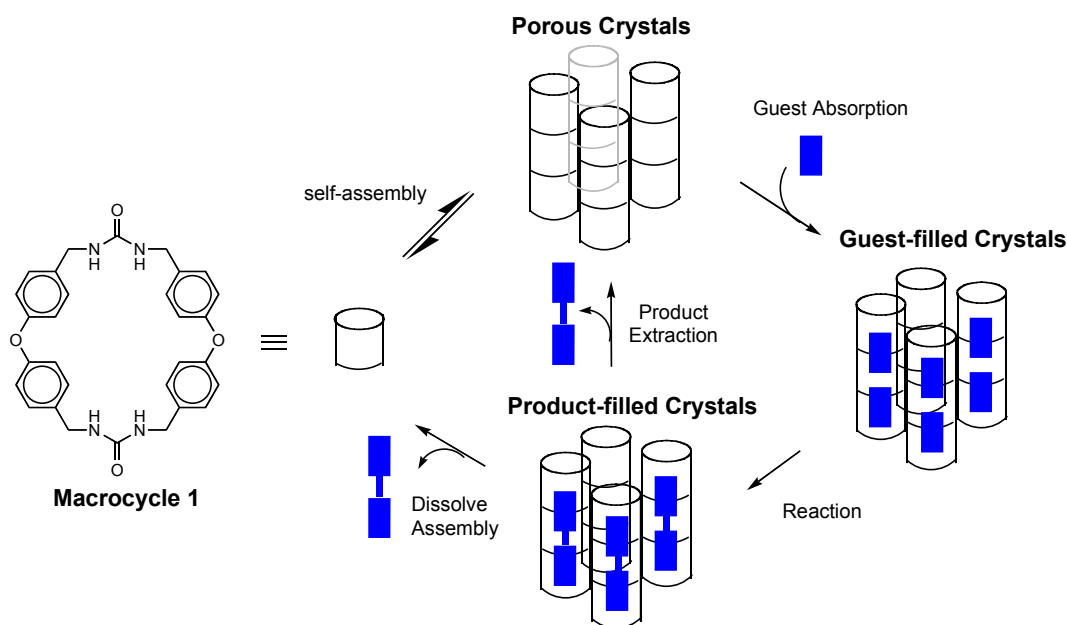


Macrocyclic ureas: A simple building block for supramolecular structures

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Abstract: There is great interest in developing new building blocks that predictably self-assemble into well-defined supramolecular structures. We have utilized the self-assembly of simple, rigid macrocyclic bis-ureas to reliably form columnar structures. Larger macrocycles assemble into porous crystals containing channels of predetermined dimensions. The self-assembly of these monomers is directed by the formation of strong urea-urea hydrogen bond and by the stacking of the aromatic surfaces in the linkers. This approach is innovative because it allows the rational design of the size, structure, and functionality of the channel by altering the structure of a small molecule, a macrocyclic bis-urea. We have examined a series of bis-ureas varying the size, shape and interior functional groups to probe the limits of this structural motif. Several of these derivatives form porous crystals that display a type 1 gas adsorption isotherm consistent with microporous materials. These microporous crystals show reversibly absorption of guest molecules, much like zeolites. In fact, crystalline **1** can be used as a container for reactions, promoting highly stereoselective head-to-tail [2+2] photodimerizations of α,β -unsaturated ketones in high conversion.

Publications:

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