Redox-Switchable Cavitands: Molecular Grippers

Significance: Here, a diquinone-based resorcin[4]arene cavitand goes from a kite to a vase form when reduced. The vase forms via hydrogen bonding between the central diols and the oxygens of the amides. This vase is stable even at –80 °C and can be used to capture the small molecule guests shown above. The molecules are shown in order of increasing association constant $K_a$. The vase cavitand releases the guests upon oxidation.

Comment: Both the kite and vase form are stable in deuterated chloroform, tetrahydrofuran, and mesitylene. After two to four days, the reduced form reverts into the oxidized form. A crystal structure of the reduced form has a 7.3° cavity, which allows it to encapsulate the solvent molecule mesitylene, as well as the larger guest molecules.

Small molecule guests:

order of increasing association constant ($K_a$)