

Supplementary materials

Structure and Properties of a New Double-Stranded $[\text{Cu}^{\text{II}}_2]_2$ Cluster Helicate

Manindranath Bera,^a Guillem Aromi,^b Wing Tak Wong^c and Debashis Ray^{*,a}

Preparation of 1: To a solution of H_2L (0.5 g, 1.09 mmol) in methanol (30 ml) was added dropwise an aqueous solution of $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.789 g, 2.18 mmol) with magnetic stirring during 15 min. After $\frac{1}{2}$ an hr., an aqueous solution of NEt_3 (0.17 g, 1.16 mmol) was slowly added to the previous solution during 10 min. The reaction mixture was then stirred for another 30 min. The resulting dark green solution was then kept in air. The green microcrystalline solid compound was separated out, collected by filtration through glass frit and washed thoroughly with hexane. The compound was finally dried in vacuo over P_4O_{10} . The single crystals suitable for X-ray analysis was obtained from 1:1(v/v) MeOH- H_2O during 6 days. Yield: 0.836 g (80 %). Anal. Calcd for $\text{C}_{28}\text{H}_{52}\text{N}_{12}\text{O}_{22}\text{Cl}_4\text{Cu}_4$: C 25.77, H 4.02, N 12.88, Cu 19.48. Found: C 25.41, H 3.98, N 12.51, Cu 19.42 %. IR (KBr, cm^{-1}): $\nu = 3424(\text{b}), 3287(\text{b}), 1623(\text{vs}), 1589(\text{s}), 1383(\text{s}), 1203(\text{s}), 1082(\text{s}), 963(\text{s}), 815(\text{s}), 738(\text{s})$. Molar conductance, Λ_M : (MeCN solution) $465 \text{ ohm}^{-1} \text{ cm}^2 \text{ mol}^{-1}$. UV-vis spectra [λ_{max} , nm (ϵ , $\text{lmol}^{-1}\text{cm}^{-1}$): (MeCN solution) 549 (1770), 457 (580), 269 (18470), 235 (17575). Room temperature μ_{eff} (tot.): $2.90\mu_B$; $\mu_{\text{eff}} / \text{Cu}$: $1.45\mu_B$.

Figures with captions

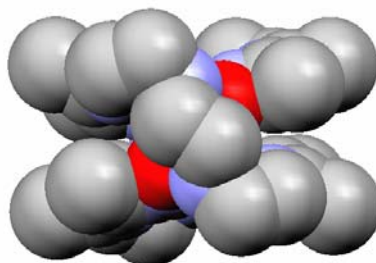


Fig. S1 Space filling representation of $[\text{Cu}_4(\mu_4\text{-L})_2]^{4+}$ showing the double-stranded helix.

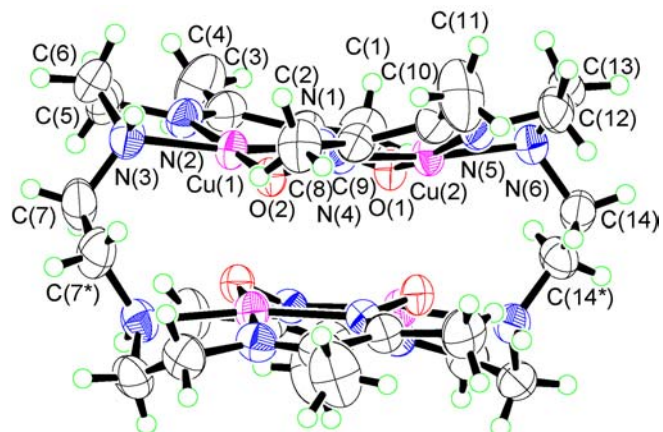


Fig. S2 Side view of $[\text{Cu}_4(\mu_4\text{-L})_2]^{4+}$. Hydrogen atoms were shown as circles of arbitrary size.

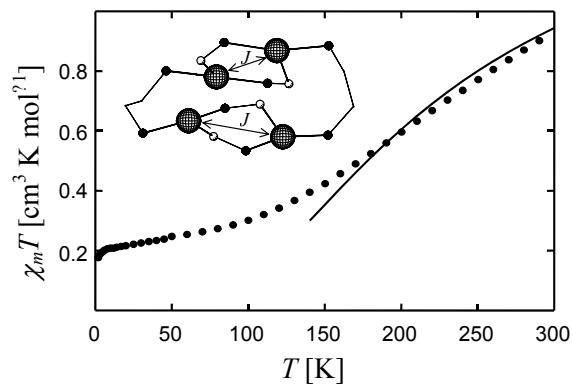


Fig. S3 Plot of experimental $\chi_m T$ vs T for $[\text{Cu}_4(\mu_4\text{-L})_2]^{4+}$. The solid line is a fit to the high temperature experimental data (See text for details). In the inset is a PLATON representation of the core of the complex.