

Supplementary material for

**Three novel cation-Templated metal thiocyanates with 1-2D
 polypseudorotaxane frameworks**

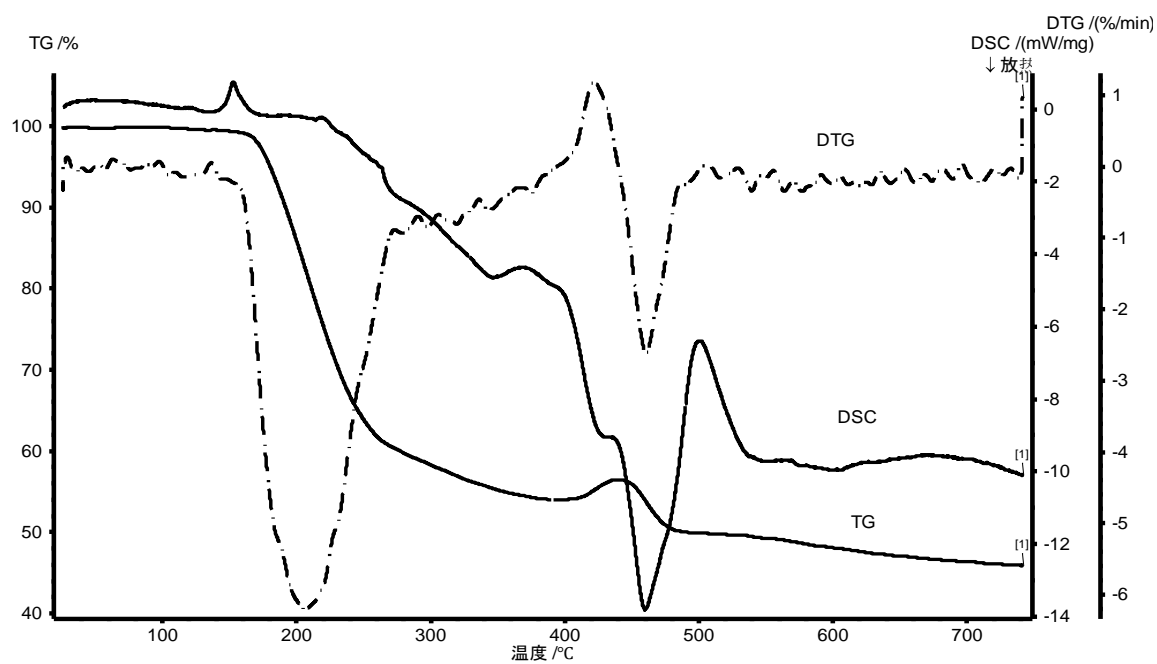
Yong-Zhen Qiao, Jun-Ming Yue, Xiu-Cun Liu, and Yun-Yin Niu

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

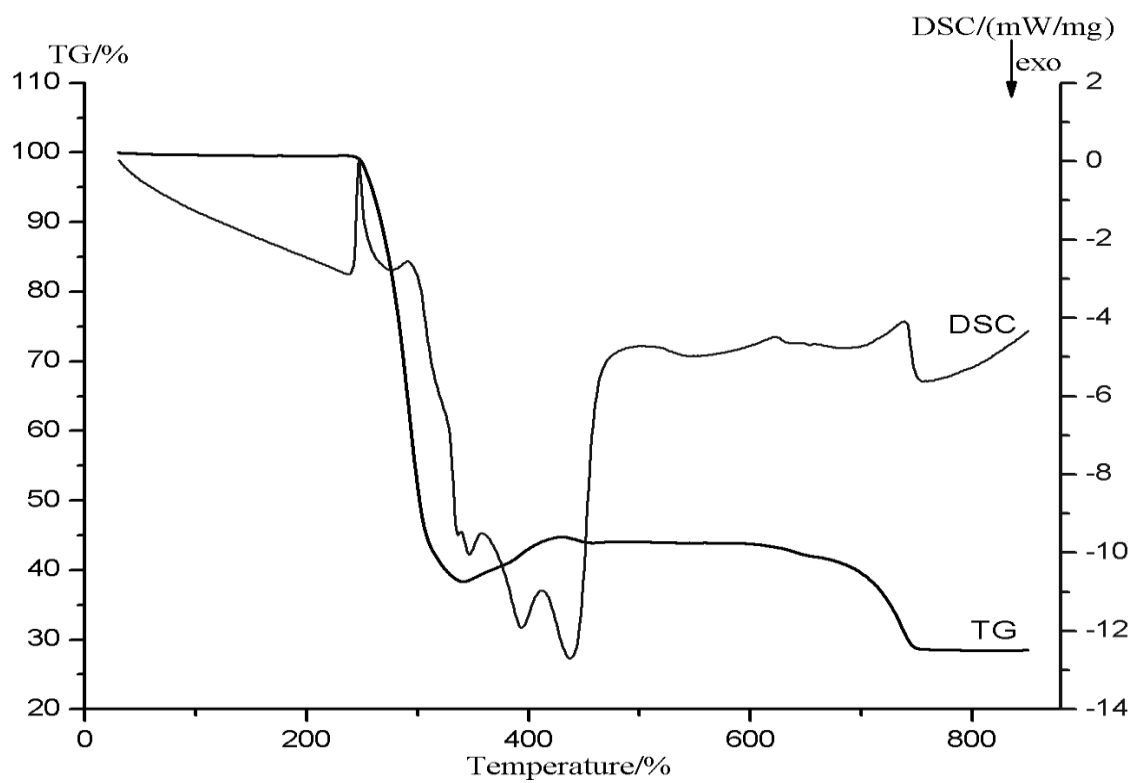
Compound 1					
Ag(1)-N(6)#1	2.255(4)	Ag(1)-S(1)	2.5402(11)	Ag(1)-S(2)	2.5547(11)
Ag(1)-Br(1)	2.7684(5)	Ag(2)-S(3)	2.5462(11)	Ag(2)-Br(2)#2	2.6907(6)
Ag(2)-Br(2)	2.7498(6)	Ag(2)-Br(1)	2.7529(6)	Br(2)-Ag(2)#2	2.6907(6)
N(6)#1-Ag(1)-S(1)	123.30(10)	N(6)#1-Ag(1)-S(2)	111.04(9)	S(1)-Ag(1)-S(2)	103.95(4)
N(6)#1-Ag(1)-Br(1)	100.53(9)	S(1)-Ag(1)-Br(1)	104.87(3)	S(2)-Ag(1)-Br(1)	113.22(3)
S(3)-Ag(2)-Br(2)#2	114.54(3)	S(3)-Ag(2)-Br(2)	117.86(3)	Br(2)#2-Ag(2)-Br(2)	102.848(17)
S(3)-Ag(2)-Br(1)	102.28(3)	Br(2)#2-Ag(2)-Br(1)	117.535(19)	Br(2)-Ag(2)-Br(1)	101.745(18)
Ag(2)-Br(1)-Ag(1)	160.76(2)	Ag(2)#2-Br(2)-Ag(2)	77.152(17)	C(19)-S(1)-Ag(1)	98.86(14)
C(20)-S(2)-Ag(1)	97.50(15)	C(21)-S(3)-Ag(2)	98.15(13)		
Compound 2					
Cu(1)-N(2)#1	1.906(3)	Cu(1)-N(3)#2	1.934(3)	Cu(1)-S(2)	2.4116(11)
Cu(1)-S(1)	2.5862(9)				
N(2)#1-Cu(1)-N(3)#2	133.63(11)	N(2)#1-Cu(1)-S(2)	111.99(8)	N(3)#2-Cu(1)-S(2)	99.76(9)
N(2)#1-Cu(1)-S(1)	100.11(8)	N(3)#2-Cu(1)-S(1)	103.19(8)	S(2)-Cu(1)-S(1)	105.19(3)
C(8)-S(1)-Cu(1)	97.92(10)	C(9)-S(2)-Cu(1)	98.75(12)		
Compound 3					
Cu(1)-N(2)	1.926(3)	Cu(1)-N(3)	1.932(3)	Cu(1)-S(2)	2.3757(11)
Cu(1)-S(1)	2.6486(10)				
N(2)-Cu(1)-N(3)	132.80(13)	N(2)-Cu(1)-S(2)	112.74(9)	N(3)-Cu(1)-S(2)	101.97(10)
N(2)-Cu(1)-S(1)	101.07(8)	N(3)-Cu(1)-S(1)	99.94(9)	S(2)-Cu(1)-S(1)	104.61(4)
C(11)-S(1)-Cu(1)	95.28(10)	C(12)-S(2)-Cu(1)	100.90(12)		

Fig. S1

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



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



(b) The TG-DSC curves of compound 3

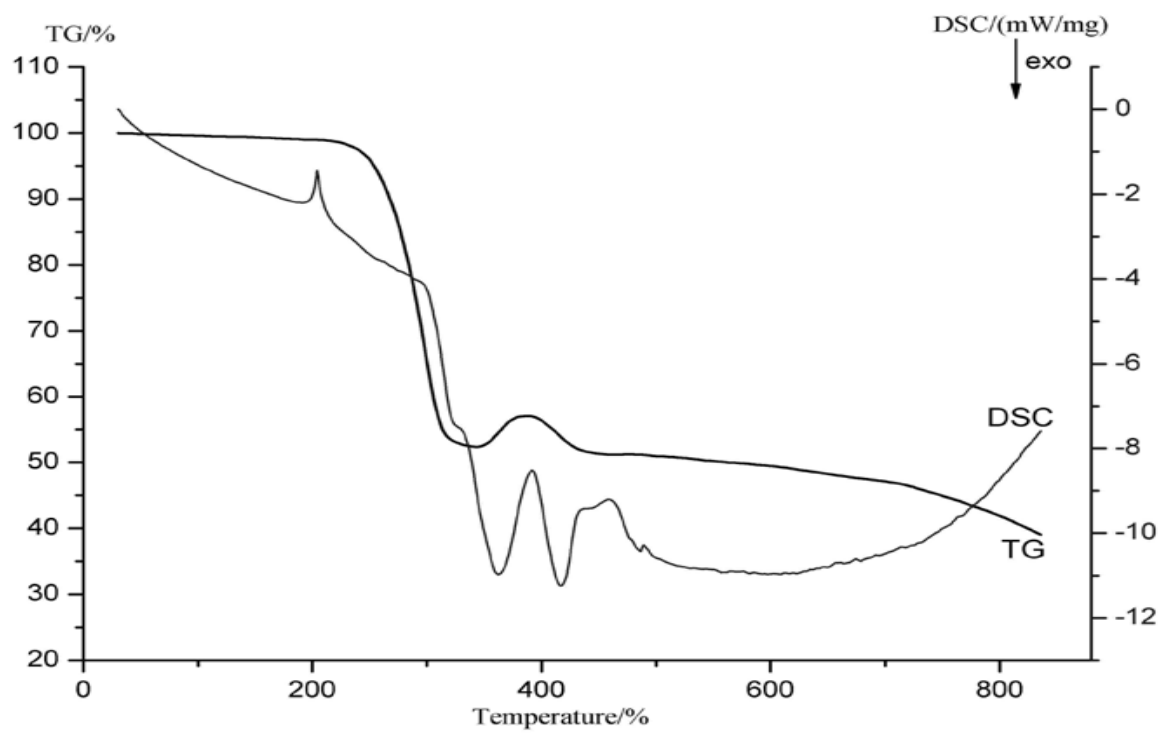
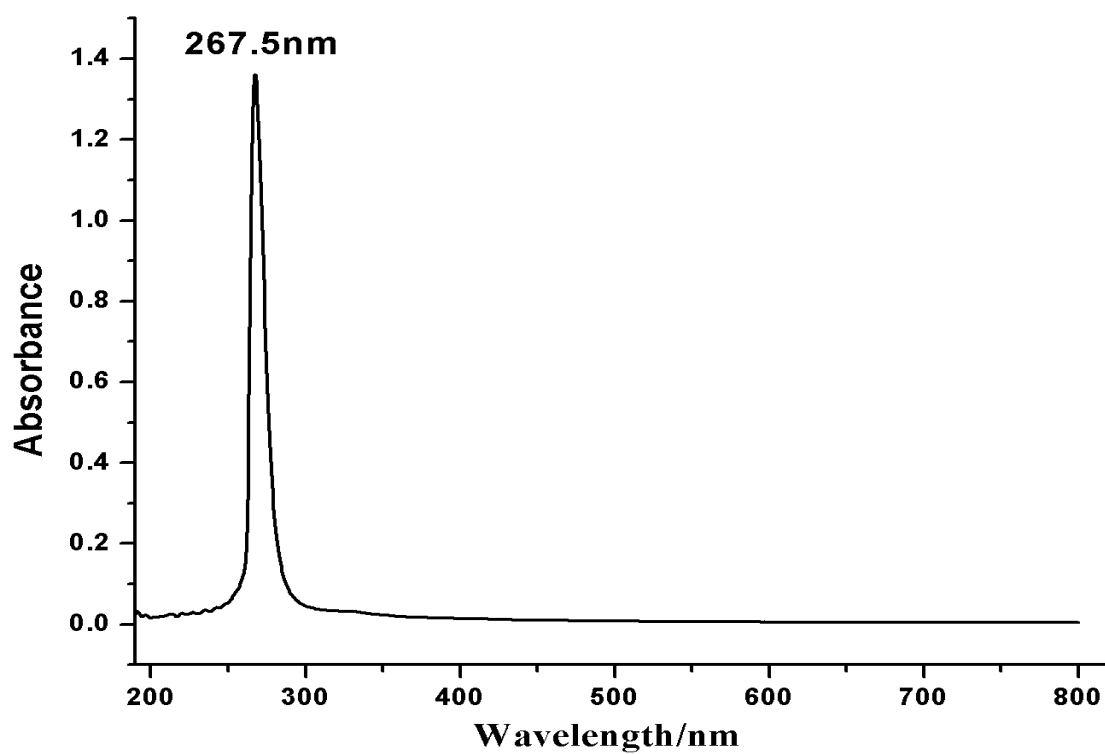
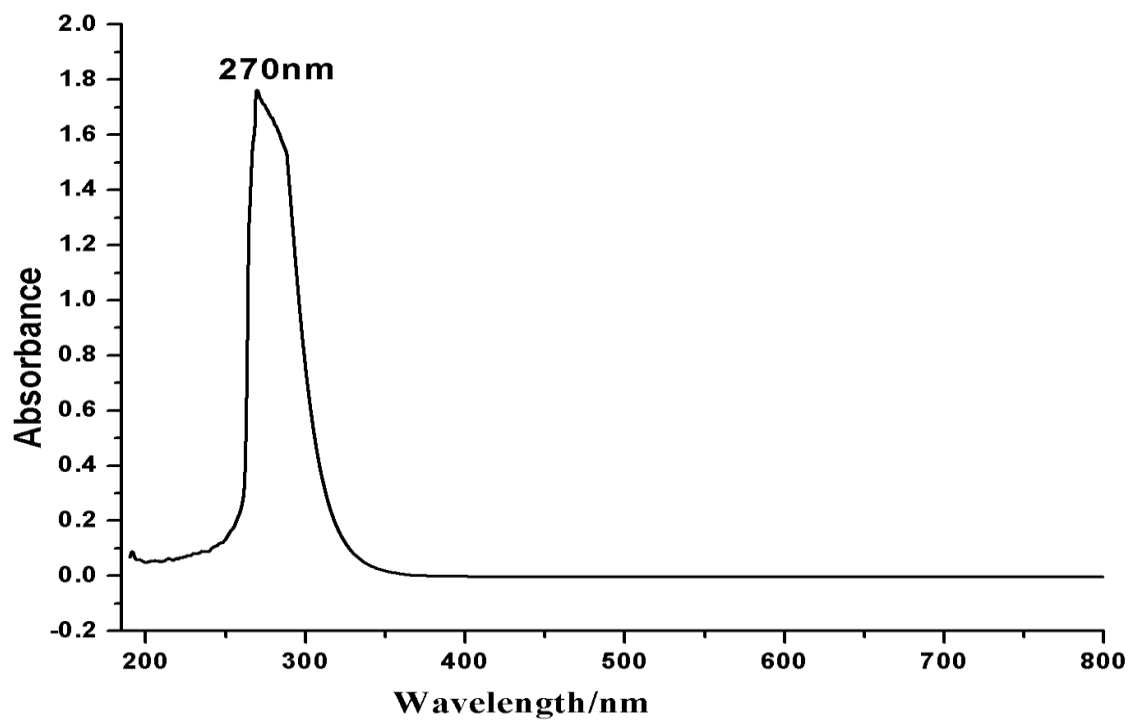


Fig. S2

(a) UV-vis curve for the DMF solution of 10^{-5} M for **1**.



(b) UV-vis curve for the DMF solution of 10^{-5} M for **2**.



(c) UV-vis curve for the DMF solution of 10^{-5} M for **3**.

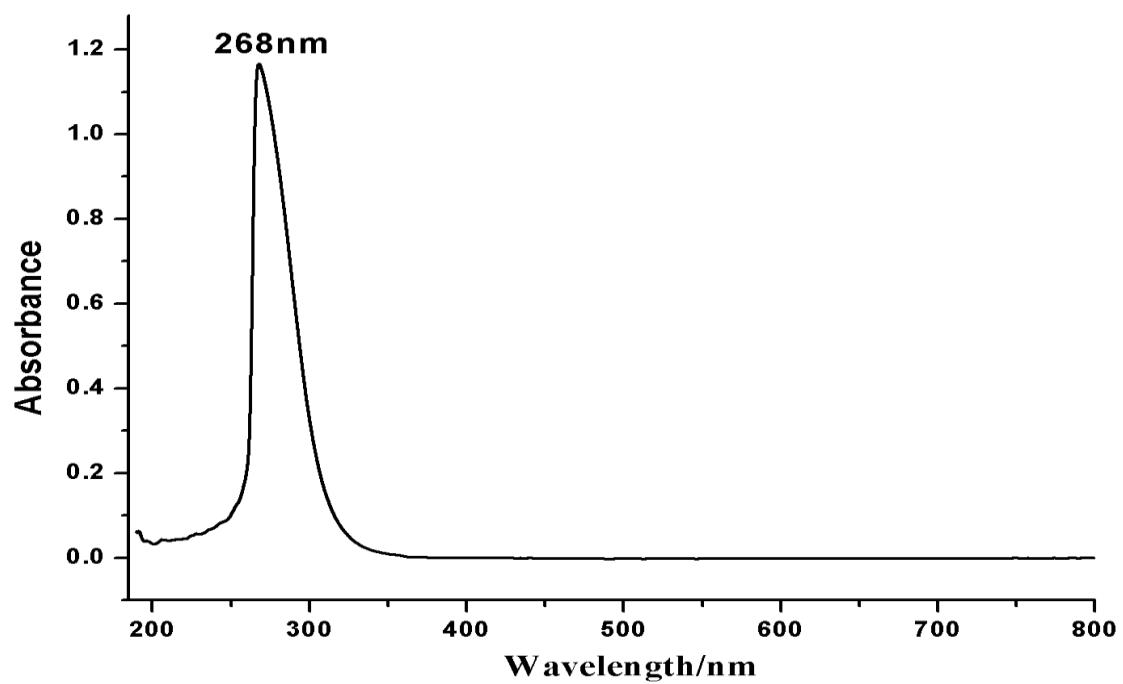
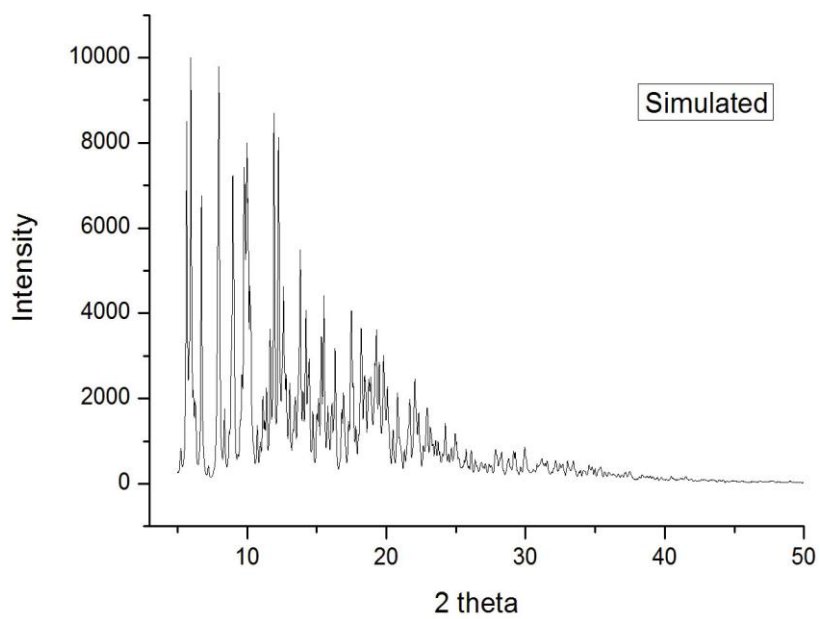


Fig. S3 Simulated and experimental PXRD pattern of compound **1**.



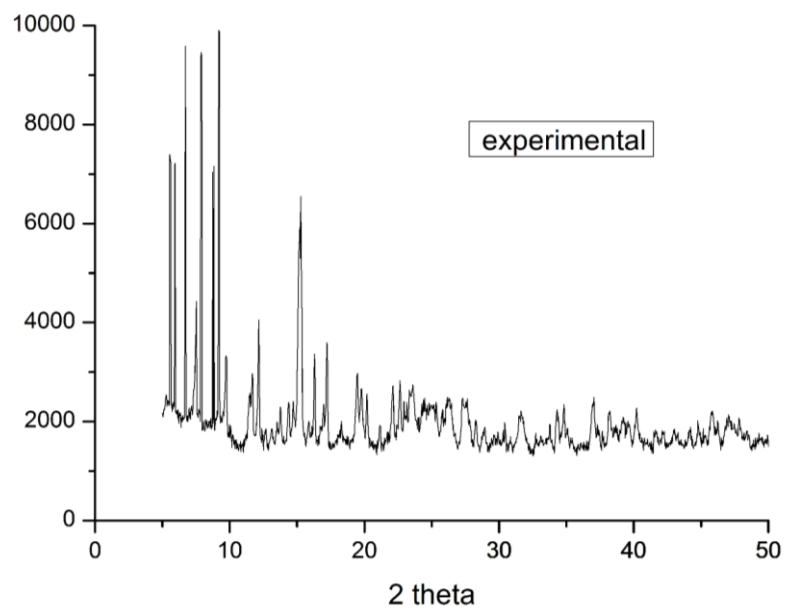


Fig. S4 Simulated and experimental PXRD pattern of compound **2**.

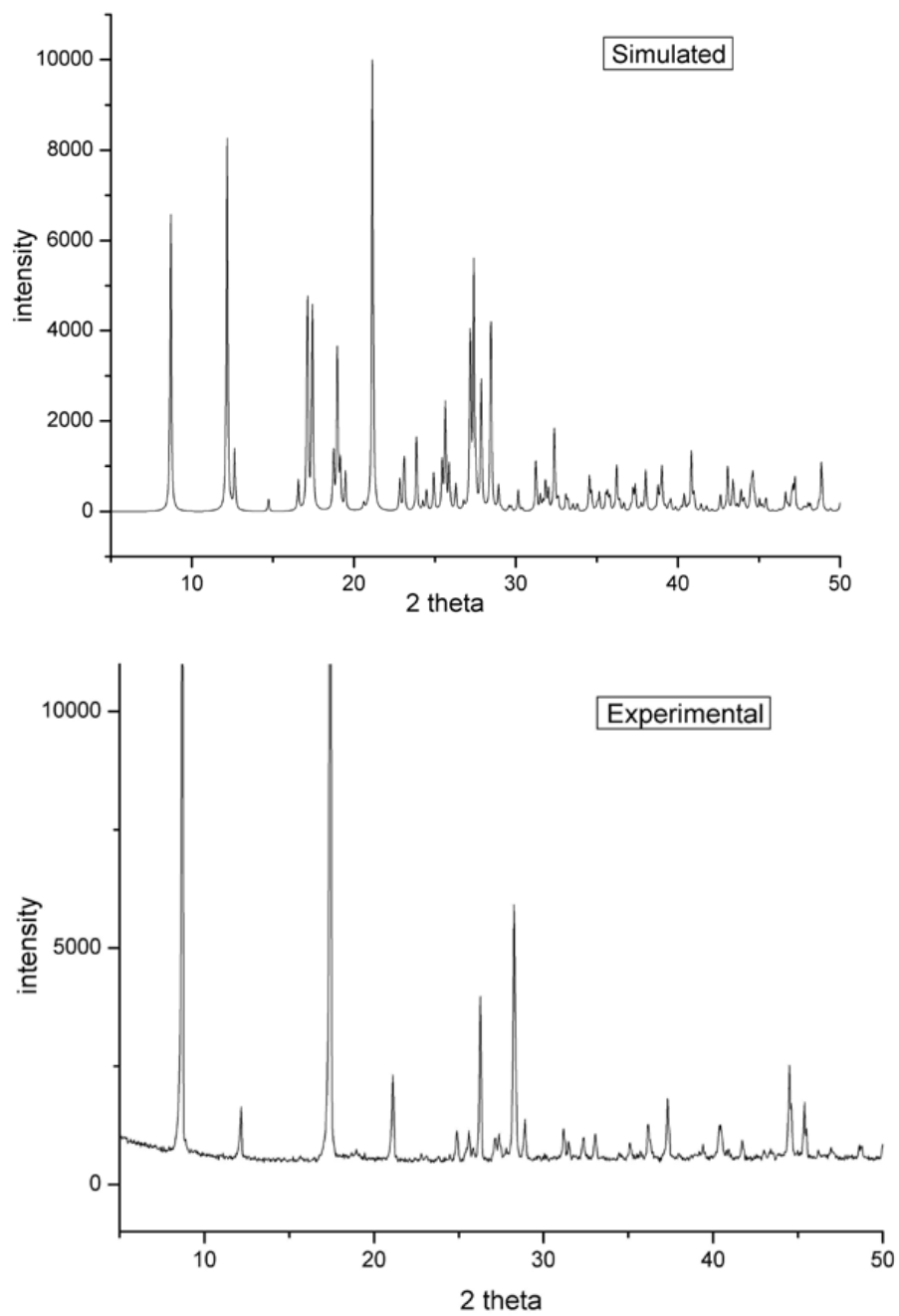


Fig. S5 Simulated and experimental PXRD pattern of compound **3**.

