Electronic Supplementary Material (ESI) for Chemical Communications


# Supporting Information for

# Fluorene-based Cu(II)-MOF: A visual colorimetric anion sensor and separator based on anion-exchange approach

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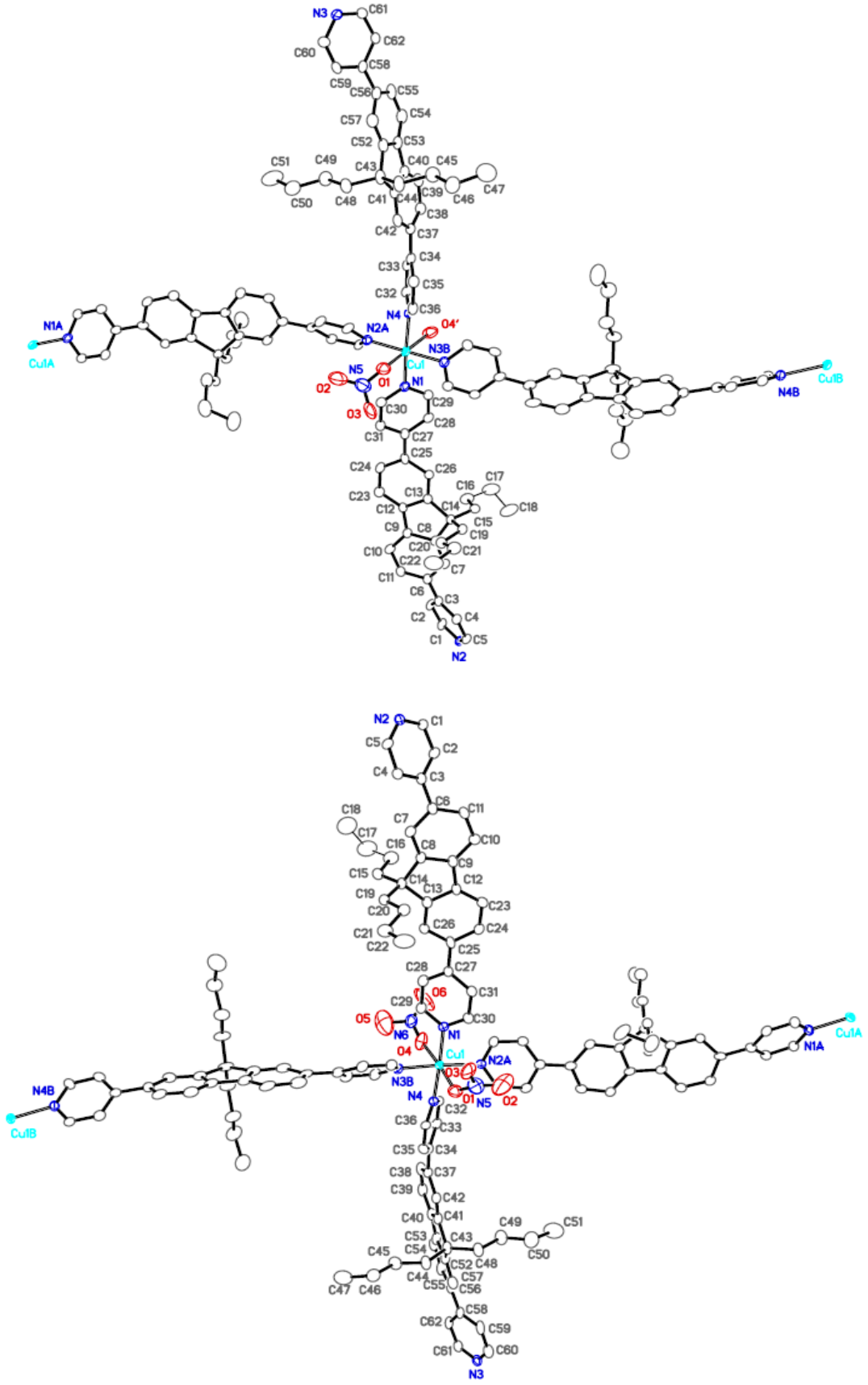



**Figure S1.** ORTEP figure of **1** (displacement ellipsoids drawn at the 50 % probability level, the H atoms, solvent, and uncoordinated nitrate not shown for clarity).

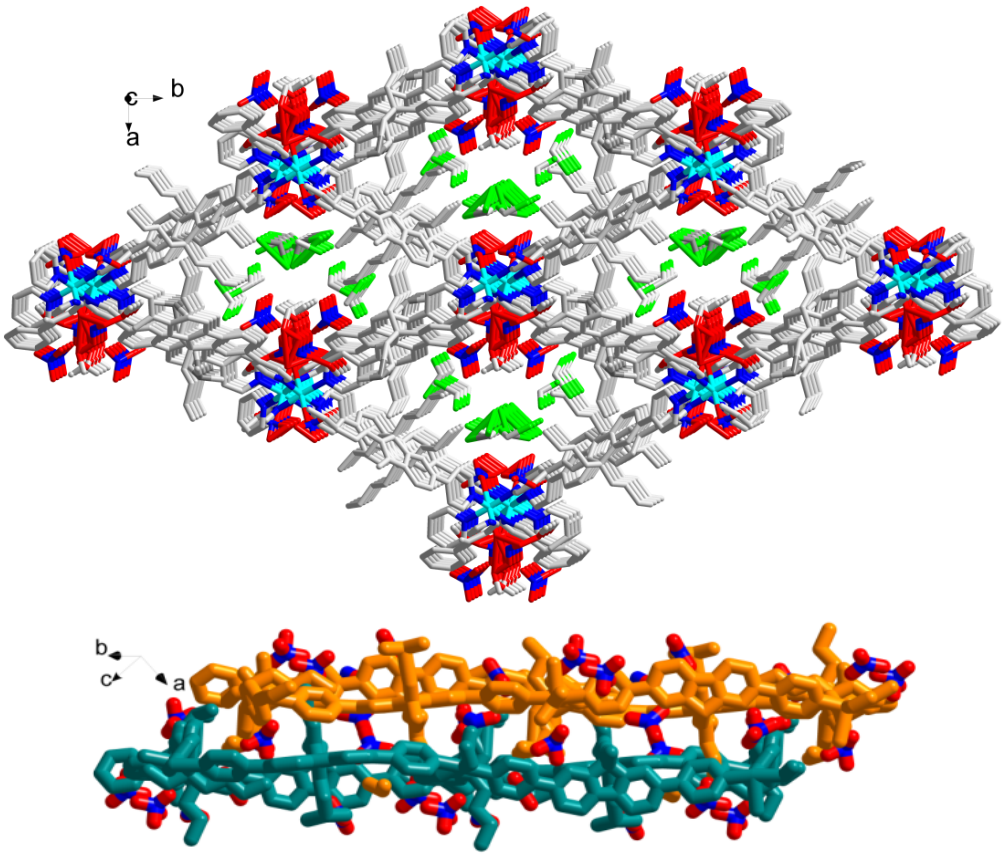



**Figure S2.** Top (up) and side (bottom) views of 2D networks stack in an –ABAB- fashion along the crystallographic *c* axis to generate rhombus-like 1D channels. The disordered solvent molecules (MeOH and $CH_2Cl_2$) and nitrate anions are located inside. The different layers in side view are shown in different colors.

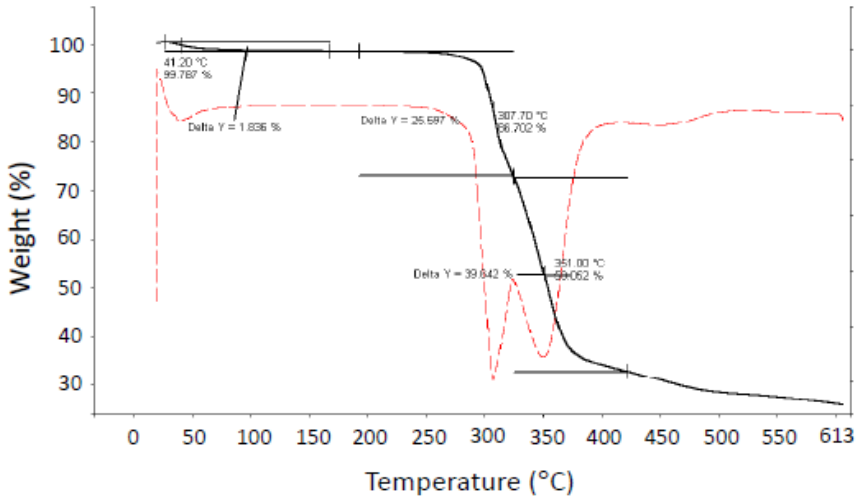



**Figure S3.** TGA trace of **1'**. The weight loss around 50°C is corresponding to the loss of coordinating water molecules. The observed mass loss is 1.84 % and the calculated mass loss is 1.68 %.

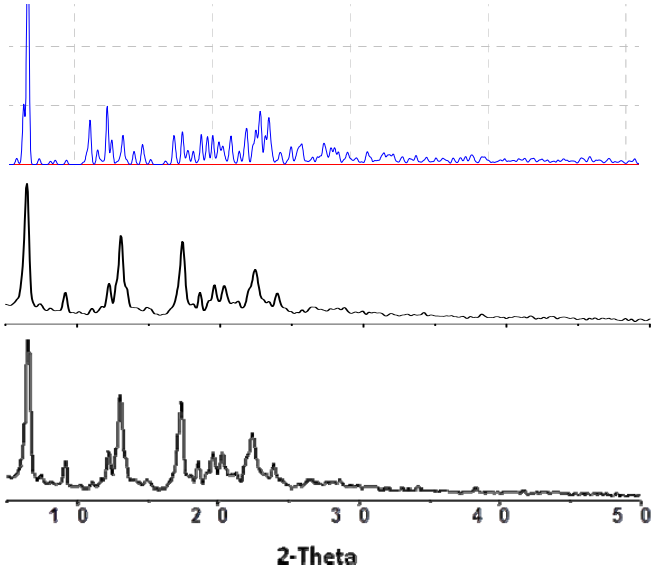



**Figure S4.** XRPD pattern of **1'** (middle) is identical to those of **1** (bottom) and simulated one (up), indicating the framework is stable after loss the uncoordinated solvent guests.

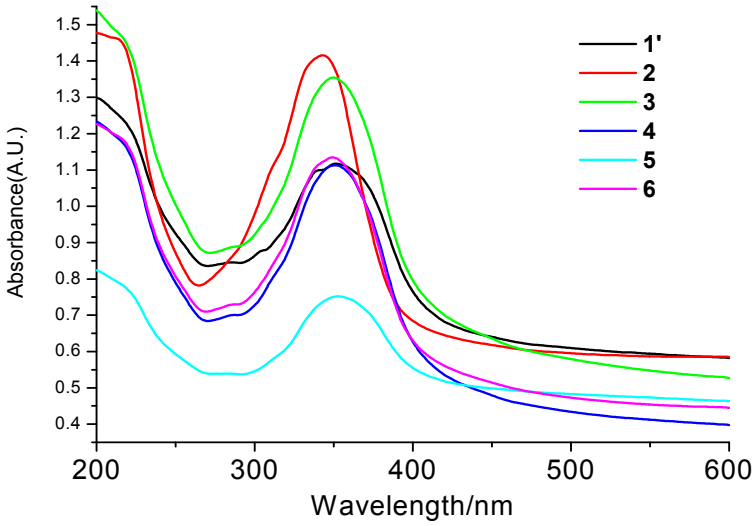



**Figure S5.** Solid-state UV-vis spectra of **1'-6**.

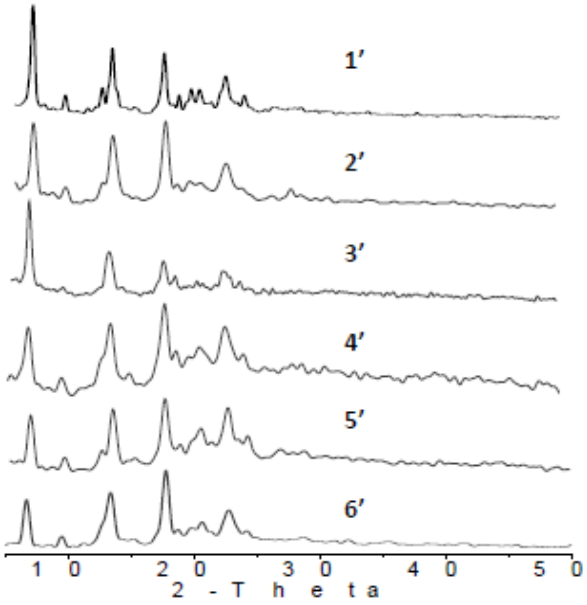



**Figure S6.** XRPD patterns of **1'-6'**.

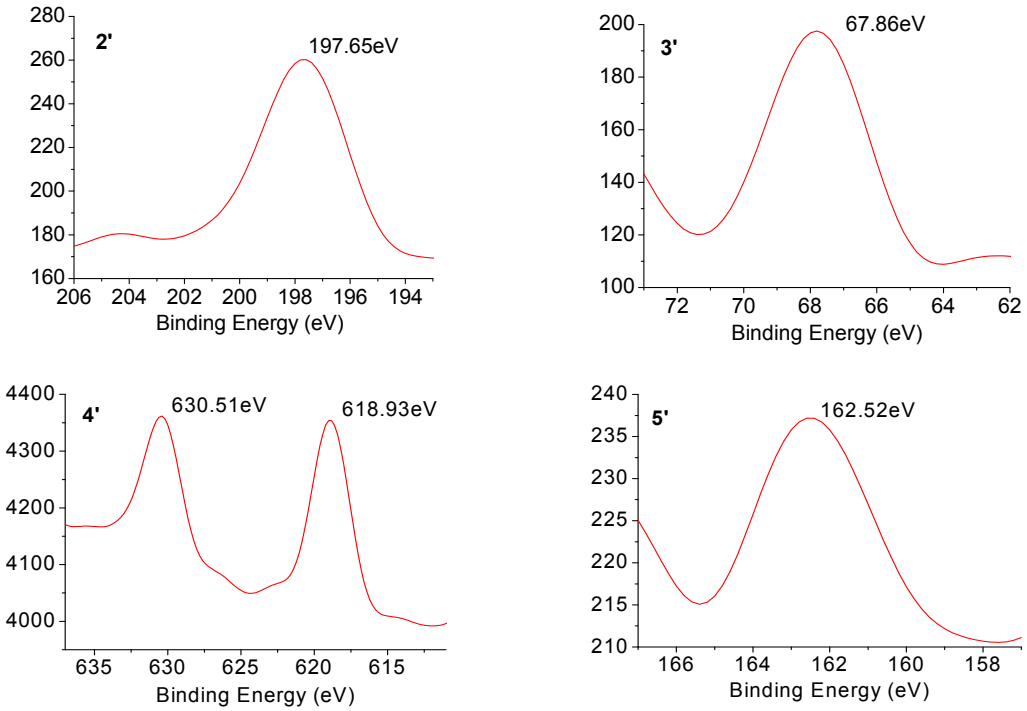



**Figure S7.** XPS spectra of **2'** (Cl 2p, 197.65 eV), **3'** (Br 3d, 67.86 eV), **4'** (I 3d, 618.93 eV), and **5'** (S 2p, 162.52 eV).

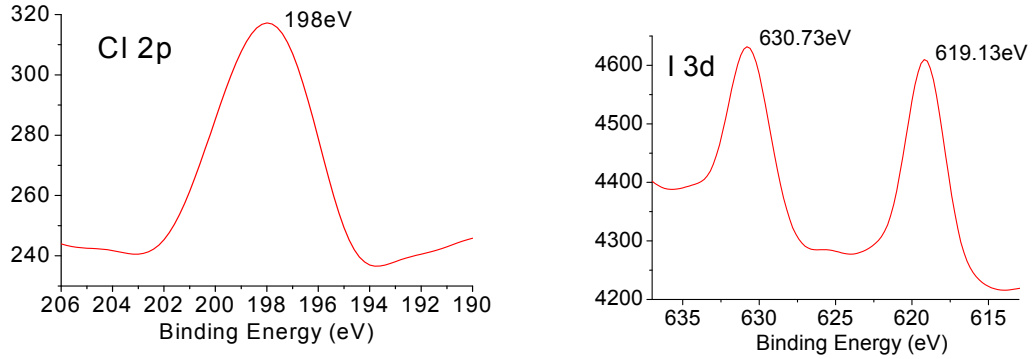
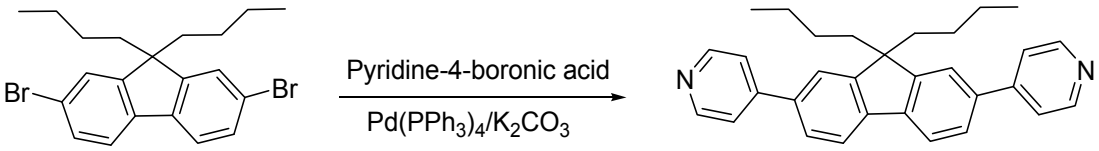



**Figure S8.** Left: XPS spectrum obtained from the sample which **1'** was immersed in an aqueous solution of equimolar NaCl and KBr (0.2mol/L). Right: XPS spectrum obtained from the sample which **1'** was immersed in an aqueous solution of equimolar NaBr and KI (0.2mol/L). No peak related to $Br^-$ was detected.

**Experimental Section.** Infrared (IR) samples were prepared as KBr pellets, and spectra were obtained in the 400-4000 $cm^{-1}$ range using a Perkin-Elmer 1600 FTIR spectrometer. Elemental analyses were performed on a Perkin-Elmer Model 2400 analyzer. Thermogravimetric analyses were carried out using a TA Instrument SDT 2960 simultaneous DTA-TGA under flowing nitrogen at a heating rate of 10°C/min. XPS spectra were obtained from THI5300 (PE) and $^1H$ NMR data were collected using an AM-300 spectrometer. Chemical shifts are reported in $\delta$ relative to TMS.

**Synthesis of L.**




**A** **L**

A solution of **A** (4.36 g，10 mmol), pyridine-4-boronic acid (3.05 g, 25 mmol), $K_2CO_3$ (17.2 g, 125 mmol) and $Pd(PPh_3)_4$ (1.2 g, 1 mmol) in toluene/EtOH/$H_2O$ was refluxed (monitored by TLC). The obtained sample was purified by column to generate light yellow crystalline

solids 3.9 g (Yield, 90 %). $^{1}$H NMR (300 MHz, DMSO, 25°C TMS): $\delta$ = 8.65 (d, 4H, -$C_5H_4N$), 8.00 (d, 2H,-$C_6H_3$), 7.95 (s, 2H,-$C_6H_3$), 7.79-7.84 (m, 2H, -$C_6H_3$; 4H, -$C_5H_4N$), 2.14 (t, 4H, -$CH_2CH_2CH_2CH_3$), 1.15-0.99 (m, 4H, -$CH_2CH_2CH_2CH_3$), 0.62-0.51 (m, 10H, -$CH_2CH_2CH_2CH_3$). IR (KBr pellet cm$^{-1}$ ): 3022(m), 2952(s), 1593(s), 1465(s), 1190(s), 120(s), 807(s), 722(s), 542(s). Elemental analysis (%) Calcd. for $C_{31}H_{32}N_2$: C 86.11, H 7.41, N 6.48; Found: C 85.56, H 7.32, N 6.15.

**Synthesis of 1.** A solution of $Cu(NO_3)_2$ (15 mg, 0.062 mmol) in $CH_3OH$ (7 mL) was layered onto a solution of **L** (10 mg, 0.023 mmol) in $CH_2Cl_2$ (6 mL). The solutions were left for about one week at room temperature, and bright blue block-like crystals (7.5 mg) were obtained. Yield, 54 %. IR (KBr pellet, cm$^{-1}$): 3441.22(m), 2953.49(m), 2927.40(m), 2856.65(m), 1612.36(s), 1544.48(w), 1509.25(w), 1465.69(m), 1384.35(s), 1304.96(m), 1222.47(m), 1069.07(w), 1024.28(w), 811.13(s), 718.65(m), 631.14(m), 491.02(w). Elemental analysis (%) Calcd. for $C_{62}H_{67}N_6O_{7.5}$ (desolvated sample): C 68.92, H 6.20, N 7.78. Found: C 67.16, H 5.83, N 7.31.

**Synthesis of 2-6**. The crystals of **1'** were immersed in an aqueous solution (0.20 mol/L, 20 mL) of NaCl, KBr, KI, KSCN and $NaN_3$ for two weeks, respectively. The ion-exchanged products of **2-6** were obtained.

**2** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{0.68}Cl_{1.32})\cdot H_2O$: IR (KBr pellet, cm$^{-1}$): 3439.26(m), 2953.45(m), 2927.35(s), 2857.08(m), 1610.41(s), 1543.59(w), 1507.96(w), 1465.14(s), 1411.32(m), 1383.88(m), 1287.09(w), 1261.37(w), 1221.35(w), 1138.50(w), 1068.85(m), 1022.44(m), 893.85(w), 845.44(w), 811.54(s), 718.25(s), 625.99(w), 567.94(w), 491.55(w). Elemental analysis (%) Calcd. For $C_{62}H_{67}N_{4.68}O_{3.54}Cl_{1.32}Cu$: C 71.23, H 6.41, N 6.22; Found: C 70.72, H

6.48, N 6.22.

**3** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{0.27}Br_{1.73})\cdot H_2O$: IR (KBr pellet, $cm^{-1}$): 3442.30(m), 2953.41(m), 2926.86(s), 2856.57(m), 1609.38(s), 1543.16(w), 1507.89(w), 1464.96 (s), 1411.46(m), 1384.10(m), 1260.82(w), 1221.64(m), 1068.56(m), 1022.28(w), 894.22(w), 811.32(s), 718.19(s), 626.19(w), 492.17 (w). Elemental analysis (%) Calcd. For $C_{62}H_{67}N_{4.27}O_{2.31}Br_{1.73}Cu$: C 67.03, H 6.04, N 5.38; Found: C 66.73, H 6.11, N 5.49.

**4** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.16}I_{0.84})\cdot H_2O$: IR (KBr pellet, $cm^{-1}$): 3446.16(m), 2952.43(m), 2926.05(s), 2855.81(m), 1604.40(s), 1541.70(w), 1464.35(s), 1410.64(m), 1384.12(m), 1259.54(w), 1220.97(m), 1067.41(m), 1021.12(w), 810.14(s), 717.26(s), 628.89(w). Elemental analysis (%) Calcd. For $C_{62}H_{67}N_{5.16}O_{4.98}I_{0.84}Cu$: C 65.60, H 5.91, N 6.37; Found: C 65.39, H 5.98, N 6.36.

**5** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.36}(SCN)_{0.64})\cdot 2H_2O$: IR (KBr pellet, $cm^{-1}$): 3442.31(m), 2953.80(m), 2927.84(s), 2856.98(m), 2072.92(m), 1612.40(s), 1544.25(m), 1509.09(w), 1465.81(s), 1384.29(m), 1305.99(m), 1222.69(s), 1139.03(w), 1111.43(w), 1069.37(m), 1024.58(m), 894.36(w), 847.73(w), 812.02(s), 744.83(w), 719.76(s), 667.90(w), 631.71(m), 593.29(w), 569.59(w), 543.83(w), 491.63(m), 430.49(w). Elemental analysis (%) Calcd. For $C_{62.64}H_{69}N_6O_{6.58}S_{0.64}Cu$: C 68.63, H 6.30, N 7.67, S 1.87; Found: C 68.51, H 6.94, N 8.02, S 1.97.

**6** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.37}(N_3)_{0.63})\cdot 2H_2O$: IR (KBr pellet, $cm^{-1}$): 3443.27(m), 2953.67(m), 2927.79(s), 2856.86(m), 2039.16(m), 1612.07(s), 1545.23(w), 1510.71(w), 1465.81(s), 1384.31(s), 1306.37(m), 1222.65(m), 1069.31(m), 1024.46(w), 811.70(s), 719.60(s), 631.58(w), 569.58(w), 491.15(w). Elemental analysis (%) Calcd. For $C_{62}H_{69}N_{7.26}O_{6.51}Cu$: C

68.57, H 6.36, N 9.36; Found: C 68.68, H 6.29, N 9.40.

**Synthesis of 2'-6'**. The crystals of **1'** were immersed in an aqueous solution ($10^{-3}$ mol/L, 20 mL) of NaCl, KBr, KI, KSCN and $NaN_3$ for two weeks, respectively. The ion-exchanged products of **2'-6'** were obtained.

**2'** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{0.77}Cl_{1.23})\cdot H_2O$: IR (KBr pellet, $cm^{-1}$): 3440.79(m), 2953.62(m), 2927.88(s), 2856.71(m), 1611.54(s), 1543.95(w), 1508.41(w), 1465.80(s), 1384.31(m), 1306.08(m), 1260.18(w), 1222.27(w), 1069.26(m), 1024.274(m), 894.25(w), 810.11(s), 755.70(w), 718.98(s), 631.54(w), 568.91(w), 490.29(w). Elemental analysis (%) Calcd. For $C_{62}H_{67}N_{4.77}O_{3.81}Cl_{1.23}Cu$: C 71.23, H 6.41, N 6.22; Found: C 70.72, H 6.48, N 6.22.

**3'** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{0.83}Br_{1.17})\cdot H_2O$: IR (KBr pellet, $cm^{-1}$): 3440.42(m), 2953.51(m), 2927.46(s), 2856.70(m), 1611.47(s), 1543.81(w), 1508.97(w), 1465.63(s), 1384.310(m), 1306.06(m), 1222.56(m), 1069.17(m), 1023.94(w), 894.01(w), 847.09(w), 811.66(s), 719.53(s), 631.37(w), 569.52(w), 491.71(w). Elemental analysis (%) Calcd. For $C_{62}H_{67}N_{4.83}O_{3.99}Br_{1.17}Cu$: C 67.22, H 6.05, N 6.11; Found: C 66.88, H 6.20, N 6.07.

**4'** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.79}I_{0.21})\cdot 2H_2O$: IR (KBr pellet, $cm^{-1}$): 3441.56(m), 2953.83(m), 2927.92(s), 2857.00(m), 1612.32(s), 1544.10(w), 1509.11(w), 1465.87(s), 1384.32(m), 1306.24(w), 1222.91(m), 1069.39(m), 1024.69(w), 894.26(w), 811.92(s), 719.816(s), 631.78(w), 569.74(w), 491.66(w). Elemental analysis (%) Calcd. For $C_{62}H_{69}N_{5.79}O_{7.87}I_{0.21}Cu$: C 66.96, H 6.20, N 7.29; Found: C 67.20, H 6.25, N 7.32.

**5'** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.61}(SCN)_{0.39})\cdot 2H_2O$: IR (KBr pellet, $cm^{-1}$): 3425.04(m), 2953.80(m), 2927.84(s), 2856.98(m), 2072.92(m), 1612.40(s), 1544.25(m), 1509.09(w), 1465.81(s), 1384.29(m), 1305.99(m), 1222.69(s), 1139.03(w), 1111.43(w), 1069.37(m), 1024.58(m),

894.36(w), 847.73(w), 812.02(s), 744.83(w), 719.76(s), 667.90(w), 631.71(m), 593.29(w), 569.59(w), 543.83(w), 491.63(m), 430.49(w). Elemental analysis(%) Calcd. For $C_{62.39}H_{69}N_6O_{7.33}S_{0.39}Cu$: C 68.31, H 6.30, N 7.66, S: 1.14; Found: C 68.72, H 7.13, N 7.65, S 1.52.

**6'** ($[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.63}(N_3)_{0.37})\cdot 2H_2O$: IR (KBr pellet, $cm^{-1}$): 3439.45(m), 2953.67(m), 2927.79(s), 2856.86(m), 2039.16(m), 1612.07(s), 1545.23(w), 1510.71(w), 1465.81(s), 1384.31(s), 1306.37(m), 1222.65(m), 1069.31(m), 1024.46(w), 811.70(s), 719.60(s), 631.58(w), 569.58(w), 491.15(w). Elemental analysis(%) Calcd. For $C_{62}H_{69}N_{6.74}O_{7.39}Cu$: C 68.25, H 6.33, N: 8.66; Found: C 68.51, H 6.35, N 8.69.

**Anion separation.**

**Separation of $Cl^-$ and $Br^-$ based on 1'**: The crystals of **1'** were immersed in an aqueous solution (20 mL) of equimolar NaCl (0.2 mol/L) and KBr (0.2 mol/L) for two weeks, the color of crystals changed from blue to green and generated $[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.09}Cl_{0.91}\cdot H_2O$. IR (KBr pellet, $cm^{-1}$): 3423.82(m), 2953.50(m), 2927.57(s), 2856.61(m), 1612.57(s), 1544.30(m), 1508.82(w), 1465.89(s), 1384.37(m), 1306.47(m), 1222.82(s), 1069.45(m), 1024.81(m), 812.00(s), 719.92(s), 631.85(m), 569.88(w), 491.73(m). Elemental analysis(%) Calcd. For $C_{62}H_{67}N_{5.09}O_{4.57}Cl_{0.91}Cu$: C 70.45, H 6.34, N 6.75; Found: C 68.93, H 6.08, N: 6.63.

**Separation of $I^-$ and $Br^-$ based on 1'**: The crystals of **1'** were immersed in an aqueous solution (20 mL) of KI (0.2 mol/L) and KBr (0.2 mol/L) for two weeks, the color of crystals changed from blue to deep brown and generated $[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)_{1.34}I_{0.66}\cdot H_2O$. IR (KBr pellet, $cm^{-1}$): 3421.79(m), 2953.76(m), 2927.82(s), 2856.79(m), 1612.47(s), 1544.37(m),

1508.78(w), 1465.93(s), 1384.41(m), 1305.36(m), 1222.80(s), 1069.44(m), 1024.80(m), 894.37(w), 847.98(w), 811.88(s), 719.90(s), 631.83(m), 569.82(w), 491.59(m). Elemental analysis(%) Calcd. For $C_{62}H_{67}N_{5.34}O_{5.52}I_{0.66}Cu$: C 66.29, H 5.96, N 6.66; Found: C 65.93, H 6.08, N 6.63.

**Separation of $SCN^-$ and $N_3^-$ based on 1'**: The crystals of **1'** were immersed in an aqueous solution (20 mL) of KSCN (0.2 mol/L) and $NaN_3$ (0.3 mol/L) for two weeks, the color of crystals changed from blue to blackish green and generated $[Cu(\mathbf{L})_2(H_2O)_{0.5}](NO_3)(SCN)\cdot H_2O$. IR (KBr pellet, $cm^{-1}$): 3418.92(m), 2954.12(m), 2927.89(s), 2857.16(m), 2071.45(m), 1611.21(s), 1544.17(m), 1508.38(w), 1465.46(s), 1384.57(m), 1304.76(m), 1221.66(s), 1138.68(w), 1069.15(m), 1023.76(m), 894.77(w), 846.60(w), 811.44(s), 744.91(w), 719.19(s), 630.90(m), 569.31(w), 491.33(m). Elemental analysis (%) Calcd. For$C_{63}H_{67}N_6O_{4.5}Cu$: C 70.29, H 6.23, N 7.81, S 2.98, Found: C 70.42, H 7.16, N 7.84, S 3.01.

**Single-Crystal Structure Determination.** Suitable single crystal of **1** was selected and mounted in air onto thin glass fibers. X-ray intensity data of **1** were measured at 123(2) K on a Bruker SMART APEX CCD-based diffractometer (Mo K$\alpha$ radiation, $\lambda$ = 0.71073 Å). The raw frame data for **1** was integrated into SHELX-format reflection files and corrected for Lorentz and polarization effects using SAINT.[1] Corrections for incident and diffracted beam absorption effects were applied using SADABS.[1] The crystal showed no evidence of crystal decay during data collection. The structure was solved by a combination of direct methods and difference Fourier syntheses and refined against $F^2$ by the full-matrix least squares technique. Systematic absences in the intensity data were consistent with the

space group P2(1)/c. The structure was solved by a combination of direct methods and difference Fourier syntheses, and refined by full-matrix least-squares against $F^2$, using the SHELXTL software package.[1] Upon successfully solved and refined the structure in *P2(1)/c*, a check for missed symmetry was performed with ADDSYM / PLATON,[3] which verified the space group choice. The asymmetric unit contains a Cu(II) atom, two coordinated **L** ligands, a coordinated disordered nitrate, half a coordinated nitrate, half a coordinated water molecule (the coordinated nitrate and $H_2O$ are disordered over two closely separated positions in a 1:1 ratio), half an uncoordinated nitrate, half uncoordinated water molecule (the uncoordinated nitrate and $H_2O$ are also disordered over two closely separated positions in a 1:1 ratio), half a methanol and 3.25 $CH_2Cl_2$ molecules. In an attempt to remove split position / disorder problems, the structure was also solved and refined in the lower symmetry space group *P-1*, the nitrate and water species were also disordered. Therefore the split position / disorder model in *P2(1)/c* was retained. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model. A restrained model involving ½ a nitrate disordered together with a water molecule (distributed over two independent half-occupied sites) was employed, and the other nitrate coordinated to Cu was refined as disordered over two orientations. The two part of the methanol molecules were also refined as disordered over two orientations, the C-Cl bonds of $CH_2Cl_2$ molecules were refined in 1.664 ~1.783 Å distance restraint and the C-O bonds of methanol molecules were refined in 1.436 ~1.448 Å distance restraint, the N-O bonds of uncoordinated nitrate ion were refined in 1.229 ~1.254 Å distance restraint.

The atoms N5', O13', O4', C17 and C64 was constrained to have the same ADPs as the atoms N5, O13, O4, C17' and C64'. The ADPs of C65, C66, C67, C69, O10, O4, O4', O9, O10, O12 and O13 were restrained to be isotropic within a standard deviation of 0.007 $Å^2$. In total 76 restraints were used in modeling the disorder. Crystal data, data collection parameters, and refinement statistics for **1** are listed in Tables S1. Relevant interatomic bond distances and bond angles for **1** are given in Tables S2. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no CCDC 852758. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44)1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

**Table S1**. Crystal data and structure refinement for **1**.

| | |
|---|---|
| Identification code | **1** |
| Empirical formula | $C_{66.25}\ H_{76.50}\ Cl_{6.50}\ Cu\ N_6\ O_8$ |
| Formula weight | 1378.80 |
| Temperature | 123(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, P2(1)/c |
| Unit cell dimensions | a = 15.679(4) Å alpha = 90 deg. |
| | b = 27.788(7) Å beta = 105.515(4) deg. |
| | c = 17.240(5) Å gamma = 90 deg. |
| Volume | 7237(3) $Å^3$ |
| Z, Calculated density | 4, 1.265 Mg/m^3 |
| Absorption coefficient | 0.596 $mm^{-1}$ |
| F(000) | 2878 |
| Crystal size | 0.42 x 0.31 x 0.12 mm |
| Theta range for data collection | 1.43 to 25.50 deg. |
| Limiting indices | -18<=h<=18, -33<=k<=30, -16<=l<=20 |
| Reflections collected / unique | 35528 / 13325 [R(int) = 0.0799] |

| | |
|---|---|
| Completeness to theta = 25.50 | 99.0 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9321 and 0.7883 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 13325 / 76 / 925 |
| Goodness-of-fit on F^2 | 1.026 |
| Final R indices [I>2sigma(I)] | R1 = 0.0995, wR2 = 0.2849 |
| R indices (all data) | R1 = 0.1350, wR2 = 0.3091 |
| Largest diff. peak and hole | 1.104 and -1.008 e.Å $^{-3}$ |

**Table S2.** Interatomic Distances (Å) and Bond Angles (°) with esds () for **1**.

| | | | |
|---|---|---|---|
| Cu(1)-N(3)#1 | 2.009(4) | Cu(1)-N(1) | 2.018(4) |
| Cu(1)-N(2)#2 | 2.023(4) | Cu(1)-N(4) | 2.035(4) |
| Cu(1)-O(1) | 2.391(5) | Cu(1)-O(4) | 2.52(2) |
| N(2)-Cu(1)#3 | 2.023(4) | N(3)-Cu(1)#4 | 2.009(4) |
| N(3)#1-Cu(1)-N(1) | 90.34(17) | N(3)#1-Cu(1)-N(2)#2 | 176.43(19) |
| N(1)-Cu(1)-N(2)#2 | 91.85(17) | N(3)#1-Cu(1)-N(4) | 89.68(17) |
| N(1)-Cu(1)-N(4) | 174.25(19) | N(2)#2-Cu(1)-N(4) | 88.44(17) |
| N(3)#1-Cu(1)-O(1) | 85.43(18) | N(1)-Cu(1)-O(1) | 96.38(18) |
| N(2)#2-Cu(1)-O(1) | 91.52(17) | N(4)-Cu(1)-O(1) | 89.36(17) |
| N(3)#1-Cu(1)-O(4) | 95.3(5) | N(1)-Cu(1)-O(4) | 83.5(5) |
| N(2)#2-Cu(1)-O(4) | 87.7(5) | N(4)-Cu(1)-O(4) | 90.8(5) |
| O(1)-Cu(1)-O(4) | 179.2(5) | C(29)-N(1)-Cu(1) | 120.0(4) |
| C(30)-N(1)-Cu(1) | 123.0(4) | C(1)-N(2)-Cu(1)#3 | 117.6(4) |
| C(5)-N(2)-Cu(1)#3 | 124.6(4) | C(61)-N(3)-Cu(1)#4 | 122.4(4) |
| C(60)-N(3)-Cu(1)#4 | 119.9(4) | C(36)-N(4)-Cu(1) | 124.1(4) |
| C(32)-N(4)-Cu(1) | 117.6(3) | | |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+1/2 #2 -x,y+1/2,-z+3/2 #3 -x,y-1/2,-z+3/2 #4 -x+1,y+1/2,-z+1/2

Reference

(1) Sheldrick, G. M. SHELXTL Version 5.12; Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, 1997.

(2) Sheldrick, G. M. SHELXTL Version 5.12; Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, 1997.

(3) Spek, A. L. PLATON, A Multipurpose Crystallographic Tool. University of Utrecht, Utrecht, The Netherlands, 1998.