

TOWARDS AN ALLOSTERICALLY CONTROLLED SYNTHESIS OF A [2]ROTAXANE

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Rotaxanes are molecular assemblies belonging to the family of mechanically interlocked molecules (MIMs).^[1] In the case of [2]rotaxanes, they are composed of a macrocycle threaded by a linear axle with two bulky end groups to prevent the dissociation of the subcomponents.^[2]

The goal of this project is to synthesize a [2]rotaxane (Fig.1c) in which the traditional macrocycle is replaced by a molecular cage described in the laboratory.^[3,4] This cage is composed with two zinc porphyrins as recognition sites for guest molecules, and triazoles as allosteric sites to control the opening/closing of the molecular cage.^[5] This allows the transition from a so-called flattened conformation to an open conformation by the addition of four equivalents of silver(I) ions that are coordinated to the triazoles (Fig.1a).

The assembly of the pseudo-rotaxane will take advantage of this allosteric control by threading a monostoppered axle into the cage only once the cage is in its open conformation (Fig.1b). This step is followed by the addition of the second stopper to form the [2]rotaxane.

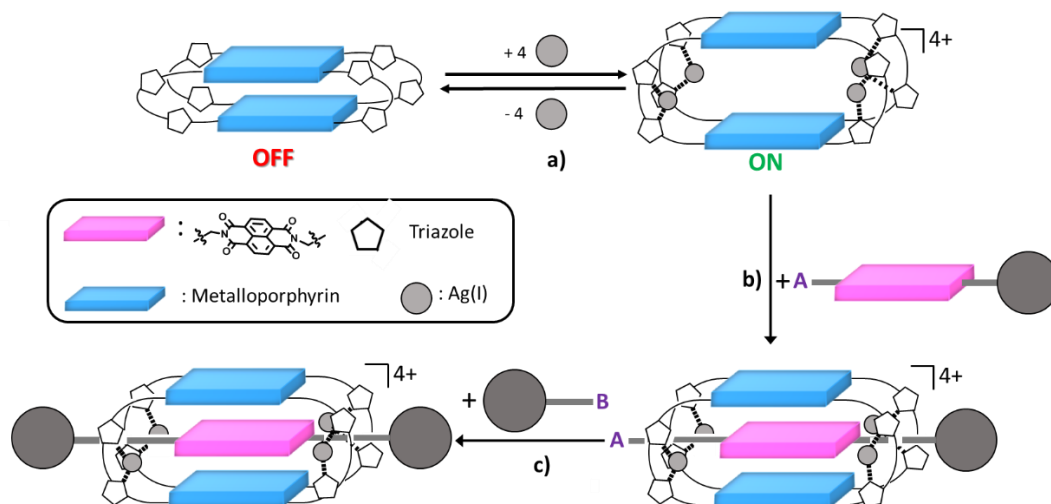


Figure 1. Scheme of the targeted [2]rotaxane

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