14th INTERNATIONAL SYMPOSIUM ON MACROCYCLIC AND SUPRAMOLECULAR CHEMISTRY

JUNE 2-6, 2019 LECCE, ITALY

BOOK OF ABSTRACTS

From Discrete Crates to 3D Racks: Piling Blue Boxes with Iodide Anions

M. Savastano,[a] C. Bazzicalupi,[a] A. Bianchi [a]

[a] *Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 3-13, 50019, Sesto Fiorentino (FI), Italy.*
E-mail: matteo.savastano@unifi.it

Cyclobis(paraquat-p-phenylene), also known as Blue Box (BB) or Stoddart's BB, is one of the everyone's favourite building blocks for the construction of supramolecular assemblies. Its inventor, one of the major scholars in the field besides, noted how iodine-based species have the ability to trigger ring opening and reforming under heating,[1] a strategy that has been successfully applied to the synthesis of mechanically interlocked systems. On the other hand, recognition of such reactivity somewhat hindered the appreciation of the unique structural properties that can be obtained by pairing BB with iodide counterions under mild conditions. Due to the polarizability and scarce tendency of the iodide anion to give rise to directional forces, the resulting three-dimensional architectures, that we dare to call Supramolecularly Organised Framerworks (SOFs), are constituted by rigid BB scaffolds which are free to orient and adjust "rolling over" the bulky counteranions: contrarily to MOFs or COFs architectures here we do not have strict requirements about the mutual localization of the different molecular components. This ultimately results in hollow structures constituted by channels made up of piled BB molecules, Figure 1, whose overall packing can be tuned depending on the conditions and nature of the crystallization medium.

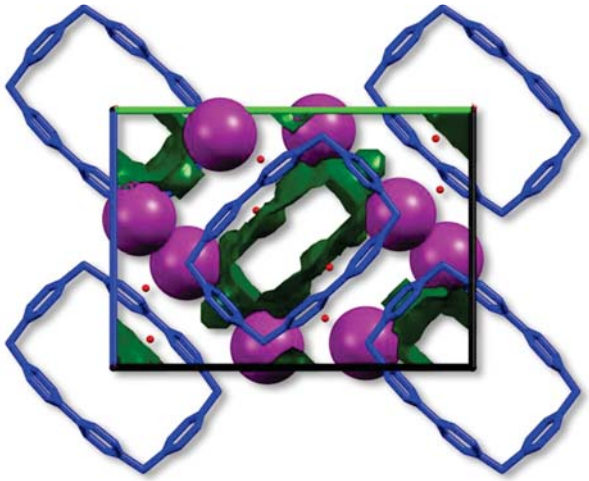

Figure 1. Crystal structure of $[BB(I)_4].6H_2O$. Green blobs are a visual representation of the void space inside the channels of piled BB molecules.

References

[1] Patel, K.; Miljanić, O. Š; Stoddart, J. F. *Chem. Commun.* **2008**, *0*, 1853-1855.