

Heterocyclic Supramolecules II

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Preface

Explanation of the structure-property relationship of a given molecule is generally simple because the characteristics of the atomic groups and chemical bonds and the effects emerging from their interaction have long been known, both from theoretical studies and numerous experimental results. In contrast, it is often difficult to analyze, estimate, and account for the structure-properties relationship in supramolecules. The characteristics of supramolecules are governed both by the nature of the constituent molecules and by their configuration while the characteristics of the constituent molecules are usually evident as mentioned above; their configurations are difficult to control, predict, and accurately estimate because of insufficient knowledge regarding the intermolecular forces. Moreover, since most of the intermolecular forces constructing supramolecules are weak, the supramolecular structure may vary depending on various factors, such as modification of the molecular structure, auxiliaries, and experimental conditions. Thus, in order to obtain supramolecules with the desired structures and properties, theoretical investigations on the intermolecular forces and accumulation of experimental studies on the relationship between the supramolecular structure and properties are both important.

In line with this, the present volume, *Topics in Heterocyclic Chemistry: Supramolecular Chemistry II*, which is a continuation of *Supramolecular Chemistry I*, is a review of recent studies on intermolecular interactions connecting (and occasionally repelling) the molecules together with a few individual topics including formation, structure, and function of crystalline-state host-guest supramolecular systems and intelligent supramolecular nano assemblies and highly stereoselective 1,3-dipolar cycloaddition catalyzed by supramolecular complex. In all chapters, the unique characteristics of heterocyclic moieties play a significant role.

The first chapter, “X/ π Interactions in Aromatic Heterocycles: Basic Principles and Recent Advances” by N. Hayashi, H. Higuchi, and K. Ninomiya, reviews recent theoretical and (partly) experimental studies on inter- and intramolecular interactions as the constructing forces of the supramolecules, which include π/π , CH/ π , cation/ π , anion/ π , OH/ π , NH/ π , and lone-pair/ π interactions, and the interplay of π/π interaction and hydrogen bonding. Unlike the other chapters in Volumes I and II, which have no apparent relationship, this chapter can be regarded as an introduction to the overall theoretical fundamentals.

The second chapter, “Supramolecular Host–Guest Chemistry of Heterocyclic V-Shaped Molecules” by R. Bishop, describes crystalline-state inclusion behavior of C_2 -symmetrical V-shaped host compounds consisting of heterocyclic moieties. The guidelines of the design and synthesis of the host molecules are also documented.

The third chapter, “Inclusion and Optical Resolution of Guest Molecules by Selected Synthetic Dihydroxy- and Trihydroxy-Host Compounds Containing Heterocyclic Scaffolds” by M. Caira and K. Tanaka, describes inclusion properties and crystal structures of TADDOL host compounds, which have a heterocyclic backbone and bear two or more hydroxy groups. The optical resolution of guest components is also discussed with reference to the structure of the host molecules.

The fourth chapter, “Supramolecular Structures and Nanoassemblies of Oligothiophenes and Tetrathiafulvalenes” by M. Iyoda, T. Nishinaga, and M. Takase, describes structure, conductivities, and optical properties of intelligent supramolecular nano-self-assemblies (nanofibers, nanoparticles, etc.) consisting of oligothiophenes and tetrathiafulvalene (TTF) derivatives. The results will provide important information for developing molecular electronics based on organic molecules.

In the final chapter, “Asymmetric 1,3-Dipolar Cycloaddition Reactions Catalyzed by Heterocycle-Based Metal Complexes” by H. Suga, highly enantioselective 1,3-dipolar cycloadditions are described, where the supramolecular catalysts consisting of metal cation and chiral heterocyclic ligands play a significant role.

This volume was originally edited by Professor Kiyoshi Matsumoto, who was also an Editor of *Topics in Heterocyclic Chemistry: Supramolecular Chemistry I*. Unfortunately, however, he died in the summer of 2008, before its completion. It was then taken over by us and completed according to his original plan, except for the missing chapter by Prof. Matsumoto himself. This volume, as well as *Supramolecular Chemistry I*, incorporates all the latest advances in heterocyclic supramolecular chemistry. We believe that the articles published in the two volumes will encourage progress in this area, and are sure that they will become an enduring monument of Prof. Matsumoto, a great master of heterocyclic supramolecular chemistry.

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