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Electronic Supplementary Information

Magnetic Properties of Manganese based One-dimensional Spin Chains

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TOPOS analysis for compound **1**

####################

1:C25 H29 Mn2 N3 O13

####################

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	
Mn 2	0.2205	0.4914	0.0942	(0 0 0)	3.670A	1
Mn 2	0.2795	0.9914	0.0942	(0 0 0)	5.510A	1
Mn 1	0.2237	0.8067	-0.4106	(0 1-1)	9.648A	1
Mn 1	0.2237	0.8067	0.5894	(0 1 0)	9.648A	1
Mn 2	0.2795	0.5086	-0.4058	(0 1-1)	9.972A	1
Mn 1	-0.2763	0.6933	0.4106	(-1 0 0)	10.952A	1
Mn 1	0.7237	0.6933	0.4106	(0 0 0)	10.952A	1
Mn 2	0.2205	1.0086	0.5942	(0 1 0)	11.107A	1
Mn 2	0.7205	0.4914	0.4058	(0 0 0)	11.457A	1
Mn 2	-0.2795	0.4914	0.4058	(-1 0 0)	11.549A	1

Topology for Mn2

Atom Mn2 links by bridge ligands and has

Common vertex with					R(A-A)	
Mn 1	0.2237	0.6933	0.0894	(0 0 0)	3.670A	1
Mn 1	0.2763	0.1933	0.0894	(0-1 0)	5.510A	1
Mn 2	0.2795	0.5086	-0.4058	(0 1-1)	9.492A	1

Mn 2 0.2795 0.5086 0.5942 (0 1 0) 9.492A 1

Mn 1 0.2763 0.3067 0.5894 (0 1 0) 9.972A 1

Mn 2 0.7205 0.4914 0.4058 (0 0 0) 10.853A 1

Mn 2 -0.2795 0.4914 0.4058 (-1 0 0) 10.853A 1

Mn 1 0.2237 0.8067 -0.4106 (0 1-1) 11.107A 1

Mn 1 -0.2763 0.6933 0.4106 (-1 0 0) 11.457A 1

Mn 1 0.7237 0.6933 0.4106 (0 0 0) 11.549A 1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Mn

Coordination sequences

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

Num 10 40 92 162 252 362 492 642 812 1002

Cum 11 51 143 305 557 919 1411 2053 2865 3867

Rad 9.4(2.7) 15.1(3.9) 21.9(4.7) 29.0(5.6) 36.1(6.5) 43.2(7.6) 50.3(8.6) 57.4(9.7) 64.5(10.8) 71.6(11.9)

Cmp Mn10 Mn40 Mn92 Mn162 Mn252 Mn362 Mn492 Mn642 Mn812 Mn1002

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

Num 10 40 92 162 252 362 492 642 812 1002

Cum 11 51 143 305 557 919 1411 2053 2865 3867

Rad 9.4(2.7) 15.1(3.8) 21.9(4.8) 29.0(5.6) 36.1(6.6) 43.2(7.6) 50.3(8.7) 57.4(9.7) 64.5(10.8) 71.6(11.9)

Cmp Mn10 Mn40 Mn92 Mn162 Mn252 Mn362 Mn492 Mn642 Mn812 Mn1002

TD10=3867

Vertex symbols for selected sublattice

Mn1 Point symbol:{3^12.4^24.5^8.6}

Extended point symbol:[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(3).4(3).4(3).4(3).5.5.5.5(2).5(3).5(3).5(4).5(5).6(10)]

Mn2 Point symbol:{3^12.4^24.5^8.6}

Extended point symbol:[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(3).4(3).4(3).4(3).5.5.5.5(2).5(3).5(3).5(4).5(5).6(10)]

Point symbol for net: {3^12.4^24.5^8.6}

10-c net; uninodal net

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Elapsed time: 68.60 sec.

TOPOS analysis for compound **2**

####################

1:C22 H22 Mn2 N2 O10

####################

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 2	0.8477	0.9298	1.0196	(1 1 2)	6.302A	1
Mn 1	0.6100	1.4203	0.5342	(1 0 1)	9.697A	1
Mn 1	0.6100	0.4203	0.5342	(1-1 1)	9.697A	1
Mn 2	0.1523	0.4298	0.4804	(0 0-1)	10.427A	1
Mn 2	0.1523	1.4298	0.4804	(0 1-1)	10.522A	1
Mn 2	0.8477	0.5702	0.5196	(1 0 1)	10.739A	1
Mn 2	0.1523	1.4298	1.4804	(0 1 0)	11.012A	1
Mn 1	0.3900	1.5797	0.4658	(0 2-1)	11.123A	1
Mn 1	0.3900	1.5797	1.4658	(0 2 0)	11.123A	1
Mn 2	-0.1523	0.5702	0.5196	(0 0 1)	11.331A	1
Common edge with					R(A-A)	
Mn 1	0.6100	1.0797	1.0342	(1 2 2)	3.610A	2
Common face with					R(A-A)	
Mn 2	0.1523	1.0702	0.9804	(0 1 0)	3.597A	3

Topology for Mn2

Atom Mn2 links by bridge ligands and has

Common vertex with R(A-A) f

Mn 1 0.6100 0.0797 1.0342 (1 1 2) 6.302A 1

Mn 2 0.1523 0.4298 0.4804 (0 0-1) 9.580A 1

Mn 2 0.1523 0.4298 1.4804 (0 0 0) 9.580A 1

Mn 1 0.3900 -0.4203 1.4658 (0 0 0) 10.427A 1

Mn 2 -0.1523 0.5702 0.5196 (0 0 1) 10.443A 1

Mn 2 -0.1523 -0.4298 0.5196 (0-1 1) 10.443A 1

Mn 1 0.3900 0.5797 1.4658 (0 1 0) 10.522A 1

Mn 1 0.6100 0.4203 0.5342 (1-1 1) 10.739A 1

Mn 2 0.1523 -0.5702 1.4804 (0-1 0) 11.006A 1

Mn 2 0.1523 -0.5702 0.4804 (0-1-1) 11.006A 1

Mn 1 0.3900 0.5797 0.4658 (0 1-1) 11.012A 1

Mn 1 -0.3900 0.4203 0.5342 (0-1 1) 11.331A 1

Common edge with R(A-A)

Mn 2 -0.1523 -0.0702 1.0196 (0 0 2) 4.457A 2

Common face with R(A-A)

Mn 1 0.3900 -0.0797 0.9658 (0-1 0) 3.597A 3

Structural group analysis

Structural group No 1

Structure consists of 3D framework with MnO2

Coordination sequences

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

Num 12 52 124 217 346 499 682 889 1132 1397

Cum 13 65 189 406 752 1251 1933 2822 3954 5351

Rad 9.1(2.9) 15.1(4.0) 21.9(4.7) 29.4(5.3) 36.5(6.3) 43.9(7.3) 51.2(8.2) 58.6(9.3) 65.9(10.3) 73.3(11.3)

Cmp Mn12 Mn52 Mn124 Mn217 Mn346 Mn499 Mn682 Mn889 Mn1132 Mn1397

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

Num 14 55 122 222 347 500 682 895 1130 1398

Cum 15 70 192 414 761 1261 1943 2838 3968 5366

Rad 9.3(2.6) 15.3(4.0) 22.4(4.6) 29.5(5.4) 36.8(6.4) 44.1(7.3) 51.4(8.3) 58.7(9.4) 66.1(10.4) 73.4(11.5)

Cmp Mn14 Mn55 Mn122 Mn222 Mn347 Mn500 Mn682 Mn895 Mn1130 Mn1398

TD10=5358

Vertex symbols for selected sublattice

Mn1 Point symbol:{3^23.4^41.5^2}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).5(7).5(7)]

Mn2 Point symbol:{3^25.4^53.5^12.6}

Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(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(2).4(2).4(2).4(2).4(3).4(3).4(3).4(3).4(3).4(3).4(3).4(3).5.5(2).5(3).5(4).5(4).5(4).5(4).5(5).5(5).5(7).5(8).5(16).6(31)]

Point symbol for net: {3^23.4^41.5^2}{3^25.4^53.5^12.6}

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

TOPOS analysis for compound **3**

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1:C17 H17 Mn1.50 N O7

####################

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 2	0.5000	0.2864	0.7500	(0 0 0)	6.296A	1
Mn 1	0.3246	-0.1857	0.1114	(0-1 0)	9.428A	1
Mn 1	0.3246	0.8143	0.1114	(0 0 0)	9.428A	1
Mn 2	0.0000	-0.2136	-0.2500	(0 0 0)	10.622A	1
Mn 2	0.5000	0.7136	0.2500	(0 0 0)	10.665A	1
Mn 1	0.1754	-0.3143	-0.1114	(0 0-1)	11.032A	1
Mn 1	0.1754	-0.3143	0.8886	(0 0 0)	11.032A	1
Mn 2	0.0000	-0.2136	0.7500	(0 0 1)	11.207A	1

Common edge with					R(A-A)	
Mn 1	0.3246	0.1857	0.6114	(0 0 1)	3.507A	2

Common face with					R(A-A)	
Mn 2	0.0000	0.2136	0.2500	(0 0 0)	3.536A	3

Topology for Mn2

Atom Mn2 links by bridge ligands and has

Common vertex with					R(A-A)	f
Mn 1	0.3246	0.1857	0.6114	(0 0 1)	6.296A	1

Mn 1 -0.3246 0.1857 -0.1114 (-1 0-1) 6.296A 1

Mn 1 0.1754 -0.3143 0.8886 (0 0 0) 10.622A 1

Mn 1 -0.1754 -0.3143 -0.3886 (0 0 0) 10.622A 1

Mn 1 0.3246 -0.1857 0.1114 (0-1 0) 10.665A 1

Mn 1 -0.3246 -0.1857 0.3886 (-1-1 0) 10.665A 1

Mn 1 0.1754 -0.3143 -0.1114 (0 0-1) 11.207A 1

Mn 1 -0.1754 -0.3143 0.6114 (0 0 1) 11.207A 1

Common edge with R(A-A)

Mn 2 0.0000 -0.2136 0.7500 (0 0 1) 9.824A 2

Mn 2 0.0000 -0.2136 -0.2500 (0 0 0) 9.824A 2

Common face with R(A-A)

Mn 1 0.1754 0.3143 0.3886 (0 0 0) 3.536A 3

Mn 1 -0.1754 0.3143 0.1114 (0 0 0) 3.536A 3

Structural group analysis

Structural group No 1

Structure consists of 3D framework with MnO2

Coordination sequences

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

Num 10 37 86 154 232 351 448 630 734 989

Cum 11 48 134 288 520 871 1319 1949 2683 3672

Rad 8.7(3.1) 14.1(3.6) 20.0(5.0) 26.5(5.8) 32.9(6.9) 39.3(8.0) 45.8(9.2) 52.1(10.3) 58.9(11.6) 65.0(12.7)

Cmp Mn10 Mn37 Mn86 Mn154 Mn232 Mn351 Mn448 Mn630 Mn734 Mn989

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

Num 12 36 92 148 244 336 474 596 782 932

Cum 13 49 141 289 533 869 1343 1939 2721 3653

Rad 8.7(2.9) 14.6(3.4) 20.1(4.9) 26.7(5.7) 33.0(6.9) 39.4(8.0) 46.0(9.1) 52.2(10.4) 59.0(11.4) 65.1(12.8)

Cmp Mn12 Mn36 Mn92 Mn148 Mn244 Mn336 Mn474 Mn596 Mn782 Mn932

TD10=3665

Vertex symbols for selected sublattice

Mn1 Point symbol:{3^18.4^22.5^5}
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(2).4(3).5.5(3).5(3).5(3).5(3)]

Mn2 Point symbol:{3^24.4^34.5^8}
Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4.4(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)]

Point symbol for net: {3^18.4^22.5^5}2{3^24.4^34.5^8}
10,12-c net with stoichiometry (10-c)2(12-c); 2-nodal net
Database with topological types was not loaded. Check 'Classification' flag.
Elapsed time: 15.22 sec.

Table S1.Crystallographic parameters for compounds **1** -**3**.

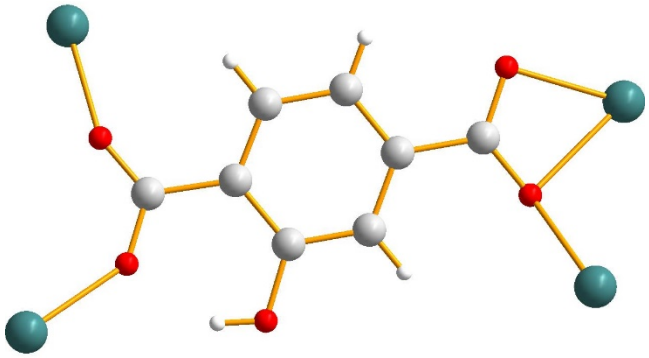
Parameters	**Compound 1**	**Compound 2**	**Compound 3**
Empirical formula	$C_{25}H_{29}Mn_2N_3O_{13}$	$C_{22}H_{22}Mn_2N_2O_{10}$	$C_{17}H_{17}Mn_{1.5}NO_7$
Formula weight	689.39	584.29	429.72
Crystal System	Orthorhombic	Monoclinic	Monoclinic
Space Group	*Pbca* (no.61)	$P2_1/c$ (no. 14)	$C2/c$ (no.15)
a(Å)	18.2507(9)	13.6353(3)	24.7417(14)
b(Å)	18.1651(6)	10.2259(3)	10.8825(6)
c(Å)	18.8518(7)	17.6925(4)	17.3105(18)
α(°)	90	90	90
β(°)	90	90.7040(10)	129.637(2)
γ(°)	90	90	90
Volume(Å^3)	6249.9(4)	2466.74(11)	3589.3(5)
Z	8	4	8
Calculated density, Mg/m^3	1.465	1.573	1.590
Crystal size, mm	0.200 x 0.150 x 0.150	0.200 x 0.200 x 0.150	0.200 x 0.150 x 0.100
θ range (deg)	2.489 to 28.247	1.494 to 26.370	2.138 to 28.280
F (000)	2832	1192	1756
Absorption coefficient (mm^{-1})	0.874	1.082	1.111
Reflections collected	30880	19737	14859
Unique reflections	7521	5036	4402
Goodness-of-fit	1.003	1.114	1.046
Number of parameters	390	329	242
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1225	R1 = 0.0308, wR2 = 0.0787	R1 = 0.0543, wR2 = 0.1128
R indices (all data)	R1 = 0.0895, wR2 = 0.1528	R1 = 0.0432, wR2 = 0.0911	R1 = 0.1007, wR2 = 0.1352
Largest diff. peak and hole e Å^{-3}	1.537 and -0.424	0.442 and -0.368	0.912 and -0.655

[a]$R_1 = \Sigma||F_0| - |F_c||/ \Sigma|F_0|$; $wR_2 = \{[w(F_0^2 - F_c^2)^2]/ [w(F_0^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_0)^2 + (aP)^2 + bP]$; $P = [\max(F_0^2,0) + 2(F_c)^2]/3$, where a = 0.0834 and b = 2.7271 for compound **1**, a = 0.0488 and b = 0.5342 for compound **2**, and a = 0.0508 and b = 11.5053 for compound **3**, respectively.

Table S2. Selected Bond lengths for compounds **1** – **3**.

Moiety	Bond lengths (Å)
Compound 1	
Mn(2)-O(11)	2.126(2)
Mn(2)-O(7)	2.156(2)
Mn(2)-O(9)	2.167(2)
Mn(2)-O(10)	2.179(2)
Mn(2)-O(6)	2.1921(19)
Mn(2)-O(8)	2.213(2)
Mn(1)-O(5)	2.094(2)
Mn(1)-O(3)	2.107(2)
Mn(1)-O(2)	2.112(2)
Mn(1)-O(4)	2.203(2)
Mn(1)-O(1)	2.232(3)
Mn(1)-O(6)	2.358(2)
Compound 2	
Mn(1)-O(2)	2.0855(16)
Mn(1)-O(3)	2.1038(16)
Mn(1)-O(9)#1	2.1480(15)
Mn(1)-O(1)	2.1660(17)
Mn(1)-O(4)	2.2234(15)
Mn(1)-O(9)#2	2.4579(16)
Mn(2)-O(7)	2.0816(16)
Mn(2)-O(10)#3	2.1080(15)
Mn(2)-O(6)	2.1426(18)
Mn(2)-O(5)	2.1740(15)
Mn(2)-O(8)	2.2047(18)
Mn(2)-O(4)	2.4335(15)
Compound 3	
Mn(1)-O(3)	2.091(3)
Mn(1)-O(1)	2.158(3)
Mn(1)-O(2)#1	2.171(2)
Mn(1)-O(5)	2.179(3)
Mn(1)-O(2)	2.322(2)
Mn(1)-O(4)	2.387(2)
Mn(2)-O(7)	2.118(3)
Mn(2)-O(7)#2	2.119(3)
Mn(2)-O(6)	2.170(3)
Mn(2)-O(6)#2	2.170(3)
Mn(2)-O(4)#2	2.284(2)
Mn(2)-O(4)	2.284(2)

(a)



(b)

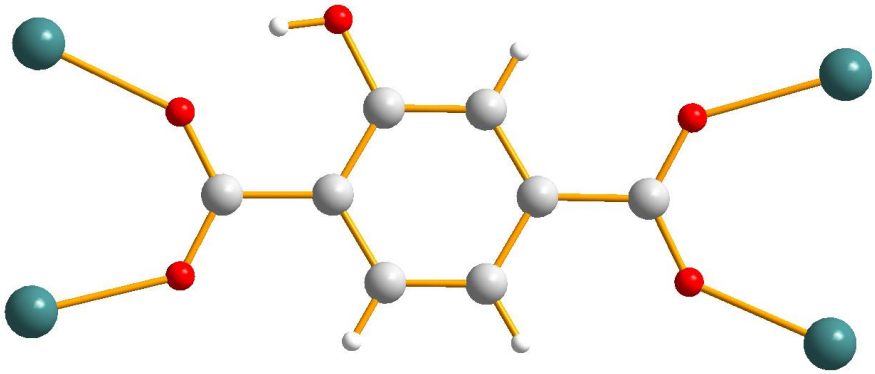


Figure S1: (a) acid-1 and (b) acid-2 connectivity of OH-BDC anion in **1**.

(a)

(b)

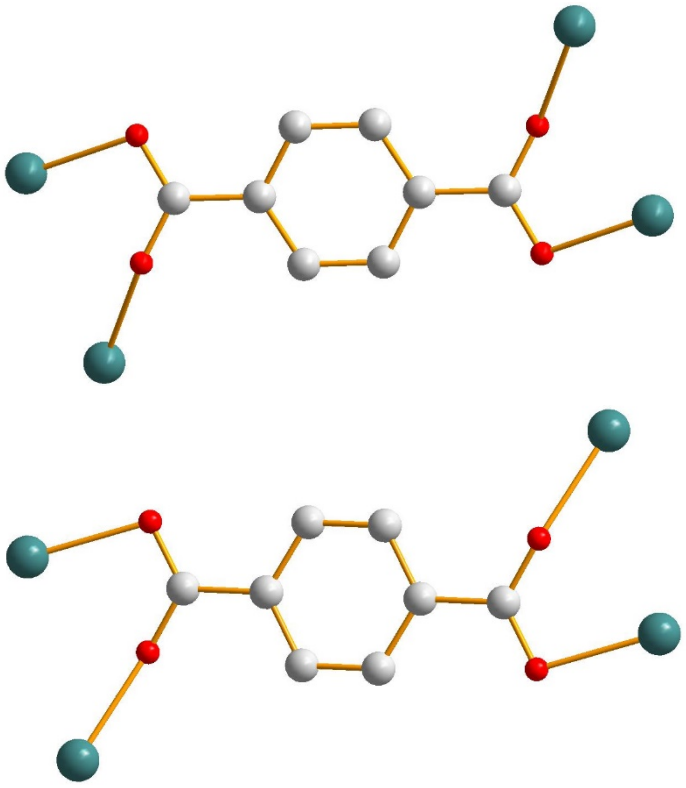


Figure S2: (a) acid-1 and (b) acid-2 connectivity of BDC anion in **2**.

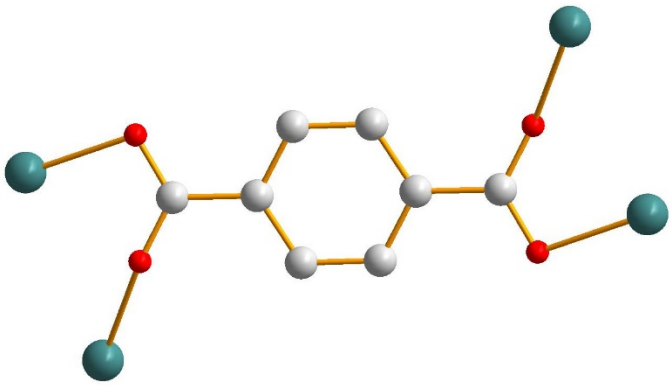


Figure S3: Acid connectivity of BDC anion in **3**.

PXRD Characterization

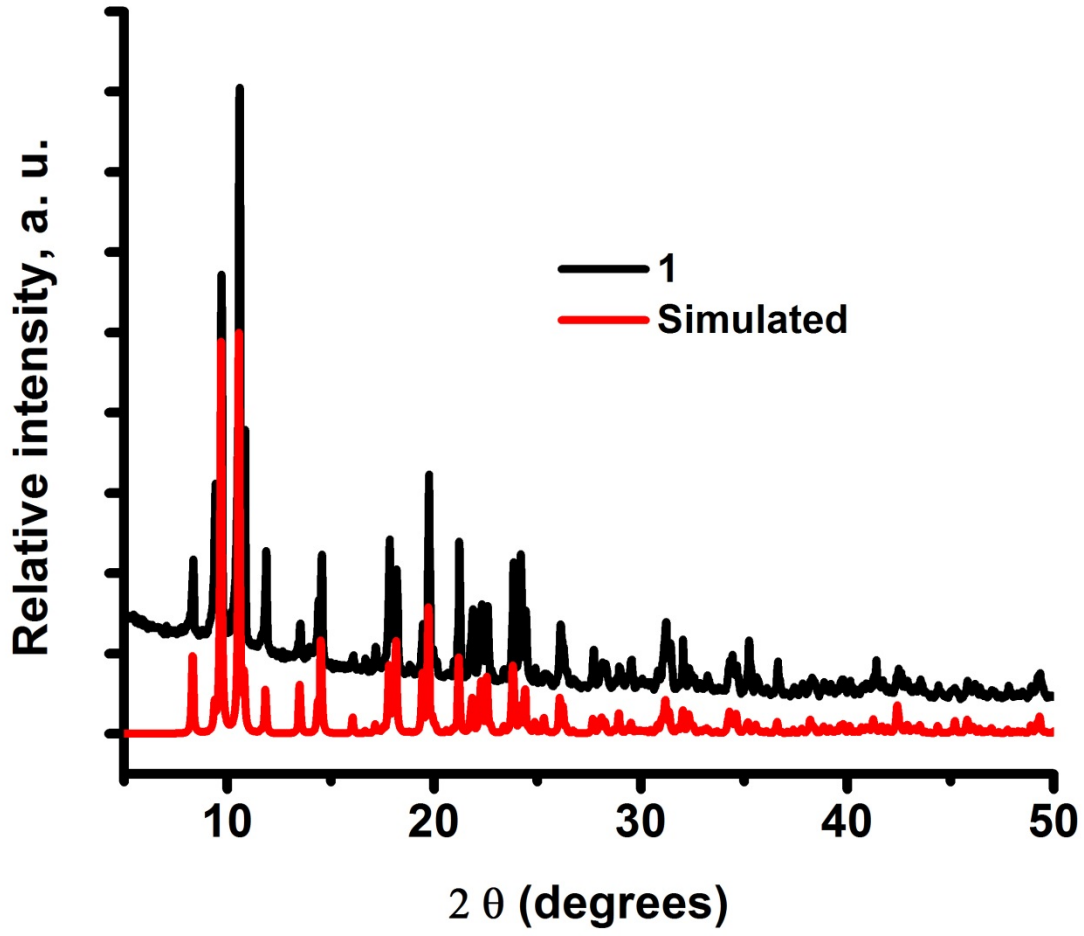


Figure S4: PXRD analysis of compound **1**.

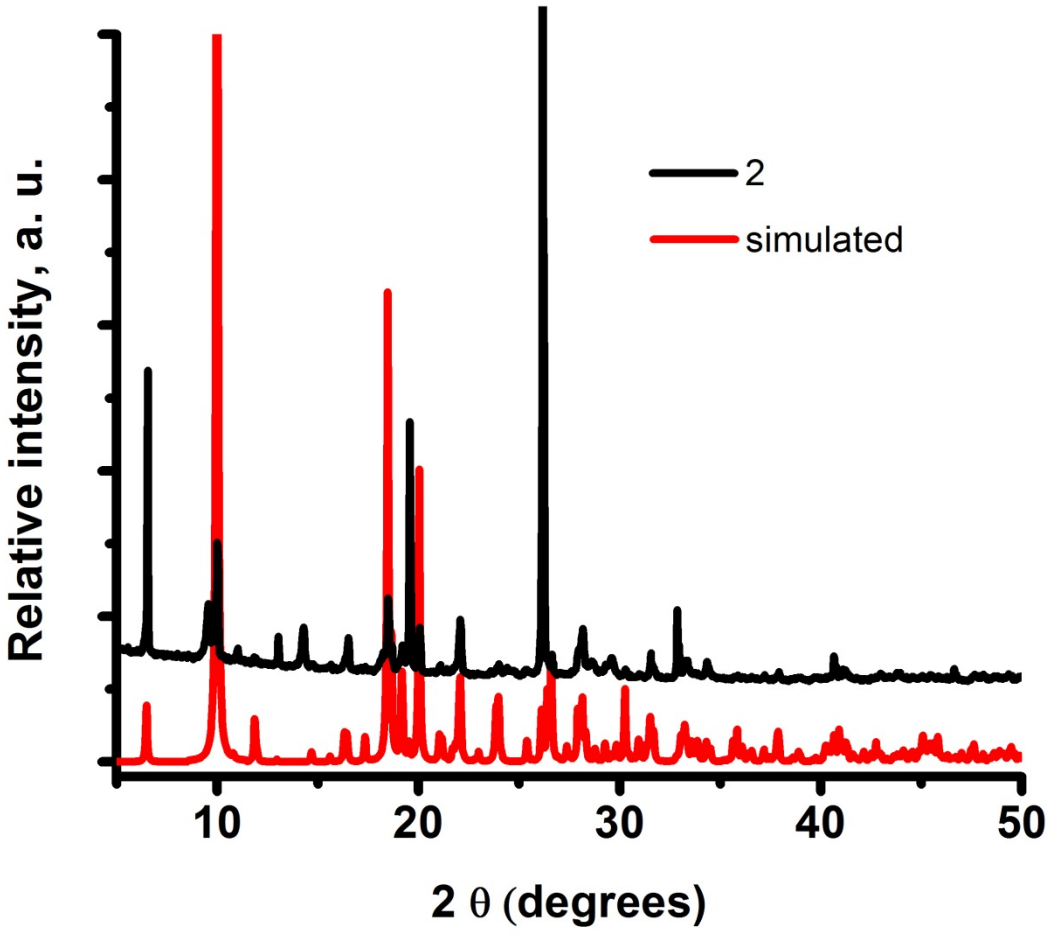


Figure S5: PXRD analysis of compound **2**.

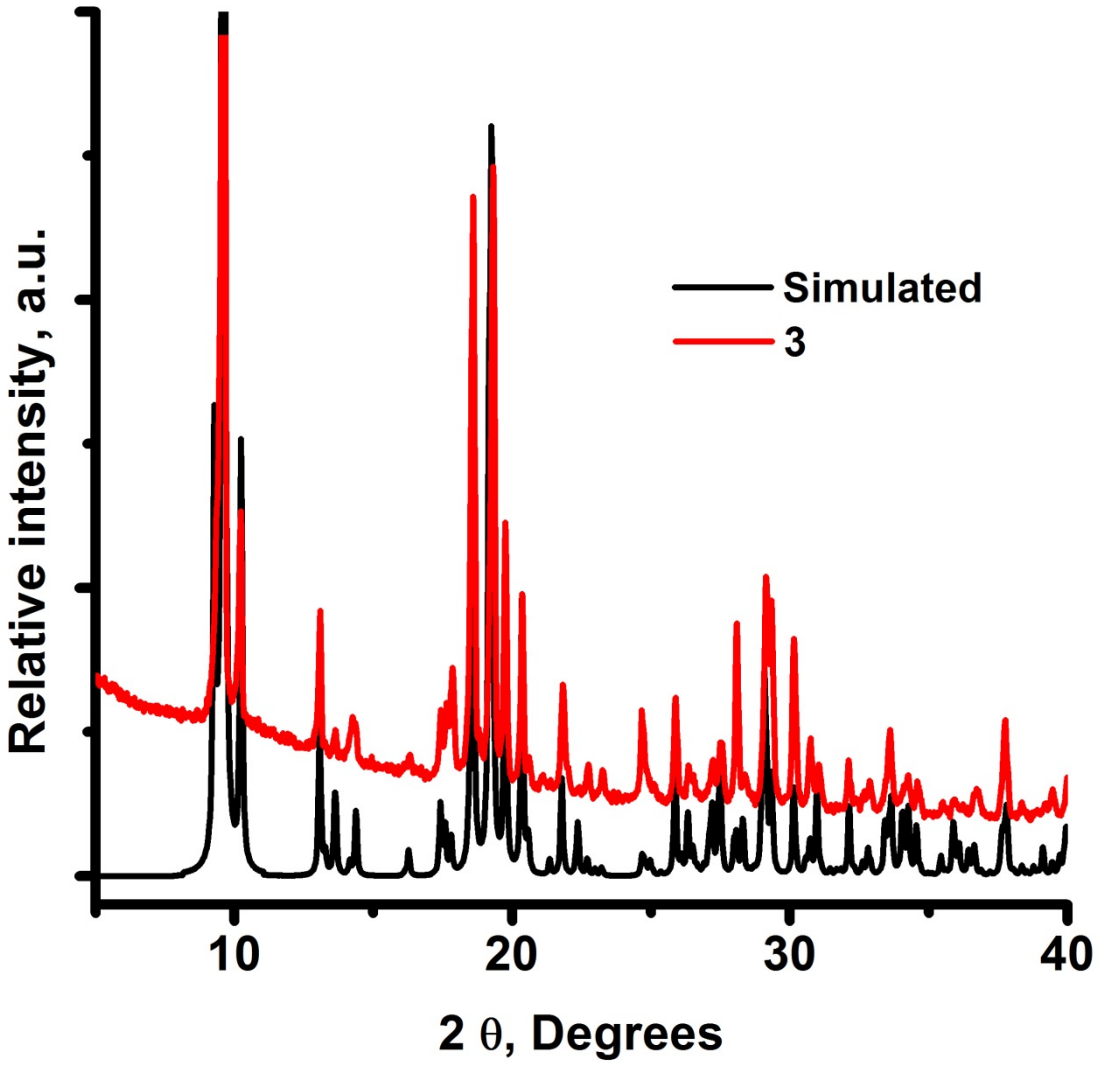


Figure S6: PXRD analysis of compound **3**.

Thermo gravimetric analysis

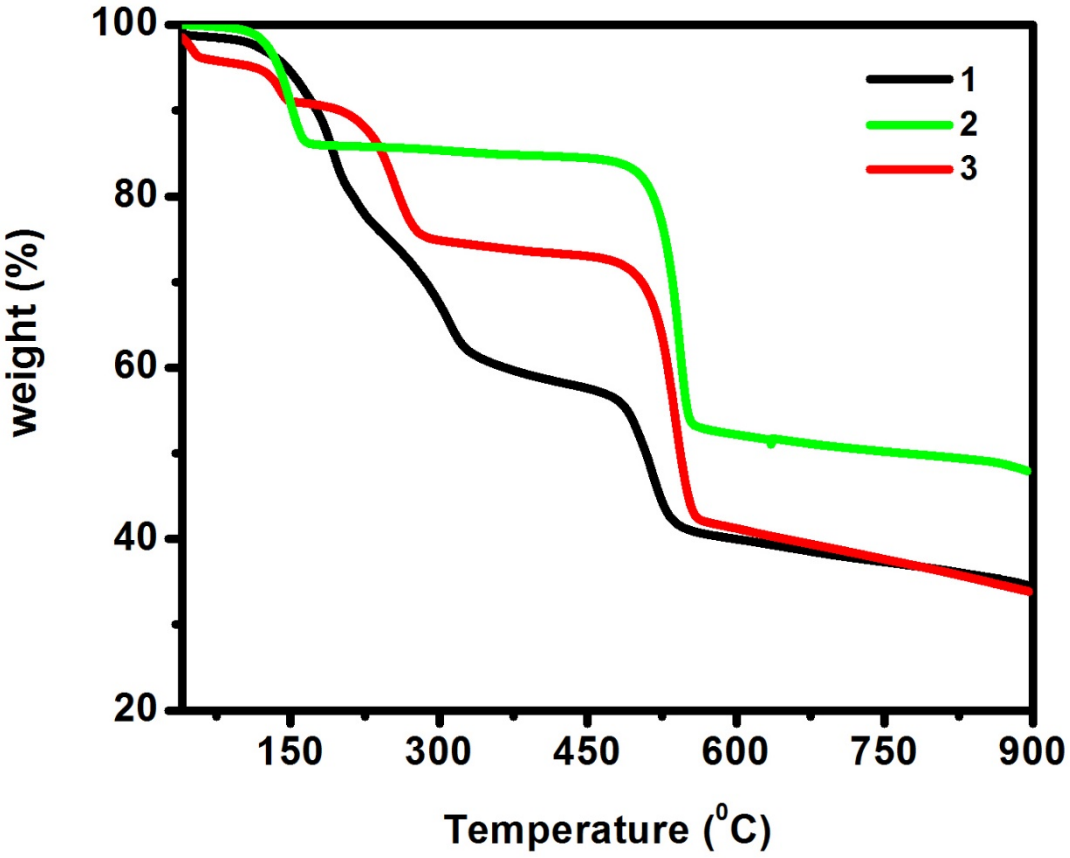


Figure S7: TGA analysis of compound **1**, **2**, and **3**, respectively.

IR analysis

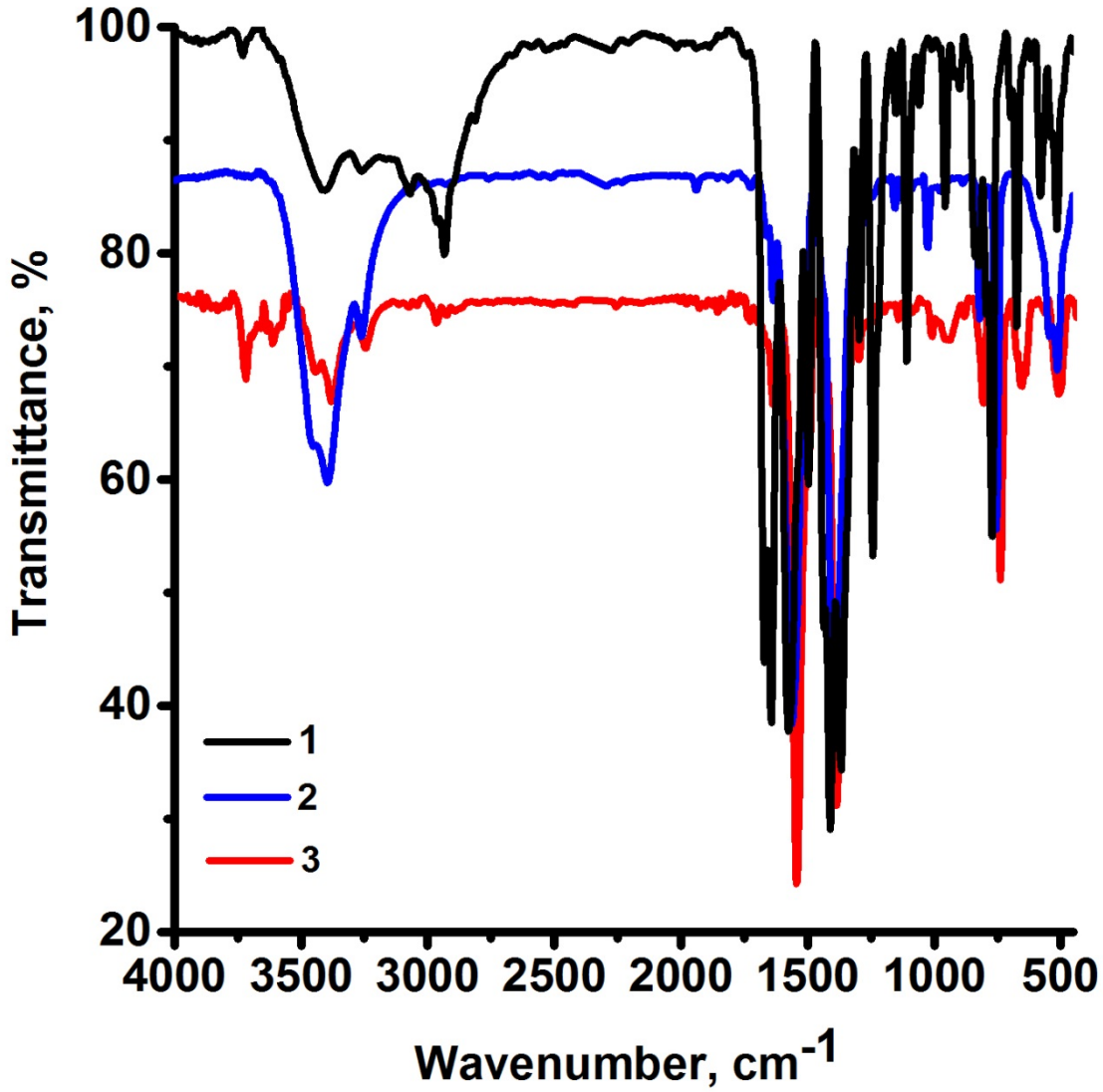


Figure S8: IR spectra for compound **1** (ν (O-H), broad = 3000-3400 cm^{-1}, ν (C=O), strong = 1642 cm^{-1}), **2** (ν (H_2O) = 3395 cm^{-1}, ν (C=O) = 1560 cm^{-1}) and **3** (ν (H_2O), weak = 3400 cm^{-1}, ν (C=O) = 1550 cm^{-1}).