

Supporting information's for the manuscript

Structural diversities in Cu(I) and Ag(I) sulfonate coordination polymers and anion exchange properties

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Table S1: TGA analysis for the compounds

Compounds	Temperature (°C)	Wt % loss (calc % loss)	Corresponding moieties
1	30-100	2.9 (2.5)	H ₂ O
	330-366	29.7 (27)	H ₂ O + 4,4'-Bipyridyl
	366-420	72	All H ₂ O and organic moieties
2	30-118	4.4 (4.5)	2H ₂ O
	231-367	44.7 (43.5)	2(4,4'-Bipyridyl)
	267-473	73	All H ₂ O and organic moieties
3	30-246	4.6 (4.58)	4H ₂ O
	291-359	17.8 (18.5)	2H ₂ O + 4,4'-Azobipyridyl
	359-598	69.4 (68.7)	3(4,4'-Azobipyridyl) + bds
	600-710	74.2	All H ₂ O and organic moieties
4	30-100	6.3 (6)	3H ₂ O
	244-327	28.6 (28.4)	H ₂ O + 4,4'-Azobipyridyl
	327-460	49.5 (49.3)	4,4'-Azobipyridyl
	460-621	73.8	All H ₂ O and organic moieties
5	30-95	6.1 (6.2)	3H ₂ O
	306-435	47.6 (48.5)	BPE
	435-560	69	All H ₂ O and organic moieties
6	3-100	3.1 (2.9)	3H ₂ O
	320-368	30.1 (30)	6H ₂ O + 2TBP
	368-420	72.7	All H ₂ O and organic moieties

Table S2: UV-visible bands for **1-6**

Compounds	Absorption bands (nm)
1	420(broad), 327(shoulder) and 248
3	324 and 250
2	486(broad), 329(shoulder) and 248
4	492, 375 and 259
5	461(broad), 352, 250
6	438, 275

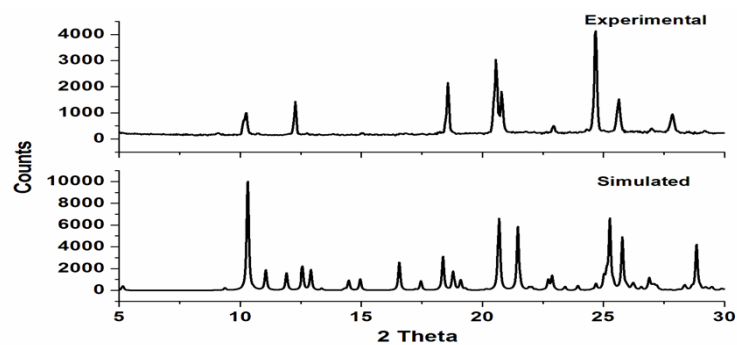
Table S3: Selected bond lengths and bond angles for **1-6**

Compounds	Bond length (Å)	Bond angle (°)
1	Cu1-N1 1.910(6)	N1-Cu1-N2 169.5(2)
	Cu1-N2 1.915(6)	O1-Cu1-O_1 98.13
	Cu1-O1 2.561	N4-Cu2-N3 171.1(2)
	Cu_1-O1 2.490	O4-Cu2-Ow1 80.40
	Cu2-N3 1.911(6)	
	Cu2-N4 1.903(6)	
	Cu2-O2 2.771	
	Cu2-Ow1 2.563	
2	Ag1-N1 2.149(2)	N1-Ag1-N2 170.80(8)
	Ag1-N2 2.156(2)	O1-Ag1-O_1 103.98
	Ag2-N4 2.151(2)	O1-Ag1-N1 92.29
	Ag2-N3 2.154(2)	O1-Ag1-N2 94.08
	Ag1-O1 2.670	O_1-Ag1-N1 100.50
	Ag1-O_1 2.682	O_1-Ag1-N2 84.39
	Ag2-O4 2.862	N4-Ag2-N3 173.88(9)
	Ag2-Ow1 2.780	O4-Ag2-Ow1 178.02
	Ag1-Ag1 3.296(5)	O4-Ag2-N3 90.99
	O4-Ag2-N4 86.57	
	Ow1-Ag2-N3 87.73	
	Ow1-Ag2-N4 94.55	
3	Cu1-N1 1.909(3)	N8-Cu1-N1 164.70(17)
	Cu1-O7 2.376(4)	N8-Cu1-O7 97.06(15)
	Cu2-N5 1.907(4)	N1-Cu1-O7 98.13(15)
	Cu2-N4 1.917(4)	N5-Cu2-N4 165.1(2)
	Cu2-O1 2.317(4)	N5-Cu2-O1 98.89(17)
	Cu3-N12 1.907(3)	N4-Cu2-O1 96.00(17)

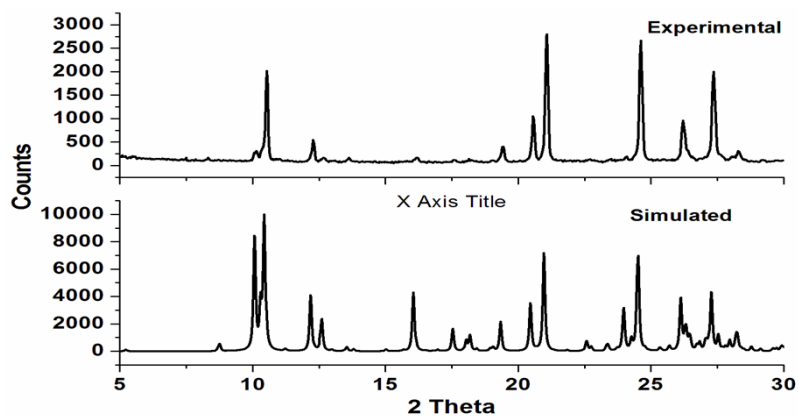
	Cu3-N13 1.911(3)	N12-Cu3-N13 166.33(17)
	Cu3-O11 2.339(4)	N12-Cu3-O11 99.10(15)
	Cu4-N16 1.895(4)	N13-Cu3-O11 94.52(16)
	Cu4-N9 1.897(4)	N16-Cu4-N9 168.37(19)
4	Ag1-N1 2.149(4)	N1 Ag1 N4 174.76(1)
	Ag1-N4 2.150(4)	O1-Ag1-N1 89.93
	Ag1-O1 2.794	O1-Ag1-N1 92.10
	Ag2-N5 2.139(4)	N5 Ag2 N8 174.91(1)
	Ag2-N8 2.145(4)	O6-Ag2-N5 91.71
	Ag2-O6 2.786	O6-Ag2-N8 89.69
5	Ag1-N1 2.133(10)	N1-Ag1-N2 174.7(4)
	Ag1-N2 2.127(10)	Ow1-Ag1-N1 92.38
	Ag1-Ow1 2.838	Ow1-Ag1-N2 91.75
	Ag1-Ag_1 3.3537(11)	
6	Ag1-N1 2.146(5)	N1-Ag1-N2 164.7(2)
	Ag1-N2 2.151(5)	O1-Ag1-N1 102.12
	Ag1-O1 2.633	O1-Ag1-N1 93.14
	Ag1-Ag1 3.211(10)	N3 Ag2 N4 166.96(2)
	Ag2-N3 2.153(5)	O4-Ag2-N3 100.03
	Ag2-N4 2.161(5)	O4-Ag2-N4 92.88
	Ag2-O4 2.688	N6-Ag3-N5 171.80(2)
	Ag3-N6 2.133(5)	O7-Ag3-N5 97.43
	Ag3-N5 2.143(5)	O7-Ag3-N6 90.51
	Ag3-Ag2 3.236(8)	N8-Ag4-N7 171.81(19)
	Ag3-O7 2.817	O11-Ag4-N7 94.11
	Ag4-N8 2.124(5)	O11-Ag4-N8 87.18
	Ag4-N7 2.130(5)	
	Ag4-O11 2.824	
	Ag4-Ag4 3.162(12)	

Table S4: Hydrogen bond parameters

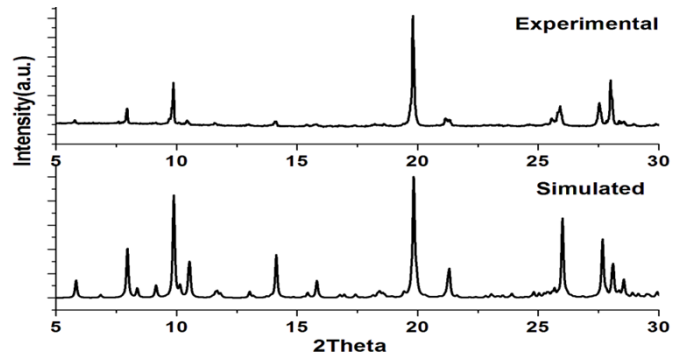
Compounds	<i>D-H</i> ⋯ <i>A</i>	<i>H</i> ⋯ <i>A</i> (Å)	<i>D</i> ⋯ <i>A</i> (Å)	<i>D-H</i> ⋯ <i>A</i> (°)
4	Ow3-H7A⋯Ow4	1.86	2.699(9)	171
	Ow3-H7B⋯Ow2	2.03	2.839(8)	158
	Ow4-H8A⋯O6	2.23	3.078(7)	172
	Ow2-H9A⋯Ow1	1.85	2.679(8)	164
	Ow2-H9B⋯O3	2.33	3.160(7)	166
	Ow1-H10A⋯Ow4	2.03	2.873(8)	169
	Ow1-H10B⋯O2	2.14	2.941(8)	158
6	Ow5-H00A⋯O8	2.11	2.940(6)	165
	Ow5-H00B⋯O3	2.04	2.853(6)	161
	Ow7-H00D⋯Ow6	2.02	2.835(4)	161
	Ow8-H00H⋯Ow9	2.04	2.812(6)	151
	Ow6-H00L⋯Ow7	2.07	2.835(4)	149



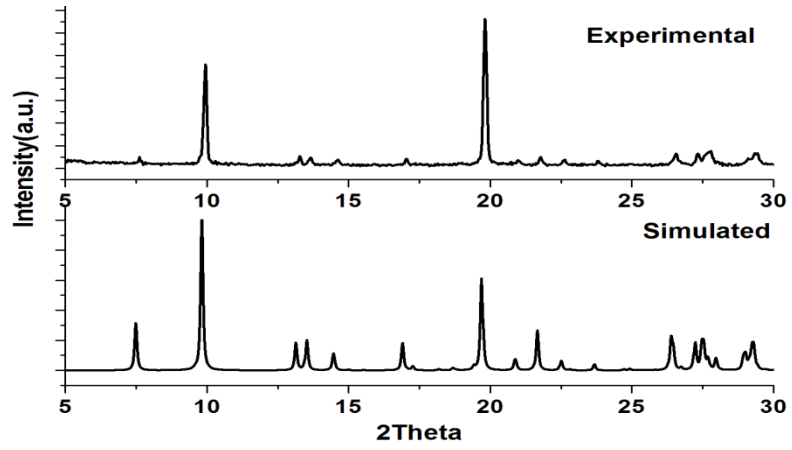
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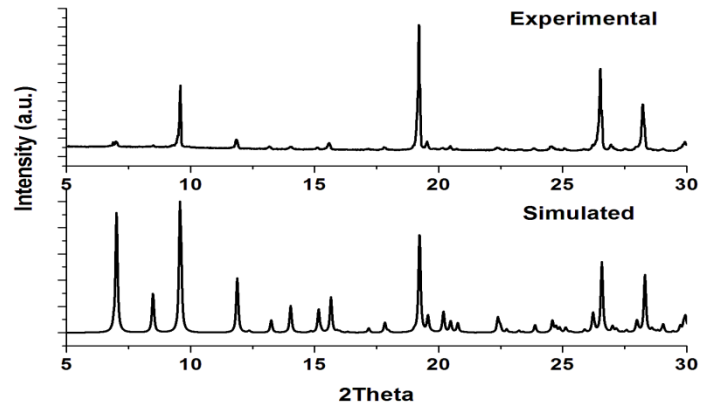
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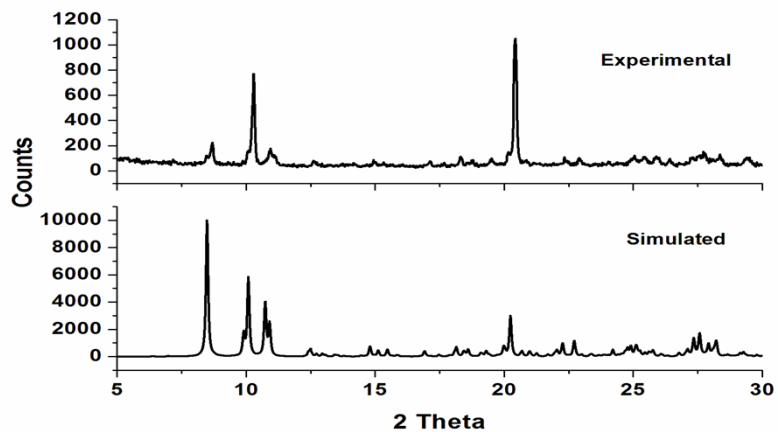
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4



5



6

Figure S1 PXR D pattern of compounds 1-6

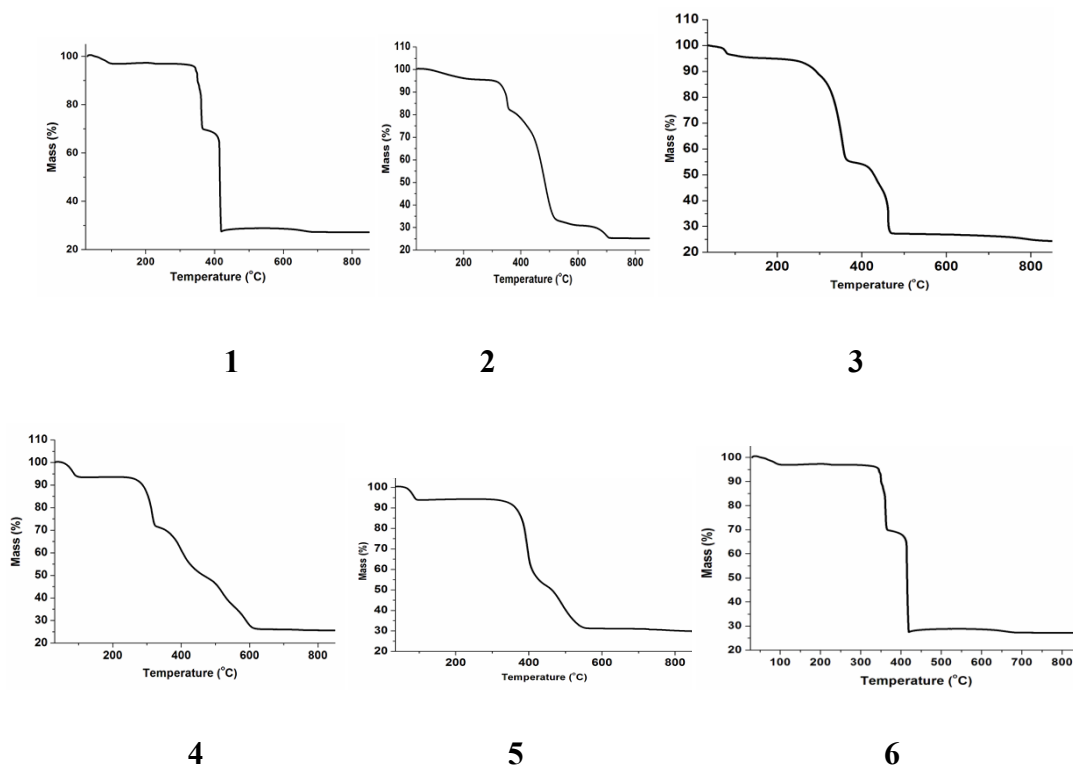


Figure S2 TGA plots for 1-6

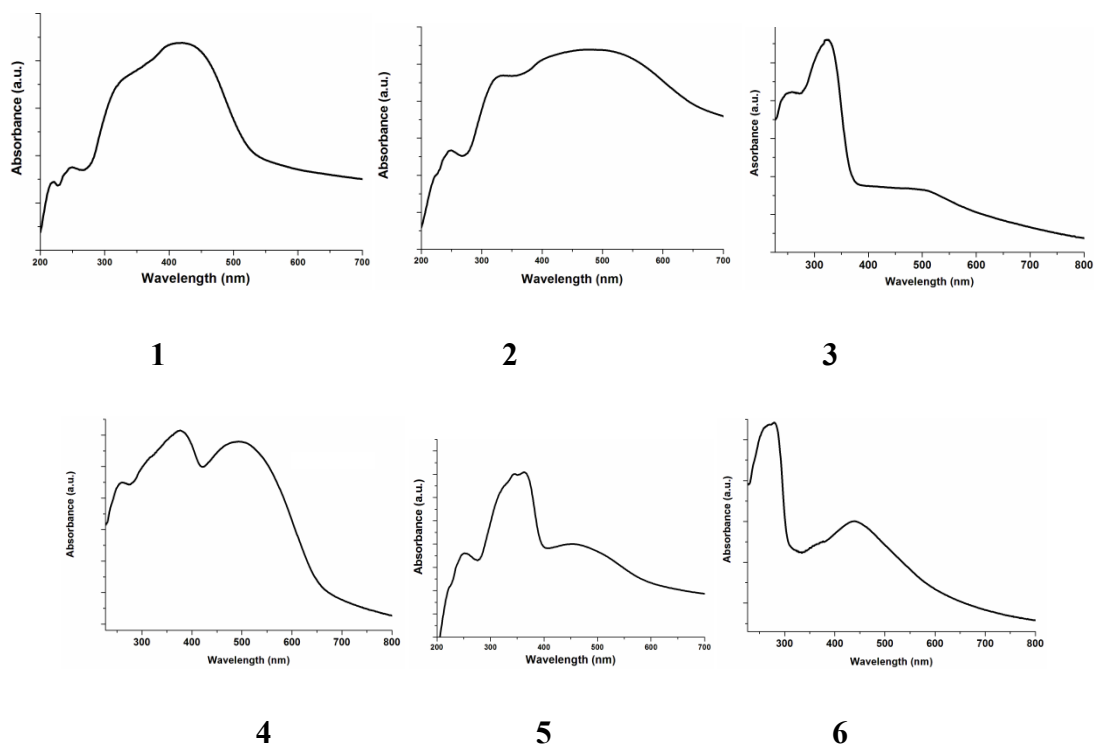


Figure S3 UV-Visible spectra of 1-6

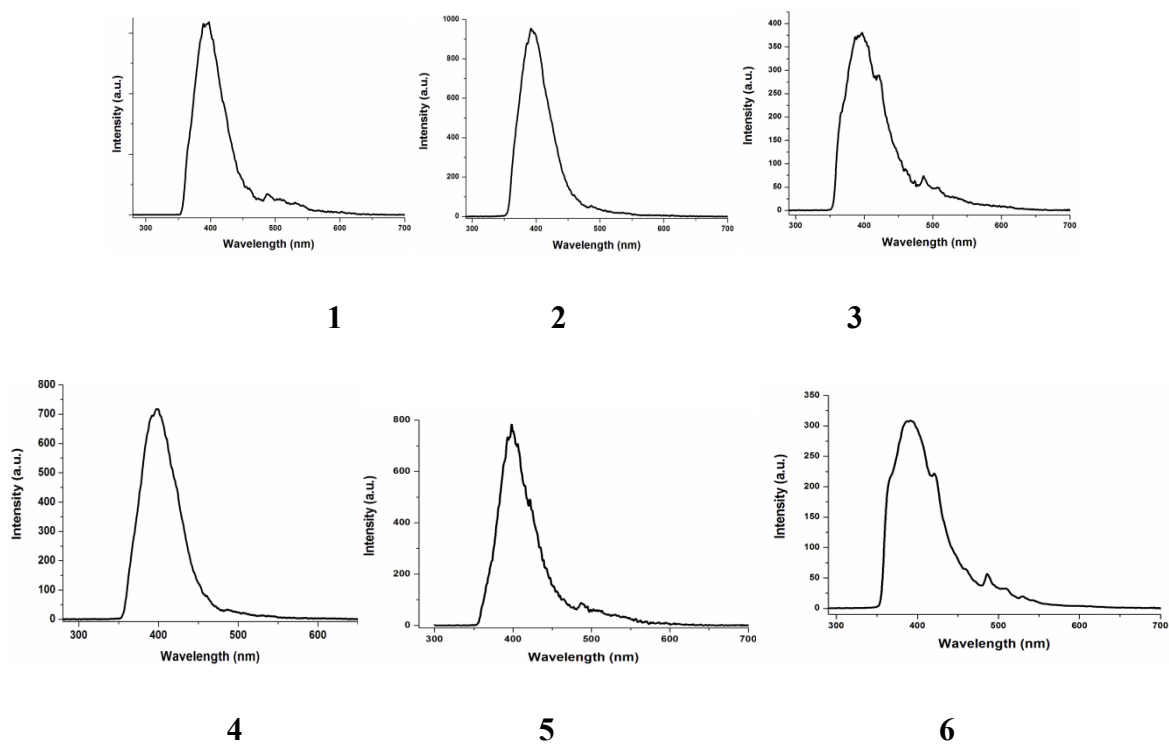


Figure S4 PL spectra of 1-6

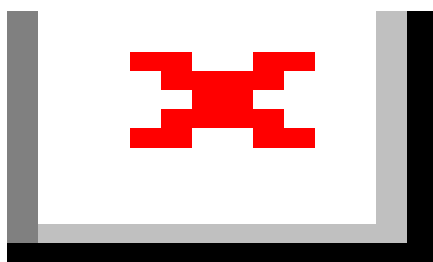


Figure S5 ^1H NMR spectra of the ketal product (2-ethyl-2-methyl-[1,3]-dioxolane, δ 3.92-4.00, m, 4H) from 2-butanone and ethylene glycol (δ 3.73-3.77, m, 4H). The integration of ketal product and precursor peak areas were used to determine yields

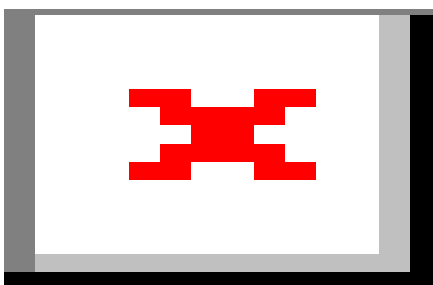


Figure S6 ^1H NMR spectra of the ketal product (δ 3.93-3.96, m, 4H) from 3-pentanone and ethylene glycol (δ 3.73-3.758, m, 4H). The integration of ketal product and precursor peak areas were used to determine yields

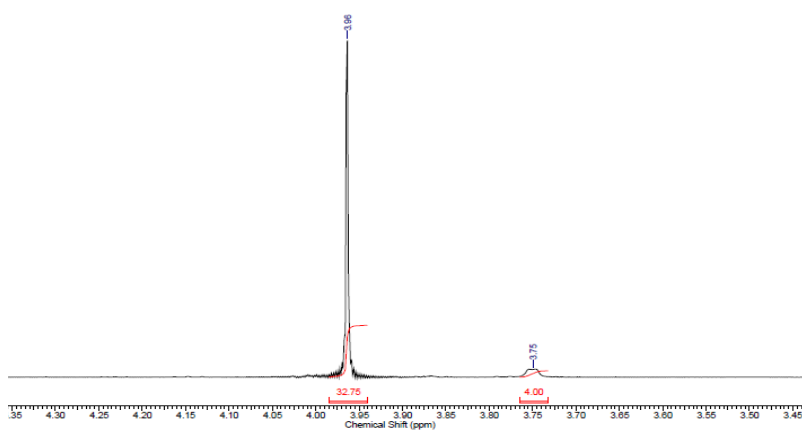


Figure S7 ^1H NMR spectra of the ketal product (δ 3.93-3.98, m, 4H) from acetone and ethylene glycol (δ 3.73-3.77, m, 4H). The integration of ketal product and precursor peak areas were used to determine yields

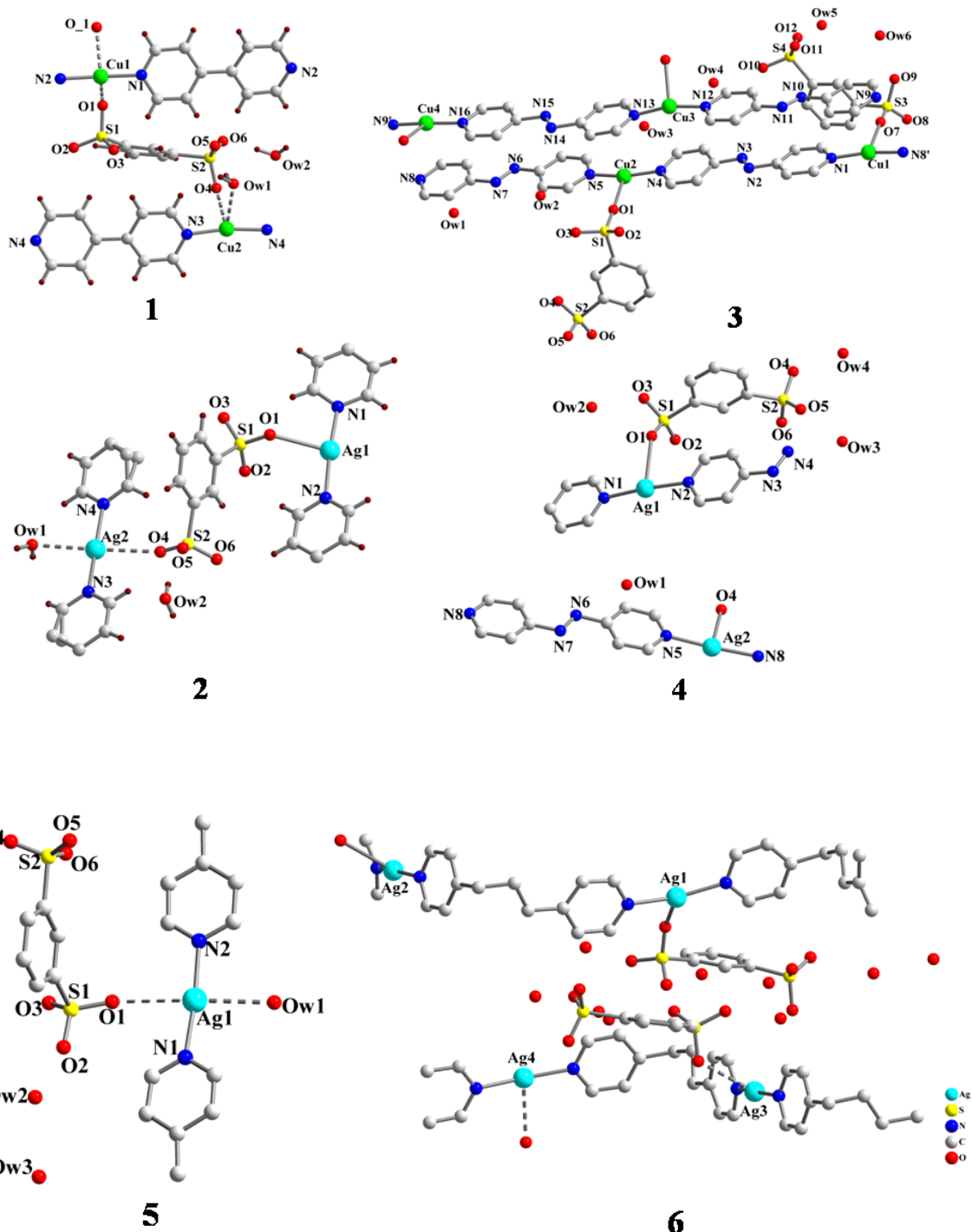
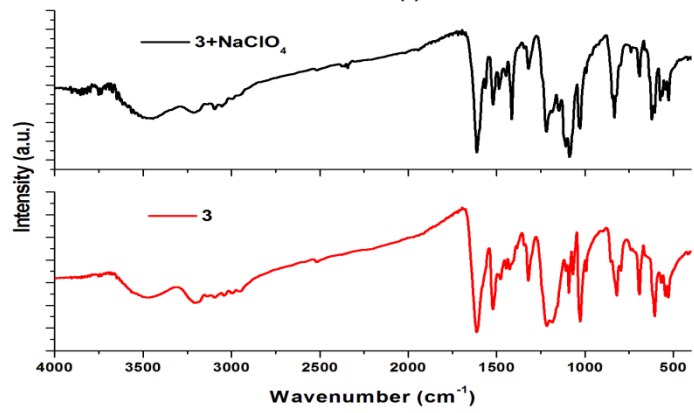
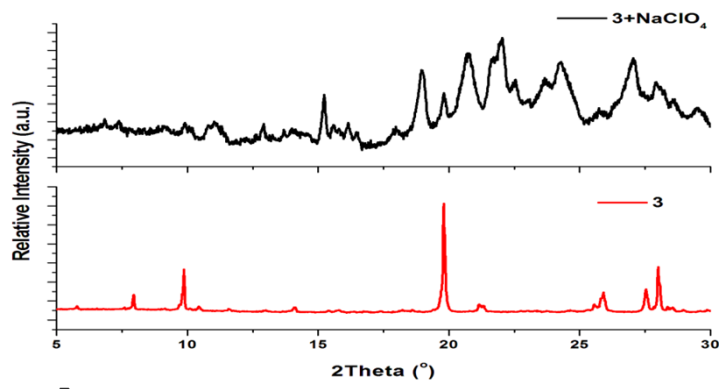
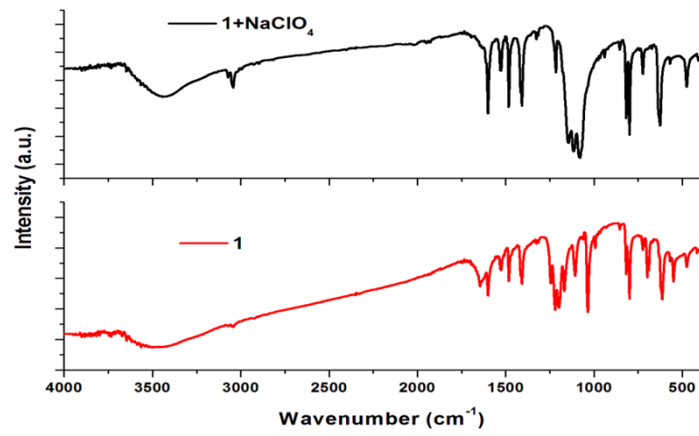
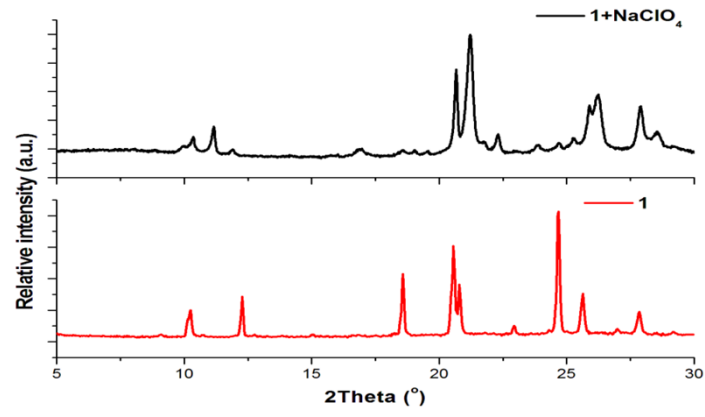
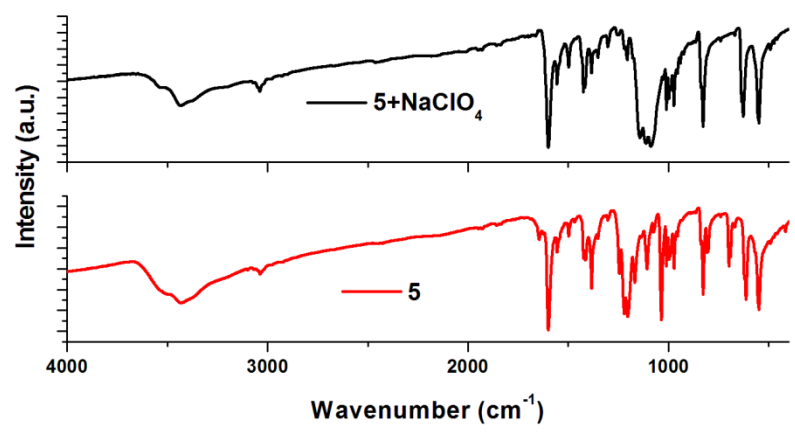
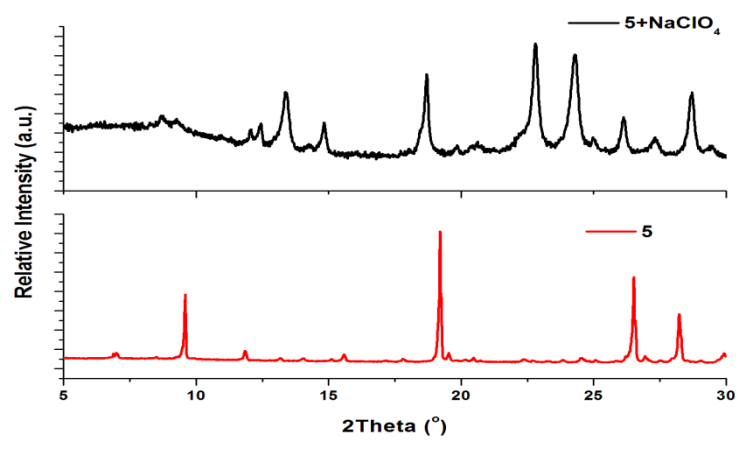
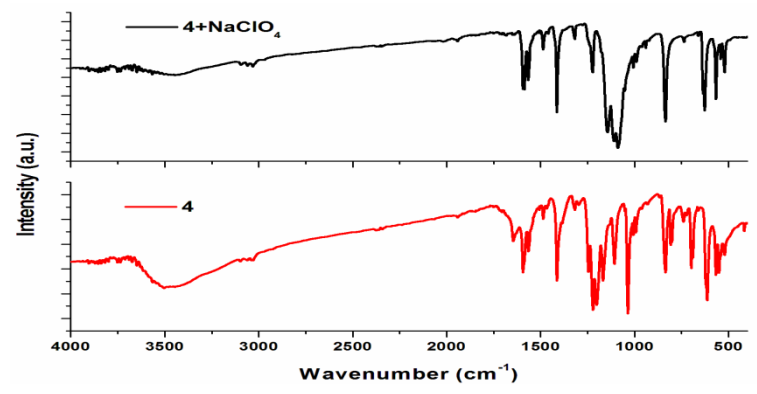
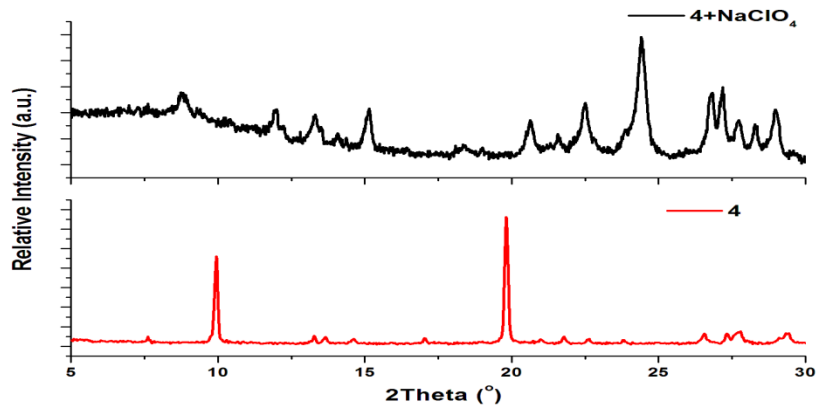


Figure S8 Asymmetric unit of 1-6





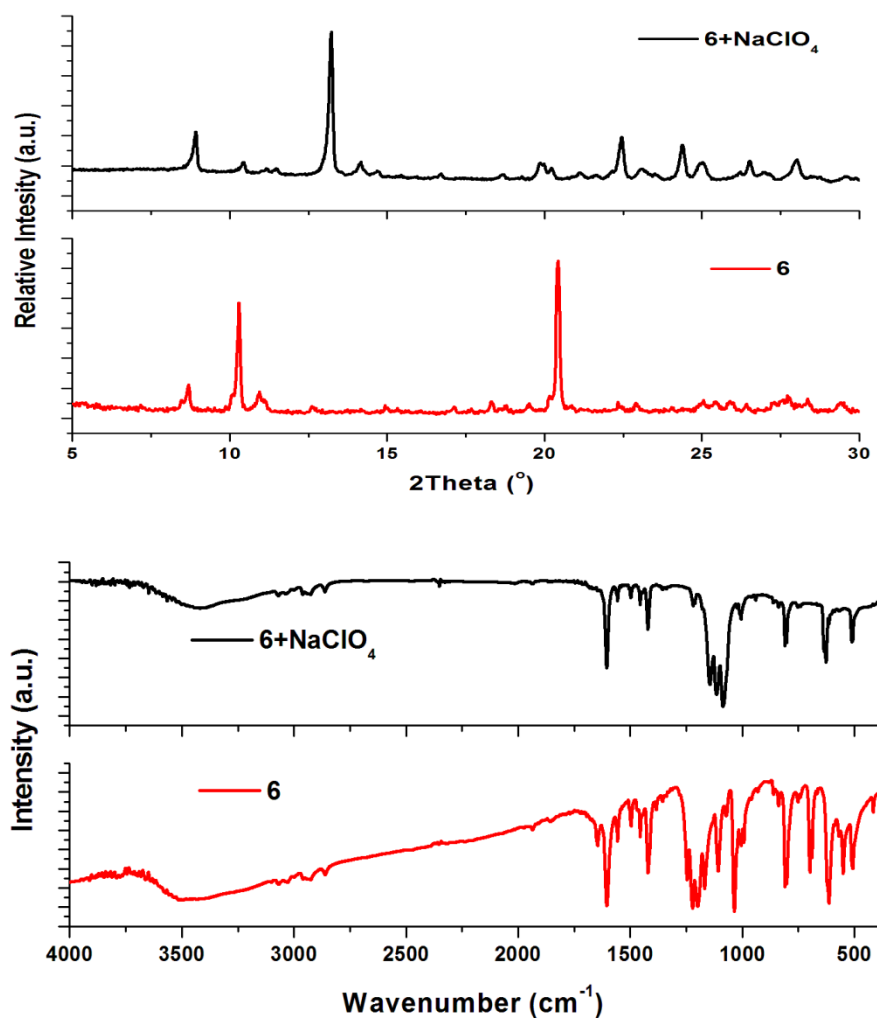


Figure S9 PXRD and FTIR of **1** and **3-6** for anion exchange with perchlorate. (a) Initial compound (red) (b) exchange products with ClO_4^- (black)

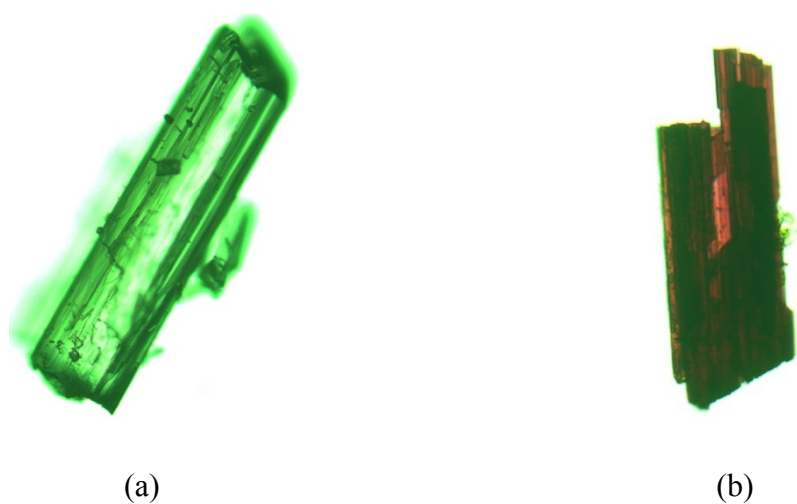


Figure S10 Color of crystal (a) **2** (b) after exchange with MnO_4^-