

s9.m3.p15 **Catenanes, Rotaxanes and Knots: From Small Building Blocks to Mechanically Interlocked Molecules.** M. Nieger^{a)}, F. Vögtle^{b)}, ^{a)Institut für Anorganische Chemie und} ^{b)Kekulé-Institut für Organische Chemie und Biochemie der Universität Bonn, Gerhard-Domagk-Str. 1, D-53121 Bonn.}

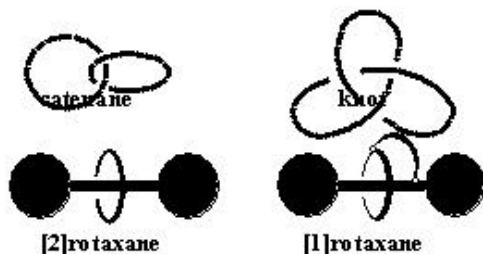
Keywords: supramolecular chemistry, mechanical interlocked molecules, non-covalent interaction.

The design of mechanically interlocked molecules such as catenanes, rotaxanes and knots present a range of novel structural and chiroptical properties and nonclassical type of chiralities. They represent intertwined polymembered rings and interlocked species and are fascinating because they are tied together in an unusual way.^[1]

The crystal structures of amide type (CONH) based catenanes, rotaxanes and knots are presented. They are synthesized from a limited number of small building blocks. The hydrogen bond pattern and non-covalent interaction are discussed in detail.

The crystal structures of the out/out and in/out isomer of amide based furano-catenanes,^[2] amide based catenanes and catenanes, where an amide group is substituted by a sulfonamide group,^[3] are presented and compared.

For the first time X-ray crystal structures of amide based [1]rotaxanes and the [2]rotaxane from which they were derived are shown.^[4] Typical non-covalent interactions as a basis of molecular recognition are observed in the crystal structure of a pyridino-[2]rotaxane. This is also an important pattern in the crystal structure of the first knot with 12 amide groups.^[5]



s9.m3.p16 **Calix[6]Arenes : A Supramolecular Approach For The Modeling Of The Active Site Of Metalloenzymes.** M. Giorgi[A], O. Seneque[B], M.-N. Rager[B] and O. Reynaud[B]. *a) Laboratoire de Cristallogénie, UMR 6517, Centre Scientifique de Saint-Jérôme, av. Escadrille Normandie Niemen, 13397 Marseille cedex 20, France. b) Laboratoire de Chimie et de Biochimie des Complexes Moléculaires, UMR CNRS 7576, ENSCP, 11 rue Pierre et Marie Curie, 75231 Paris cedex 05, France.*

Keywords: zinc-containing enzymes, calix[6]arenes, X-ray structures.

A great number of biological processes are controlled by metal-containing enzymes and it has become a challenge to understand the mechanism involved in these reactions.

In order to understand the catalytic mechanism of a family of Zinc-containing enzymes (carboxypeptidase, carbonic anhydrase, adamalysin II... which share a common structural motif : a mononuclear metal center coordinated to three histidines and a water molecule)[ref.1], a strategy based on the synthesis of calix[6]arene ligands bearing three imidazol groups has been elaborated as a logical development of previous works on mononuclear enzymes models[ref.2].

The advantage of this novel family of ligands is to provide a constrained tetrahedral environment for the cation as well as a conic hydrophobic cavity in which an organic substrate can selectively interact with the metal.

The work presented here will focus on the X-ray structures resolved for Zn- and Cu-calix[6]arene complexes obtained with different organic coordinating substrates.

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