***Pseudocryptand-type [3]Pseudorotaxane and “Hook-Ring”
Polypseudo[2]catenane Based on a Bis(meta-phenylene)-32-crown-10
Derivative and Bisparaquat Derivatives***

*Zhenbin Niu, Carla Slebodnick, and Harry W. Gibson**

*Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, Virginia,
24061*

E-mail hwgibson@vt.edu

Contents

1. Materials and methods.....	S2
2. Determination of Δ_0 for 1c₂·2	S2
3. Determination of Δ_0 for 1c·3	S2
4. Mass spectrum of 1c₂·2	S3
5. Mass spectrum of 1c·3	S3
6. Crystal structure of 1c·3	S4

1. Materials and methods

BMP32C10 derivative **1c**,¹ bisparaquat **2**² and **CBPQT 3**³ were prepared according to literature procedures. Solvents were either used as purchased or dried according to literature procedures. ¹H-NMR spectra were obtained on JEOL ECLIPSE-500 and INOVA-400 spectrometers with internal standard TMS. HR-MS were obtained by employing an Agilent LC-ESI-TOF.

2. Determination of Δ_0 for **1c**·**2**

Figure S1. Determination of Δ_0 of **1c**·**2** in acetone- d_6 . $[2]_0 = 0.50$ mM. $\Delta_0 = 0.137$ ppm.

3. Determination of Δ_0 for **1c**·**3**

Figure S2. Determination of Δ_0 of **1c**·**3** in acetonitrile- d_3 . $[1c]_0 = 0.85$ mM. $\Delta_0 = 0.930$ ppm.

4. Mass spectrum of **1c₂·2**

Figure S3. Electrospray ionization (ESI) mass spectrum of **1c₂·2**.

5. Mass spectrum of **1c·3**

Figure S4. Electrospray ionization (ESI) mass spectrum of **1c·3**.

6. Crystal structure of **1c**·**3**

Figure S5. Another view of the X-ray structure of poly(**1c**·**3**). **1c** is red. **3** is blue. Solvent molecules, PF_6^- ions and hydrogen atoms except the ones involved in hydrogen bonding have been omitted for clarity. Hydrogen bonds shown in Figure 5 were omitted for clarity. Selected hydrogen-bond parameters: H $\cdots$ O(F, N) distances (Å), C $\cdots$ O(F, N) distances (Å), C-H $\cdots$ O(F, N) angles (deg): k 2.61, 3.35, 135; l 2.66, 3.36, 131; m 2.41, 3.10, 130; n 2.29, 3.13, 146.

References:

- (1) Niu, Z.; Slebodnick, C.; Schoonover, D.; Azurmendi, H.; Harich, K.; Gibson, H. W. *Org. Lett.* DOI [10.1021/ol201502r](https://doi.org/10.1021/ol201502r).
- (2) Huang, F.; Fronczek, F. R.; Gibson, H. W. *J. Am. Chem. Soc.* **2003**, *125*, 9272-9273.
- (3) Odell, B.; Reddington, M. V.; Slawin, A. M. Z.; Spencer, N.; Stoddart, J. F.; Williams, D. J. *Angew. Chem. Int. Ed.* **1988**, *27*, 1547-1550.