Electronic Supplementary Information for

Cationic all-halogen bonding rotaxanes for halide anion recognition

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1. Spectral Characterization of Rotaxanes 3.PF_6, 4.PF_6, 7, 8.PF_6

Cationic Rotaxane **3.PF_6**

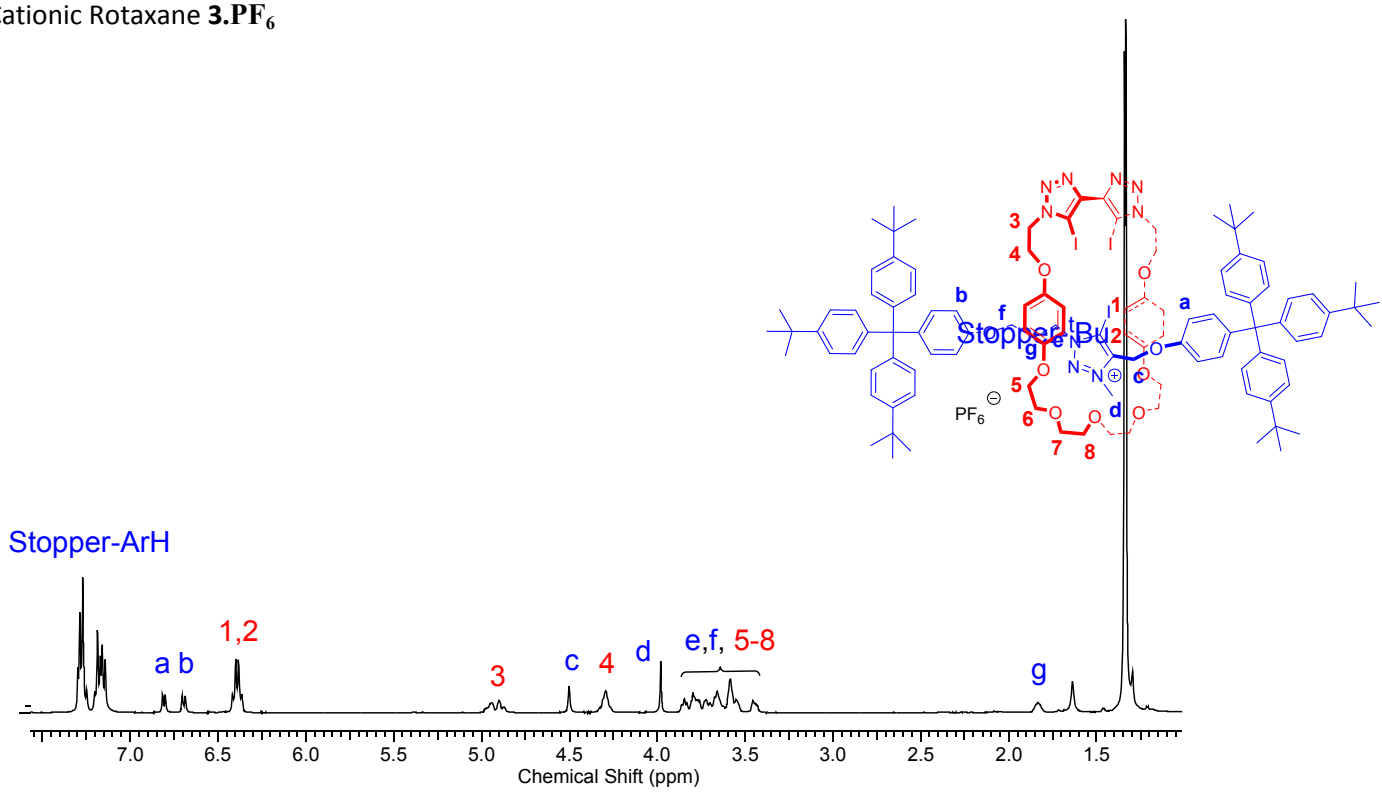


Figure S1-1. ^{1}H NMR of [2]rotaxane **3.PF_6** in $CDCl_3$ at 298 K (500 MHz).

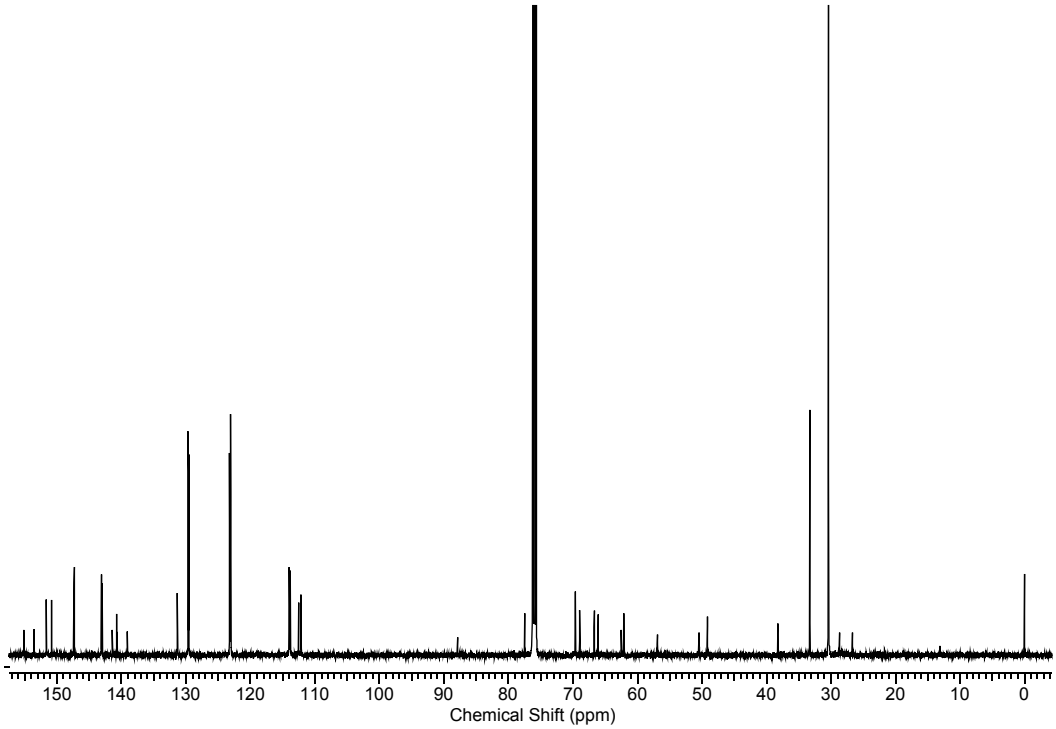
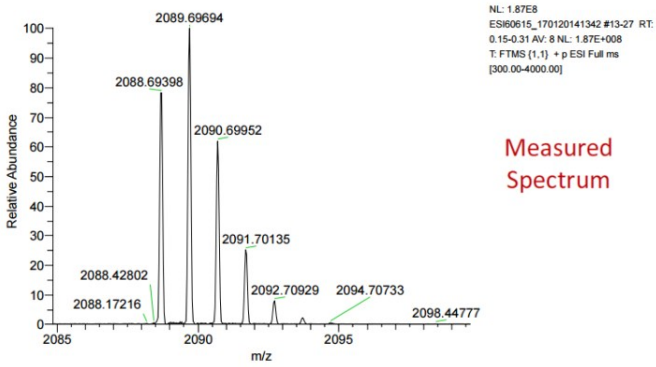


Figure S1-2. ^{13}C NMR of [2]rotaxane **3.PF_6** in $CDCl_3$ at 298 K (125 MHz).


NL: 1.87E8
ESI60615_170120141342 #13-27 RT:
0.15-0.31 AV: 8 NL: 1.87E+008
T: FTMS {1,1} + p ESI Full ms
[300.00-4000.00]
Relative Abundance
m/z
2089.69694
2088.69398
2090.69952
2091.70135
2088.42802
2088.17216
2092.70929
2094.70733
2098.44777
Measured Spectrum

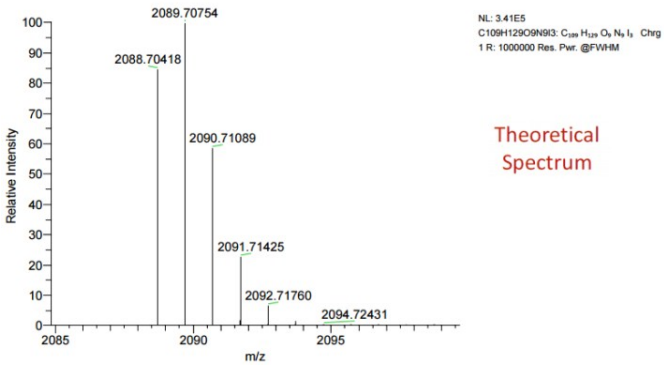

NL: 3.41E5
C109H129O9N9I3: C109 H129 O9 N9 I3 Chrg
1 R: 1000000 Res. Pwr. @FWHM
Relative Intensity
m/z
2089.70754
2088.70418
2090.71089
2091.71425
2092.71760
2094.72431
Theoretical Spectrum

Fig S1-3. High-resolution mass spectrum of rotaxane **3.PF$_6$**. Left: measured spectrum; Right: theoretical isotope model.

Cationic Re^{I}-Rotaxane **4.PF$_6$**

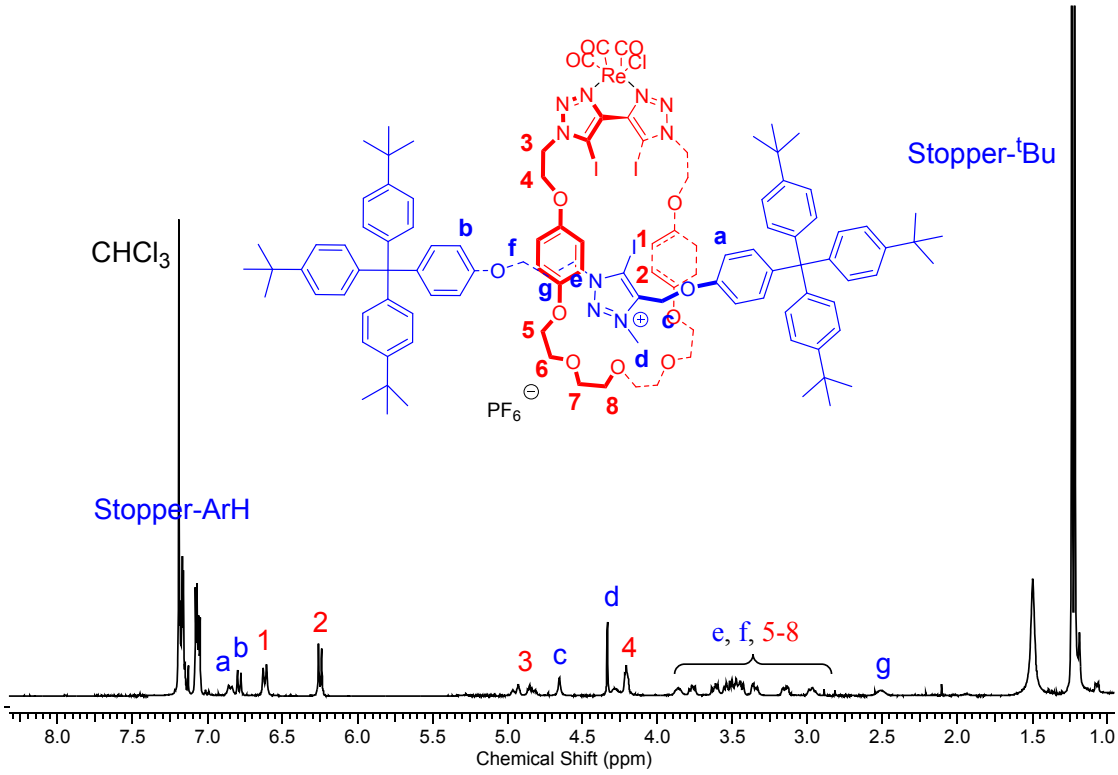


Figure S1-4. ^{1}H NMR of [2]rotaxane **4.PF$_6$** in $CDCl_3$ at 298 K (500 MHz).

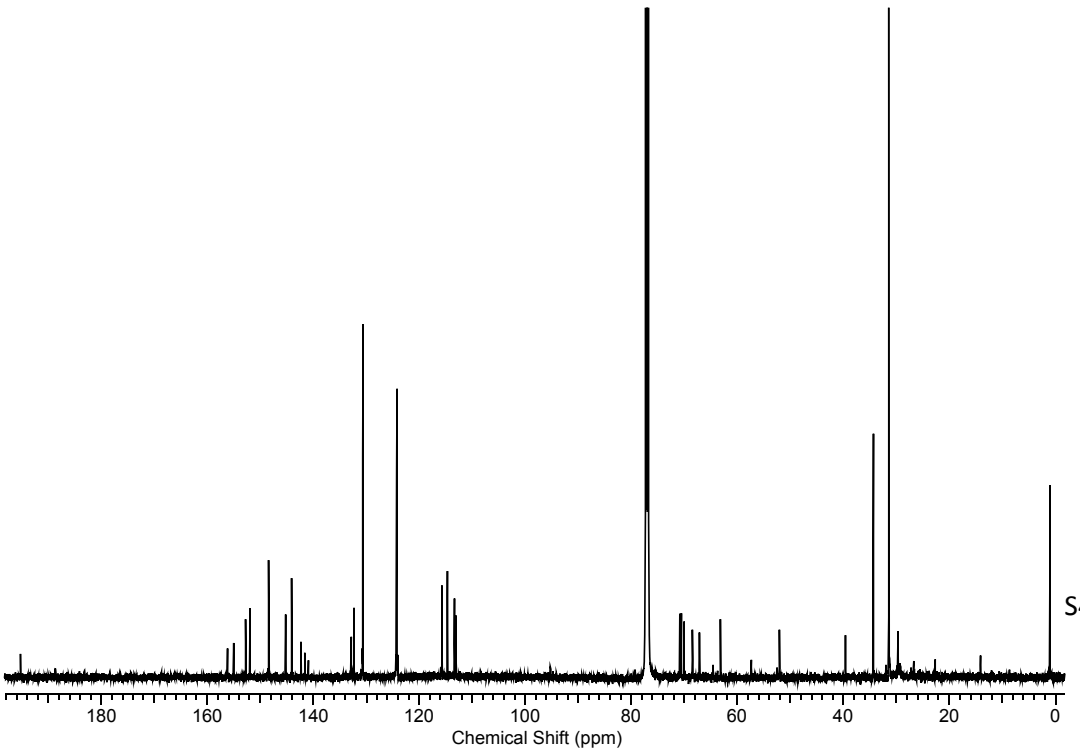


Figure S1-5. ^{13}C NMR of [2]rotaxane **4.PF_6** in $CDCl_3$ at 298 K (500 MHz).

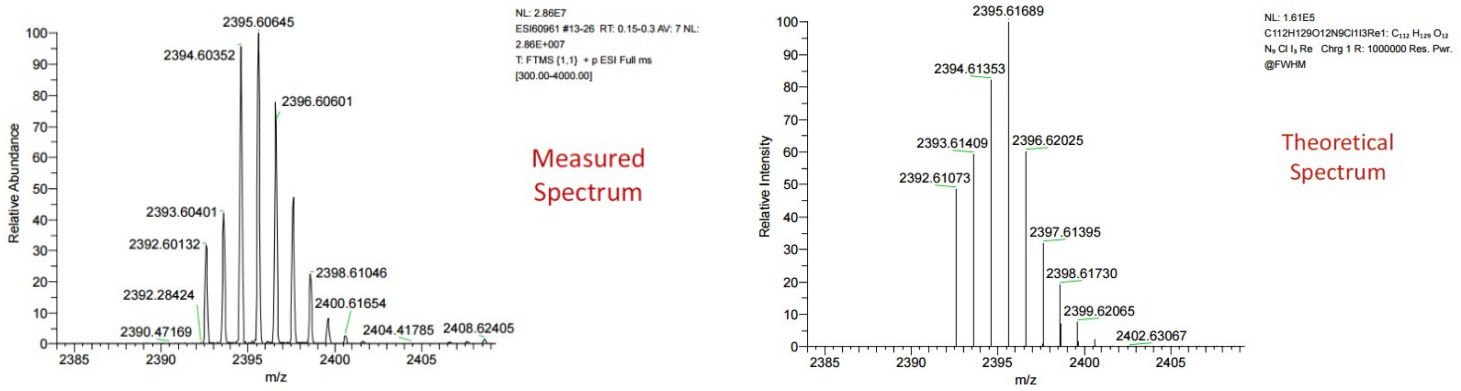


Fig S1-6. High-resolution mass spectrum of rotaxane **4.PF$_6$**. Left: measured spectrum; Right: theoretical isotope model.

Neutral Rotaxane **7**

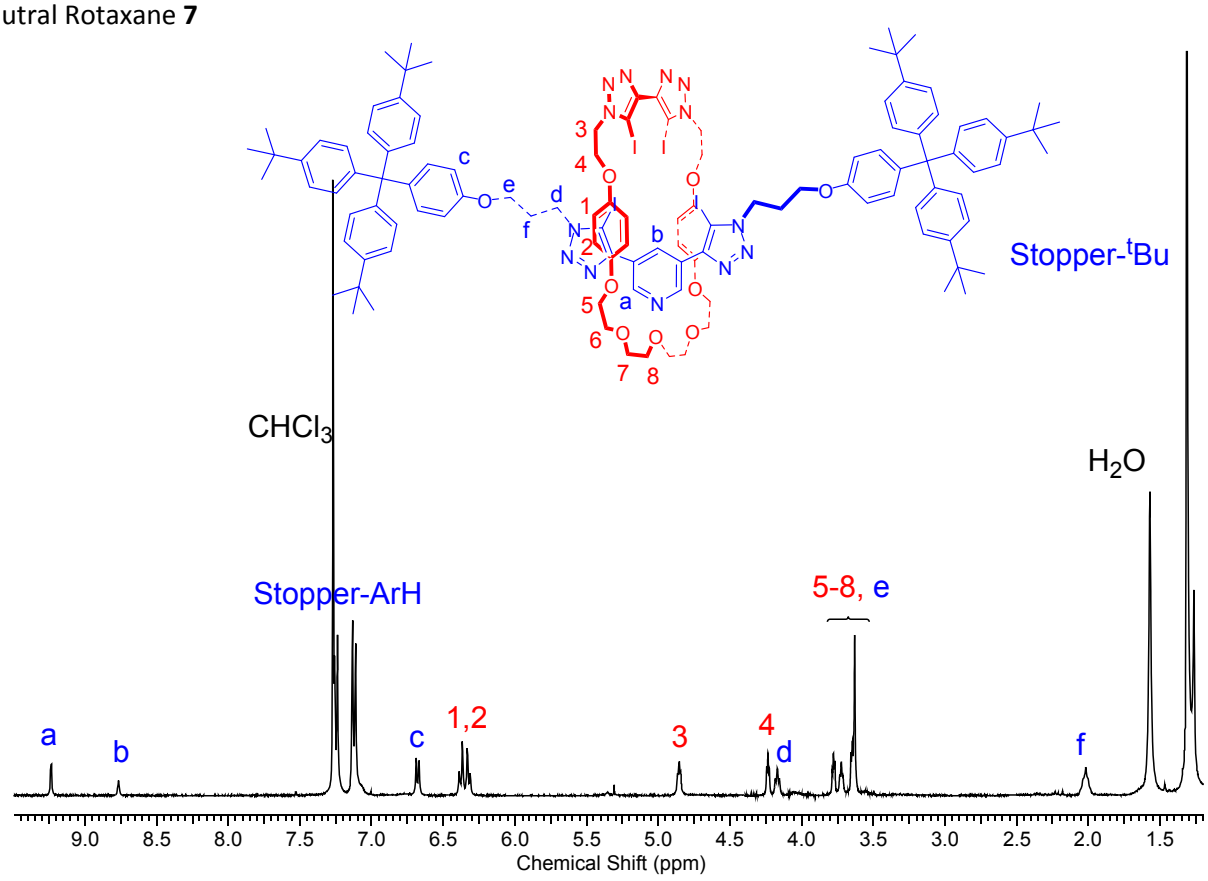


Figure S1-7. ^{1}H NMR of [2]rotaxane **7** in $CDCl_3$ at 298 K (500 MHz).

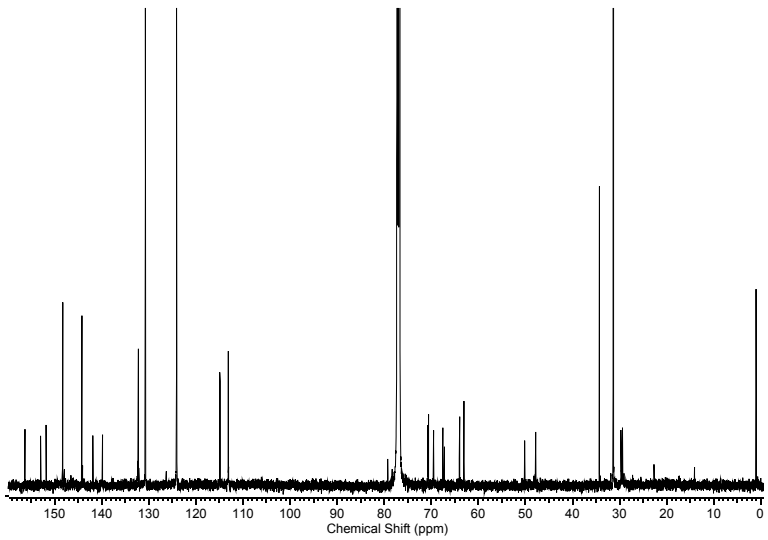


Figure S1-8. ^{13}C NMR of [2]rotaxane **7** in $CDCl_3$ at 298 K (500 MHz).

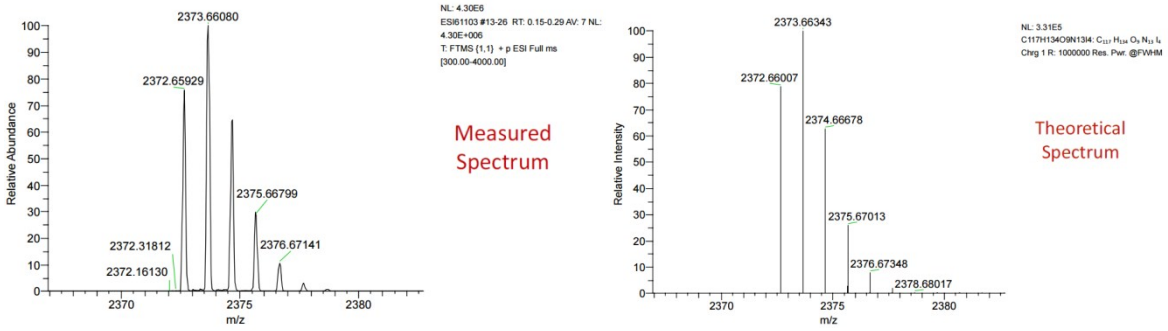


Fig S1-9.

High-resolution mass spectrum of rotaxane **7**. Left: measured spectrum; Right: theoretical isotope model.

^{1}H-^{1}H ROESY NMR

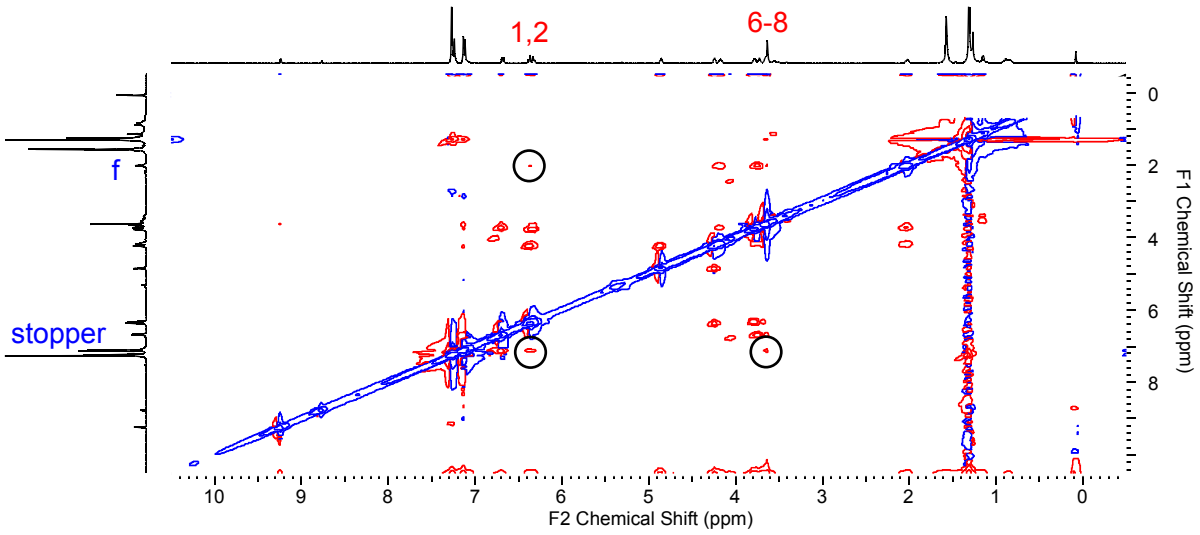


Fig. S1-10. ^{1}H ROESY spectrum of rotaxane **7** in $CDCl_3$ at 298 K (500 MHz). Cross peaks indicative of the interlocked nature of the rotaxane are circled in black.

Cationic Rotaxane **8.PF$_6$**

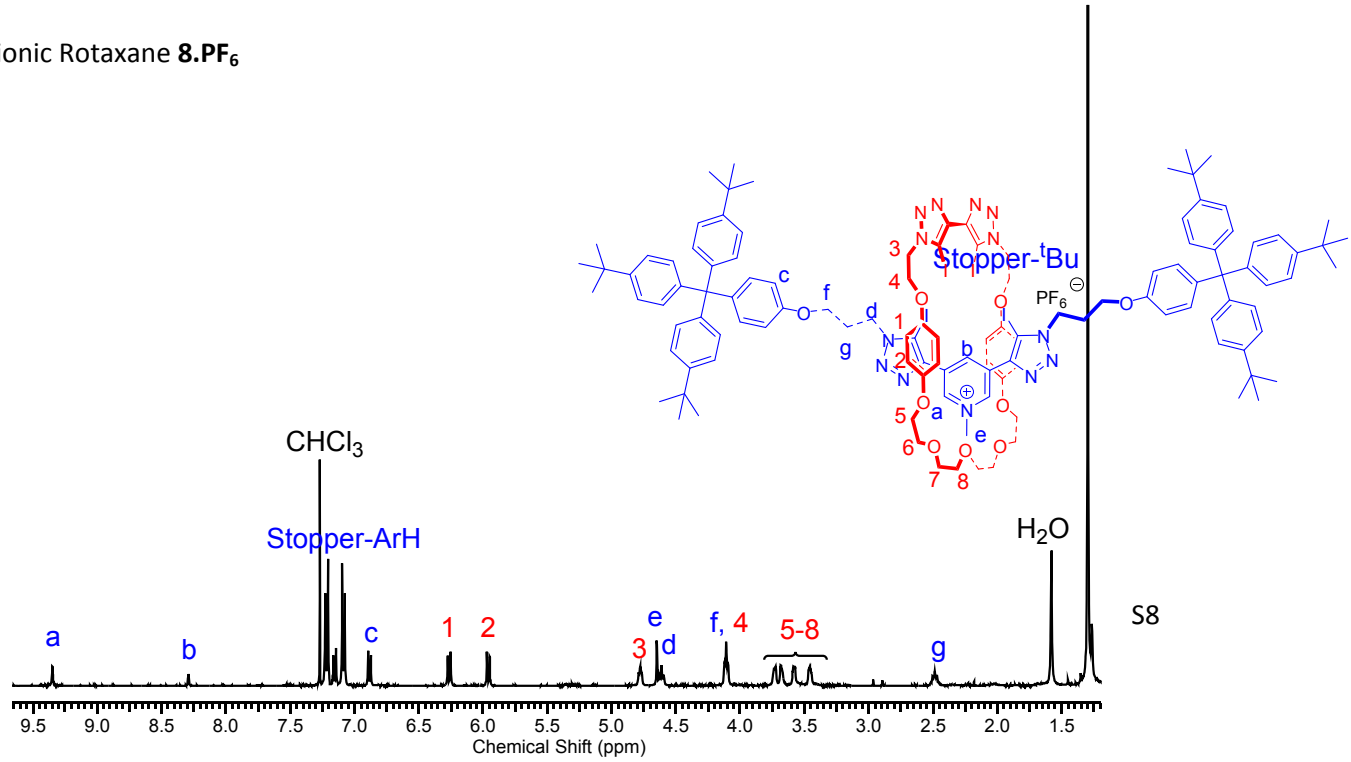


Figure S1-11. ^{1}H NMR of [2]rotaxane **8.PF$_6$** in $CDCl_3$ at 298 K (500 MHz).

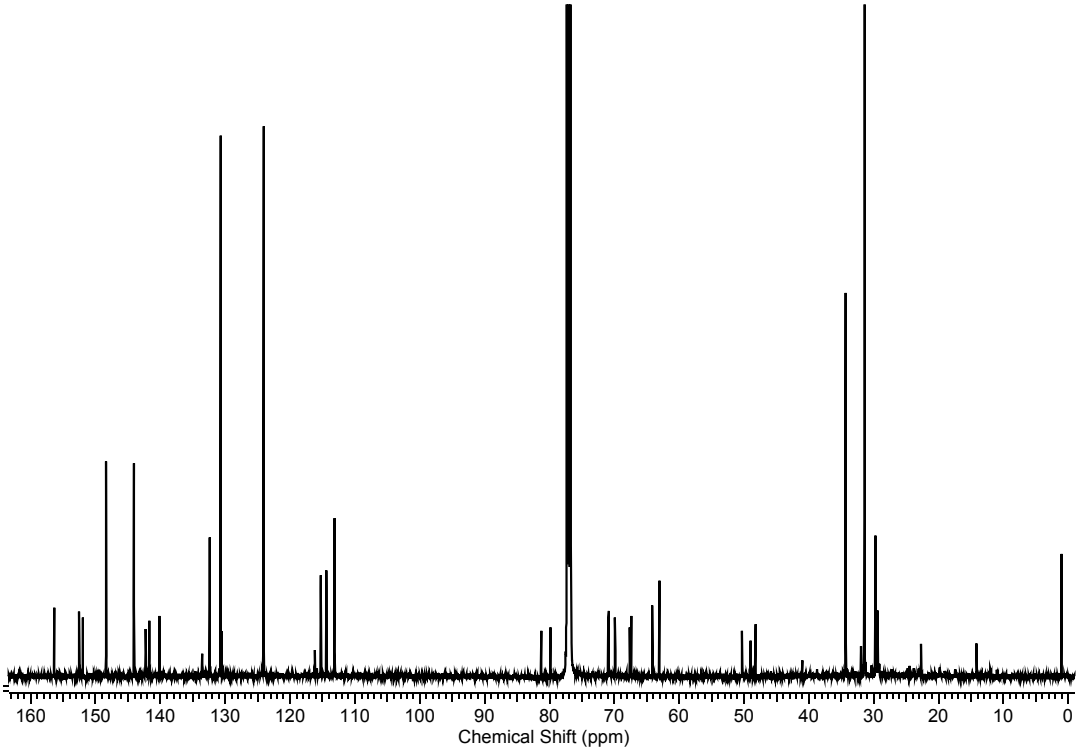


Figure S1-12. ^{13}C NMR of [2]rotaxane **8.PF$_6$** in $CDCl_3$ at 298 K (500 MHz).

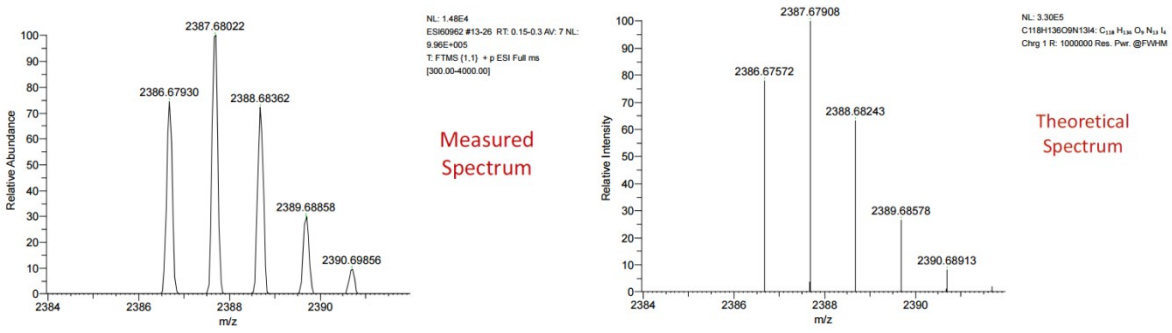


Fig S1-13. High-resolution mass spectrum of rotaxane **8.PF$_6$**. Left: measured spectrum; Right: theoretical isotope model.

2. Anion Recognition Studies of [2]Rotaxanes by ^{1}H NMR Titrations

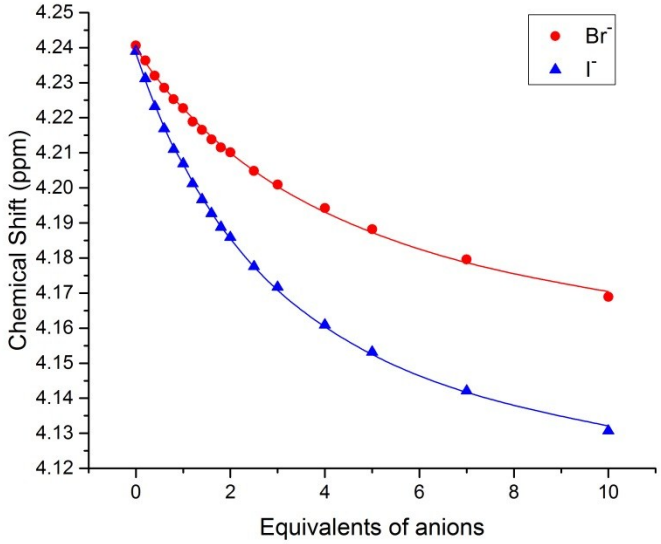


Figure S2-1. Changes in chemical shift of methyl group protons upon addition of increasing quantities of TBA salt to the NMR solution of rotaxane **3.PF$_6$**.

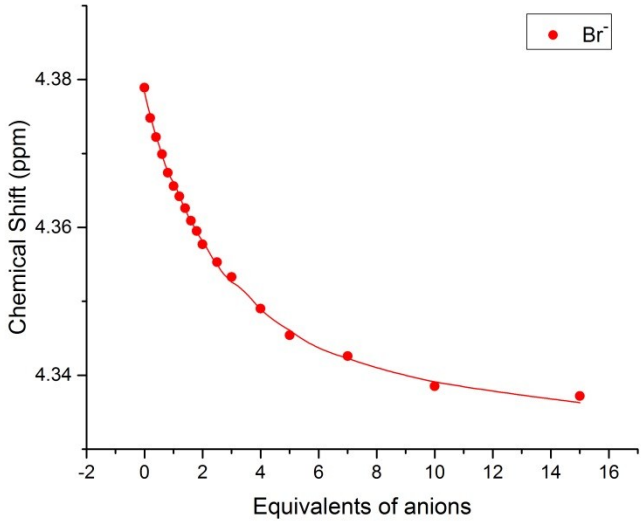


Figure S2-2. Changes in chemical shift of methyl group protons upon addition of increasing quantities of TBA salt to the NMR solution of rotaxane **4.PF_6**.