Electronic Supplementary Information

A series of Mn(II)/Mg(II)/Zn(II) coordination polymers with azo/alkene functionalized ligands

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Contents

3. Figures

1. Experimental section

1.1. Magnetic Measurements

Magnetic susceptibility χ(T) as a function of temperature was measured at an applied field of H = 1 T. Zero-field-cooled (ZFC), and field cooled (FC) susceptibilities were measured at a low field of H = 100 Oe. For both the measurements, a vibrating sample magnetometer (VSM) attachment to the PPMS was used.

The equation used for magnetic fitting:

The χ(T) data were fitted using one-dimensional (1D) chain model

$\chi(T) = \chi_0 + \chi_{spin}$ (T), …… (1)

Where χ_{spin} is the spin susceptibility of the S = 5/2 one-dimensional (1D) chain model. The high-temperature series expansion (HTSE) of χ_{spin} for the S = 5/2 Heisenberg 1D chain is given by Dingle et al.[1]

$\chi_{spin}(T) = \frac{N_A g^2 \mu_B^2}{3K_B T} S(S+1) \frac{1+u(K)}{1-u(K)}$……..(2)

Where, $u(K) = cothK - \frac{1}{K}$and $K = \frac{-2JS(S+1)}{K_B T}$.

Our $\chi(T)$ data were fitted well by the Eq. (1), indicating the 1D nature of these compounds.

1.2. Optical band gap measurements

We have measured the optical band gaps of all these materials using diffuse reflectance spectroscopy and the Kubelka–Munk model.$BaSO_4$ was used as the reference material for the spectral measurements. The intersection point between the energy axis and the line extrapolated from the linear portion of the absorption edge from a plot of Kubelka–Munk function *vs*. energy is taken and confirmed as the optical band gap energy. The two-flux model, which considers only diffuse light, is used to determine the absorption coefficient from a surface that both scatters and absorbs incident radiation. For a crystalline solid with a band gap (E_{bg}), the frequency (ν) dependence of the absorption coefficient (κ) can be approximated as

$$\kappa(\upsilon) = \frac{B_T(\mathrm{h}\upsilon - E_{Bg})}{\mathrm{h}\upsilon}$$

Where, B_T is a constant derived from the square of the averaged dipolar momentum matrix element, and n is equal to 0.5 and 2 for direct and indirect band gap transitions, respectively.[2-5] The absorption coefficient (κ) can be measured from the reflectance (R) and expressed as $\kappa = (1 - R)^2/(2R)$.The band gap of a material can be obtained by extrapolating to zero with the linear fit to a plot of $(\mathrm{kh}\nu)^{1/n}$ vs. hν. By this method, we have measured the lowest electronic transition between valence and conduction bands via absorption, which reflects the optical band gap of the material. The absorption coefficient (κ) can be measured from the reflectance (R) and expressed as $\kappa = (1 - R)^2/(2R)$.

2. Tables

Table S1a. Crystallographic parameters for the compounds **1**–**3**, respectively[a]

Parameters	**[Mn(ABDCA)(DPE)$_{0.5}$ DMF].DMF, (1)**	**[Mn$_{1.5}$ (ABDCA)$_{1.5}$ (DMF)$_2$].DMF, (2)**	**[Mg$_3$ ABDCA$_3$ (DMF)$_4$]. 4DMF, (3)**
Empirical formula	$C_{26}H_{27}N_5O_6Mn$	$C_{30}H_{33}Mn_{1.50}N_6O_9$	$C_{54}H_{54}Mg_3N_{10}O_{16}$
Formula weight	560.46	704.03	1172.00
Crystal System	Triclinic	Monoclinic	Monoclinic
Space Group	*P*(-1) (no. 2)	$P2_1/n$ (no. 14)	$P2_1/n$ (no. 14)
a(Å)	8.234(5)	14.772(3)	15.10(2)
b(Å)	11.911(5)	17.531(4)	17.634(5)
c(Å)	15.189(5)	16.603(3)	17.002(9)
?(?)	102.883(5)	90	90
?(?)	99.718(5)	114.524(7)	114.26(2)
?(?)	106.220(5)	90	90
Volume(Å3)	1351.2(11)	3911.7(13)	4128(3)
Z	2	2	2
Calculated density (g/cm^3)	1.378	1.195	0.943
? range (?)	1.419 to 28.427	2.676to 28.356	2.348 to 27.933
Absorption coefficient (mm^{-1})	0.537	0.543	0.090
Reflections collected	24518	34173	62305
Unique reflections	6712	9580	9623
Goodness -of-fit	0.933	1.022	0.986
Number of parameters	327	398	381
Final R indices [I>2sigma(I)]	R_1 = 0.0628, wR_2 = 0.1768	R_1 = 0.0792 , wR_2 = 0.2348	R_1 = 0.0880, wR_2 = 0.2462
Largest diff. peak and hole e Å^{-3}	1.657 and -0.716	1.336and -0.632	0.542 and -0.407

Table S1b. Crystallographic parameters for the compounds 4 - 6 respectively[a]

Parameters	**[Zn(ABDCA)(2,2'-BPY)]. H_2O, (4)**	**[$Zn_{0.5}$($SDCA)_{0.5}$(2,2'-$BPy)_{0.5}$] (5)**	**[$Zn_{0.5}$ ($ABDCA)_{0.5}$ (4,4'-$BPy)_{0.5}$]. $DMF_{0.5}$, (6)**
Empirical formula	$C_{12}H_8N_2O_3Zn_{0.5}$	$C_{12}H_8N_2O_2Zn_{0.50}$	$C_{13.50}H_8N_{2.50}O_{2.50}Zn_{0.50}$
Formula weight	260.89	244.89	277.91
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	*C*2/*c*(no. 15)	*C*2/*c*(no. 15)	*C*2/*c*(no. 15)
a(Å)	17.0178(10)	17.75(4)	29.082(3)
b(Å)	33.0702(19)	32.29(8)	6.0970(7)
c(Å)	7.3279(4)	7.651(18)	17.5730(18)
α(^{0})	90	90	90
β(^{0})	94.744(3)	90.51(4)	104.874
γ(^{0})	90	90	90
Volume(Å^3)	4109.9(4)	4384 (18)	3011.5(6)
Z	8	8	8
Calculated density (g/cm^3)	0.843	0.742	1.226
θ range (^{0})	3.008 to 28.396	3.455 to 28.360	2.463 to 25.998
Absorption coefficient (mm^{-1})	0.625	0.580	0.856
Reflections collected	18348	35153	13339
Unique reflections	5018	5327	3627
Goodness-of-fit	1.057	1.062	1.012
Number of parameters	159	150	196
Final R indices [I>2sigma(I)]	R_1 = 0.0886, wR_2 = 0.2351	R_1 = 0.0811, wR_2 = 0.2014	R_1 = 0.0816, wR_2 = 0.2376
Largest diff. peak and hole e Å^{-3}	1.166 and -0.647	1.331 and -0.627	1.182 and -0.771

[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(Å)**
Mn(1) - O(1)	2.109(2)
Mn(1)-O(3)	2.234(2)
Mn(1)-O(4)	2.326(2)
Mn(1)-O(5)	2.165(2)
Mn(1)-N1	2.247(3)
Mn(1) -O(2)#1	2.106(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

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

Compound 2	**Bond Length(Å)**
Mn(1) - O(4)	2.269(2)
Mn(1)-O(3)	2.267(3)
Mn(1)-O(7)	2.103(3)
Mn(1)-O(6)	2.124(3)
Mn(1)-O(6)	2.123(4)
Mn(1)- O(1)	2.099(3)
Mn(2) -O(4)	2.193(2)
Mn(2) -O(2)	2.134(2)
Mn(2) -O(8)	2.141(3)
Mn(2)-O(2)#4	2.134(2)
Mn(2)-O(8)#4	2.142(3)

Mn(2)-O(4)#4	2.193(2)

Symmetry transformations used to generate equivalent atoms: #4 -x,-y,-z

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

Compound 3	**Bond Length(Å)**
Mg(1) - O(1)	2.224 (13)
Mg(1)-O(2)	2.198 (3)
Mg(1)-O(4)	2.068 (4)
Mg(1)-O(5)	2.163 (5)
Mg(1)-O(7)	2.041 (3)
Mg(1) - O(8)	2.084 (14)
Mg(2)-O(1)	2.120 (4)
Mg(2) - O(1)#1	2.120 (4)
Mg(2) - O(3)	2.105 (11)
Mg(2) - O(3) #1	2.105 (11)
Mg(2) - O(6)	2.072 (3)
Mg(2)-O(6)#1	2.072 (3)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z

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

Compound 4	**Bond Length(Å)**
Zn(1) - O(1)	2.294(15)
Zn(1)-O(2)	2.047(12)
Zn(1)-O(4)	2.395(12)

Zn(1)-O(6)	2.003(9)
Zn(1)-N(3)	2.065(12)
Zn(1)-N(4)	2.074(17)

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

Compound 5	**Bond Length(Å)**
Zn (1) - O(1)	2.025(5)
Zn(1) - O(2)	2.445(5)
Zn(1)- N(1)	2.095(5)
Zn (1) - O(1) #1	2.025(5)
Zn (1) - O(2) #1	2.445 (5)
Zn (1) - N(1) #1	2.095 (5)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z

Table S7. Selected bond lengths of compound **6**.

Compound 6	**Bond Length(Å)**
Zn(1)-N(1)	2.062(3)
Zn(1)-N(1) #1	2.062(3)
Zn(1)-O(1)	1.943(3)
Zn(1)-O(1)#1	1.943(3)

Symmetry transformations used to generate equivalent atoms:#1-x+2,-y+1,-z+1

2.2. Topos

2.2.1. Topos for compound 1

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 1	0.9704	-0.3860	0.4169	(1 0 1)	13.674A	1
Mn 1	0.9704	1.6140	1.4169	(1 2 2)	15.979A	1
Mn 1	1.0296	1.3860	1.5831	(1 1 1)	16.208A	1
Mn 1	-0.9704	-0.6140	-0.4169	(-1-1-1)	16.208A	1
Mn 1	-0.0296	-0.3860	1.4169	(0 0 2)	17.225A	1
Mn 1	-1.0296	-0.3860	-0.5831	(-1 0 0)	17.457A	1
Common edge with					R(A-A)	
Mn 1	-0.0296	0.6140	0.4169	(0 1 1)	4.167A	2

Structural group analysis

Structural group No 1

Structure consists of 3D framework with $MnO_5N_4C_{23}H_{20}$

There are 3 interpenetrating nets

FIV: Full interpenetration vectors

[1,0,0] (8.23A)

PIC: [3,0,0][1,1,1][1,-1,0] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences

Mn1: 1 2 3 4 5 6 7 8 9 10

Num 7 22 47 82 127 182 247 322 407 502

Cum 8 30 77 159 286 468 715 1037 1444 1946

TD10=1946

Vertex symbols for selected sub lattice

Mn1 Point symbol:{$3^6.4^8.5^6.6$}

Extended point symbol:[3.3.3.3.3.3.4.4.4.4.4.4.4.4.5.5.5.5.5(2).5(2).6(5)]

Point symbol for net: {3^6.4^8.5^6.6};7-c net; uninodal net

2.2.2. Topos for compound 2

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 2	0.5000	1.5000	-0.5000	(0 1-1)	16.393A	1
Mn 2	0.0000	0.0000	0.0000	(0 0 0)	16.846A	1
Mn 1	-0.2411	0.0599	-0.1669	(0 1 0)	16.934A	1
Mn 1	0.7411	1.5599	-0.3331	(0 2-1)	17.101A	1
Mn 1	-0.2589	1.5599	0.6669	(-1 2 0)	17.101A	1
Mn 2	-0.5000	1.5000	0.5000	(-1 1 0)	17.235A	1
Common face with					R(A-A)	
Mn 2	0.0000	1.0000	0.0000	(0 1 0)	3.643A	3

Topology for Mn2

Atom Mn2 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 2	-0.5000	-0.5000	0.5000	(-1-1 0)	15.849A	1
Mn 2	0.5000	0.5000	-0.5000	(0 0-1)	15.849A	1
Mn 2	-0.5000	0.5000	0.5000	(-1 0 0)	15.849A	1

Mn 2 0.5000 -0.5000 -0.5000 (0-1-1) 15.849A 1

Mn 1 -0.2589 0.5599 0.6669 (-1 1 0) 16.393A 1

Mn 1 0.2589 -0.5599 -0.6669 (0-2-1) 16.393A 1

Mn 1 -0.2411 -0.9401 -0.1669 (0 0 0) 16.846A 1

Mn 1 0.2411 0.9401 0.1669 (0 0 0) 16.846A 1

Mn 1 -0.7411 -0.5599 0.3331 (-1-2 0) 17.235A 1

Mn 1 0.7411 0.5599 -0.3331 (0 1-1) 17.235A 1

Mn 2 0.0000 -1.0000 0.0000 (0-1 0) 17.531A 1

Mn 2 0.0000 1.0000 0.0000 (0 1 0) 17.531A 1

Common face with R(A-A)

Mn 1 0.2411 -0.0599 0.1669 (0-1 0) 3.643A 3

Mn 1 -0.2411 0.0599 -0.1669 (0 1 0) 3.643A 3

Structural group analysis

Structural group No 1

Structure consists of layers (1 0 1) with Mn3O16N10C54H56

Coordination sequences

Mn1: 1 2 3 4 5 6 7 8 9 10

Num 7 31 54 72 90 108 126 144 162 180

Cum 8 39 93 165 255 363 489 633 795 975

Mn2: 1 2 3 4 5 6 7 8 9 10

Num 14 36 54 72 90 108 126 144 162 180

Cum 15 51 105 177 267 375 501 645 807 987

TD10=979

Vertex symbols for selected sublattice

Mn1 Point symbol:{3^9.4^12}

Extended point symbol:[3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4(3).4(3).4(3)]

Mn2 Point symbol:{3^24.4^48.5^16.6^3}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).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).5(2).5(2).5(2).5(2).5(2).5(2).5(6).5(6).5(6).5(6).5(6).5(6).5(6).5(12).5(12).5(12).6(12).6(12).6(12)]

Point symbol for net: {3^24.4^48.5^16.6^3}{3^9.4^12}2

7,14-c net with stoichiometry (7-c)2(14-c); 2-nodal net

2.2.3. Topos for compound 3

Topology for Mg1

Atom Mg1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 1	0.7500	1.2500	0.0000	(1 2 0)	15.180A	1
Mg 1	-0.2500	0.2500	0.0000	(0 1 0)	15.180A	1
Mg 2	0.6712	1.2988	-0.2155	(1 2 0)	15.669A	1
Mg 2	-0.1712	0.2012	0.2155	(-1-1 0)	15.669A	1
Mg 2	0.1712	-0.2012	-0.2155	(0 0 0)	16.928A	1
Mg 2	0.3288	1.7012	0.2155	(0 1 0)	16.928A	1
Mg 2	0.8288	0.7988	-0.2845	(0 1-1)	16.955A	1
Mg 2	-0.3288	0.7012	0.2845	(0 0 0)	16.955A	1
Mg 1	0.2500	-0.2500	0.0000	(0-1 0)	17.423A	1
Mg 1	0.2500	1.7500	0.0000	(0 1 0)	17.423A	1
Mg 1	0.7500	0.7500	-0.5000	(1 0-1)	17.697A	1
Mg 1	-0.2500	0.7500	0.5000	(0 0 0)	17.697A	1

Common face with					R(A-A)	
Mg 2	0.1712	0.7988	-0.2155	(0 1 0)	3.554A	3
Mg 2	0.3288	0.7012	0.2155	(0 0 0)	3.554A	3

Topology for Mg2

Atom Mg2 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mg 1	0.7500	1.2500	0.0000	(1 2 0)	15.669A	1
Mg 2	-0.3288	0.7012	0.2845	(0 0 0)	16.856A	1
Mg 2	0.6712	1.2988	-0.2155	(1 2 0)	16.907A	1
Mg 1	0.2500	-0.2500	0.0000	(0-1 0)	16.928A	1
Mg 1	-0.2500	0.7500	0.5000	(0 0 0)	16.955A	1
Mg 2	0.1712	-0.2012	-0.2155	(0 0 0)	17.170A	1

Common face with					R(A-A)	
Mg 1	0.2500	0.7500	0.0000	(0 0 0)	3.554A	3

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Mg3O16N10C54H48

Coordination sequences

Mg1:	1	2	3	4	5	6	7	8	9	10
Num	14	54	134	252	410	604	834	1100	1402	1740
Cum	15	69	203	455	865	1469	2303	3403	4805	6545

Mg2:	1	2	3	4	5	6	7	8	9	10
Num	7	37	109	221	374	561	787	1045	1343	1673
Cum	8	45	154	375	749	1310	2097	3142	4485	6158

TD10=6287

Vertex symbols for selected sublattice

Mg1 Point symbol:{3^18.4^36.5^22.6^14.7}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(3).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(2).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).5(4).6(4).6(6).6(6).6(8).6(8).6(8).6(8).6(12).6(12).6(12).6(12).6(16).6(16).6(16).7(40)]

Mg2 Point symbol:{3^9.4^12}

Extended point symbol:[3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4(2).4(2).4(3)]

Point symbol for net: {3^18.4^36.5^22.6^14.7}{3^9.4^12}2

7,14-c net with stoichiometry (7-c)2(14-c); 2-nodal net

2.2.4. Topos for compound 6

Topology for Zn1

Atom Zn1 links by bridge ligands and has

Common vertex with				R(A-A)	f
Zn 1	0.0000	2.0712	-0.2500 (0 3 0)	11.213A	1
Zn 1	0.0000	2.0712	0.7500 (0 3 1)	11.213A	1
Zn 1	0.5000	-0.4288	0.7500 (0 0 0)	17.075A	1
Zn 1	-0.5000	-0.4288	-0.2500 (-1 0-1)	17.075A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with ZnO4N4C24H16

There are 5 interpenetrating nets

FIV: Full interpenetration vectors

[0,1,0] (6.10A)

PIC: [5/2,5/2,0][0,0,1][1,0,0] (PICVR=5)

Zt=5; Zn=1

Class Ia Z=5

Coordination sequences

Zn1:	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

TD10=981

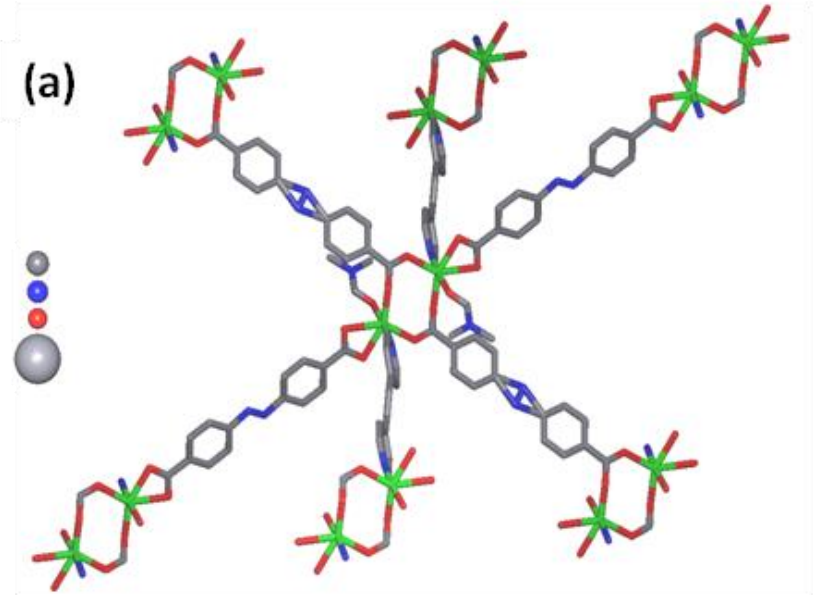
Vertex symbols for selected sublattice

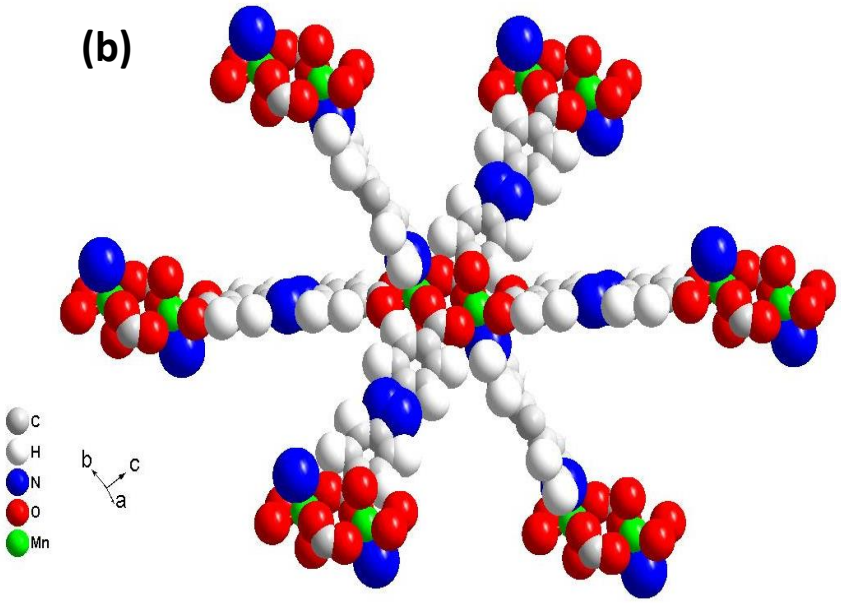
Zn1 Point symbol:{6^6}

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

Point symbol for net: {6^6}

4-c net; uninodal net




(b)
C
H
N
O
Mn
b
c
a

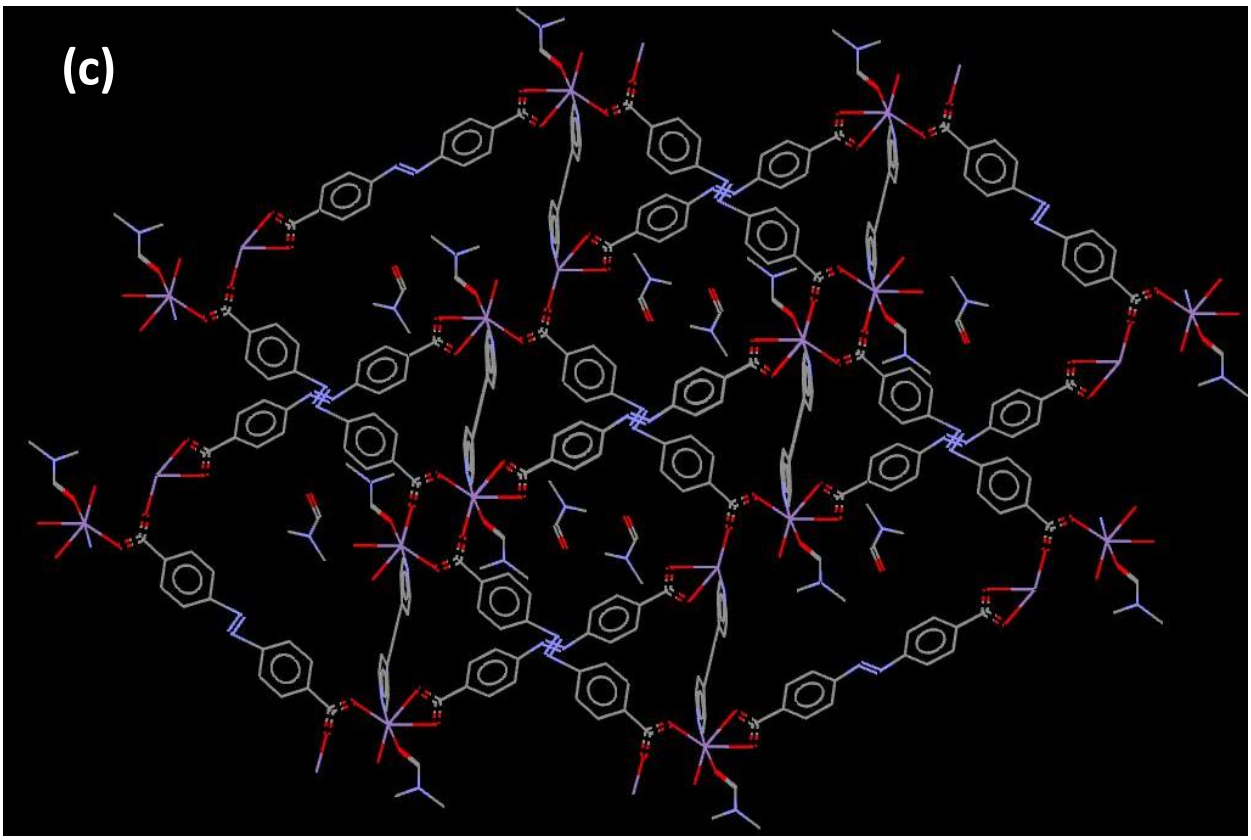


Figure. S1. (a) The manganese dimer connectivity with the ABDCA ligands, (b) space-filling model of dimer's connectivity and (c) the parallel orientation of the N=N bond of ABDCA in compound **1**.

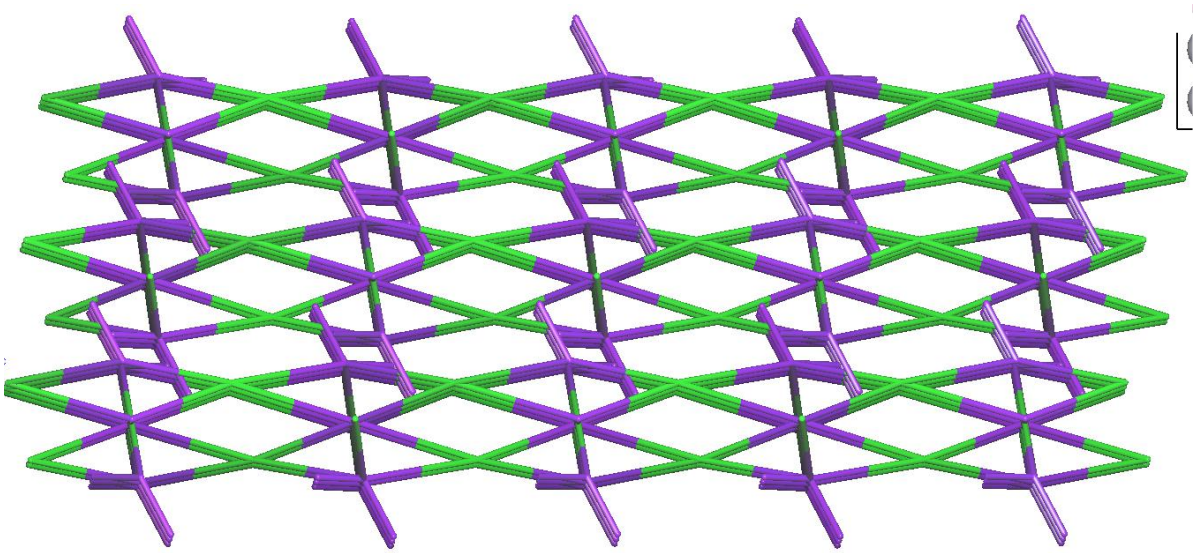


Figure. S2.Topological representation (metal and ligand connectivity) of compound **2**.

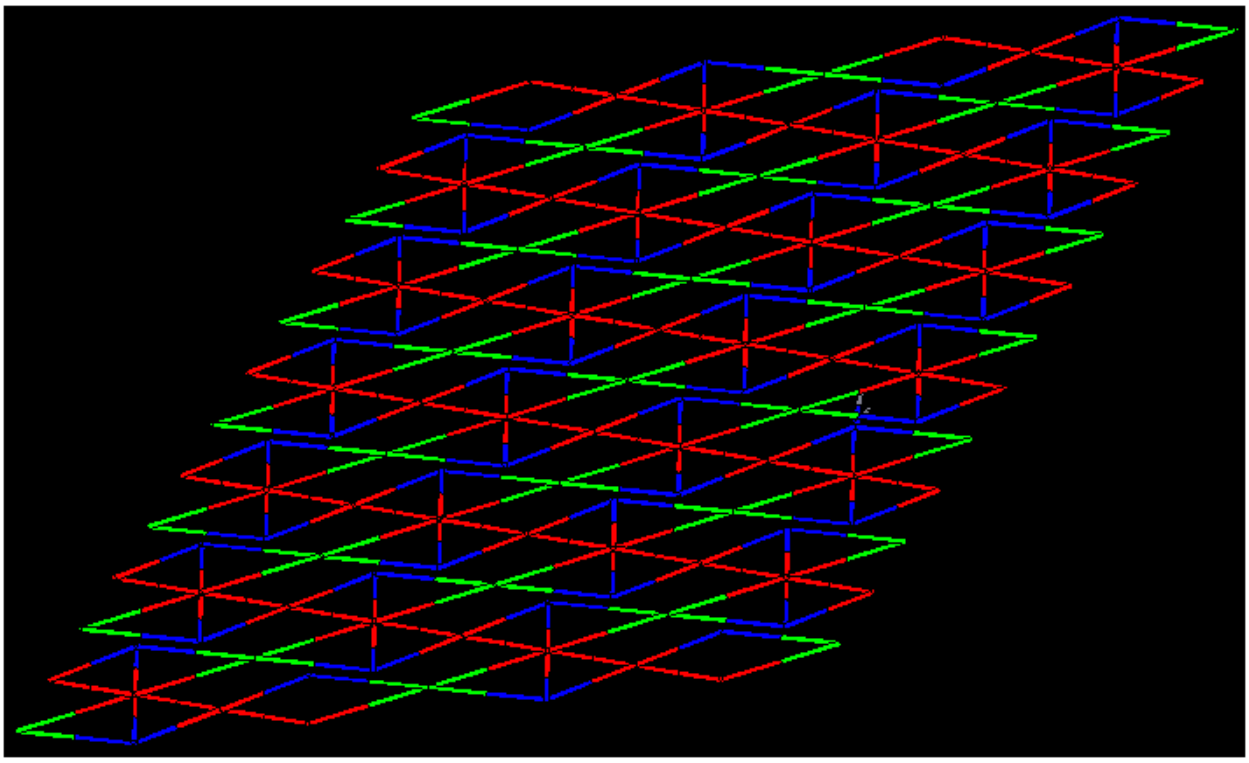


Figure. S3.Topological representation (metal and ligand connectivity)in compound **3**.

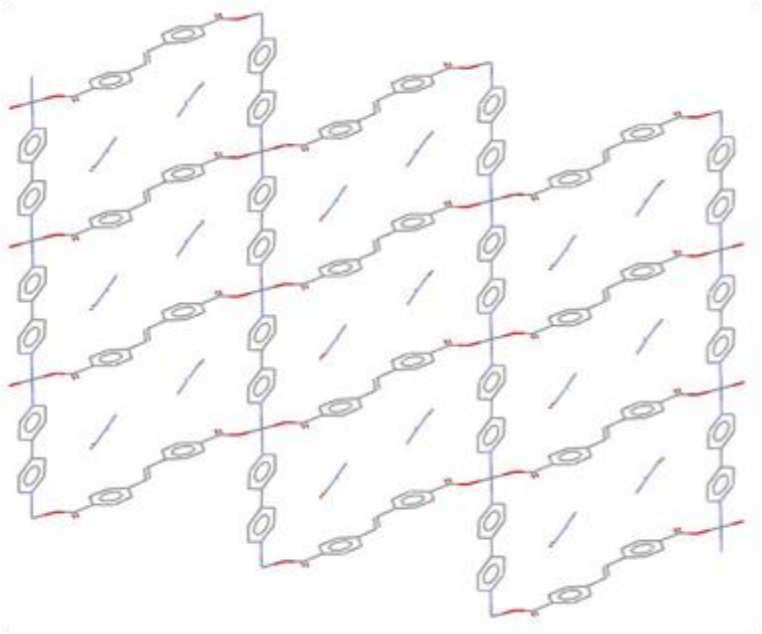
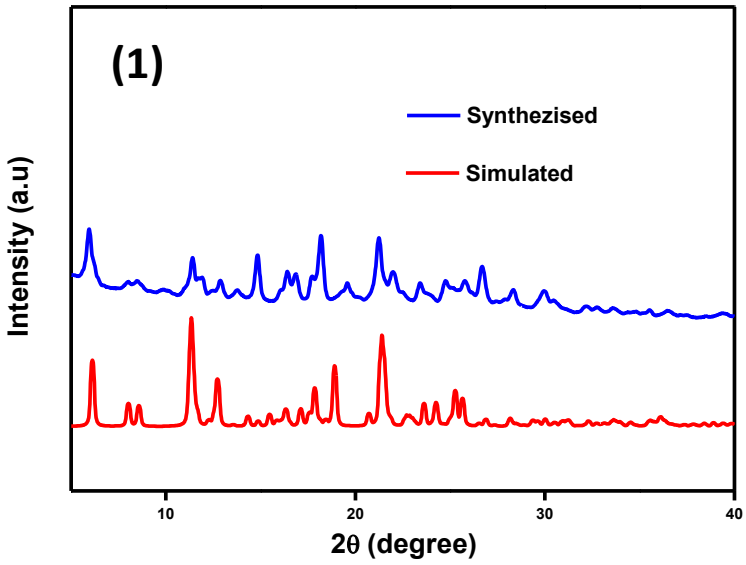
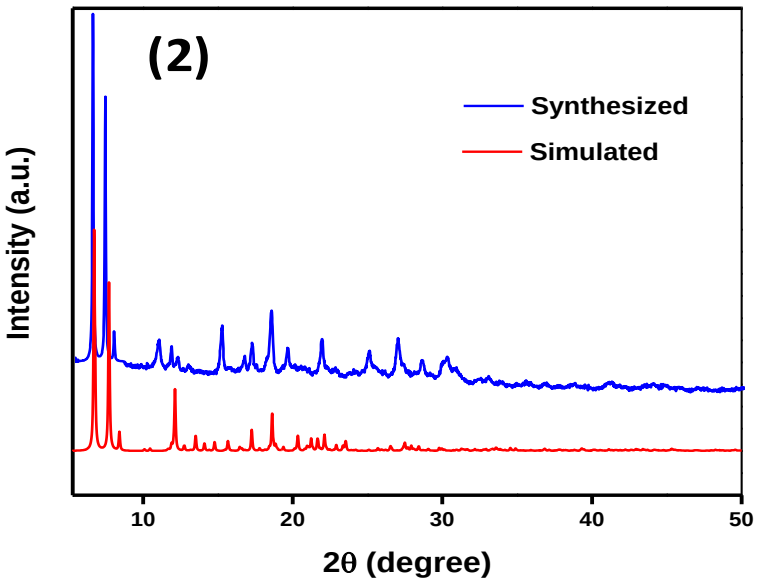
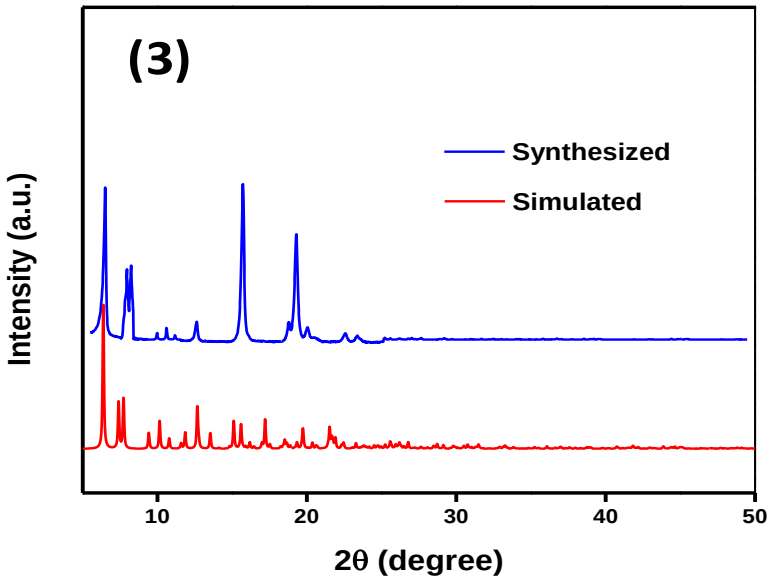
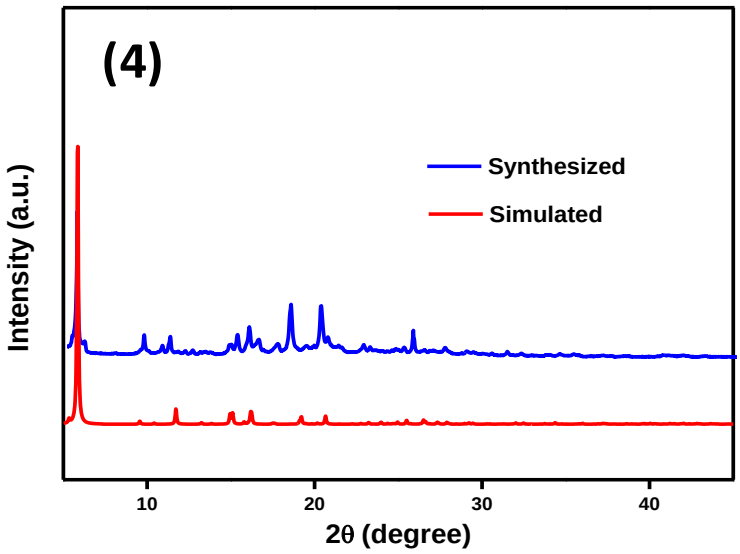


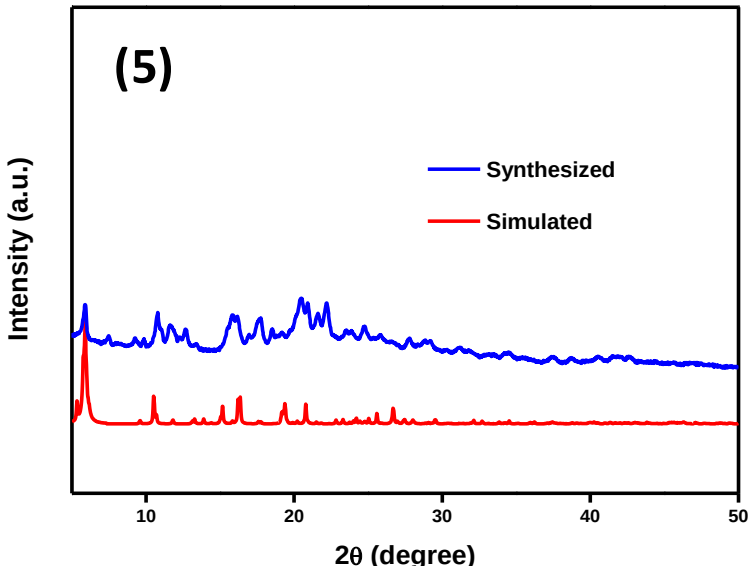
Figure. S4. Three -dimensional structure of compound **6**.


(1)
Synthezised
Simulated
Intensity (a.u)
10
20
30
40
2θ (degree)


(2)
Synthesized
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (degree)


(3)
Synthesized
Simulated
Intensity (a.u.)
10
20
30
40
50
2θ (degree)


(4)
Synthesized
Simulated
Intensity (a.u.)
10
20
30
40
2θ (degree)



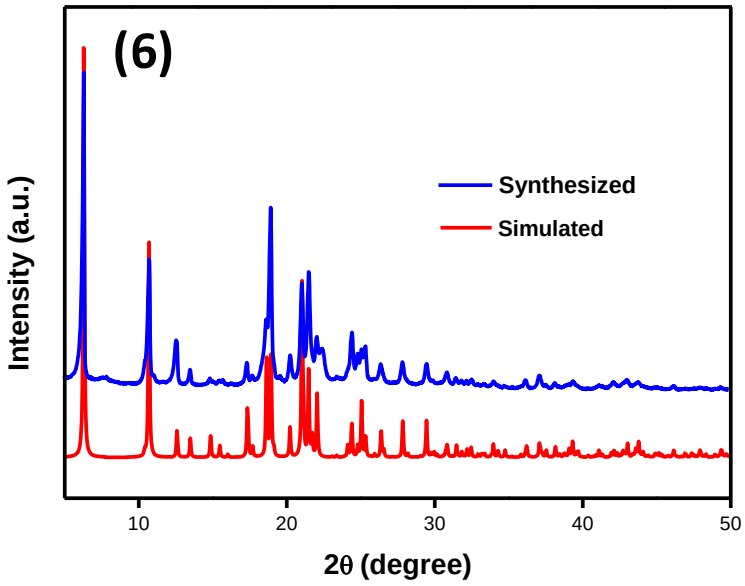
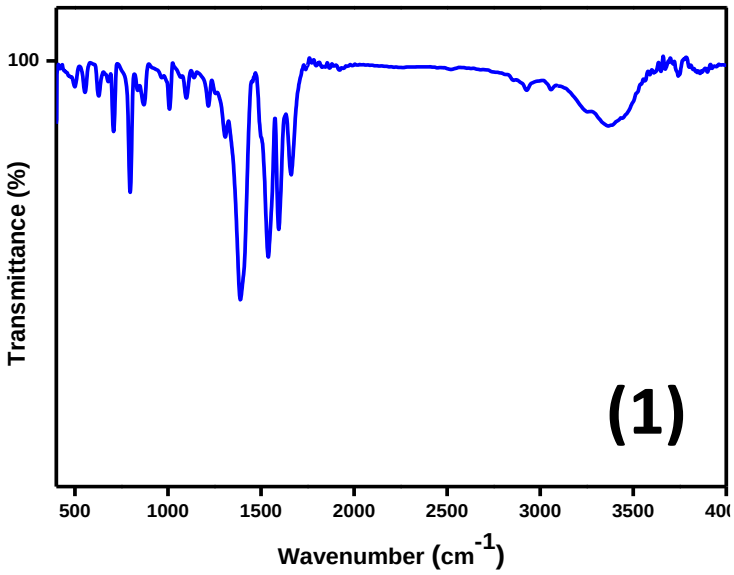
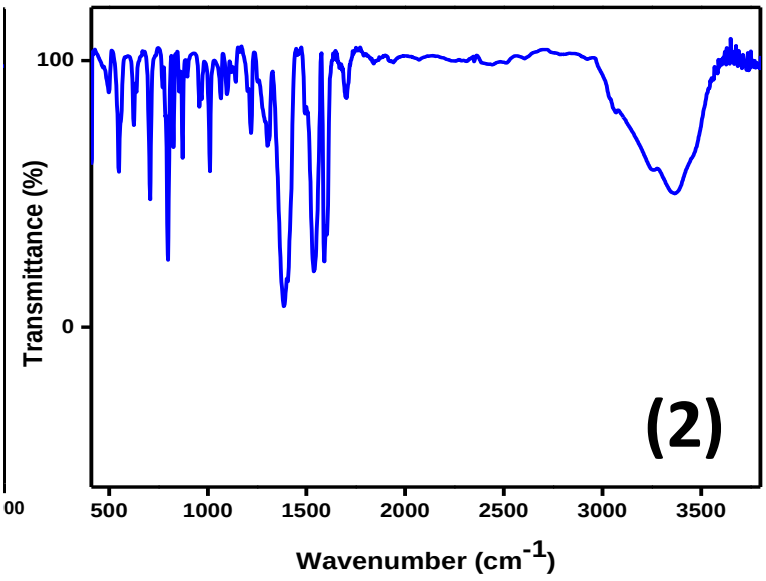
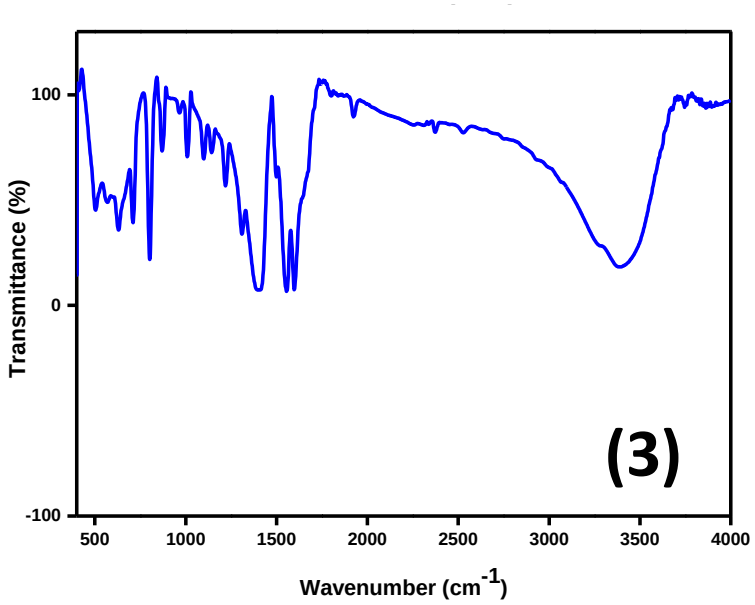
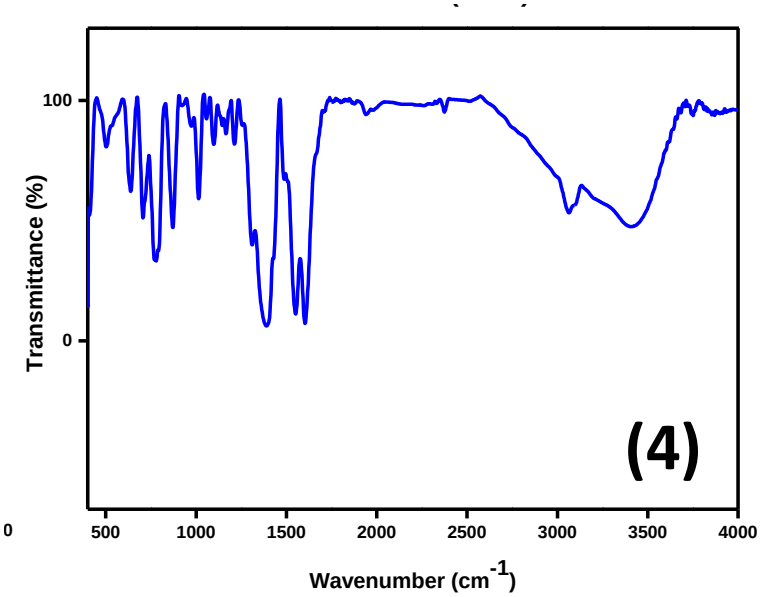


Figure S5. Powder XRD plots of the compounds **1**-**6**.


100
Transmittance (%)
(1)
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)


100
0
Transmittance (%)
(2)
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)


100
0
-100
Transmittance (%)
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)
(3)


100
0
Transmittance (%)
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)
(4)

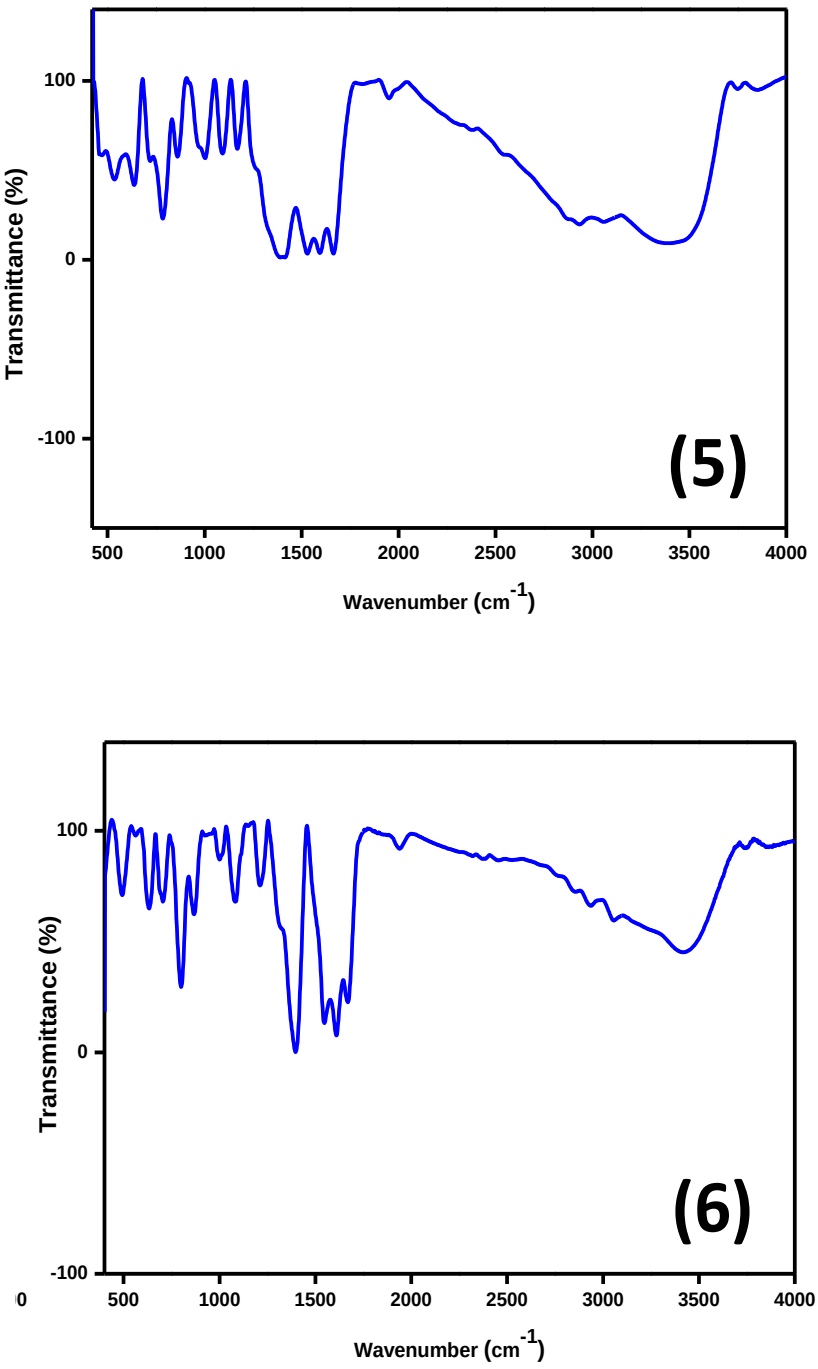
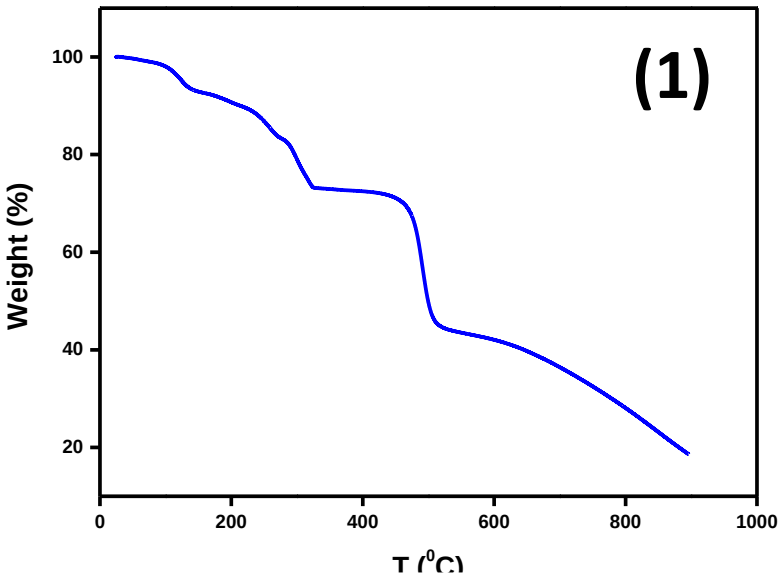


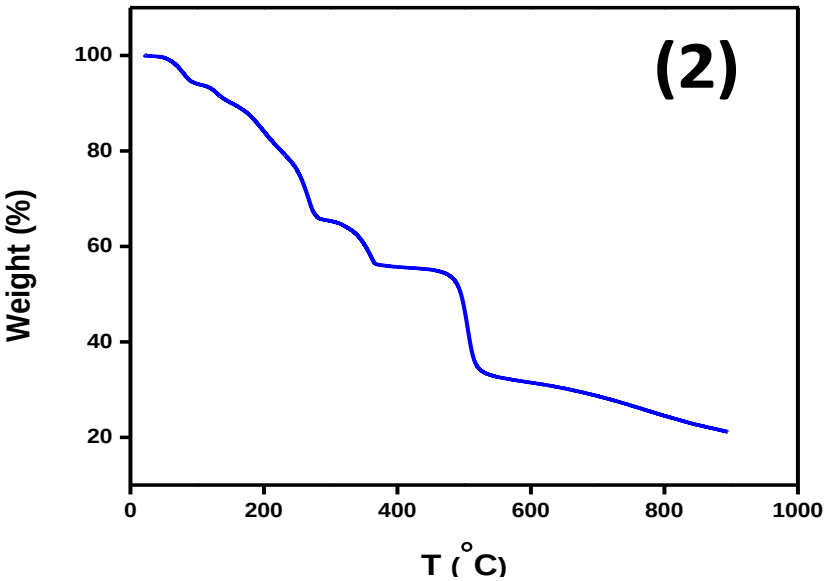
Figure S6. IR plots of the compounds **1**-**6**.

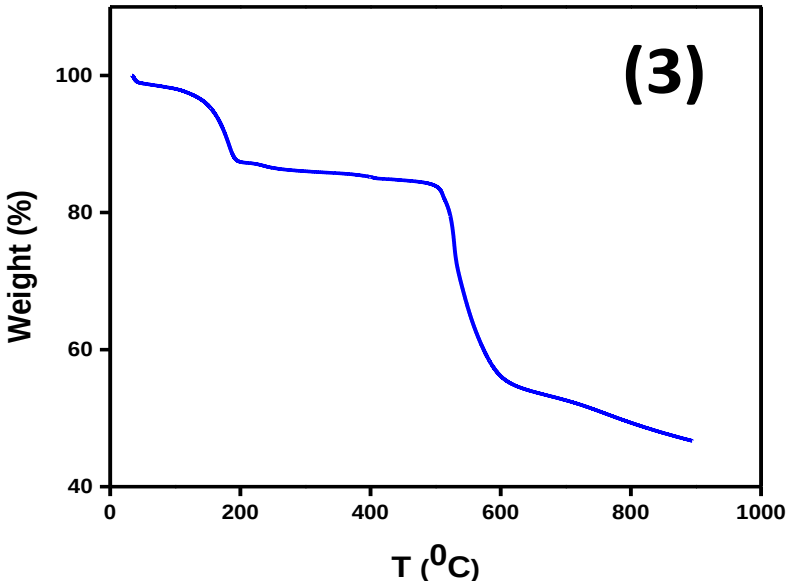
Table S8. Selected IR frequencies of the compounds **1-6**.

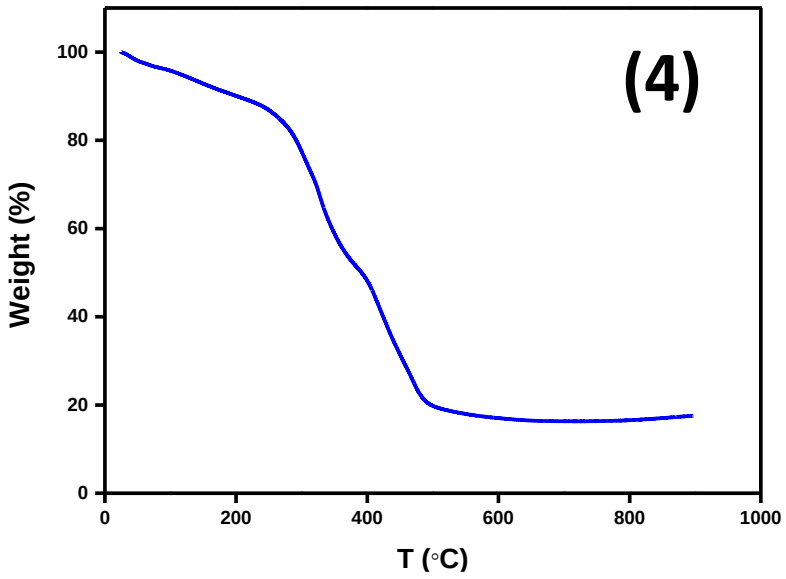
Sl. No.	Material	Stretching frequencies (cm^{-1})	Bonds
1	Compound 1	3385	-OH
		1669	-C=O
		1591	-N-H
		1540	-C=C-
		1308	-N=N-
		1206	-C-O
		1103	-C-N
		793	Aromatic
		785	-C-H
		699	-NH
2	Compound 2	3364	-OH
		1598	-C=C-
		1306	-N=N-
		1705	-C=O
		801	Aromatic
		629	-N-H
3	Compound 3	3394	-OH
		1597	-NH
		1555	-C=C-
		1399	-C-H
		1304	-N=N-
		805	Aromatic
		708	-CH
		631	-NH

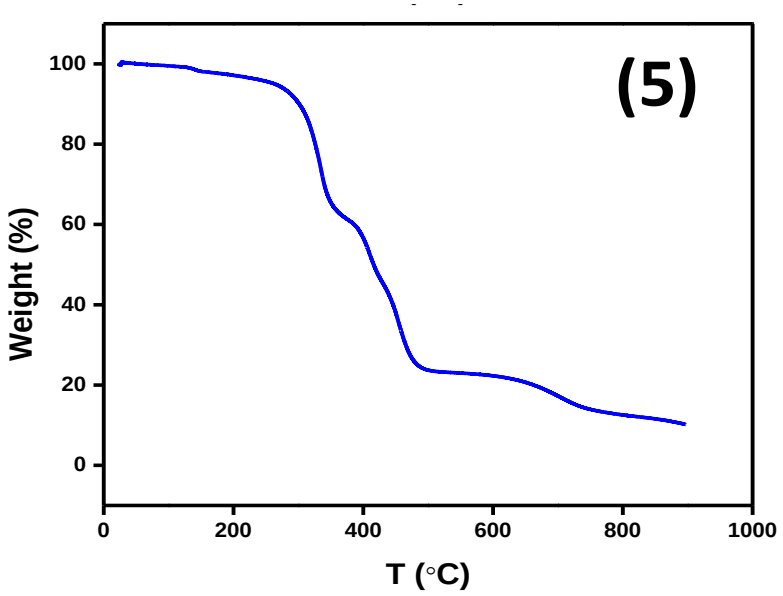
4	Compound 4	3394	-OH
		1607	-NH
		1555	-C=C-
		1313	-N=N-
		865	Aromatic
		768	-CH
		631	-NH
5	Compound 5	3390	-OH
		1672	-C=O
		1535	-C=C-
		1165	-C-O
6	Compound 6	3422	-OH
		1555	-C=C-
		1304	-N=N-
		795	Aromatic
		701	-CH
		631	-NH


(1)
Weight (%)
100
80
60
40
20
0
200
400
600
800
1000
T (0C)


(2)
Weight (%)
100
80
60
40
20
0
200
400
600
800
1000
T (°C)


(3)
Weight (%)
100
80
60
40
0
200
400
600
800
1000
T (0C)


(4)
Weight (%)
100
80
60
40
20
0
0
200
400
600
800
1000
T (◦C)



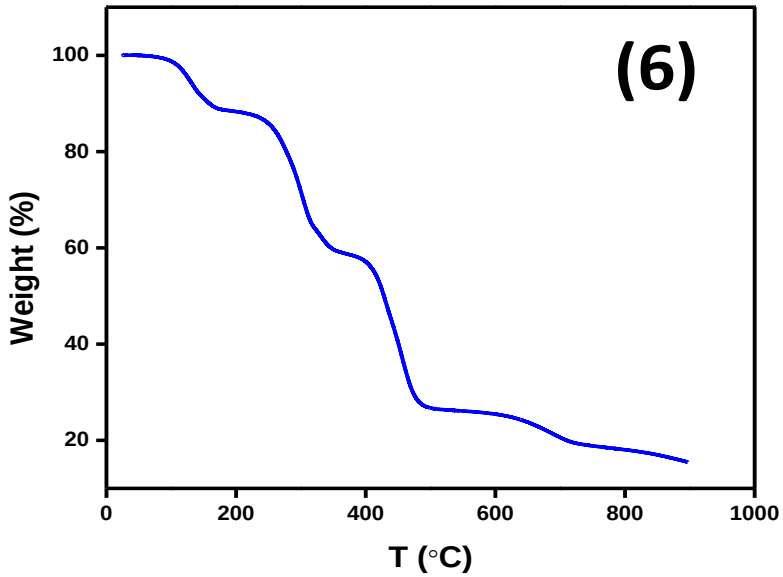
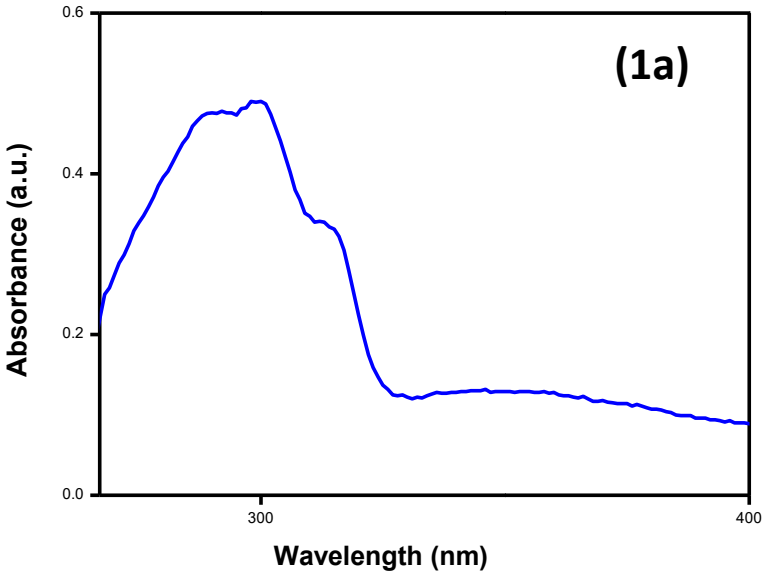
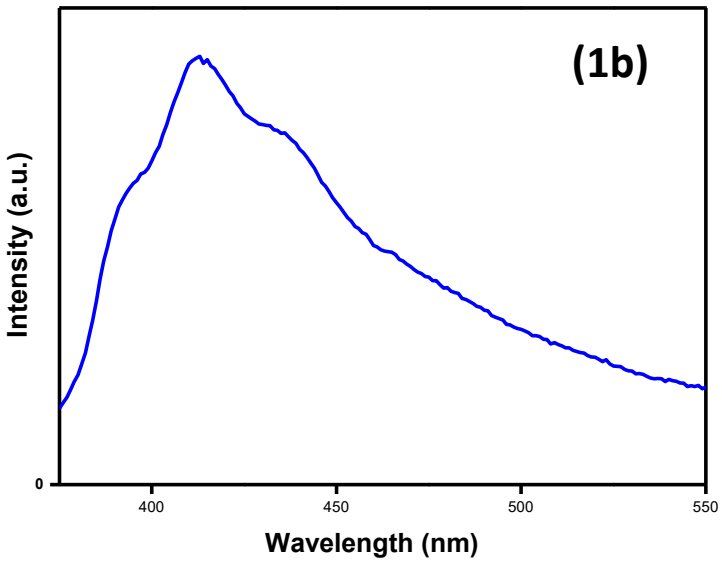
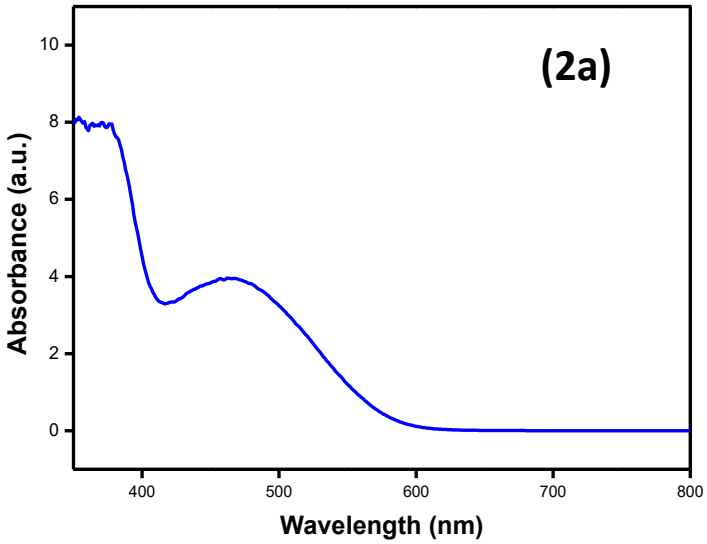
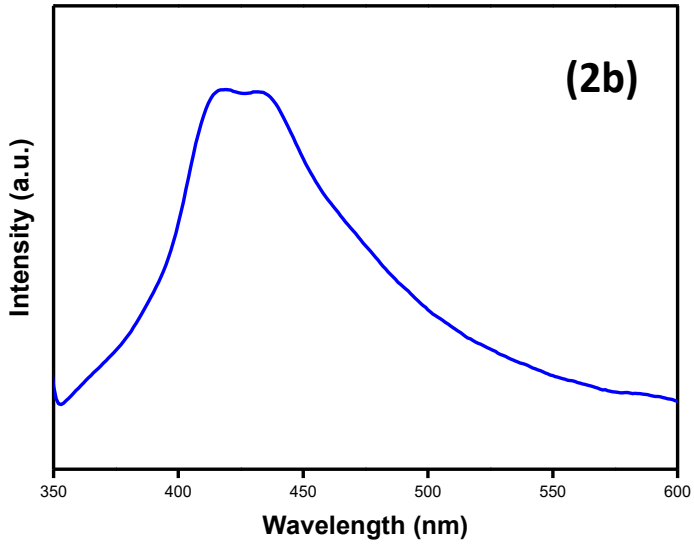


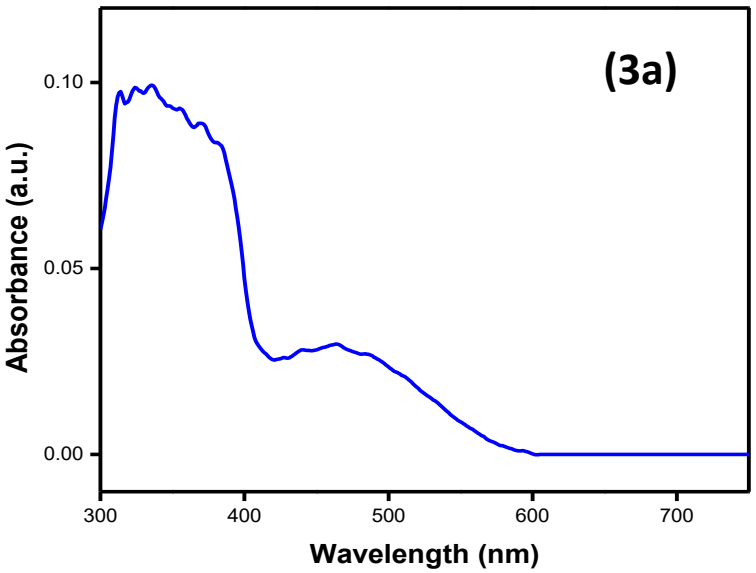
Figure S7. TGA plots of the compounds **1**-**6**.

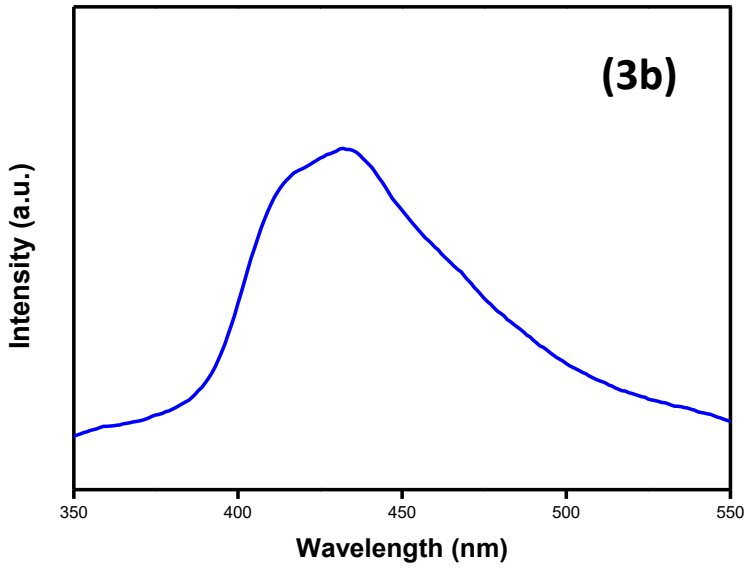

(1a)
Absorbance (a.u.)
0.6
0.4
0.2
0.0
300
400
Wavelength (nm)

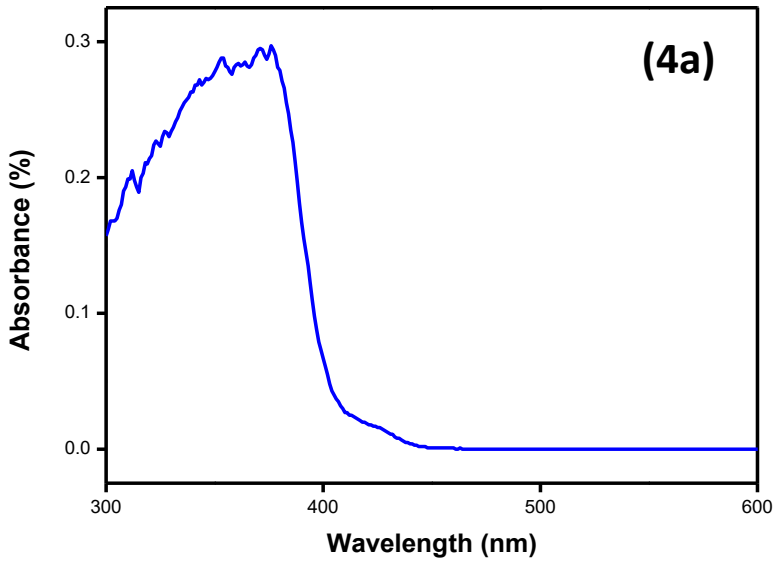

(1b)
Intensity (a.u.)
0
400
450
500
550
Wavelength (nm)

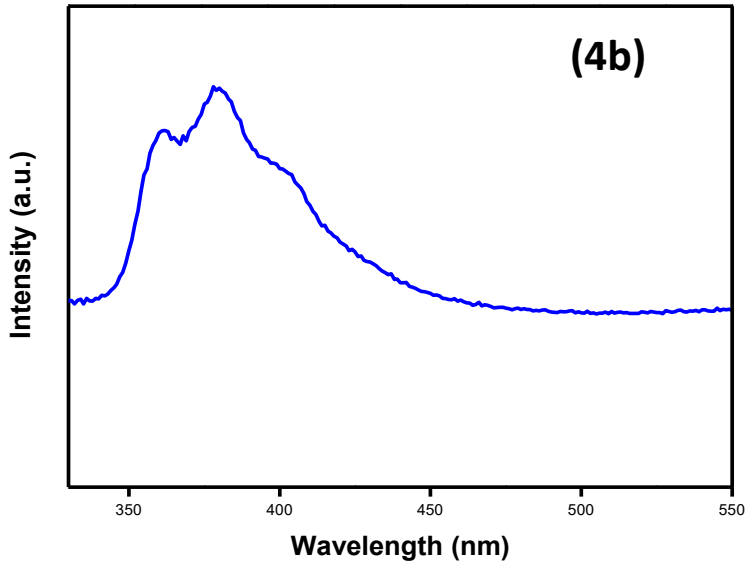

(2a)
Absorbance (a.u.)
10
8
6
4
2
0
400
500
600
700
800
Wavelength (nm)

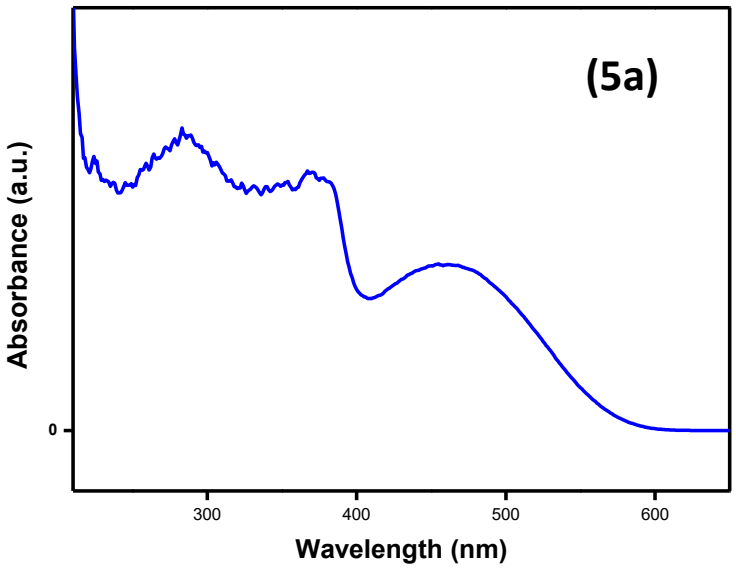

(2b)
Intensity (a.u.)
350
400
450
500
550
600
Wavelength (nm)

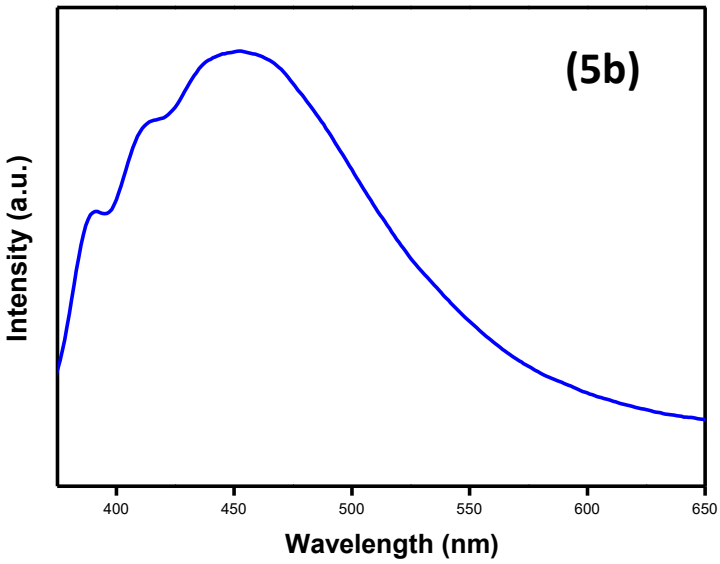

(3a)
0.10
0.05
0.00
Absorbance (a.u.)
300
400
500
600
700
Wavelength (nm)


(3b)
Intensity (a.u.)
350
400
450
500
550
Wavelength (nm)


(4a)
Absorbance (%)
0.3
0.2
0.1
0.0
300
400
500
600
Wavelength (nm)


(4b)
Intensity (a.u.)
350
400
450
500
550
Wavelength (nm)


(5a)
Absorbance (a.u.)
0
300
400
500
600
Wavelength (nm)


(5b)
Intensity (a.u.)
400
450
500
550
600
650
Wavelength (nm)

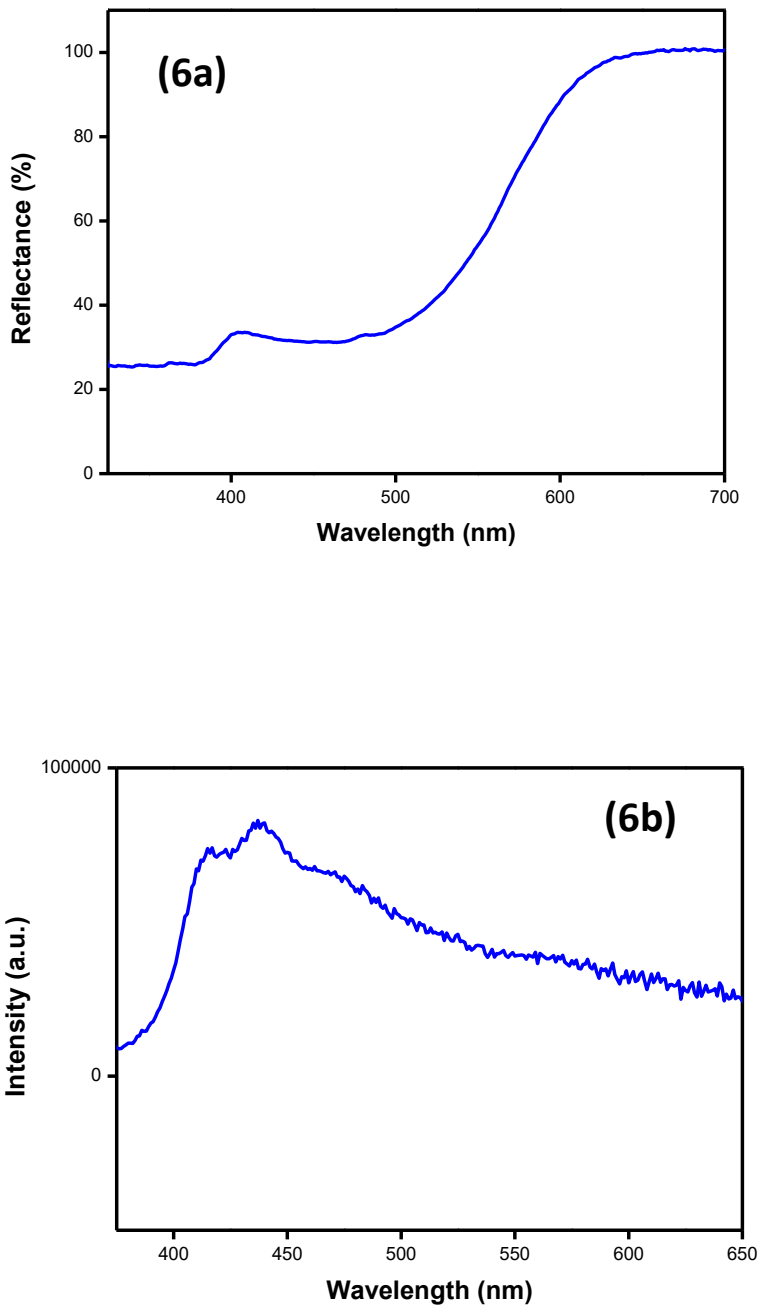


Figure S8. (a)Absorbance and (b) photoluminescence spectra of the compounds **1**-**6**.

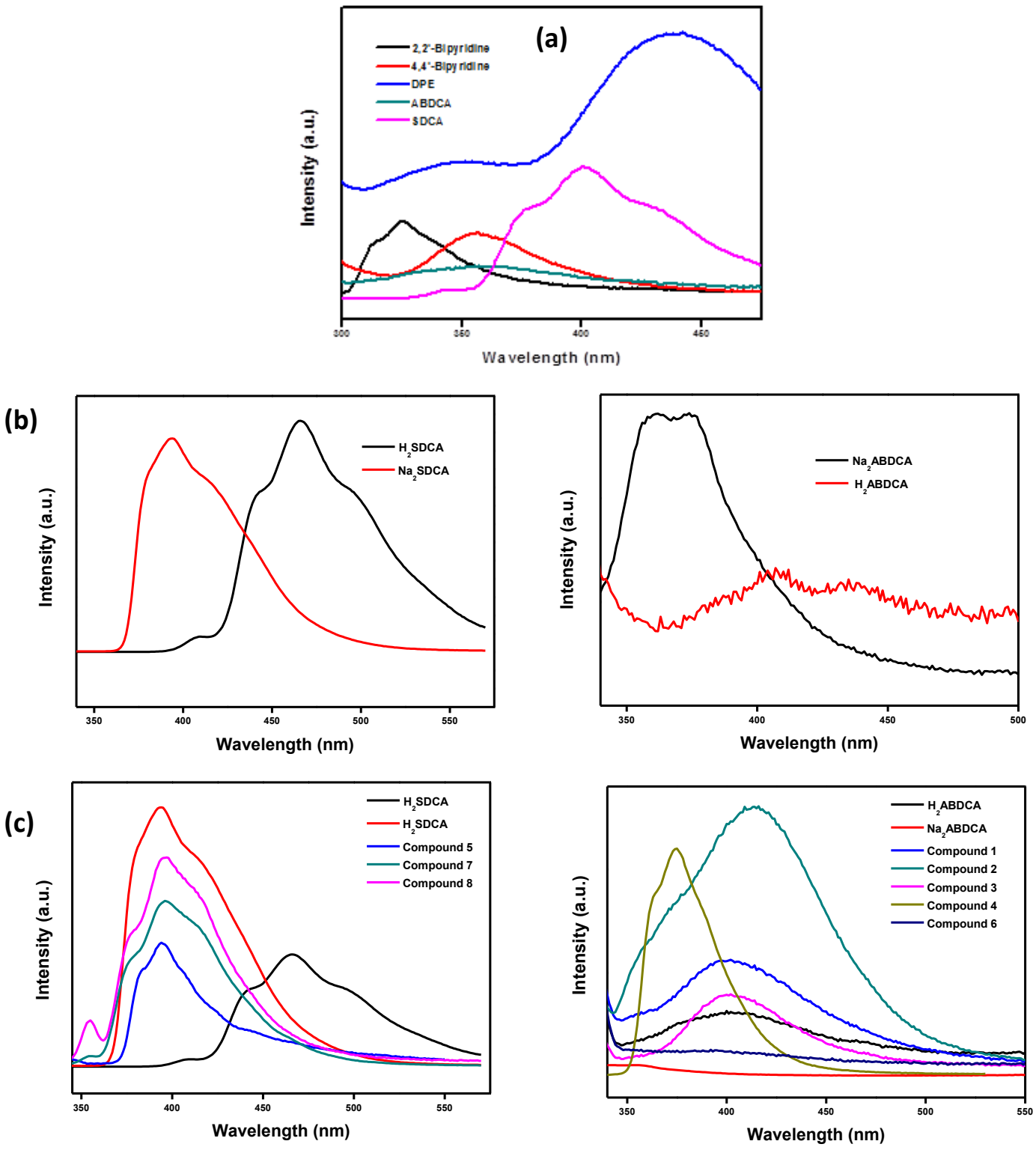
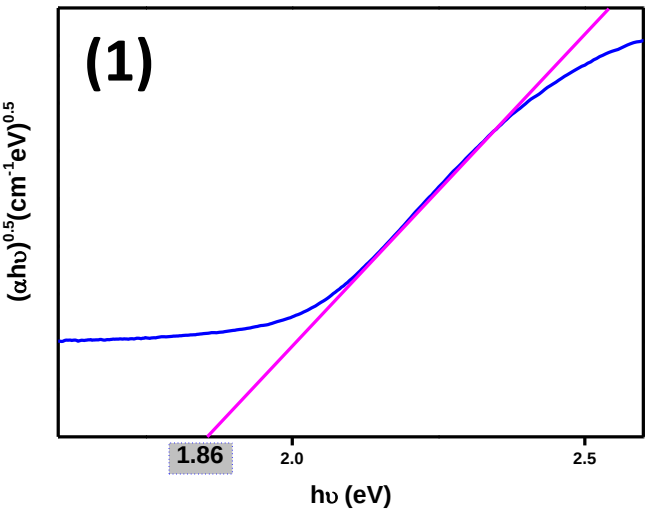
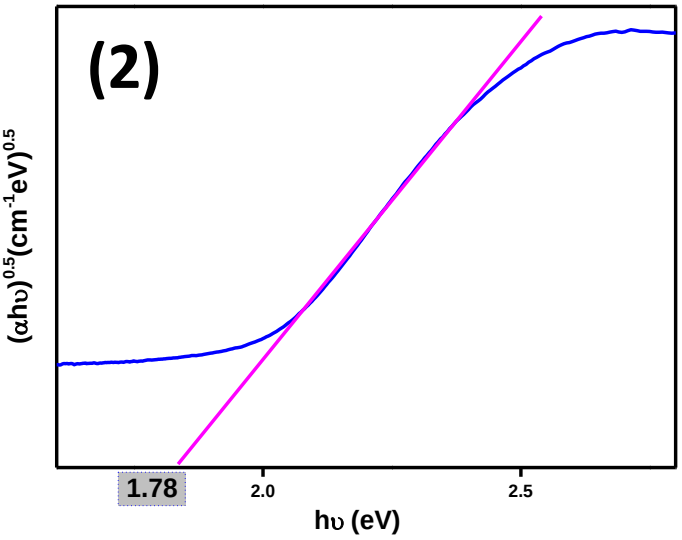
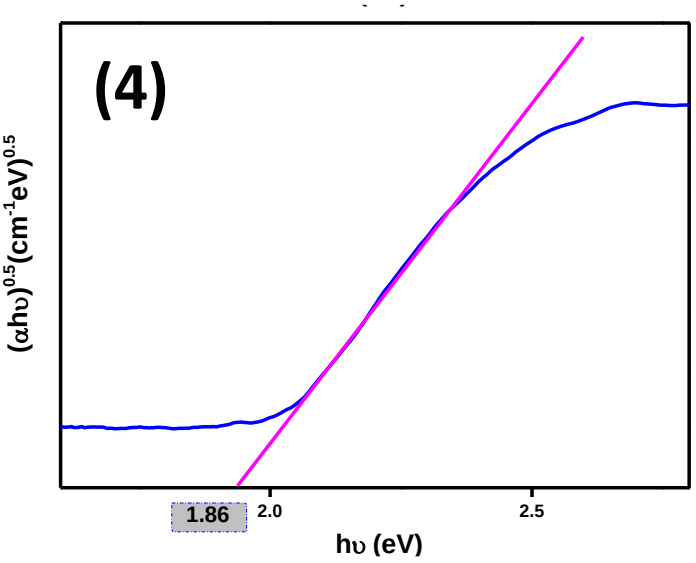
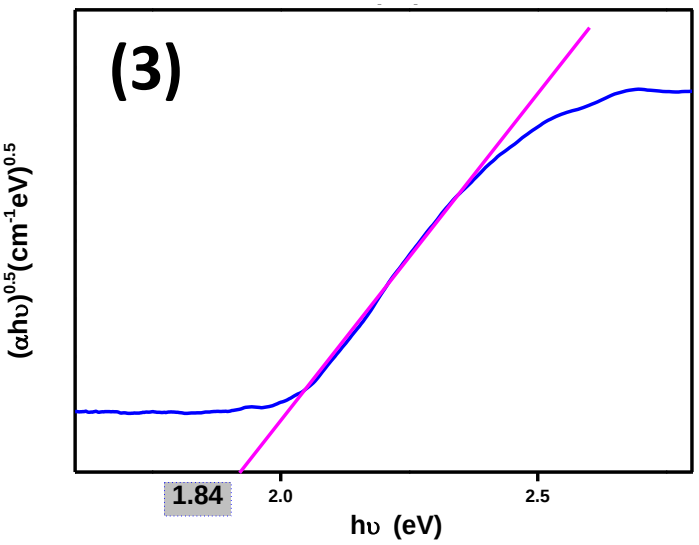


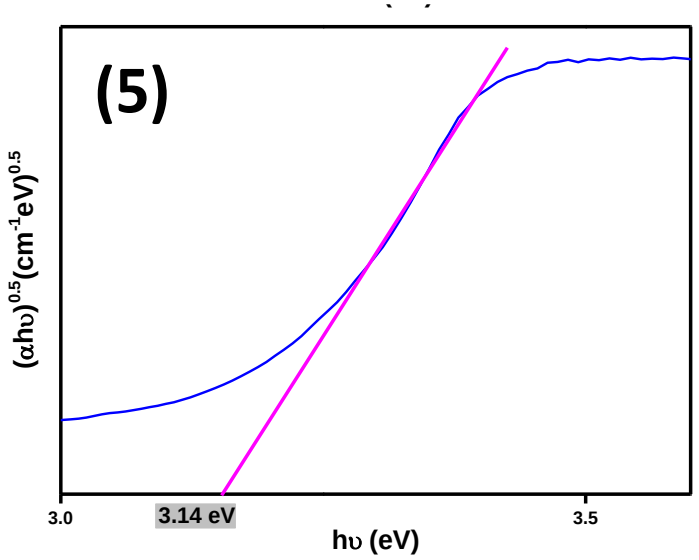
Figure S9. Photoluminescence spectra of (a) all the ligands, (b) H_2L and Na_2L and (c) the compounds **1-6** compared with the H_2L and Na_2L.


(1)
(αhυ)^0.5(cm^-1eV)^0.5
1.86
2.0
2.5
hυ (eV)


(2)
(αhυ)^0.5(cm^-1eV)^0.5
1.78
2.0
2.5
hυ (eV)


(4)
(αhυ)^0.5(cm^-1eV)^0.5
1.86
2.0
2.5
hυ (eV)


(3)
(αhυ)^0.5(cm^-1eV)^0.5
1.84
2.0
2.5
hυ (eV)



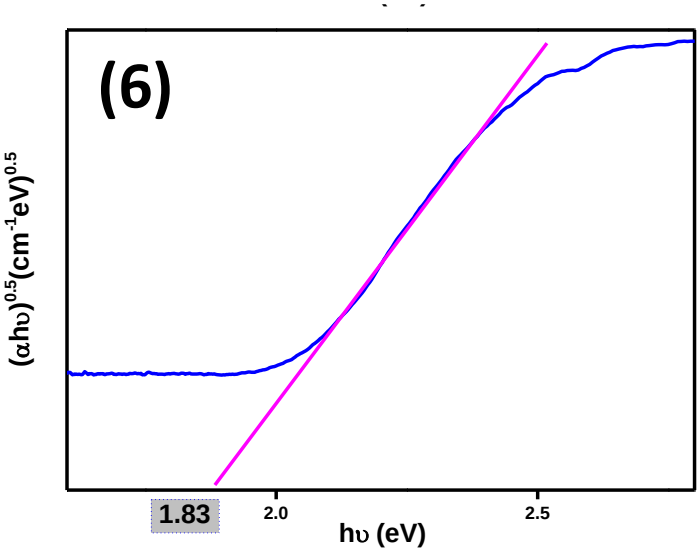


Figure S10. Tauc plot of the compounds **1**-**6**.

Table S9. The bandgaps of compounds and the acid ligands.

Sl. No.	Name of the Compound	Band gap energy (eV)
1	Na_2ABDCA	1.89
2	Na_2SDCA	3.84
3	Compound **1**	1.86
4	Compound **2**	1.78
5	Compound **3**	1.86
6	Compound **4**	1.84
7	Compound **5**	3.14
8	Compound **6**	1.83

4. References

(1) Dingle, R.; Lines, M. E.; Holt, S. L. Linear-Chain Antiferromagnetism in $[(CH_3)_4N]$ $[MnCl_3]$. *Phys. Rev.* **1969**, *187*, 643.

(2) Kubelka, P. New Contributions to the Optics of Intensely Light-Scattering Materials. Part I. *J. Opt. Soc. Am.***1948**, *38*, 448.

(3) Kubelka, P. New Contributions to the Optics of Intensely Light-Scattering Materials. Part II: Nonhomogeneous Layers. *J. Opt. Soc. Am.* **1954**, *44*, 330.

(4) Murphy A. B. Modified Kubelka-Munk Model for Calculation of the Reflectance of Coatings with Optically-Rough Surfaces. *J. Phys. D:Appl. Phys.***2006**, *39*, 3571.

(5) Laidani, N.; Bartali, R.; Gottardi, G.; Anderle, M. Optical Absorption Parameters of Amorphous Carbon Films fromForouhi–Bloomer andTauc–Lorentz Models: a comparative study. *J. Phys.: Condens. Matter*. **2008**, *20*, 15216.