A Supramolecular Poly[3]pseudorotaxane from Self-Assembly of a Homoditopic Cylindrical Bis(crown ether) Host and a Bisparaquat Derivative

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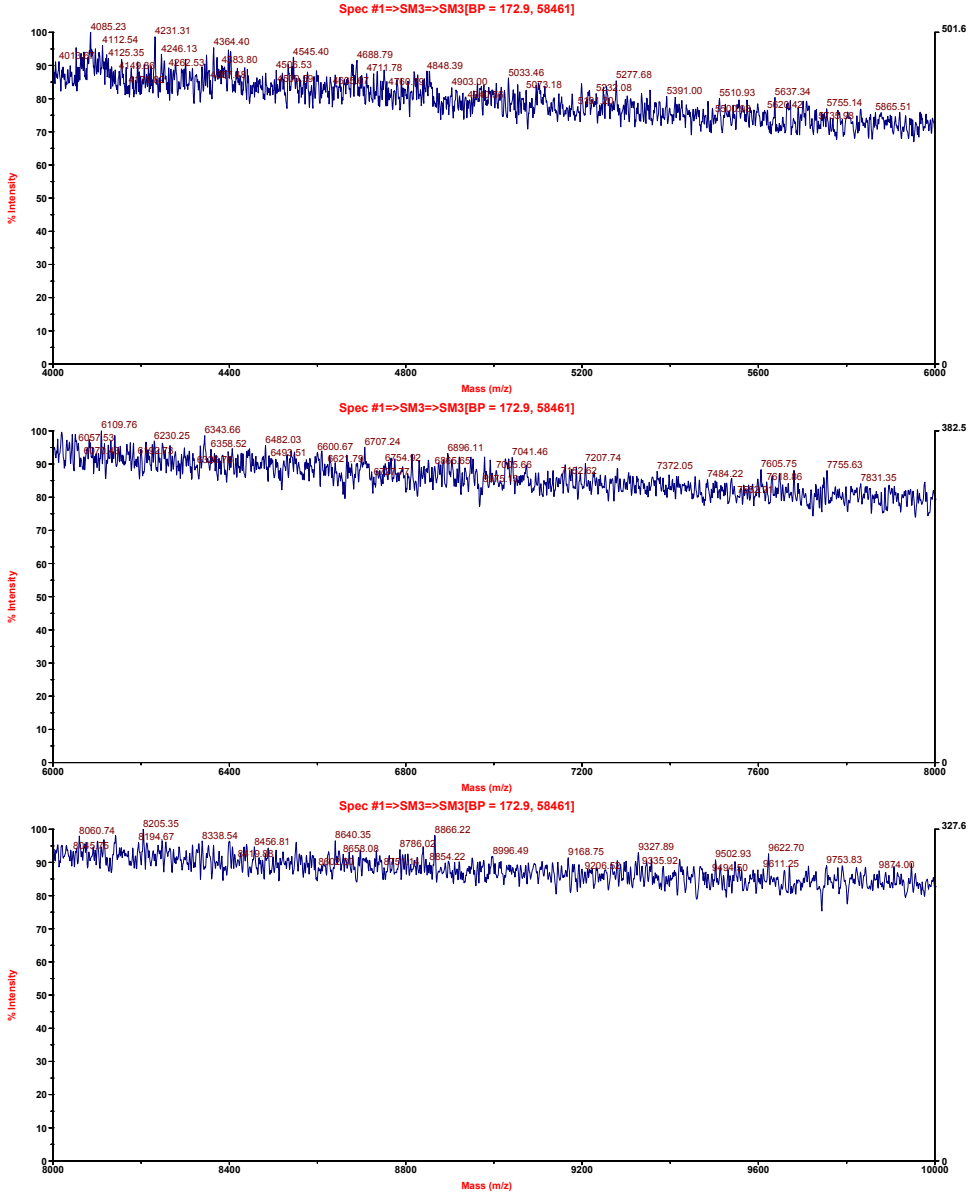
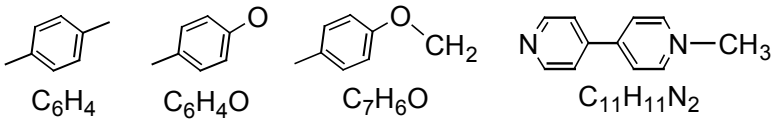
Supplemental Material (2 pages)

Some other parts of the MALDI-TOF mass spectrum of ***4***: The spectrum was measured in the positive-ion mode using 2,5-dihydroxbenzoic acid as the matrix and acetone as the solvent.



Assignments of some peaks:



1) Five more peaks for dimer (**1**•**3**)$_2$: *m/z* 4688.79 [(**1**•**3**)$_2$ - 3CH$_3$]$^+$, 4545.40 [(**1**•**3**)$_2$ - PF$_6$ - 3CH$_3$ + H]$^+$, 4364.40 [(**1**•**3**)$_2$ - 2HPF$_6$ - C$_6$H$_4$ - H]$^+$, 4231.31 [(**1**•**3**)$_2$ - 3PF$_6$ - C$_7$H$_6$O + K]$^+$, and 4085.23 [(**1**•**3**)$_2$ - 3PF$_6$ - C$_7$H$_6$O - HPF$_6$ + K]$^+$.
2) Peaks for **3**•(**1**•**3**)$_2$: *m/z* 4848.39 [**3**•(**1**•**3**)$_2$ - 3PF$_6$ - 3HPF$_6$ - C$_6$H$_4$ + K]$^+$ and 5033.46 [**3**•(**1**•**3**)$_2$ - 4PF$_6$ - HPF$_6$]$^+$.
3) Peaks for trimer (**1**•**3**)$_3$: *m/z* 6707.24 [(**1**•**3**)$_3$ - PF$_6$ - HPF$_6$ - C$_6$H$_4$O]$^+$, 6482.03 [(**1**•**3**)$_3$ - 3PF$_6$ - HPF$_6$ - C$_6$H$_4$ + K]$^+$, 6343.66 [(**1**•**3**)$_3$ - 4PF$_6$ - HPF$_6$ - 2CH$_3$]$^+$, 6109.76 [(**1**•**3**)$_3$ - 2PF$_6$ - 4HPF$_6$ - C$_7$H$_6$O]$^+$, 5865.51 [(**1**•**3**)$_3$ - C$_{11}$H$_{11}$N$_2$ - 3PF$_6$ - 4HPF$_6$ - 3CH$_3$]$^+$, 5755.14 [(**1**•**3**)$_3$ - C$_{11}$H$_{11}$N$_2$ - 8PF$_6$ - CH$_3$ + H]$^+$, 5637.34 [(**1**•**3**)$_3$ - 10PF$_6$ - CH$_3$ + H]$^+$, and 5277.68 [(**1**•**3**)$_3$ - C$_{11}$H$_{11}$N$_2$ - 8PF$_6$ - 3HPF$_6$ - C$_6$H$_4$O + K]$^+$.
4) Peaks for **3**•(**1**•**3**)$_3$: *m/z* 7605.75 [**3**•(**1**•**3**)$_3$ - C$_{11}$H$_{11}$N$_2$ - 2PF$_6$ - 4CH$_3$]$^+$ and 7372.05 [**3**•(**1**•**3**)$_3$ - 3HPF$_6$ - PF$_6$ - C$_{11}$H$_{11}$N$_2$]$^+$.
5) Peaks for (**1**•**3**)$_3$•**1**: *m/z* 7755.63 [(**1**•**3**)$_3$•**1** - C$_7$H$_6$O - 4PF$_6$ + H]$^+$ and 7041.46 [(**1**•**3**)$_3$•**1** - 2HPF$_6$ - 7PF$_6$ - C$_6$H$_4$O]$^+$.
6) Peaks for tetramer (**1**•**3**)$_4$: *m/z* 8866.22 [(**1**•**3**)$_4$ - 4HPF$_6$ - CH$_4$]$^+$, 8640.35 [(**1**•**3**)$_4$ - C$_{11}$H$_{11}$N$_2$ - 4PF$_6$ - C$_6$H$_4$ + H]$^+$, 8205.35 [(**1**•**3**)$_4$ - C$_{11}$H$_{11}$N$_2$ - 7PF$_6$ - C$_6$H$_4$ + H]$^+$, and 8060.74 [(**1**•**3**)$_4$ - C$_{11}$H$_{11}$N$_2$ - 8PF$_6$ - C$_6$H$_4$ + H]$^+$.
7) A peak for **3**•(**1**•**3**)$_4$: *m/z* 9622.70 [**3**•(**1**•**3**)$_4$ - 6PF$_6$]$^+$.
8) Peaks for (**1**•**3**)$_4$•**1**: *m/z* 9502.93 [(**1**•**3**)$_4$•**1** - 9PF$_6$]$^+$, 9327.89 [(**1**•**3**)$_4$•**1** - 10PF$_6$ - 2CH$_3$]$^+$, and 9168.75 [(**1**•**3**)$_4$•**1** - 12PF$_6$ + H]$^+$.
9) A peak for **3**•(**1**•**3**)$_4$: *m/z* 9753.83 [**3**•(**1**•**3**)$_4$ - 5PF$_6$ - CH$_3$ + H]$^+$.

*Determination of Δ_0 of H_1 on **3**:*