New and old driving forces for host-guest complexation

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The mechanistic investigation of host-guest complexation phenomena in aqueous solution aims at the identification of the dominant driving force. In the absence of electrostatic and induction interactions, only the hydrophobic effect[1] and dispersion interactions[2] are thought to prevail. However, exactly these two have proven difficult to dissect, because large alkyl residues (encountered in high-affinity binding motifs such as adamantyl or ferrocenyl) show not only higher hydrophobicity but also stronger dispersion interactions: Both driving forces operate "in the same direction", their contributions are therefore difficult to pin-point, and it is difficult to identify which one dominates. We have now constructed an aqueous host-guest system in which dispersion interactions can be readily isolated and their absolute values compared with gas-phase quantum-chemical calculations. In addition to dispersion interactions, we will show that cavitation energy recovery can become the dominant driving force for host-guest complexation.

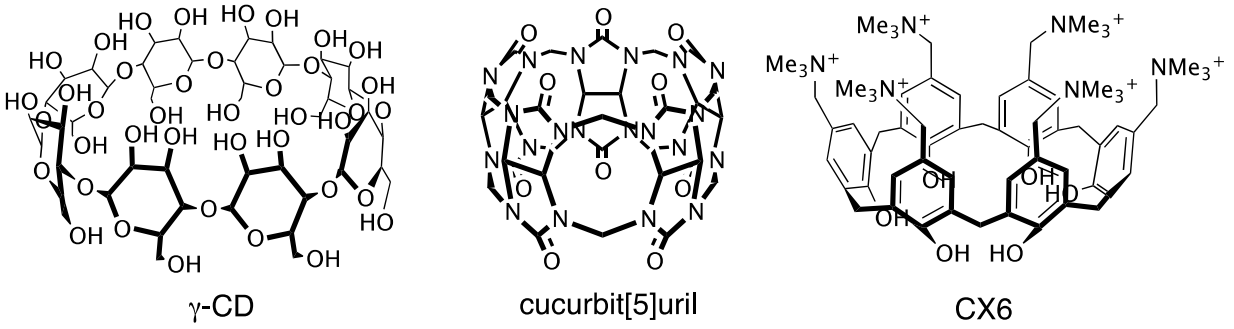

Figure 1. Water-soluble macrocycles capable of encapsulating guest molecules.

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