Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Orientational isomers of α-cyclodextrin [2]semi-rotaxanes with asymmetric dicationic threads

Andrew J. Baer† and Donal H. Macartney*

Department of Chemistry, Queen's University, Kingston, ON Canada K7L 3N6. E-mail: donal@chem.queensu.ca; Fax: +1 613 533 6669; Tel: +1 613 533 2617

Table S1. The observed rate constants for the formation of the α-CD [2]semi-rotaxane $\{3,5\text{-Lut}(CH_2)_{10}N(CH_3)_3\bullet\ \alpha\text{-CD}\}^{2+}$ at 25 °C in D_2O.[a]

10^3 [α-CD], mol dm^{-3}	$10^5\ k_2^{obs}$, s^{-1}	$10^5\ k_1^{obs}$, s^{-1}
2.09	5.52	15.3
6.13	14.3	36.2
10.1	14.6	38.2
14.8	26.1	60.0
20.6	38.5	85.3

[a] I = 0.10 mol dm^{-3} (NaCl), $[[3,5\text{-Lut}(CH_2)_{10}N(CH_3)_3]^{2+}]$ = 9.91 x 10^{-4} mol dm^{-3}.

Table S2. The observed rate constants for the formation of the α-CD [2]semi-rotaxane $\{3,5\text{-Lut}(CH_2)_{10}N(CH_3)_2CH_2CH_3\bullet\ \alpha\text{-CD}\}^{2+}$ at 25 °C in D_2O.[a]

10^3 [α-CD], mol dm^{-3}	$10^5\ k_2^{obs}$, s^{-1}	$10^5\ k_1^{obs}$, s^{-1}
10.7	0.572	1.11
22.2	2.01	3.40
31.0	2.77	4.51
40.7	3.23	5.15

[a] I = 0.10 mol dm^{-3} (NaCl), $[[3,5\text{-Lut}(CH_2)_{10}N(CH_3)_2CH_2CH_3]^{2+}]$ = 2.59 x 10^{-3} mol dm^{-3}.

Table S3. The observed rate constants for the formation of the α-CD [2]semi-rotaxane $\{Quin(CH_2)_{10}N(CH_3)_3\bullet\ \alpha\text{-CD}\}^{2+}$ at 25 °C in D_2O.[a]

10^3 [α-CD], mol dm^{-3}	$10^5\ k_2^{obs}$, s^{-1}	$10^5\ k_1^{obs}$, s^{-1}
5.14	9.59	26.2
8.57	14.8	38.8
15.1	27.8	66.7
17.4	30.2	73.0

[a] I = 0.10 mol dm^{-3} (NaCl), $[[Quin(CH_2)_{10}N(CH_3)_3]^{2+}]$ = 2.74 x 10^{-3} mol dm^{-3}.

Table S4. The observed rate constants for the formation of the α-CD [2]semi-rotaxane $\{Quin(CH_2)_{10}N(CH_3)_2CH_2CH_3\bullet\ \alpha\text{-CD}\}^{2+}$ at 25 °C in D_2O.[a]

10^3 [α-CD], mol dm^{-3}	$10^5\ k_2^{obs}$, s^{-1}	$10^5\ k_1^{obs}$, s^{-1}
10.8	1.34	1.65
22.6	2.39	3.24
40.9	6.73	9.02

[a] I = 0.10 mol dm^{-3} (NaCl), $[[Quin(CH_2)_{10}N(CH_3)_2CH_2CH_3]^{2+}]$ = 2.59 x 10^{-3} mol dm^{-3}.

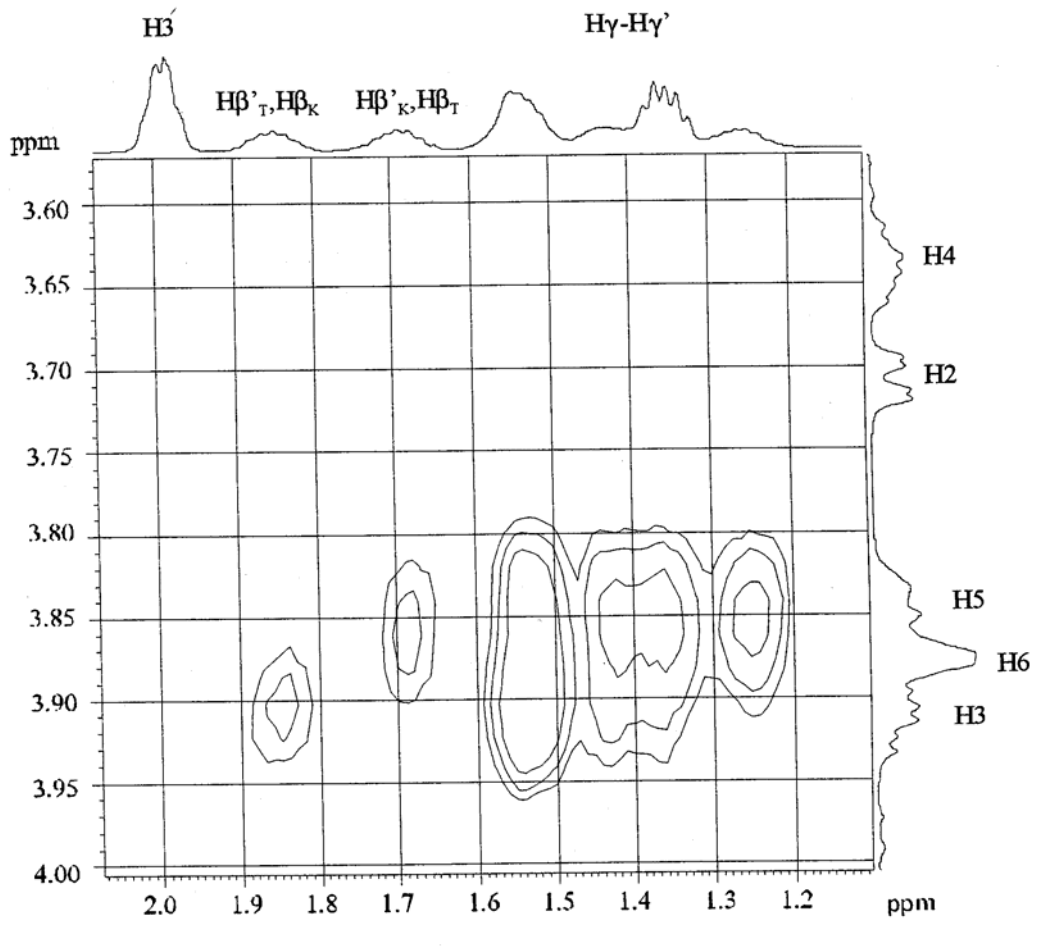

Figure S1. A portion of the $^{1}H - {}^{1}H$ ROESY NMR spectrum of the [2]semi-rotaxane $[\{Quin(CH_2)_{10}N(CH_3)_2(CH_2CH_3)\bullet\alpha\text{-}CD\}]^{2+}$ showing the NOE signals from the H3 and H5 protons of α-CD to protons on the guest (see Figure 1 for proton labelling scheme)