In Silico Design of Cylindrophanes: The Role of Functional Groups in a Fluoride Selective Host

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Molecular recognition is the key driver in the formation of supramolecular complexes, enabling the selective encapsulation of specific guests. Here, we explore the delicate balance between different energetic terms in the formation of an efficient host for fluoride anions based on a cylindrophane structure, which can be achieved by the incorporation of ligand sites into a cyanuric acid based cyclophane framework, resulting a close proximity between the ammonium hydrogens and the anion. This study describes the character and contribution of different energetic and repulsive terms that favor the efficient inclusion of fluoride. Our findings are useful for further rational design and synthesis of efficient and highly selective fluoride hosts, which have been generally less well described than complexing agents for other halides. © 2020 Wiley-VCH GmbH

Anion-?

cylindrophanes

fluoride hosts

hydrogen bond

non-covalent interactions

Negative ions

Close proximity

Complexing agents

Cyanuric acids

Cyclophanes

Fluoride anions

Rational design

Selective encapsulation

Supramolecular complexes

Fluorine compounds