Synthesis of a [2]Catenane with Guanidine Groups for Ion Binding

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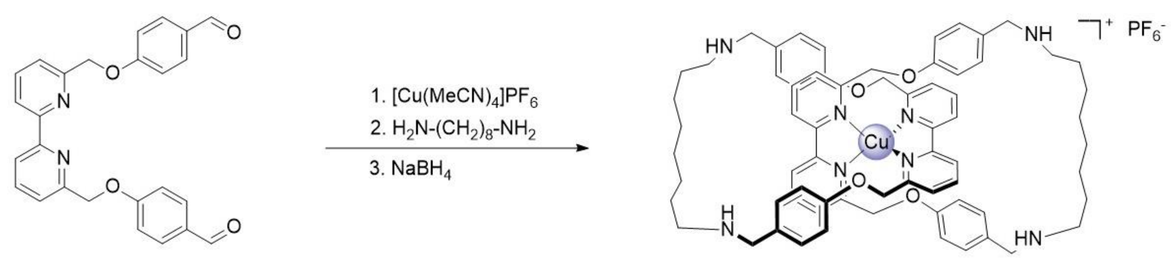
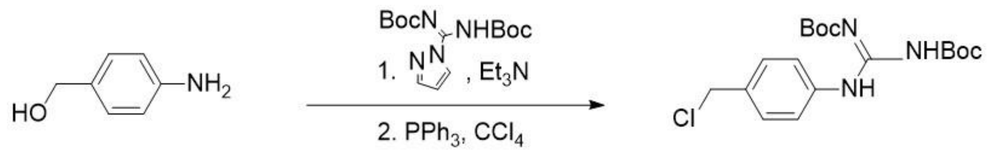
Introduction

A [2]catenane is a molecule with two macrocycles that are mechanically interlocked. In this project, a copper(I)-bipyridine [2]catenane **(A)** was used to perform a SN reaction with *N*,*N'*-bis-(tert-butoxycarbonyl)-N''-(4-chloromethyl-phenyl)-guanidine **(B).** The resulting [2]catenane with guanidine groups **(E)**, after Boc-group deprotection and demetallation, is expected to act as a molecular receptor for various ionic guests.

Synthesis of **A** and **B**

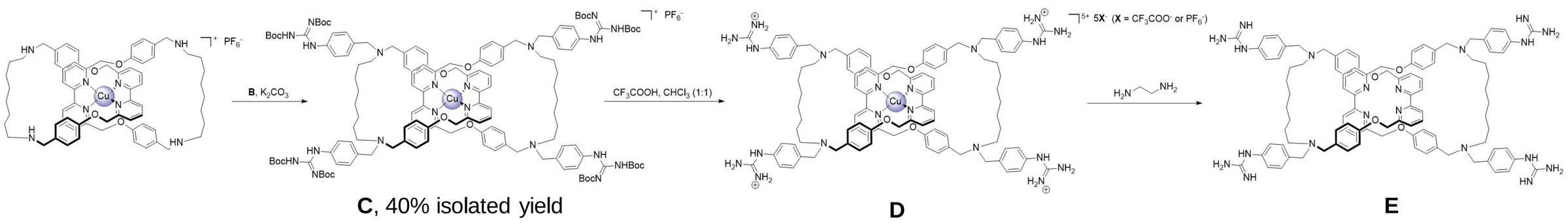


A, 36% isolated yield



B, 24% isolated yield

Synthesis of **E**

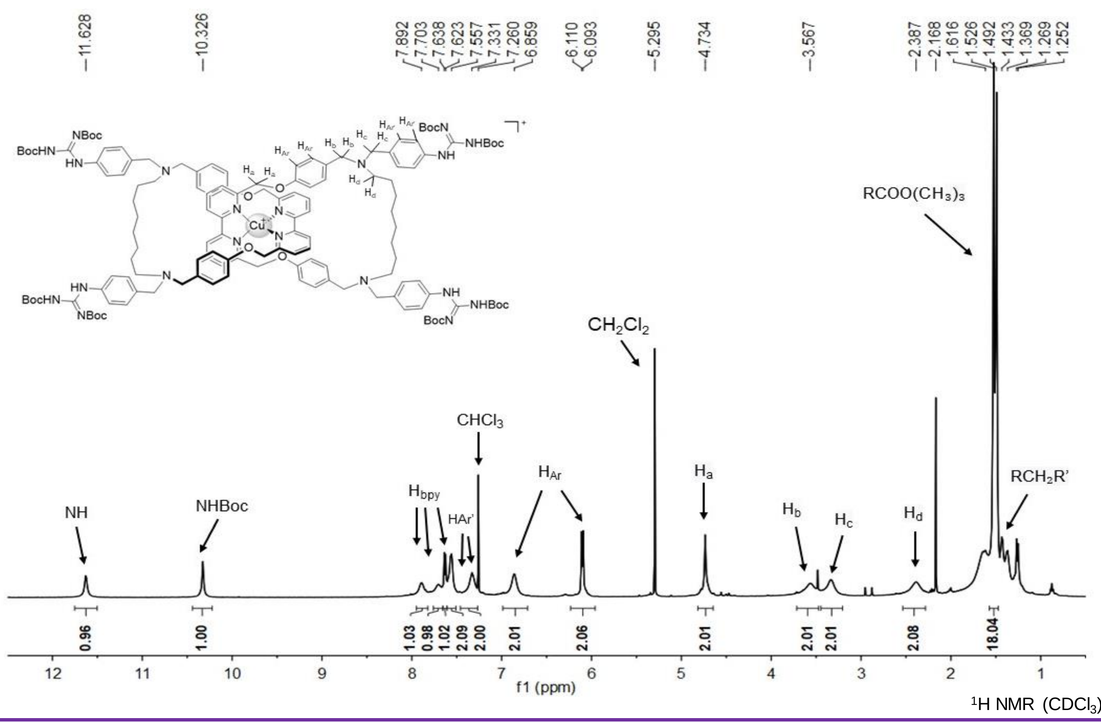


C, 40% isolated yield

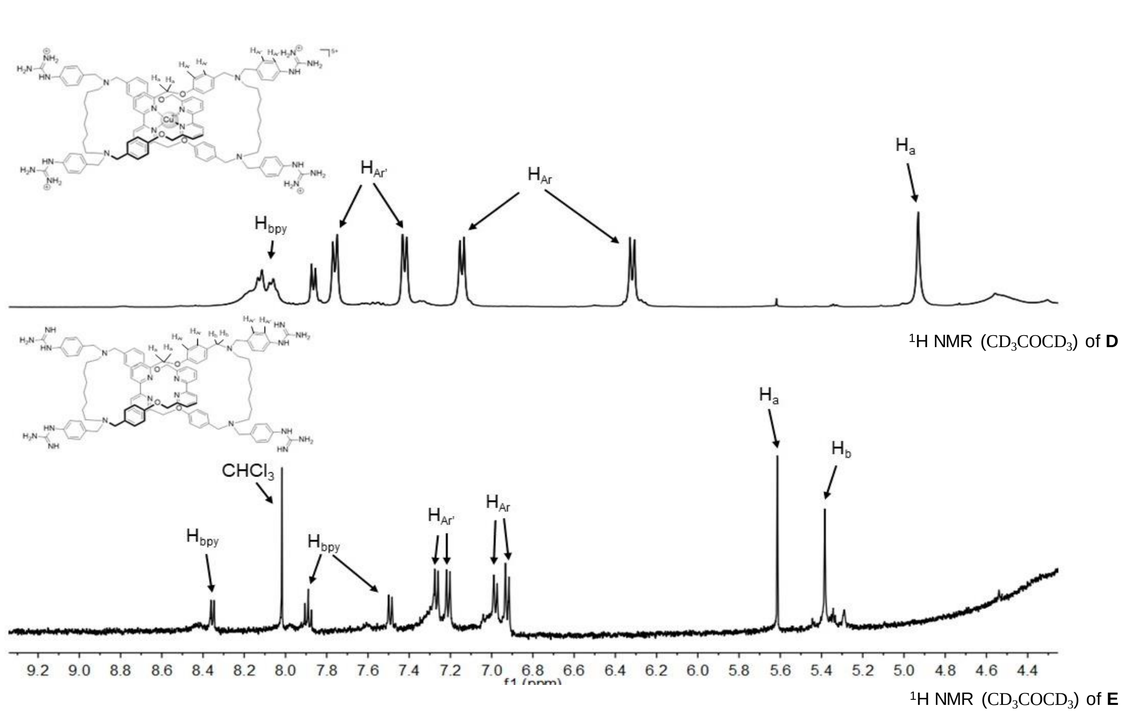
D

E

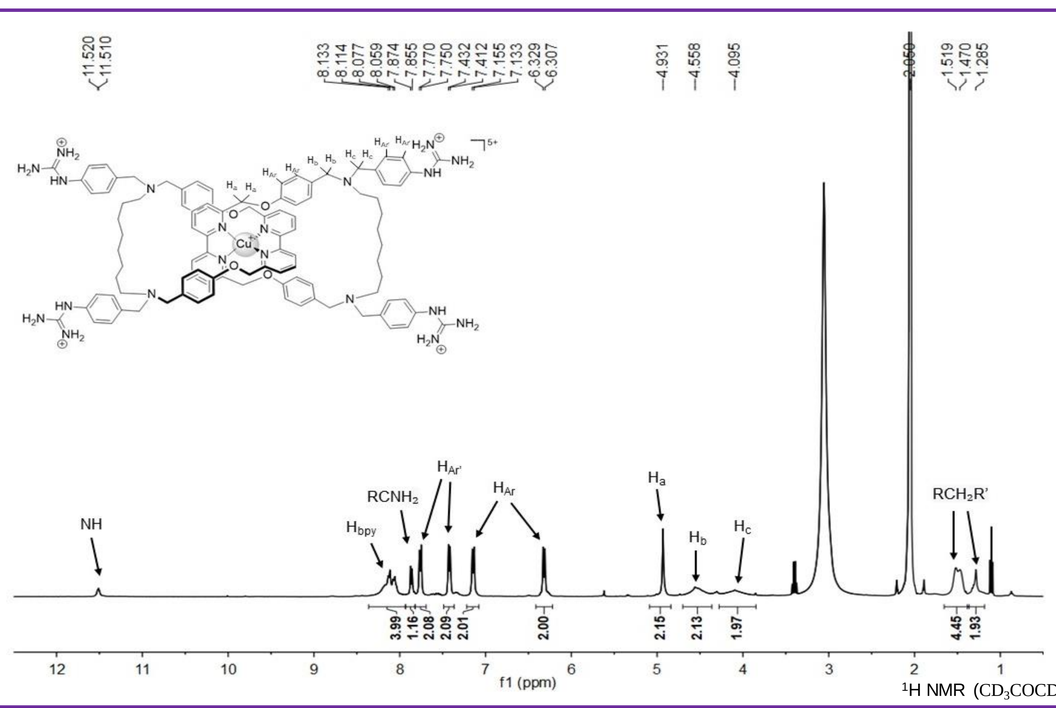
^{1}H NMR Characterization



^{1}H NMR ($CDCl_3$) of **C**



^{1}H NMR (CD_3COCD_3) of **D**



^{1}H NMR (CD_3COCD_3) of **E**

Potential Ion Binding

The mechanically interlocked **E** is expected to bind various ionic guests, with different binding affinities, as measured by ^{1}H NMR titration. It is also anticipated to undergo potential guest-induced co-conformational changes, making it suitable for the development of sensors, transporters, ion-controlled molecular switches, etc.

Acknowledgement

Thanks for the support from The University of Hong Kong and the EUREKA Project.