Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

for

pH-Controlled Crystal Growth of Copper/Gemini Surfactant Complexes with Bipyridine Groups

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Supporting Figures

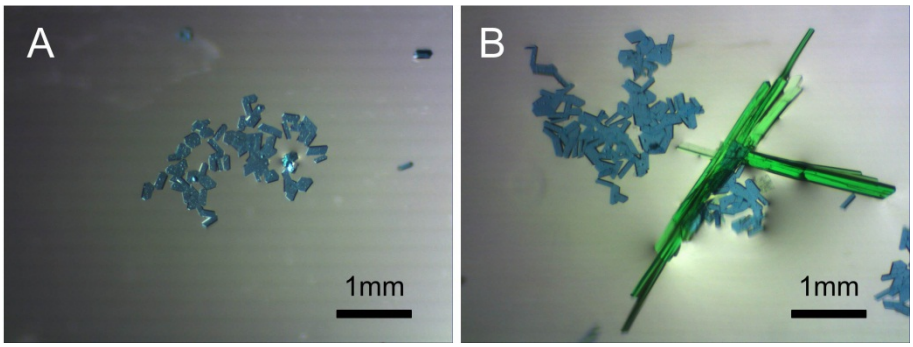

Figure S1. Crystallization form 12Bpy/$CuBr_2$ mixed solution. (A) The formation of blue crystals at pH = 4.8; (B) The coexistence of blue and green crystals at pH = 4.2.

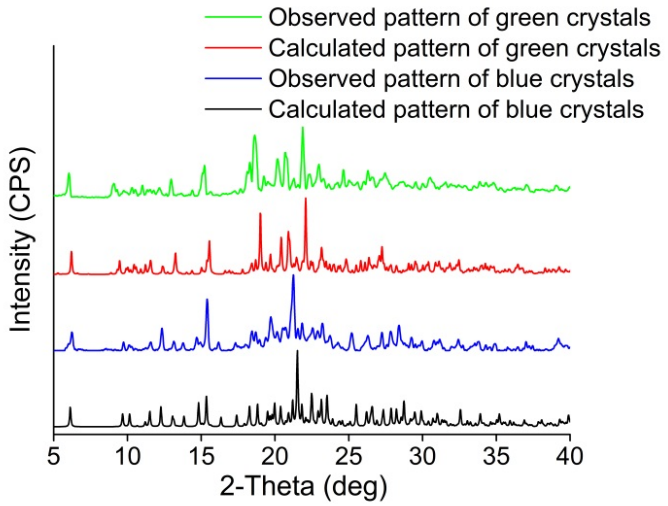

Figure S2. The powder XRD patterns of the blue crystal and green crystal based on both observed measurement and calculated simulation from the single crystalline data.

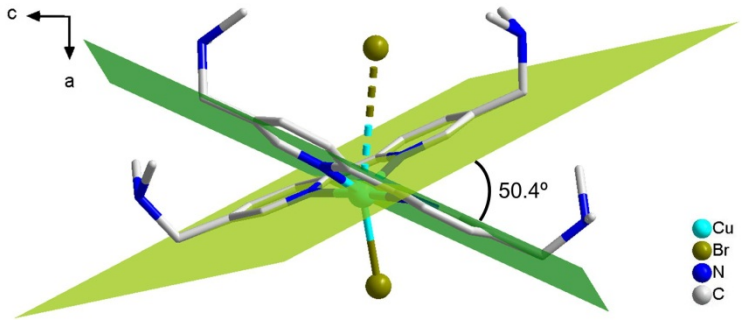

Figure S3. The dihedral angle between two bipyridine planes.

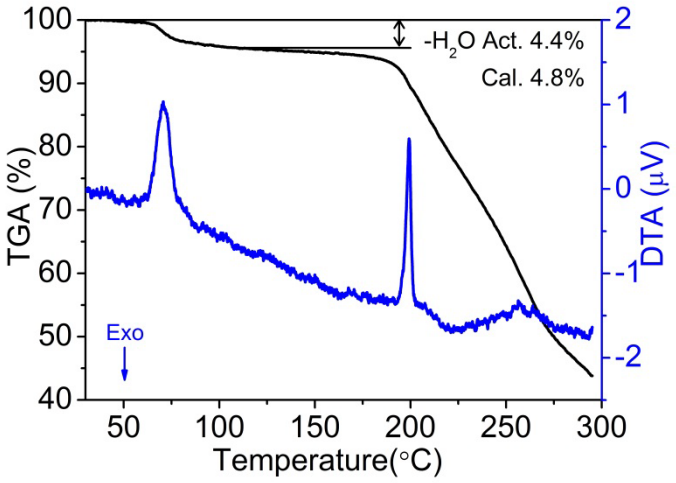

Figure S4. Thermogravimetric analysis together with the differential thermal analysis of green crystals. A 4.4% mass loss before 100 °C in TGA curve is roughly consistent with the crystal water content (4.8%), which can be attributed to the evaporation of water. In addition, the decomposition of complex crystals takes place around 200 °C.

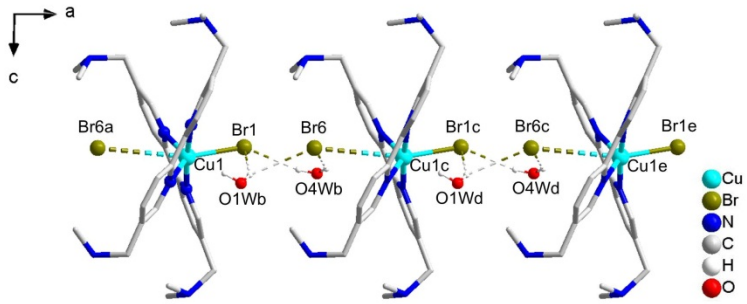

Figure S5. A supramolecular long chain along the a-axis connected with the interactions of O-H⋯Br hydrogen bonds and Cu-Br coordination. Symmetry codes: (a) -1+x, y, z; (b) x, y, 1+z; (c) 1+x, y, z; (d) 1+x, y, 1+z; (e) 2+x, y, z.

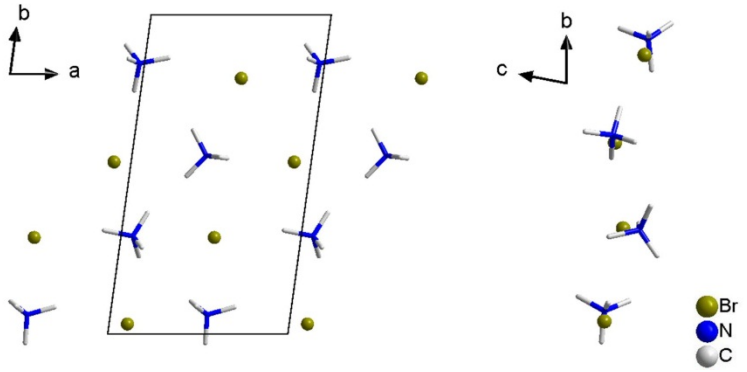

Figure S6. The location of quaternary ammonium head groups and bromide counter ions in the *aob* projection plane.

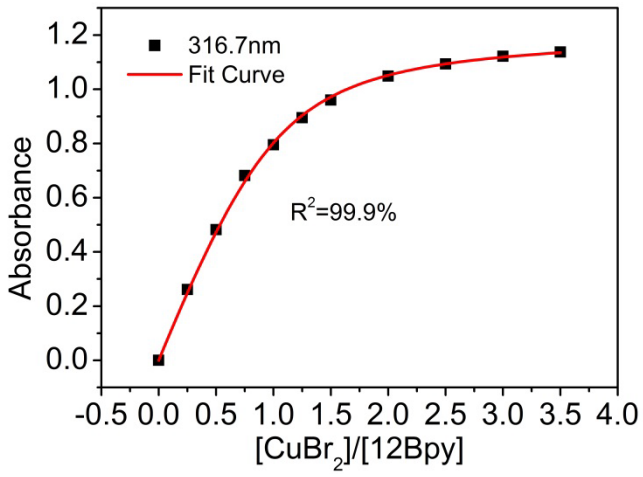

Figure S7. Binding constant estimation by the nonlinear least-squares regression method.

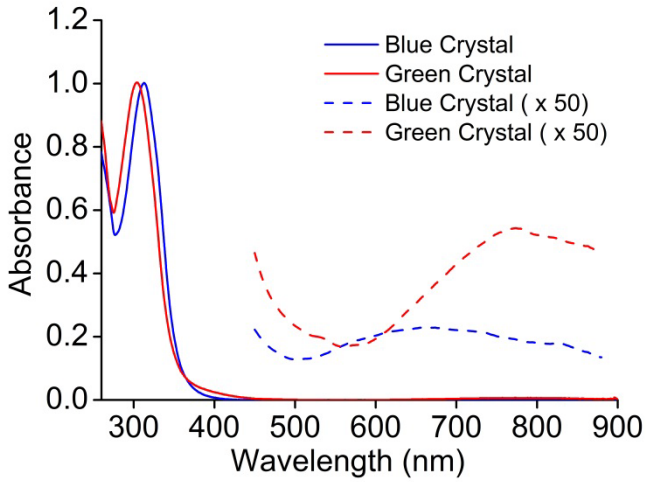

Figure S8. The UV-Vis spectra of blue and green crystals in $CHCl_3$ solution.

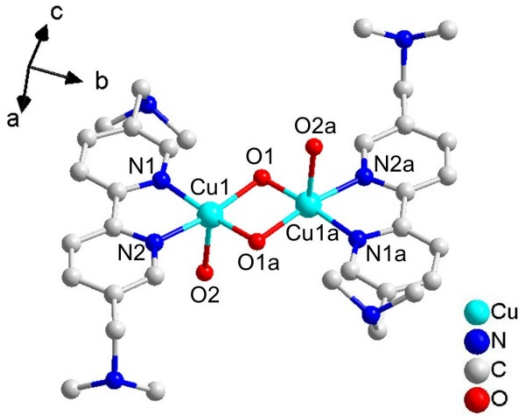

Figure S9. The coordination of Cu(II) ion in the blue crystal showing a square pyramidal geometry with $\tau = 0.044$. H atoms and alkyl chains are omitted for clarity. Symmetry codes: (a) 1-x, -y, 1-z.

Supporting Tables

Table S1. Crystal data and structure refinement

Crystal reference	Blue Crystal	Green Crystal
Empirical formula	C80 H166 Br6 Cu2 N8 O12	C80 H154 Br6 Cu N8 O5
Formula weight	2038.74	1851.11
Temperature	130 K	143K
Wavelength	1.54178 Å	1.54178 Å
Crystal system	Monoclinic	triclinic
Space group	P21/c(14)	$P\bar{1}$(2)
Unit cell dimensions	a=30.2435(5)Å b=9.4252(2)Å c=18.2742(3)Å α=90° β=107.5450(10)° γ=90°	a=9.4175(5)Å b=17.1528(9)Å c=28.9801(16)Å α=79.223(3)° β=89.723(4)° γ=82.329(3)°
Volume	4966.75(16) $Å^3$	4556.6(4) $Å^3$
Z	2	2
Density (calculated)	1.363 Mg/m3	1.349 Mg/m3
Absorption coefficient	3.788 mm^{-1}	3.795 mm^{-1}
F(000)	2132	1938
Crystal size	0.2 x 0.11 x 0.03 mm^3	0.26 x 0.15 x 0.06 mm^3
Theta range for data collection	1.532 to 69.592°	2.65 to 69.3°
Index ranges	-36<=h<=35, -11<=k<=10, -20<=l<=21	-10<=h<=10, -19<=k<=19, -33<=l<=0
Reflections collected	26082	14818
Independent reflections	8946[R(int) = 0.0527]	14818[R(int) = 0.1011]
Completeness to theta	97.6 % (to 67.679°)	98.2% (to 64.00°)
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7532 and 0.4104	0.4386 and 0.8043
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data / restraints / parameters	8946 / 0 / 506	14818 / 0 / 913
Goodness-of-fit on F2	1.025	1.113
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.1537	R1 = 0.0919, wR2 = 0.2301
R indices (all data)	R1 = 0.0633, wR2 = 0.1608	R1 = 0.1011, wR2 = 0.2348
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	1.816 and -1.619 e.$Å^{-3}$	1.156 and -0.974 e.$Å^{-3}$