Electronic Supporting Information

The Structural Diversity, Band Gap Energy and Photoluminescence Properties of Thiophenedicarboxylate based Coordination Polymers

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Table S1. Crystallographic parameters for compounds **1 - 5** respectively[a].

Parameters	Compound 1	Compound 2	Compound 3	Compound 4	Compound 5
Empirical formula	$C_6H_7Mg_{1.5}O_7S$	$C_{14}H_4Mg_{1.5}NO_8S_2$	$C_{18}H_{18}Mg_2N_2O_{10}S_2$	$C_{26}H_{16}N_3O_{8.50}S\,Zn_2$	$C_7H_2In_{0.50}N_{0.50}O_4S$
Formula weight	259.64	414.77	535.08	701.28	246.56
Crystal System	Monoclinic	Triclinic	Monoclinic	Monoclinic	Tetragonal
Space Group	$P\,2_1/c$ (No.14)	P -1 (No.2)	P 21/n	C 2/c	P 43 22
a(Å)	6.4499 (3)	9.6615 (3)	10.0483(2)	34.681(3)	13.5642(13)
b(Å)	19.1637 (8)	10.4900 (3)	13.4969(3)	15.3678(13)	13.5642(13)
c(Å)	8.0685 (3)	11.9404 (3)	16.7346(4)	13.7141(10)	15.6425(12)
$\alpha(^0)$	90	110.2950 (10)	90	90	90
$\beta(^0)$	96.557	91.8750 (10)	93.6830(10)	112.169(4)	90
$\gamma(^0)$	90	114.8600 (10)	90	90	90
Volume (Å³)	990.77 (7)	1006.93 (5)	2264.87(9)	6768.9(9)	2878.0(6)
Z	4	2	4	8	8
Calculated density (g/cm³)	1.741	1.368	1.569	1.376	1.138
θ range (^{0})	2.125to28.427	1.860 to 28.573	1.940 to 28.320	1.268 to 24.351	3.006 to 28.282
Absorption coefficient (mm^{-1})	0.436	0.349	0.349	1.587	0.992
Reflections collected	9372	17817	22714	21964	13786
Unique reflections	2468	5058	5637	5487	3579
Goodness-of-fit	1.166	1.112	1.039	1.069	1.071
Number of parameters	145	241	311	388	119
Final R indices [I>2sigma(I)]	R1= 0.0392, wR2= 0.1014	R1= 0.0733, wR2= 0.2561	R1=0.0511, wR2= 0.1339	R1=0.0515, wR2 = 0.1855	R1=0.0364, wR2= 0.0959

[a]$R_1 = \Sigma||F_0| - |F_c||/ \Sigma|F_0|$; $wR_2 = \{[w(F_0^2 - F_c^2)^2]/ [w(F_0^2)^2]\}^{1/2}$;

$w = 1/[\sigma^2(F_0)^2 + (aP)^2 + bP]$; $P = [max(F_0^2,0) + 2(F_c)^2]/3$

Table S2: Selected bond lengths of compound **1**.

Compound **1**	Bond Length
Mg(1)-O(2) #1	2.0499(15)
Mg(1)-O(2)	2.0500(15)
Mg(1)-O(1)	2.0711(15)
Mg(1)-O(1) #1	2.0711(15)
Mg(1)-O(7) #2	2.1078(15)
Mg(1)-O(7) #3	2.1078(15)
Mg(2)-O(2) #5	2.0508(17)
Mg(2)-O(2)	2.0550(16
Mg(2)-O(6) #6	2.0787(17)
Mg(2)-O(5)	2.0937(17)
Mg(2)-O(3)	2.5680(17)
Mg(2)-O(4)	2.1861(19)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z   #2 -x-1,-y,-z   #3 -x,-y,-z

#4 x,y+1,z   #5 -x-1,-y,-z+1   #6 x+1,y,z

Table S3: Selected bond lengths of compound **2**.

Compound **2**	Bond Length
Mg(1)-O(3)	1.998(3)
Mg(1)-O(5) #1	2.016(3)
Mg(1)-O(1)	2.043(3)
Mg(1)-O(4)	2.051(3)
Mg(1)-O(2)	2.162(3)
Mg(1)-O(7)	2.220(2)
Mg(2)-O(8) #2	2.056(2)
Mg(2)-O(8)	2.056(2)
Mg(2)-O(6) #3	2.073(2)
Mg(2)-O(6) #1	2.073(2)
Mg(2)-O(7) #2	2.121(2)
Mg(2)-O(7)	2.121(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z   #2 x,-y+1/2,z-1/2   #3 -x,y+1/2,-z+1/2

Table S4: Selected bond lengths of compound **3**.

Compound **3**	Bond Length
Mg(1)-O(2)#2	1.986(2)
Mg(1)-O(5)#3	2.042(2)
Mg(1)-O(6)	2.043(2)
Mg(1)-O(1)	2.044(2)
Mg(1)-O(3)	2.070(2)
Mg(1)-O(4)	2.2124(19)
Mg(1)-Mg(2)	3.4897(12)
Mg(2)-O(8)#3	2.0226(19)
Mg(2)-O(10)	2.040(2)
Mg(2)-O(9)	2.043(2)
Mg(2)-O(7)	2.062(2)
Mg(2)-O(9)#4	2.2004(19)
Mg(2)-O(4)	2.323(2)
Mg(2)-C(3)	2.614(3)
Mg(2)-C(2)	2.714(3)
Mg(2)-O(6)	2.725(3)
Mg(2)-Mg(2)#4	3.2974(17)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,z+1/2   #2 -x+1,-y+1,-z

#3 -x+1/2,y-1/2,-z+1/2   #4 -x+1,-y,-z

#5 -x+1/2,y+1/2,-z+1/2   #6 x-1/2,-y+1/2,z-1/2

Table S5: Selected bond lengths of compound **4**.

Compound **4**	Bond Length
Zn(1)-N(1)	2.019(5)
Zn(1)-O(8)	2.028(4)
Zn(1)-O(1)	2.031(4)
Zn(1)-O(5)	2.030(4)
Zn(1)-O(4)	2.067(5)
Zn(1)-Zn(2)	3.0152(9)
Zn(2)-N(2)	2.029(5)
Zn(2)-O(7)	2.030(4)
Zn(2)-O(6)	2.034(4)
Zn(2)-O(3)	2.044(4)
Zn(2)-O(2)	2.048(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y,z+1/2   #2 x,-y+1,z+1/2   #3 x,-y+1,z-1/2

#4 x,-y,z-1/2   #5 x-1/2,-y+1/2,z-1/2

#6 x+1/2,-y+1/2,z+1/2   #7 -x,y,-z+1/2

Table S6: Selected bond lengths of compound **5**.

Compound **5**	Bond Length
In(1)-O(2)#1	2.212(4)
In(1)-O(2)	2.212(4)
In(1)-O(3)	2.231(4)
In(1)-O(3)#1	2.231(4)
In(1)-O(4)	2.328(4)
In(1)-O(4)#1	2.329(4)
In(1)-O(1)#1	2.375(4)
In(1)-O(1)	2.375(4)
In(1)-C(1)#1	2.631(5)
In(1)-C(1)	2.631(5)
In(1)-C(2)#1	2.634(6)
In(1)-C(2)	2.634(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z   #2 -y+1,x-1,z-1/4   #3 y+1,-x+1,z+1/4   #4 x,-y,-z+1/2

Topos for compound **1**

Topology for Mg1

Atom Mg1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 2	-0.4742	0.9819	-0.3155	(-1 1-1)	9.967A	1
Mg 2	0.4742	0.0181	0.3155	(1-1 0)	9.967A	1
Mg 1	0.0000	1.0000	-0.5000	(0 0-1)	10.396A	1
Mg 1	0.0000	0.0000	0.5000	(0-1 0)	10.396A	1
Mg 1	0.0000	0.0000	-0.5000	(0-1-1)	10.396A	1
Mg 1	0.0000	1.0000	0.5000	(0 0 0)	10.396A	1
Mg 2	0.5258	-0.0181	-0.3155	(0 0-1)	10.887A	1
Mg 2	-0.5258	1.0181	0.3155	(0 0 0)	10.887A	1

Common edge with					R(A-A)	
Mg 2	0.5258	0.5181	0.1845	(0 0 0)	3.562A	2
Mg 2	-0.5258	0.4819	-0.1845	(0 1 0)	3.562A	2
Mg 2	0.4742	0.4819	-0.1845	(1 1 0)	3.568A	2
Mg 2	-0.4742	0.5181	0.1845	(-1 0 0)	3.568A	2

Topology for Mg2

Atom Mg2 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 2	0.4742	1.0181	0.3155	(1 0 0)	9.650A	1
Mg 2	0.4742	0.0181	0.3155	(1-1 0)	9.650A	1
Mg 1	1.0000	1.0000	0.5000	(1 0 0)	9.967A	1
Mg 1	0.0000	0.0000	0.5000	(0-1 0)	10.887A	1

Common edge with					R(A-A)	
Mg 2	0.4742	0.4819	-0.1845	(1 1 0)	3.038A	2
Mg 1	0.0000	0.5000	0.0000	(0 0 0)	3.562A	2
Mg 1	1.0000	0.5000	0.0000	(1 0 0)	3.568A	2

Structural group analysis

Structure consists of 3D framework with S2Mg3O14C12H14

Coordination sequences

Mg1: 1 2 3 4 5 6 7 8 9 10

Num 12 48 118 192 330 432 650 768 1078 1200

Cum 13 61 179 371 701 1133 1783 2551 3629 4829

Mg2: 1 2 3 4 5   6   7   8   9   10

Num   7 37 100 194 290 456 576 826 958 1304

Cum   8 45 145 339 629 1085 1661 2487 3445 4749

TD10=4775

Vertex symbols for selected sublattice

Mg1 Point symbol:{3^14.4^18.5^18.6^14.7^2}

Extended point
symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.5(3).5(3).5(3).5(3).5(4).5(4).5(4).5(4).5(
3).5(3).5(3).5(3).4.4.4.4.5.5.5.5.5(2).5(2).6(4).6(4).6(4).6(4).6(4).6(4).6(4).6(4).6(6).6(6).6(8).6(8).6(8
).6(8).7(10).7(10)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.5.5.5.5.5.5.5.5.5.5.5.5.5(2).5(2).5(2).5(2).*.*.*.*.*.*.*.
..*.*.*.*.*.*.*.*.*.*.*.*.*.*.*.*]

Rings with types:
[3a.3b.3c.3a.3b.3c.3b.3a.3d.3b.3a.3d.3e.3e.4a.4a.4b.4c.4a.4a.4b.4c.4b.4b.5c.5c.5e.5e.5a.5a.5a.5a.5b.5
d.5b.5d.(5c,5d).(5c,5d).(5b,5e).(5b,5e).*]

Mg2 Point symbol:{3^8.4^8.5^5}

Extended point symbol:[3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.5(4).5(4).4.5(4).5(4).5(2)]

Vertex symbol: [3.3.3.3.3.3.3.3.4.4.4.5.5.5.5.5.5.5(2).5(2).5(2).*]

Rings with types: [3c.3a.3d.3d.3b.3c.3e.3e.4c.4b.4b.5a.5f.5a.5f.5c.5e.(5c,5e).(5d,5f).(5b,5f).*]

Point symbol for net: {3^14.4^18.5^18.6^14.7^2}{3^8.4^8.5^5}2

7,12-c net with stoichiometry (7-c)2(12-c); 2-nodal net

Topos for compound **2**

Topology for Mg1

Atom Mg1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 1	-0.4714	0.0844	0.3266	(-1 0 0)	9.661A	1
Mg 1	1.5286	0.0844	0.3266	(1 0 0)	9.661A	1
Mg 2	-0.5000	0.0000	0.0000	(-1 0 0)	10.120A	1
Mg 2	0.5000	1.0000	1.0000	(0 1 1)	10.285A	1
Mg 1	0.5286	-0.9156	0.3266	(0-1 0)	10.490A	1
Mg 1	0.5286	1.0844	0.3266	(0 1 0)	10.490A	1
Mg 2	1.5000	0.0000	0.0000	(1 0 0)	10.538A	1
Mg 2	0.5000	-1.0000	0.0000	(0-1 0)	10.545A	1

Common edge with					R(A-A)	
Mg 1	0.4714	-0.0844	0.6734	(1 0 1)	5.001A	2
Mg 1	0.4714	0.9156	0.6734	(1 1 1)	8.522A	2

Common face with					R(A-A)	
Mg 2	0.5000	0.0000	0.0000	(0 0 0)	3.660A	3

Topology for Mg2

Atom Mg2 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 1	-0.5286	-0.0844	-0.3266	(0 0 0)	10.120A	1
Mg 1	1.5286	0.0844	0.3266	(1 0 0)	10.120A	1
Mg 1	0.5286	-0.9156	-0.6734	(0-1-1)	10.285A	1
Mg 1	0.4714	0.9156	0.6734	(1 1 1)	10.285A	1
Mg 1	1.4714	-0.0844	-0.3266	(2 0 0)	10.538A	1
Mg 1	-0.4714	0.0844	0.3266	(-1 0 0)	10.538A	1
Mg 1	0.4714	-1.0844	-0.3266	(1-1 0)	10.545A	1
Mg 1	0.5286	1.0844	0.3266	(0 1 0)	10.545A	1

Common edge with					R(A-A)	
Mg 2	-0.5000	0.0000	0.0000	(-1 0 0)	9.661A	2
Mg 2	1.5000	0.0000	0.0000	(1 0 0)	9.661A	2

Common face with   R(A-A)

Mg 1   0.4714   -0.0844   -0.3266   (1 0 0)   3.660A   3

Mg 1   0.5286   0.0844   0.3266   (0 0 0)   3.660A   3

Structural group analysis

Structure consists of 3D framework with S4Mg3O16C24H8

Coordination sequences

Mg1: 1 2   3   4   5   6   7   8   9   10

Num 11 46 95 178 263 398 515 706 851 1102

Cum 12 58 153 331 594 992 1507 2213 3064 4166

Mg2: 1 2   3   4   5   6   7   8   9   10

Num 12 44 102 170 278 380 542 674 894 1052

Cum 13 57 159 329 607 987 1529 2203 3097 4149

TD10=4160

Vertex symbols for selected sublattice

Mg1 Point symbol:{3^15.4^33.5^7}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(3).4.5(4).5(4).5(6).5(6).5(8).4.4.4.4.4.4.4.4.4.4.5.5(2)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).5.5.5.5.5.5(2).5(3).*.*.*.*.*.*.*.*.*.*.*]

Mg2 Point symbol:{3^18.4^36.5^11.6}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4.4.4.4.5(2).5(2).5(6).5(6).5(3).5(3).5(3).5(3).4.4.4.4.4.4.4(2).4(2).5(2).5(2).5(2).6(16)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).5.5.5.5.5.5.5.5.6.6.6.6.6(2).6(2).*.*.*.*.*.*.*.*.*]

Point symbol for net: {3^15.4^33.5^7}2{3^18.4^36.5^11.6}

11,12-c net with stoichiometry (11-c)2(12-c); 2-nodal net

Topos for compound **3**

Atom Mg1 links by bridge ligands and has

Common vertex with   R(A-A)   f

Mg 2   0.4707   -0.1029   -0.0512   (1 0 0)   6.205A   1

Mg 2   0.0293   0.3971   -0.4488   (-1 0-1)   8.610A   1

Mg 2   -0.0293   0.6029   0.4488   (0 0 0)   9.254A   1

Mg 2   0.9707   0.6029   0.4488   (1 0 0)   9.445A   1

Mg 1   0.9078   0.1562   0.5257   (0 0 0)   9.811A   1

Mg 1   -0.0922   0.1562   -0.4743   (-1 0-1)   9.811A   1

Mg 1   0.9078   0.1562   -0.4743   (0 0-1)   10.347A   1

Mg 1   -0.0922   0.1562   0.5257   (-1 0 0)   10.347A   1

Mg 2   1.0293   0.3971   -0.4488   (0 0-1)   10.437A   1

Mg 2   1.0293   0.3971   0.5512   (0 0 0)   10.479A   1

Mg 1   0.0922   -0.1562   0.4743   (0-1 0)   10.724A   1

Mg 1   0.0922   0.8438   0.4743   (0 0 0)   10.724A   1

Common edge with   R(A-A)

Mg 1   0.5922   0.6562   -0.0257   (1 1 0)   4.708A   2

Common face with   R(A-A)

Mg 2   0.5293   0.1029   0.0512   (0 0 0)   3.490A   3

Topology for Mg2

Atom Mg2 links by bridge ligands and has

Common vertex with   R(A-A)   f

Mg 1   0.5922   -0.3438   -0.0257   (1 0 0)   6.205A   1

Mg 1   0.9078   0.1562   0.5257   (0 0 0)   8.610A   1

Mg 1   0.0922   -0.1562   0.4743   (0-1 0)   9.254A   1

Mg 1   1.0922   -0.1562   0.4743   (1-1 0)   9.445A   1

Mg 2   0.0293   0.3971   -0.4488   (-1 0-1)   10.277A   1

Mg 2   1.0293   0.3971   0.5512   (0 0 0)   10.277A   1

Mg 2   0.9707   -0.3971   0.4488   (1-1 0)   10.280A   1

Mg 2   0.9707   0.6029   0.4488   (1 0 0)   10.280A   1

Mg 1   -0.0922   0.1562   0.5257   (-1 0 0)   10.437A   1

Mg 1   -0.0922   0.1562   -0.4743   (-1 0-1)   10.479A   1

Common edge with   R(A-A)

Mg 2   0.4707   -0.1029   -0.0512   (1 0 0)   3.297A   2

Common face with   R(A-A)

Mg 1   0.4078   0.3438   0.0257   (0 0 0)   3.490A   3

Structural group analysis

Structural group No 1

Structure consists of 3D framework with SMgO5NC9H9

Coordination sequences

Mg1: 1 2 3 4 5 6 7 8 9 10

Num 14 55 124 225 351 503 690 900 1137 1409

Cum 15 70 194 419 770 1273 1963 2863 4000 5409

Rad 8.9(2.4) 14.8(3.7) 21.5(4.2) 28.5(4.9) 35.6(5.7) 42.7(6.5) 49.7(7.4) 56.8(8.3) 63.9(9.3) 71.0(10.2)

Cmp Mg14 Mg55 Mg124 Mg225 Mg351 Mg503 Mg690 Mg900 Mg1137 Mg1409

Mg2: 1 2 3 4 5 6 7 8 9 10

Num 12 52 122 224 347 505 685 899 1137 1407

Cum 13 65 187 411 758 1263 1948 2847 3984 5391

Rad 8.5(2.7) 14.4(3.5) 21.2(4.2) 28.1(4.8) 35.3(5.5) 42.4(6.4) 49.5(7.3) 56.7(8.2) 63.8(9.1) 70.9(10.1)

Cmp Mg12 Mg52 Mg122 Mg224 Mg347 Mg505 Mg685 Mg899 Mg1137 Mg1407

TD10=5400

Vertex symbols for selected sublattice

Mg1 Point symbol:{3^25.4^55.5^11}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4.4.4.4.4.5(8).4.4.4.4.4(2).5(6).5(8).5(12).4.4.4.4.5.4.4.4.4.4.4.4.4.4.4(2).4(2).5.5(4).5(4).5(5).5(7).5(10)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).5.5.5.5.5.5.5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(3).5(6).6.6.6.*.*.*.*.*.*.*.*.*.*.*.*.*.*.*]

Rings with types:
[3a.3b.3c.3d.3e.3f.3g.3h.3b.3i.3j.3g.3k.3d.3e.3l.3m.3n.3n.3o.3l.3i.3m.3n.3o.4h.4i.4i.4o.4n.4r.4d.4e.4f.4g.4g.4p.4k.4m.4l.4g.4p.4e.4a.(4j,4k).(4f,4l).(4f,4j).(4d,4m).(4b,4c).(4m,4n).(4d,4l).(4b,4q).(4k,4l).(4i,4o).(4p,4r).5a.5b.5f.5j.5h.5i.(5c,5d).(5e,5f).(5k,5l).(5q,5v).(5t,5u).(5w,5x).(5g,5h).(5c,5v).(5n,5r,5s).(5j,5m,5n,5o,5p,5q).6a.6b.6b.*.*.*.*.*.*.*.*.*.*.*.*.*.*.*.*]

ATTENTION! Some rings * are bigger than 6, so likely no rings are contained in that angle

Mg2 Point symbol:{3^23.4^39.5^4}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).4.4.4.4.4.4.4.4(2).5(7).4.4.4(2).4(2).4.4.5(5).4.5(4).4.4.4.4.4.4.4.4.5(6)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).5.5.5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(3).5(4).5(4).5(4).6.6.6(2).6(3).6(3).*.*.*.*.*.*.*.*]

Rings with types:
[3h.3b.3j.3i.3c.3p.3a.3d.3p.3a.3j.3f.3k.3e.3p.3h.3c.3k.3f.3g.3m.3o.3l.4s.4c.4g.4a.4e.4e.4a.4j.4f.4j.4p.(4b,4d).(4a,4s).(4h,4i).(4m,4q).(4b,4k).5n.5p.(5n,5o).(5aa,5ab).(5b,5e).(5c,5m).(5e,5f).(5r,5t).(5x,5y).(5b,5e,5w).(5j,5p,5s,5u).(5c,5d,5v,5z).(5aa,5ab,5r,5t).6f.6a.(6b,6d).(6c,6d,6e).(6a,6b,6e).*.*.*.*.*.*.*.*.*.*]

Point symbol for net: {3^23.4^39.5^4}{3^25.4^55.5^11}

12,14-c net with stoichiometry (12-c)(14-c); 2-nodal net

Topos for compound **4**

Atom Zn1 links by bridge ligands and has

Common vertex with   R(A-A)   f

Zn 1	0.1120	-0.2207	0.5658	(0 0 0)	9.645A	1
Zn 1	0.1120	-0.2207	-0.4342	(0 0 -1)	9.645A	1
Zn 2	0.2015	0.7202	0.6449	(0 1 0)	10.631A	1
Zn 2	0.2015	-0.2798	0.6449	(0 0 0)	10.642A	1
Zn 2	0.2015	0.7202	-0.3551	(0 1 -1)	10.743A	1
Zn 2	0.2015	-0.2798	-0.3551	(0 0 -1)	10.753A	1
Zn 1	0.1120	0.7793	0.5658	(0 1 0)	10.987A	1
Zn 1	0.1120	0.7793	-0.4342	(0 1 -1)	10.987A	1
Zn 2	-0.2985	0.2202	-0.3551	(-1 0 -1)	13.191A	1

Common face with   R(A-A)

Zn 2	0.2015	0.2798	0.1449	(0 0 0)	3.015A	4

Topology for Zn2

Atom Zn2 links by bridge ligands and has

Common vertex with   R(A-A)   f

Zn 2	0.2015	0.7202	0.6449	(0 1 0)	9.635A	1
Zn 2	0.2015	0.7202	-0.3551	(0 1 -1)	9.635A	1
Zn 1	0.1120	0.7793	-0.4342	(0 1 -1)	10.631A	1
Zn 1	0.1120	-0.2207	-0.4342	(0 0 -1)	10.642A	1
Zn 1	0.1120	0.7793	0.5658	(0 1 0)	10.743A	1
Zn 1	0.1120	-0.2207	0.5658	(0 0 0)	10.753A	1
Zn 2	0.2015	-0.2798	-0.3551	(0 0 -1)	10.998A	1
Zn 2	0.2015	-0.2798	0.6449	(0 0 0)	10.998A	1
Zn 1	0.6120	0.2793	0.5658	(0 0 0)	13.191A	1

Common face with   R(A-A)

Zn 1	0.1120	0.2207	0.0658	(0 0 0)	3.015A	4

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZnSO4NC12H8

There are 2 interpenetrating nets

FISE: Full interpenetration symmetry elements

1: -1

2: 2[0,1,0]

Symmetry operations

1-2 nets

1: (-x,y,1/2-z)   2[0,1,0]

2: (-x,y,1/2-z;1/2,1/2,0)   2[0,1,0]

3: (-x,-y,-z)   -1

4: (-x,-y,-z;1/2,1/2,0)   -1

PIC: [0,0,1][0,1,0][1/2,1/2,0] (PICVR=1)

Z_t=1; Z_n=2

Class IIa Z=2

Coordination sequences

Zn1: 1 2 3 4 5 6 7 8 9 10

Num 10 30 66 114 178 254 346 450 570 702

Cum 11 41 107 221 399 653 999 1449 2019 2721

Rad 10.0(2.6) 17.8(2.5) 24.9(3.7) 32.8(4.1) 40.4(4.9) 48.3(5.5) 56.1(6.3) 64.1(6.9) 71.9(7.7) 79.8(8.4)

Cmp Zn10 Zn30 Zn66 Zn114 Zn178 Zn254 Zn346 Zn450 Zn570 Zn702

Zn2: 1 2 3 4 5 6 7 8 9 10

Num 10 30 66 114 178 254 346 450 570 702

Cum 11 41 107 221 399 653 999 1449 2019 2721

Rad 10.0(2.6) 17.8(2.5) 24.9(3.7) 32.8(4.1) 40.4(4.9) 48.3(5.5) 56.1(6.3) 64.1(6.9) 71.9(7.7) 79.8(8.4)

Cmp Zn10 Zn30 Zn66 Zn114 Zn178 Zn254 Zn346 Zn450 Zn570 Zn702

TD10=2721

Vertex symbols for selected sublattice

Zn1 Point symbol:{3^12.4^28.5^5}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4.4.5.5.5.5.4.4.4.4.4.4.5(4)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).6.6.6(7).6(7).6(7).6(7).*.*.*.*.*.*]

Rings with types:
[3a.3b.3c.3b.3a.3d.3e.3f.3g.3h.3e.3g.4e.4e.4p.4p.(4a,4b).(4c,4d).(4a,4f).(4b,4g).(4f,4g).(4h,4i).(4j,4k).(4l,4m).(4a,4c).(4b,4d).(4j,4n).(4l,4o).(4i,4q).(4g,4m).(4d,4o).(4b,4l).6d.6h.(6a,6b,6c,6d,6e,6f,6g).(6e,6f,6g,6h,6i,6j,6k).(6a,6b,6c,6h,6l,6m,6n).(6d,6i,6j,6k,6l,6m,6n).*.*.*.*.*.*.*]

ATTENTION! Some rings * are bigger than 6, so likely no rings are contained in that angle

Zn2 Point symbol:{3^12.4^28.5^5}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4.4.5.5.5.5.4.4.4.4.4.4.5(4)]

Vertex symbol:
[3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).6.6.6(7).6(7).6(7).6(7).*.*.*.*.*.*.*]

Rings with types:
[3c.3a.3d.3d.3b.3c.3h.3f.3g.3h.3e.3f.4p.4p.4e.4e.(4j,4l).(4k,4m).(4f,4h).(4g,4i).(4n,4o).(4q,4r).(4k,4r).(4m,4q).(4c,4h).(4d,4i).(4n,4r).(4o,4q).(4h,4r).(4f,4k).(4c,4n).(4a,4j).6d.6h.(6a,6d,6g,6i,6n,6o,6p).(6c,6g,6h,6j,6n,6p,6q).(6c,6d,6e,6j,6l,6q,6r).(6a,6e,6h,6i,6l,6o,6r).*.*.*.*.*.*.*]

Point symbol for net: {3^12.4^28.5^5}

10-c net; uninodal net

Topos for compound **5**

Atom In1 links by bridge ligands and has

Common vertex with   R(A-A)   f

In 1   -0.0766   0.5000   -0.2500   (0 1-1)   10.462A   1

In 1   1.0766   0.5000   0.2500   (1 0 0)   10.462A   1

In 1   0.0766   -0.5000   0.2500   (0-1 0)   10.462A   1

In 1   0.9234   -0.5000   -0.2500   (1 0-1)   10.462A   1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with InS2O8C12H4

There are 2 interpenetrating nets

FIV: Full interpenetration vectors

 [0,1,0] (13.56A)

[1,0,0] (13.56A)

[0,1,1] (20.70A)

[0,1,-1] (20.70A)

[1,0,1] (20.70A)

[1,0,-1] (20.70A)

PIC: [0,2,0][0,0,1][1,1,0] (PICVR=2)

Zt=2; Zn=1

Class Ia Z=2

Coordination sequences

In1: 1 2 3 4 5 6 7 8 9 10

Num   4 12 24 42 64 92 124 162 204 252

Cum   5 17 41 83 147 239 363 525 729 981

Rad 10.5(0.0) 16.9(2.0) 22.8(4.4) 29.6(5.0) 36.1(6.2) 43.1(6.8) 49.8(8.0) 56.9(8.7) 63.7(9.8) 70.7(10.7)

Cmp In4 In12 In24 In42 In64 In92 In124 In162 In204 In252

TD10=981

Vertex symbols for selected sublattice

In1 Point symbol:{6^6}

Extended point symbol:[6(2).6(2).6(2).6(2).6(2).6(2)]

Rings coincide with circuits

Rings with types: [6a(2).6a(2).6a(2).6a(2).6a(2).6a(2)]

Point symbol for net: {6^6}

4-c net; uninodal net
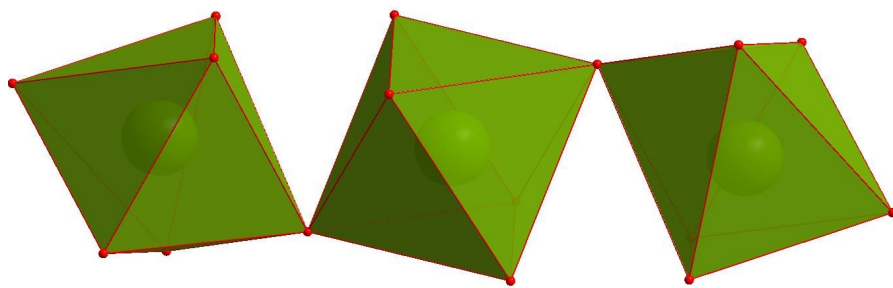
Fig. S1. The Mg$_3$O$_{16}$ cluster present in compound **2**. Green: Mg and Red; Oxygen ions, respectively.
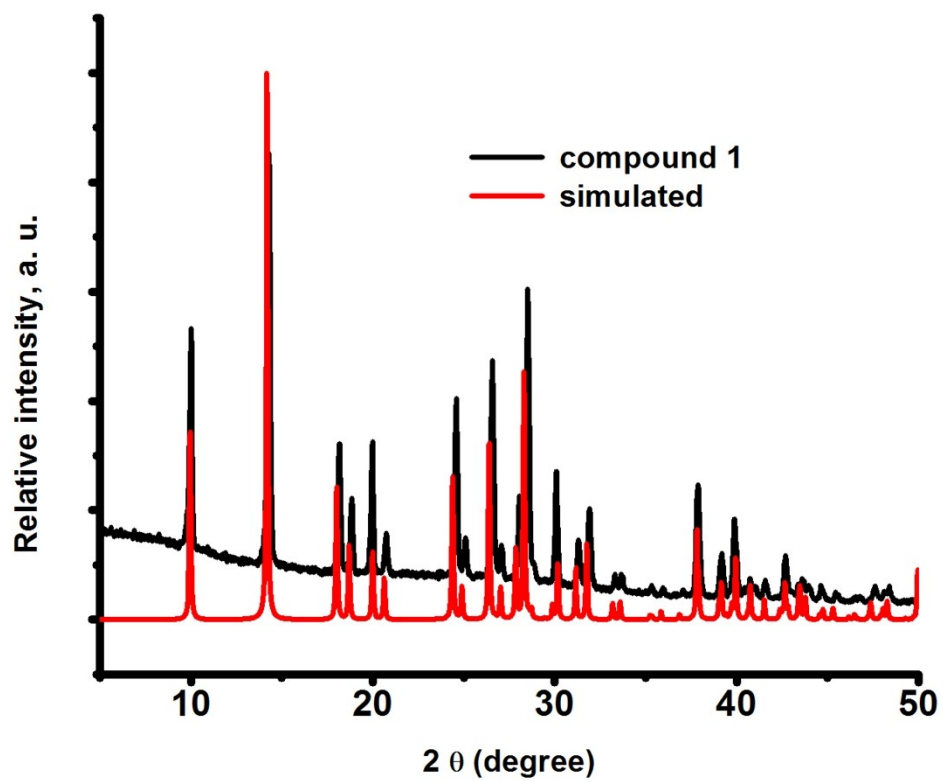
Fig. S2. Powder XRD pattern of compound **1**.
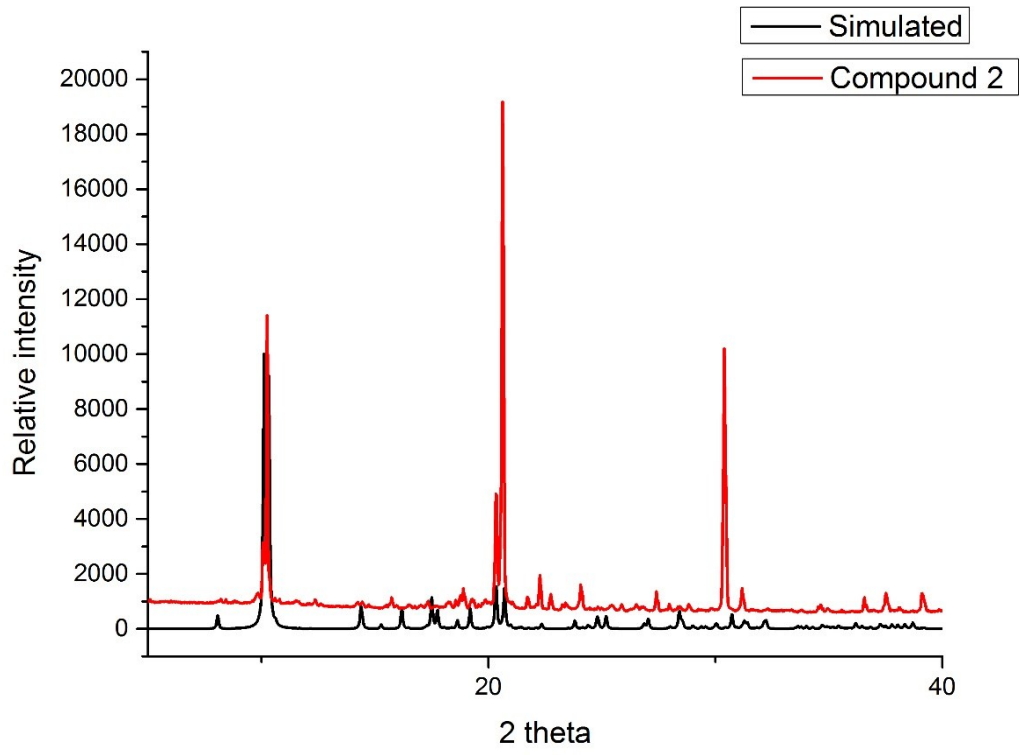
Fig. S3. Powder XRD pattern of compound **2**.
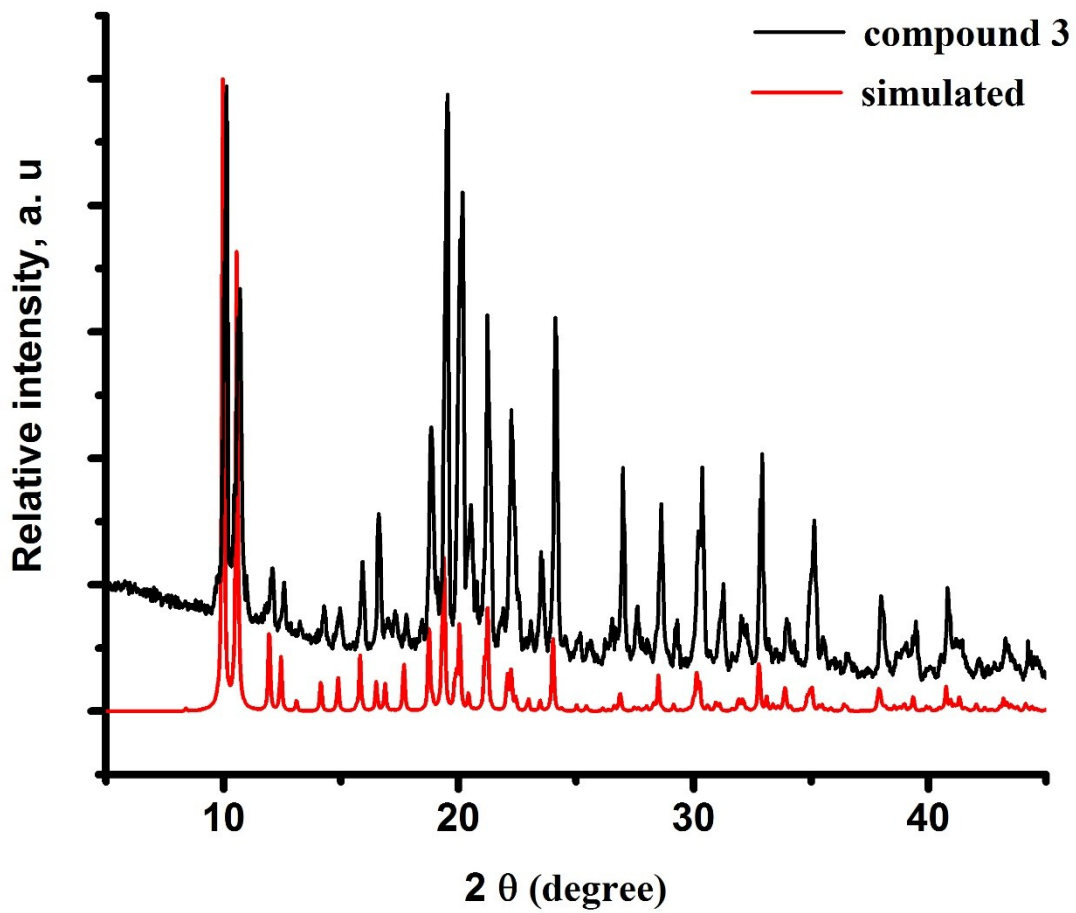
Fig. S4. Powder XRD pattern of compound **3**.
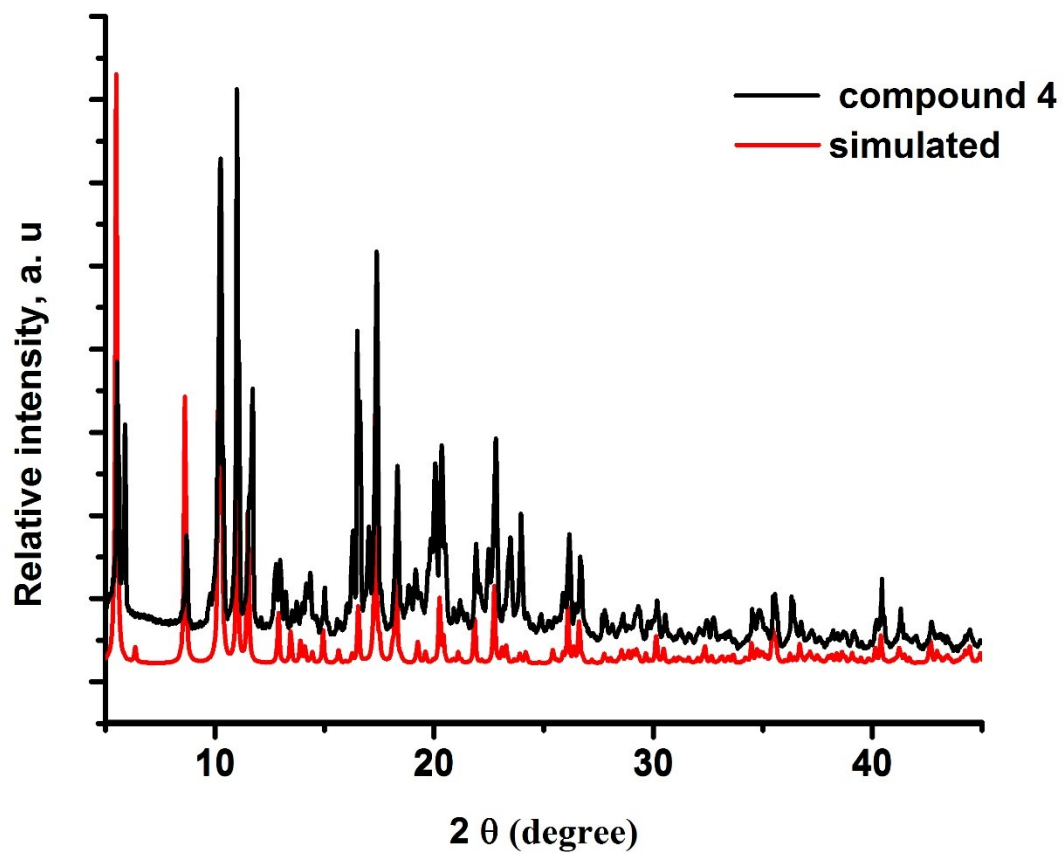
Fig S5. Powder XRD pattern of compound **4**.
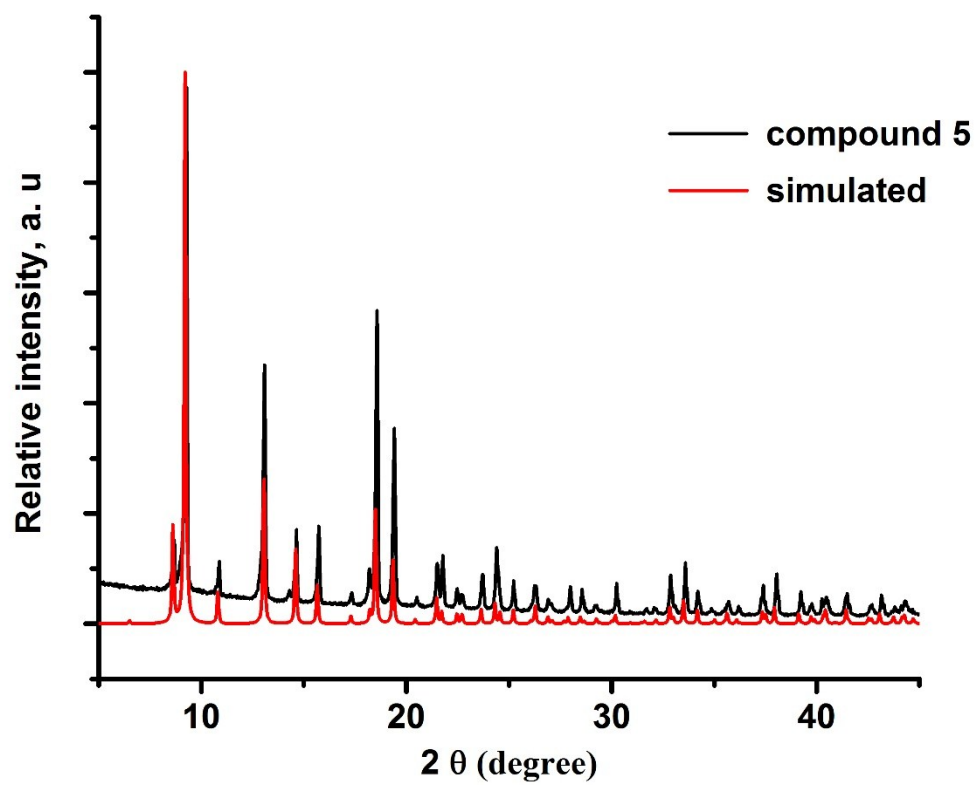
Fig S6. Powder XRD pattern of compound **5**.
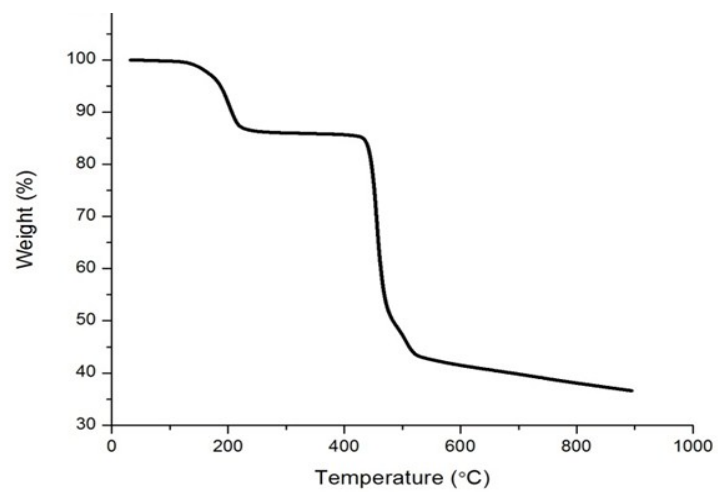
Fig. S7.Thermogravimetric analysis plot of compound **1**.
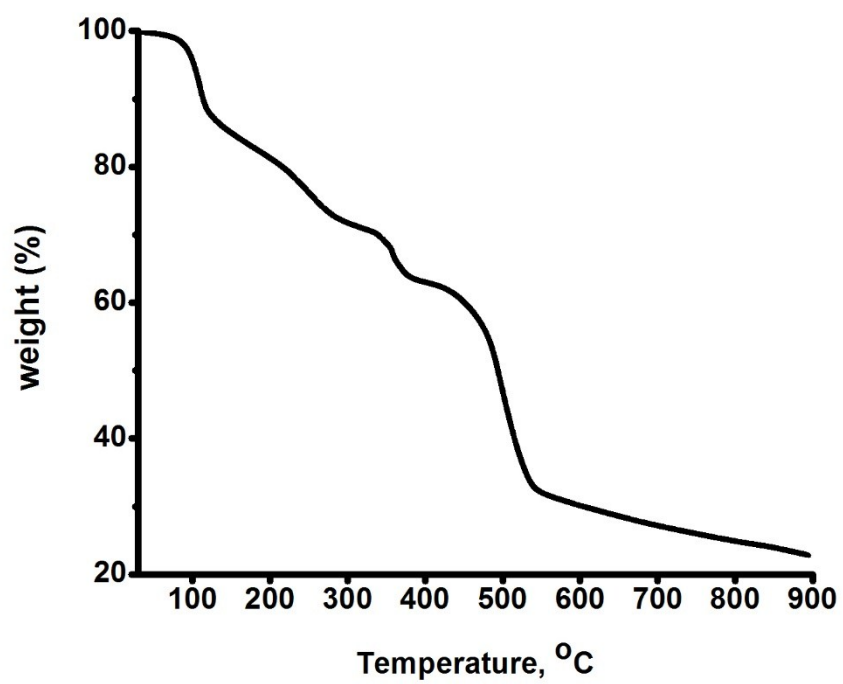
Fig. S8.Thermogravimetric analysis plot of compound **2**.
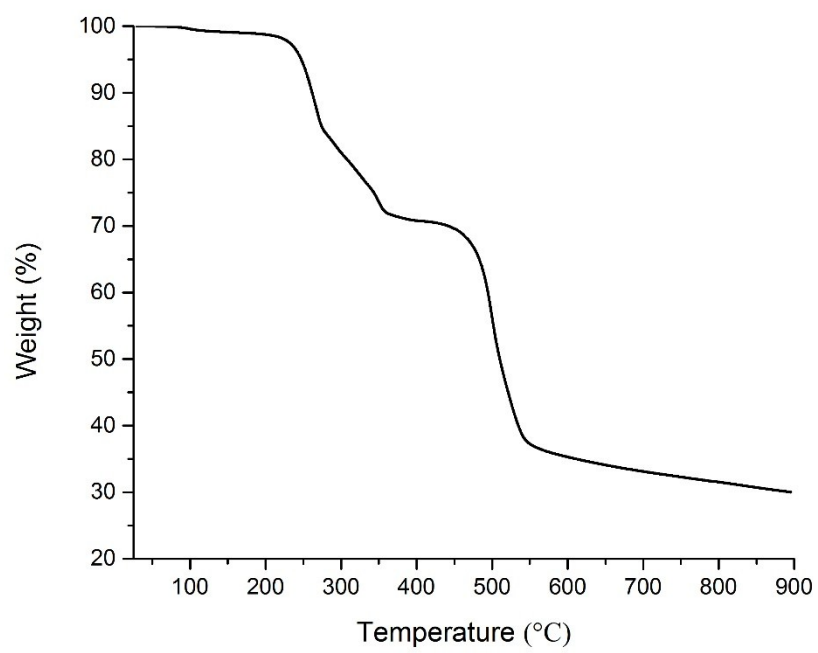
Fig. S9.Thermogravimetric analysis plot of compound **3**.
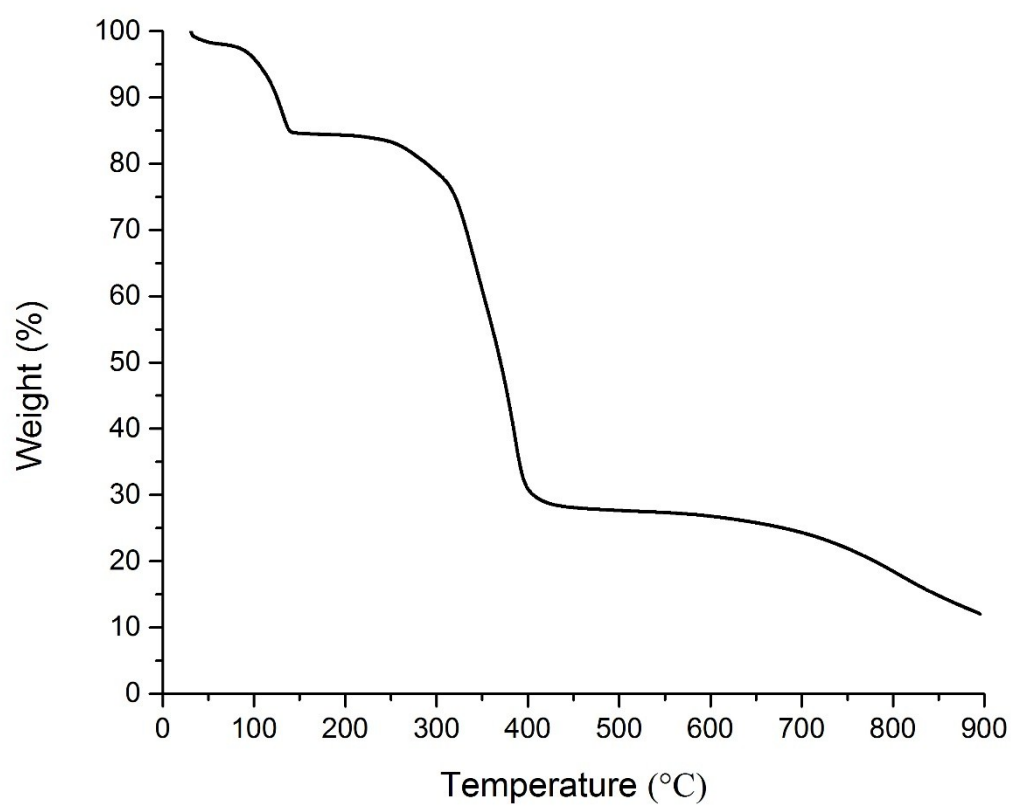
Fig. S10.Thermogravimetric analysis plot of compound **4**.
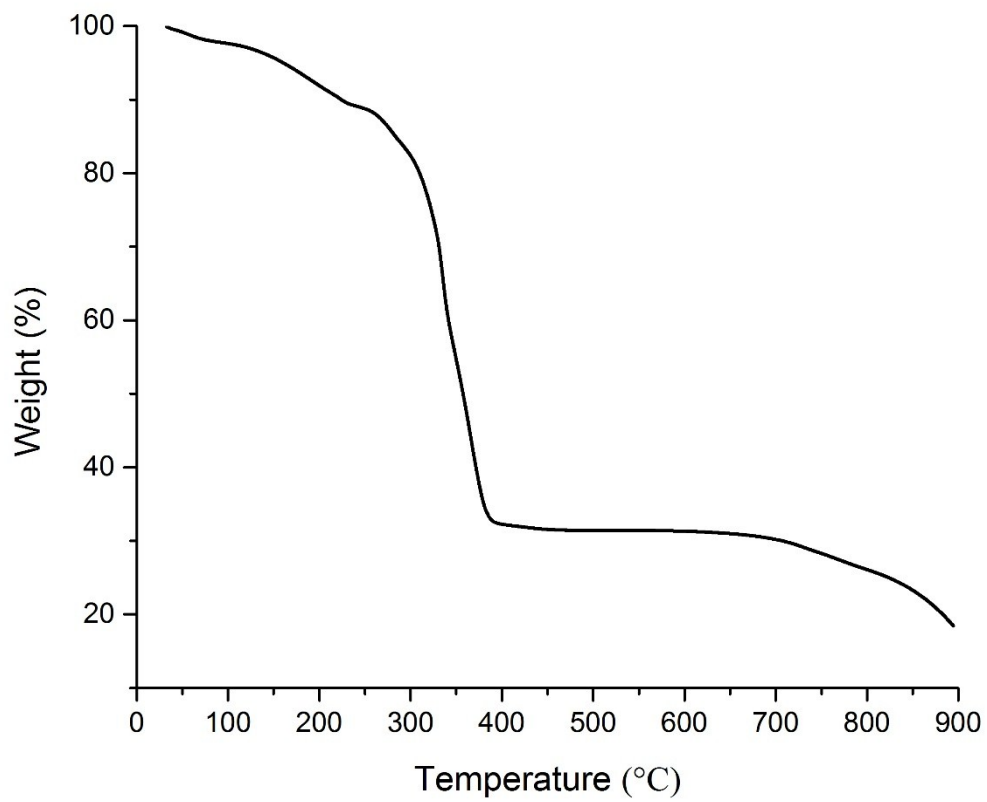
Fig. S11.Thermogravimetric analysis plot of compound **5**.
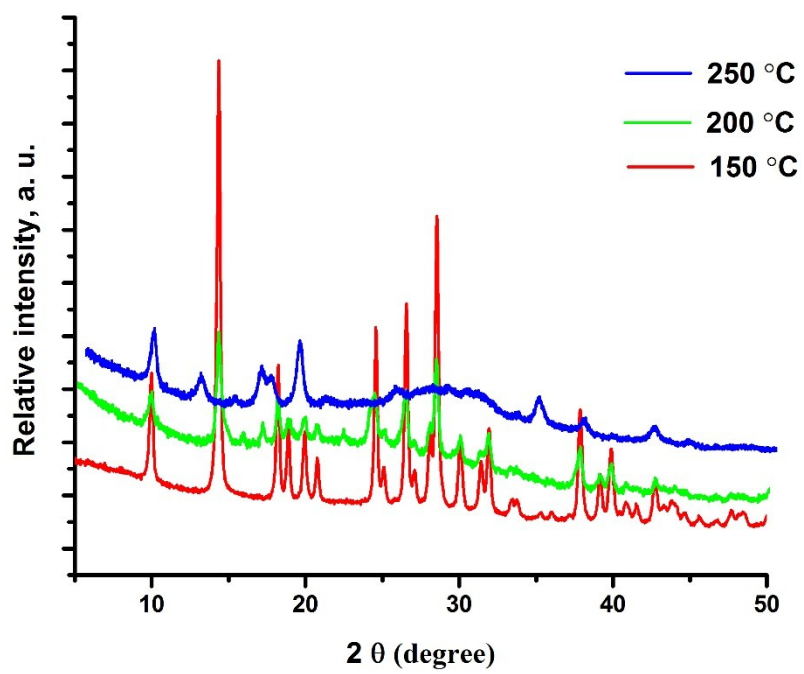
Fig. S12. PXRD pattern at different temperatures for compound **1**.
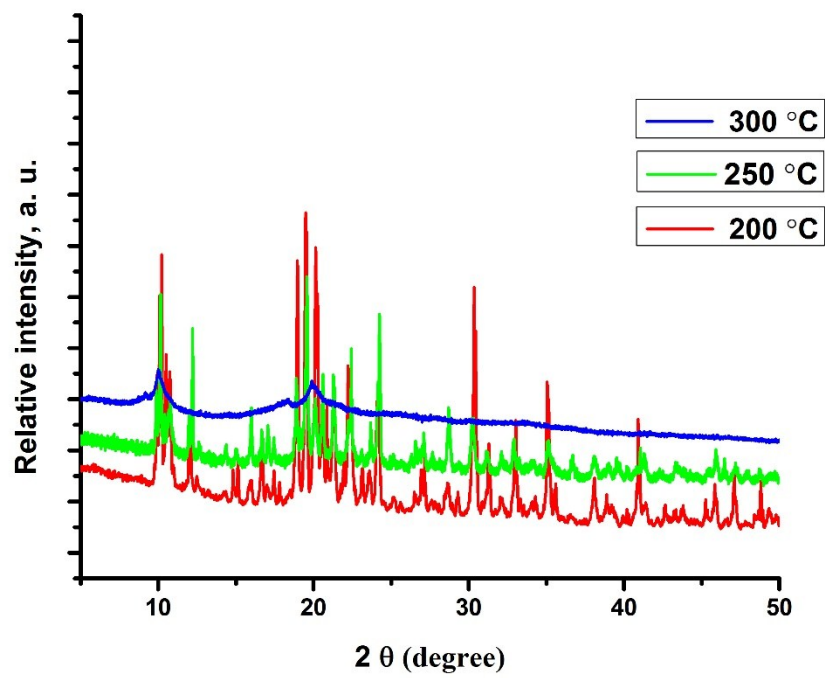
Fig. S13. PXRD pattern at different temperatures for compound **3**.
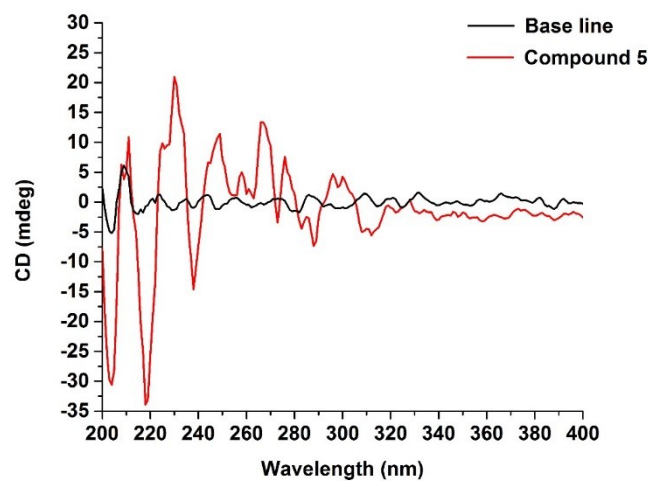
Fig. S14. The solid CD spectra of compound **5** (red line) and KBr pellet (black line).
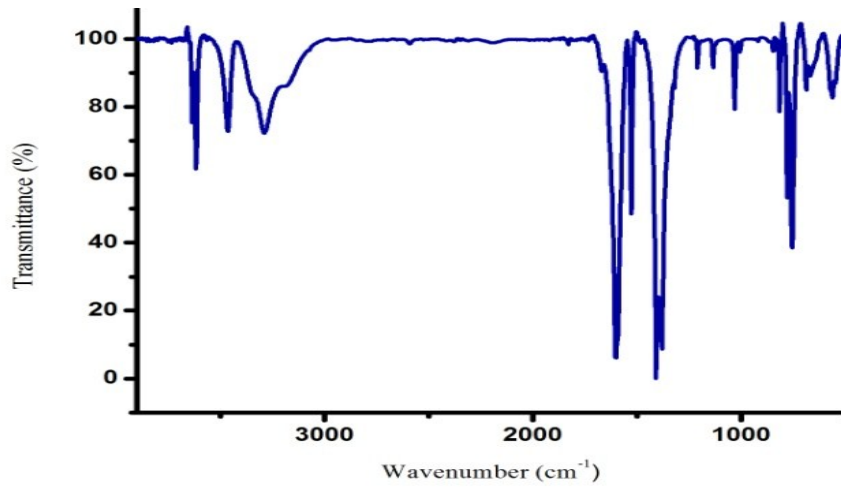
Fig. S15. Characteristic IR spectra of compound **1**.
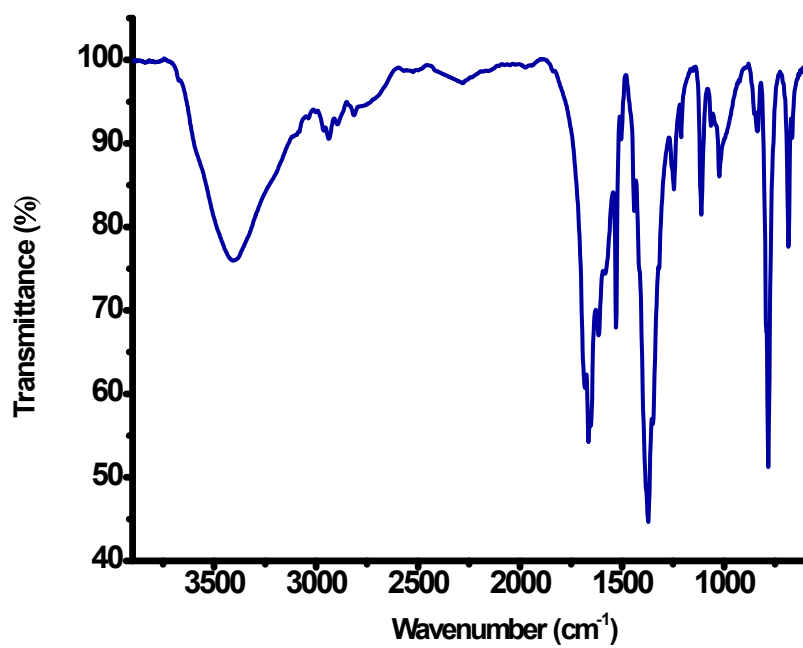
Fig. S16. Characteristic IR spectra of compound **2**.
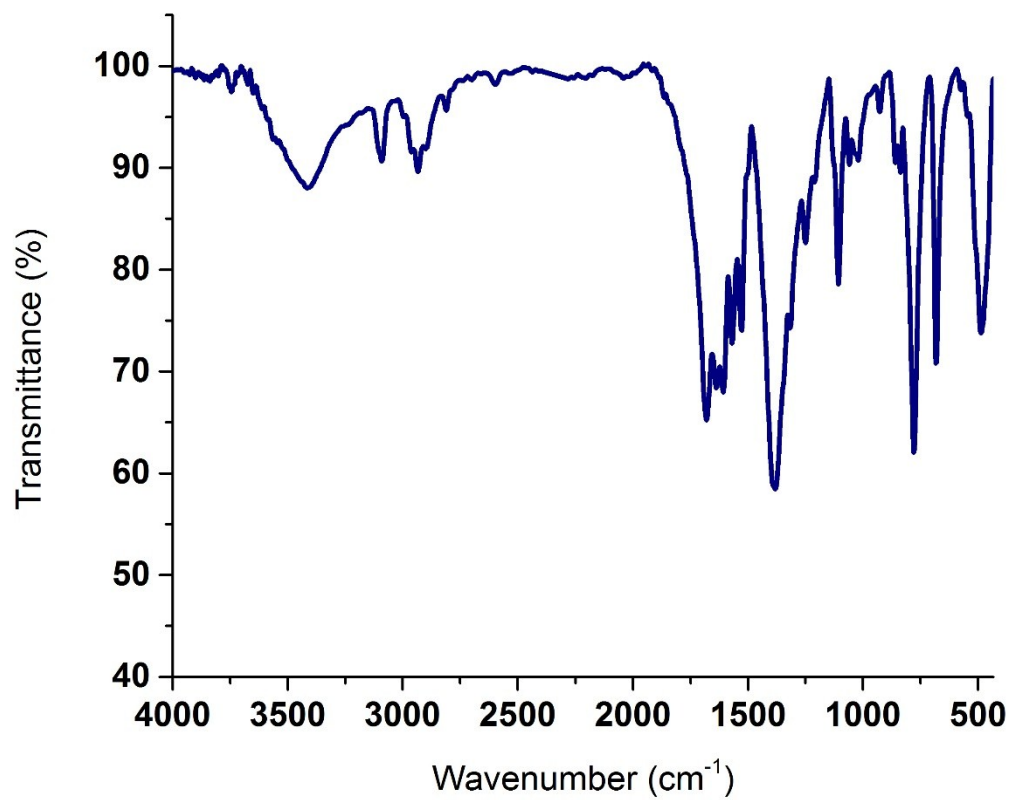
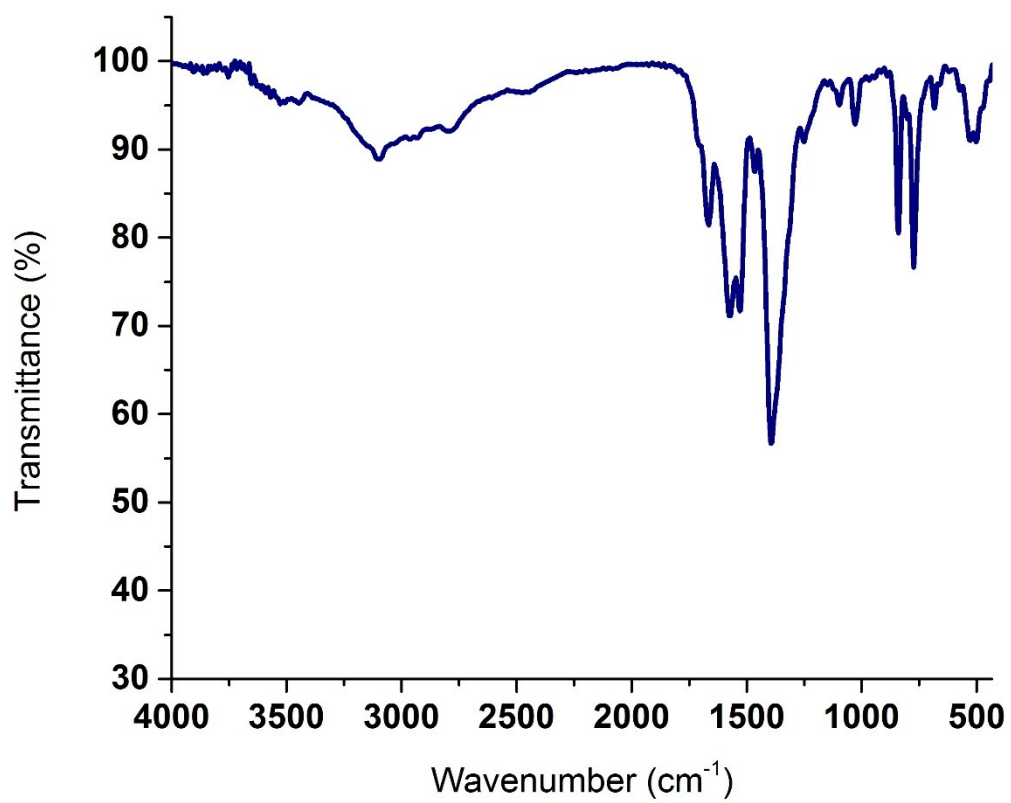Fig. S17. Characteristic IR spectra of compound **3**.
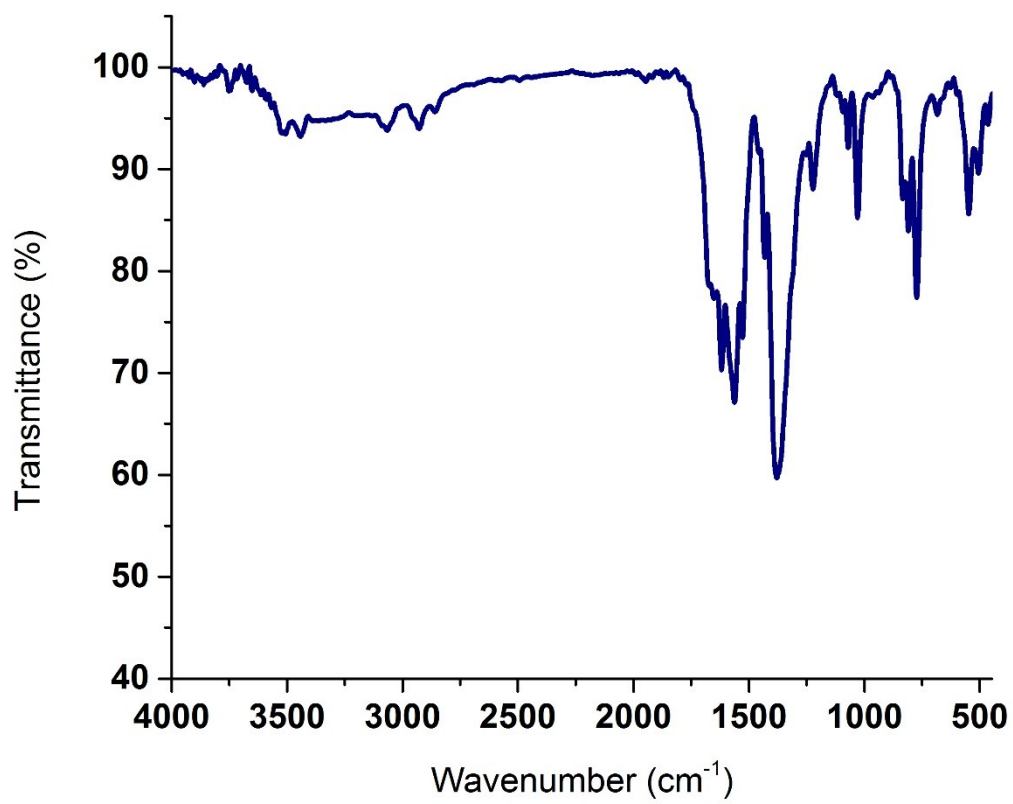
Fig. S18. Characteristics IR spectra of compound **4**.

Fig. S19. Characteristics IR spectra of compound **5**.