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Title:Novel Macrocyclic Compounds as Building Blocks in Supramolecular Chemistry

Resorcinarenes and pyrogallolarenes have been used as building blocks for novel synthetic receptors and supramolecular self-assemblies. Introduction of functionalities such as nitro, cyano, and amido groups into the resorcin[4]arene molecule can significantly change the chemical properties of these macrocycles. The spectroscopic data and X-ray crystal structures of the new tetracyano resorcin[4]arenes show that these compounds adopt a crown conformation. No hydrogen-bonded self-assembly is observed. The complex of silver(I) ion and tetracyano resorcin[4]arene is a polymer in which the silver center is coordinated by three cyano groups of the macrocycle and possesses an unusual trigonal planar geometry. No new tetranitro and tetracamido resorcin[4]arenes were synthesized under the studied conditions.

Additionally, molecular hosts with a spacious inner cavity have also received a lot of interest because of their ability to encapsulate several guest molecules. To obtain such valuable receptors, the Suzuki-Miyaura cross coupling and the aldehyde-amine condensation are used as the synthetic pathways to functionalize calix[4]arenes and cavitands with a trimethoxyphenyl moiety. Unfortunately, both synthetic approaches afford only mixtures of products and no pure desired macrocycles can be isolated.

Finally, a new calix[4]arene derivative possessing the versatile 2,4-diamino-1,3,5-triazine moieties has been prepared. Its ability to participate in a large hydrogen-bonded system and to serve as a potential ligand for transition metal complexes was examined by X-ray crystal structure analysis and 1H-NMR titration. No hydrogen-bonded network is detected for this new macrocycle. Dimethylsulfoxide may disturb the formation of a hydrogen-bonded assembly, even in the presence of compatible barbituric acid and a zinc ion.