

Chemistry inside the cavity of a flexible coordination cage

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The hydrophobic cavities of water-soluble coordination cages often serve as minimal models of enzymatic active sites; however, most cages investigated so far are relatively rigid. In this talk, I will review our studies of a Pd₆L₄ coordination cage that combines high water solubility, high conformational flexibility, and a readily accessible hydrophobic cavity. Owing to its flexible structure, the cage can adapt to and stabilize a variety of structurally diverse organic guests, as well as structurally different isomers of photoresponsive molecules, such as spiropyrans and azobenzenes, thus supporting their reversible photoswitching. Small aromatic guests, such as anthracenes and BODIPYs dyes, are encapsulated as dimers to afford inclusion complexes of a 2:1 stoichiometry; such noncovalent dimerization can significantly affect the optical properties of the encapsulated molecules. In the presence of two small guest molecules, ternary complexes are possible, whereby the cage facilitates the noncovalent dimerization of, e.g., BODIPYs with anthracenes. Taking advantage of the reversible, light-induced anthracene dimerization, we developed a light-controlled fluorescence switch whereby BODIPY's emission can be toggled between high and low values through rapid guest exchange between the cages.

