

Supporting information for: Calixarene supported enneanuclear Cu(II) clusters

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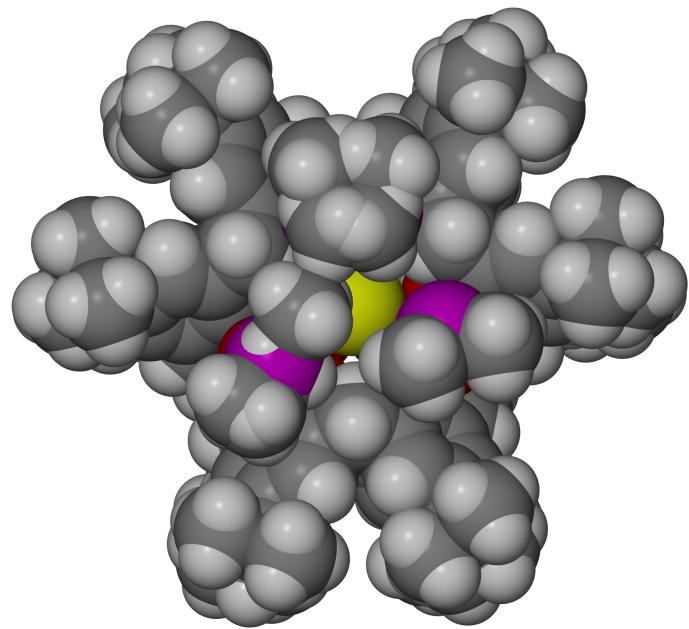


Figure S1. Space filling representation of the Cl^- anion residing in the pocket generated by ligated solvent molecules on the Cu centres of the trigonal prsim in cation **1**.

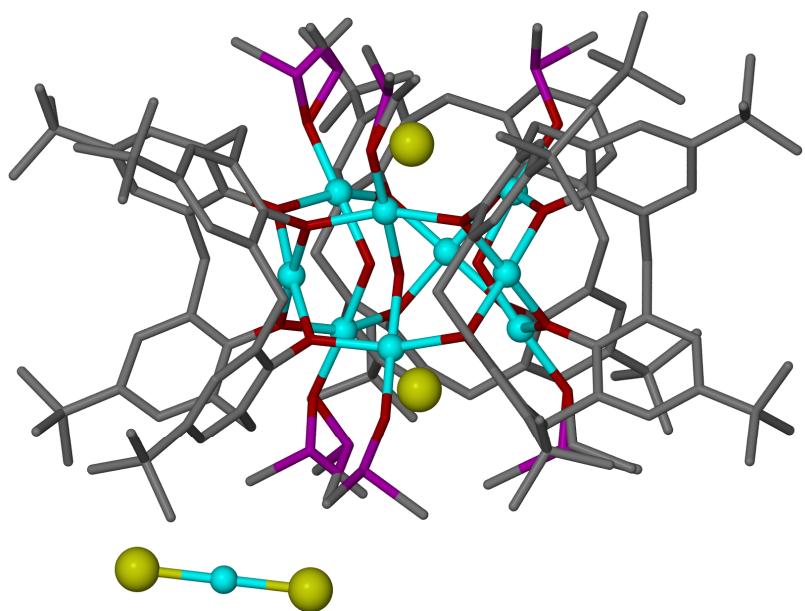
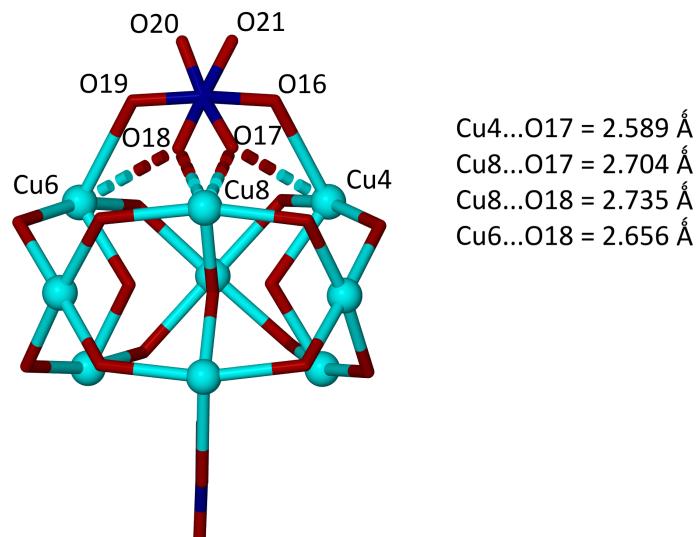


Figure S2. Cluster and the $\text{Cu}^{\text{I}}\text{Cl}_2$ counterion found in the single crystal structure of **1**.



$\text{Cu4...O17} = 2.589 \text{ \AA}$
 $\text{Cu8...O17} = 2.704 \text{ \AA}$
 $\text{Cu8...O18} = 2.735 \text{ \AA}$
 $\text{Cu6...O18} = 2.656 \text{ \AA}$

Figure S3. Detailed information relating to the coordination and long contacts associated with the disordered NO_3^- anion in the cation found in **2**.

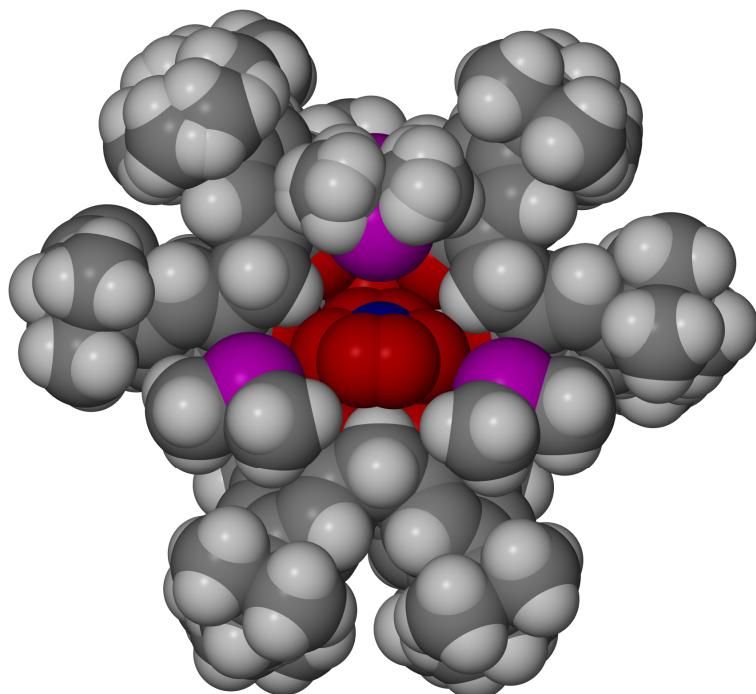


Figure S4. Space filling representation of the disordered NO_3^- anion residing in the pocket generated by ligated DMSO molecules on the Cu centres of the trigonal prsim in cation **2**.

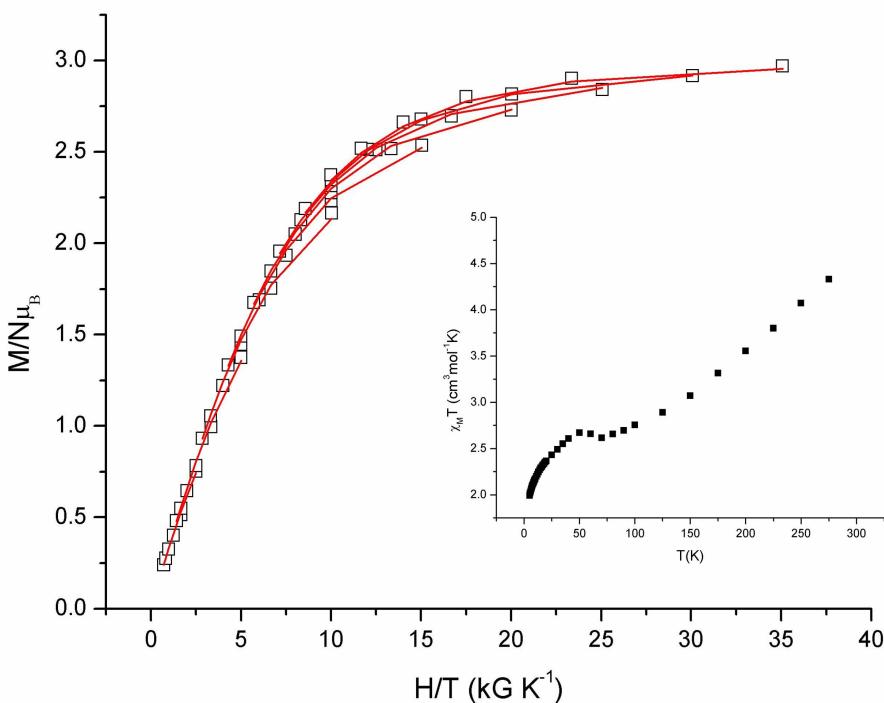


Figure S5. Plot of reduced magnetisation ($M/N\mu_B$) versus H/T for complex **1** measured in the 0.5 - 7 T field range between 2 - 7 K. The red lines represent the fit of the experimental data by a matrix diagonalization method employing the Hamiltonian $\hat{H} = D(\hat{S}_z^2 - S(S+1)/3) + \mu_B g H \hat{S}$. This gives an $S = 3/2$ ground state with $g = 2.02$ and $D = -0.1 \text{ cm}^{-1}$. The inset shows a plot of $\chi_M T$ versus T for **1** in the 300 - 5 K temperature range using an applied field of 0.1 T. Attempts to fit the data to isotropic 1, 2 and 3J models were unsuccessful.