

Supplementary Materials:

Bidimensional Polyiodide Netting Stabilized by a Cu(II) Macrocylic Complex

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Figure S1. Pocket hosting the ClO ₄ ⁻ anion in the [Cu(L)Cl]ClO ₄ ·CH ₃ CN crystal structure.	S2
Figure S2. Views representing steric hindrance generated by tosyl groups around Cu-bound iodide. .	S3
Figure S3. Cell content of crystallized impurity identified as 1,4-ditosylpiperazine.	S4

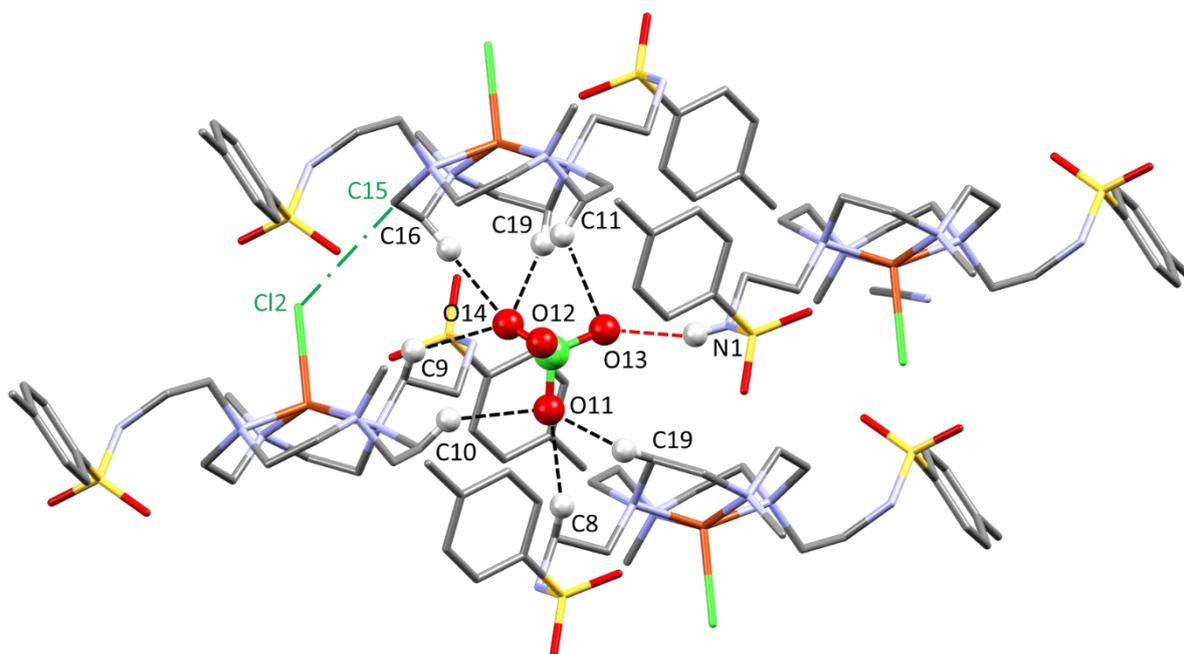


Figure S1. Pocket hosting the ClO₄⁻ anion in the [Cu(L)Cl]ClO₄·CH₃CN crystal structure. Multiple CH...anion contacts (black) plus an NH...O H-bond (red) are established. Green: detail of the third Cl2 contact, Cl2...HC15.

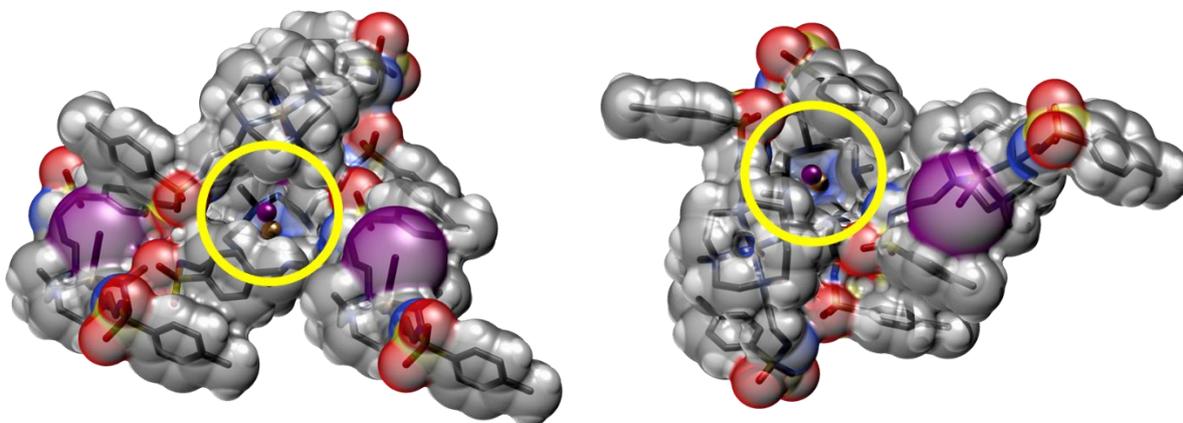


Figure S2. Views representing a central $[\text{Cu}(\text{L})\text{I}]^+$ unit (ball and stick) surrounded by its H-bonded partners (surface). For both copper-coordinated iodides, I1 (left) and I2 (right), it is observed that the resulting H-bonded network entirely buries the iodide ligand in a pocket, preventing I...I contacts.

Identification and Crystal structure of the impurity (1,4-ditosylpiperazine)

As mentioned, an impurity was found in our synthetic batch prior to recrystallization. Since it segregated giving single crystals, although of poor quality, it was possible to assess its nature. Our partial data indicate a triclinic (P-1) unit cell with $a = 9.1030(17) \text{ \AA}$, $b = 10.686(2) \text{ \AA}$, $c = 10.953(2) \text{ \AA}$, $\alpha = 101.676(16)^\circ$, $\beta = 100.638(15)^\circ$, $\gamma = 108.221(15)^\circ$, $V = 955.299 \text{ \AA}^3$. Preliminary data show that 1,4-ditosylpiperazine has been obtained by dimerization of N-tosylaziridine (Figure S4), crystal quality does not allow for full refinement. The impurity is successfully eliminated by recrystallization.

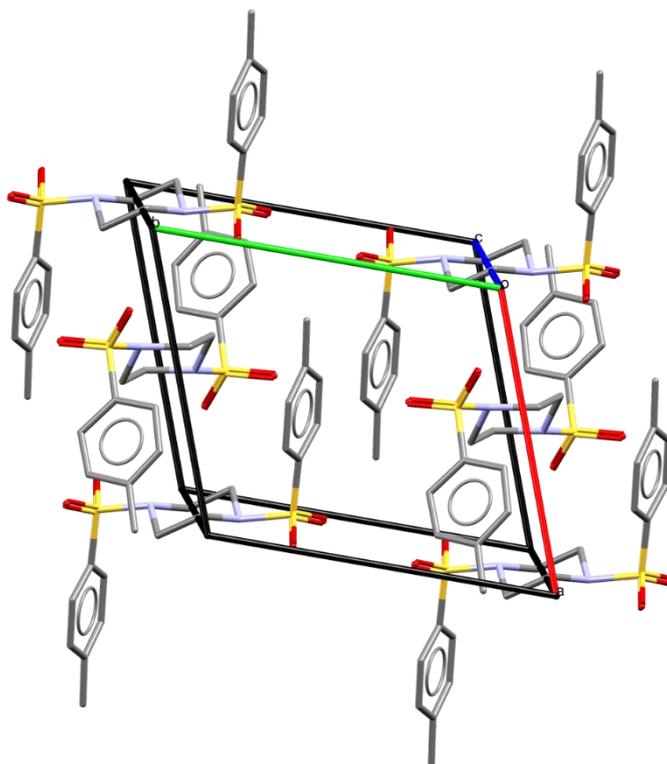


Figure S3. Cell content of crystallized impurity identified as 1,4-ditosylpiperazine. Cell axes shown: *a* red, *b* green, *c* blue.