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Preface

The investigation of molecular container compounds and of their encapsulated guest(s) has become one of the most fascinating areas of research in organic chemistry. Molecular container chemistry belongs to the highly interdisciplinary field of host–guest chemistry or supramolecular chemistry, pioneered by Donald J. Cram, Jean-Marie Lehn, and Charles J. Pedersen. Molecular containers are unique spherical, hollow hosts with cavities that are large enough to encapsulate one or more guest molecules. The first molecular containers were developed about 25 years ago by Donald J. Cram (carcerands and hemicarcerands) and by André Collet (cryptophanes). Cram coined the name ‘molecular container compounds’ for these host molecules. Carcerands permanently encapsulate their guests, whereas hemicarcerands and cryptophanes have larger pores in their shell, through which guests may slowly exit or enter the inner cavity. Guests are held inside the container by intrinsic binding interactions between the guest and inner host surfaces and by constrictive binding energy, which is a form of mechanical binding and describes the steric repulsion and increased conformational energy as a guest passes through an opening in the host shell. The development of self-assembled molecular containers, pioneered by Julius Rebek, Jr., who is one of the contributors to this symposium, has led to an explosive growth of the field and of its importance. Formation of these capsules is thermodynamically controlled. They assemble spontaneously with high precision and efficiency from up to 50 smaller building blocks, thus paralleling similar capsule assembly processes in nature, such as that of virus capsids, chaperon protein complexes or the iron storage protein ferritin. Since Rebek’s first report of a hydrogen bonded dimeric capsule, a multitude of discrete self-assembled capsules, held together by non-covalent interactions, such as hydrogen bonds, metal–ligand bonds or van der Waals forces,

have been developed or serendipitously discovered. In fact, the reader will find that many of the contributions to this symposium describe preparation, properties and/or applications of self-assembled capsules.

Much of the attractive character and fascination of molecular container chemistry lies in the design and synthesis of novel containers, in the exploration of their structural, dynamic, and molecular recognition properties and in the investigation of the guest’s properties and reactivities. Most remarkable, in my opinion, is the use of covalent and self-assembled container molecules as nanoreactors. As such, molecular containers allow generation and stabilization of otherwise fleeting reactive intermediates and have catalyzed and completely changed the course of chemical reactions. This special issue highlights some of these aspects in container chemistry and provides the reader with a snapshot of the current status of this rapidly expanding field.

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