RECOGNITION WITHIN REVERSED MOLECULAR CAPSULES

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Molecule-sized synthetic container molecules (capsules and cavitands) have been of continuing interest to many researchers because they provide a specific, confined nanospace as a site for recognition and catalysis. Their unique constrictive internal environment and ability to eliminate solvent's influence have been sown to cause stabilization of unusual conformations, transition states and reaction intermediates. These features can be exploited for the construction of selective sensors, gas storage media, reaction nanovessels.

Most of the currently known synthetic container molecules (capsules and cavitands) have walls composed of aromatic rings. Therefore they have smooth and hydrophobic interiors incapable of directional interactions with guests, recognition of polar guests, distinguishing of enantiomers, performing in asymmetric reactions or generation of unidirectional motion. Their nonpolar interiors are also disadvantageous for catalytic purposes. Synthetic container molecules with chiral, polar walls capable of directional interactions with guests can potentially overcome these drawbacks and therefore are of great interest.

We have succeeded in the synthesis of a series of capsular dimers with hydrophobic outer surfaces and polar and chiral interiors. High kinetic stability of the resulting polar capsules requires a non-covalent approach to the synthesis and isolation. We will discuss various aspects of supramolecular synthesis of the polar capsules and show their applications and use for basic research. For example:

- extraction and encapsulation of biologically relevant polar molecules from water phase;
- differentiation of enantiomers with detailed interaction studies based on X-ray analysis;
- model studies on the influence of water molecules on recognition;
- model studies on the guests' dynamics in restricted polar environment.

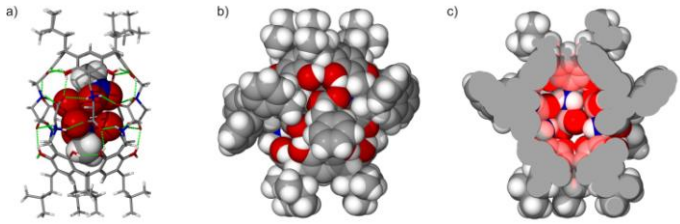

Fig. 1. X-ray structure of capsular dimer with polar cavity.

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