

**MS33-2-1 Quasi-pentagonal shape of carboxylated pillar[6]arene in its host-guest crystalline complexes**  
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**Abstract**

Carboxylated Pillar[6]arene (CPA6), first reported by Guocan Yu in 2012 [1], is highly symmetrical pillar-shaped macrocyclic compound, composed of six hydroquinone units linked by methylene bridges at the para-positions, modified by twelve carboxylic acid groups. Its hydrophobic, electron-rich cavity combined with its water solubility makes it great candidate as host molecule for various electron-deficient guest or other cationic molecules. Moreover, carboxyl groups, that can take part in proton transfer, are located at the terminal positions of flexible aliphatic chains, so they can adjust to the size and shape of guests.

All we know about the shape of CPA6 or its host-guest complexes is based on the theory, solution studies or relying on the crystal structures of already known members of pillar[6]arene derivatives. But can we believe the assumptions?

Herein, we want to present, for the very first time, our results on the X-ray structures of CPA6 in the form of its host-guest complexes with N,N'-dimethyl-4,4'-bipyridinium cation (paraquat) and pentamidine. Our studies show that roughly hexagonal molecule can change shape and simulate the symmetry of a pentagon, adapting to the shape of the guest molecule. These results shed a new light on the self-assembly and properties of the host-guest complexes of CPA6 in the solid state.

**References**

[1] Yu G., Xue M., Zhang Z., Li J., Han C., Huang F., *J. Am. Chem. Soc.* 2012, **134**, 19489–19497