Rotaxane building-blocks for the easy and straightforward synthesis of interlocked molecular shuttles

Interlocked molecular machines are very appealing molecular architectures because they contain several elements that can move the ones with respect to others. The accurate control of the motions of elements in an interlocked molecule leads to, what we call, molecular shuttles, and for which the localization of each element is responsible for the physical and chemical properties of the interlocked molecule. In the field of interlocked molecules, rotaxanes hold a particular place: they consist of a molecular axle that is surrounded by a macrocycle. The two components are not covalently linked (i.e. a strong link), although they can interact through weak bonds (H bond, ion-dipole, …). Because of the high potential of such sophisticated interlaced compounds, efforts have still to be made in order to improve the ability to access to these interlaced molecules.

Fig. 1. Synthesis of a palindromic molecular shuttle (compounds 3 and 4) from an easy to make activated rotaxane building-block (compound 2)

In our recent paper, we investigated a new straightforward and very easy access to rotaxane building-blocks that can be used as “lego® blocks” for the synthesis of more sophisticated...
molecular shuttles. In particular, we report the formation of an isolable [2]rotaxane building-block (compound 2, Fig. 1) through the slipping strategy (i.e. a way that necessitates heat to make the macrocycle going through the axle extremity until it surrounds the molecular axle). The further elongation of the axle of the isolated interlocked building block 2 was then achieved with the aim of obtaining [2] and [3]molecular shuttles (i.e. an axle that is encircled by respectively one or two macrocycles and that contains several sites of interactions of different tunable affinities for the macrocycle). More particularly, the synthesis of a palindromic [3]rotaxane (i.e. a molecules 3 and 4 that can identically be “read” from the left to the right or from right to the left, and whose molecular machinery, that is to say the motion of the macrocycles, is symmetrical) was reported and its pH-sensitive molecular machinery actuated and accurately studied.

This chemical method paves the way to the easy and straightforward synthesis of various sophisticated molecular shuttles that could perform tasks.

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