

Supplementary Materials

The Role of Anions on the Crystal Structures of Copper(II) and Zinc(II) Complexes of a Tunable Butterfly Cyclophane Macrocyclic

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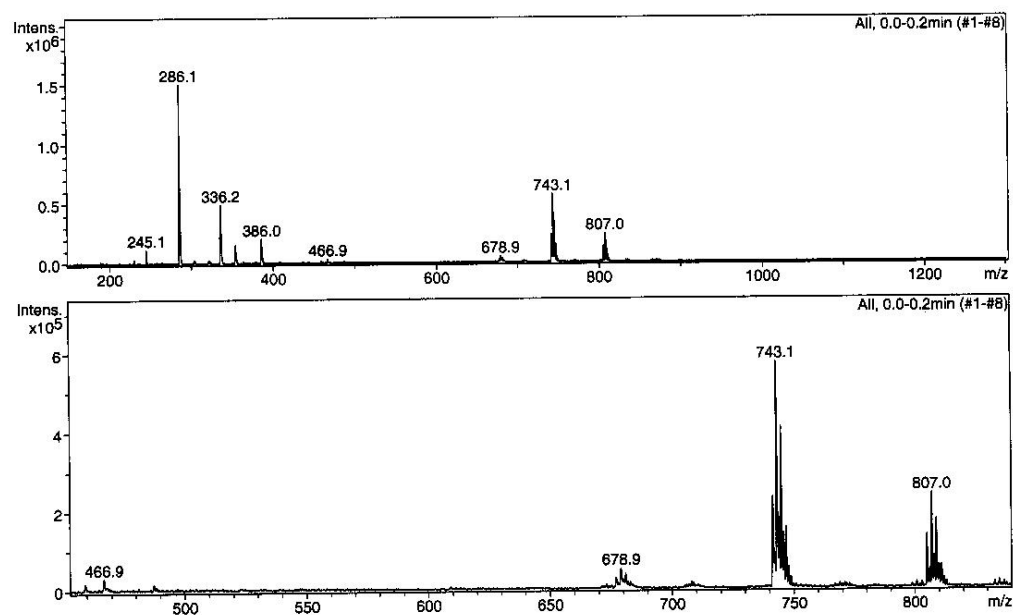


Figure S1. ESI spectrum of solutions containing $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ and $\text{L} \cdot 8\text{HCl} \cdot 2\text{H}_2\text{O}$ at $\text{pH} = 8$.

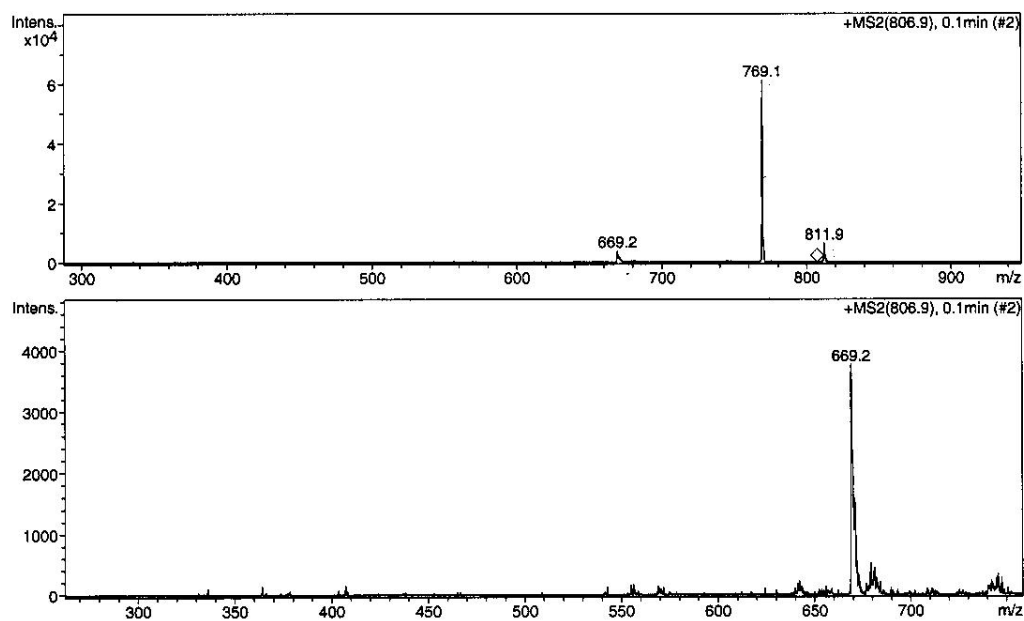


Figure S2. Fragmentation of the peak at $m/z = 807.0$

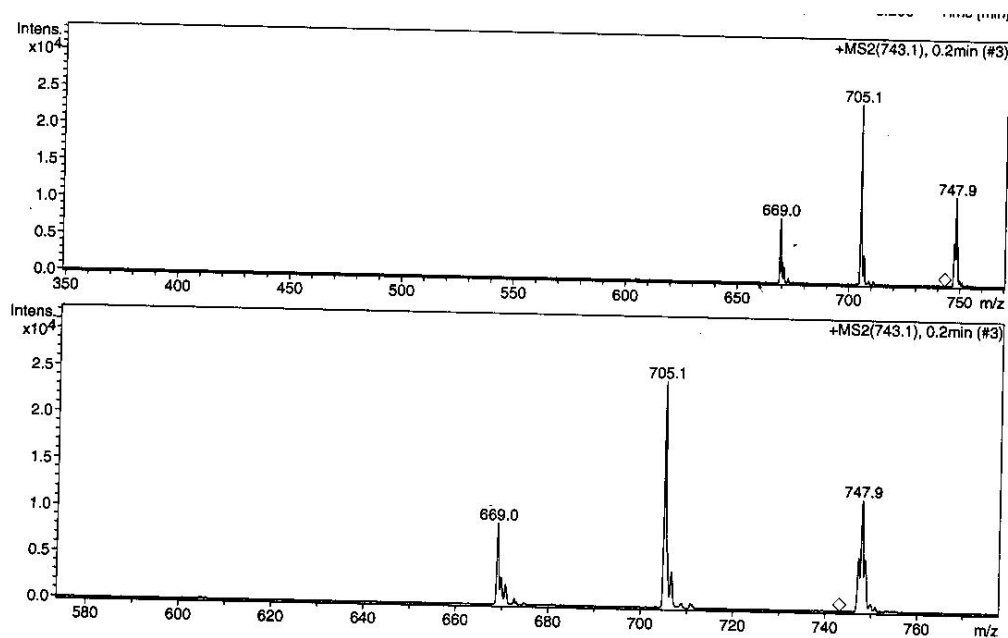


Figure S3. Fragmentation of the peak at $m/z=743.1$

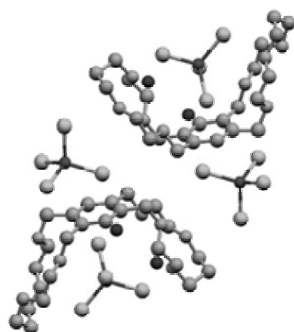


Figure S4.- View of the packing of [H₄L](ZnCl₄)₂·2H₂O (**1**) showing the two types of ZnCl₄²⁻ anions.

NMR Measurements

The ^1H and ^{13}C NMR spectra were recorded on a Bruker AV 400 spectrometer operating at 399.913 MHz for ^1H . Adjustments to the desired pH were made adding drops of DCl or NaOD solutions. The pD was calculated from the measured pH values using the correlation $\text{pH}=\text{pD}-0.4$.

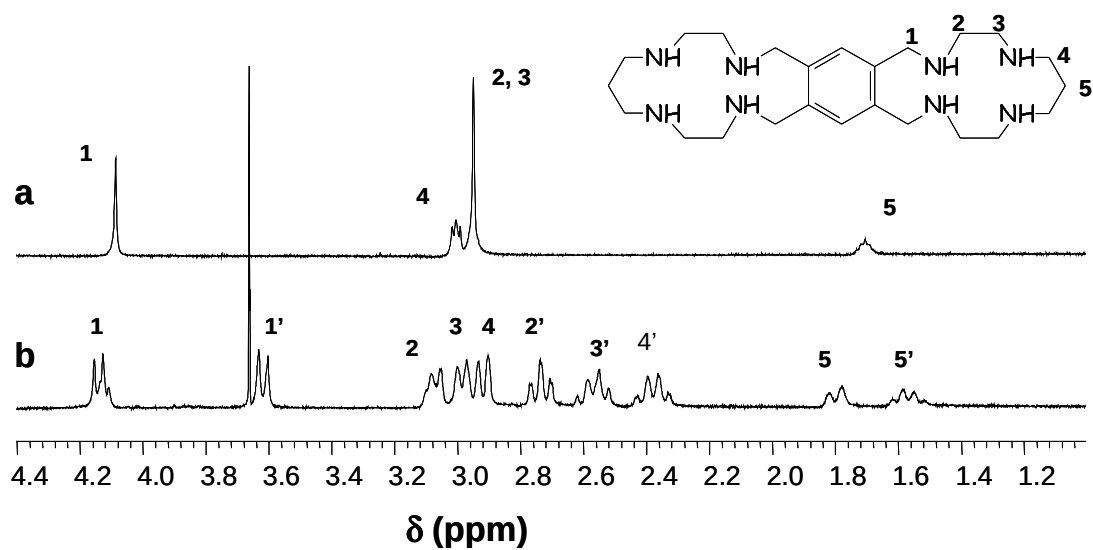


Figure S5. (a) ^1H NMR spectrum of **L** at pD 7.4 in D_2O . (b) ^1H NMR spectrum of **L**: Zn^{2+} (1:2) at pD 7.4 in D_2O .