Binding and release of Sulfide and Hydrosulfide Anions in Water by Bambusuril Macrocycles

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Abstract

Hydrogen sulfide (**H**₂**S**) has become an important target for research due to its physiological properties and potential applications in medicine.¹⁻³ Many synthetic molecules have been reported as exogenous H₂S sources, which rely on chemical reactions for the delivery of the H₂S.⁴⁻⁶ Bambusurils (**BU**) are a family of host macrocycles that bind inorganic and organic anions with high affinity and selectivity in both organic and aqueous media.⁷⁻⁹ In this work, supramolecular binding of sulfide (**S**²⁻) and hydrosulfide (**HS**⁻) anions by a synthetic receptor in water have been studied for the first time. Bambusuril macrocycles (**BU**) were used to stabilize these anions in its cavity following by their release into water.¹⁰

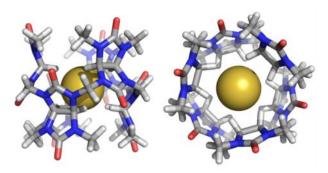


Figure 1. Energy-optimized geometry of the Bambusuril complex with sulfide anion.

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