

Supporting Information

Cucurbituryl Complexes of Viologens Bound to TiO₂ Films

*Marina Freitag and Elena Galoppini**

Chemistry Department, Rutgers University, 73 Warren Street, Newark, New Jersey

07102

Page, List of Contents:

- S2. UV-Vis of **1** and **2** in solution in the absence and presence of CB[7] (Figs S1 and S2)
- S3. FT-IR-ATR of CB[7]
- S3. ¹H NMR of methylviologen dicloride (MV²⁺, **1**).
- S3. ¹H NMR of Cucur[7]bituril (CB[7]) in D₂O.
- S4. ¹H NMR of MV²⁺@CB[7] in D₂O.
- S4. ¹H NMR of 1-(2,4-dinitrophenyl)-4-(pyridin-4-yl) pyridinium chloride (**3**) in D₂O.
- S4. ¹³C NMR of 1-(2,4-dinitrophenyl)-4-(pyridin-4-yl) pyridinium chloride (**3**) in D₂O.
- S5. ¹H NMR of 4-(pyridin-4-yl)-1-*p*-tolylpyridinium chloride (**4**) in D₂O.
- S5. ¹³C NMR of 4-(pyridin-4-yl)-1-*p*-tolylpyridinium chloride (**4**) in D₂O.
- S5. ¹³C NMR of MTV²⁺ (**2**) in D₂O.
- S6. Binding constant determination: absorbance spectra of MTV²⁺ after addition of CB[7] aliquotes
- S6. Fitted experimental absorbance data at 218 nm
- S6. Movie of Color Changes in Electrochromic Windows prepared from MTV²⁺@CB[7] (see Figs 10 and 11) in manuscript (real time).

* Corresponding author; email: galoppin@rutgers.edu

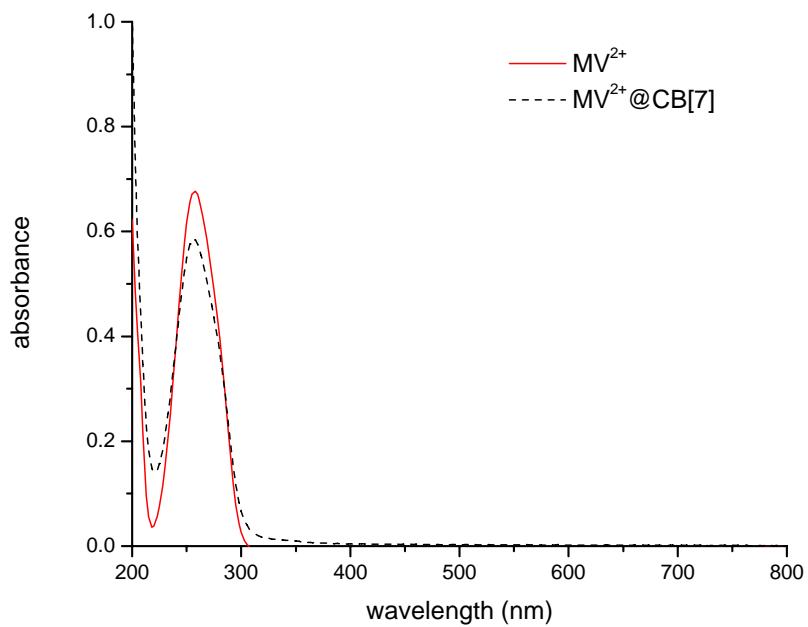


Figure S1. Absorption spectra of MV^{2+} and $\text{MV}^{2+}@CB[7]$ in aqueous solutions.

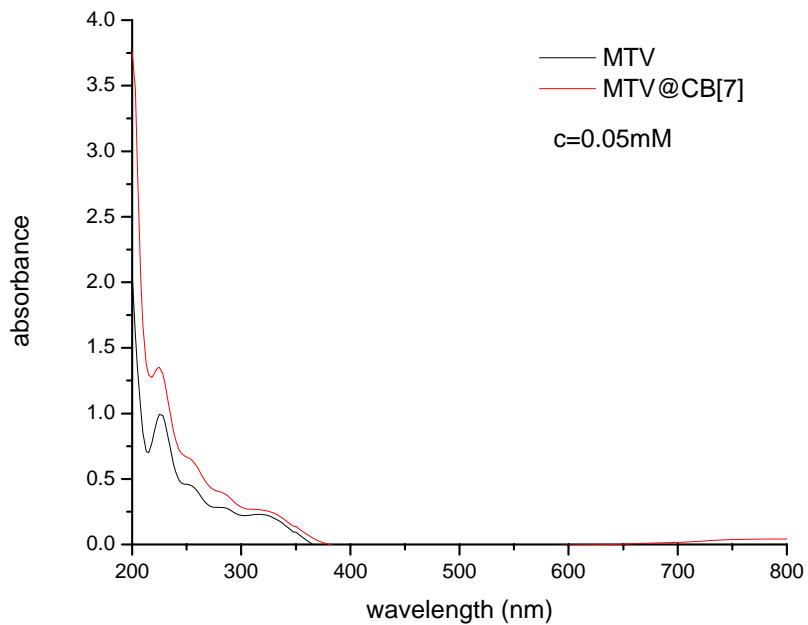


Figure S2. Absorption spectra of MTV^{2+} and $\text{MTV}^{2+}@CB[7]$ in aqueous solutions.

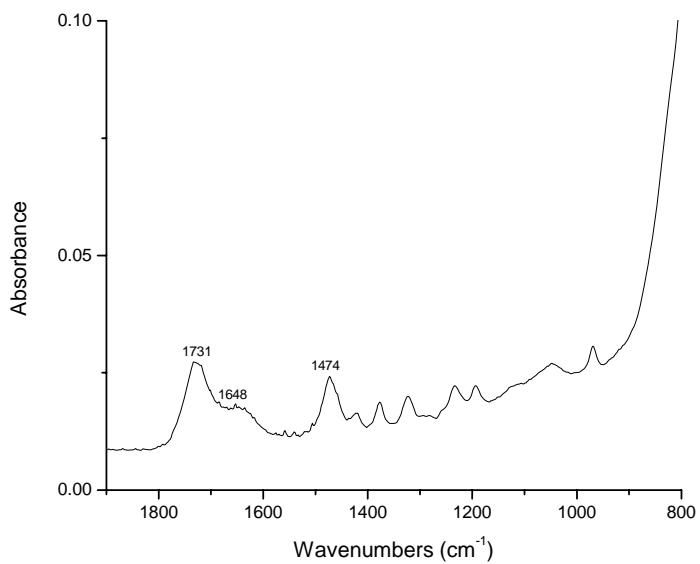


Figure S3. FT-IR-ATR of CB[7]

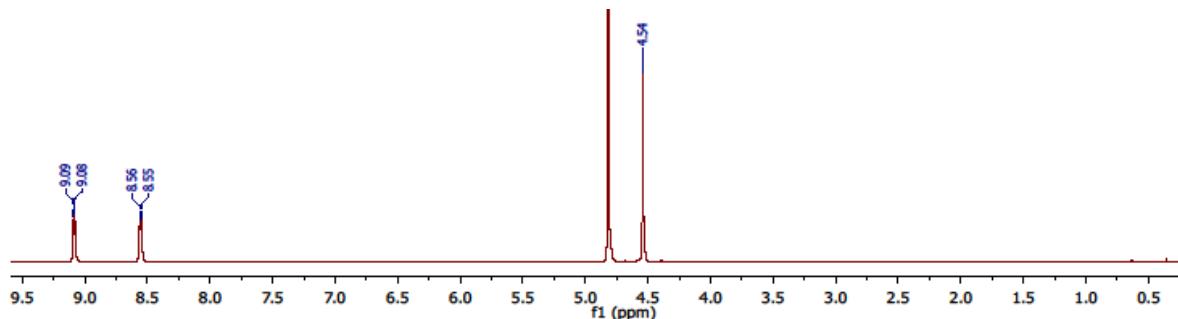


Figure S4. ^1H NMR of methylviologen dicloride (MV^{2+} , **1**) in D_2O .

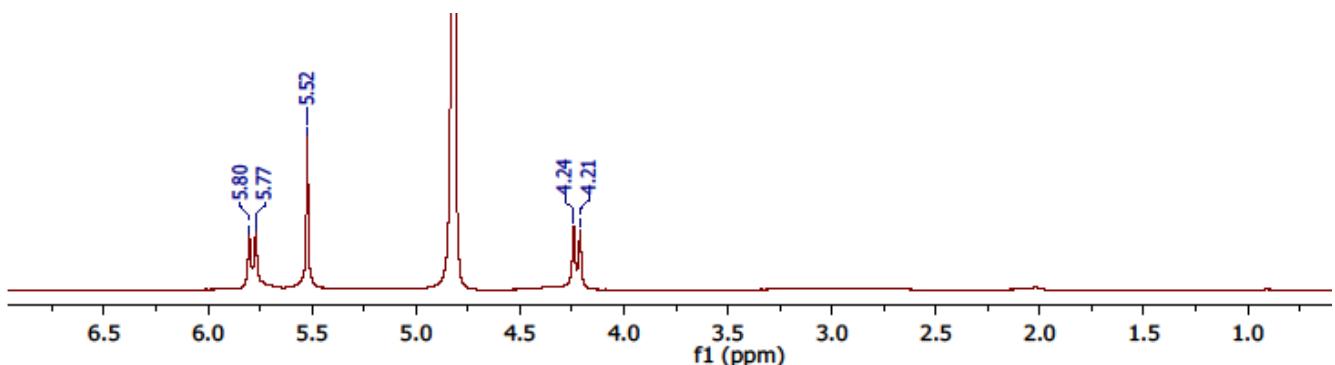


Figure S5. ^1H NMR of Cucur[7]bituril (CB[7]) in D_2O .

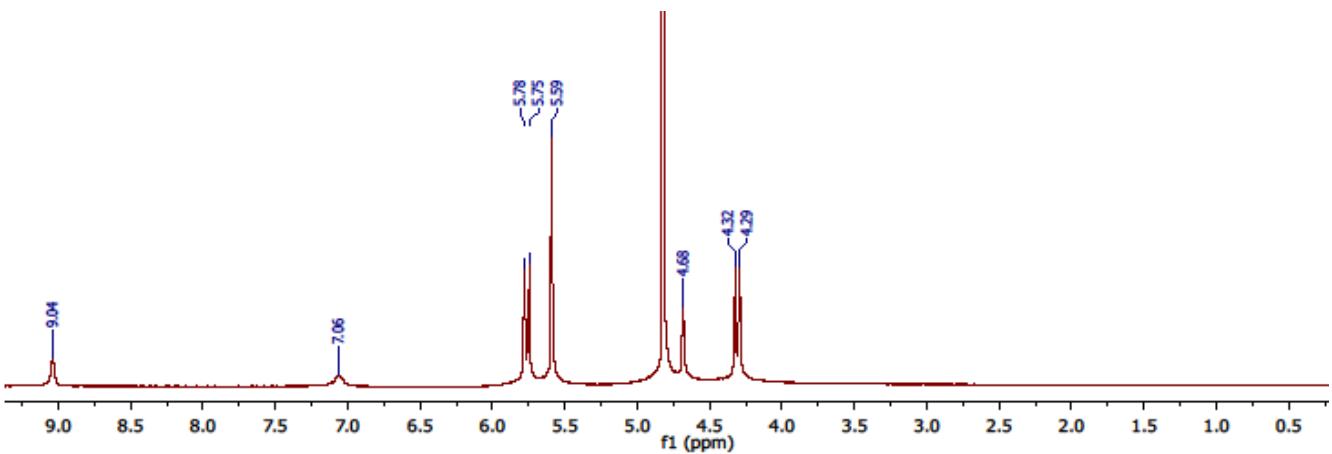


Figure S3. ^1H NMR of $\text{MV}^{2+}@\text{CB}[7]$ in D_2O .

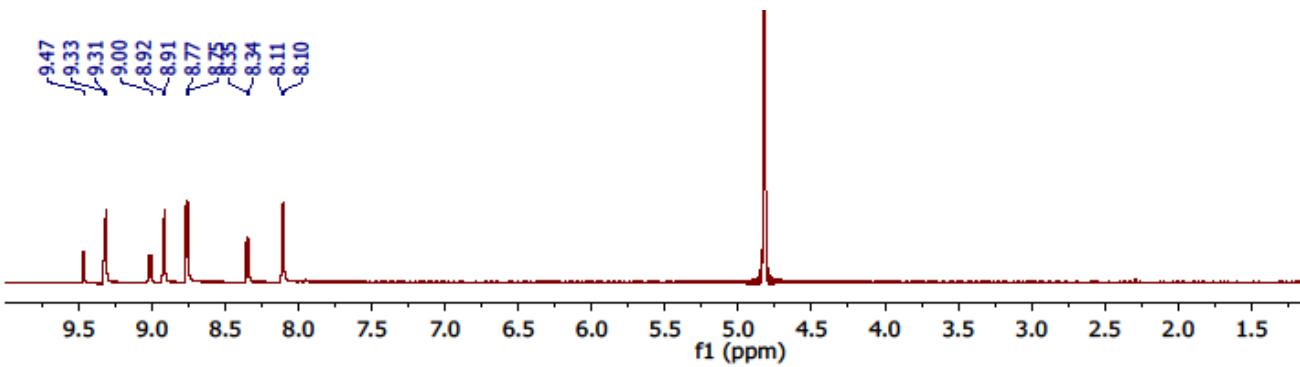


Figure S4. ^1H NMR of 1-(2,4-dinitrophenyl)-4-(pyridin-4-yl) pyridinium chloride (**3**) in D_2O .

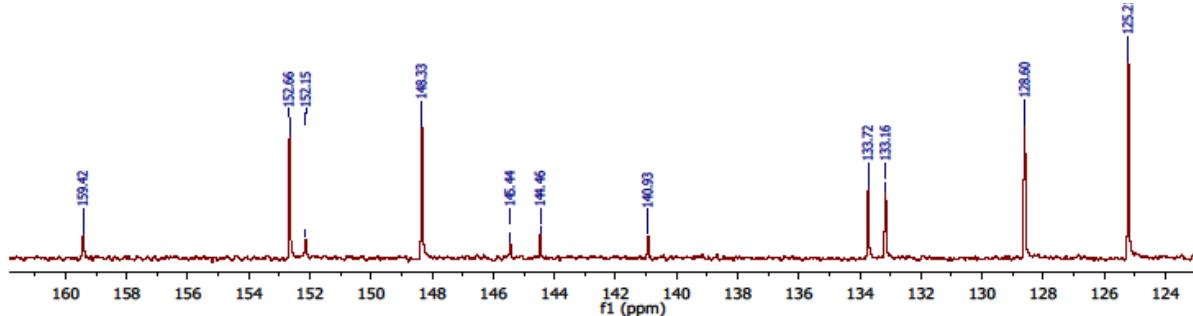


Figure S7. ^{13}C NMR of 1-(2,4-dinitrophenyl)-4-(pyridin-4-yl) pyridinium chloride (**3**) in D_2O .

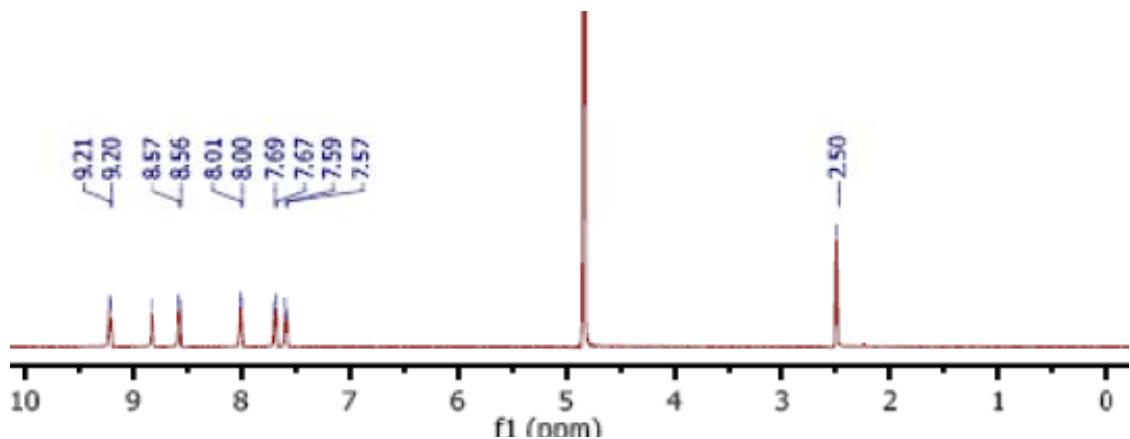


Figure S8. ^1H NMR of 4-(pyridin-4-yl)-1-*p*-tolylpyridinium chloride (**4**) in D_2O .

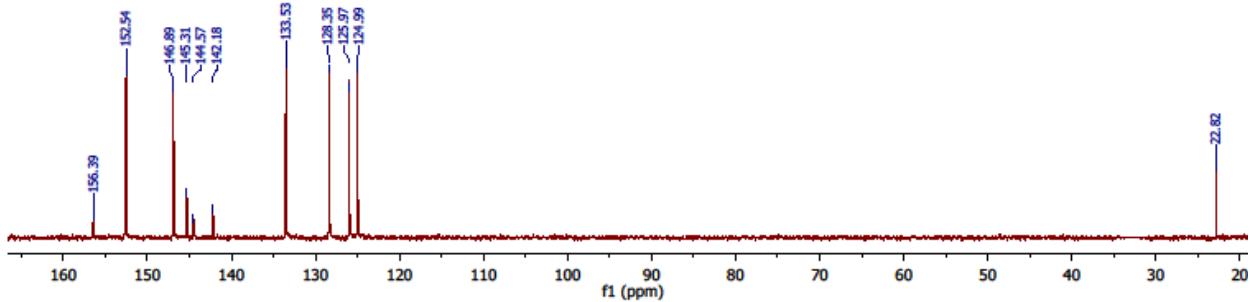


Figure S9. ^{13}C NMR of 4-(pyridin-4-yl)-1-*p*-tolylpyridinium chloride (**4**) in D_2O .

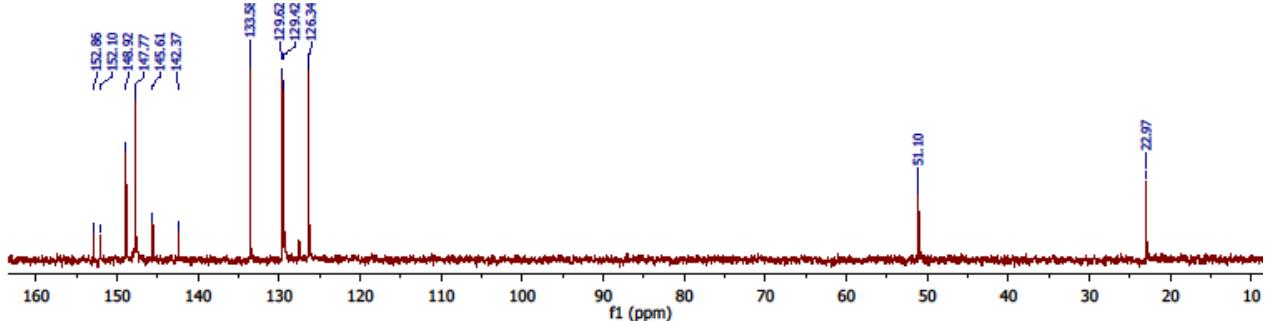


Figure S10. ^{13}C NMR of MTV $^{2+}$ (**2**) in D_2O .

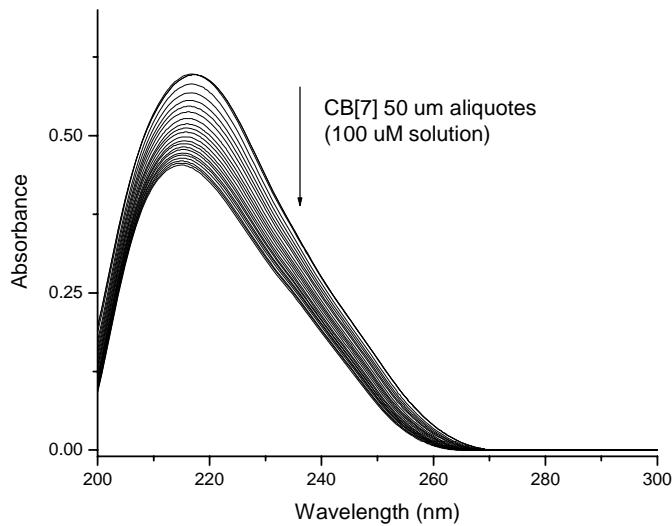


Figure S11. Changes in the absorption spectra of a 1000 μl aqueous solution (0.1 M phosphate buffer) of 30 μM MTV^{2+} upon addition of 50 μl aliquotes of a 100 μM aqueous solution of CB[7].

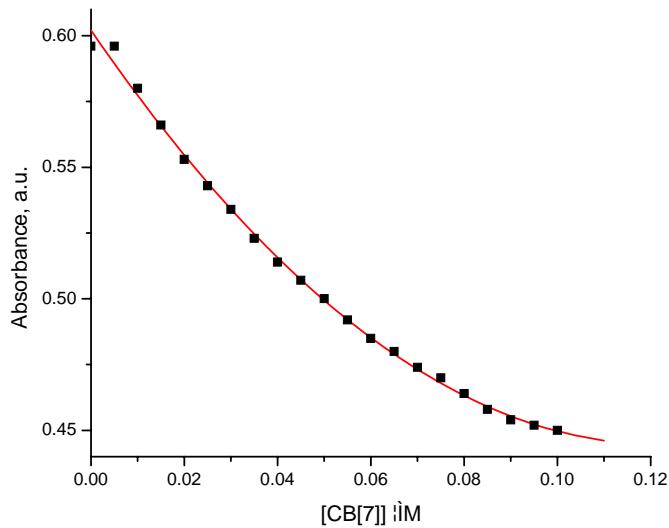


Figure S12. Fitted (red solid line) experimental data (squares) of absorbance of MTV^{2+} at 218 nm against concentration of CB[7] (see Figure S11)

Click on the Icon for Movie of Color Changes in Electrochromic Windows prepared from MTV^{2+} @CB[7] (real time).



P6110507.avi