

Abstract

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

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Mechanically interlocked molecules (MIMs) are an important class of compounds used for the construction of artificial molecular machines.¹ Within MIMs, rotaxane and pseudorotaxane classes are especially interesting, comprising a macrocyclic wheel threaded by the axle, with numerous applications.² Recently, we have reported a novel [2]rotaxane system³ coupling hypervalent iodine reversible covalent bond with anion recognition properties of bambus[6]uril macrocycles.

Herein, we report the [1]rotaxanes consisted of racemic mono-functionalized bambus[6]uril appended with a single aliphatic carboxylate arm (Fig. 1). The arm is engaged in the formation of a bis(acyloxy)iodate(I) anionic moiety threading through the bambus[6]uril cavity. We investigated the possibility of component exchange to facilitate triggered release of carboxylic acids.

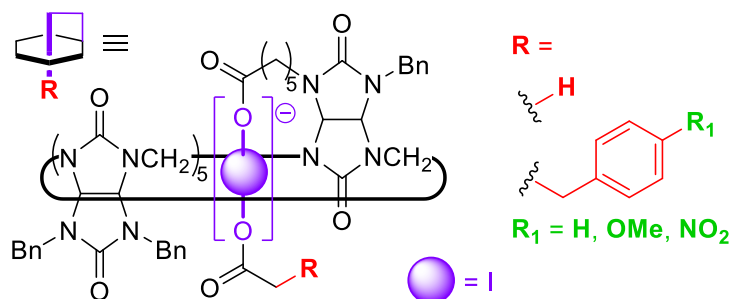


Fig. 1 Representation of the prepared [1]rotaxanes.

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1 Erbas-Cakmak, S.; Leigh, D. A.; McTernan, C. T.; Nussbaumer, A. L. Artificial Molecular Machines. *Chemical Reviews* **2015**, *115* (18), 10081–10206. <https://doi.org/10.1021/acs.chemrev.5b00146>.

2 Xue, M.; Yang, Y.; Chi, X.; Yan, X.; Huang, F. Development of Pseudorotaxanes and Rotaxanes: From Synthesis to Stimuli-Responsive Motions to Applications. *Chemical Reviews* **2015**, *115* (15), 7398–7501. <https://doi.org/10.1021/cr5005869>.

3 Kandrnálová, M.; Kokan, Z.; Havel, V.; Nečas, M.; Šindelář, V. Hypervalent Iodine Based Reversible Covalent Bond in Rotaxane Synthesis. *Angew. Chem. Int. Ed.* **2019**, *58* (50), 18182–18185. <https://doi.org/10.1002/anie.201908953>.