

The condensation of imines has been of great importance to chemists for over a century. This reaction is widely used to obtain not only huge macrocycles, but also to obtain large organic cages with well-defined shapes and sizes. Organic imine cages (OICs) and related amine macrocycles have gained attention in the field of synthetic organic chemistry for their strikingly beautiful structures and valuable applications.

Extensive research has shown that properly designed starting materials using the self-sorting process together with electronic, steric and solvent effects have a huge impact on the formation of the desired structures with the valuable functions. Such self-sorting / self-selecting procedures have the amazing ability to steer a system towards creating a specific product from a complex set encompassing a multitude of equally likely other possible architectures.

Research interest in this area has grown steadily since the discovery of organic imine cages as porous materials. In addition to the porosity and structural beauty of these compounds, the importance of OICs mainly lies in their good solubility in common organic solvents; which facilitates their processing and the preparation of complex materials for the separation of small molecules, detection, obtaining nano-particle templates or as molecular building blocks for the synthesis of polymers. In the last few years, a great number of research has been published on shape-persistent three-dimensional metallocsupramolecular systems and imine cages constructed of di- / trialdehyde and di- / triamine cores.

Some supramolecular cage compounds show remarkable properties: they can, for example, stabilize reactive molecules such as white phosphorus, or allow "extraordinary reactions" such as the Diels-Alder reactions running with unusual regioselectivity. Among the wide variety of organic cages in existence, imine-based structures are among the most attractive due to their easy formation, made possible by the truly dynamic nature of imine bonds. Due to this nature of imine bonds, the process of "self-healing" of the formed molecules becomes possible, consisting in the formation of the most thermodynamically stable structures. These types of compounds can also be thought of as molecular boxes or capsules that have the property of storing other smaller molecules, enabling nano-reactions, mimicking enzymes and targeted delivery of e.g., drugs.

The scientific goal of the project is to synthesize and study the properties of molecular cages derived from tetraaldehydes and mainly di- and triamines, therefore the second goal is the synthesis of appropriate tetraaldehydes on a preparative scale. Such molecular cages will be tested for binding guest molecules, and also checked to see if they complex metal ions, which is another goal of the project. It should be emphasized that, at present, there are few examples of such cage compounds. The reason is probably the commercial unavailability and difficult synthesis of tetraaldehyde precursors. The rarity of such structures was the reason for undertaking this research.

Preparation of molecular cages will include two methods: 1) Direct condensation of tetraaldehydes with polyamine compounds carried out under variable conditions (solvent, temperature and template) will provide polyimine cages that will be reduced to appropriate amine derivatives. 2) Step-wise synthesis will be the expansion of tetraaldehydes to primary tetraamines using Boc-protected diamine or triamine compounds, followed by reduction of the imine bonds and deprotection of the Boc groups. This approach will enable formation of extended tetraamines. Subsequent condensation of this expanded precursor with another tetraaldehyde molecule and reduction should yield the desired amine cage.

We are particularly interested in chiral imine and amine cages, which will be tested for their fundamental properties, molecular (and / or chiral) recognition, as porous materials or for detecting harmful organic pollutants. The final goal of the project is to try to complex cage compounds with metal ions. We hope to obtain various multinuclear complexes with interesting magnetic, luminescent or redox properties. At the moment, it is difficult to predict the exact properties and potential application of the cage compounds that do not exist yet, but it should be emphasized that such structures are still published in "top journals".