Supplementary material for

The side chain template effect in viologen on the formation of polypseudorotaxane architecture: six novel metal coordination polymers and their properties

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1-3**

Compound **1**					
Cu(1)-N(2)	1.928(4)	Cu(1)-N(1)#1	1.931(4)	Cu(1)-S(1)	2.409(1)
Cu(1)-S(2)#2	2.530(2)	N(1)-Cu(1)#3	1.931(4)	S(2)-Cu(1)#2	2.530(2)
N(2)-Cu(1)-N(1)#1	131.3(2)	N(2)-Cu(1)-S(1)	112.0(1)	N(1)#1-Cu(1)-S(1)	100.0(1)
N(2)-Cu(1)-S(2)#2	103.2(1)	N(1)#1-Cu(1)-S(2)#2	101.5(1)	S(1)-Cu(1)-S(2)#2	106.48(6)
C(7)-N(1)-Cu(1)#3	165.5(4)	C(8)-N(2)-Cu(1)	161.9(4)	C(7)-S(1)-Cu(1)	100.1(2)
C(8)-S(2)-Cu(1)#2	95.4(2)				
Compound 2					
Cu(1)-N(1)#1	1.976(4)	Cu(1)-N(2)#2	1.977(4)	Cu(1)-S(2)	2.398(1)
Cu(1)-S(1)	2.401(1)	N(1)-Cu(1)#2	1.976(4)	N(2)-Cu(1)#1	1.977(4)
N(1)#1-Cu(1)-N(2)#2	116.3(2)	N(1)#1-Cu(1)-S(2)	102.1(1)	N(2)#2-Cu(1)-S(2)	118.5(1)
N(1)#1-Cu(1)-S(1)	109.0(1)	N(2)#2-Cu(1)-S(1)	102.1(1)	S(2)-Cu(1)-S(1)	108.63(5)
C(1)-S(1)-Cu(1)	98.6(2)	C(2)-S(2)-Cu(1)	98.7(1)	C(1)-N(1)-Cu(1)#2	158.8(3)
C(2)-N(2)-Cu(1)#1	158.7(3)				
Compound 3					
Cu(1)-N(1)#1	1.976(4)	Cu(1)-N(2)#2	1.977(4)	Cu(1)-S(2)	2.398(1)
Cu(1)-S(1)	2.401(1)	N(1)-Cu(1)#2	1.976(4)	N(2)-Cu(1)#1	1.977(4)
N(1)#1-Cu(1)-N(2)#2	116.3(2)	N(1)#1-Cu(1)-S(2)	102.1(1)	N(2)#2-Cu(1)-S(2)	118.5(1)

N(1)#1-Cu(1)-S(1)	109.0(1)	N(2)#2-Cu(1)-S(1)	102.1(1)	S(2)-Cu(1)-S(1)	108.63(5)
C(1)-S(1)-Cu(1)	98.6(2)	C(2)-S(2)-Cu(1)	98.7(1)	C(1)-N(1)-Cu(1)#2	158.8(3)
C(2)-N(2)-Cu(1)#1	158.7(3)				
Compound 4					
Cu1- S1	2.407(1)	Cu1- S2	2.498(1)	Cu1- $N1^{1}$	1.977(3)
Cu1- N4	2.034(3)	Cu2- S1	2.659(1)	Cu2- S2	2.451(1)
Cu2- $N2^{2}$	1.934(4)	Cu2- N3	1.938(4)	N1- $Cu1^{3}$	1.977(3)
N2- $Cu2^{2}$	1.934(4)	S1- Cu1- S2	98.52(4)	$N1^{1}$- Cu1- S1	119.5(1)
$N1^{1}$- Cu1- S2	99.3(1)	$N1^{1}$- Cu1- N4	117.0(1)	N4- Cu1- S1	111.7(1)
N4- Cu1- S2	107.2(1)	S1- Cu1- S2	93.27(4)	$N2^{2}$-Cu2- S1	106.9(1)
$N2^{2}$-Cu2- S2	102.8(1)	$N2^{2}$-Cu2- N3	128.1(2)	N3- Cu2- S1	105.1(1)
N3- Cu2- S2	115.1(1)	Cu1- S1-Cu2	80.07(4)	C1- S1- Cu1	112.5(1)
C1- S1- Cu2	100.5(1)	Cu2- S2- Cu1	82.54(4)	C2- S2- Cu1	97.7(2)
C2- S2- Cu2	99.5(1)	C1- N1- $Cu1^{3}$	170.9(3)	C2- N2- $Cu2^{2}$	157.7(3)
C3- N3- Cu2	164.6(4)	C4- N4- Cu1	121.8(3)	C8- N4- Cu1	122.2(3)
Compound 5					
Cu(1)-N(2)	1.912(2)	Cu(1)-N(1)	1.918(2)	Cu(1)-S(2)	2.3742(9)
Cu(1)-S(1)	2.800(1)				
N(2)-Cu(1)-N(1)	136.1(1)	N(2)-Cu(1)-S(2)	110.78(8)	N(1)-Cu(1)-S(2)	105.63(8)
N(2)-Cu(1)-S(1)	98.80(8)	N(1)-Cu(1)-S(1)	95.65(9)	S(2)-Cu(1)-S(1)	103.61(3)
C(2)#1-N(1)-Cu(1)	166.7(3)	C(1)-N(2)-Cu(1)	166.2(2)	C(1)#2-S(1)-Cu(1)	95.1(1)
C(2)-S(2)-Cu(1)	101.4(1)				
Compound 6					
Cu1-S1	2.421(2)	Cu1-S2	2.383(2)	Cu1-$N2^{1}$	2.004(5)
Cu1-$N3^{2}$	1.995(5)	N2-$Cu1^{2}$	2.004(5)	N3-$Cu1^{1}$	1.995(5)
S2-Cu1-S1	107.89(6)	$N2^{1}$-Cu1-S1	115.5(2)	$N2^{1}$-Cu1-S2	103.3(1)
$N3^{2}$-Cu1-S2	115.4(2)	$N3^{2}$-Cu1-$N2^{1}$	113.7(2)	C11-S1-Cu1	99.0(2)
C12-S2-Cu1	97.3(2)	C11-N2-$Cu1^{2}$	156.5(5)	C12-N3-$Cu1^{1}$	157.1(4)

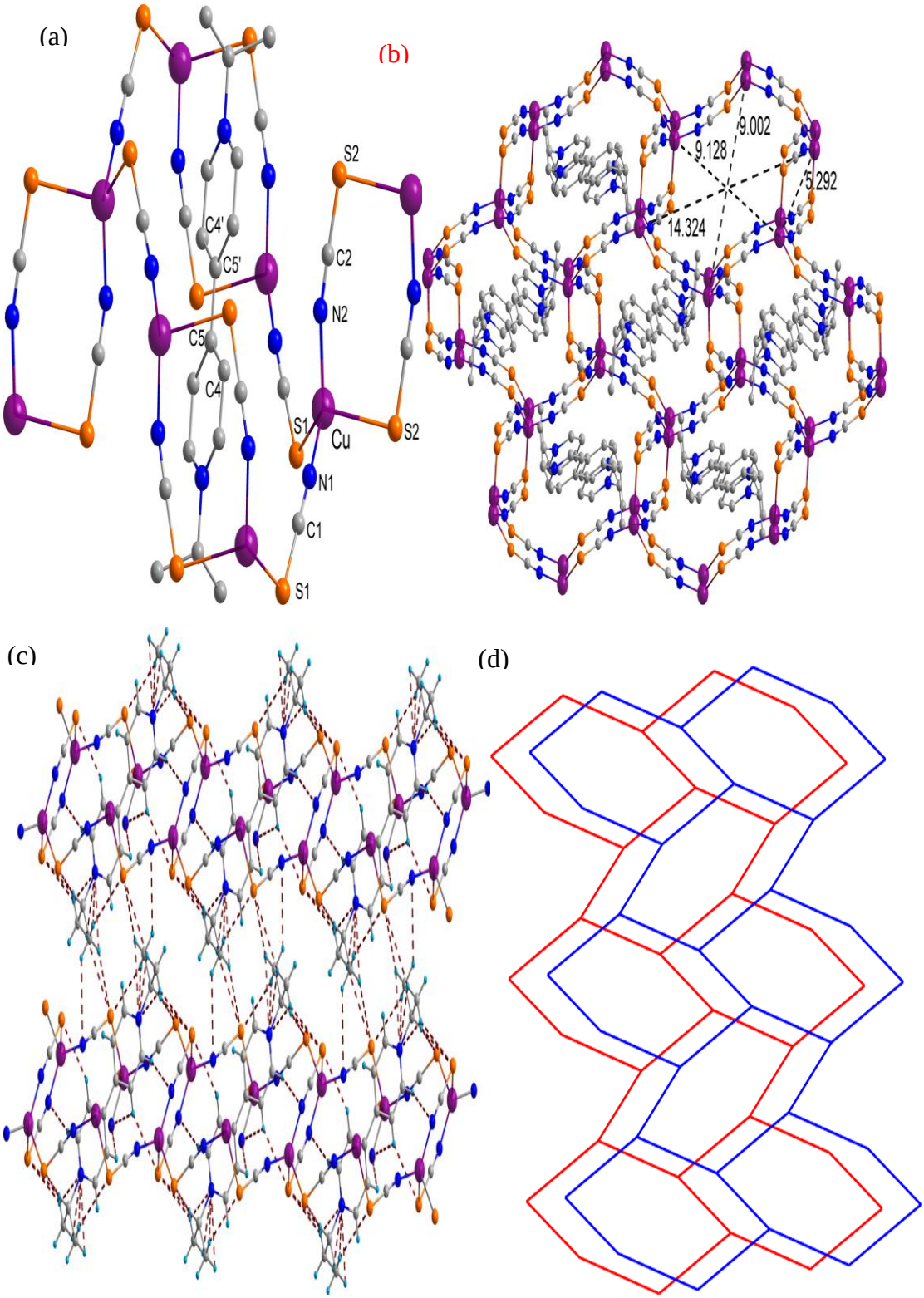


Fig. S1 (a) The structure unit diagram of **3** (#1 -x+2,-y+2,-z #2 x,-y+3/2,z+1/2 #3 x,-y+3/2,z-1/2 #4 -x,-y+2,-z+1)**.** (The H atoms were omitted for clarity) (b) Structure showing the accumulation in space of **3** viewed along *a* -derection. (c) The diagram of weak interactions in complex **3**. (d) The topology of compound **3**.(Distinct colour shows different layer)

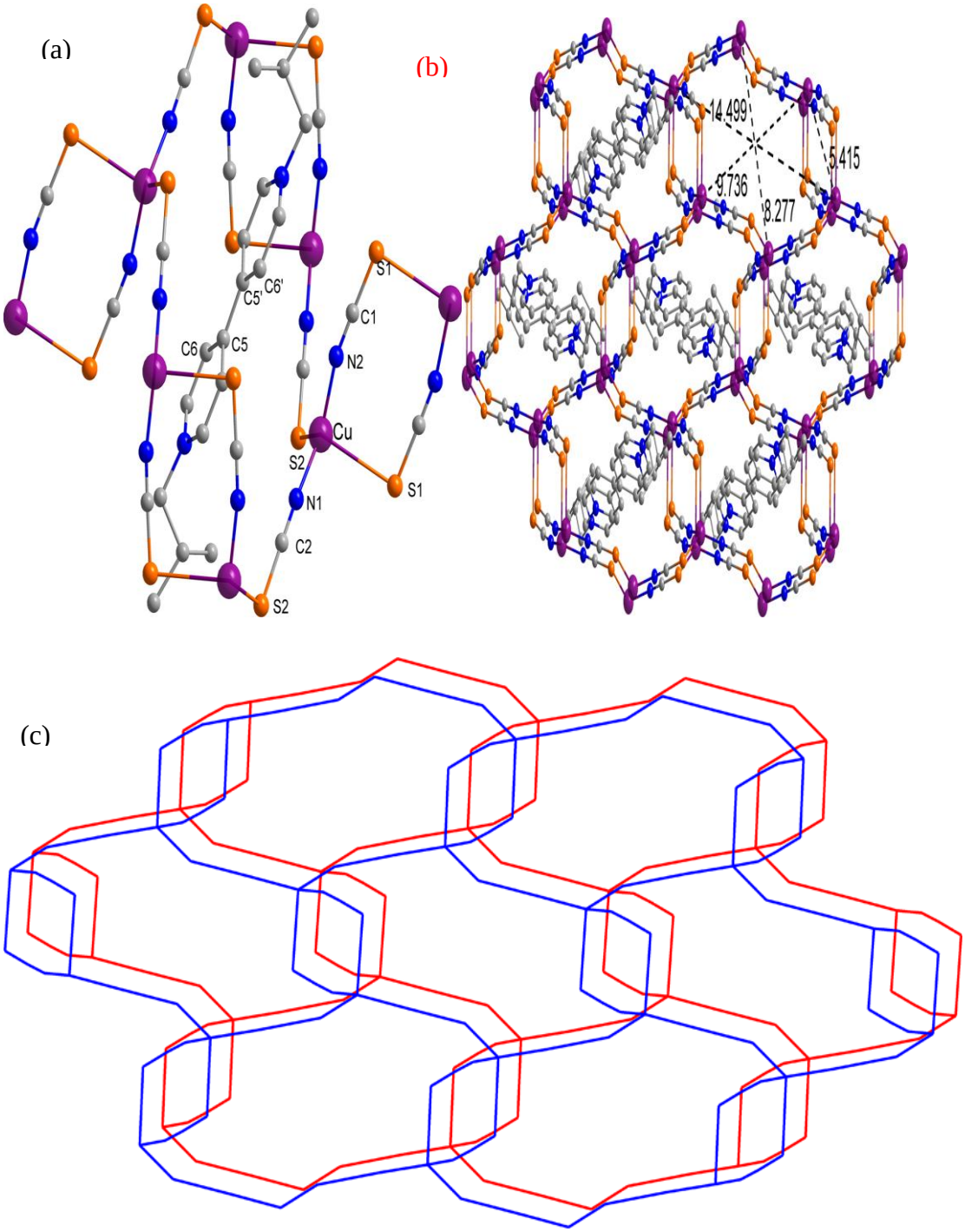


Fig. S2 (a) The structure unit diagram of **5** (#1 x,-y+3/2,z-1/2 #2 -x+1,-y+2,-z+2 #3 x,-y+3/2,z+1/2 #4 -x+1,-y+1,-z+2). (The H atoms were omitted for clarity) (b) Structure showing the accumulation in space of **5** viewed along *a* -derection. (c) The topology of compound **3**(distinct colour shows different layer).

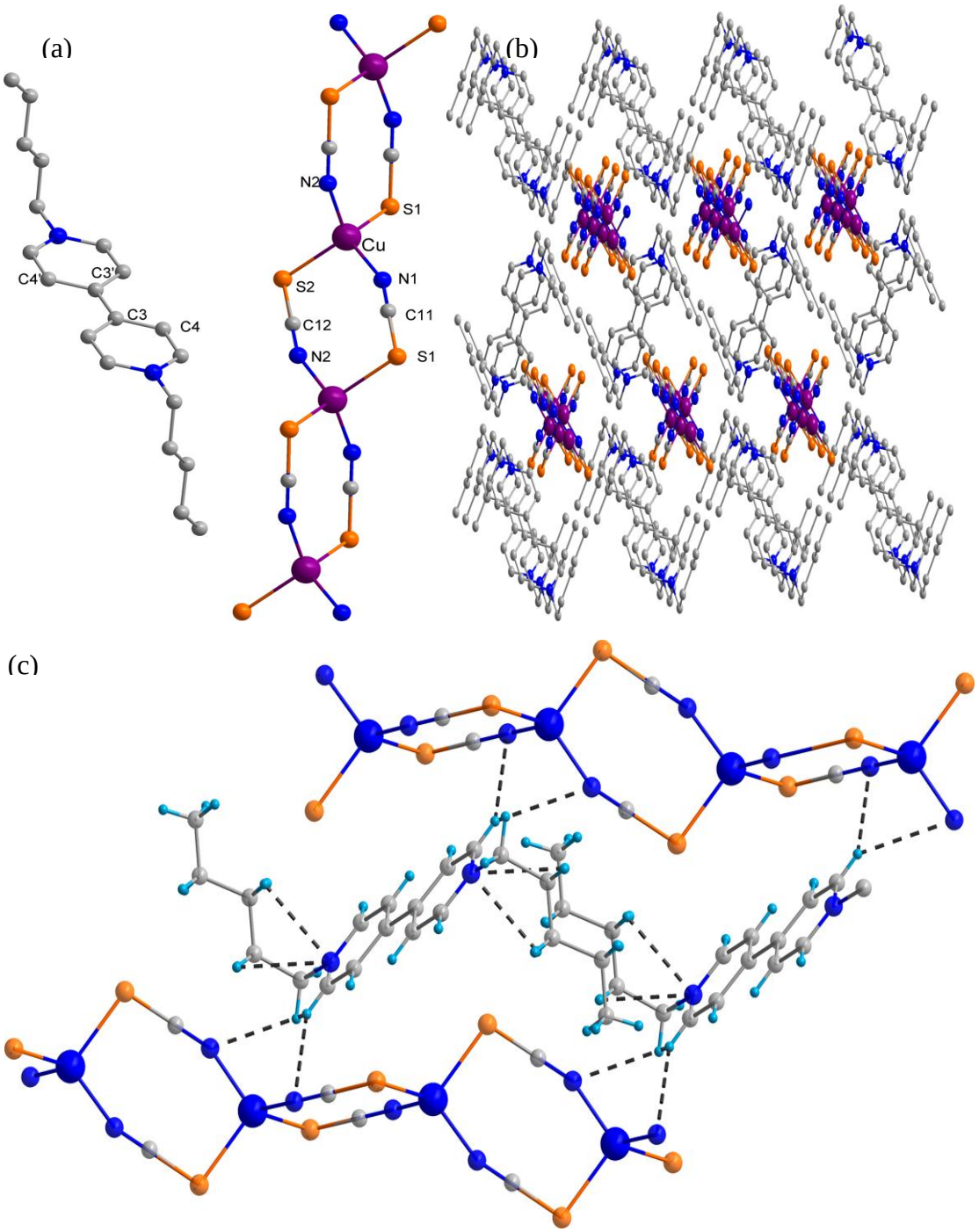
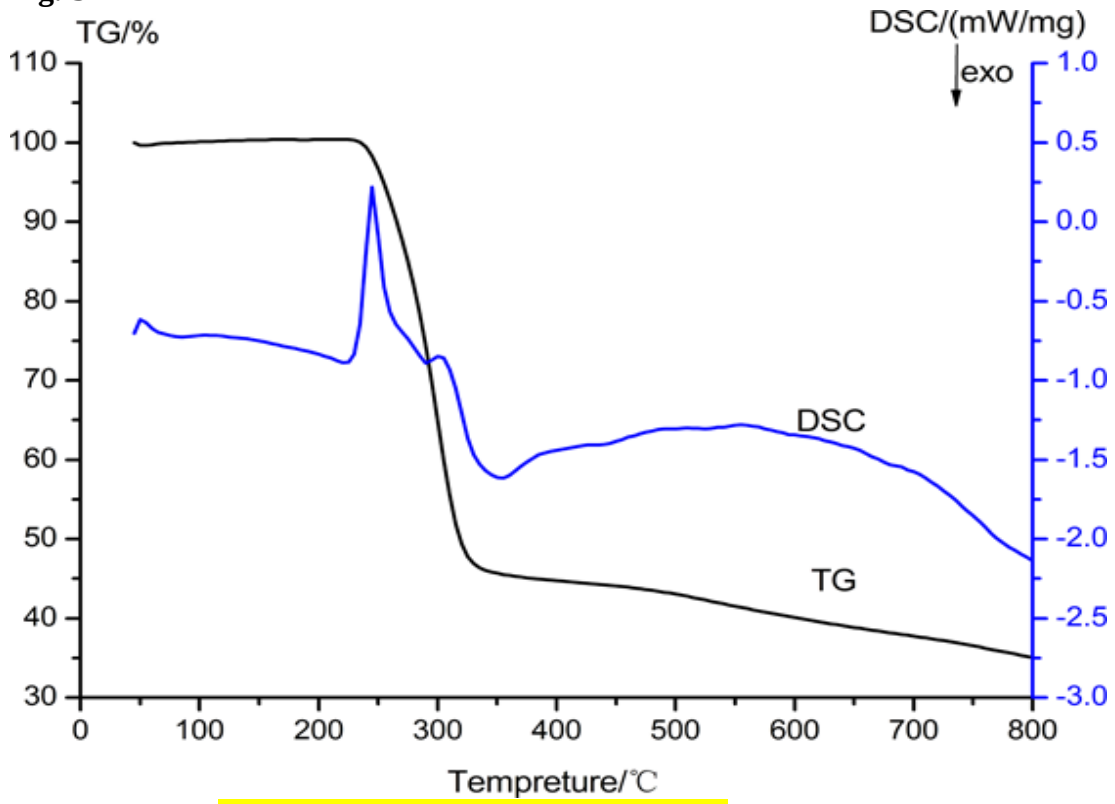
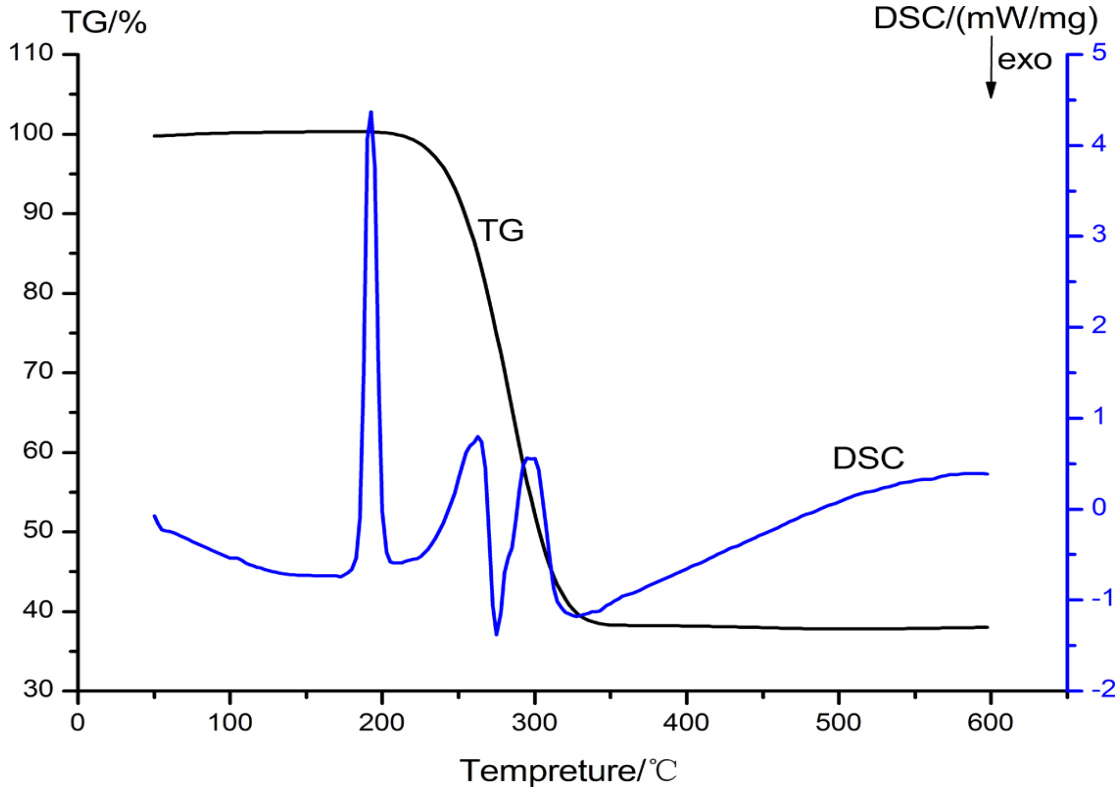


Fig. S3 (a) The structural diagram of **6** ([1]+X,1/2-Y,-1/2+Z; [2]+X,1/2-Y,1/2+Z; [3]1-X,1-Y,1-Z)**.**(The H atoms were omitted for clarity) (b) Structure showing the unit-cell packing and one-dimensional chain of **6** viewed along *a*-direction. (c) The diagram of weak interactions in complex **6**.

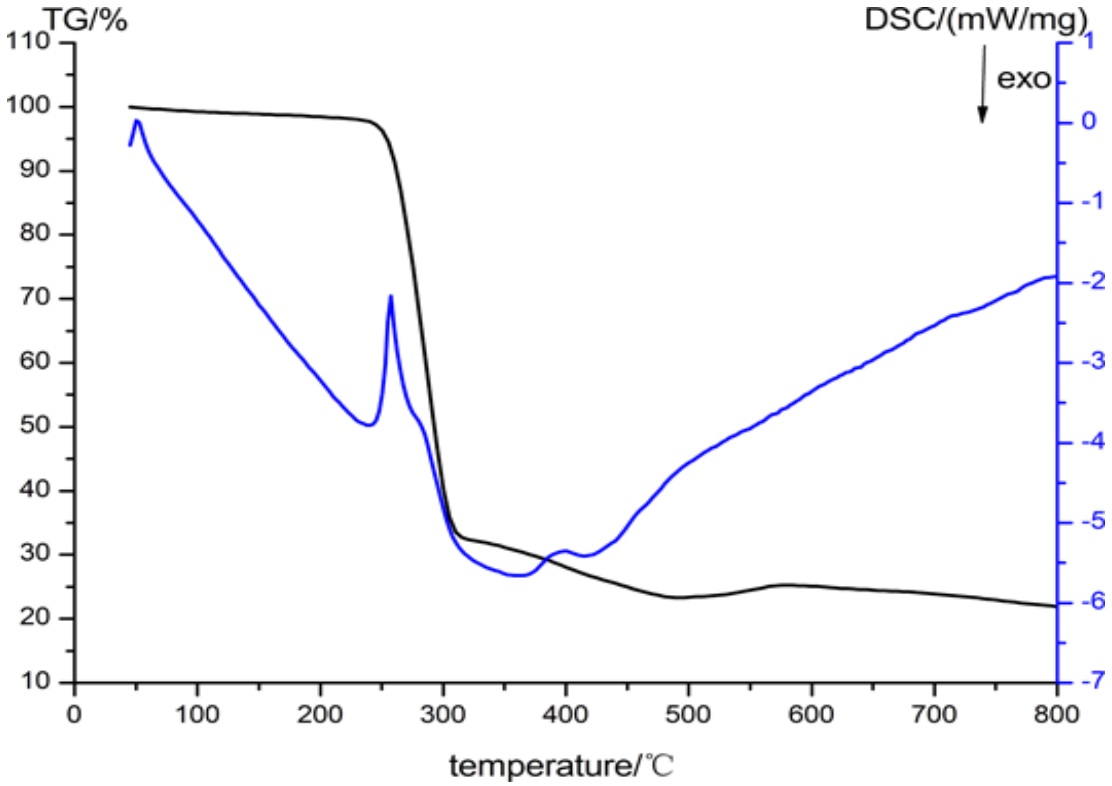
Fig. S4



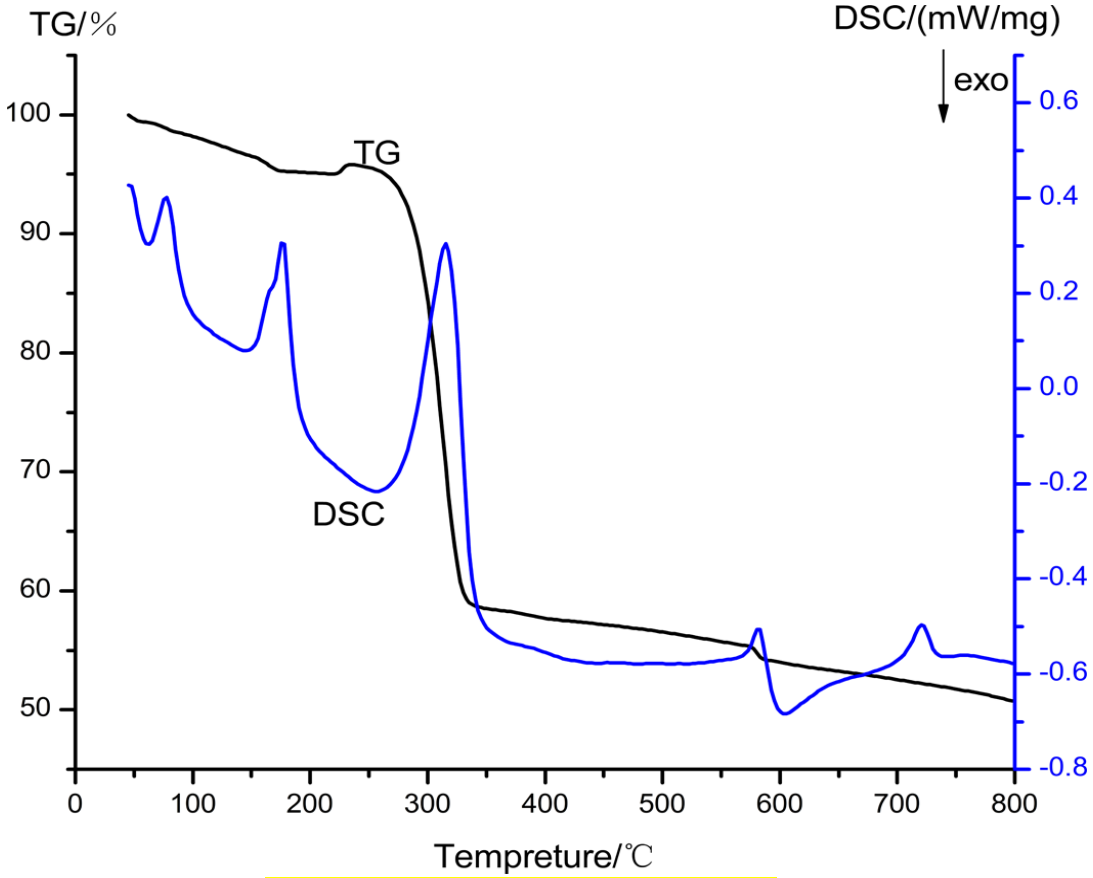
(a) The TG-DSC curves of compound **1**



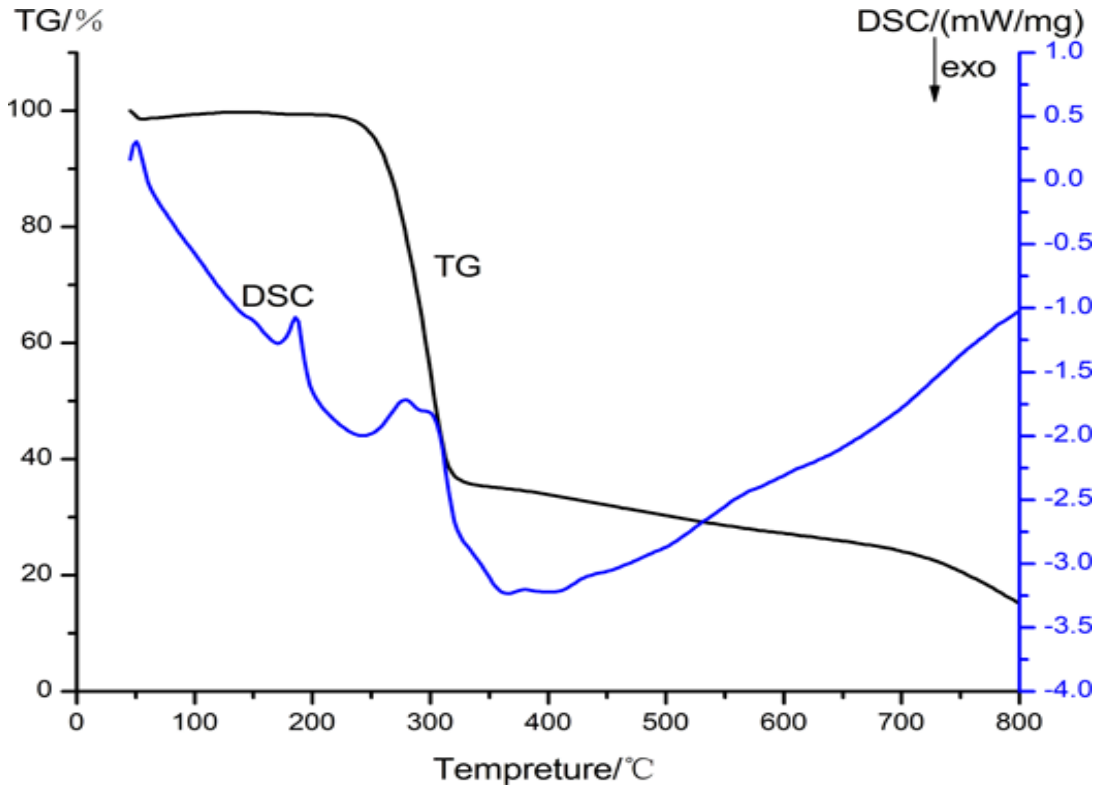
(b) The TG-DSC curves of compound **2**



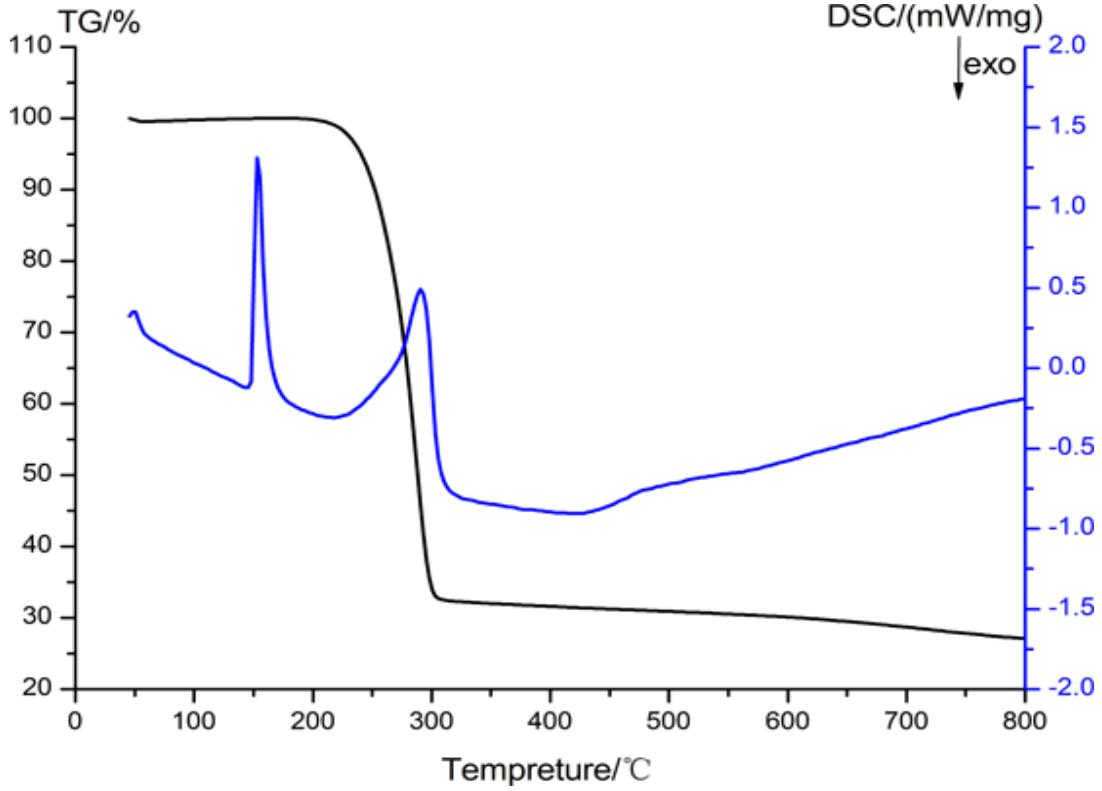
(c) The TG-DSC curves of compound **3**



(d) The TG-DSC curves of compound **4**



(e) The TG-DSC curves of compound **5**



(f) The TG-DSC curves of compound **6**

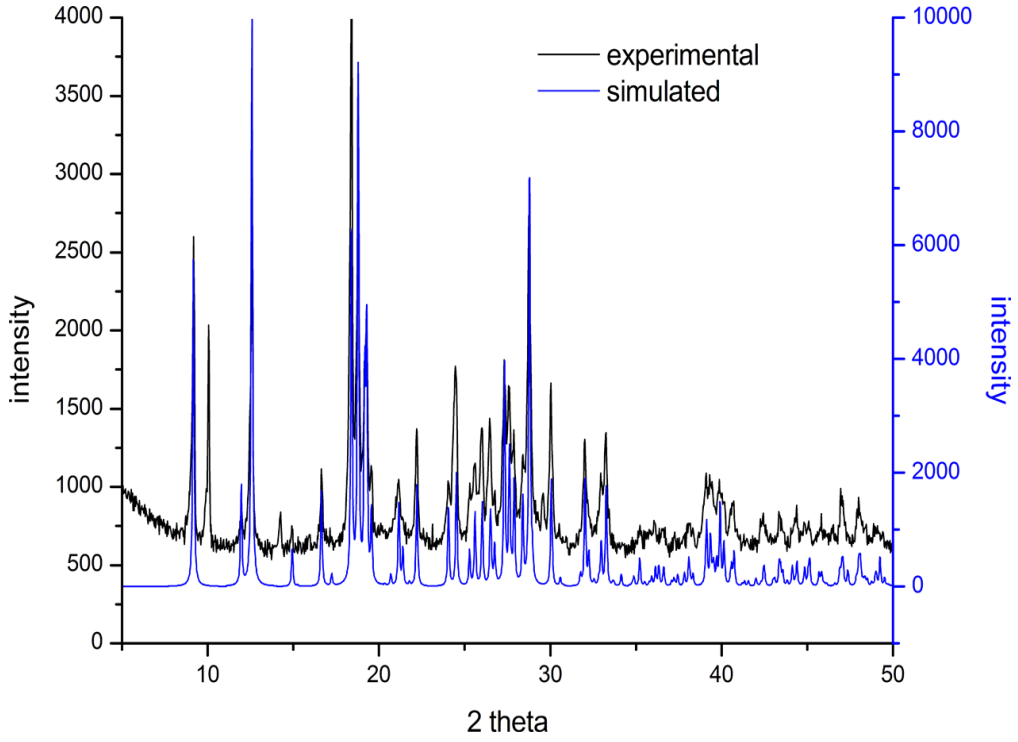


Fig. S5 Simulated and experimental PXRD pattern of compound **1.**

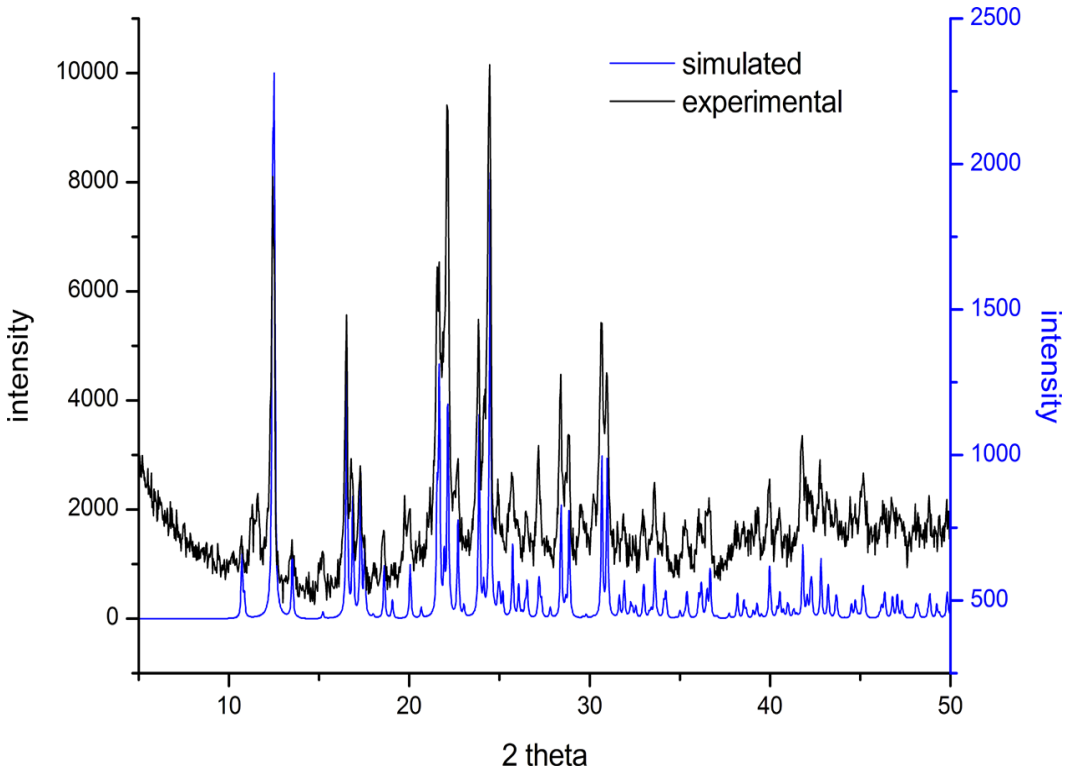


Fig. S6 Simulated and experimental PXRD pattern of compound **2.**

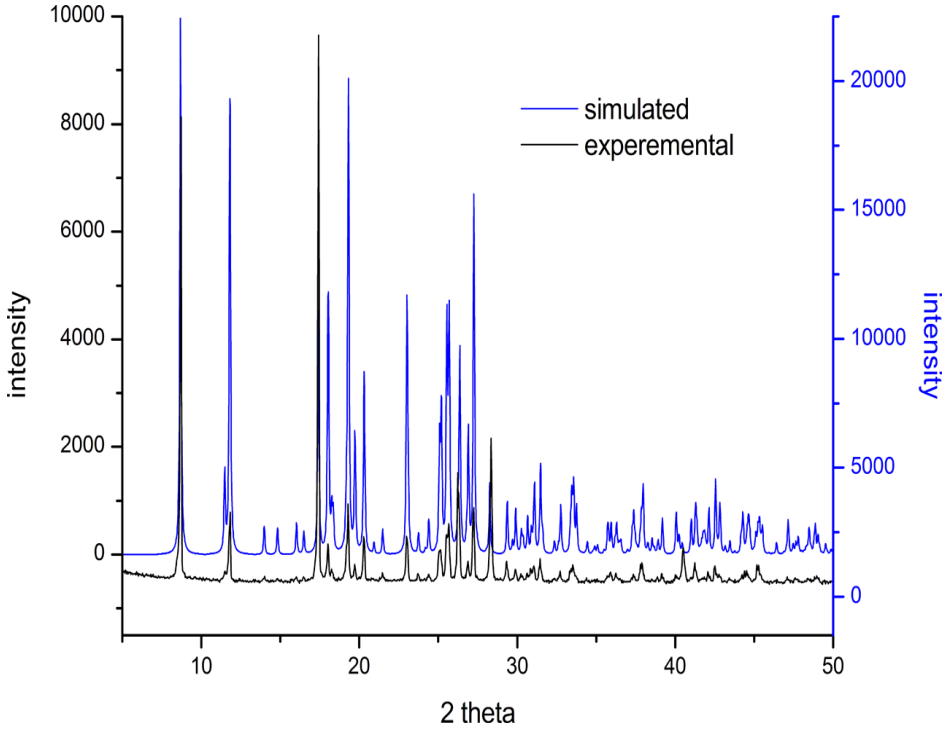


Fig. S7 Simulated and experimental PXRD pattern of compound **3.**

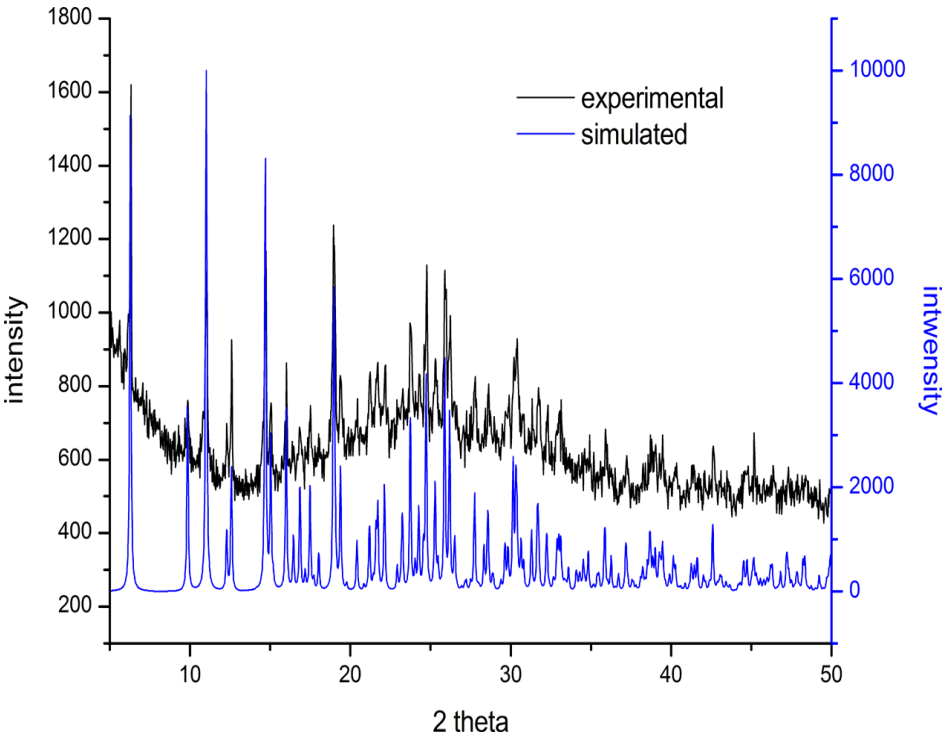


Fig. S8 Simulated and experimental PXRD pattern of compound **4.**

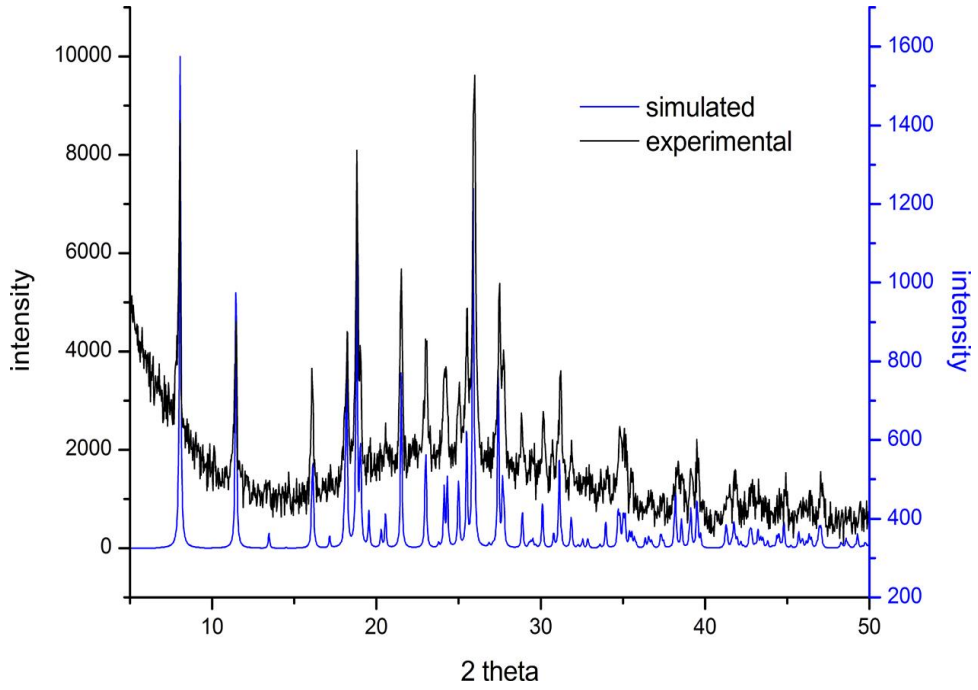


Fig. S9 Simulated and experimental PXRD pattern of compound **5.**

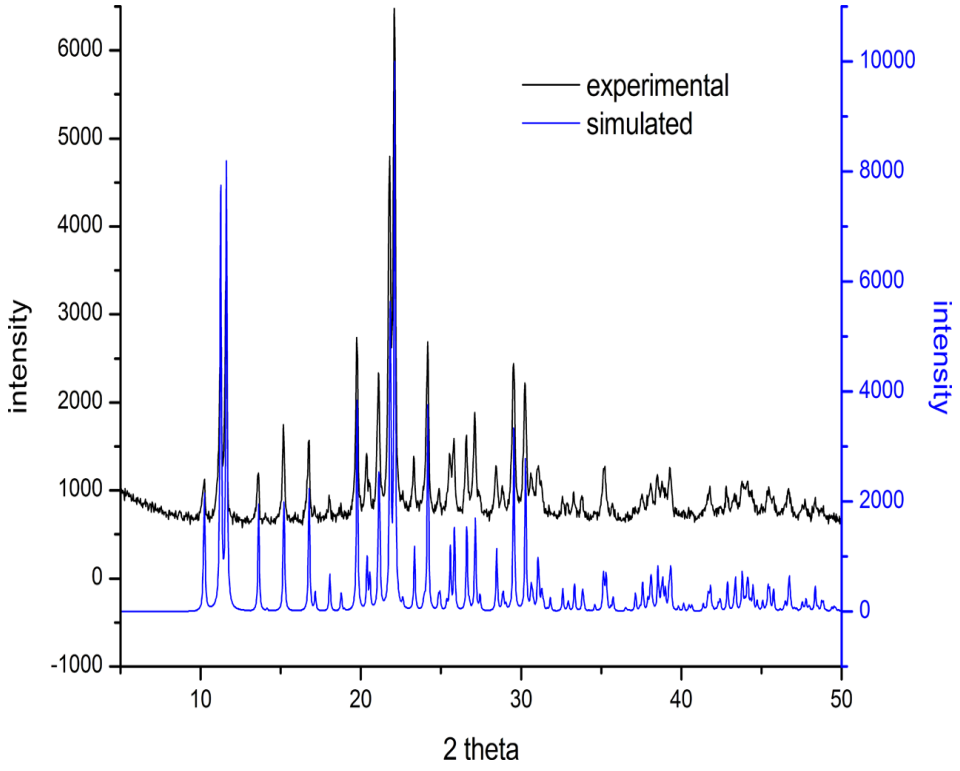


Fig. S10 Simulated and experimental PXRD pattern of compound **6**