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Properties and patterns in anion-receptors: a closer look at**Bambusurils**

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Abstract

The recently discovered glycoluril-based macrocycles, bambusurils, have been recognized as effective anion containers and electron donors, playing an important role in a variety of systems with technological and biological relevance. The potential use of bambusurils in energy-storage systems and in processes related to ion-channel diseases are undoubtedly examples of emerging applications. Their multifaceted properties are, so far, very little explored and recent efforts have set the basis for a better understanding of the binding behavior of bambusuril derivatives, able to form stable complexes with various anionic molecules. This review focuses on the key advances pertaining to bambusurils, including structural variations, methods of synthesis and corresponding physical and chemical properties. The main factors affecting the stability and structure of the respective inclusion complexes are outlined. Challenges regarding computational approaches for predicting properties of these host-guest systems are also discussed. Computational insight is particularly valuable to improve and fine-tune the conformation and ion affinity of bambusurils, being crucial to reinforce anion recognition properties.

Keywords

Bambusurils; Anion receptors; Host-guest systems; Supramolecular chemistry.

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