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Confinement and Catalysis in Chiral, Self-Assembled, Nanoscale Flasks

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The metal-ligand host shown below binds cationic guests selectively and strongly in water (K_a up to 10⁵ M⁻¹) [1, 2]. Isotope effects on guest binding and exchange are observed [3]. Applied and solvent internal pressures are shown to increase the barrier to bond rotation in encapsulated guests [4]. This host is shown to catalyze the cyclization of monoterpene derivatives while excluding water from reactive intermediates. This property is also observed in an enyne cyclization by an encapsulated gold catalyst [5]. Moreover, the host is used to increase the rate, turnover and stability of encapsulated transition metal catalysts in aqueous solution [6, 7]. Encapsulation of these catalysts is also shown to improve the yields and enantioselectivities of tandem catalytic processes with enzymes [8]. The high affinity of polyamine ligands for the host interior is used to drive their coencapsulation with transition metal cations [9].



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