Shielded alkyl-functionalised rotaxane host cavities for improved anion recognition

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Electronic Supporting Information

¹H NMR spectral characterisation of alkyl-functionalised rotaxanes

Figure S1. Partial ¹H NMR spectra of a) pyridinium chloride thread **13**·PF₆, b) 1:1:1 **13**·PF₆:Cl⁻:**14** 'pseudo[2]rotaxane', c) macrocycle **14**. (300 MHz, CD₂Cl₂, 293 K).

Figure S2. Partial ^1H NMR spectra of a) pyridinium chloride axle **18-Cl**, b) rotaxane **19-Cl**, c) macrocycle precursor. (300 MHz, acetone- d_6 , 293 K).

Figure S3. ^1H - ^1H ROESY NMR spectrum of rotaxane **19-Cl**. Assignable inter-component through-space interactions are highlighted (500 MHz, 1:1 CDCl_3 : CD_3OD , 298 K).

Figure S4. ^1H NMR spectra of a) pyridinium chloride axle **27·Cl**, b) [2]rotaxane **29·Cl**, c) macrocycle precursor. (500 MHz, CD_2Cl_2 , 298 K).

Figure S5. ^1H - ^1H ROESY spectrum of rotaxane **29·Cl**. Assignable inter-component through-space interactions are highlighted (500 MHz, acetone- d_6 , 298 K).