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ACCEPTED MANUSCRIPT

Communication

Selective recognition of aromatic hydrocarbons by endo-functionalized molecular tubes *via* C/N-H···π interactions

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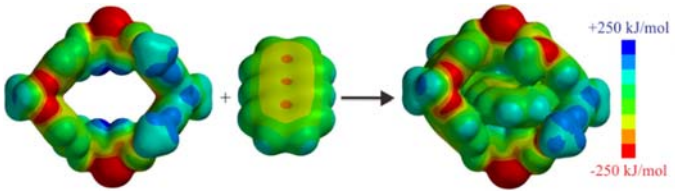
Graphical abstract



Aromatic hydrocarbons can be selectively recognized by four *endo*-functionalized molecular tubes through C/N-H···π interactions in nonpolar media with binding constants up to 1580 L/mol.

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ABSTRACT

Molecular recognition of aromatic hydrocarbons by four *endo*-functionalized molecular tubes has been studied by ^{1}H NMR spectroscopy, computational methods, and single crystal X-ray crystallography. The binding selectivity is rationalized by invoking shape complementarity and dipole alignment. The non-covalent interactions are proved to predominantly be C/N-H···π interactions.

Molecular recognition [1] is the basis of numerous biological phenomena and synthetic supramolecular chemistry, and plays pivotal roles in sensing, assembly, transport, and catalysis. During the last half of a century, most of the attention has been paid to molecular recognition of ions and functional molecules, and less synthetic receptors can selectively recognize hydrocarbons through non-covalent interactions in nonpolar media [2].

Aromatic hydrocarbons [3] are probably the largest and most structurally diverse class of organic molecules known, representing a wide range of molecular sizes and structural types. This class of molecules are considered to be highly carcinogenic [4]. Detection and removal would require efficient receptors. However, synthetic receptors for aromatic hydrocarbons are still rare [5-7]. In the crystal structures of these molecules, three interaction geometries are possible (Fig. 1a). But parallel-displaced π···π interaction [8] and edge to face C-H···π interactions [9] are the preferred geometries. Among the known synthetic receptors for aromatic hydrocarbons, π···π interaction and/or charge-transfer interaction are often harnessed and cyclophane structures are employed to position two aromatic subunits in parallel and in a well-defined distance for the intercalation of planar aromatic hydrocarbons (Fig. 1b). The prominent examples are Stoddart's ExBoxes and ExCages [6], and Würthner's perylene bisimide cyclophanes [7]. In contrast, biological receptors used C/N-

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