Electronic Supporting Information

For

Solvent/temperature-dpendent assemblies of several high-dimensional supramolecular networks containing quinoline-2,3-dicarboxylic acid

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Contents

Table S**1.** Crystal data and structure refinement for complexes **1**-**4**.

Complexes	**1**	**2**	**3**	**4**
Empirical formula	$C_{22}H_{16}N_2O_{10}Zn$	$C_{26}H_{24}N_2O_{10}S_2Zn$	$C_{28}H_{22}N_2O_{10}Zn$	$C_{22}H_{12}N_2O_8Zn$
Formula weight	533.74	653.96	611.85	497.71
Temperature	298(2) K	298(2) K	298(2) K	298(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	triclinic	triclinic	monoclinic	monoclinic
Space group	*P*-1	*P*-1	*C*2/*c*	$P2_1/n$
a (Å)	7.4062(17)	8.453(5)	17.912(4)	12.693(4)
b (Å)	9.136(2)	9.025(5)	7.1061(15)	5.7903(19)
c (Å)	9.415(3)	9.160(6)	20.966(4)	13.581(5)
α (º)	110.466(4)	76.339(8)	90	90
β (º)	98.320(4)	85.010(9)	107.440(2)	115.966(4)
γ (º)	111.664(3)	73.885(8)	90	90
V (Å^3)	526.6(2)	652.2(7)	2545.9(9)	897.4(5)
Z	1	1	4	2
ρ (cald.) (mg m^{-3})	1.683	1.665	1.596	1.842
μ (m^{-1})	1.232	1.166	1.031	1.431
F(000)	272	336	1256	504
Crystal size (mm)	0.26 × 0.18 × 0.11	0.18 × 0.15 × 0.09	0.22 × 0.16 × 0.09	0.25 × 0.21 × 0.16
θ range for data collection (°)	2.43 to 25.20	2.29 to 25.19	2.04 to 25.20	1.83 to 25.20
h/*k*/*l* (max, min)	-6 , 8/-10, 10/ -10, 11	-9, 10/-10, 10/ -8, 10	-18, 21/-8, 6/ -24, 25	-12, 15/-6, 6/ -16, 14
Reflections collected	2731	3366	6252	4341
Unique	1861 [R(int) = 0.0250]	2307 [R(int) = 0.0307]	2300[R(int) = 0.0306]	1609 [R(int) = 0.0583]
Completeness to θ = 27.13	98.0 %	98.4 %	99.7 %	99.3 %
Absorption correction	empirical	empirical	empirical	empirical
Max. and min. transmission	full-matrix	full-matrix	full-matrix	full-matrix
	least-squares on F^2	least-squares on F^2	least-squares on F^2	least-squares on F^2
Data / restraints / parameters	1861 / 3 / 165	2307 / 0 / 190	2300 / 4 / 195	1609 / 1 / 155
Goodness-of-fit on F^2	1.074	1.047	1.099	1.003
Final $R1^a$,$wR2^b$ indices [$I > 2\sigma(I)$]	0.0543, 0.1331	0.0576, 0.1265	0.0594, 0.1812	0.0496, 0.1038
	0.0650, 0.1408	0.0857, 0.1442	0.0800, 0.1979	0.0864, 0.1206
*R*1, *wR*2 indices (all data)	0.383 / -0.709	0.397 / -0.650	0.706 /-0.656	0.409 /-0.550
Largest diff. Peak/ hole(e Å^{-3})				

[a] $R = \Sigma \big| |F_o| - |F_c| \big| / S|F_o|$. [b] $wR = [\Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2)+(0.0433P)^2+1.8091P]$ for **1**, $1/[\sigma^2(F_o^2)+(0.0491P)^2+1.3878P]$ for **2**, $1/[\sigma^2(F_o^2)+(0.1077P)^2+15.9016P]$ for **3** and $w = 1/[\sigma^2(F_o^2)+(0.0393P)^2+2.0990P]$ for **4**, $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Selected Bond Distances (Å) and Angles (°) for complexes **1-4***.

		1	
Zn(1)-O(2)	2.031(3)	O(2)-Zn(1)-N(1)	75.25(12)
Zn(1)-O(3)	2.091(3)	O(2)-Zn(1)-N(1)#1	104.75(12)
Zn(1)-N(1)	2.221(3)	O(3)-Zn(1)-N(1)	90.72(13)
O(2)-Zn(1)-O(3)	89.79(13)	O(3)-Zn(1)-N(1)#1	89.28(13)
O(2)-Zn(1)-O(3)#1	90.21(14)		
		2	
Zn(1)-O(1)	2.000(3)	O(6)-Zn(1)-N(1)#2	88.19(15)
Zn(1)-O(5)	2.110(4)	O(1)-Zn(1)-N(1)	77.05(14)
Zn(1)-N(1)	2.126(4)	O(6)-Zn(1)-N(1)	91.81(15)
O(1)-Zn(1)-O(6)#2	86.02(15)	O(1)-Zn(1)-N(1)#2	102.95(14)
O(1)-Zn(1)-O(6)	93.97(15)		
		3	
Zn(1)-O(1)	2.034(3)	O(1)-Zn(1)-N(1)	74.24(14)
Zn(1)-O(3)	2.052(4)	O(3)-Zn(1)-N(1)	91.64(15)
Zn(1)-N(1)	2.254(4)	O(1)-Zn(1)-N(1)#2	105.76(14)
O(1)-Zn(1)-O(3)#2	91.67(16)	O(3)-Zn(1)-N(1)#2	88.36(15)
O(1)-Zn(1)-O(3)	88.33(16)		
		4	
Zn(1)-O(1)	1.892(3)	O(1)-Zn(1)-N(1)#3	98.55(14)
Zn(1)-N(1)	2.127(3)	O(1)-Zn(1)-N(1)	81.45(14)
Zn(1)-O(3)#4	2.476(3)	O(1)-Zn(1)-O(3)#5	90.19(13)
Zn(1)-O(3)#5	2.476(3)	N(1)-Zn(1)-O(3)#4	85.30(12)
N(1)-Zn(1)-O(3)#5	94.70(12)		

*Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1; #2 -x+1,-y+1,-z; #3 -x+2,-y,-z+2; #4 -x+3/2,y+1/2,-z+3/2; #5 x+1/2,-y-1/2,z+1/2.

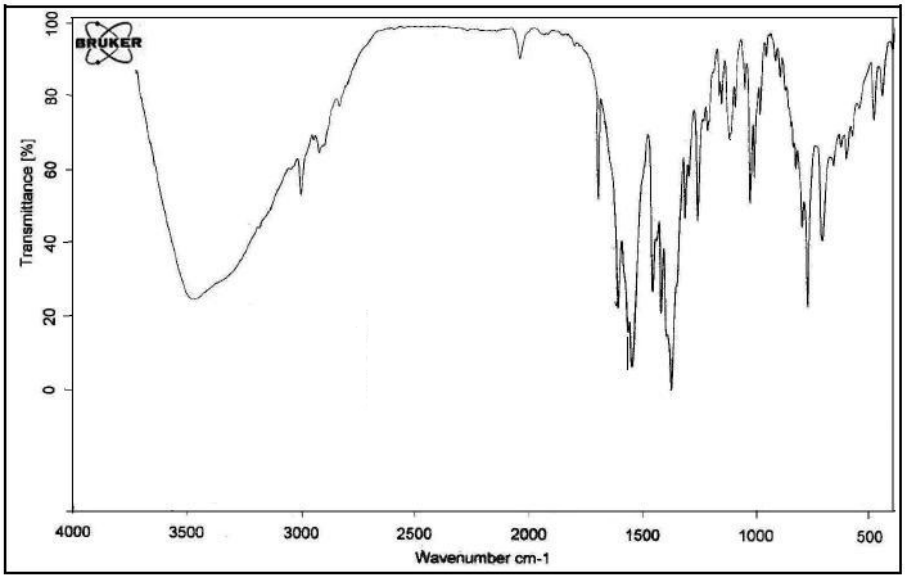
Table **S3.** Distances (Å) and angles (°) of hydrogen bonds for the compounds **1**-**4***.

D-H···A	d(H···A)	d(D···A)	∠D-H···A
		1	
O4-H4···O1	1.55	2.387(5)	176
O3-H3A···O5#1	1.94	2.743(5)	165
O3-H3B···O4#2	1.97	2.795(4)	177
C8-H8···O1#3	2.52	3.385(5)	136
π···π[a]	3.58		
		2	
O3-H3···O2	1.63	2.444(6)	173
C12-H12A···O4#4	2.52	3.425(6)	157
C13-H13C···O4#4	2.71	3.572(6)	145
C13-H13B···O1#5	2.66	3.582(5)	160
C13-H13B···O2#5	2.63	3.486(6)	148
C8-H8···O3#6	2.48	3.267(5)	142
C9-H9···O2#6	2.68	3.572(5)	161
π···π[a]	3.71		
		3	
O3-H3A···O5#7	1.94	2.747(5)	144
O3-H3A···O3#8	2.33	3.130(4)	154
O4-H4···O2	1.69	2.386(5)	165
C8-H8···O4#9	2.63	3.430(5)	145
C9-H9···O2#9	2.69	3.515(6)	148
C7-H7···π[b]	2.63		
π···π[b]	3.56		
		4	
O3-H3···O2#10	1.74	2.570(5)	171
C10-H10···O4#11	2.68	2.723(3)	156

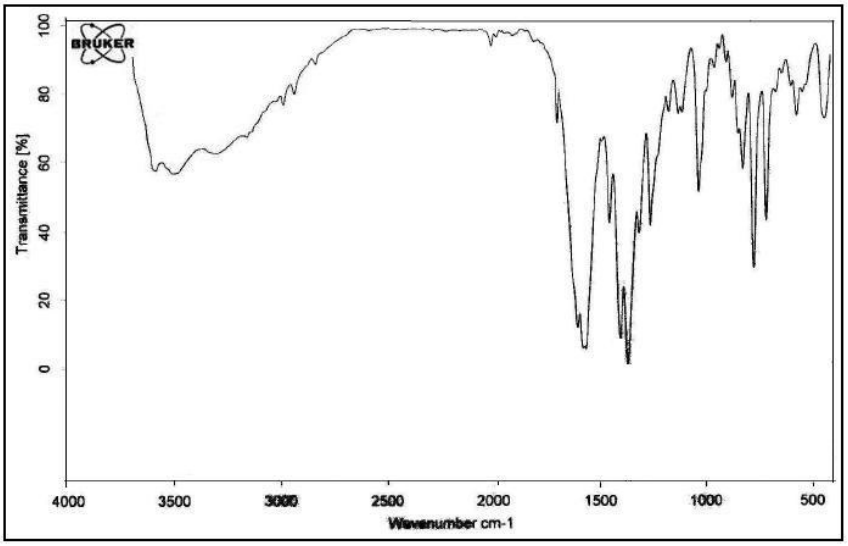
*Symmetry transformation used to generate equivalent atoms: #1 x-1,y-1,z; #2 -x, -y+1, -z+1; #3 –x-2, y-1/2, -z+1/2; #4 –x-1, y-1/2, -z+1/2; #5 –x,-y,-z+1; #6 x-1,y,z; #7 x-1/2,y+1/2,z; #8 -x+1,-y+2,-z; #9 -x-1,-y,-z; #10 -x+3/2,y+1/2, -z+3/2; #11 x-1/2,y,-z+1/2. [a]Denotes distances between the centroids of quinoline rings, [b]denotes the shortest distance between two quinoline rings in crystal lattice of compound **3**.

Figure S1

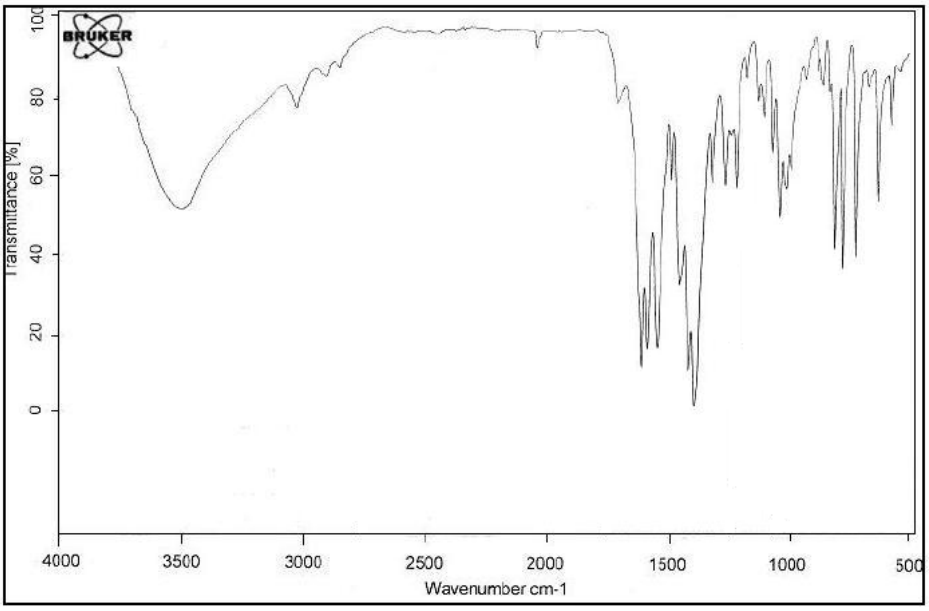
(a) For compound **1**



(b) For compound **2**



(c) For compound **3**



(d) For compound **4**

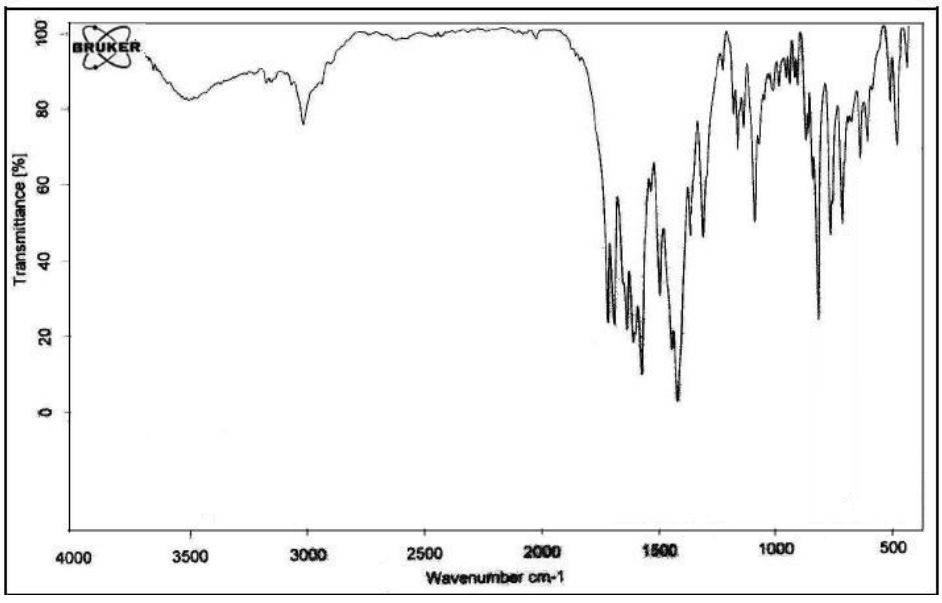
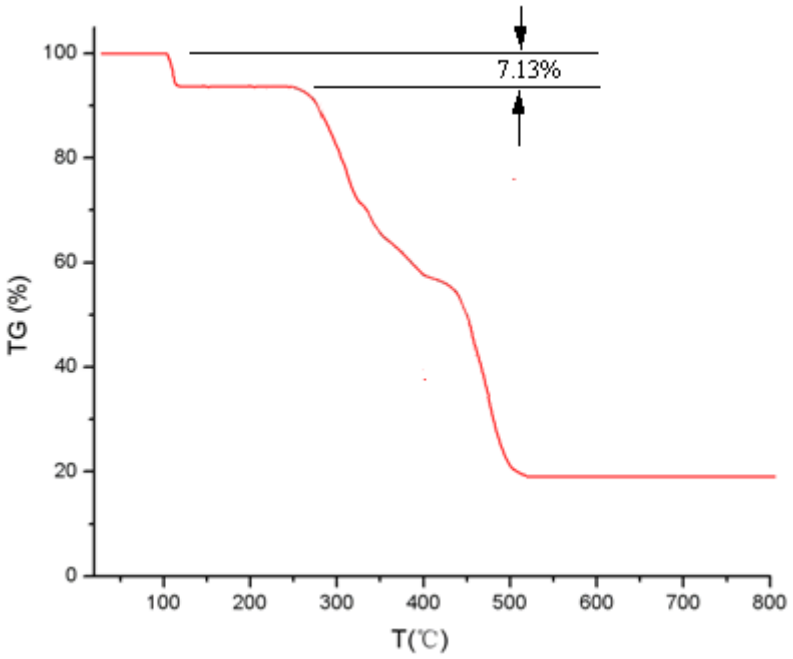
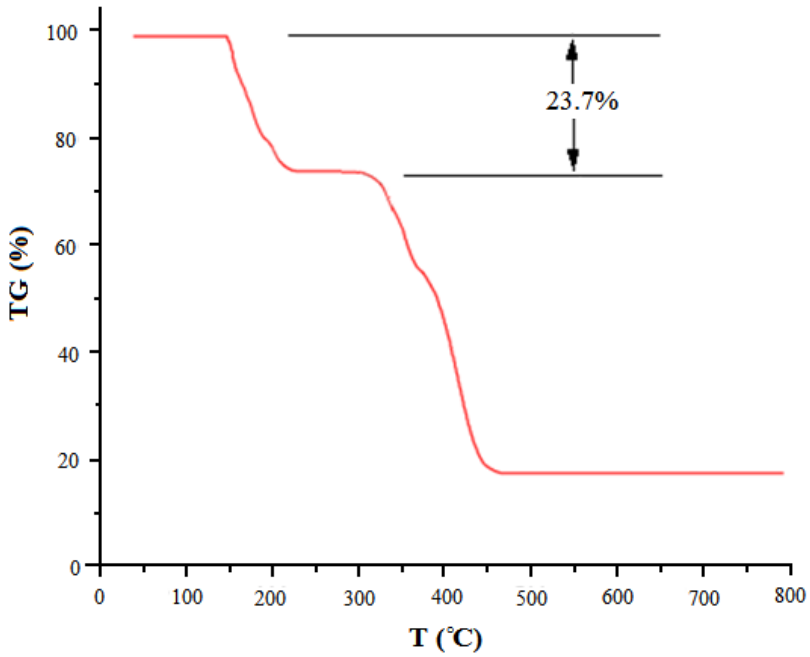


Figure S2

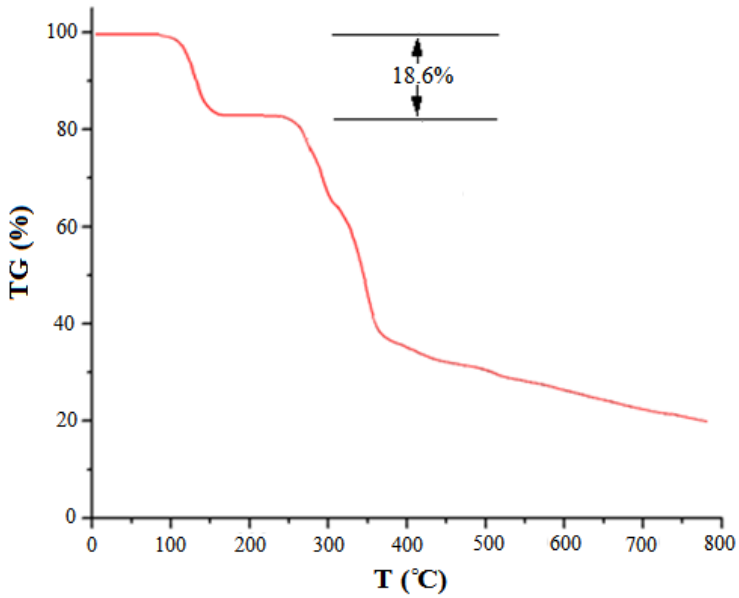
(**a**) for compound **1**



(**b**) for compound **2**



(**c**) for compound **3**



(**d**) for compound **4**

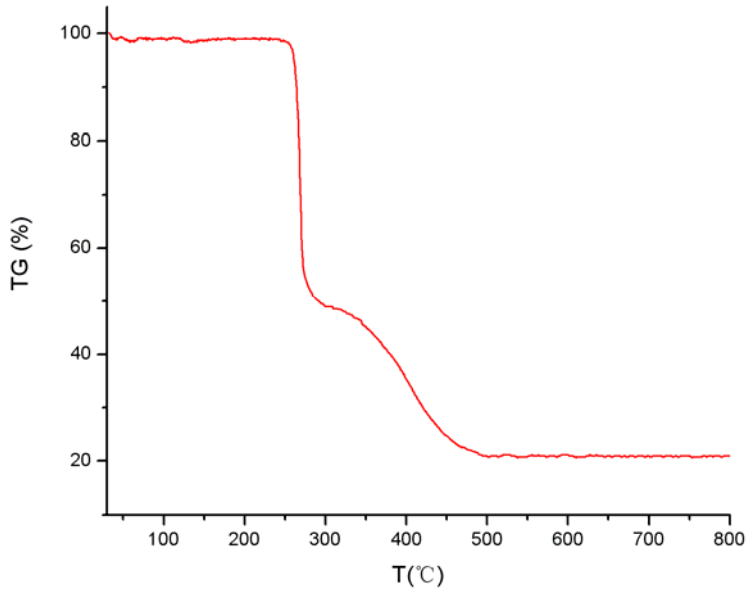


Figure S3

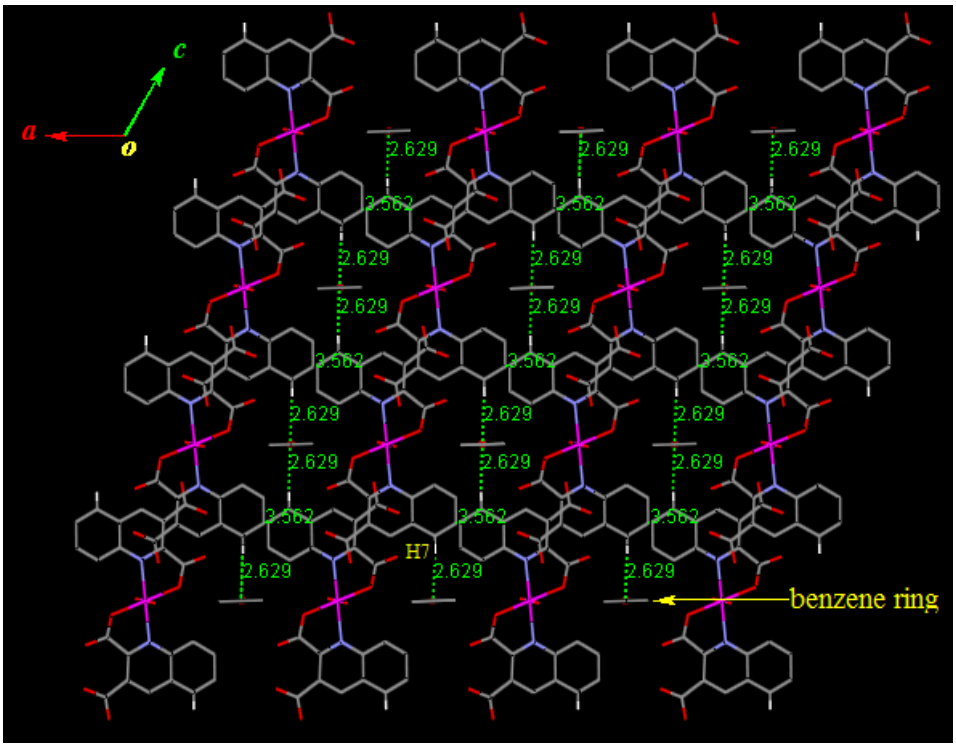
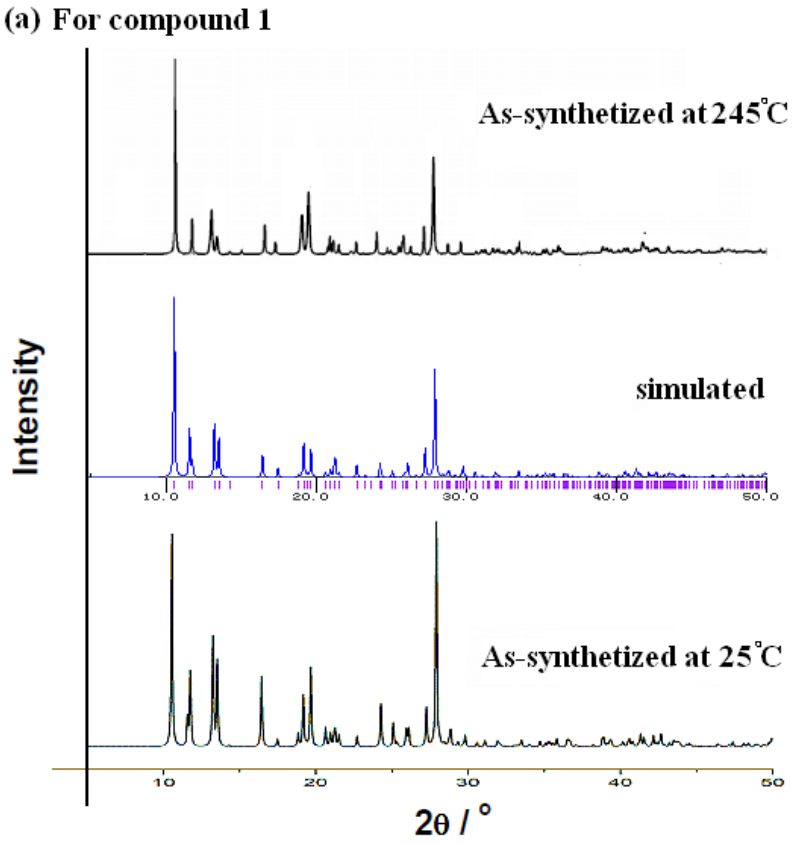
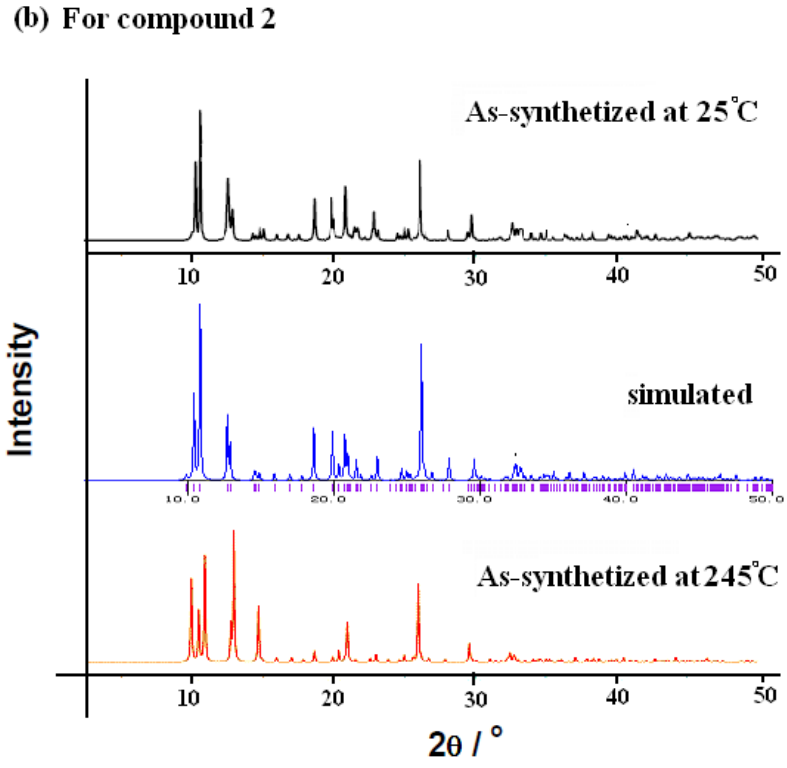
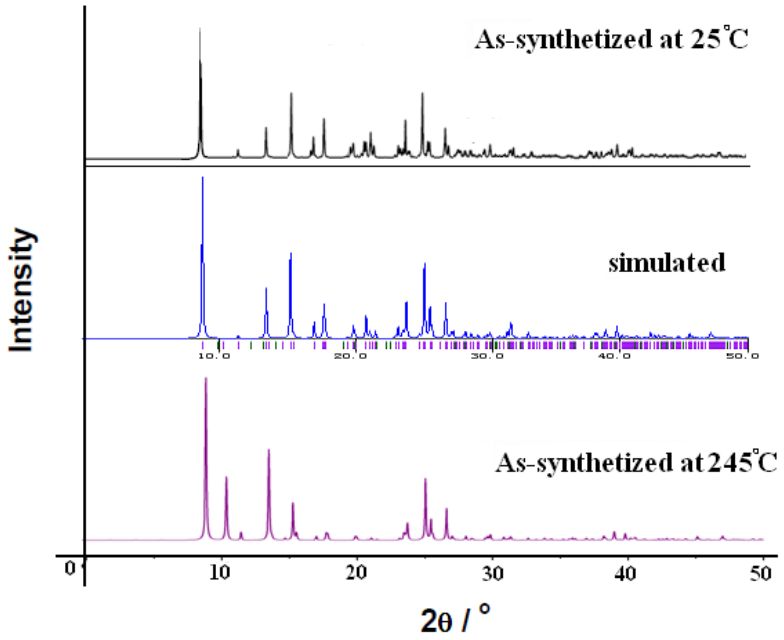


Figure S4





(c) For compound 3



(d) compound 4