Imine-bridged Rotaxanes: Structural Effects toward Imine-directed Threading and Hydrolytic Equilibrium

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Development of diverse protocols for the preparation of interlocked molecules are increasing in importance because of their promising applications as molecular devices.

We previously reported novel rotaxane synthesis based on imine bond between hydrindacene axle molecule 3A and a ring molecules 4a,b, for which we can control the subunit mobility between 1Ab and 2Ab based on hydrolytic equilibrium of imine bonds\textsuperscript{[1]}.

Here we report adaptability of imine-directed threading and hydrolytic equilibrium by using various axles (3A-C) and rings (4a-e).

Studies of threading process by using a axle 3A and rings 4a-e or 3B/4b, 3C/4a,b, revealed that the rigidities of an axle and a ring were important and the electronic effect of an aniline moiety could also affect. In equilibrium between imine-bridged rotaxane 1 and [2]rotaxane 2 under acidic hydrolytic conditions (wet CDCl\textsubscript{3}, TFA), the equilibrium ratio of [2]rotaxane was higher for the hexahydropyrene-type 2Cb than for the hydrindacene-type 2Ab, due to the increased steric hindrance between axle and macrocycle in the imine-bridged rotaxane 1Cb.

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