Supplementary materials for

The anion exchange reaction of bis(isoquinoline) ionic liquids: self-assembly, crystal structures and thermal properties of ten novel d^{10} metal (Cu, Ag) halide/thiocyanate supramolecular polymers

Li-Sha Song，Hong-Mei Wang, Yun-Yin Niu,* Hong-Wei Hou,*and Yu Zhu

College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China

Table S1

Selected bond lengths (Å) and bond angles (°) within the coordination spheres around the metal centers in complex **1-10.**

		{(BIQPT)$_2$[Ag$_2$I$_6$]} (1)			
I1-Ag1	2.8246(5)	I3-Ag1	2.8203(5)	Ag1-I2^1	2.9568(6)
I2-Ag1	2.8968(5)	I2- Ag1^1	2.9568(5)	Ag1-I2-Ag1^1	85.162(14)
I1-Ag1-I2^1	109.434(16)	I1-Ag1-I2	117.369(17)	I2-Ag1-I2^1	94.837(14)
I3-Ag1-I1	113.056(16)	I3-Ag1-I2^1	113.695(17)	I3-Ag1-I2	107.273(16)
		{(BIQBT)[CuI$_3$]} (2)			
Cu1-I1	2.5174(11)	Cu1–I2	2.5096(10)	Cu1–I3	2.4973(11)
I2-Cu1-I1	121.26(4)	I3-Cu1-I1	122.60(4)	I3-Cu1–I2	116.12(4)
		{(BIQHX)[Cu$_4$I$_8$]·DMF} (3)			
I1-Cu1^1	2.6186(9)	I2-Cu1	2.7500(10)	I2-Cu2	2.5827(9)
I1-Cu1	2.6800(9)	I3-Cu1	2.7314(9)	I3-Cu2	2.5768(9)

I4-Cu2	2.4777(9)	Cu1-I1^{1}	2.6187(9)	Cu1-Cu2	2.6309(12)
Cu1^{1} -I1-Cu1	70.67(3)	Cu2-I2-Cu1	59.02(3)	Cu2-I3-Cu1	59.34(3)
I1^{1-}Cu1-I1	109.33(3)	I1^{1} -Cu1-I1	111.93(3)	I1-Cu1-I2	109.16(3)
I1^{1} -Cu1-I3	114.57(3)	I1-Cu1-I3	109.13(3)	I1^{1} -Cu1-Cu2	159.56(4)
I3-Cu1-I2	102.45(3)	Cu2-Cu1-I1	91.04(3)	Cu2-Cu1-I2	57.32(3)
Cu2-Cu1-I3	57.41(3)	I2-Cu2-Cu1	63.66(3)	I3-Cu2-I2	111.85(3)
I3-Cu2-Cu1	63.26(3)	I4-Cu2-I2	123.23(4)	I4-Cu2-I3	123.81(4)
I4-Cu2-Cu1	152.64(5)				
		{(BIQBT)$_{1.5}$[MoOS$_3$Cu$_3$I$_4$]·DMF} (4)			
I1-Cu1	2.414(2)	I2-Cu1	2.950(2)	I3-Cu2	2.427(19)
I4-Cu3	3.3863(19)	Mo1-Cu1	2.6744(19)	Mo1-Cu2	2.6667(18)
Mo1-Cu3	2.6431(18)	Mo1-S1	2.272(3)	Mo1-S2	2.267(3)
Mo1-S3	2.268(3)	Mo1-O1	1.706(8)	Cu1-S1	2.283(3)
Cu1-S2	2.279(3)	Cu2-S2	2.274(3)	Cu2-S3	2.272(3)
Cu3-S1	2.263(4)	Cu3-S3	2.258(4)	Cu2-Mo1-Cu1	81.33(6)
Cu3-Mo1-Cu1	83.69(7)	Cu3-Mo1-Cu2	82.50(6)	S1-Mo1-Cu1	54.25(9)
S1-Mo1-Cu2	117.41(9)	S1-Mo1-Cu3	54.20(9)	S2-Mo1-Cu1	54.17(9)
S2-Mo1-Cu2	54.17(9)	S2-Mo1-Cu3	120.36(10)	S3-Mo1-Cu1	118.74(10)
S3-Mo1-Cu2	54.11(9)	O1-Mo1-Cu1	130.7(3)	O1-Mo1-S1	109.4(3)
I1-Cu1-Mo1	149.44(10)	I1-Cu1-I2	117.97(8)	Mo1-Cu1-I2	92.57(6)
S1-Cu1-I1	119.20(11)	S1-Cu1-Mo1	53.85(9)	S2-Cu1-I1	119.66(11)
S1-Cu1-Mo1	53.76(8)	S2-Cu1-S1	107.47(12)	Cu3-S3-Cu2	101.22(14)
Cu3-S3- Mo1	71.47(10)	Mo1-S2-Cu1	72.07(10)	Mo1-S2-Cu2	71.92(10)
		{(BIQHX)[Ag$_4$Br$_6$]}$_n$ (5)			
Ag1-Br1	2.6665(10)	Ag1-Br2#2	2.7113(14)	Ag1-Br2	2.7180(12)
Ag1-Br1#3	2.7467(10)	Ag1-Ag1#2	3.2121(13)	Br1-Ag1#3	2.7467(10)
Br2-Ag1#2	2.7113(14)	Br1-Ag1-Br2#2	121.12(3)	Br1-Ag1-Br2	116.73(3)
Br2#2-Ag1-Br2	95.79(4)	Br1-Ag1-Br1#3	102.54(3)	Br2#2-Ag1-Br1#3	109.35(4)
Br2-Ag1-Br)#3	111.45(4)	Br1-Ag1-Ag1#2	108.081(19)	Br2#2-Ag1-Ag1#2	53.83(3)

Ag1-Br1-Ag1#3	77.46(3)	Br1#3-Ag1-Ag1#2	149.38(2)	Br2-Ag1-Ag1#2	53.63(3)
Ag1#2-Br2-Ag1	72.54(3)				
		{(BIQHX)[Ag_4I_6]}$_n$ (6)			
I1-Ag1	2.8625(6)	I2-Ag1	2.8238(5)	I2-Ag1^2	2.9360(7)
I1-Ag1^1	2.8641(7)	Ag1-Ag1^1	3.3166(10)	I2-Ag1-Ag1^1	111.907(14)
I2^2-Ag1-Ag1^1	151.905(13)	Ag1-I1-Ag1^1	70.78(2)	Ag1-I2-Ag1^2	84.098(17)
I1-Ag1-I1^1	99.876(18)	I1^1-Ag1-I2^2	120.96(2)	I1-Ag1-I2^2	105.055(19)
I1-Ag1-Ag1^1	54.632(17)	I1^1-Ag1-Ag1^1	54.588(16)	I2-Ag1-I1^1	108.881(19)
I2-Ag1-I1	128.19(2)	I2-Ag1-I2^2	95.901(17)		
		{(BIQHX)[$Cu_2(SCN)_4$]}$_n$ (7)			
Cu1-S1	2.4318(19)	Cu1-S2^1	2.4578(19)	Cu1-N1^2	1.973(5)
Cu1-N2	1.966(6)	C14-N2-Cu1	160.9(5)	C13-N1-Cu1^2	157.3(5)
S1-Cu1-S2^1	109.26(7)	N1^2 -Cu1-S1	100.96(16)	N1^2 -Cu1-S2^1	114.26(15)
N2-Cu1-S1	110.92(18)	N2-Cu1-S2^1	100.35(17)	N2-Cu1-N1^2	121.1(2)
C13-S1-Cu1	100.8(2)	C14-S2-Cu1^1	98.9(2)		
		{(BIQBT)[$Cu_2(SCN)_4$]}$_n$ (8)			
Cu1-N2#1	1.984(2)	Cu1-N3#2	1.999(2)	Cu1-S2	2.4101(7)
Cu1-S1	2.4408(7)	N2-Cu1#1	1.984(2)	N3-Cu1#2	1.999(2)
N2#1-Cu1-N3#2	119.14(9)	N2#1-Cu1-S2	110.76(7)	N3#2-Cu1-S2	101.75(6)
N2#1-Cu1-S1	103.74(6)	N3#2-Cu1-S1	111.40(6)	S2-Cu1-S1	110.08(3)
C12-N2-Cu1#1	161.40(19)	C13-N3-Cu1#2	153.54(18)	C12-S1-Cu1	95.25(8)
C13-S2-Cu1	98.63(8)				
		{(BIQPP)[$Cu_2(SCN)_4$]}$_n$ (9)			
Cu1-S1	2.4755(12)	Cu1-S2	2.5018(12)	Cu1-N2^1	1.956(4)
Cu1-N3^2	1.944(3)	N2-Cu1^1	1.956(4)	N3-Cu1^3	1.944(3)
S1-Cu1-S2	102.71(4)	N2^1 -Cu1-S1	100.63(9)	N2^1 -Cu1-S2	108.78(11)
N3^2 -Cu1-S1	105.34(11)	N3^2 -Cu1-S2	108.40(10)	N3^2 -Cu1-N2^1	127.88(14)
C12-S1-Cu1	98.43(12)	C13-S2-Cu1	106.85(13)	C12-N2-Cu1^1	159.4(3)
C13-N3-Cu1^3	170.4(3)				

{(BIQEH)[$Cu_2(SCN)_4$]]}$_n$ (10)					
Cu1- S1	2.3984(8)	Cu1-S2	2.3980(8)	Cu1- $N2^1$	2.012(3)
Cu1- $N3^2$	1.960(2)	N2- $Cu1^1$	2.012(3)	N3- $Cu1^3$	1.960(2)
S2- Cu1- S1	96.58(3)	$N3^2$- Cu1- S1	121.77(8)	$N3^2$- Cu1-$N2^1$	113.44(11)
$N2^1$- Cu1- S1	106.02(7)	$N3^2$- Cu1- S2	103.37(9)	C11-S1-Cu1	96.57(9)
$N2^1$- Cu1- S2	114.77(8)	C12-S2-Cu1	100.07(10)	C11-N2-$Cu1^1$	158.1(2)
C12-N3-$Cu1^3$	160.5(3)				

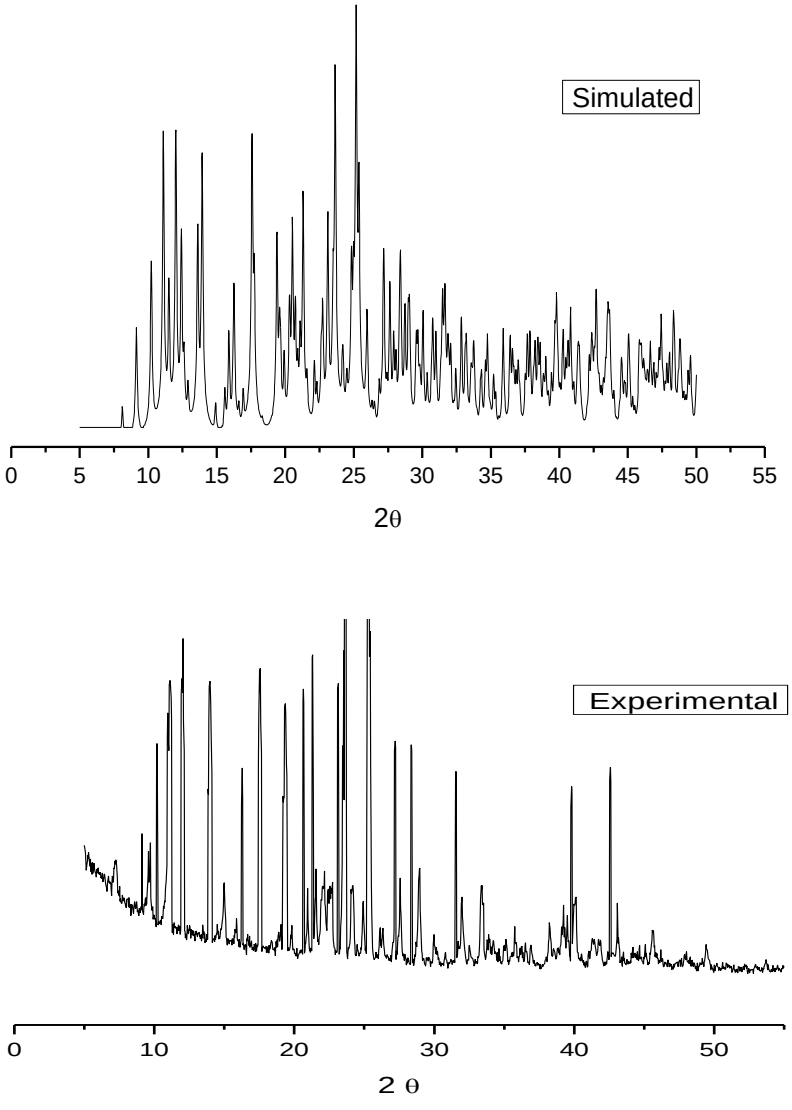
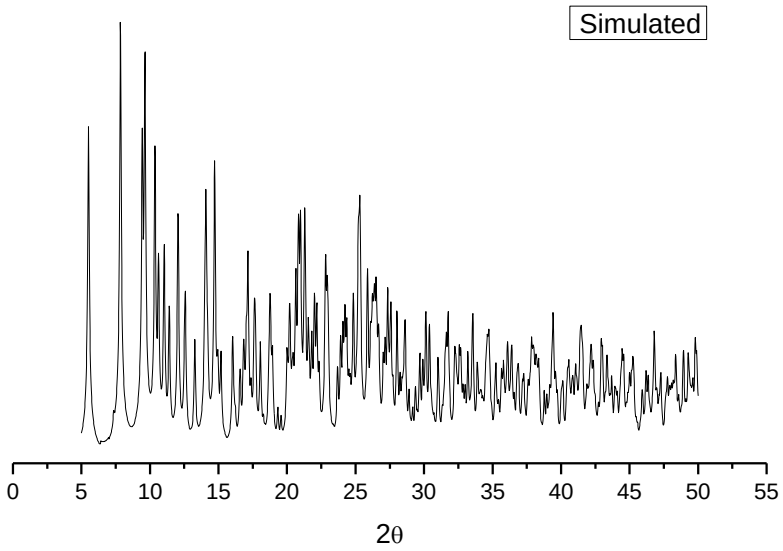


Fig. S1 Simulated and experimental PXRD pattern of compound **2.**



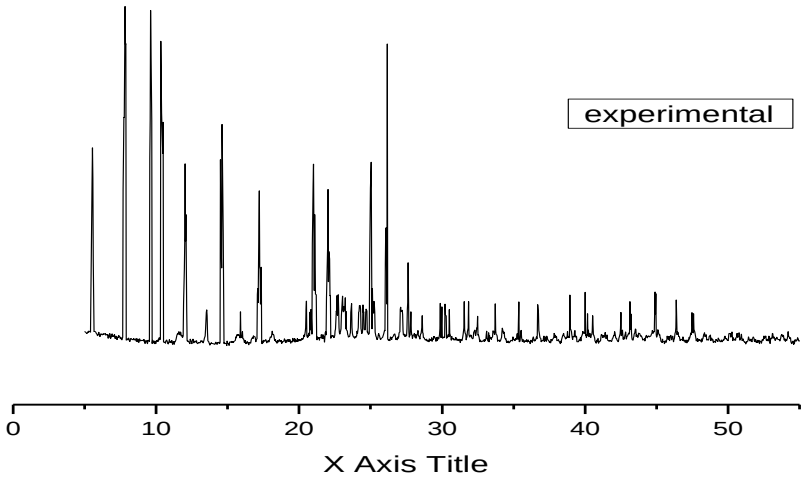


Fig. S2 Simulated and experimental PXRD pattern of compound **4.**

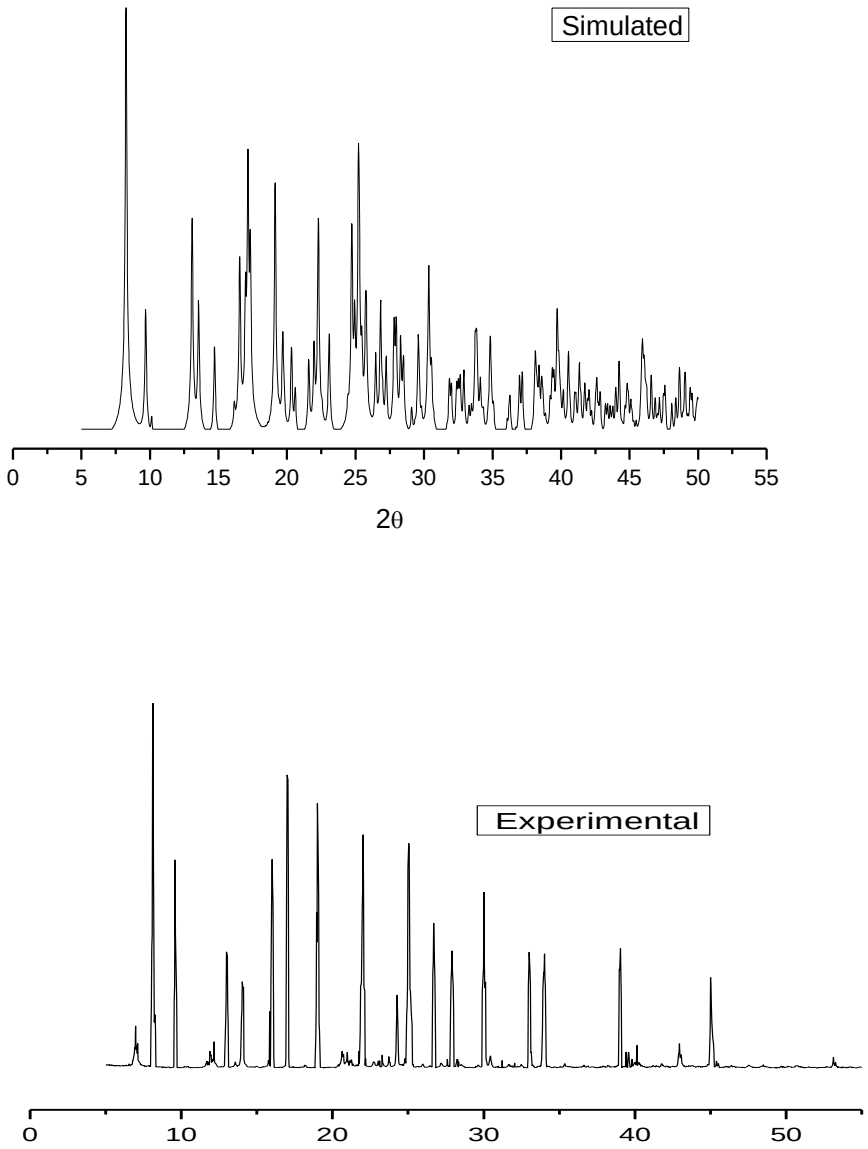


Fig. S3 Simulated and experimental PXRD pattern of compound **10.**