Supplementary Material (ESI) for New Journal of Chemistry

Coordination polymers of various architectures built with mixed imidazole/benzimidazole and carboxylate donor ligands and different metal ions: syntheses, structural features and magnetic properties

Arshad Aijaz[a] , Prem Lama[a], E. Carolina Sañudo[b], Rupali Mishra[a], Parimal K. Bharadwaj[a*]

[a]Chemistry Department, Indian Institute of Technology Kanpur, 208016, India, E-mail: pkb@iitk.ac.in
[b]Departament de Química Inorgànica. Universitat de Barcelona
Diagonal, 647, 08028-Barcelona – Spain

Supporting Informations

Table S1. Selected Bond Angles and Bond Distances in **1-10.**

Compound 1

Cd1 O1 2.261(3)	Cd1 O2 2.451(4)	Cd1 N1 2.261(3)
O1 Cd1 O1 127.7(2)	O1 Cd1 N1 92.74(17)	N1 Cd1 O2 85.47(14)
O1 Cd1 O2 55.34(16)	O1 Cd1 N1 125.31(13)	N1 Cd1 O2 133.81(12)
O1 Cd1 O2 100.82(11)	O2 Cd1 O2 128.79(19)	N1 Cd1 N1 89.59(16)

Compound 2

Cu1 O1 1.971(3)	Cu1 N1 1.978(4)	
O1 Cu1 O1 180	O1 Cu1 N1 90.47(13)	N1 Cu1 N1 180
O1 Cu1 N1 89.53(13)		

Compound 3

Cd1 O1 2.376(3)	Cd1 N3 2.261(3)	Cd2 O5 2.410(3)
Cd1 O2 2.336(3)	Cd1 OW1 2.293(3)	Cd2 O7 2.252(3)
Cd1 O4 2.411(3)	Cd2 O3 2.468(3)	Cd2 O8 2.286(3)
Cd1 O5 2.242(3)	Cd2 O4 2.355(3)	Cd2 N1 2.245(3)
O1 Cd1 O4 94.77(10)	O7 Cd2 O3 109.13(10)	N1 Cd2 O8 111.76(11)
O2 Cd1 O1 55.78(10)	O7 Cd2 O4 156.11(11)	N3 Cd1 O1 90.94(11)
O2 Cd1 O4 94.42(10)	O7 Cd2 O5 87.61(10)	N3 Cd1 O2 146.67(12)
O4 Cd2 O3 54.84(9)	O7 Cd2 O8 85.23(10)	N3 Cd1 O4 89.64(11)
O4 Cd2 O5 73.59(10)	O8 Cd2 O3 78.25(10)	N3 Cd1 OW1 94.25(12)
O5 Cd1 O1 158.42(10)	O8 Cd2 O4 105.98(10)	OW1 Cd1 O1 90.05(11)
O5 Cd1 O2 105.05(11)	O8 Cd2 O5 156.09(10)	OW1 Cd1 O2 85.00(11)
O5 Cd2 O3 82.64(10)	N1 Cd2 O3 153.45(11)	O5 Cd1 O4 75.58(11)
OW1 Cd1 O4 173.76(10)	N1 Cd2 O4 98.65(11)	Cd1 O5 Cd2 105.01(12)

O5 Cd1 N3 107.99(12)	N1 Cd2 O5 91.68(11)	Cd2 O4 Cd1 101.55(11)
O5 Cd1 OW1 98.55(11)	N1 Cd2 O7 96.45(11)	

Compound 4

Cd1 O1 2.333(11)	Cd1 N5 2.256(11)	Cd2 O7 2.347(9)
Cd1 O2 2.360(8)	Cd1 N7 2.268(10)	Cd2 O8 2.377(10)
Cd1 O3 2.362(8)	Cd2 O5 2.337(10)	Cd2 N1 2.259(12)
Cd1 O4 2.397(8)	Cd2 O6 2.417(8)	Cd2 N3 2.276(10)

O1 Cd1 O2 55.1(3)	O7 Cd2 O8 55.6(3)	N3 Cd2 O8 84.0(3)
O1 Cd1 O3 92.0(3)	O8 Cd2 O6 147.8(3)	N5 Cd1 O1 144.4(3)
O1 Cd1 O4 85.6(3)	N1 Cd2 O5 136.6(3)	N5 Cd1 O2 89.9(3)
O2 Cd1 O3 143.1(3)	N1 Cd2 O6 82.4(3)	N5 Cd1 O3 118.4(3)
O2 Cd1 O4 100.9(3)	N1 Cd2 O7 96.0(4)	N5 Cd1 O4 96.2(3)
O3 Cd1 O4 55.9(3)	N1 Cd2 O8 117.3(4)	N5 Cd1 N7 95.0(4)
O5 Cd2 O7 96.7(4)	N1 Cd2 N3 91.4(4)	N7 Cd1 O1 104.7(4)
O5 Cd2 O8 104.0(4)	N3 Cd2 O5 106.0(3)	N7 Cd1 O2 114.2(3)
O5 Cd2 O6 54.6(3)	N3 Cd2 O6 122.8(3)	N7 Cd1 O3 87.9(3)
O7 Cd2 O6 99.6(3)	N3 Cd2 O7 137.7(3)	N7 Cd1 O4 143.0(3)

Compound 5

Cd1 O1 2.321(3)	Cd1 N1 2.253(3)	Cd2 O3 2.247(2)
Cd1 O4 2.373(3)	Cd2 O2 2.228(2)	

O1 Cd1 O1 81.34(15)	O2 Cd2 O3 98.79(10)	N1 Cd1 O1 98.70(10)
O1 Cd1 O4 97.85(14)	O3 Cd2 O3 145.07(13)	N1 Cd1 O4 83.61(10)
O1 Cd1 O4 177.56(8)	O4 Cd1 O4 83.05(17)	N1 Cd1 O4 86.35(10)
O2 Cd2 O2 143.41(14)	N1 Cd1 O1 91.48(10)	O2 Cd2 O3 92.04(9)
N1 Cd1 N1 166.59(15)		

Compound 6

Cd1 O1 2.488(7)	Cd1 N1 2.280(8)	Cd1 N3 2.328(13)
Cd1 O2 2.400(7)		
O1 Cd1 O1 161.3(3)	N1 Cd1 O1 87.3(3)	N1 Cd1 N1 172.3(4)
O2 Cd1 O1 53.7(2)	N1 Cd1 O1 94.0(2)	N1 Cd1 N3 93.9(2)
O2 Cd1 O1 144.9(2)	N1 Cd1 O2 88.2(3)	N3 Cd1 O1 80.64(17)
O2 Cd1 O2 91.7(3)	N1 Cd1 O2 86.4(3)	N3 Cd1 O2 134.17(17)

Compound 7

Zn1 O1 1.928(3)	Zn1 N1 2.002(3)	Zn1 N3 2.002(3)
Zn1 O3 1.948(2)		
O1 Zn1 O3 113.11(13)	O1 Zn1 N3 122.37(12)	O3 Zn1 N3 97.50(11)
O1 Zn1 N1 109.94(13)	O3 Zn1 N1 108.52(11)	N1 Zn1 N3 104.14(13)

Compound 8

Cd1 O3 2.442(3)	Cd1 N1 2.255(3)	Cd2 O7 2.280(3)
Cd1 O4 2.287(2)	Cd1 N3 2.297(3)	Cd2 O8 2.449(2)
Cd1 O5 2.354(2)	Cd2 O1 2.385(2)	Cd2 N5 2.287(3)
Cd1 O6 2.350(2)	Cd2 O2 2.298(2)	Cd2 N7 2.279(3)
O1 Cd2 O8 103.05(8)	O7 Cd2 O1 143.69(8)	O2 Cd2 O1 56.30(8)
N3 Cd1 O5 148.20(8)	O7 Cd2 O2 101.76(9)	N3 Cd1 O6 92.28(9)
O2 Cd2 O8 112.56(8)	O7 Cd2 O8 55.49(8)	N5 Cd2 O1 108.72(9)
O4 Cd1 O3 55.71(7)	O7 Cd2 N5 99.58(9)	N5 Cd2 O2 91.49(9)
O4 Cd1 O5 102.63(8)	N1 Cd1 O3 89.77(8)	N5 Cd2 O8 147.39(9)
O4 Cd1 O6 96.99(8)	N1 Cd1 O4 138.13(9)	N7 Cd2 O1 91.18(9)
O4 Cd1 N3 83.10(9)	N1 Cd1 O5 102.28(8)	N7 Cd2 O2 145.15(9)

O5 Cd1 O3 93.36(8)	N1 Cd1 O6 124.85(8)	N1 Cd1 N3 92.84(9)
O6 Cd1 O3 135.75(8)	N7 Cd2 O7 112.76(10)	N7 Cd2 O8 84.64(9)
O6 Cd1 O5 56.13(8)	N3 Cd1 O3 114.74(9)	N7 Cd2 N5 87.49(10)

Compound 9

Cd1 O1 2.205(7)	Cd2 O8 2.338(6)	Cd3 O4 2.511(7)
Cd1 O5 2.296(6)	Cd2 O9 2.523(7)	Cd3 O11 2.503(8)
Cd1 O6 2.488(6)	Cd2 O10 2.275(7)	Cd3 O12 2.351(8)
Cd1 N10 2.279(8)	Cd2 N5 2.295(8)	Cd3 N1 2.308(8)
Cd1 N11 2.210(8)	Cd2 N7 2.264(8)	Cd3 N3 2.303(8)
Cd2 O7 2.418(7)	Cd3 O3 2.369(7)	Cd3 OW1 2.296(9)

O1 Cd1 O5 89.8(2)	O12 Cd3 O4 136.8(3)	N7 Cd2 O8 102.1(3)
O1 Cd1 O6 139.4(2)	O12 Cd3 O11 52.2(3)	N7 Cd2 O9 107.1(3)
O1 Cd1 N10 116.2(3)	N1 Cd3 O3 82.5(2)	N7 Cd2 O10 126.5(3)
O1 Cd1 N11 112.2(3)	N1 Cd3 O4 135.4(2)	N7 Cd2 N5 86.6(3)
O3 Cd3 O4 53.3(2)	N1 Cd3 O11 139.6(3)	N10 Cd1 O5 92.8(3)
O3 Cd3 O11 137.8(3)	N1 Cd3 O12 87.4(3)	N10 Cd1 O6 88.0(2)
O5 Cd1 O6 55.2(2)	N3 Cd3 O3 94.3(3)	N11 Cd1 O5 142.6(2)
O7 Cd2 O9 97.7(2)	N3 Cd3 O4 93.8(3)	N11 Cd1 O6 91.3(2)
O8 Cd2 O7 55.4(2)	N3 Cd3 O11 82.0(3)	N5 Cd2 O7 78.7(3)
O8 Cd2 O9 150.6(2)	N3 Cd3 O12 85.5(3)	OW1 Cd3 O3 94.0(3)
O10 Cd2 O7 81.2(2)	N3 Cd3 N1 95.1(3)	OW1 Cd3 O4 84.5(4)
O10 Cd2 O8 104.9(2)	N11 Cd1 N10 102.9(3)	OW1 Cd3 O11 86.3(3)
O10 Cd2 O9 54.3(2)	N5 Cd2 O8 97.7(3)	OW1 Cd3 O12 87.8(3)
O10 Cd2 N5 133.0(3)	N5 Cd2 O9 86.9(3)	OW1 Cd3 N1 94.3(4)
O11 Cd3 O4 84.9(3)	N7 Cd2 O7 150.3(2)	OW1 Cd3 N3 168.2(3)
O12 Cd3 O3 169.9(3)		

Compound 10

Cd1 O1 2.3124(17)	Cd1 O2 2.3722(18)	Cd1 N1 2.285(2)

O1 Cd1 O1 153.67(9)	O2 Cd1 O2 87.31(9)	N1 Cd1 O2 96.53(7)
O1 Cd1 O2 56.32(6)	N1 Cd1 O1 92.08(7)	N1 Cd1 O2 163.87(7)
O1 Cd1 O2 103.00(6)	N1 Cd1 O1 107.57(7)	N1 Cd1 N1 84.11(10)

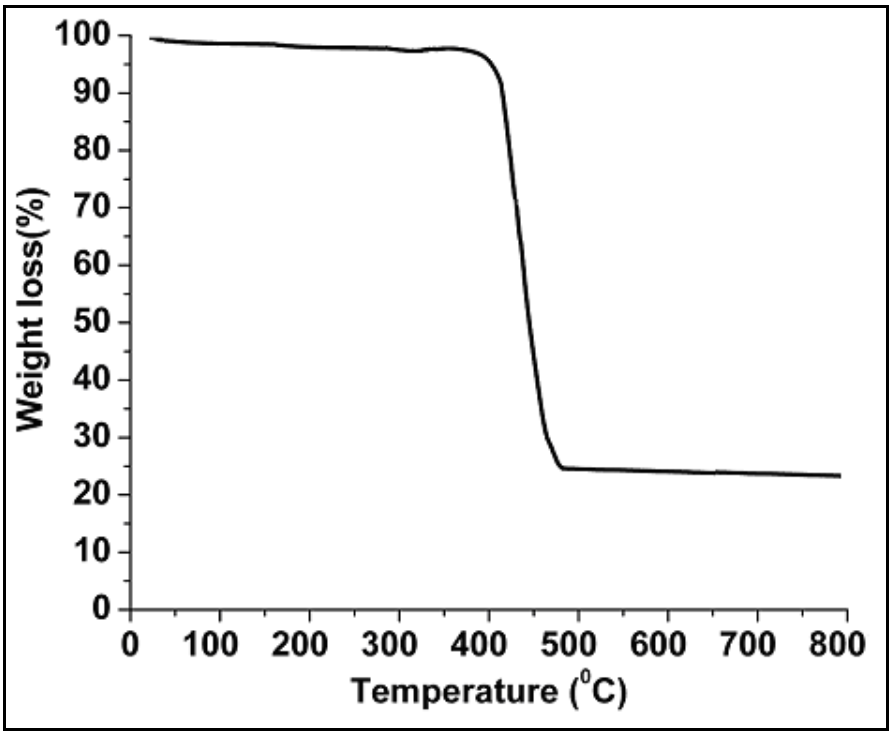

Figure S1. TGA of compound **1**.

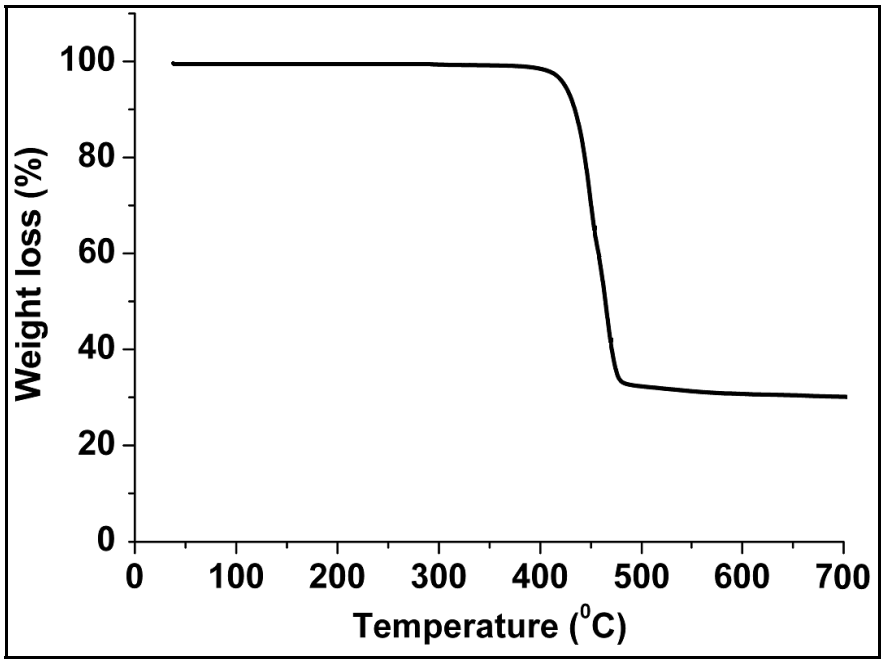

Figure S2. TGA of compound **2**.

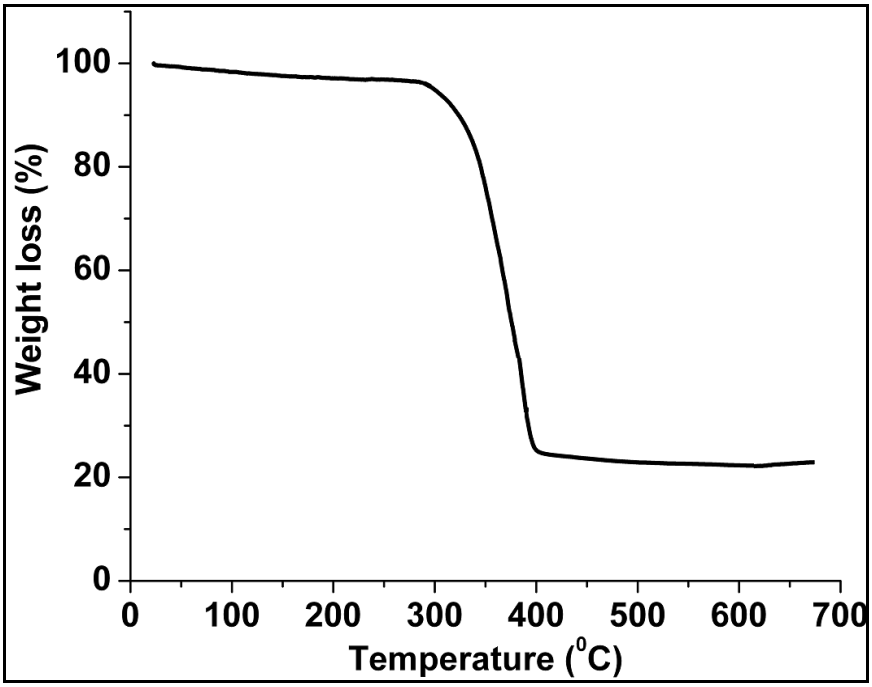

Figure S3. TGA of compound **3**.

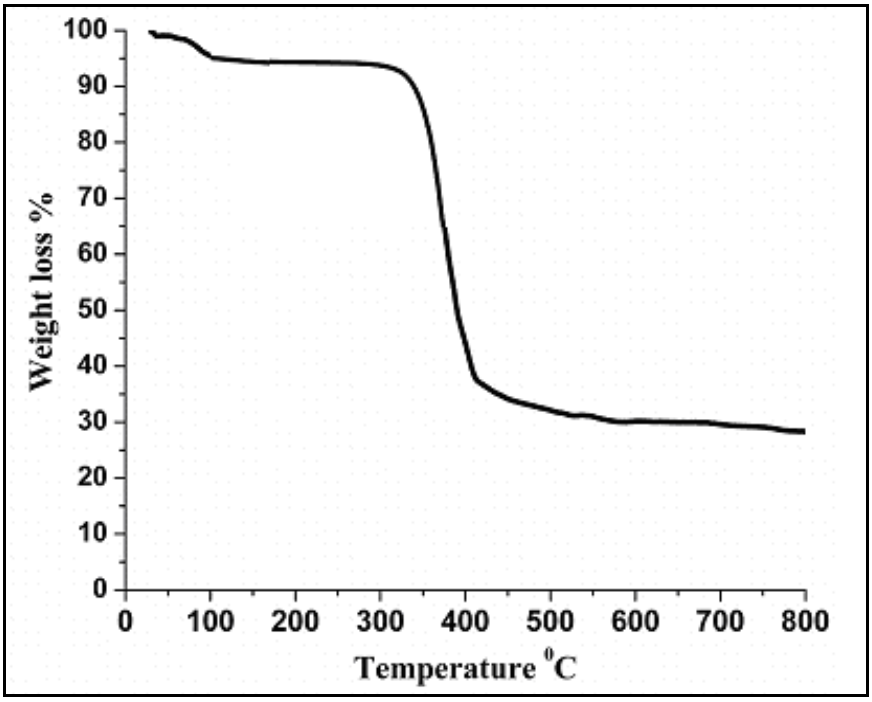

Figure S4. TGA of compound **4.**

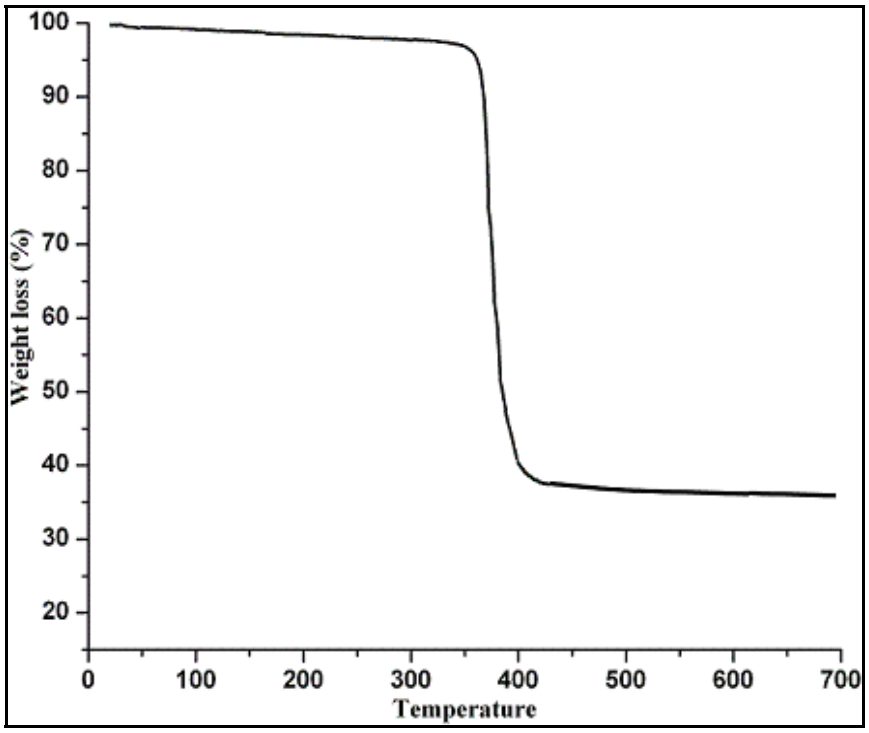

Figure S5. TGA of compound **5.**

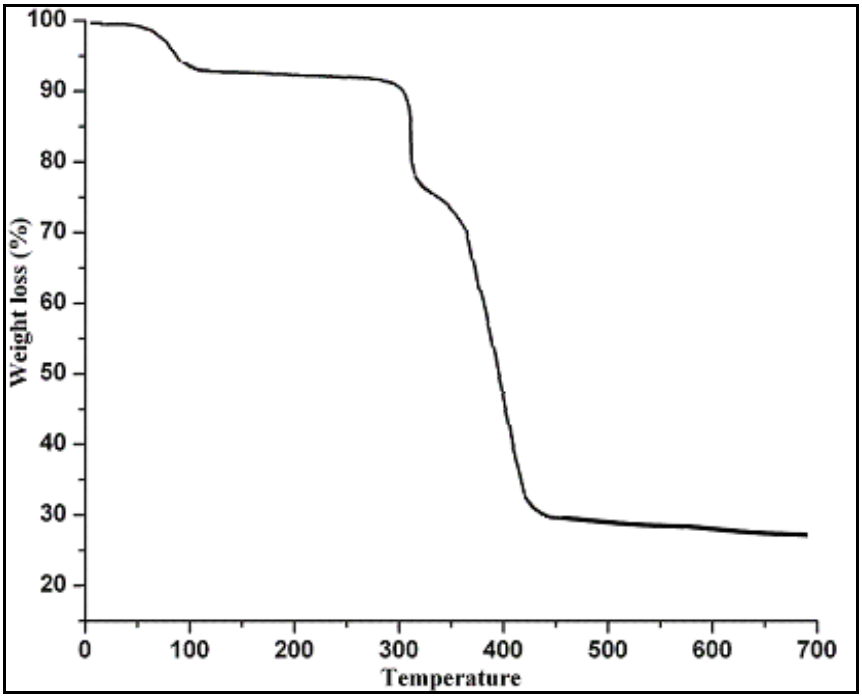

Figure S6. TGA of compound **6.**

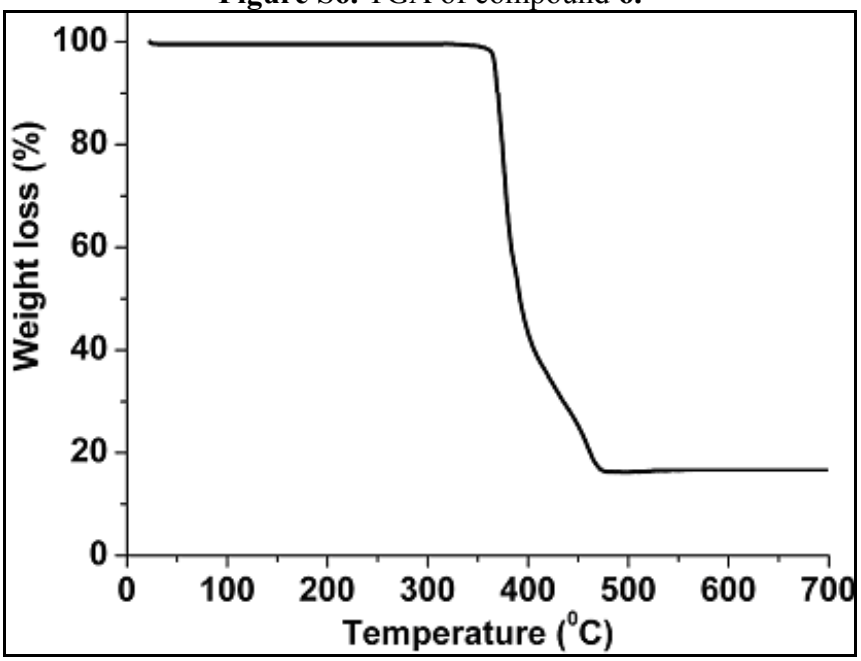

Figure S7. TGA of compound **7**.

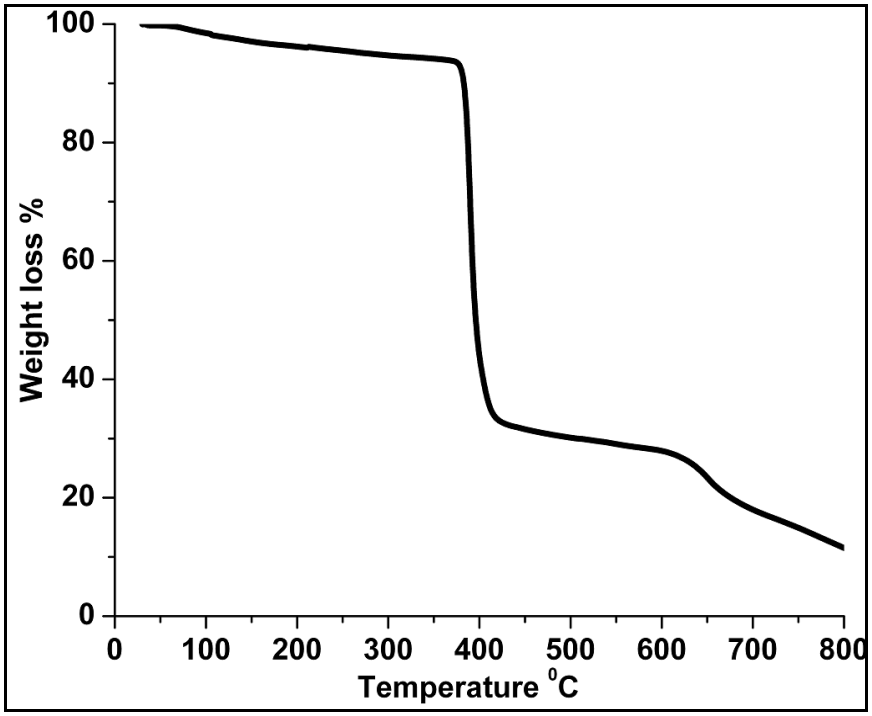

Figure S8. TGA of compound **8.**

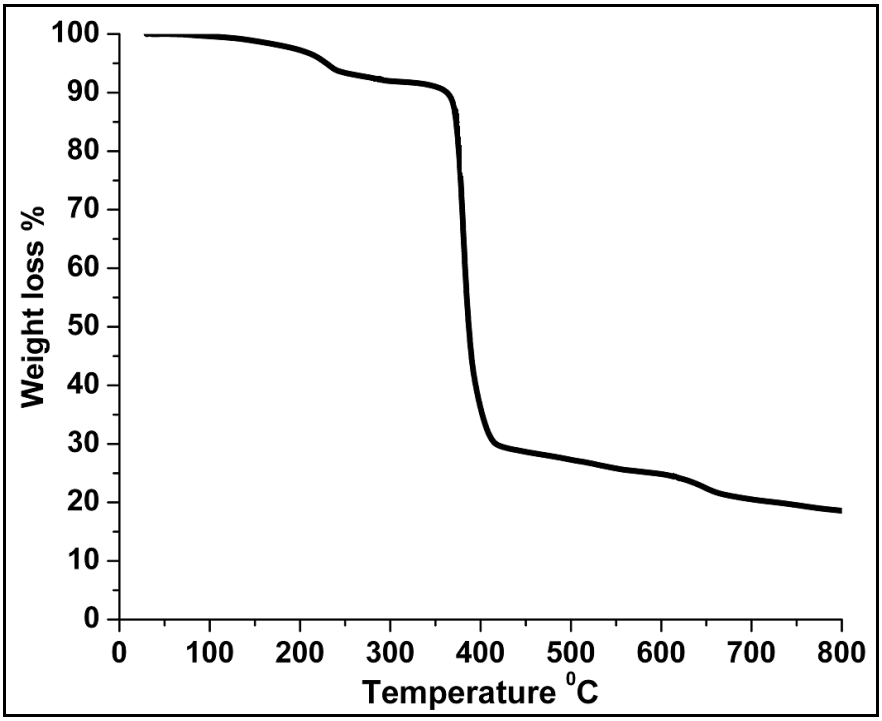

Figure S9. TGA of compound **9.**

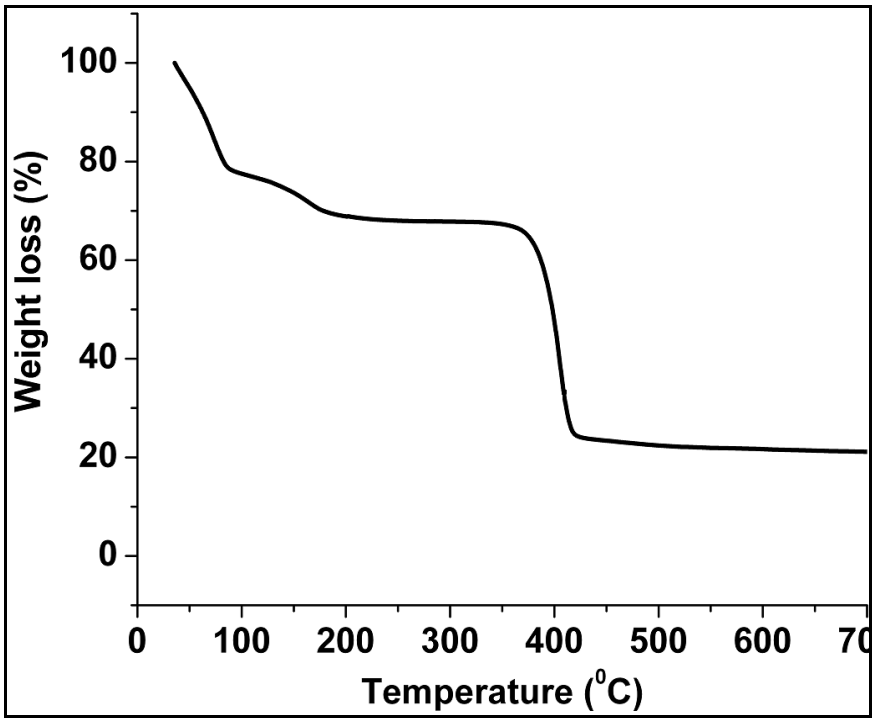

Figure S10. TGA of compound **10**.

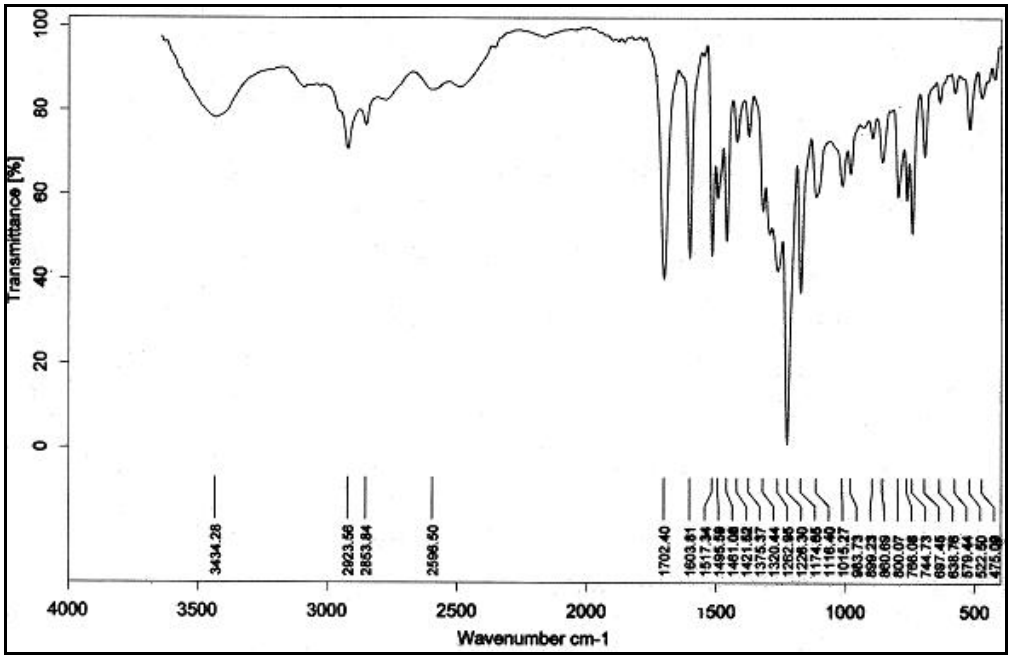

Figure S11. IR spectra of $\mathbf{HL_3}$.

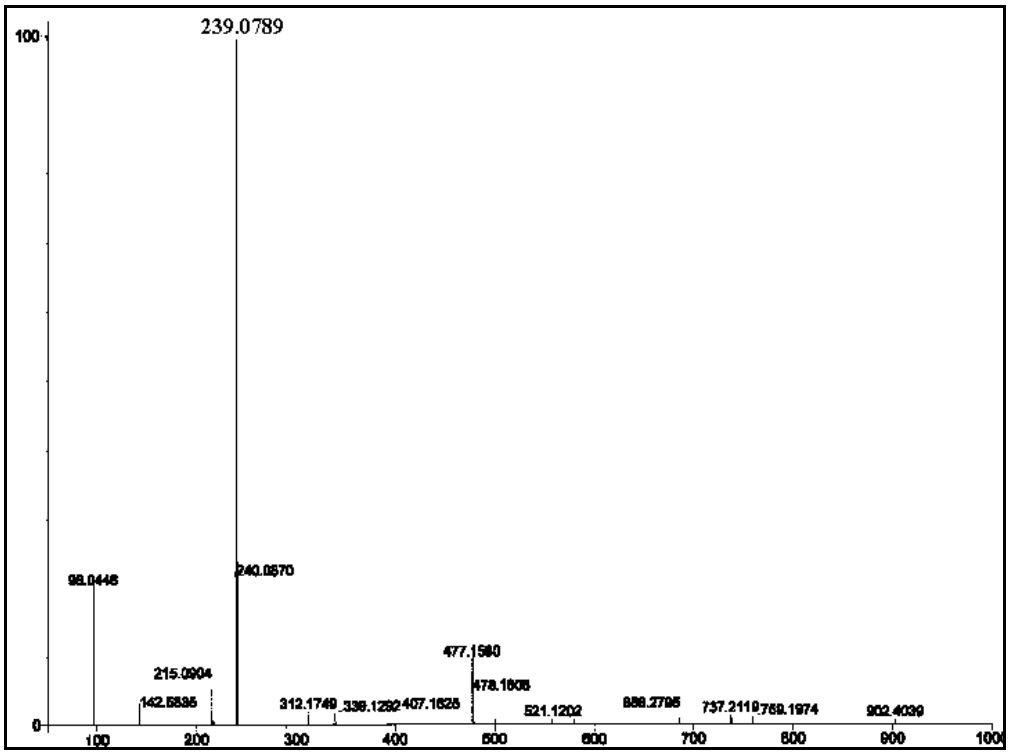

Figure S12. ESI-MS spectra of $\mathbf{HL_3}$.

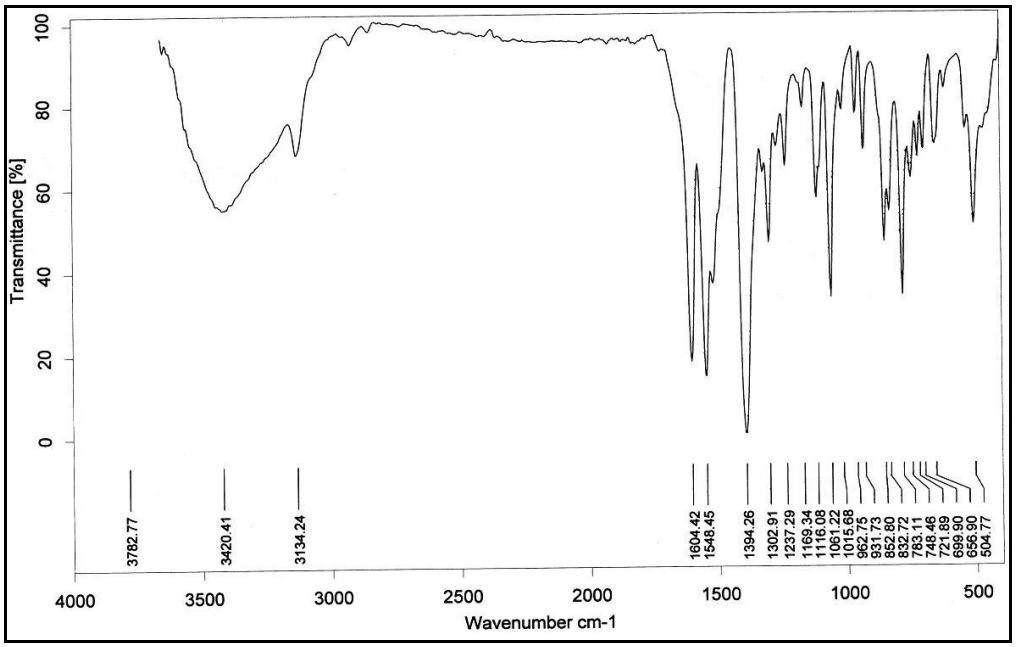

Figure S13. IR spectra of compound **1**.

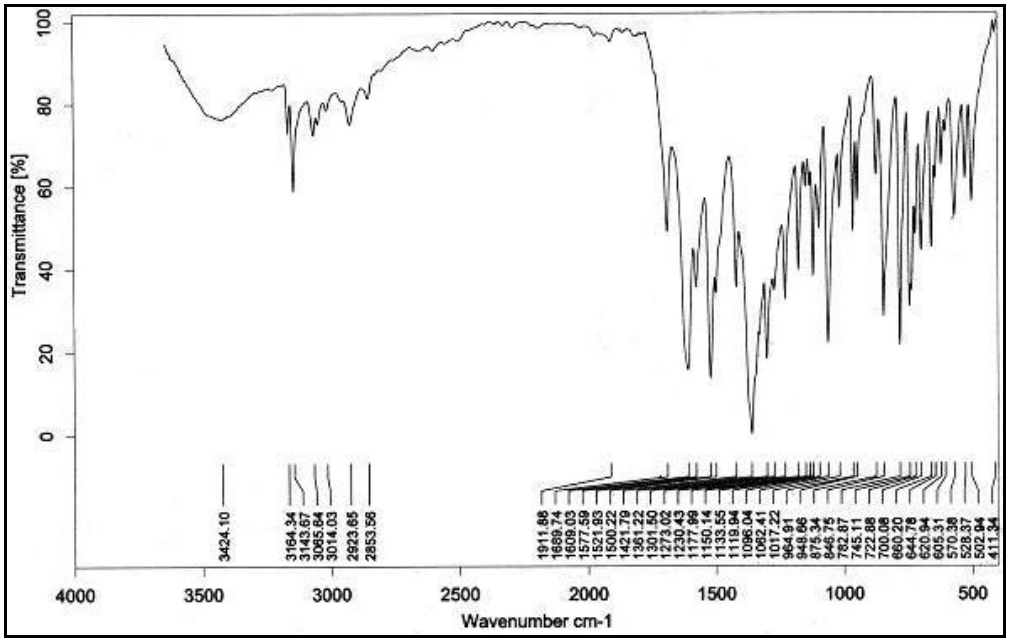

Figure S14. IR spectra of compound **2**.

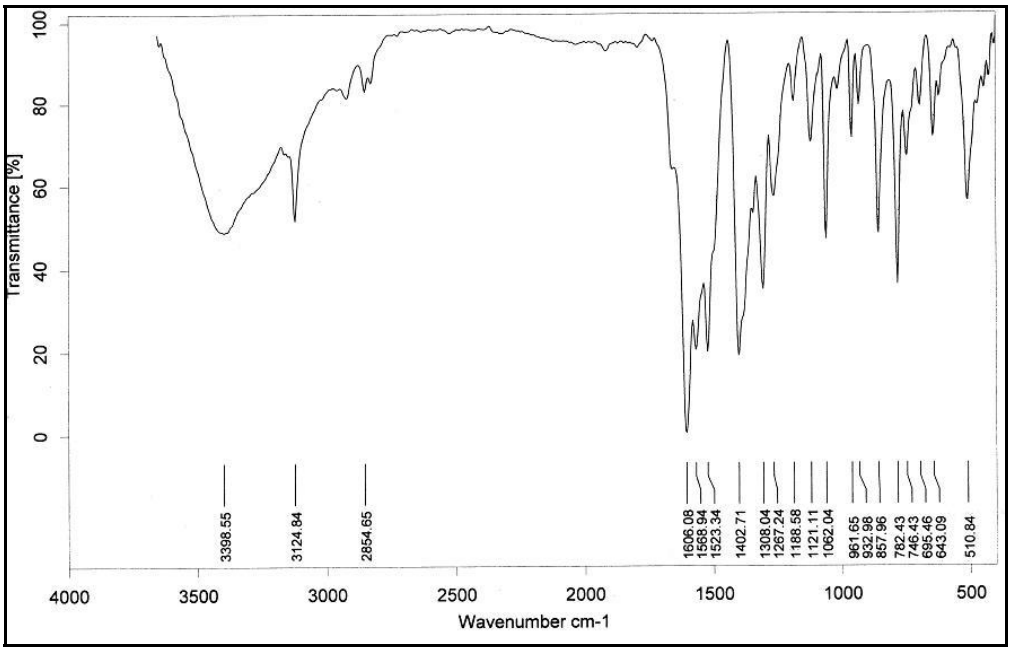

Figure S15. IR spectra of compound **3**.

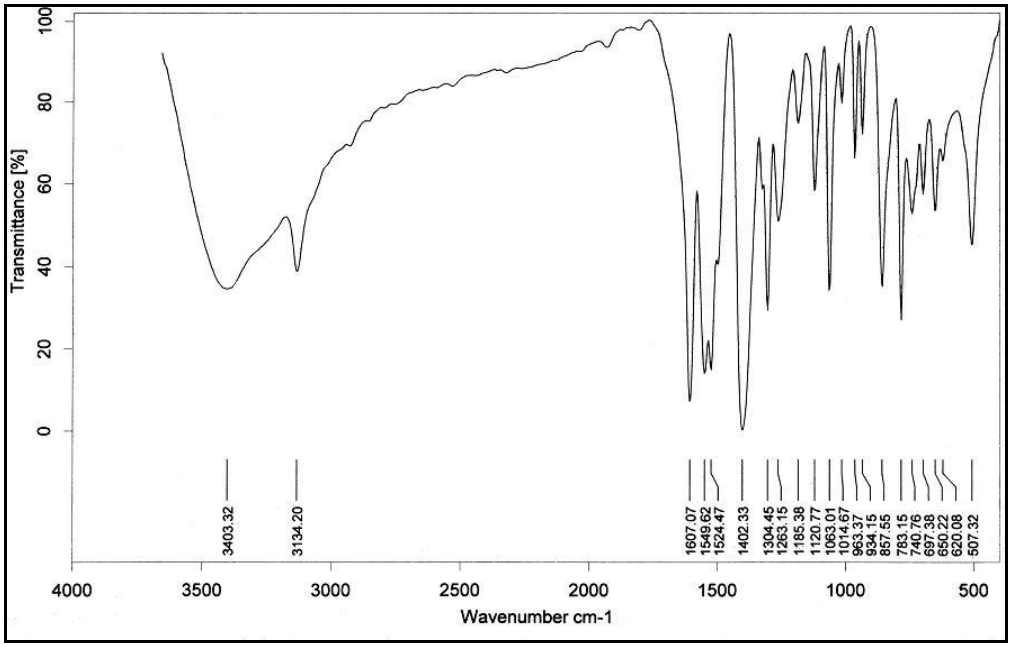

Figure S16. IR spectra of compound **4**.

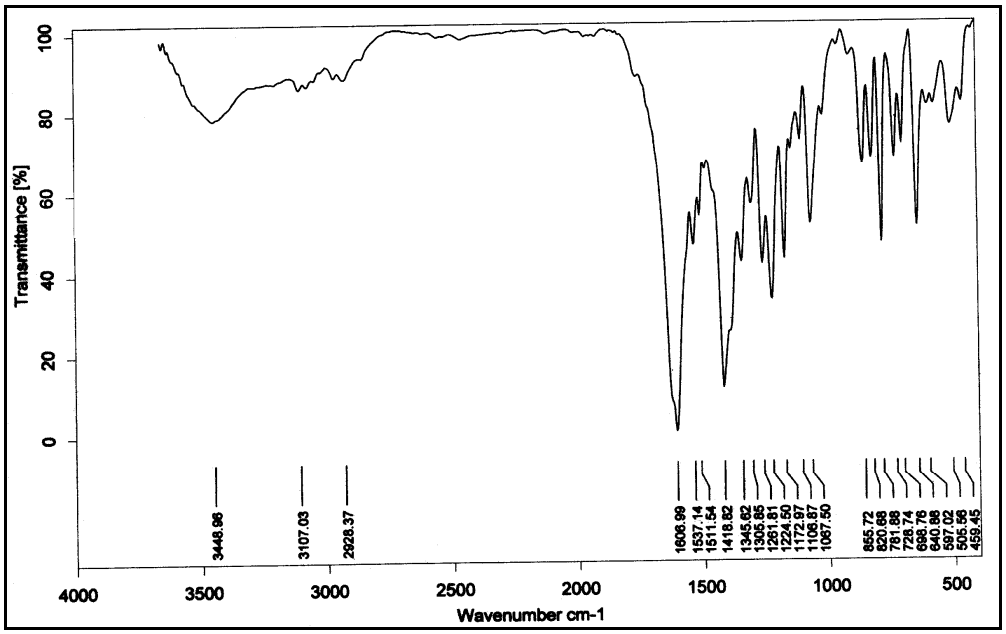

Figure S17. IR spectra of compound **5.**

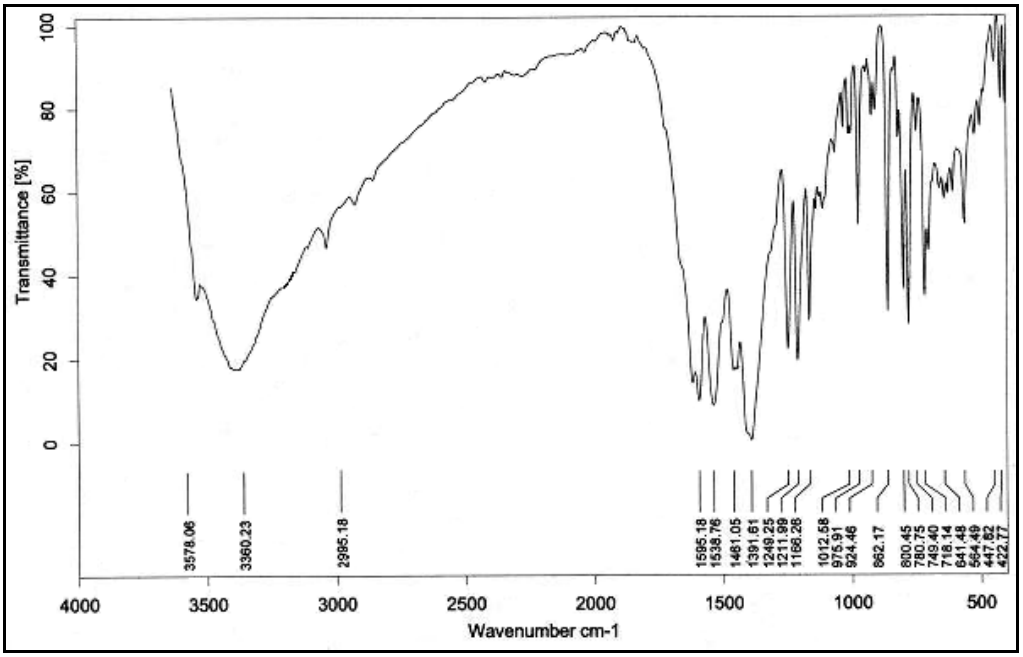

Figure S18. IR spectra of compound **6.**

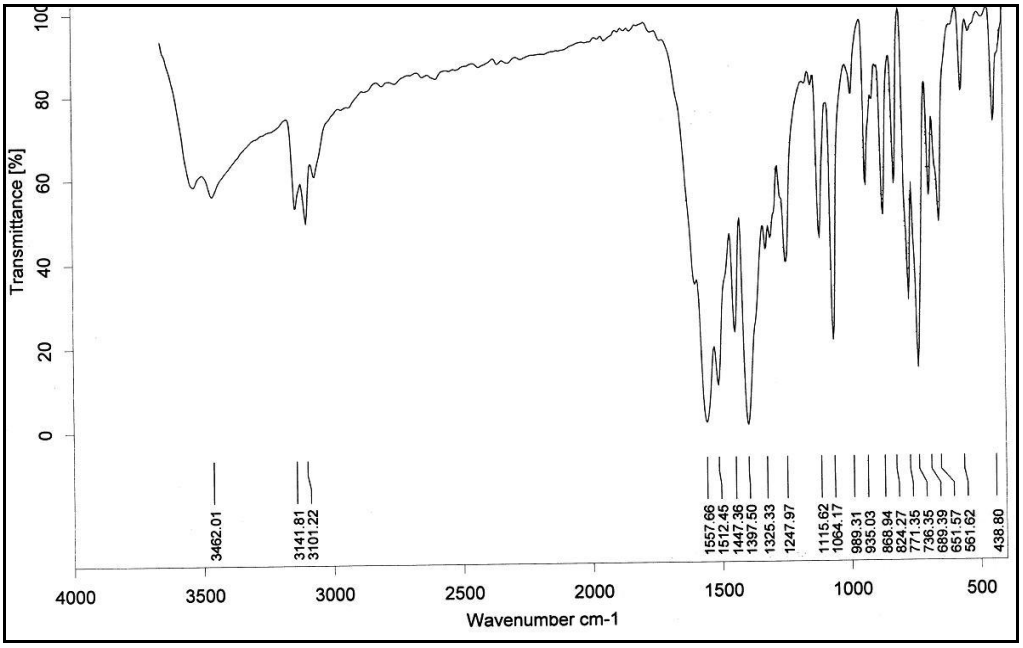

Figure S19. IR spectra of compound **7**.

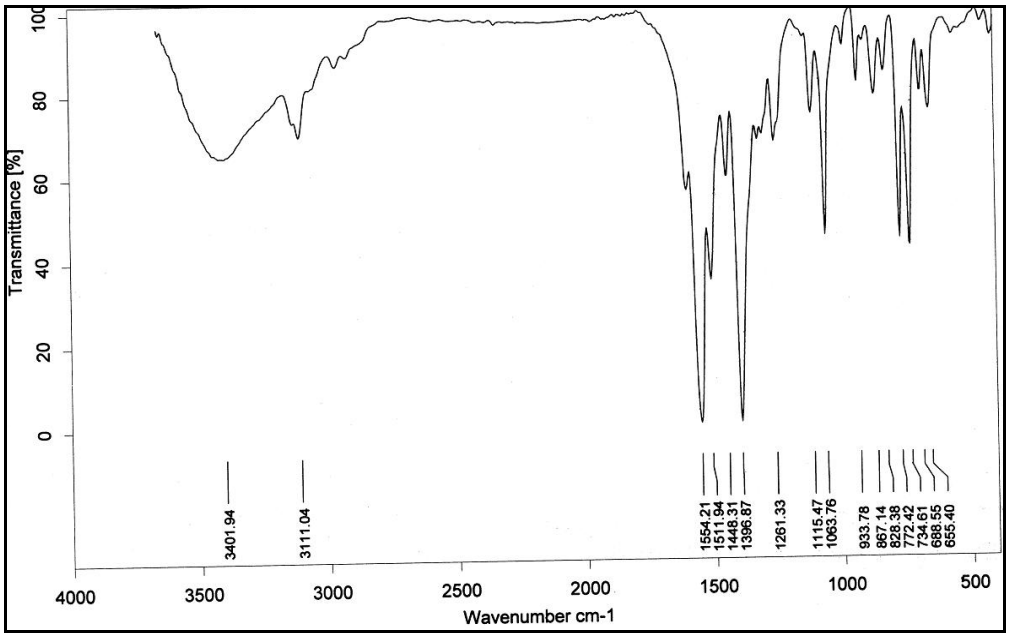

Figure S20. IR spectra of compound **8**.

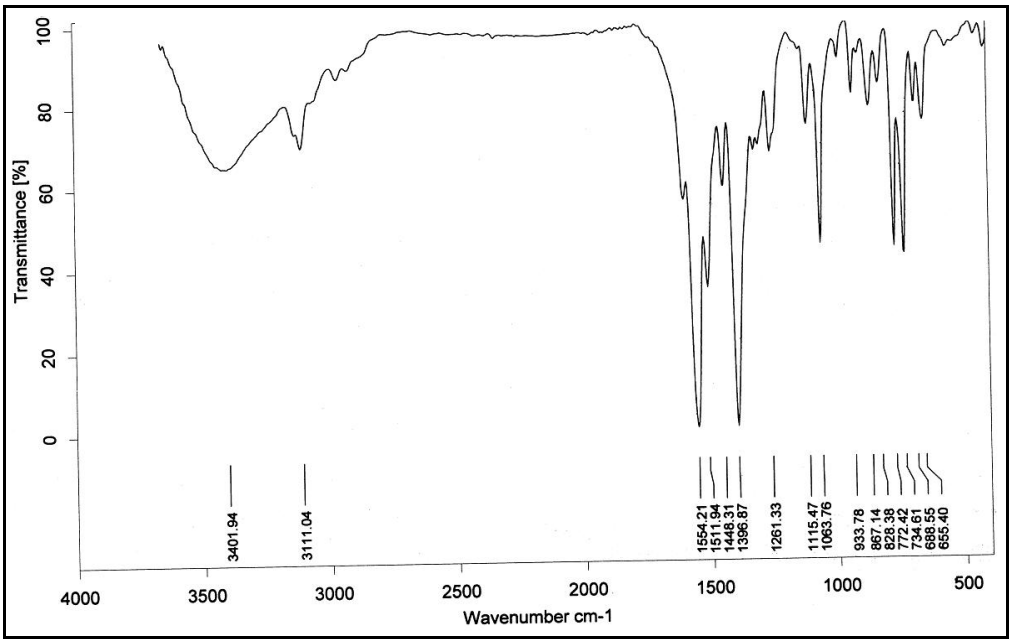

Figure S21. IR spectra of compound **9.**

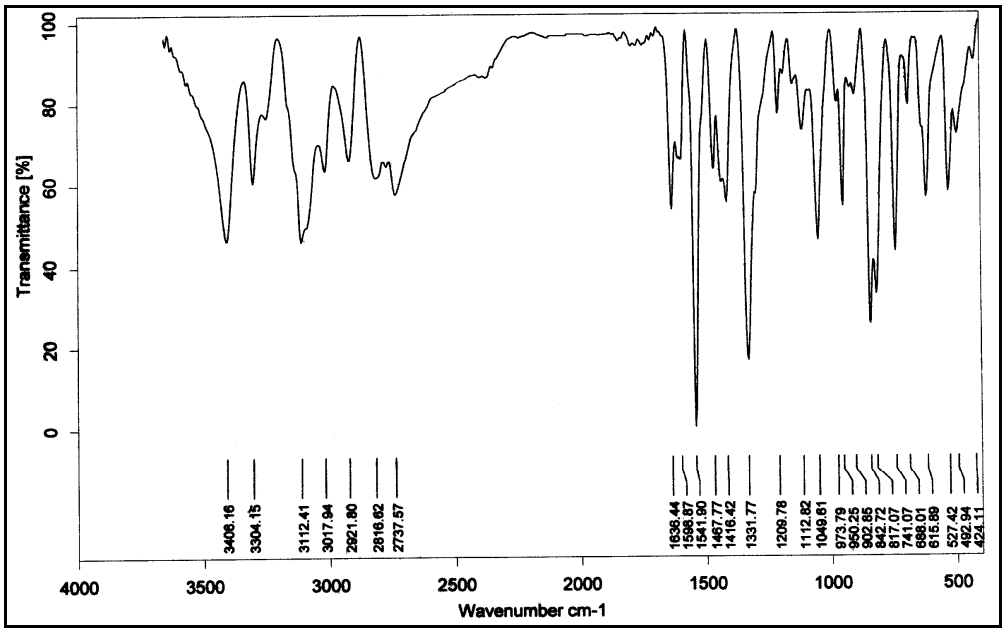

Figure S22. IR spectra of compound **10.**

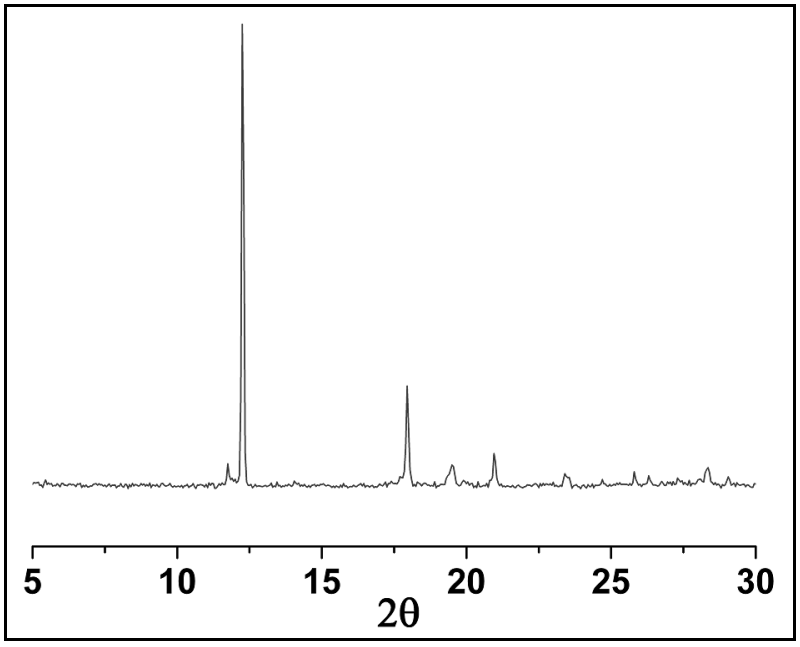

Figure S23. PXRD pattern of compound **2**.