

Contrasting Biscryptand/Dimethyl Paraquat [3]Pseudorotaxanes: Statistical vs. Anticooperative Complexation Behavior

Zhenbin Niu, Harry. W. Gibson*

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

E-mail hwgibson@vt.edu

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1. Materials and methods

The bis(*meta*-phenylene)-32-crown-10 (BMP32C10) cryptands **1** and **2**^{S1} and guest **DMP**^{S2} were prepared according to literature procedures. Solvents were either used as purchased or dried according to literature procedures. ¹H-NMR spectra were obtained on a JEOL ECLIPSE-500 spectrometer with internal standard TMS. ¹³C-NMR spectra were collected on a JEOL ECLIPSE-500 spectrometer at 125 MHz. MS were obtained by employing a Hewlett Packard MSD GCMS.

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

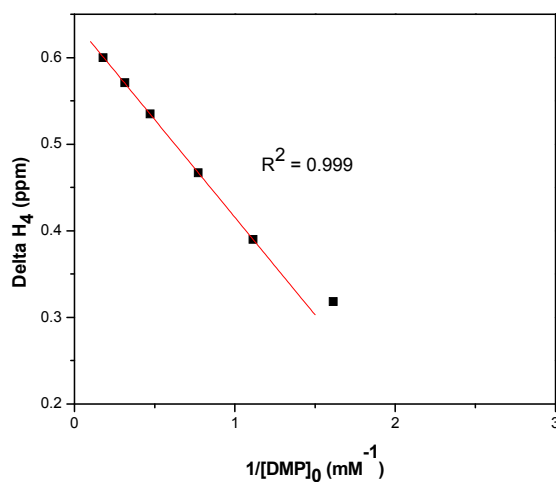


Figure S1. Determination of Δ_0 of **1**·**DMP**₂ in CDCl₃/(CD₃)₂CO = 1/3 <v/v>. [**1**]₀ = 0.34 mM. $\Delta_0 = 0.631$ ppm.

3. Determination of Δ_0 of $2 \cdot \text{DMP}_2$

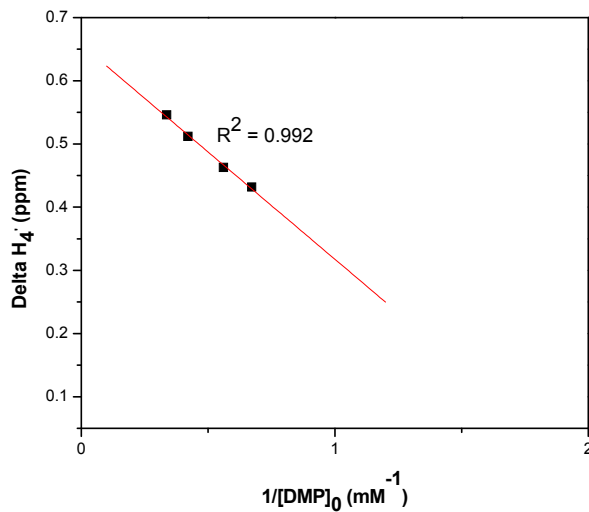


Figure S2. Determination of Δ_0 of $2 \cdot \text{DMP}_2$ in $\text{CDCl}_3/(\text{CD}_3)_2\text{CO} = 1/3$ $\langle v/v \rangle$. $[\mathbf{2}]_0 = 0.34$ mM. $\Delta_0 = 0.657$ ppm.

4. Mass spectrum of $1 \cdot \text{DMP}_2$

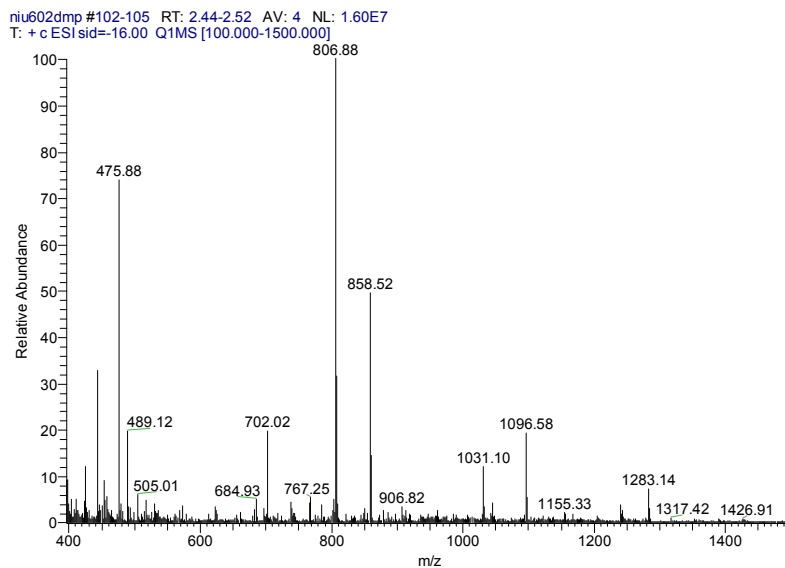


Figure S3. Electrospray ionization mass spectrum of $1 \cdot \text{DMP}_2$.

5. Mass spectrum of 2·DMP₂

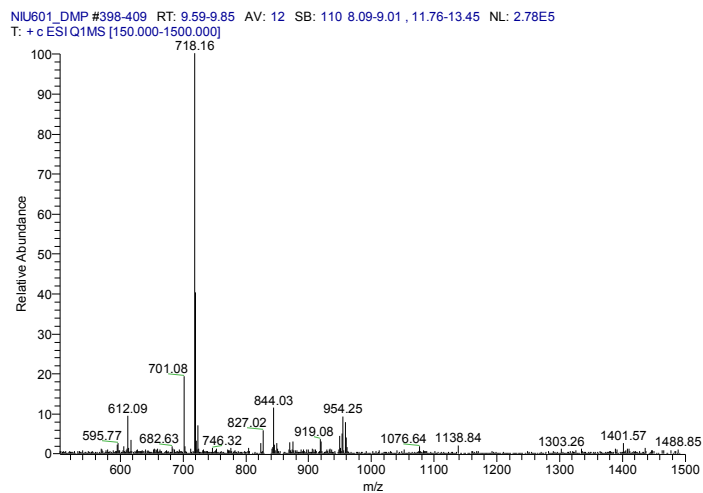


Figure S4. Electrospray ionization mass spectrum of 2·DMP₂.

References:

- (S1) Z. Niu, F. Huang and H. W. Gibson, *J. Am. Chem. Soc.*, 2011, **133**, 2836-2839.
(S2) B. L. Allwood, H. Shahriari-Zavareh, J. F. Stoddart, D. J. Williams, *Chem. Commun.* 1987, 1058-1061.