

# Supporting Information

## Three cationic non-porous Cu<sup>I</sup>-coordination polymers: structural investigation and vapor iodine capture

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

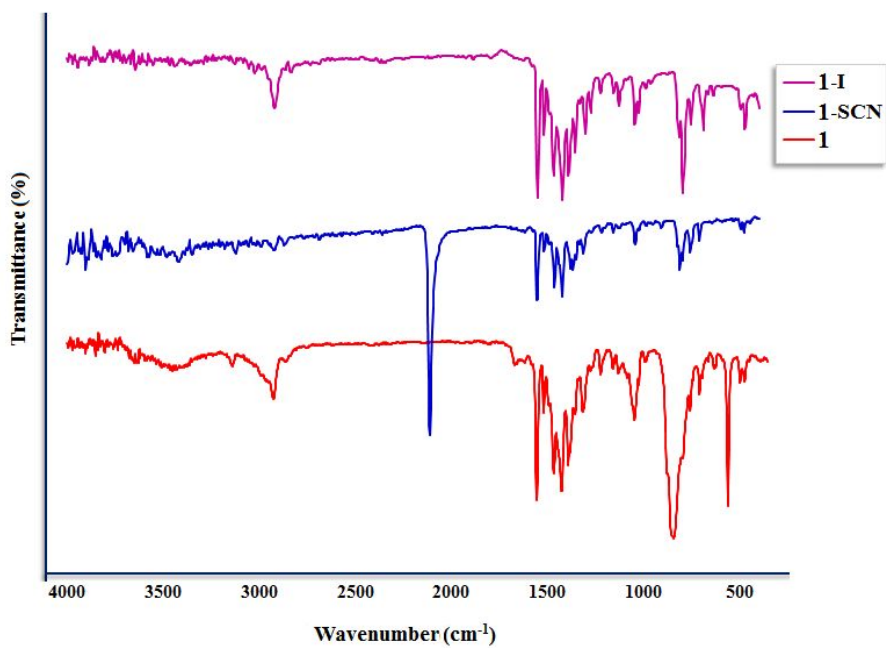
<b>(1)</b>			
Cu1-N1	1.998(2)	P1-F7	1.650(11)
Cu1-N3	1.977(2)	P1-F8	1.414(18)
Cu1-N5	1.983(2)	P1-F9	1.588(15)
P1-F1	1.588(6)	P1-F10	1.505(17)
P1-F2	1.530(8)	P1-F11	1.494(14)
P1-F3	1.529(8)	P1-F12	1.598(14)
P1-F4	1.548(6)	N1-Cu1-N3	117.86(10)
P1-F5	1.591(5)	N1-Cu1-N5	117.19(9)
P1-F6	1.590(6)	N3-Cu1-N5	124.21(10)
<b>(2)</b>			
Cu1-N1	2.0766(14)	N1-Cu1-N1a	116.19(6)
P1-F1	1.606(3)	N1-Cu1-N1b	96.74(6)
P1-F2	1.602(4)		
P1-F3	1.610(3)		
P1-F3	1.605(6)		
<b>(3)</b>			
Cu1-N1	2.074(2)	N1-Cu1-N1a	113.80(9)
P1-F1	1.615(4)	N1-Cu1-N1b	101.13(9)
P1-F2	1.605(4)		
P1-F3	1.576(2)		

**Table S2.** Hydrogen bonds in compounds **2** and **3**.

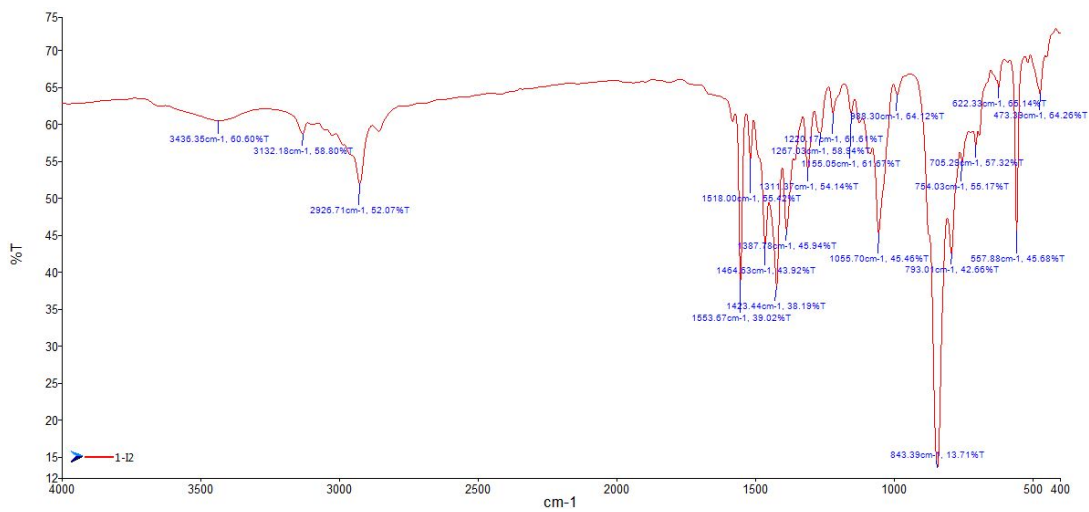
<b>D-H...A</b>	<b>D-H/Å</b>	<b>H...A/Å</b>	<b>D-A/Å</b>	<b>D-H...A/°</b>
<b>(2)</b>				
C3-H3...F3	0.9300	2.4300	3.269(3)	151.00
<b>(3)</b>				
C7-H7...N2	0.9300	2.5100	2.852(4)	102.00

**Table S3.** Gravimetric and UV-Vis determination of iodine contents for compounds **1** and **KEZXEU** in different I<sub>2</sub>(g) exposure time.

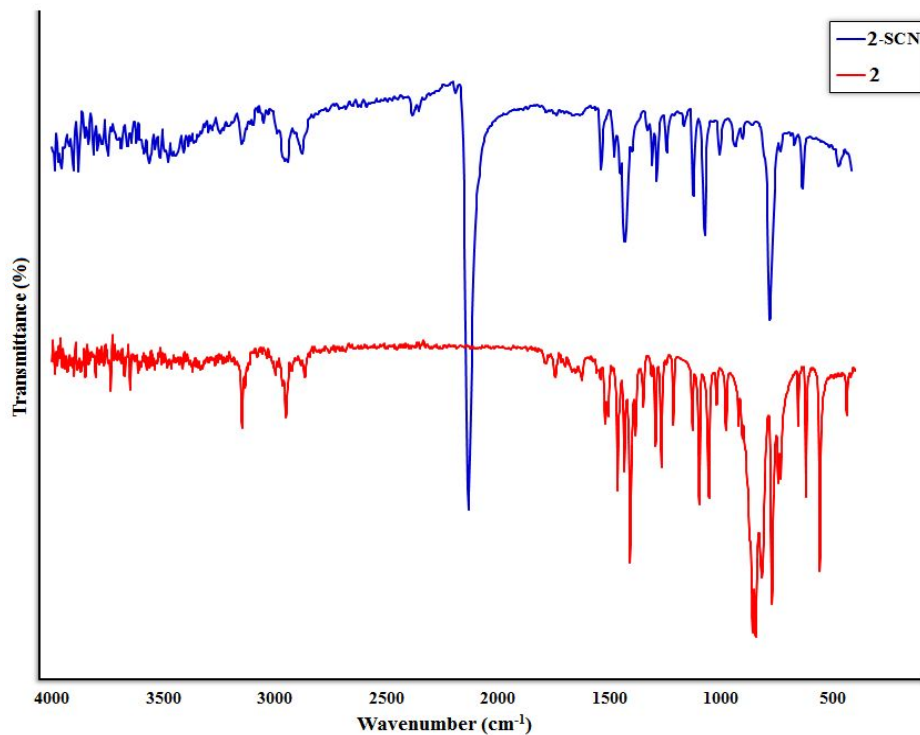
Compound	Initial weight (mg)	I <sub>2</sub> (g) Exposure time	Iodine content (mg)	Iodine wt %	Iodine content (mg)	Iodine wt %
Method	Gravimetric			UV-Vis		
<b>1</b>	15.4	30 min	1.5	9.7%	1.4	9.4%
	15.0	50 min	3.0	20.0%	4.1	27.0%
	15.5	2 h	7.3	47.0%	7.1	45.0%
<b>KEZXEU</b>	16.0	30 min	3.3	20.6%	2.8	18.0%
	16.8	50 min	5.3	31.5%	7.0	42.0%
	16.5	2 h	9.6	58.2%	10.2	62.0%



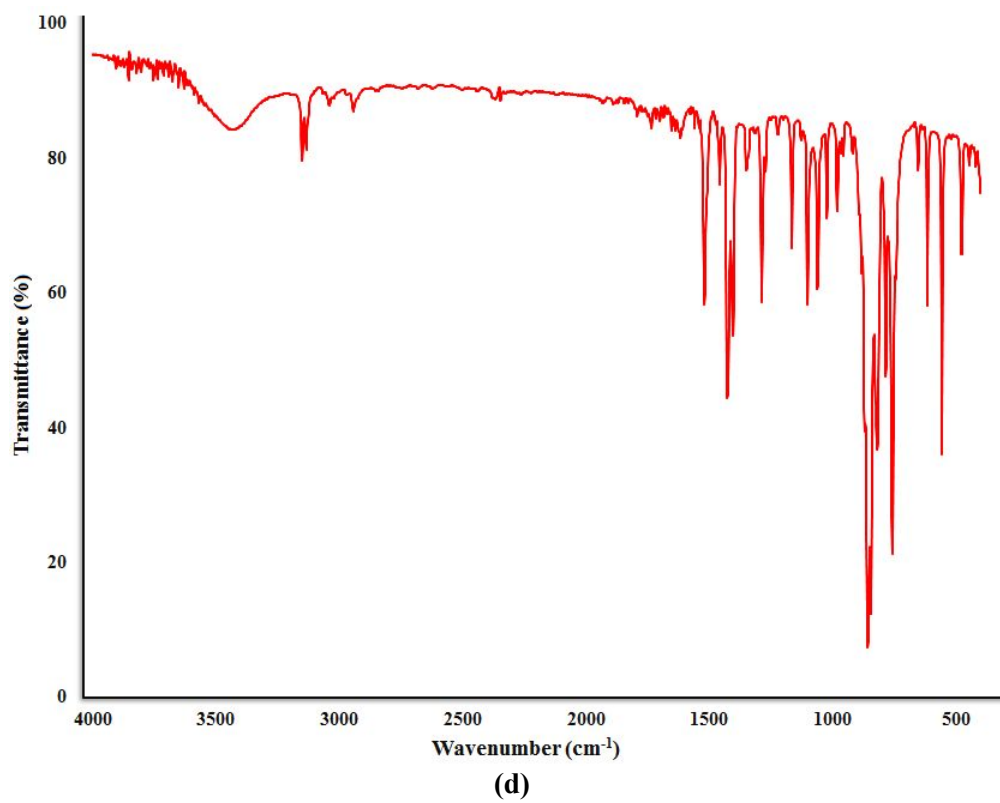
(a)



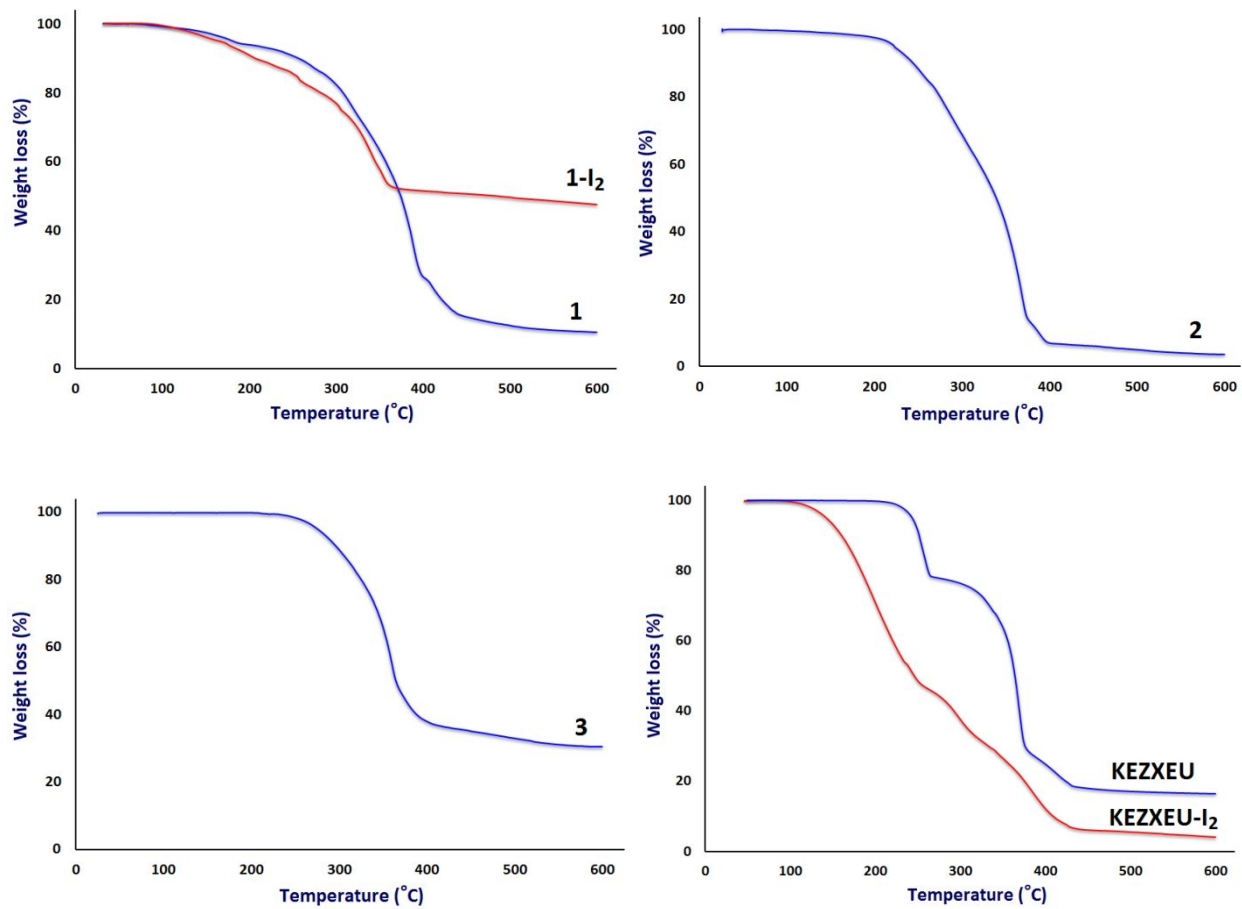
(b)



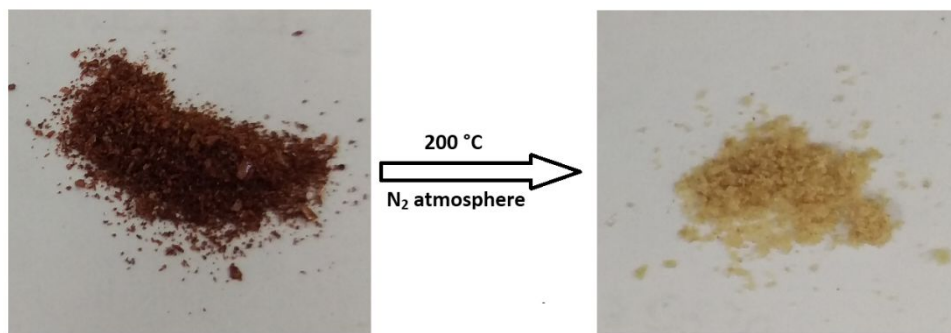
(c)



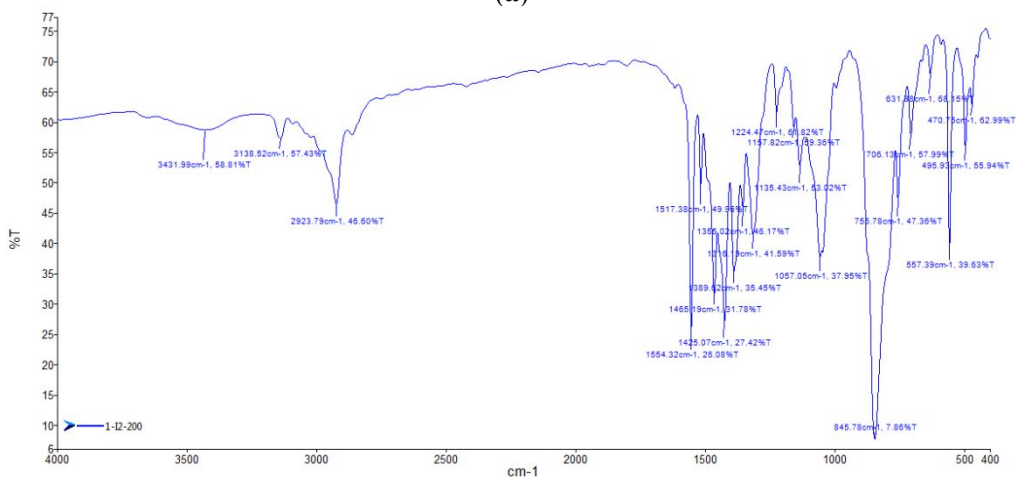
**Figure S1.** FT-IR spectra of compounds; a) **1**, **1-I** and **1-SCN**, b) **1-I<sub>2</sub>**, c) **2** and **2-SCN** and d) **3**.



**Figure S2.** TGA curves for compounds **1-3** and iodine adsorbed **1-I<sub>2</sub>** and **KEZXEU-I<sub>2</sub>**.

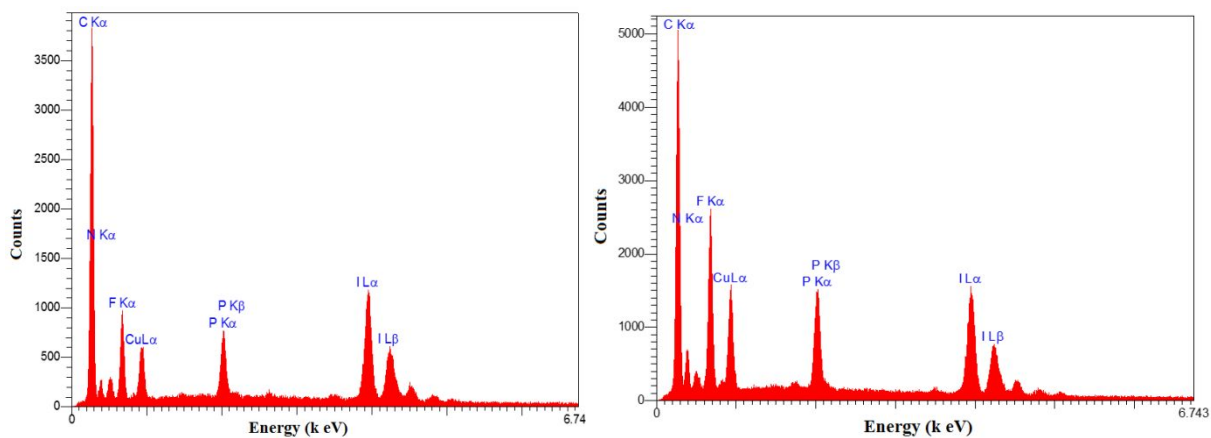


(a)



(b)

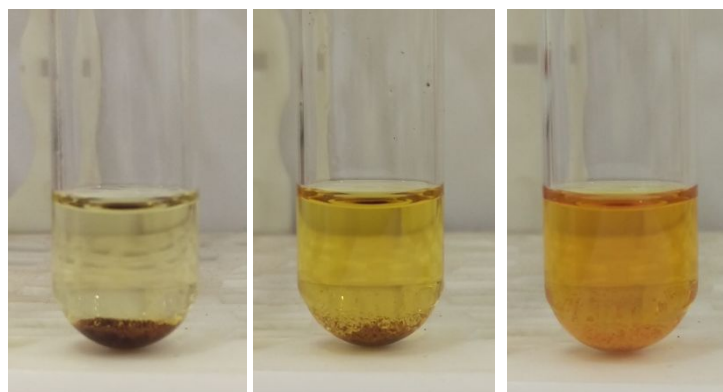
**Figure S3.** a) 1-I<sub>2</sub> before (brown) and after (yellow) heating at 200°C for 20 min in N<sub>2</sub> atmosphere and b) corresponding FT-IR spectrum of the recovered solid at 200° C.



(a)

(b)

**Figure S4.** EDX spectra of a) 1-I<sub>2</sub> and b) KEZXEU-I<sub>2</sub>.

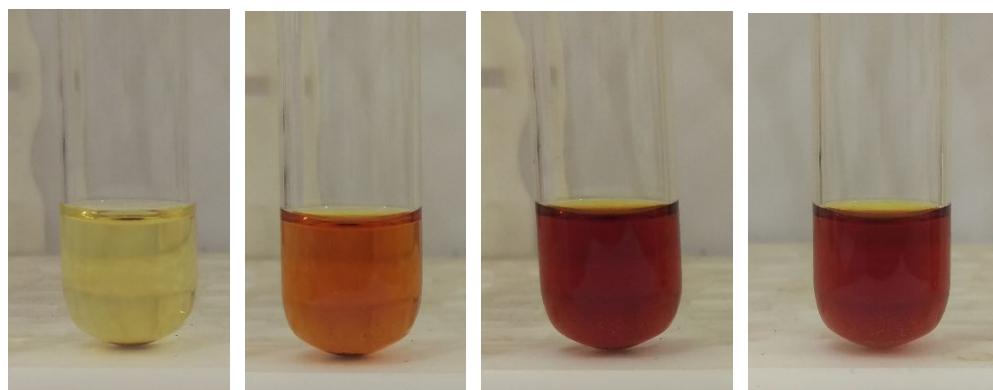


1 min.

10 min.

1 day

(a)



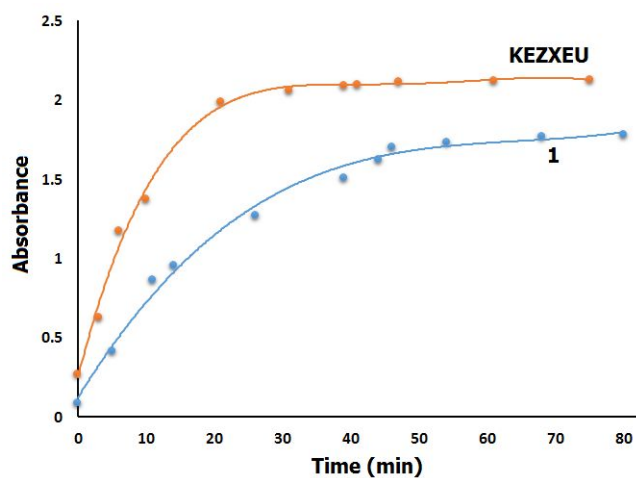
1 min.

5 min.

30 min

1 day

(b)



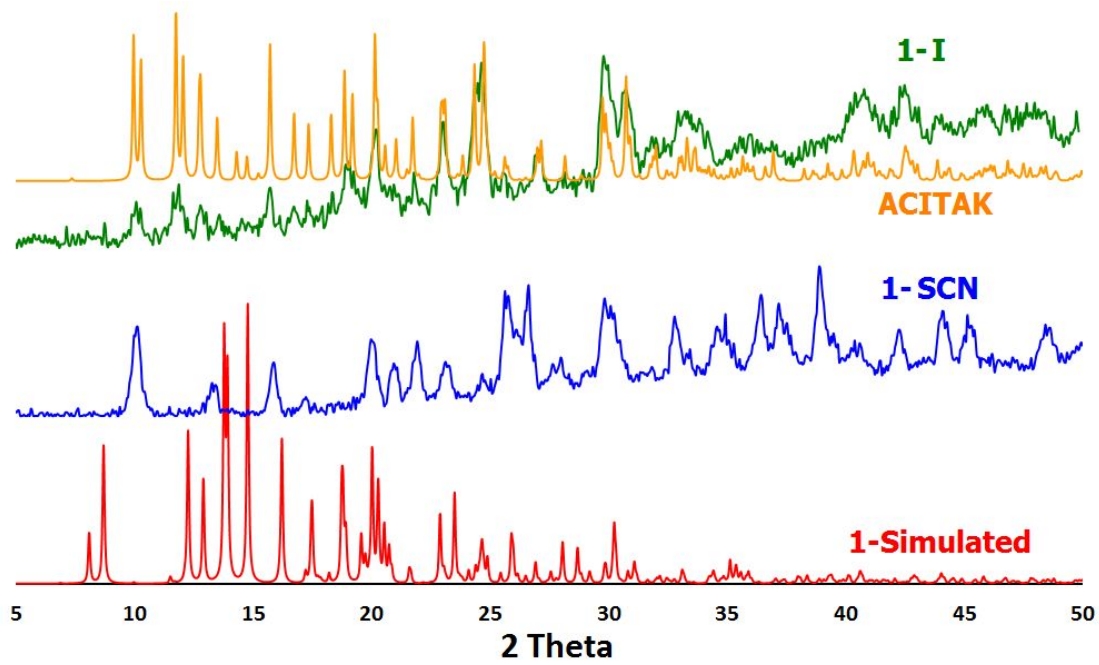
(c)



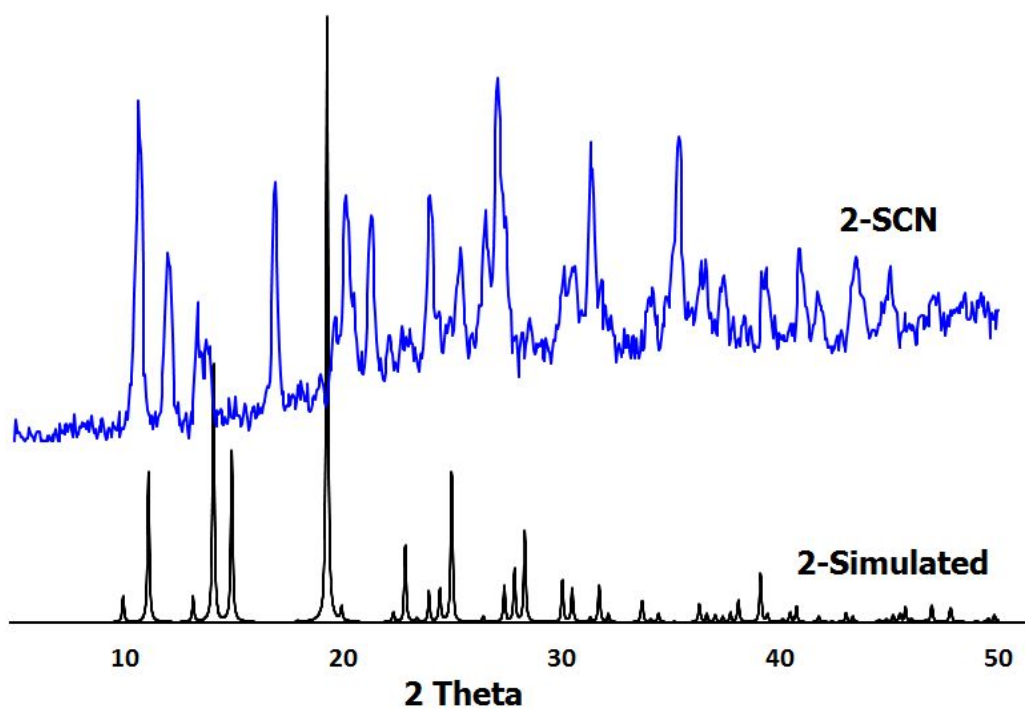
(d)

**Figure S5.** Visual detection of iodine release for 15 mg a) **1-I<sub>2</sub>** and b) **KEZXEU-I<sub>2</sub>** immersed in 2 ml EtOH. c) Absorbance-time profile for the release of iodine from 15 mg **1-I<sub>2</sub>** (blue) and **KEZXEU-I<sub>2</sub>** (orange) immersed in 3 ml EtOH. d) Solid materials of compounds **1** (left) and **KEZXEU** (right) recovered from EtOH solutions after iodine release.





(a)



(b)

**Figure S6.** Comparison between experimental PXRD patterns of the anion exchanged products a) 1-SCN and 1-I, b) 2-SCN and simulated PXRD of their pristine frameworks.