Synthesis of novel [2]rotaxanes using hydrogen-bonding template

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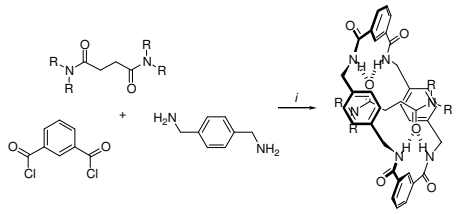
INTRODUCTION

[2]rotaxanes are mechanically interlocked molecules which and are employed in the development of new electronic devices.[1] Due to their characteristic of controlling motion (pirouetting or shuttling) the [2]rotaxanes have received much scientific interest over the last decade, especially in the development of biological machines.[1,2] Thus continuing our work[3] in this exciting area of chemistry, the aim of this study is to show the synthesis of novel [2]rotaxanes models which can later be used in molecular dynamics studies.

RESULTS AND DISCUSSION

The four novel [2]rotaxanes models were prepared by self-assembly with post-modification process through multicomponent reaction (five components). In the reactions were used different succinamides templates for the formation of amide macrocycles. In the **Scheme 1** are showed synthesis of [2]rotaxanes which exhibited different structural variations in the stoppers.



R = Pr, *i*-Pr, Bu, *i*-Bu
i = Et_3N, $CHCl_3$, 16 h, 25 °C, 17 - 29 %

Scheme 1. Synthesis of [2]rotaxanes

The [2]rotaxanes were characterized by ^{1}H NMR spectra through chemical shift differences between the thread and the [2]rotaxanes. In the **Figure 1** are showed the ^{1}H NMR spectra of **(a)** thread (R = Pr) and **(b)** [2]rotaxane (R = Pr). It is possible to establish the significant upfield shifts (e.g., δ = 0.23, 1.24, and 2.69 ppm) corresponding to the signal of hydrogens H_d, H_c, and H_b of the Pr group. The assignment is due to proximity of the meta-diamide portion of the macrocycle to the structural fragments. Additional indication of the formation of [2]rotaxane is given by chemical shift of macrocyclic methylene, $H_{E\text{-axial}}$, and $H_{E'\text{-equatorial}}$ (δ = 3.79–5.46 ppm), which are associated with the pirouetting motion between the two subunits.[3]

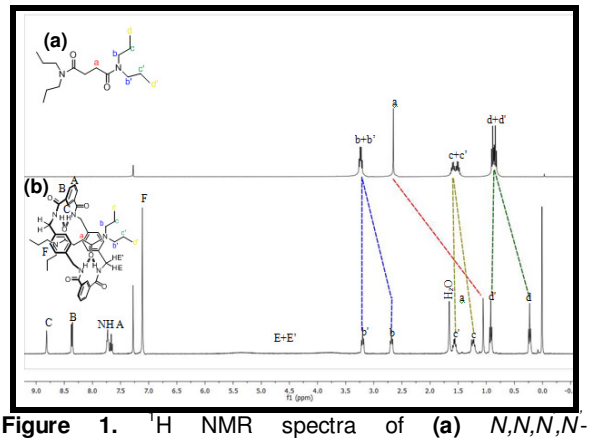


Figure 1. ^{1}H NMR spectra of **(a)** *N,N,N',N'*-tetrapropylsuccinamide and **(b)** [2]rotaxane.

CONCLUSION

In summary, we report the efficient synthesis of four [2]rotaxanes. These new compounds can be used of molecular dynamics of this rotation studies. In addition they will also use as potential models for structural and supramoleculares studies.

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