

Hydrogen-bonded microporous network, helix and 1D zigzag chains in MOFs of Zn(II): studying the effects of ligating topologies, hydrogen bonding backbone and counter-anions

D. Krishna Kumar, Amitava Das* and Parthasarathi Dastidar*

Analytical Science Discipline, Central Salt & Marine Chemicals Research Institute G. B. Marg, Bhavnagar – 364 002,
Gujarat (India) Fax: +91-278-2567562 E-mail: parthod123@rediffmail.com; dastidar@csmcri.org (PD);
amitava@csmcri.org (AD)

FT-IR for 1a-6

[{Zn(L1)(Cl)}₂].EG.MeOH]_n (1a):

FT-IR (cm⁻¹): 3373b, 2945m, 2360m, 1940w, 1737vs, 1598vs, 1526s, 1509m, 1433vs, 1335vs, 1295vs, 1195vs, 1083vs, 1043s, 1028s, 884b, 835s, 738s, 657b, 552m, 534s

[{Zn(L1)(Cl)}₂].H₂O]_n (1b):

FT-IR (cm⁻¹): 3508b, 3364w, 3309m, 3198m, 3033w, 2550w, 2513m, 2363m, 2201w, 1820w, 1748vs, 1592vs, 1515s, 1435vs, 1337vs, 1295vs, 1259s, 1182vs, 1063vs, 1026vs, 910w, 836vs, 742s, 664m, 556s, 533vs

[{Zn(L1)(OAc)}₂].H₂O]_n (2):

FT-IR (cm⁻¹): 3454m, 3292vs, 3177b, 3120w, 3085m, 3027m, 2542w, 2505m, 2361m, 2197w, 1946m, 1747vs, 1594s, 1563w, 1521s, 1414b, 1332vs, 1292vs, 1292vs, 1254s, 1183vs, 1060s, 1024vs, 934m, 906m, 852s, 834vs, 799w, 769m, 725s, 680s, 622s, 552w, 533vs, 496m

[{Zn(L1)(SO₄)}₂].EG.xH₂O]_n (3):

FT-IR (cm⁻¹): 3369b, 2946m, 2878w, 2513w, 1949b, 1731vs, 1600s, 1519b, 1439vs, 1385m, 1338vs, 1310vs, 1259w, 1197s, 1132s, 1087m, 1029vs, 983m, 881s, 837vs, 740s, 654m, 618vs, 597m, 559vs, 530vs

[{Zn(L2)(Cl)}₂]_n (4):

FT-IR (cm⁻¹): 3856w, 3751w, 3676w, 3300vs, 3105m, 3072s, 2984w, 2925m, 2740w, 2540b, 2365w, 1992w, 1945m, 1899m, 1870w, 1834m, 1704vs, 1613s, 1587vs, 1528vs, 1476vs, 1423vs, 1331vs, 1288m, 1267vs, 1214vs, 1131m, 1108s, 1059s, 948m, 914s, 861m, 822s, 784vs, 742s, 698s, 652vs, 584s, 516m, 416s

[{Zn(L2)(OAc)}₂].CHCl₃]_n (5):

FT-IR (cm⁻¹): 3285m, 3198w, 3138w, 3045m, 3001s, 2573w, 2361m, 1715vs, 1642s, 1615vs, 1551s, 1487vs, 1416s, 1331s, 1317s, 1286vs, 1254m, 1213vs, 1132vs, 1111s, 1057b, 1015m, 927s, 805s, 753vs, 701vs, 680vs, 648s, 615s, 521w, 496w, 418s

[{Zn(L2)(SO₄)(H₂O)}₃].MeOH]_n 6:

FT-IR (cm⁻¹): 3420m, 3276m, 3083w, 2829w, 2362m, 2340w, 1918w, 1878w, 1832w, 1701vs, 1619vs, 1597m, 1561vs, 1482vs, 1433vs, 1414s, 1336s, 1290vs, 1232s, 1196s, 1158s, 1058m, 1023w, 977s, 940m, 980m, 803s, 774w, 732s, 699s, 645m, 616b, 427b

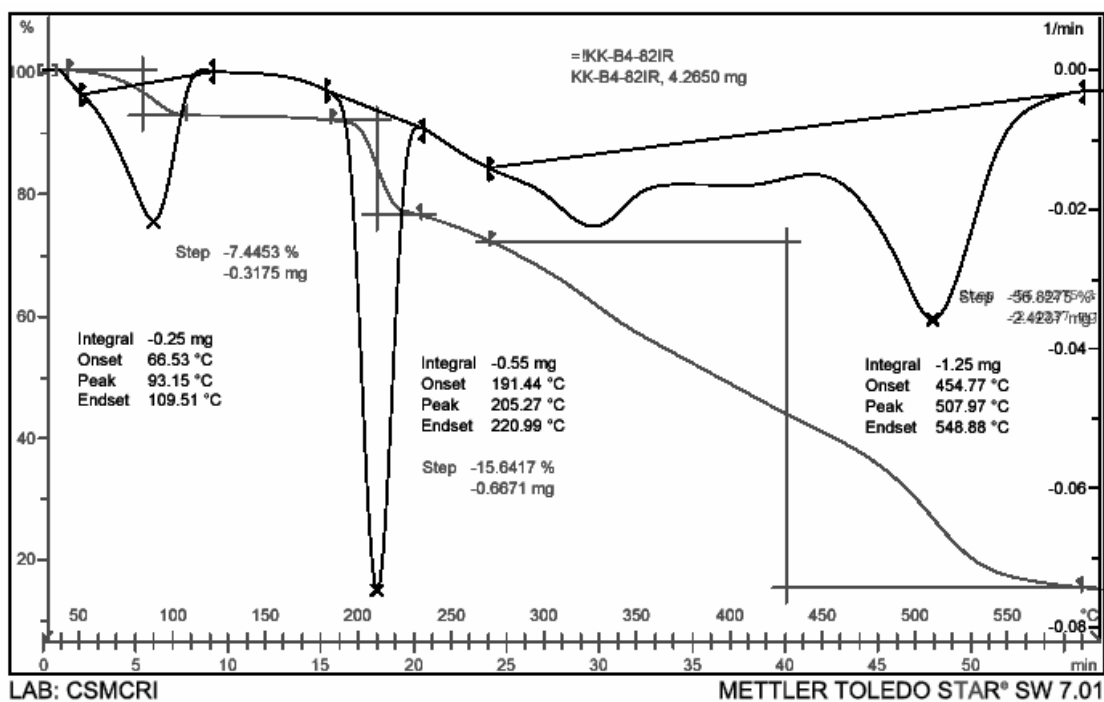
Electronic Supplementary Material for CrystEngComm
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Hydrogen Bonding Parameters for 1a-6

1a					
D-H...A	D-H/Å	H...A/Å	D...A/Å	D-H...A/⁰	Symmetry operation for A
N(7)-H(7)...O(18)	0.86	2.06	2.840(4)	151	
N(10)-H(10)...O(20A)	0.86	2.06	2.827(5)	148	
N(10)-H(10)...O(20B)	0.86	2.11	2.947(5)	164	-x, 1-y, 1-z
O(18)-H(18)...Cl(2)	0.78(6)	2.58(6)	3.327(3)	163(5)	-x, -1+y, 1/2-z
C(3)-H(3)...O(18)	0.93	2.39	3.145(5)	139	
C(12)-H(12)...O(20A)	0.93	2.54	3.265(5)	135	
1b					
N(7)-H(7)...O(17)	0.84(4)	2.44(4)	3.214(6)	153(3)	
N(7)-H(7)...O(19)	0.84(4)	2.06(4)	2.815(6)	149(3)	
N(10)-H(10)...O(19)	0.73(4)	2.22(4)	2.903(6)	157(4)	
N(10)-H(10)...O(20)	0.73(4)	2.27(4)	3.000(6)	177(4)	
C(5)-H(5)...O(17)	0.93	2.55	3.347(6)	144	
2					
N(7)-H(7)...O(19)	0.82(2)	2.14(2)	2.891(2)	153(2)	1-x, -y, 1-z
N(10)-H(10)...O(19)	0.83(2)	1.98(2)	2.786(2)	164(2)	1-x, -y, 1-z
O(25)-H(25)...O(23)	0.83(2)	2.02(2)	2.828(2)	165(2)	-x, y, 3/2-z
C(13)-H(13)...O(17)	0.93(2)	2.49(2)	3.202(2)	134(2)	1/2-x, 1/2-y, 1-z
C(16)-H(16)...O(25)	0.98(2)	2.38(2)	3.154(2)	135(2)	1-x, -y, 1-z
C(20)-H(20B)...O(23)	0.96(2)	2.52(2)	3.437(2)	158(2)	-x, y, 3/2-z
C(20)-H(20C)...O(9)	0.94(2)	2.56(2)	3.429(2)	153(2)	-1/2+x, -1/2+y, z
C(24)-H(24B)...O(21)	0.95(2)	2.58(2)	3.388(2)	143(2)	1-x, y, 3/2-z
3					
N(7)-H(7)...O(19)	0.88	2.26	3.101(5)	160	-x, 1/2+y, 1/2-z
N(10)-H(10)...O(20)	0.88	1.92	2.778(5)	164	-x, 1/2+y, 1/2-z
O(25)-H(25)...O(19)	0.84	1.93	2.756(6)	166	1-x, 1/2+y, 1/2-z
C(5)-H(5)...O(19)	0.95	2.48	3.303(6)	145	-x, 1/2+y, 1/2-z
C(15)-H(15)...O(20)	0.95	2.27	3.208(7)	168	-1+x, 1/2-y, 1/2+z
C(16)-H(16)...O(20)	0.95	2.51	3.270(6)	137	-x, 1/2+y, 1/2-z
4					
N(7)-H(7)...Cl(2)	0.86	2.53	3.310(3)	151	x,-1/2+y,1/2+z
C(4)-H(4)...O(9)	0.93	2.35	3.127(5)	141	1/4-x,1/4+y,1/4+z
5					
N(7)-H(7)...O(17)	0.88	1.97	2.782(8)	153	-x, 1/2+y, 1/2-z
N(10)-H(10)...O(21)	0.88	2.09	2.905(8)	154	-x, 1/2+y, 1/2-z
C(13)-H(13)...O(9)	0.95	2.38	3.140(10)	137	1-x, 1-y, 1-z
C(16)-H(16)...O(21)	0.95	2.51	3.305(10)	142	-x, 1/2+y, 1/2-z
C(25)-H(25)...O(23)	1.00	2.37	3.196(12)	139	1-x, 1/2+y, 1/2-z
6					
N(7)-H(7A)...O(21)	0.86	1.99	2.842(4)	169	-x, 1-y, -z
N(10)-H(10)...O(19)	0.86	2.11	2.952(4)	166	-x, 1-y, -z
O(26)-H(10A)...O(9)	0.82	1.92	2.730(5)	169	
O(22)-H(22A)...O(20)	0.82	1.93	2.745(4)	176	1+x, y, z
O(22)-H(22B)...O(26)	0.78(4)	1.90(4)	2.678(5)	176(2)	
O(23)-H(23A)...O(19)	0.82	1.98	2.739(4)	154	1+x, y, z
O(23)-H(23B)...O(20)	0.80(4)	1.91(4)	2.703(4)	171(4)	1/2-x, -1/2+y, 1/2-z

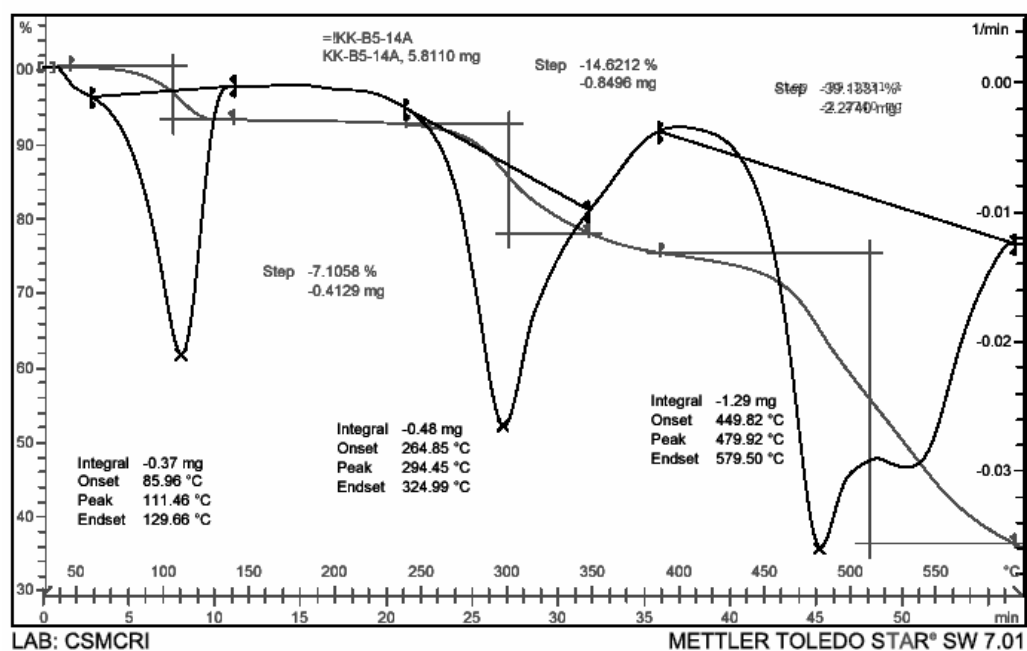
O(24)–H(24B)…O(17)	0.73(4)	2.02(4)	2.746(4)	178(7)	1/2-x, -1/2+y, 1/2-z
C(12)–H(12)…O(19)	0.93	2.56	3.357(4)	144	-x, 1-y, -z

Thermal Analyses plot for 1a-6

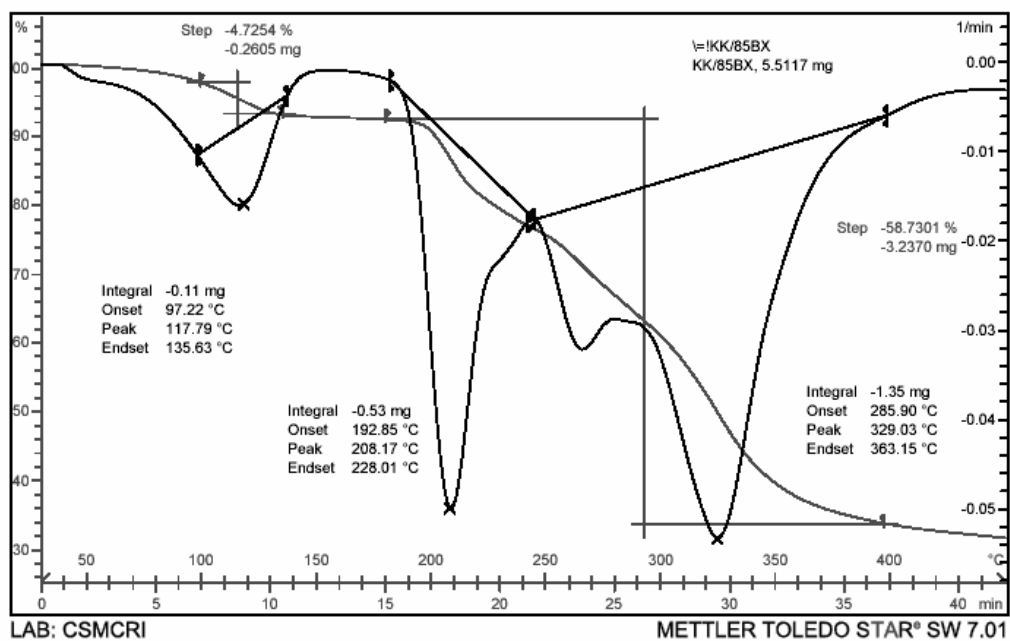
TG curve for the compound 1a



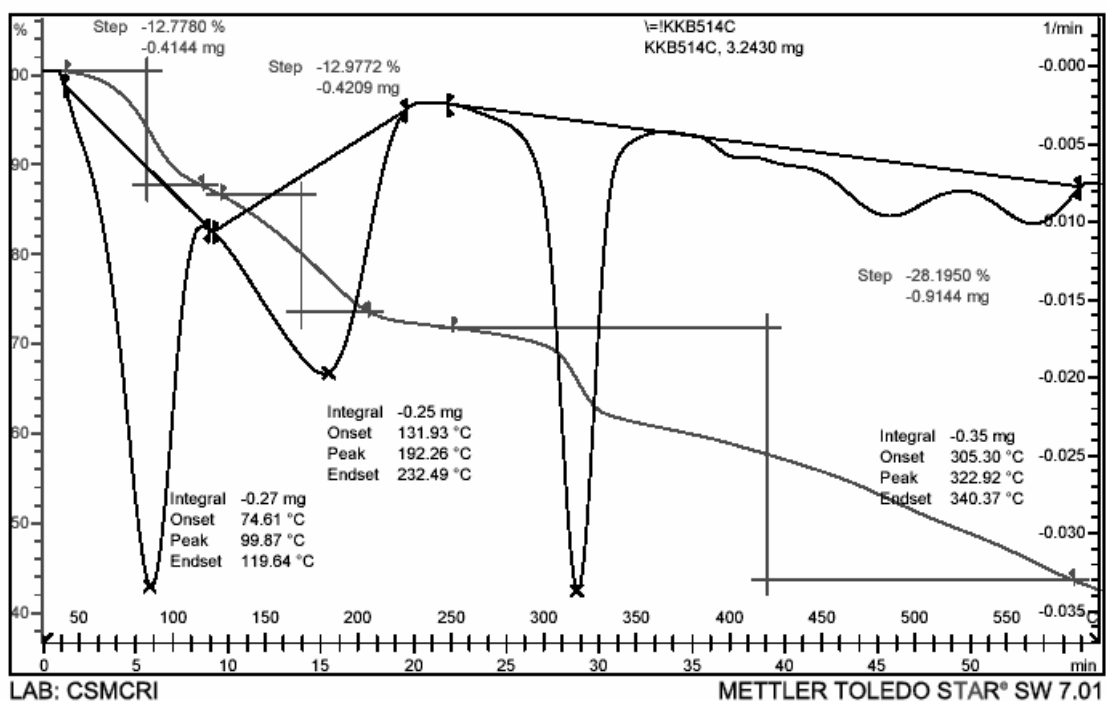
TG curve for the compound 1b



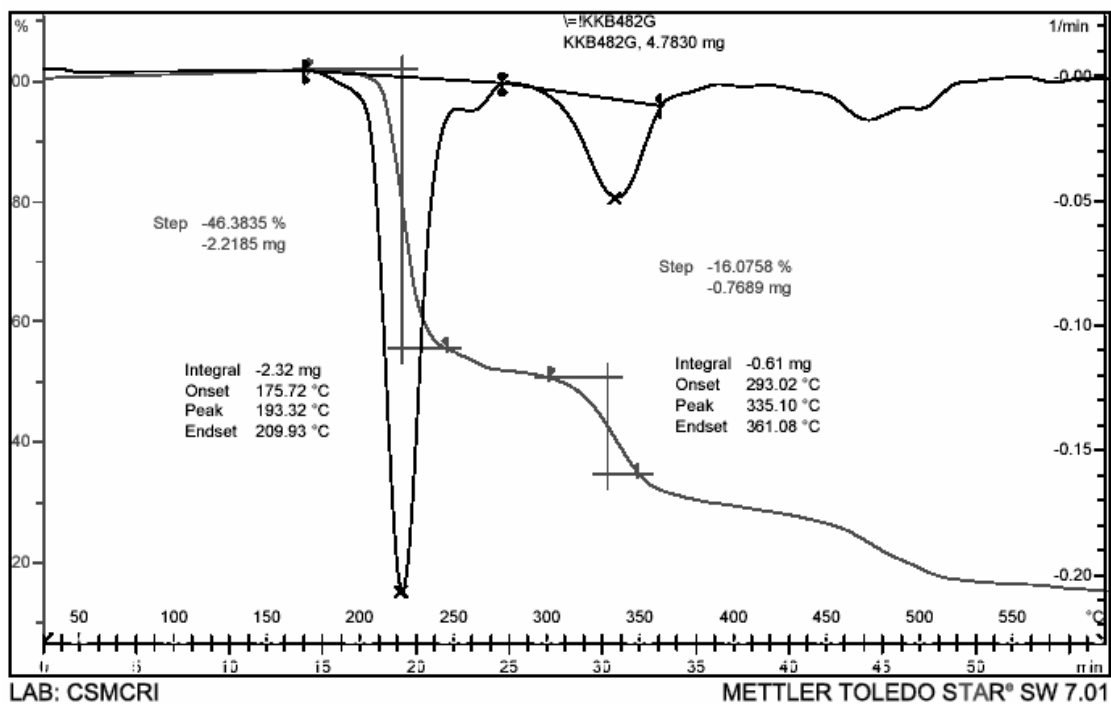
TG curve for the compound 2



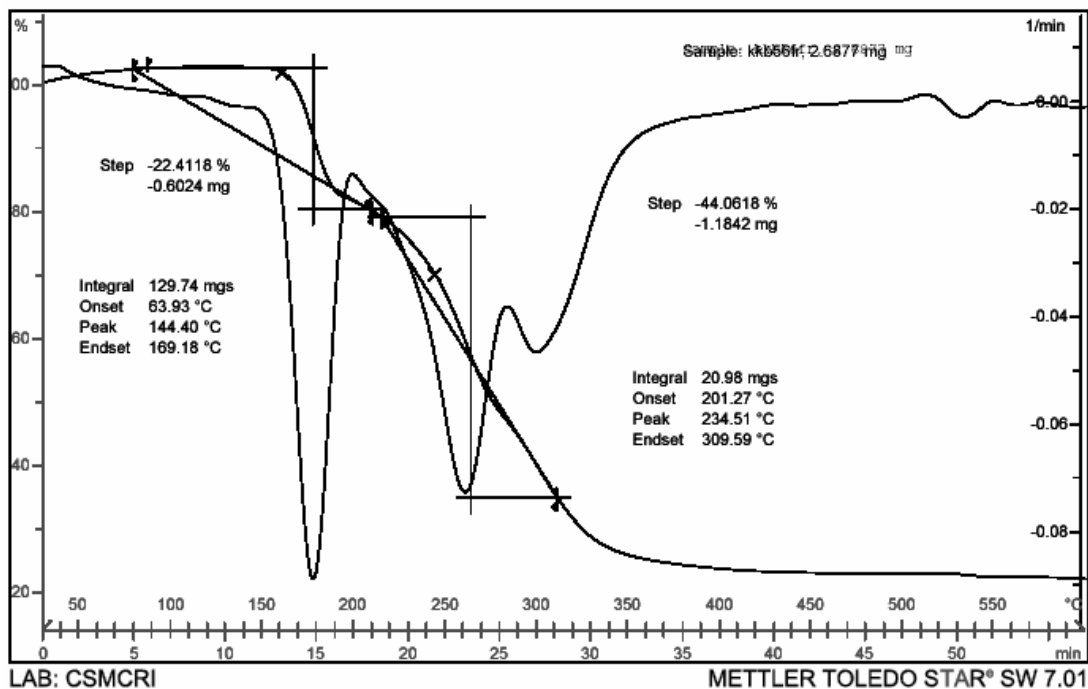
TG curve for the compound 3



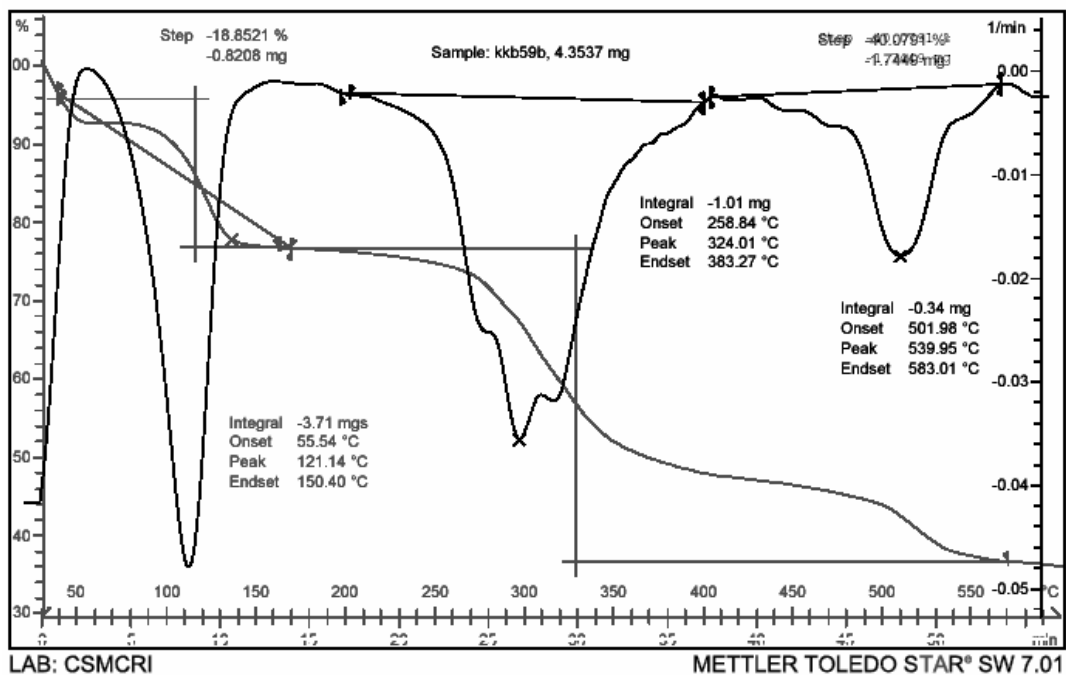
TG curve for the compound 4



TG curve for the compound 5



TG curve for the compound 6



XRPD plots for 1a-6

