

Tuning Selectivity of Bambus[6]urils toward Inorganic Anions

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Bambus[6]urils are a relatively new class of macrocycles with six glycoluril units held together by six methylene bridges.¹ These compounds are characterized by an electropositive cavity that allows them to bind to inorganic anions of different sizes, such as small fluoride and large iodide. This behavior is due to the relatively high flexibility of the macrocycle, which can adapt to anions of different sizes and shapes. The binding strength of bambus[6]urils could be modulated by different functionalization of their portals. For example, the attachment of fluorinated benzyl substituents increased the bambus[6]uril binding by several orders of magnitude.² However, the selectivity of bambus[6]urils for different anions has remained the same independently of the type of substituent attached to their portals. Recently, we reported the synthesis of chiral bambus[6]urils bearing spacious 1-phenylethyl groups, which provide the macrocycles with higher rigidity compared to the former derivatives.³ Herein, we show that these chiral bambus[*n*]urils (BU1, BU2, Fig. 1) bind inorganic anions with very different selectivity than previously reported bambus[6]urils derivatives. Moreover, association constants of the host-guest complexes determined by ¹H NMR titrations and isothermal titration calorimetry showed that the selectivity is dependent also on type of solvent.

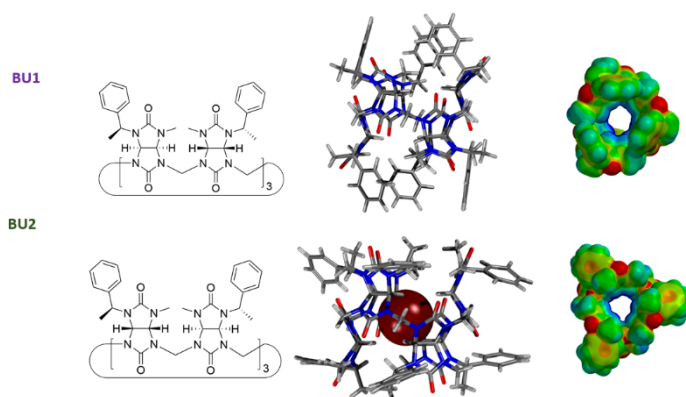


Fig. 1 Schematic representation and electrostatic surface potential of BU1 and BU2.

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