

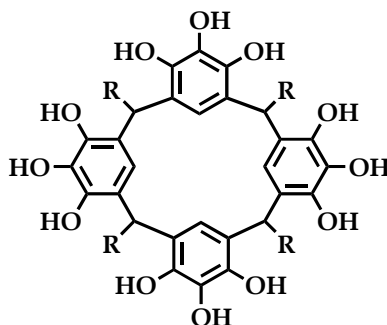
## Supplementary Information

# Pyrogallarene-based Ion-conducting Pores that Show Reversible Conductance Properties

Ruiqiong Li, †Oleg V. Kulikov, ‡ and George W. Gokel ‡\*

†Department of Chemistry, Washington University, St. Louis, MO 63130 and  
‡Departments of Chemistry & Biochemistry and Biology, Center for Nanoscience,  
University of Missouri – Saint Louis, One University Boulevard, Saint Louis, MO  
63121 USA

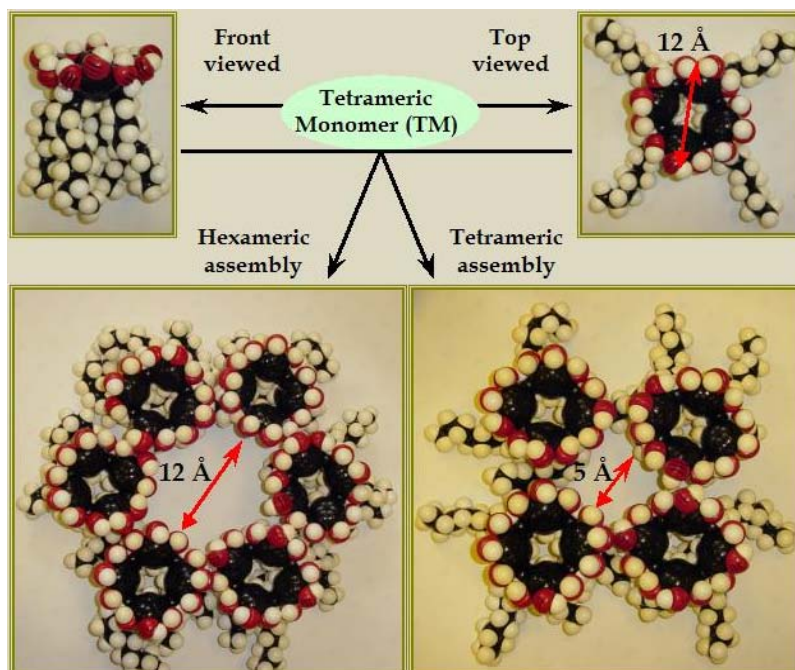
### Compounds studied:



- 1, R = C<sub>11</sub>H<sub>23</sub> ("bilayer" isolated)
- 2, R = C<sub>11</sub>H<sub>23</sub> ("capsule" isolated)
- 3, R = C<sub>3</sub>H<sub>7</sub> ("bilayer" isolated)
- 4, R = C<sub>6</sub>H<sub>13</sub> ("bilayer" isolated)

Compounds 1-3 studied in this work have been synthesized according to a general procedure for pyrogallarenes synthesis. <sup>1</sup>

### CPK models for monomers, tetrameric assembly and hexameric assembly of compound 1



---

Insert SI Figure 1 (Filename: SI Figure 1\_self-assembly for 1)

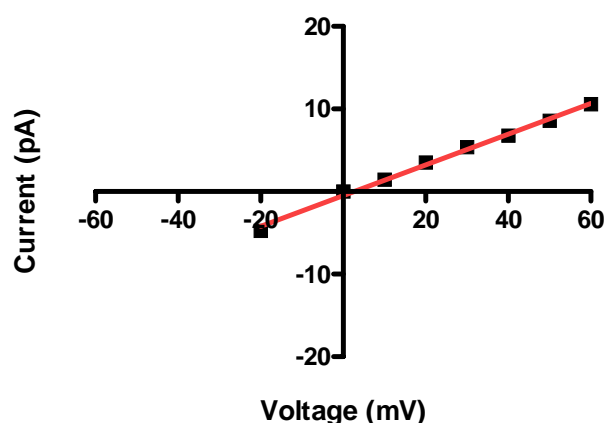
Caption: CPK models of 1 in monomeric, tetrameric and hexameric assembly with size marked.

---

#### Planar Bilayer Clamp Experiment (BLM):

All the experiments were performed at room temperature ( $25 \pm 1$  °C). Planar Bilayer Workstation from Warner Instruments, LLC was applied for the ion conductance study. Sample was dissolved in DMSO to form a suspension (1 mM) as stock solution. Chamber and delrin cuvette were filled with either symmetric buffer solution (450 mM KCl, 10 mM HEPES, pH = 7.00) or asymmetric buffer solution (*cis/trans*, 3 M/0.45 M KCl, 10 mM HEPES, pH = 7.00) for cation-anion selectivity experiment, 3 mL for each side. Membrane was made by typical lipid solution (asolectin from soybean extract dissolved in n-decane, 25 mg/mL, for regular experiment or 20 weight - % cholesterol in asolectin solution, 25 mg/mL, for steroid presence issue) painting technique through the aperture of partition on the cuvette. 9  $\mu$ L of sample suspension or solution was added into the *cis* chamber to make the final concentration of 3  $\mu$ M (the real concentration is varied because of the solubility issue) after the membrane was formed by judgment of capacitance (over 100 pF) and perfect square wave displayed on the oscilloscope (HM305 from Hameg). The mixture was stirred for ten minutes and equilibrium

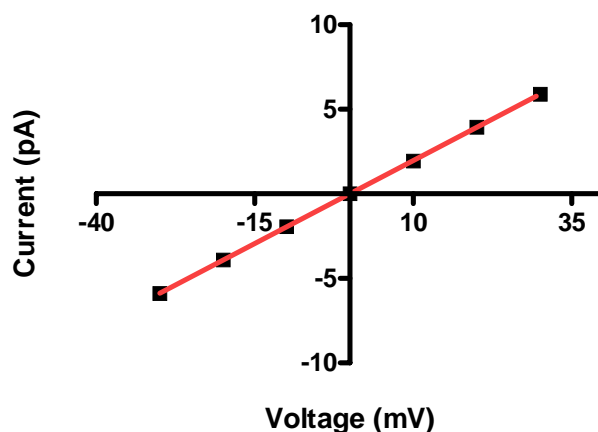
for five minutes. Specific potential was applied (*trans* connected to ground) to record the currents in Faraday cage (from Warner Instruments, LLC). The currents were amplified (amplifier BC-525 D, from Warner Instruments, LLC), filtered with a 4-pole Bessel filter at 1 kHz, digitized by Digitizer (Digidata 1322A from Axon Instruments), sampled at the 100 Hz of amplifier filter frequency and collected by pClamp 9.2 (software from Axon Instruments). The data were analyzed later using Clampfit v. 9.2 (software from Axon Instruments).



---

Insert SI Figure 2 (Filename: SI Figure 2\_I-V plot for 1)  
Caption: "I - V" plot for 1 by BLM.  $g_s = 186.3$  pS,  $R^2 = 0.995$

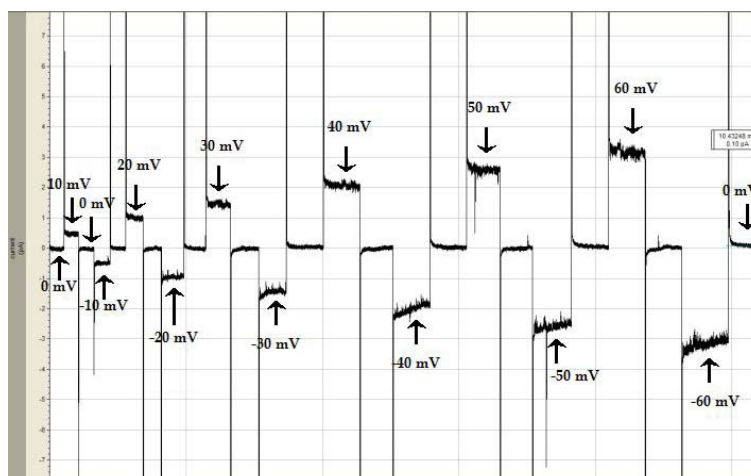
---



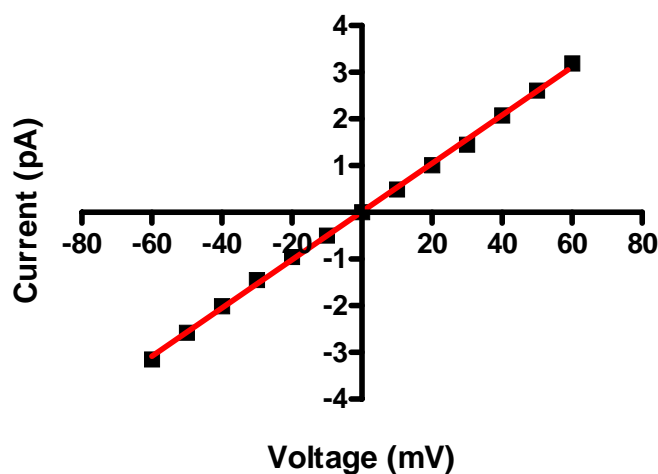
---

Insert SI Figure 3 (Filename: SI Figure 3\_V-switch I-V plot for 1)  
Caption: Voltage-switching "I - V" plot for 1 by BLM.  $g_s = 196.3$  pS,  $R^2 = 1.000$

---



Insert SI Figure 4 (Filename: SI Figure 4\_V-switch for 1 w/ cholesterol)  
Caption: Voltage-switching experiment conducted on **1** at indicated voltages in the presence of 20 weight -% cholesterol. The time scale for the experiment is 10 minutes and 30 seconds.



Insert SI Figure 5 (Filename: SI Figure 5\_V-switch I-V plot for 1 w/ cholesterol)  
Caption: Voltage-switching "I - V" plot for **1** by BLM in the presence of 20 weight -% cholesterol.  $g_s = 52$  pS,  $R^2 = 0.999$

- 1 G. W. V. Cave, S. J. Dalgarno, J. Antesberger, M. C. Farrarelli, R. M. McKinlay, J. L. Atwood, *Supramol. Chem.*, 2008, **20**, 157-159.