**Supporting information**

# Broadband Blue Light Emissions of One-Dimensional Hybrid Cu(I) Halides with Ultrahigh Anti-Water Stability

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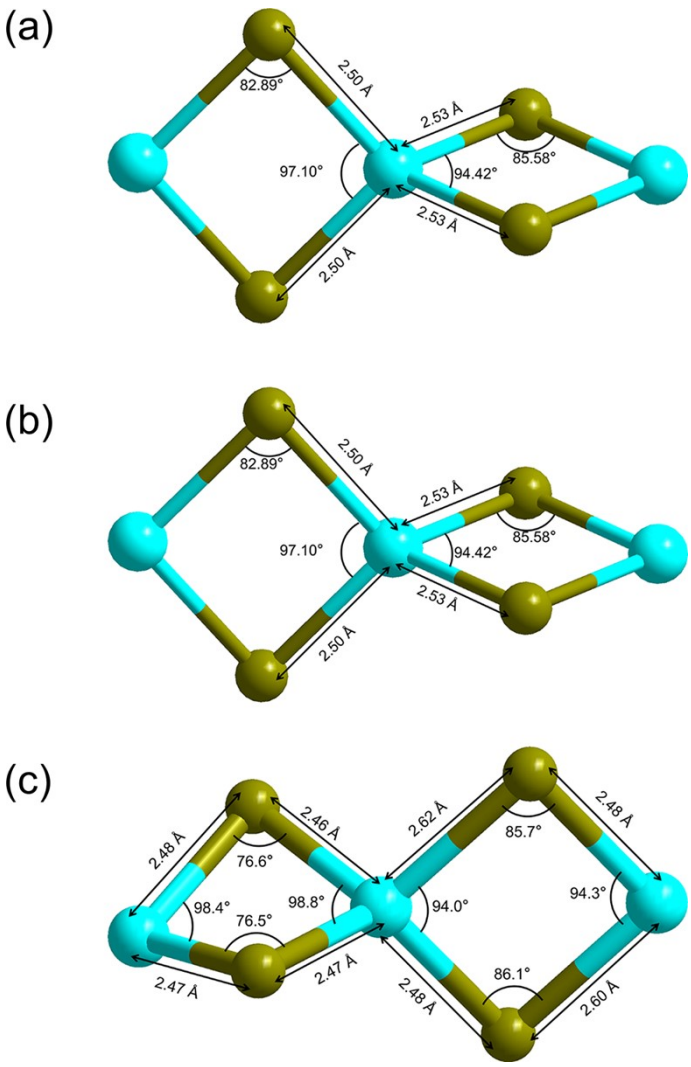


**Fig. S1** The configurations of 1D $[Cu_2Br_4]^{2-}$ chain of (a) $[(Me)_4\text{-Pipz}]Cu_2Br_4$, (b) $[BuDA]Cu_2Br_4$ and (c) $[TMEDA]Cu_2Br_4$.

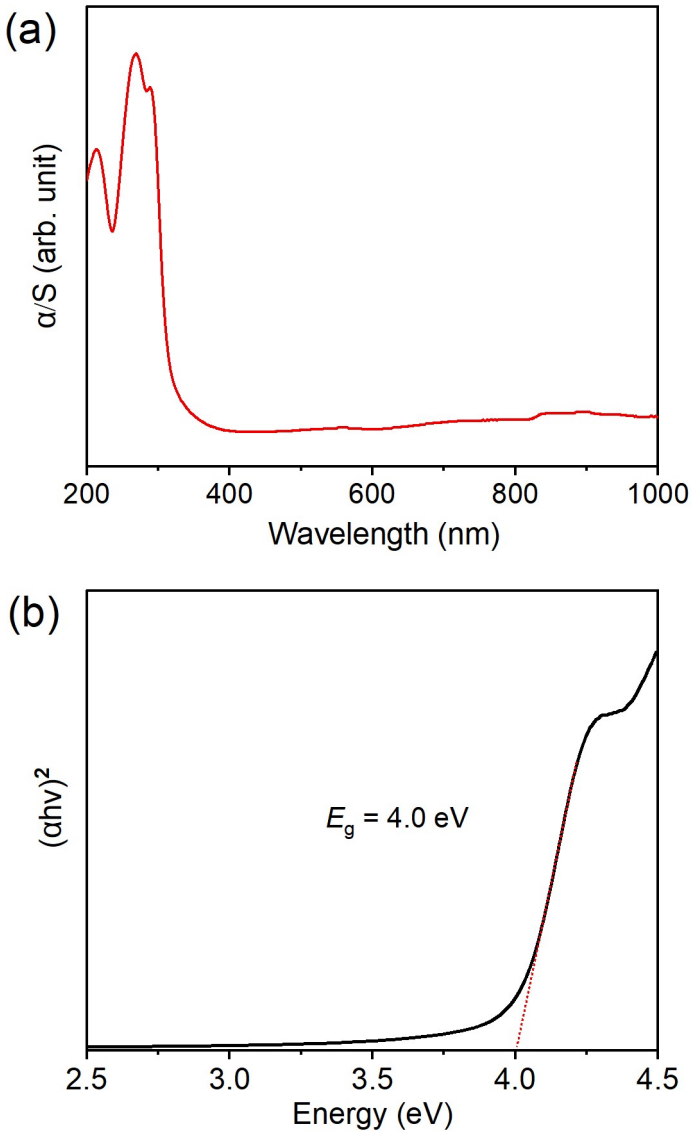


**Fig. S2** The solid state UV-vis adsorption spectrum (a) and Tauc plot for band gap (b) of [$(Me)_4$-Pipz]$Cu_2Br_4$.

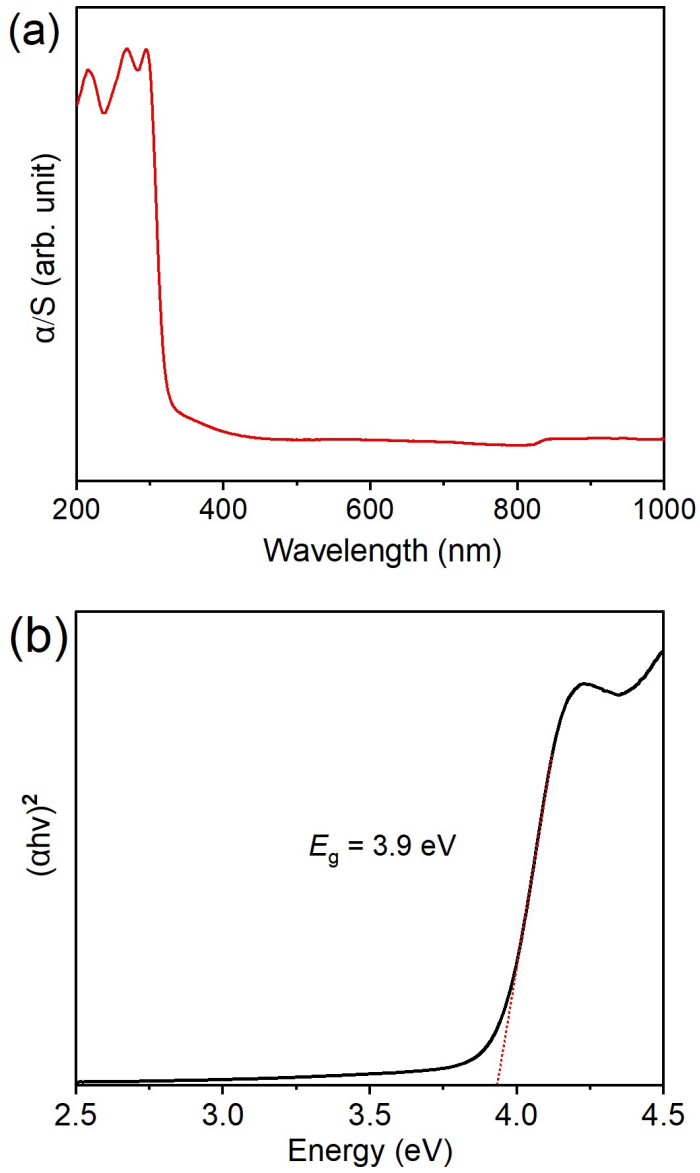


**Fig. S3** The solid state UV-vis adsorption spectrum (a) and Tauc's plot for band gap (b) of [BuDA]$Cu_2Br_4$.

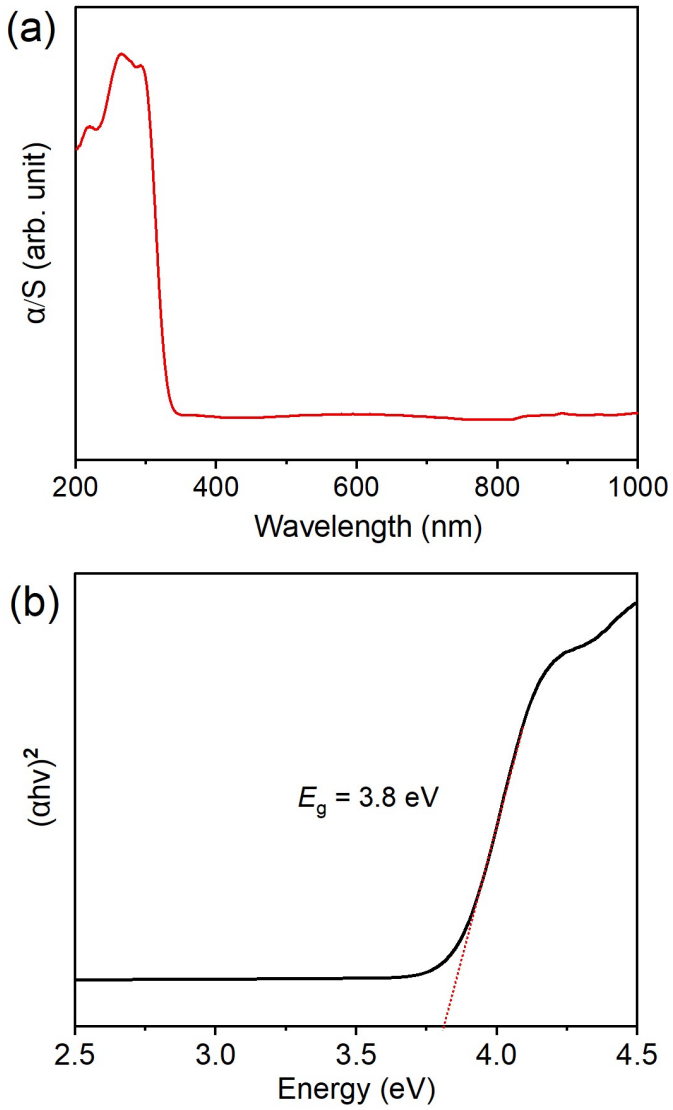


**Fig. S4** The solid state UV-vis adsorption spectrum (a) and Tauc plot for band gap (b) of [TMEDA]$Cu_2Br_4$.

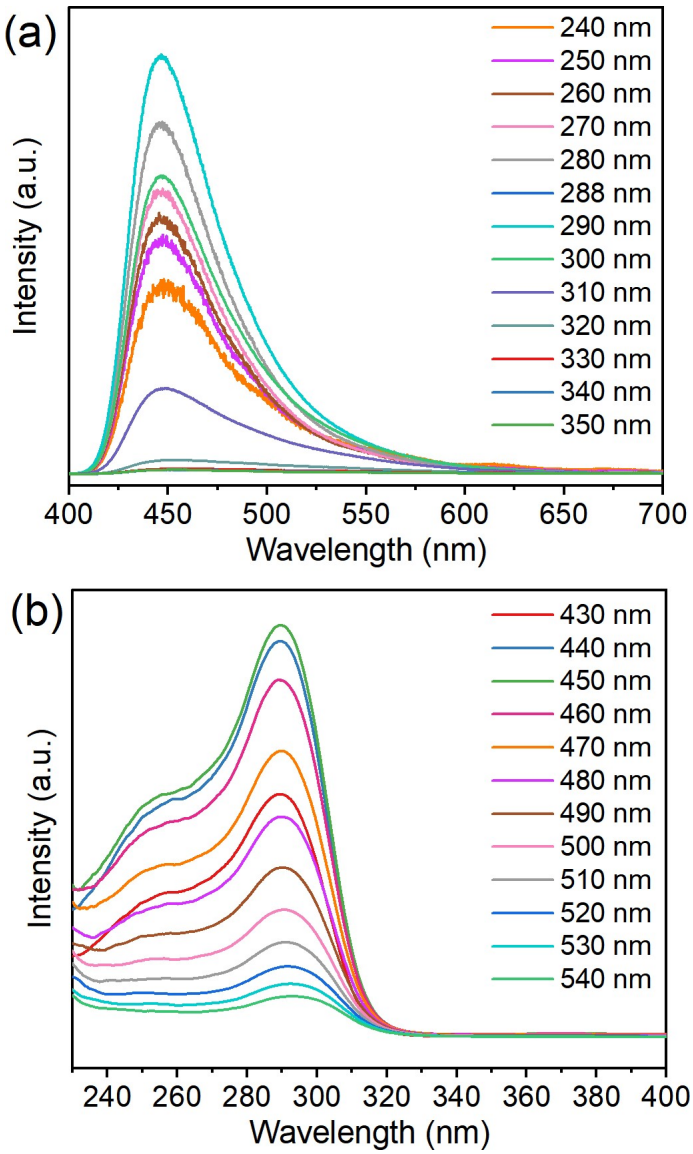


**Fig. S5** (a) The excitation wavelength dependent PL emission spectra, and (b) the emission wavelength dependent PL excitation spectra of $[(Me)_4\text{-Pipz}]Cu_2Br_4$.

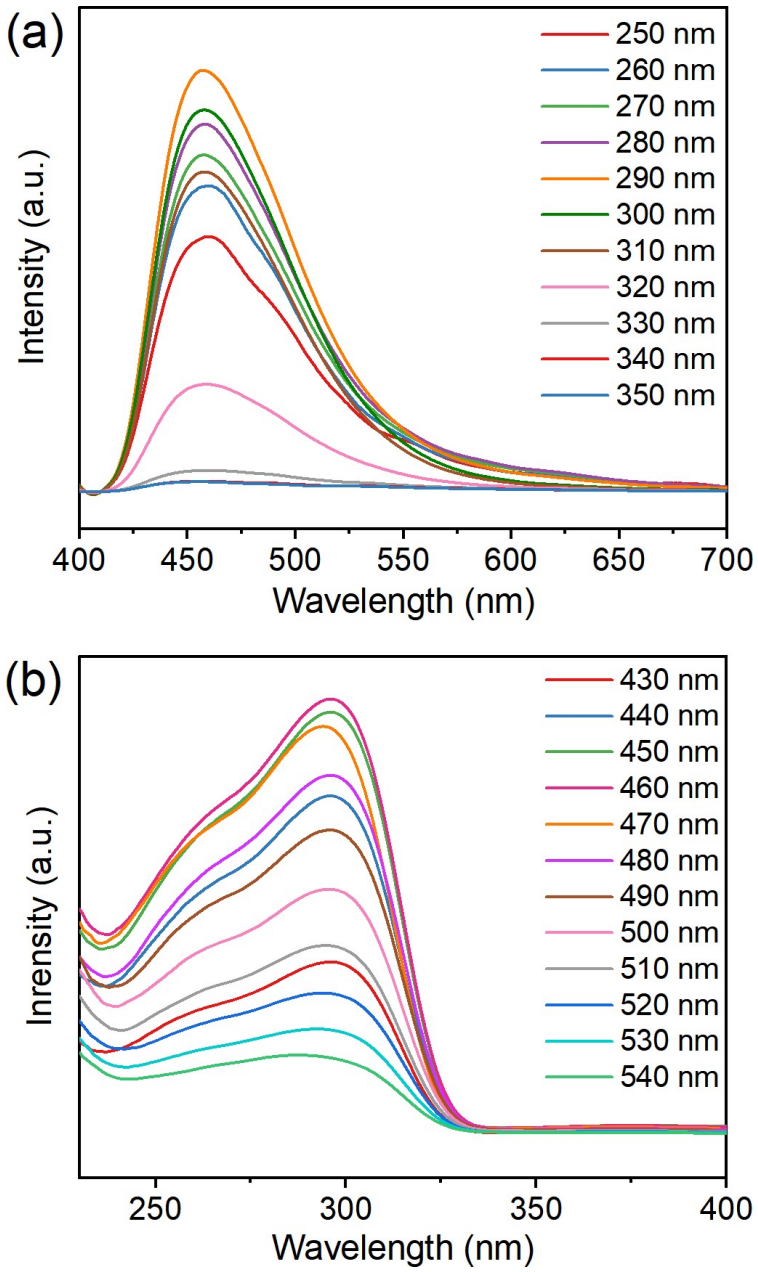


**Fig. S6** (a) The excitation wavelength dependent PL spectra and (b) the emission wavelength dependent PL excitation spectra of [BuDA]$Cu_2Br_4$.

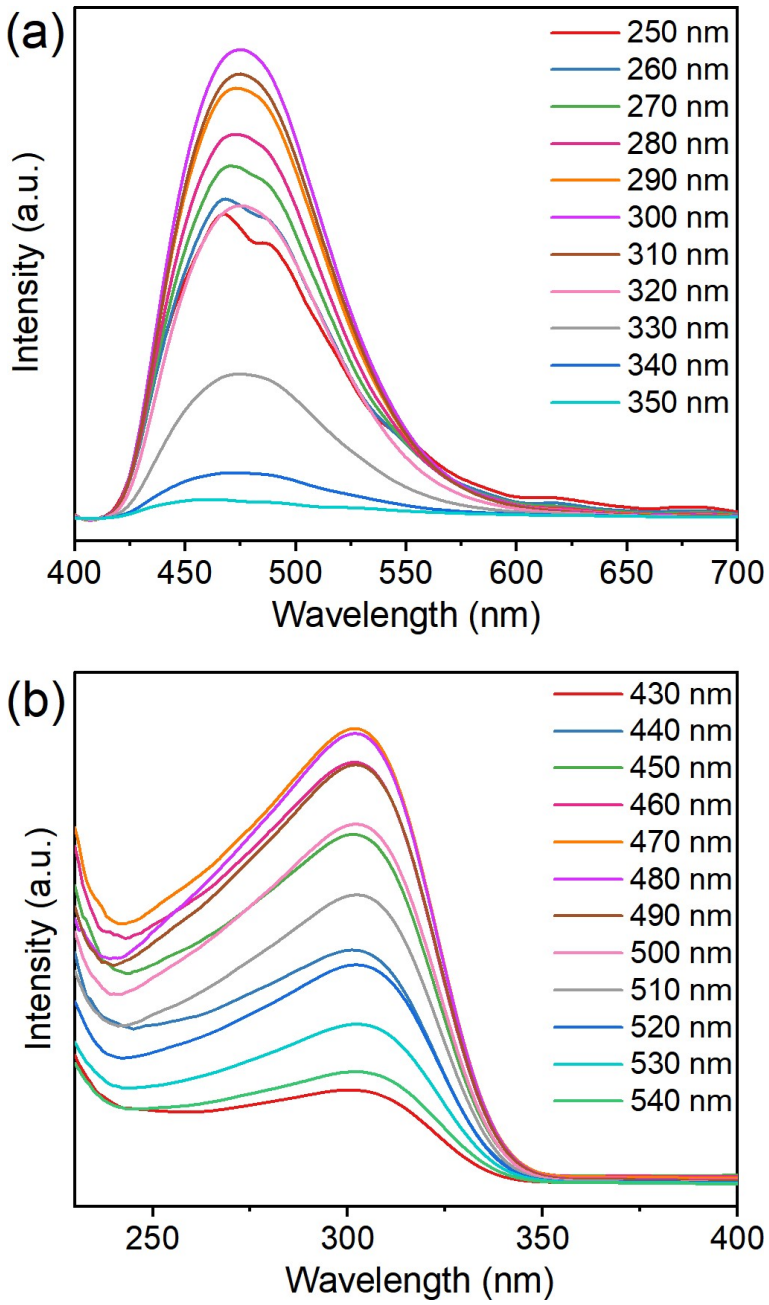


**Fig. S7** (a) The excitation wavelength dependent PL spectra and (b) the emission wavelength dependent PL excitation spectra of [TMEDA]$Cu_2Br_4$.

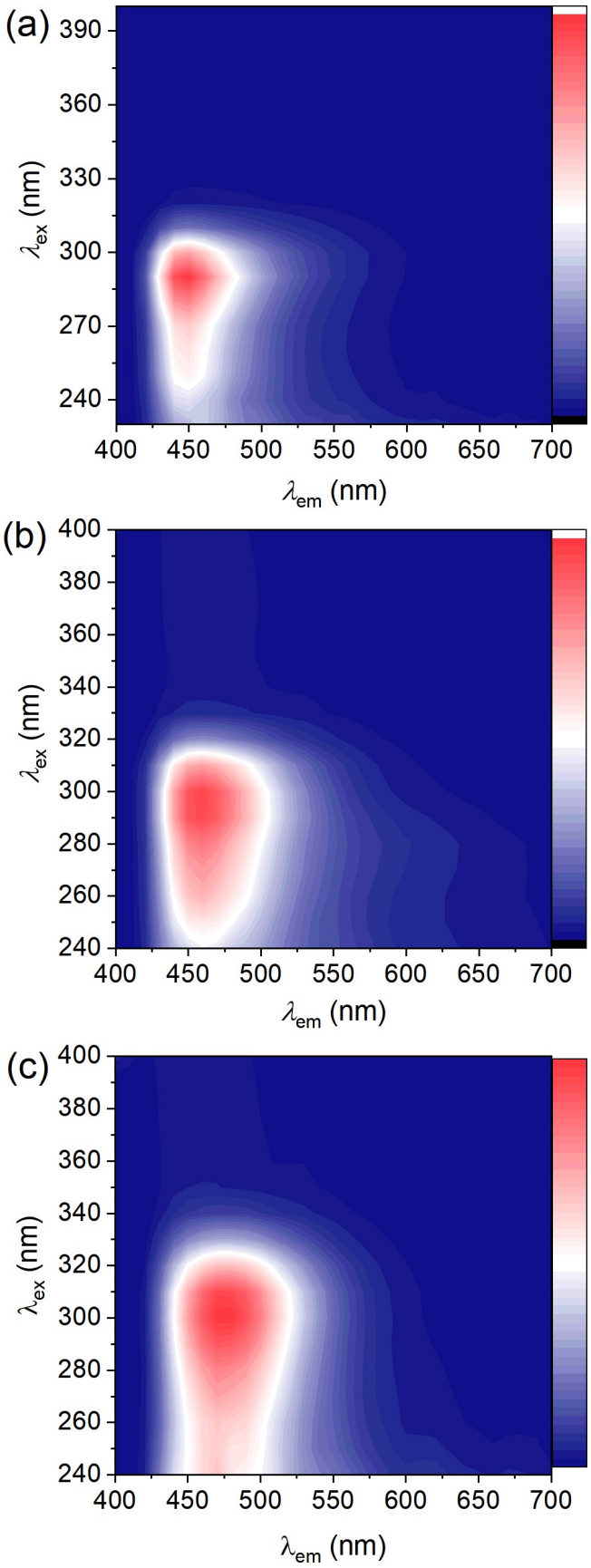


**Fig. S8** 3D consecutive PL excitation and emission correlation maps of (a) $[(Me)_4\text{-Pipz}]Cu_2Br_4$; (b) $[BuDA]Cu_2Br_4$ and (c) $[TMEDA]Cu_2Br_4$.

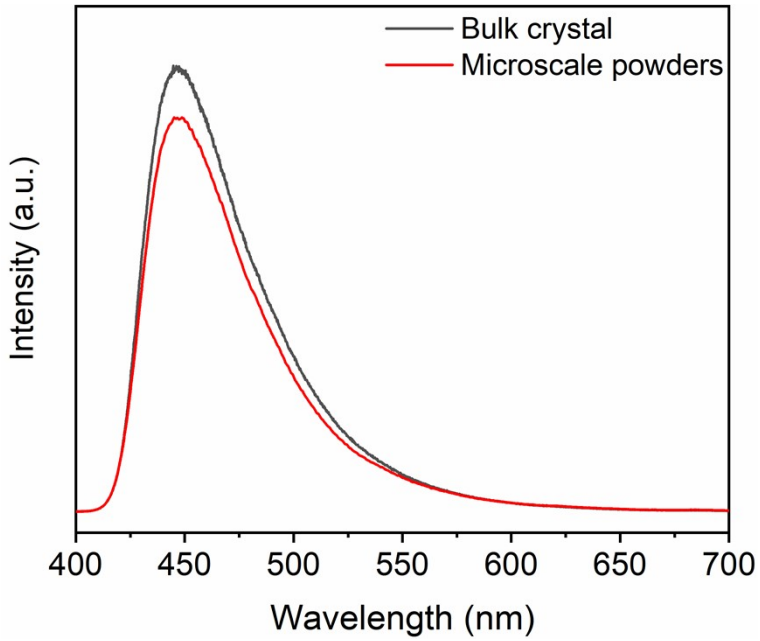


**Fig. S9** Comparison of PL emission spectra of bulk crystals and microscale powders for $[(Me)_4$-Pipz$]Cu_2Br_4$.

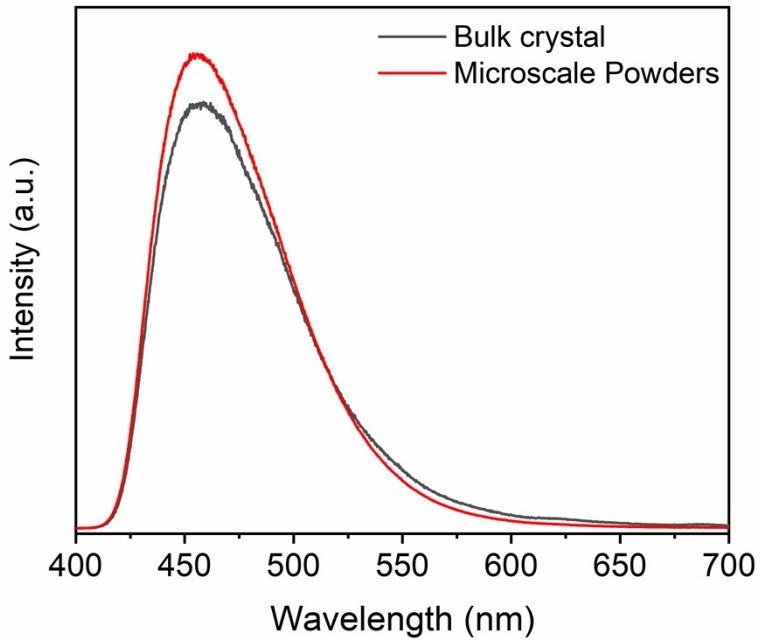


**Fig. S10** Comparison of PL emission spectra of bulk crystals and microscale powders for $[BuDA]Cu_2Br_4$.

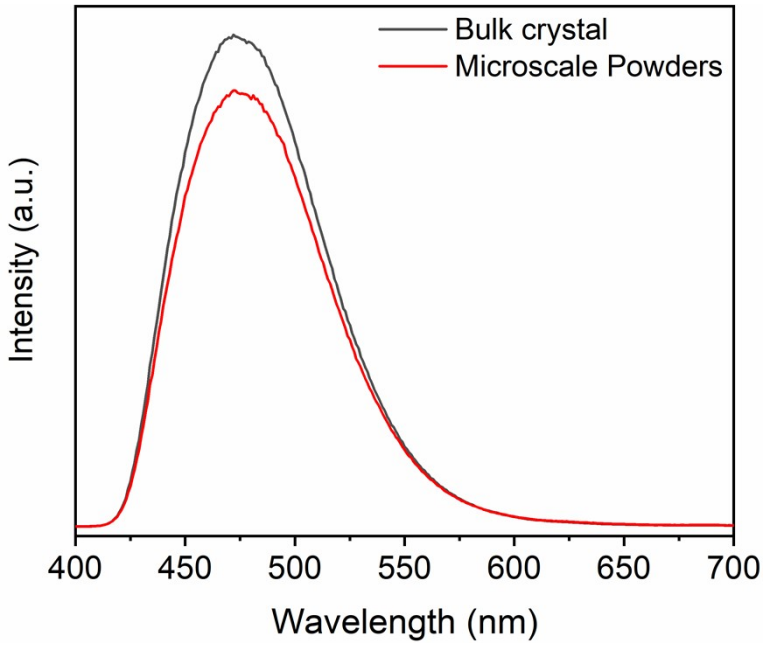


**Fig. S11** Comparison of PL emission spectra of bulk crystals and microscale powders for [TMEDA]$Cu_2Br_4$.

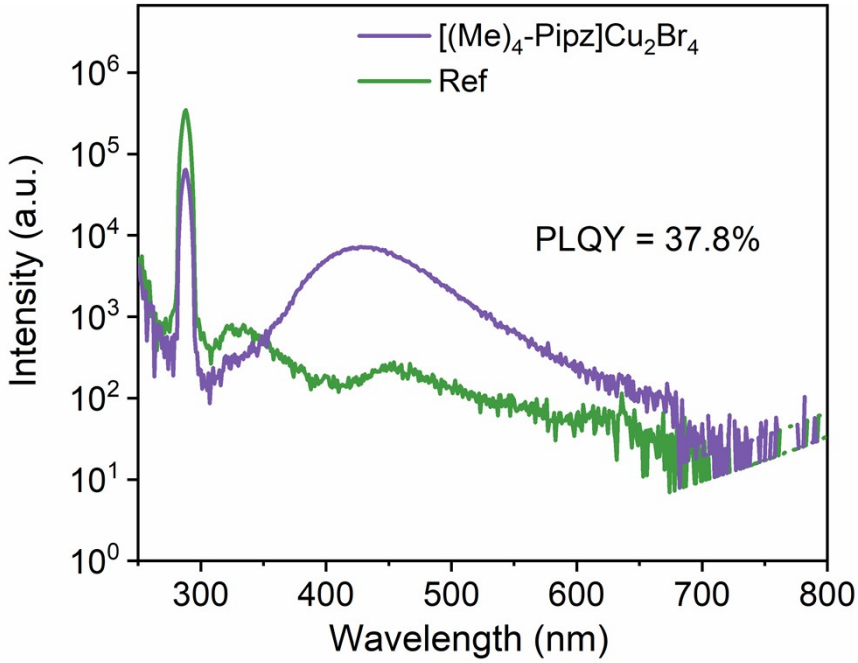


**Fig. S12** The PLQY of [$(Me)_4$-Pipz]$Cu_2Br_4$.

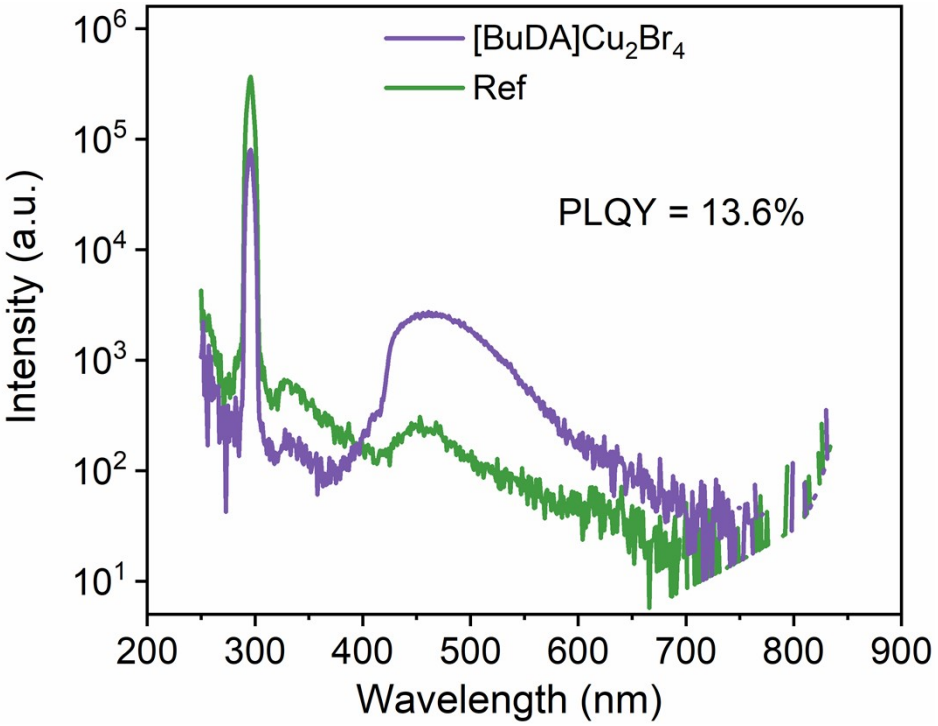


**Fig. S13** The PLQY of $[BuDA]Cu_2Br_4$.

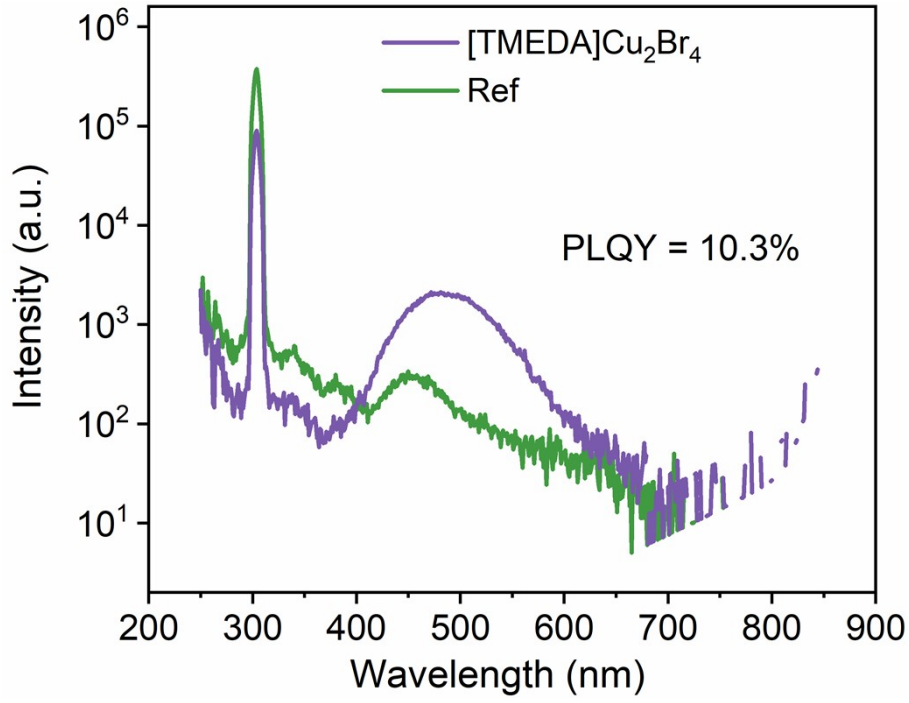


**Fig. S14** The PLQY of $[TMEDA]Cu_2Br_4$.

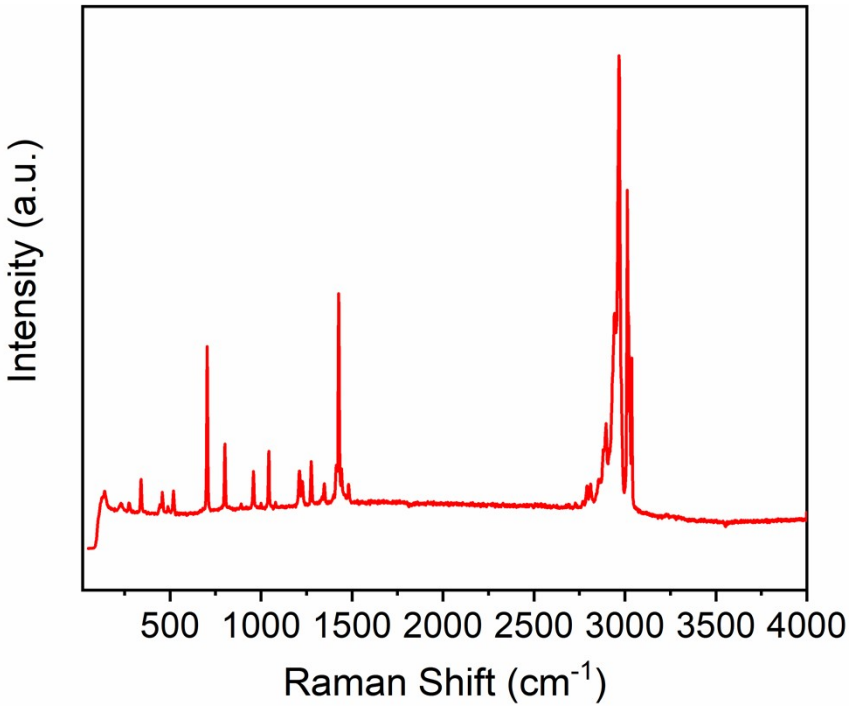


**Fig. S15** Raman spectrum of $[(Me)_4\text{-Pipz}]Cu_2Br_4$.

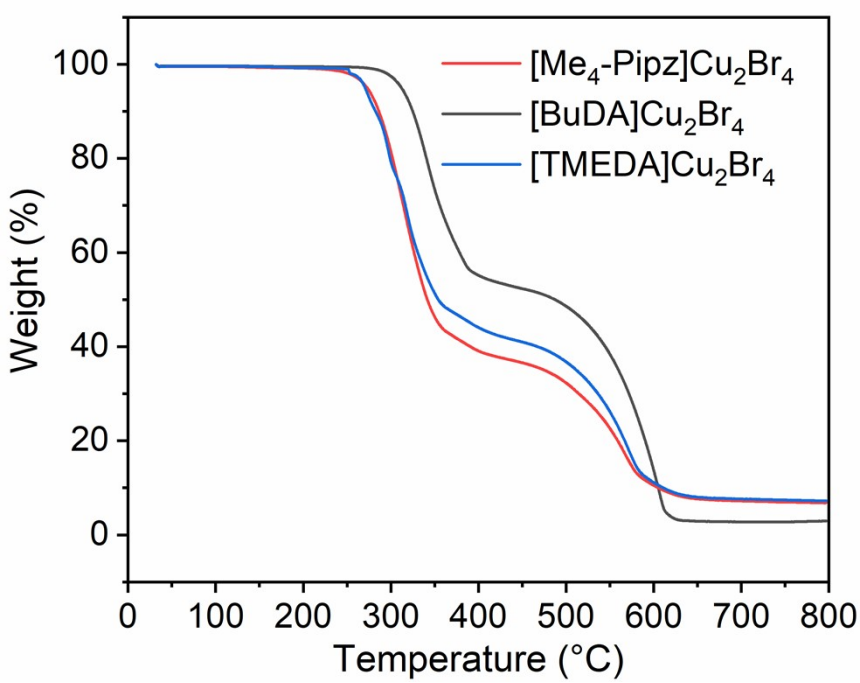


**Fig. S16** The thermogravimetric analysis (TGA) curves of $[(Me)_4\text{-Pipz}]Cu_2Br_4$, $[BuDA]Cu_2Br_4$ and $[TMEDA]Cu_2Br_4$.

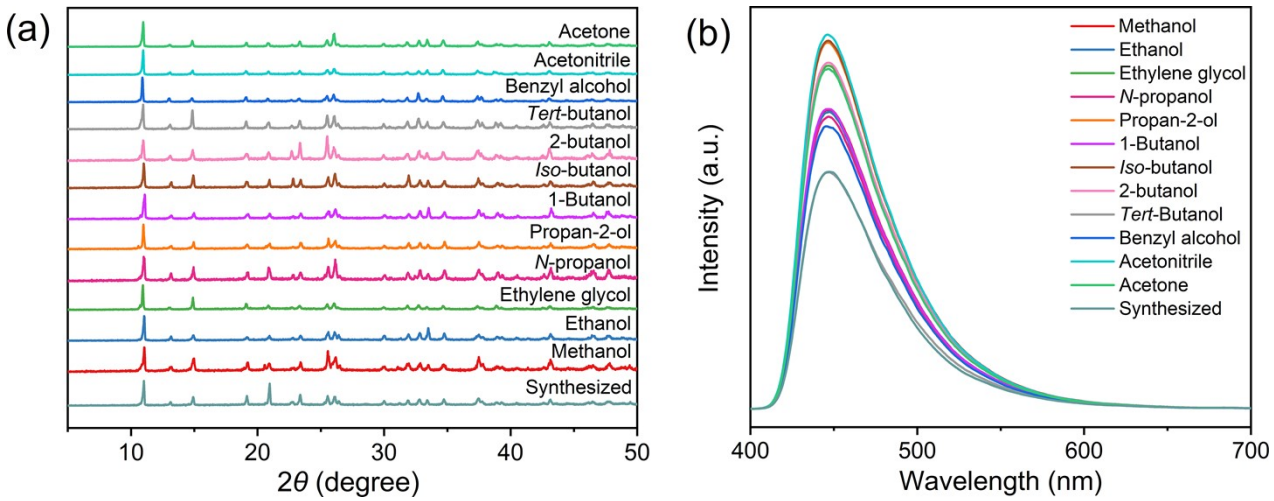


**Fig. S17** PXRD patterns and PL emission spectra of $[(Me)_4\text{-Pipz}]Cu_2Br_4$ after immersing in various organic solvents.

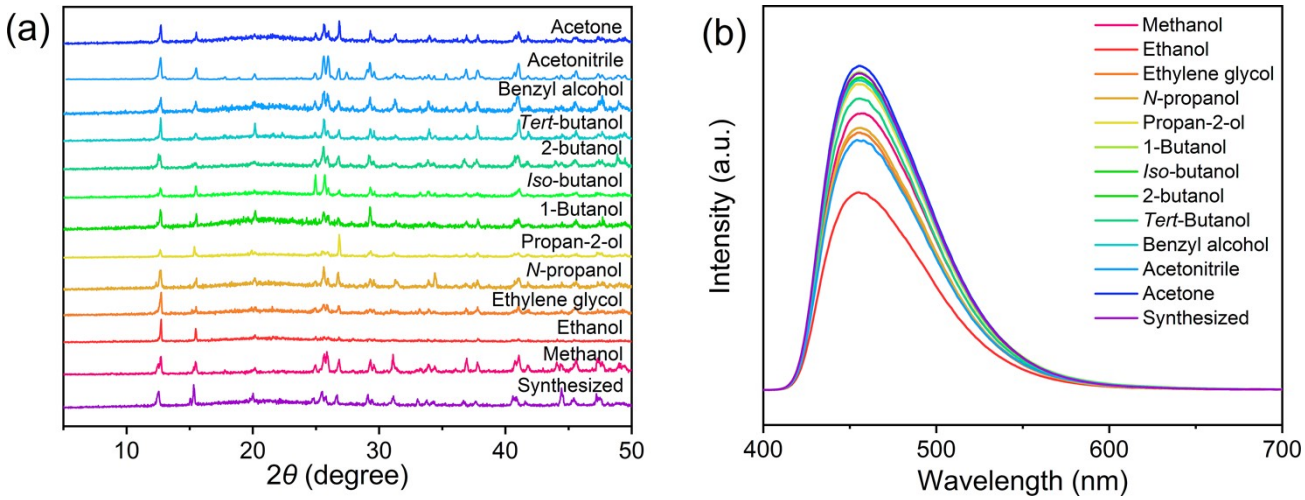


**Fig. S18** PXRD patterns and PL emission spectra of $[BuDA]Cu_2Br_4$ after immersing in various organic solvents.

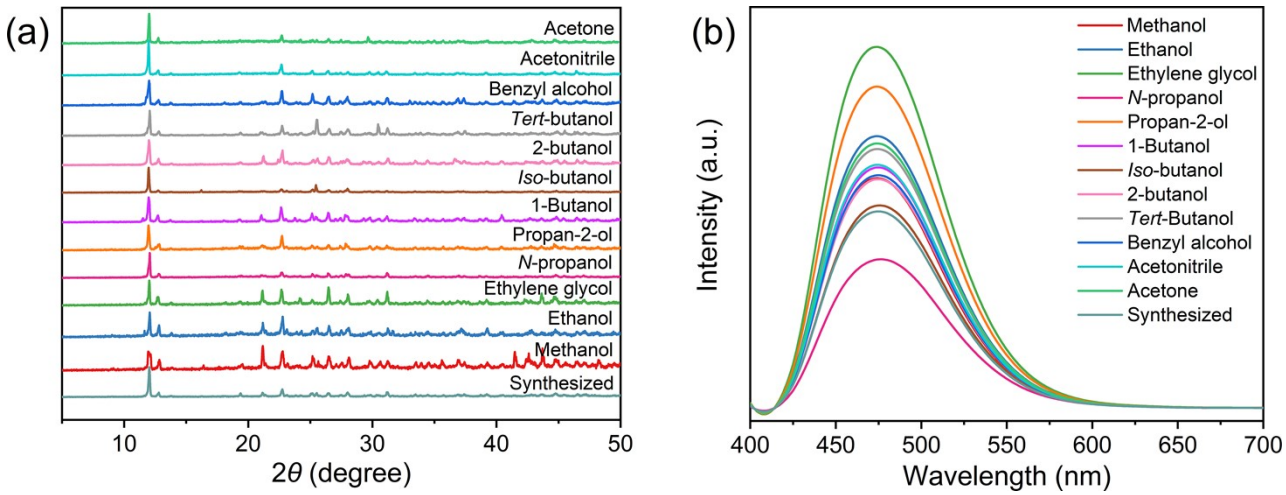


**Fig. S19** PXRD patterns and PL emission spectra of [TMEDA]$Cu_2Br_4$ after immersing in various organic solvents.

**Table S1.** Crystal Data and Structural Refinements for $[(Me)_4\text{-Pipz}]Cu_2Br_4$.

| Compound | $[(Me)_4\text{-Pipz}]Cu_2Br_4$ |
|---|---|
| Chemical formula | $C_8N_2H_{20}Cu_2Br_4$ |
| FW | 295.49 |
| Space group | *C*2/*m* |
| *a*/Å | 13.848(4) |
| *b*Å | 6.7421(19) |
| *c*/Å | 9.389(3) |
| *α*/° | 90 |
| *β*/° | 121.275(2) |
| *γ*/° | 90 |
| *V*(Å$^3$) | 749.2(4) |
| *Z* | 4 |
| $D_{calcd}$ (g·cm$^{-3}$) | 2.620 |
| Temp (K) | 296.15 |
| $\mu$(mm$^{-1}$) | 13.481 |
| *F*(000) | 560.0 |
| Reflections collected | 4263 |
| Unique reflections | 922 |
| GOF on $F^2$ | 1.131 |
| [a]$R_1$,$wR_2$ ($I > 2\sigma(I)$) | 0.0322/0.0834 |
| [b]$R_1$,$wR_2$ (all data) | 0.0361/0.0852 |

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

**Table S2.** Crystal Data and Structural Refinements for [BuDA]$Cu_2Br_4$ .

| Compound | [BuDA]$Cu_2Br_4$ |
|---|---|
| Chemical formula | $C_4N_2H_{14}Cu_2Br_4$ |
| FW | 268.45 |
| Space group | $P2_1/n$ |
| $a$/Å | 6.0905(3) |
| $b$Å | 8.8163(5) |
| $c$/Å | 11.5467(6) |
| $\alpha$/° | 90 |
| $\beta$/° | 97.583(2) |
| $\gamma$/° | 90 |
| $V$(Å$^3$) | 614.59(6) |
| $Z$ | 4 |
| $D_{calcd}$ (g·cm$^{-3}$) | 2.901 |
| Temp (K) | 273.15 |
| $\mu$(mm$^{-1}$) | 16.419 |
| $F$(000) | 500.0 |
| Reflections collected | 6960 |
| Unique reflections | 1097 |
| GOF on $F^2$ | 1.044 |
| [a]$R_1$,$wR_2$ ($I > 2\sigma(I)$) | 0.0236/0.0488 |
| [b]$R_1$,$wR_2$ (all data) | 0.0330/0.0518 |

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

**Table S3.** Crystal Data and Structural Refinements for [TMEDA]$Cu_2Br_4$.

| Compound | [TMEDA]$Cu_2Br_4$ |
|---|---|
| Chemical formula | $C_6N_2H_{18}Cu_2Br_4$ |
| FW | 564.94 |
| Space group | $P2_1/c$ |
| $a$/Å | 7.8140(7) |
| $b$Å | 14.6335(13) |
| $c$/Å | 12.9812(11) |
| $\alpha$/° | 90 |
| $\beta$/° | 93.824(3) |
| $\gamma$/° | 90 |
| $V$(Å$^3$ ) | 1481.0(2) |
| $Z$ | 4 |
| $D_{calcd}$ (g·cm$^{-3}$) | 2.534 |
| Temp (K) | 273.15 |
| $\mu$(mm$^{-1}$) | 13.633 |
| $F$(000) | 1064.0 |
| Reflections collected | 16515 |
| Unique reflections | 2616 |
| GOF on $F^2$ | 1.028 |
| [a]$R_1$,$wR_2$ ($I > 2\sigma(I)$) | 0.0345/0.0656 |
| [b]$R_1$,$wR_2$ (all data) | 0.0682/0.0762 |

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

**Table S4.** Hydrogen bonds data for $[(Me)_4\text{-Pipz}]Cu_2Br_4$.

| D-H···A | d(D-H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| C1-H2···Br2[1] | 0.96 | 3.03 | 3.772(3) | 135.5 |
| C1-H3···Br2[2] | 0.96 | 3.19 | 3.862(6) | 128.3 |
| C2-H4···Br1[3] | 0.96 | 2.89 | 3.804(7) | 159.2 |
| C2-H5···Br1 | 0.96 | 2.83 | 3.765(3) | 164.9 |
| C2-H6···Br1[4] | 0.96 | 2.89 | 3.765(3) | 152.8 |
| C3-H7···Br2[5] | 0.97 | 3.18 | 3.808(4) | 124.1 |
| C3-H8···Br2[6] | 0.97 | 2.97 | 3.633(4) | 126.5 |

[1]1/2+*x*, 1/2+y, +z; [2]1-*x*, +*y*,1 -*z*; [3]3/2-*x*, 1/2+*y*, 2-*z*; [4]+*x*, 1+*y*, +*z*; [5]1/2+*x*, -1/2+*y*, +*z*; [6]3/2-*x*, -1/2+*y*, 2-*z*