Abstract

Dynamic [1]Rotaxanes via Reversible Covalent Bond and Host-Guest Anion Recognition

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Mechanically interlocked molecules (MIMs) are a type of compound that is widely used in the construction of artificial molecular machines.[1] Among MIMs, the rotaxane and pseudorotaxane classes are particularly intriguing, consisting of a macrocyclic wheel threaded by the axle and having numerous applications.[2] We recently reported a novel [2]rotaxane system[3] that combines a reversible hypervalent iodine covalent bond with anion recognition properties of bambus[6]uril macrocycles.
We present racemic mono-functionalized bambus[6]uril appended with a single aliphatic carboxylate arm [1]rotaxanes(Fig. 1). The arm is forming a bis(acyloxy)iodate(I) anionic moiety that is threading through the bambus[6]uril cavity. We investigated the possibility of component exchange to facilitate carboxylic acid triggered release.[4] Furthmore, we create a new enantiomerically pure mono-functionalized bambus[6]uril and the first enantiomerically pure [1]rotaxanes based on hypervalent iodine axle. Following that, the [1]rotaxanes will be tested for chiral carboxylic acid recognition.

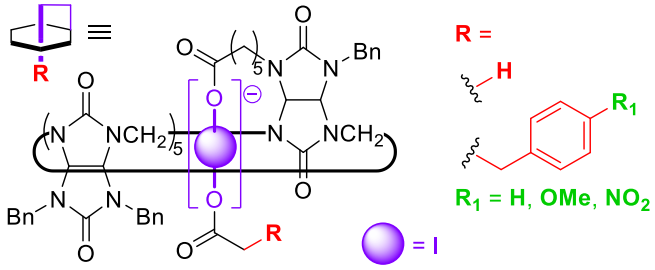

Fig. 1 Representation of the prepared [1]rotaxanes.

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(3) Kandrnálová, M.; Kokan, Z.; Havel, V.; Nečas, M.; Šindelář, V. Hypervalent Iodine Based Reversible Covalent Bond in Rotaxane Synthesis. *Angewandte Chemie International Edition* **2019**, *58* (50), 18182–18185.
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