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 CH₂Cl₂) 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 δ relative to TMS.

Synthesis of L.

A solution of A (4.36 g, 10 mmol), pyridine-4-boronic acid (3.05 g, 25 mmol), K₂CO₃ (17.2 g, 125 mmol) and Pd(PPh₃)₄ (1.2 g, 1 mmol) in toluene/EtOH/H₂O was refluxed (monitored by TLC). The obtained sample was purified by column to generate light yellow crystalline
solids 3.9 g (Yield, 90 %). ¹H NMR (300 MHz, DMSO, 25°C TMS): δ = 8.65 (d, 4H, -C₅H₄N), 8.00 (d, 2H, -C₆H₃), 7.95 (s, 2H, -C₆H₃), 7.79-7.84 (m, 2H, -C₆H₃; 4H, -C₅H₄N), 2.14 (t, 4H, -CH₂CH₂CH₂CH₃), 1.15-0.99 (m, 4H, -CH₂CH₂CH₂CH₃), 0.62-0.51 (m, 10H, -CH₂CH₂CH₂CH₃).

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 C₃₁H₃₂N₂: 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(NO₃)₂ (15 mg, 0.062 mmol) in CH₃OH (7 mL) was layered onto a solution of L (10 mg, 0.023 mmol) in CH₂Cl₂ (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).


**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 NaN₃ for two weeks, respectively. The ion-exchanged products of 2-6 were obtained.

2 ([Cu(L)₂(H₂O)₀.₅][NO₃]₀.₆₅Cl₁.₃₂)·H₂O: 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 C₆₂H₆₇N₄.₆₈O₃.₅₄Cl₁.₃₂Cu: C 71.23, H 6.41, N 6.22; Found: C 70.72, H
6.48, N 6.22.

3 \( \text{[Cu} (\text{L})_{2} (\text{H}_{2}\text{O})_{0.5}] (\text{NO}_{3})_{0.27}\text{Br}_{1.73} \) \( \cdot \) \text{H}_{2}\text{O} \text{: IR (KBr pellet, cm}^{-1} \text{): 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 \( \text{C}_{62}\text{H}_{67}\text{N}_{4.27}\text{O}_{2.31}\text{Br}_{1.73}\text{Cu} \): C 67.03, H 6.04, N 5.38; Found: C 66.73, H 6.11, N 5.49.

4 \( \text{[Cu} (\text{L})_{2} (\text{H}_{2}\text{O})_{0.5}] (\text{NO}_{3})_{1.16}\text{I}_{0.84} \) \( \cdot \) \text{H}_{2}\text{O} \text{: IR (KBr pellet, cm}^{-1} \text{): 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 \( \text{C}_{62}\text{H}_{67}\text{N}_{5.16}\text{O}_{4.98}\text{I}_{0.84}\text{Cu} \): C 65.60, H 5.91, N 6.37; Found: C 65.39, H 5.98, N 6.36.

5 \( \text{[Cu} (\text{L})_{2} (\text{H}_{2}\text{O})_{0.5}] (\text{NO}_{3})_{1.36}\text{(SCN)}_{0.64} \) \( \cdot \) \text{H}_{2}\text{O} \text{: IR (KBr pellet, cm}^{-1} \text{): 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 \( \text{C}_{62.64}\text{H}_{69}\text{N}_{6}\text{O}_{6.58}\text{S}_{0.64}\text{Cu} \): 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 \( \text{[Cu} (\text{L})_{2} (\text{H}_{2}\text{O})_{0.5}] (\text{NO}_{3})_{1.37}\text{(N}_{3}\text{)}_{0.63} \) \( \cdot \) \text{H}_{2}\text{O} \text{: IR (KBr pellet, cm}^{-1} \text{): 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 \( \text{C}_{62}\text{H}_{69}\text{N}_{7.26}\text{O}_{6.51}\text{Cu} \): C

**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 NaN₃ for two weeks, respectively. The ion-exchanged products of 2'-6' were obtained.

2' ([Cu(L)₂]₂[N₃]₀.₇₇Cl₁.₂₃)·H₂O: 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), 1024.27(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 C₆₂H₆₇N₄.77O₃.81Cl₁.₂₃Cu: C 71.23, H 6.41, N 6.22; Found: C 70.72, H 6.48, N 6.22.

3' ([Cu(L)₂]₂[H₂O]₀.₅][NO₃]₀.₈₃Br₁.₁₇)·H₂O: 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), 1384.30(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 C₆₂H₆₇N₄.8₃O₃.₉₉Br₁.₁₇Cu: C 67.22, H 6.05, N 6.11; Found: C 66.88, H 6.20, N 6.07.

4' ([Cu(L)₂][H₂O]₀.₅][NO₃]₁.₇₉[SCN]₀.₃₉)·H₂O: 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 C₆₂H₆₉N₅.₇₉O₇.₈₇[SCN]₀.₃₉Cu: C 66.96, H 6.20, N 7.29; Found: C 67.20, H 6.25, N 7.32.

5' ([Cu(L)₂]₀.₅)[NO₃]₁.₆₁(SCN)₀.₃₉)·H₂O: 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), 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_{6.33}O_{7.39}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(L)_2(H_2O)_{0.5}](NO_3)_{1.63}(N_3)_{0.37})·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_{67}N_{5.69}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(L)_2(H_2O)_{0.5}](NO_3)_{1.09}Cl_{0.91}·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_{69}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(L)_2(H_2O)_{0.5}](NO_3)_{1.34}I_{0.66}·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 N₃⁻ based on 1’: The crystals of 1’ were immersed in an aqueous
solution (20 mL) of KSCN (0.2 mol/L) and NaN₃ (0.3 mol/L) for two weeks, the color of
crystals changed from blue to blackish green and generated [Cu(L)_{2}(H₂O)_{0.5}](NO₃)(SCN)·H₂O. 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. ForC_{63}H_{67}N_{6}O_{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 Kα radiation, λ = 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 F² 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\(_2\)O 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\(_2\)O are also disordered over two closely separated
positions in a 1:1 ratio), half a methanol and 3.25 CH\(_2\)Cl\(_2\) 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 \(\frac{1}{2}\) 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\(_2\)Cl\(_2\) 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.**

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<th>Identification code</th>
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<tr>
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<td>123(2) K</td>
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<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Monoclinic, P2(1)/c</td>
</tr>
</tbody>
</table>
| 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) Å³ |
| Z, Calculated density | 4, 1.265 Mg/m³ |
| 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 F²
Data / restraints / parameters   13325 / 76 / 925
Goodness-of-fit on F²    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.

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<th>Bond</th>
<th>Distances (Å)</th>
<th>Bond</th>
<th>Distances (Å)</th>
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<tr>
<td>C(32)-N(4)-Cu(1)</td>
<td>117.6(3)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

