Electrostatic self-assembly of organic crystals from charged macrocycles

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Macrocyclic host molecules are versatile building blocks in the supramolecular chemistry and crystal engineering. Depending on their structure and properties, macrocycles have found numerous applications in the host-guest systems, sensing, catalysis, design of porous materials, *etc*. Here we describe our approach towards design of molecular crystalline assemblies using oppositely charged macrocyclic building blocks, anionic *p*-sulfonatocalix[4]arene and cationic pillar[*n*]pyridiniums. *P*-Sulfonatocalix[4]arene with electron-rich basket-like cavity is well-known water-soluble supramolecular host, capable of forming various types of assemblies, such as bilayer clay-type structures, capsules, nanometer tubules, spheres or Russian-doll assemblies.[1] Pillar[*n*]pyridiniums are new family of water-soluble inherently cationic host molecules of prismatic electon-deficient cavities.[2] These two types of macrocyclic hosts are complementary in terms of charge, size and shape. Their self-assembly is guided mainly by the electrostatic attraction between anionic sulfonate groups of calix[4]arene and positive charge on the pyridinium rings of the cationic macrocycles. The crystallization in gel and liquid-liquid diffusion methods have been used for the obtaining suitable crystals build from mixed macrocycles for single crystal X-ray diffraction analysis. The structural aspects of the supramolecular architectures and main non-covalent interactions guiding the assembly will be discussed.

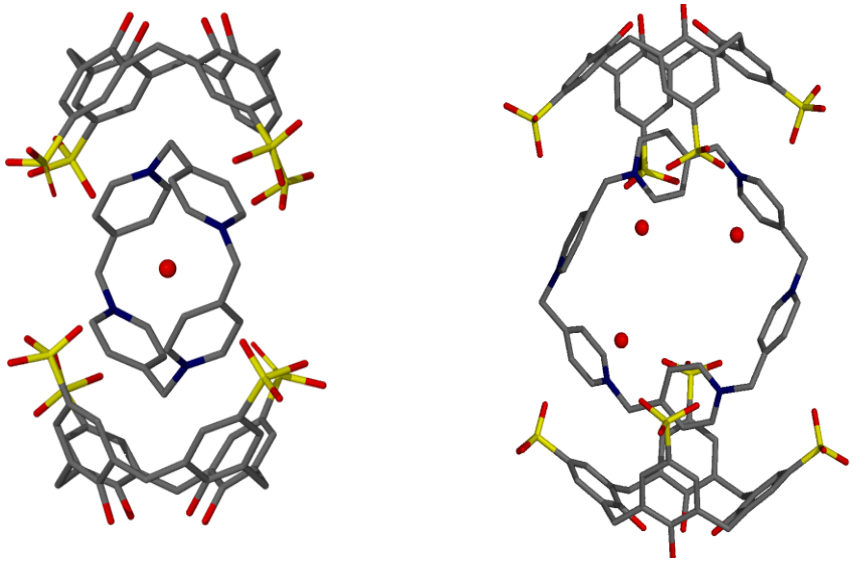

Figure 1. Complexes formed by *p*-sulfonatocalix[4]arene and pillar[*n*]pyridiniums.

[1] Scott, J., Dalgarno, M.J., Hardie, J., Mohamed, M., Colin L. R. (2003). Chem. Eur. J. **9**, 2834.

[2] Kosiorek, S., Butkiewicz, H., Danylyuk, O., Sashuk, V. (2018). Chem. Commun. **54**, 6316.

Keywords: *p*-sulfonatocalix[4]arene; pillar[*n*]pyridinium; complex.

National Science Center for funding the research Grant 2019/35/O/ST4/01865.