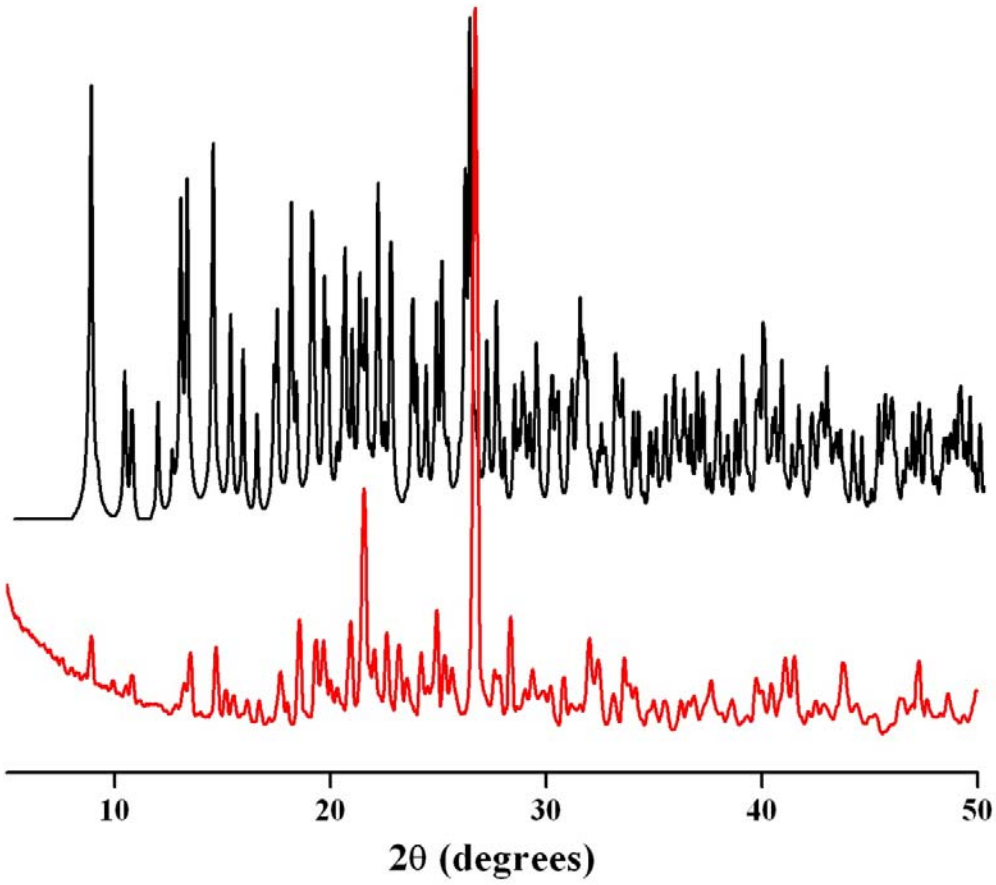


Figure SI-23. Powder XRD pattern of compound **7**, simulated (black), experimental (red)**.**

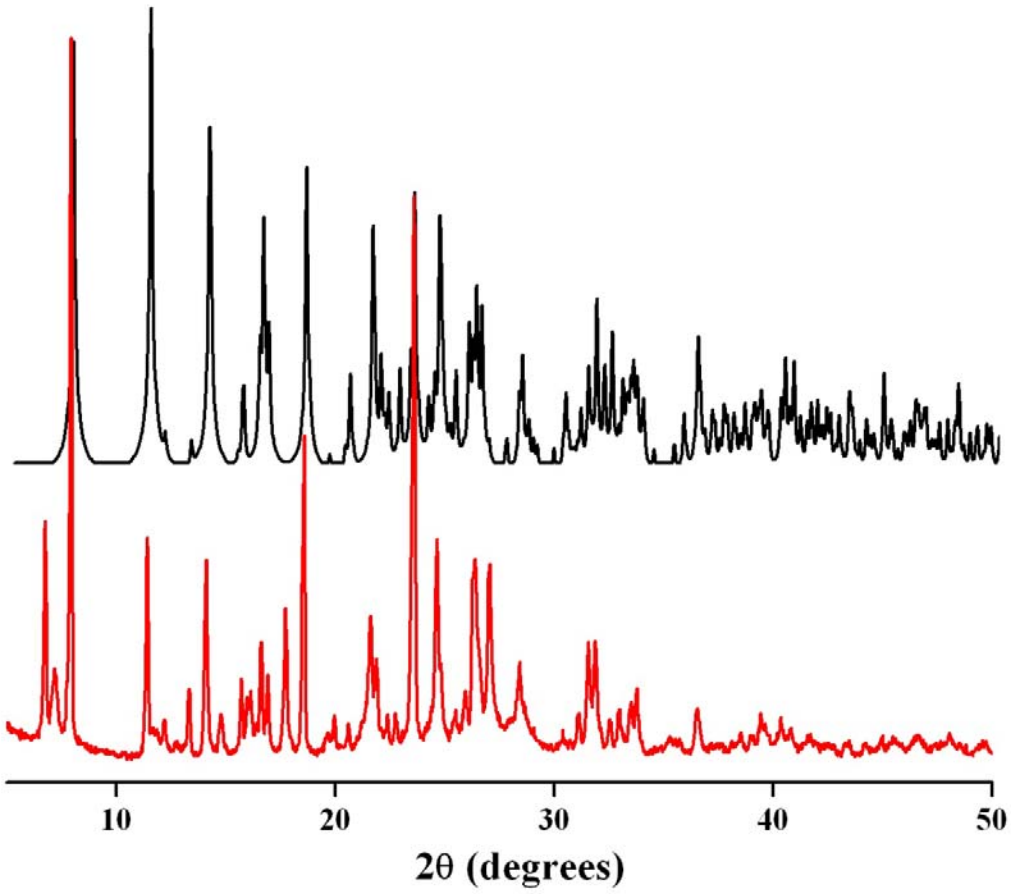


Figure SI-24. Powder XRD pattern of compound **8**, simulated (black), experimental (red)**.**

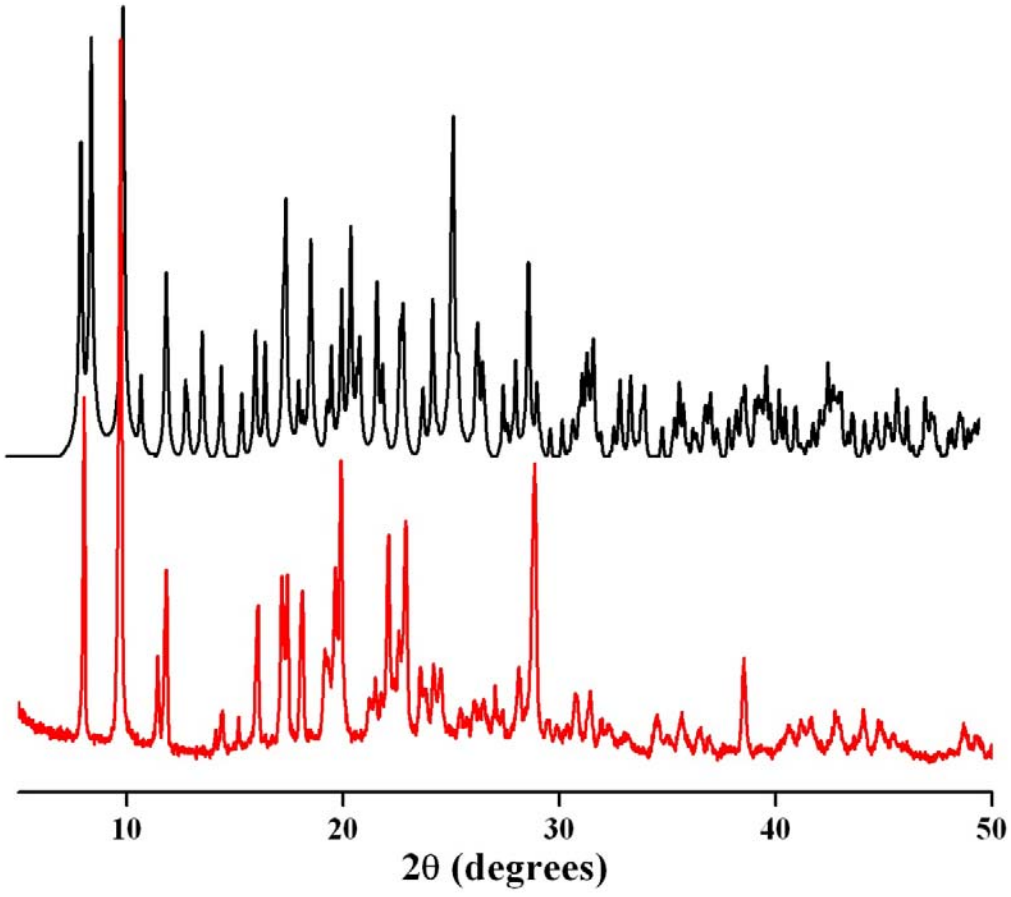


Figure SI-25. Powder XRD pattern of compound **9**, simulated (black), experimental (red)**.**

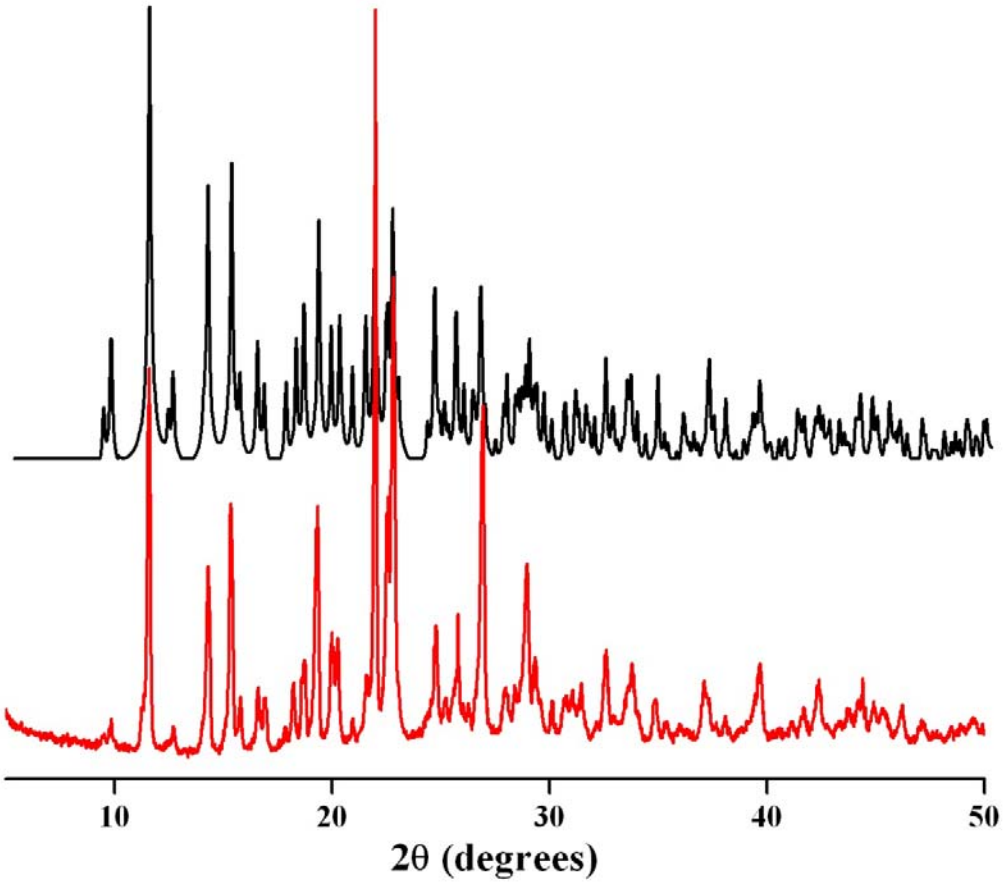
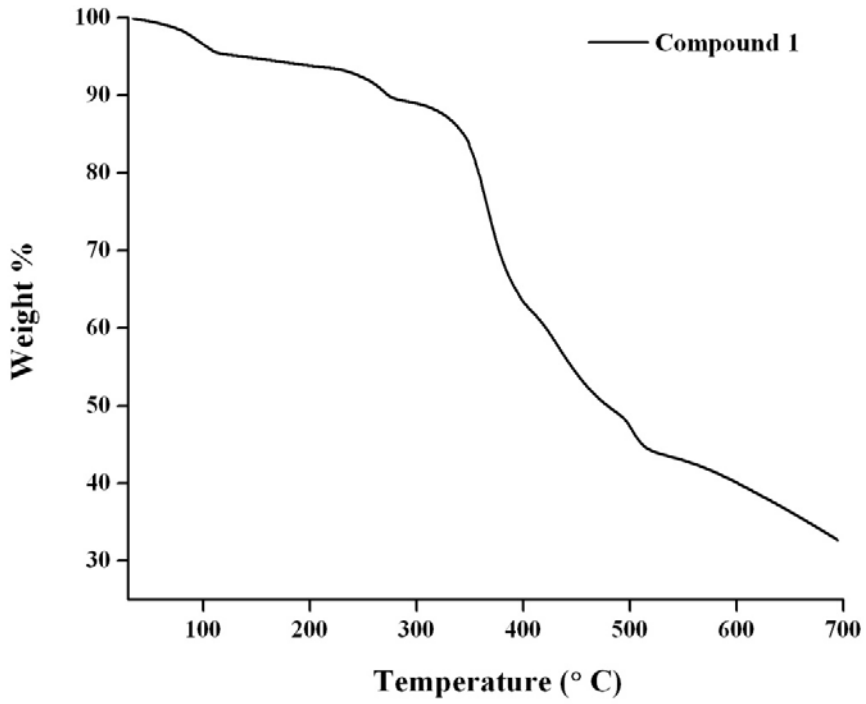
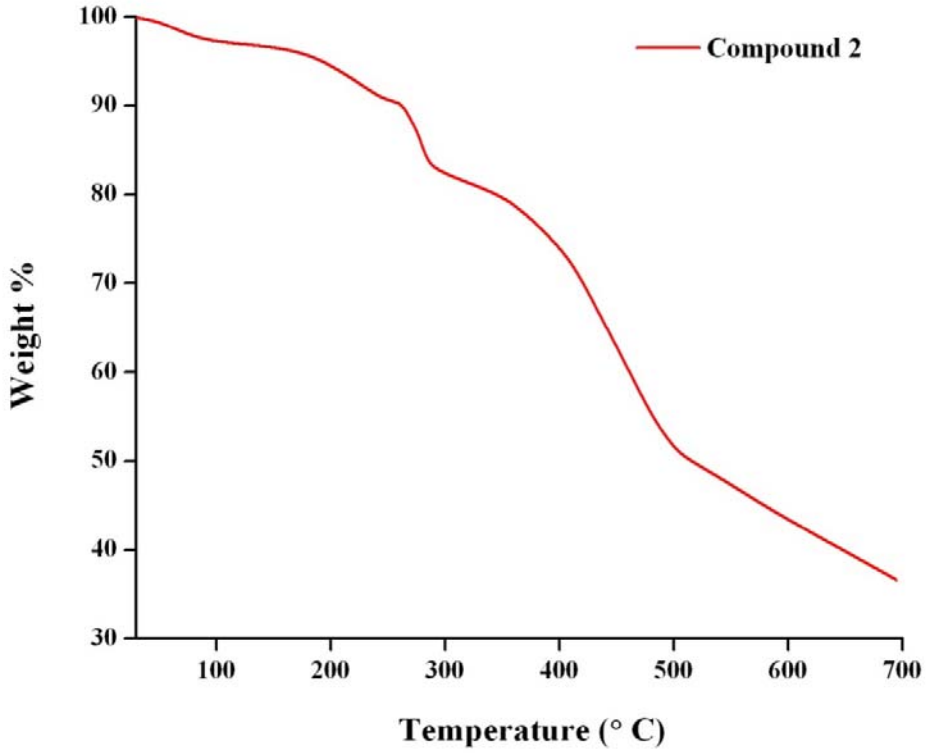
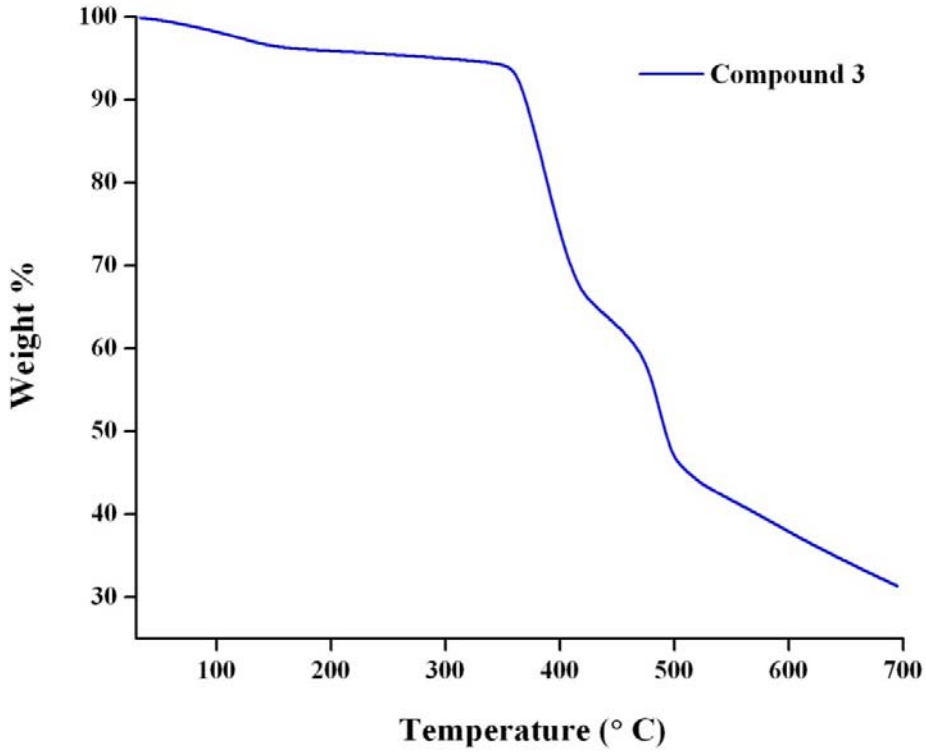
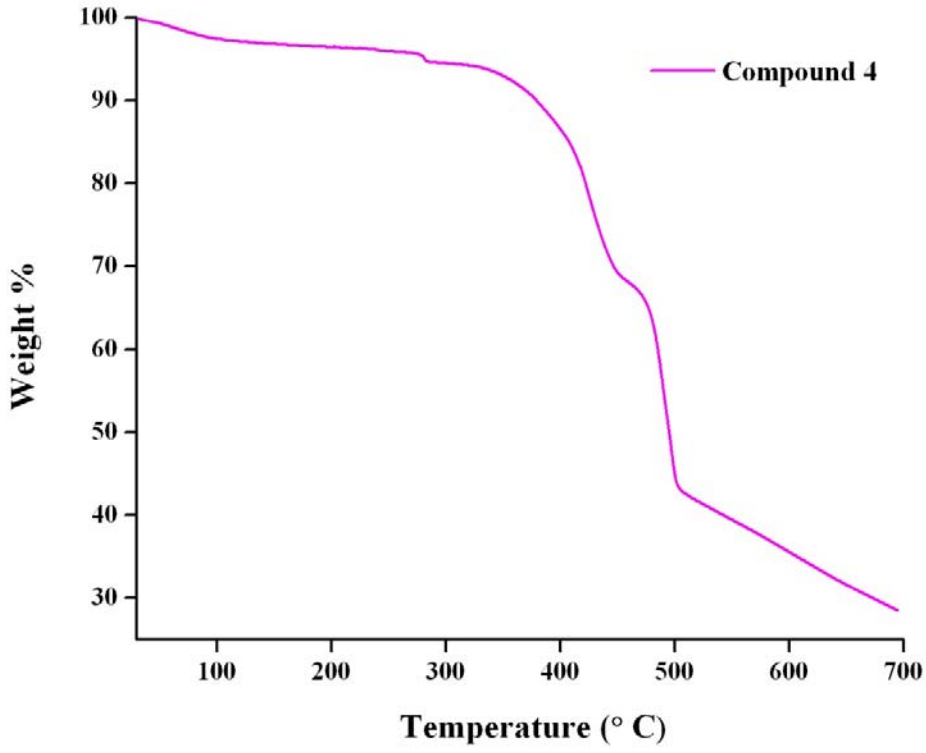


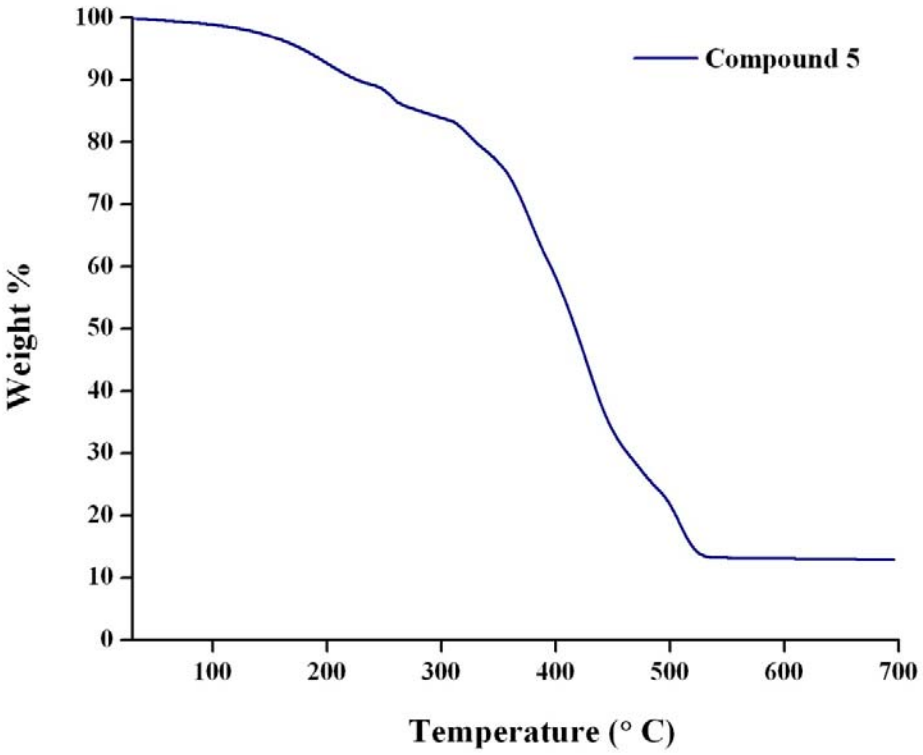
Figure SI-26. Powder XRD pattern of compound **10**, simulated (black), experimental (red)**.**

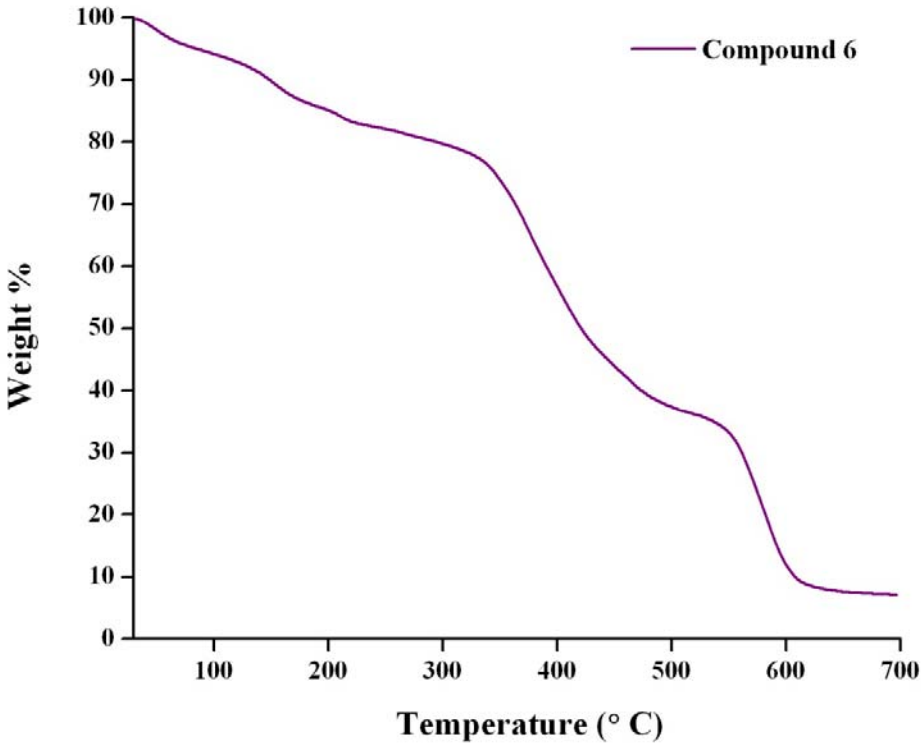


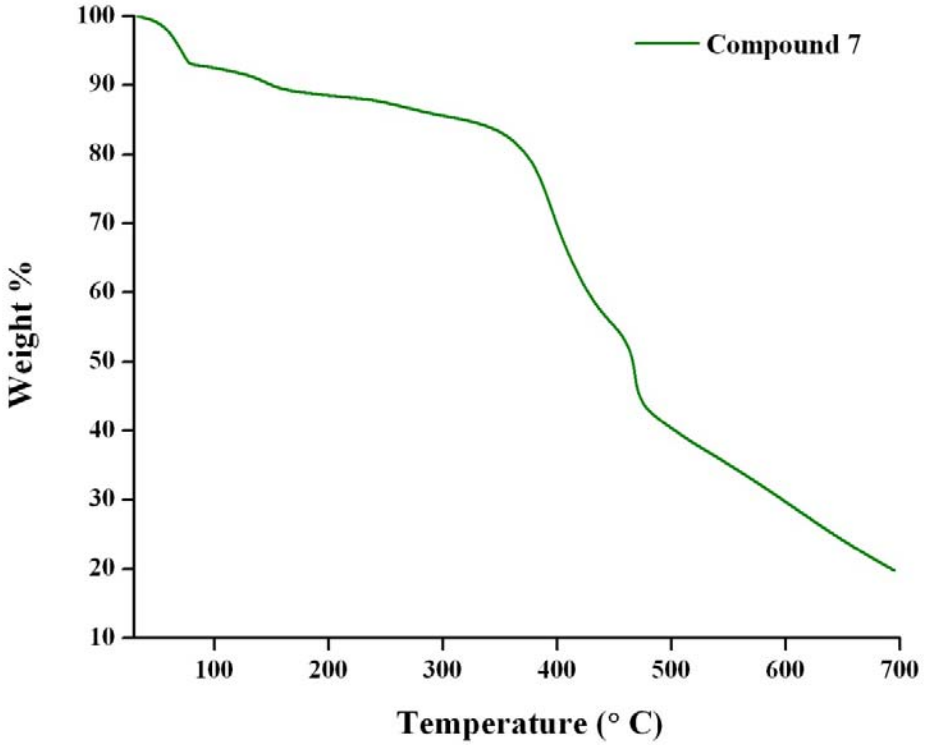


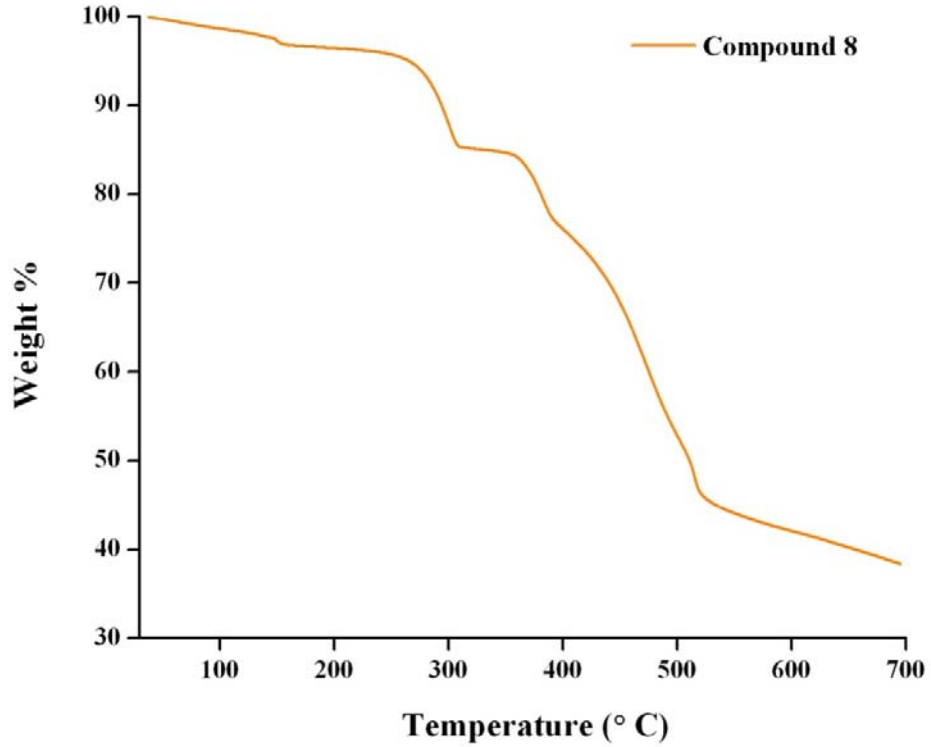












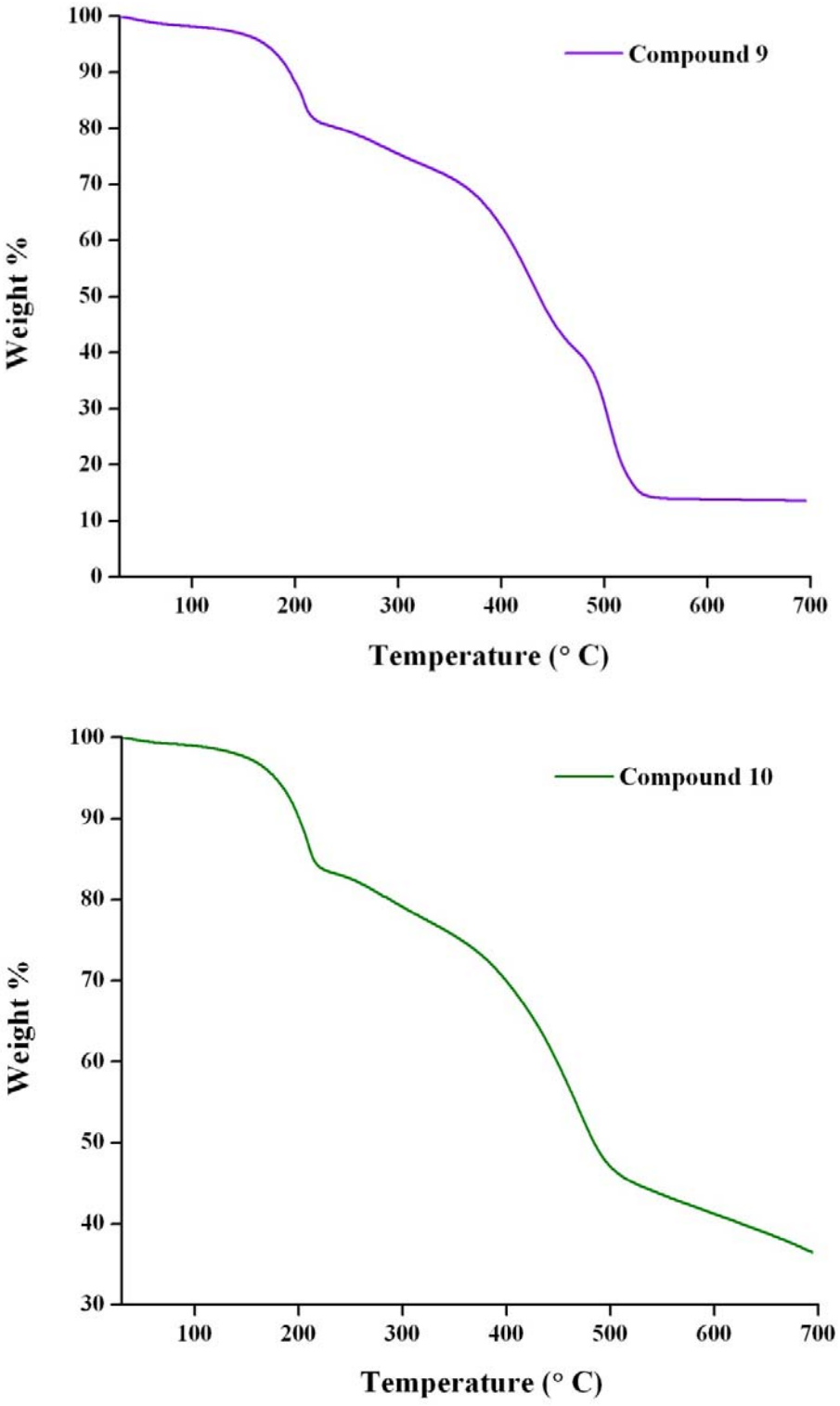


Figure SI-27. TGA plots of compound **1-10** (from top to bottom)**.**

Table SI-1: Selected Bond Lengths (A^{o}) and Angles (^{o}) for Compounds **1-6.**

Compound 1

Zn_1-O_{1A}	1.959(3)	O_{1A}-Zn_1-O_1	104.17(13)
Zn_1-O_1	1.965(2)	O_{1A}-Zn_1-N_{3A}	121.50(15)
Zn_1-N_{3A}	2.005(3)	O_1-Zn_1-N_{3A}	94.31(11)
Zn_1-N_1	2.010(4)	O_{1A}-Zn_1-N_1	109.50(14)
		O_1-Zn_1-N_1	113.82(14)
		N_{3A}-Zn_1-N_1	112.39(14)

Compound 2

Zn_1-O_1	1.976(2)	N_1-Zn_1-N_3	107.05(13)
Zn_1-N_1	2.022(3)	O_1-Zn_1-O_3	96.17(11)
Zn_1-N_3	2.037(3)	N_1-Zn_1-O_3	118.99(13)
Zn_1-O_3	2.062(3)	N_3-Zn_1-O_3	119.61(12)
Zn_1-O_4	2.326(3)	O_1-Zn_1-O_4	155.38(11)
O_1-Zn_1-N_1	104.50(12)	N_1-Zn_1-O_4	89.75(12)
O_1-Zn_1-N_3	108.36(13)	N_3-Zn_1-O_4	85.78(12)
		O_3-Zn_1-O_4	59.22(10)

Compound 3

Zn_1-O_1	1.9603(9)	O_1-Zn_1-O_3	117.98(5)
Zn_1-O_3	1.9637(11)	O_1-Zn_1-N_1	112.53(5)
Zn_1-N_1	2.0143(14)	O_3-Zn_1-N_1	107.68(5)
Zn_1-N_3	2.0269(13)	O_1-Zn_1-N_3	117.02(5)
		O_3-Zn_1-N_3	91.93(5)
		N_1-Zn_1-N_3	107.59(5)

Compound 4

Zn_1-O_4	1.9380(16)	O_4-Zn_1-O_1	101.19(7)
Zn_1-O_1	1.9475(15)	O_4-Zn_1-N_3	121.39(8)
Zn_1-N_3	2.0037(18)	O_1-Zn_1-N_3	99.29(7)
Zn_1-N_1	2.0130(17)	O_4-Zn_1-N_1	109.71(8)
		O_1-Zn_1-N_1	111.54(7)
		N_3-Zn_1-N_1	112.36(7)

Compound 6

Zn_1-O_3	1.951(3)	O_3-Zn_1-O_1	99.07(13)
Zn_1-O_1	1.954(3)	O_3-Zn_1-N_1	121.82(16)
Zn_1-N_1	1.992(4)	O_1-Zn_1-N_1	103.09(15)
Zn_1-N_3	2.003(3)	O_3-Zn_1-N_3	106.84(15)
		O_1-Zn_1-N_3	111.47(13)
		N_1-Zn_1-N_3	113.39(14)

Compound 5

Zn_1-O_5	1.955(2)	O_5-Zn_1-O_1	103.34(10)
Zn_1-O_1	1.958(2)	O_5-Zn_1-N_1	98.59(10)
Zn_1-N_1	2.008(3)	O_1-Zn_1-N_1	107.51(10)
Zn_1-N_3	2.008(3)	O_5-Zn_1-N_3	112.07(11)
		O_1-Zn_1-N_3	120.25(10)
		N_1-Zn_1-N_3	112.58(11)

Table SI-2: Selected Bond Lengths (A^o) and Angles (^{o}) for Compounds **7-10.**

Compound 7

Zn_1-O_3	1.976(3)	O_3-Zn_1-N_1	108.29(12)
Zn_1-N_1	2.008(3)	O_3-Zn_1-O_1	96.64(11)
Zn_1-O_1	2.011(3)	N_1-Zn_1-O_1	117.28(12)
Zn_1-N_3	2.014(3)	O_3-Zn_1-N_3	109.31(12)
		N_1-Zn_1-N_3	111.96(13)
		O_1-Zn_1-N_3	112.02(12)

Compound 8

Zn_1-O_4	1.939(2)	O_4-Zn_1-O_2	101.63(8)
Zn_1-O_2	1.9779(17)	O_4-Zn_1-N_1	103.26(11)
Zn_1-N_1	2.002(3)	O_2-Zn_1-N_1	124.25(12)
Zn_1-N_3	2.067(2)	O_4-Zn_1-N_3	114.37(10)
		O_2-Zn_1-N_3	103.38(9)
		N_1-Zn_1-N_3	110.12(11)

Compound 9

Zn_1-O_1	1.973(3)	O_1-Zn_1-N_1	107.78(13)
Zn_1-N_1	2.012(3)	O_1-Zn_1-O_3	95.29(11)
Zn_1-O_3	2.027(3)	N_1-Zn_1-O_3	118.11(13)
Zn_1-N_3	2.035(3)	O_1-Zn_1-N_3	112.09(13)
		N_1-Zn_1-N_3	107.49(13)
		O_3-Zn_1-N_3	115.38(13)

Compound 10

Zn_1-O_1	1.945(4)	O_1-Zn_1-N_3	110.68(19)
Zn_1-N_3	1.998(5)	O_1-Zn_1-N_1	114.2(2)
Zn_1-N_1	2.006(5)	N_3-Zn_1-N_1	106.55(19)
Zn_1-O_3	2.056(5)	O_1-Zn_1-O_3	124.5(3)
		N_3-Zn_1-O_3	89.5(2)
		N_1-Zn_1-O_3	107.6(2)

Table SI-3: π-π interactions observed in compounds 1-10

Compound	Cg (I)-Cg (J)	Cg-Cg Distance (Å)	dihedral angle (α)
Compound 1	Cg1 Cg3[1] Cg2 Cg4[2] Cg2 Cg5[2]	3.8633 3.8749 3.9197	73 65 47
Compound 2	Cg1 Cg3[1] Cg1 Cg4[1] Cg2 Cg3 Cg5 Cg5[4]	3.9539 3.9321 3.7119 3.8459	58 45 0 0
Compound 3	Cg1 Cg2[1] Cg1 Cg3[1] Cg3 Cg3[5] Cg4 Cg4[4]	3.9035 3.8545 3.9174 3.8374	66 58 0 0
Compound 4	Cg1 Cg3[1] Cg3 Cg5[4]	3.8277 3.8768	73 13
Compound 5	Cg3 Cg3[6]	3.5657	0
Compound 6	Cg1 Cg3[1] Cg1 Cg4[1] Cg4 Cg5[7]	3.9825 3.7395 3.7246	41 81 8
Compound 7	Cg1 Cg2[1] Cg1 Cg3[1] Cg3 Cg3[8] Cg4 Cg4[9]	3.9452 3.7678 3.5682 3.5692	58 62 0 0
Compound 8	Cg8 Cg8[10]	3.8388	0
Compound 9	Cg1 Cg3[1] Cg1 Cg4[1] Cg4 Cg4[10] Cg5 Cg5[5]	3.9358 3.8863 3.6002 3.7359	59 51 0 0
Compound 10	Cg1 Cg3[1] Cg5 Cg5[11]	3.8597 3.6700	74 0

(1) X,Y,Z; (2) 2-X,-1/2+Y,1-Z (3) 1-X,2-Y,-Z; (4) 1-X,1-Y,1-Z; (5) 1-X,-Y,1-Z; (6) -X,1-Y,-Z; (7) 2-X,-Y,-Z; (8) -X,-Y,-Z; (9) -X,1-Y,1-Z; (10) 1-X,1-Y,-Z; (11) 1-X,-Y,-Z

I and J denote ring numbers between which Cg-Cg distance is calculated

Table SI-4: Hydrogen bonding interactions in compounds 1-10

Compound	Donor --- H....Acceptor	D - H	H...A	D...A	D - H...A
Compound 1	O2W --H2WA ..O4A[1]	0.95	2.03	2.9728	173
	N2A --H22A ..O4A[2]	0.90	1.80	2.7043	174
	N4A --H44A ..O1	0.68	2.55	2.9723	122
	N4A --H44A ..O2W[3]	0.68	2.25	2.8100	140
	N2 --H222 ..O2	0.73	2.01	2.6909	156
	N4 --H444 ..O1W[4]	0.78	2.23	2.8567	137
Compound 2	O5 --H5 ..O1S[5]	0.75	1.89	2.6304	173
	N2 --H222 ..O3[6]	0.89	1.96	2.8400	169
	N4 --H444 ..O2	0.88	1.94	2.7431	152
Compound 3	O1W --H1WA ..O5[6]	0.93	2.50	3.0107	115
	N2 --H222 ..O2[7]	0.87	2.03	2.8252.	151
	N4 --H444 ..O4[6]	0.82	1.91	2.6991	162
Compound 4	O1S --H1S ..O2[6]	1.06	1.74	2.7658	162
	N2 --H222 ..O2	0.88	1.90	2.7381	158
	N4 --H444 ..O1S	0.92	1.88	2.7511	158
Compound 5	O 4 --H44 ..O2[8]	0.77	1.98	2.7234	161
	N 2 --H222 ..O2	0.82	2.39	3.0601	140
	N 2 --H222 ..O3[9]	0.82	2.24	2.8620	133
	N 4 --H444 ..O6	0.87	1.80	2.6409	162
Compound 6	N2 --H2A ..O1S	0.86	1.91	2.7562	166
	N4 --H4B ..O2	0.86	1.97	2.7594	151
Compound 7	O1W --H1WA ..O3W[10]	0.66	2.33	2.5790	104
	N2 --H2A ..O1[11]	0.86	2.03	2.8851	172
	O2W --H2WB ..O3W	0.80	2.09	2.6443	126
	O2W --H2WA ..O3W[10]	0.83	2.23	2.7946	126
	N4 --H4B ..O1W[12]	0.86	2.00	2.8305	162
Compound 8	O2W --H2WB ..O1W[13]	1.01	2.56	2.9843	105
	O2W --H2WA ..O1W[13]	1.02	2.48	2.9843	110
	N2 --H2A ..O1W[13]	0.86	1.89	2.7233	163
	N3 --H3AB ..O3[14]	0.92	2.14	3.0261	161
	N3 --H3AA ..O2[15]	0.83	2.27	3.0709	163
Compound 9	N(2) --H(2A) ..O(3)[16]	0.86	2.01	2.8522	166
	N(4) --H(4B) ..O(2)	0.86	2.10	2.7795	135
Compound 10	O1W --H1WA ..O3	1.02	2.52	3.5231	167
	N2 --H2A ..O2[7]	0.86	2.04	2.8648	160
	N4 --H4B ..O2	0.86	2.60	3.1031	119
	N4 --H4B ..O4[14]	0.86	1.94	2.7394	155

(1) -x,1/2+y,1-z; (2) 1-x,1/2+y,2-z; (3) 1+x,y,z; (4) x,y,1+z; (5) 2-x,1-y,1-z; (6) 1-x,1-y,1-z; (7) x,1/2-y,-1/2+z; (8) -1/2+x,1/2+y,z; (9) -x,1-y,-z; (10) 1-x,1-y,-z; (11) -x,-y,1-z; (12) -1+x,y,z; (13) 1/2-x,-1/2+y,1/2-z; (14) 1-x,-y,-z; (15) 3/2-x,-1/2+y,1/2-z; (16) 1-x,-y,1-z.