University of Salerno

Department of Chemistry and Biology "Adolfo Zambelli"



PhD Thesis in Chemistry XXXIII Cycle

Study on Calixarene Threading: Towards Molecular Machines

Tutor:

Prof. Placido Neri

PhD Student:

Veronica Iuliano

8800100034

Co-Tutor:

Prof. Carmine Gaeta Prof.ssa Carmen Talotta **Coordinator:** Prof. Claudio Pellecchia

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Abstract

Over the past three decades, the use of calixarenes as macrocyclic hosts in supramolecular chemistry has gained an increasing relevance, especially for the construction of molecular devices. Therefore, it is important to understand how to modify the supramolecular abilities of these macrocycles. In this PhD thesis, the threading abilities of calix[n] arenes with ammonium axles have been studied by modifying the calixarene scaffold. Initially, new hosts were obtained by functionalizing the upper rim, the lower rim, or the methylene bridges (**Figure 1**). From these studies, important information was gained to obtain increasingly stable interpenetrated systems.



Figure 1. Sketched functionalization for the new calixarene hosts here studied.

Subsequently, a trivalent calixarene host (**Figure 2, left**) was studied which led to the formation of multicomponent systems such as pseudo[3]- and -[4]rotaxanes. Finally, studies on self-sorting processes in pseudo[3]rotaxane systems (**Figure 2, right**) have been carried out. Thus, the peculiar ability of some diammonium axles to select the calixarene partner in the presence of other macrocycles has been highlighted. Furthermore, the selection takes place in a stereocontrolled way leading to the formation of selected stereo-adducts over those theoretically possible.

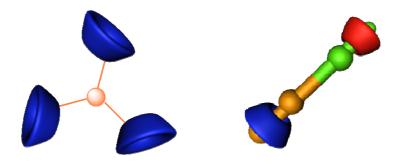


Figure 2. Studied multivalent systems.