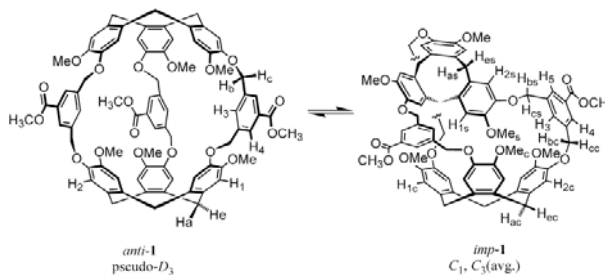


W0200

Designer Molecular Container Materials: Crystal Structures and Thermal Properties of Cryptophane Materials. S.T. Mough, J.C. Goeltz, K.T. Holman, Georgetown Univ., 37th and O St., NW, Washington, DC 20057, USA.

Cryptophanes are a class of “molecular container” molecules known to bind gases, cations and lipophilic species in solution. Their enforced cavities, highly symmetric structure, and modular design make them interesting targets for crystal engineering, particularly as porous solids. Though cryptophanes have been studied extensively in solution, little is known about the detailed structures of the corresponding encapsulated complexes, or the

kinetic stabilities of the corresponding solid-state inclusion compounds. To this end, the single X-ray crystal structures and thermal stabilities of a variety of cryptophane host-guest inclusion compounds will be reported. Notably, a solid-state atropisomerization reaction was discovered, and we report the first crystal structure of an *imploded* cryptophane.



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