

# SYNTHESIS AND CONFORMATIONAL STUDY OF NEW OXACALIX[4]ARENE MACROCYCLES

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In supramolecular chemistry, calixarenes form a class of macrocyclic host molecules that have found use in a wide range of applications. [1] Their diverse utilization is possible due to the host-guest complexation with smaller guest molecules through non-covalent interactions such as  $\pi$ - $\pi$  interactions. Oxacalix[*n*]arenes can be regarded as aromatic crown ethers that comprise the key binding motifs of calix[*n*]arenes and classical crown ethers. [2]

In this work, we present single crystal structures of the unsubstituted oxacalix[4]arene (**1a**) and investigate the weak supramolecular interactions that govern the macrocycles' packing in the solid state. [3] We further analyse the complexation properties between electron-rich host molecules **1a** and carboxyl-substituted oxacalix[4]arene **1b** with various electron-poor guests e.g benzoic acid and well-known herbicide, paraquat (Fig.1). <sup>1</sup>H NMR dilution studies of **1b** show the macrocycles' ability to change its geometry upon proton dissociation at lower concentrations.

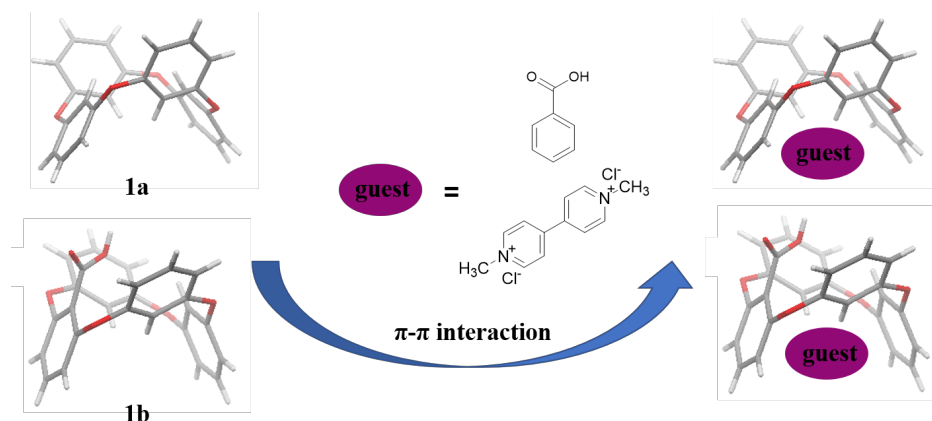


Fig.1 The crystal structures of oxacalix[4]arene macrocycles **1a** and **1b** and the graphical illustration of [**1a**-benzoic acid] and [**1b**-paraquat] host-guest complexes.

## References

1. Zhao, Y., 2015, *Chem. Rev.*, 115, 7794.
2. Dehaen, W., 2008, *Chem. Soc. Rev.*, 37, 2393.
3. Adamson, J., 2018, *ChemistrySelect*, 3, 9091.