

Electronic Supplementary Information (ESI)

Host–guest complexation of di-cyclohexanocucurbit[6]uril and hexa-cyclohexanocucurbit[6]uril with alkyldiammonium ions: A comparative study

Guo-Sheng Fang^a, Wen-Qi Sun^a, Wen-Xuan Zhao^b, Rui-Lian Lin^a, Zhu Tao^b and Jing-Xin Liu^{,a}*

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- a* G.-S. Fang, W.-Q. Sun, R.-L. Lin, J.-X. Liu
College of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan 243002, China
jxliu411@ahut.edu.cn
- b* W.-X. Zhao, Z. Tao
Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China
gzutao@263.net

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Figure S1 (a) ^1H NMR spectra (400 MHz, D_2O) of guest **5** in the absence (A) and in the presence of 0.36 (B) equiv of $\text{Cy6Q}[6]$; (b) ^1H NMR spectra (400 MHz, D_2O) of guest **6** in the absence (A) and in the presence of 0.47 (B) equiv of $\text{Cy6Q}[6]$.

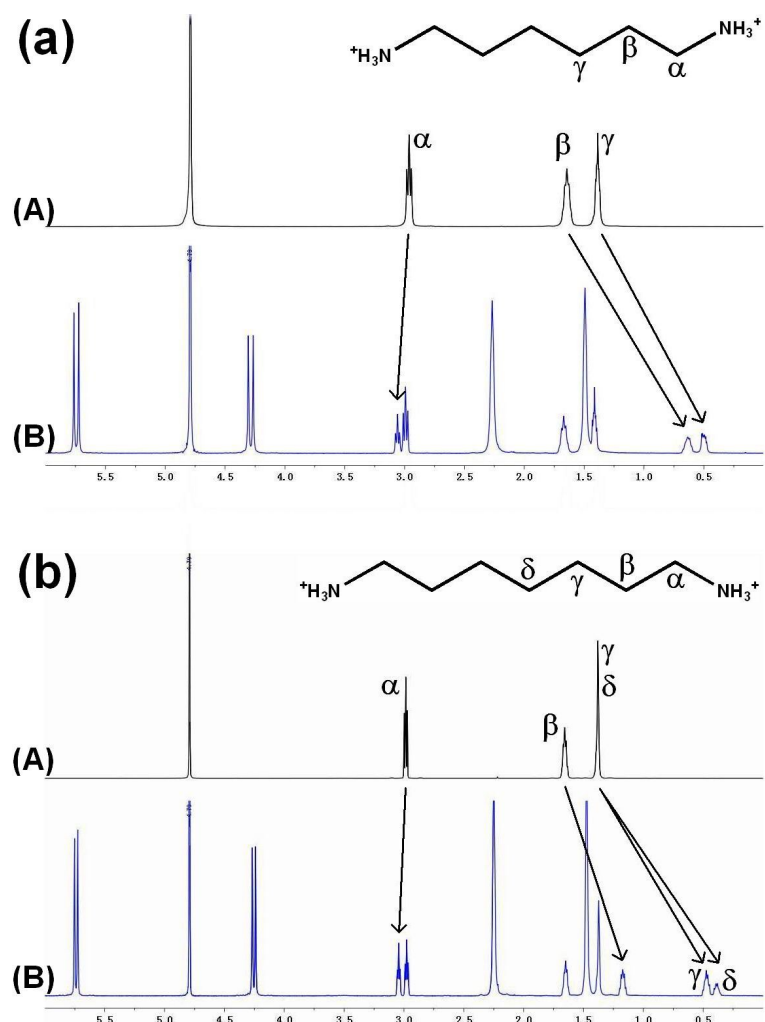


Figure S2 (a) ^1H NMR spectra (400 MHz, D_2O) of guest **5** in the absence (A) and in the presence of 0.41 equiv of Cy2Q[6]; (b) ^1H NMR spectra (400 MHz, D_2O) of guest **6** in the absence (A) and in the presence of 0.98 equiv of Cy2Q[6].

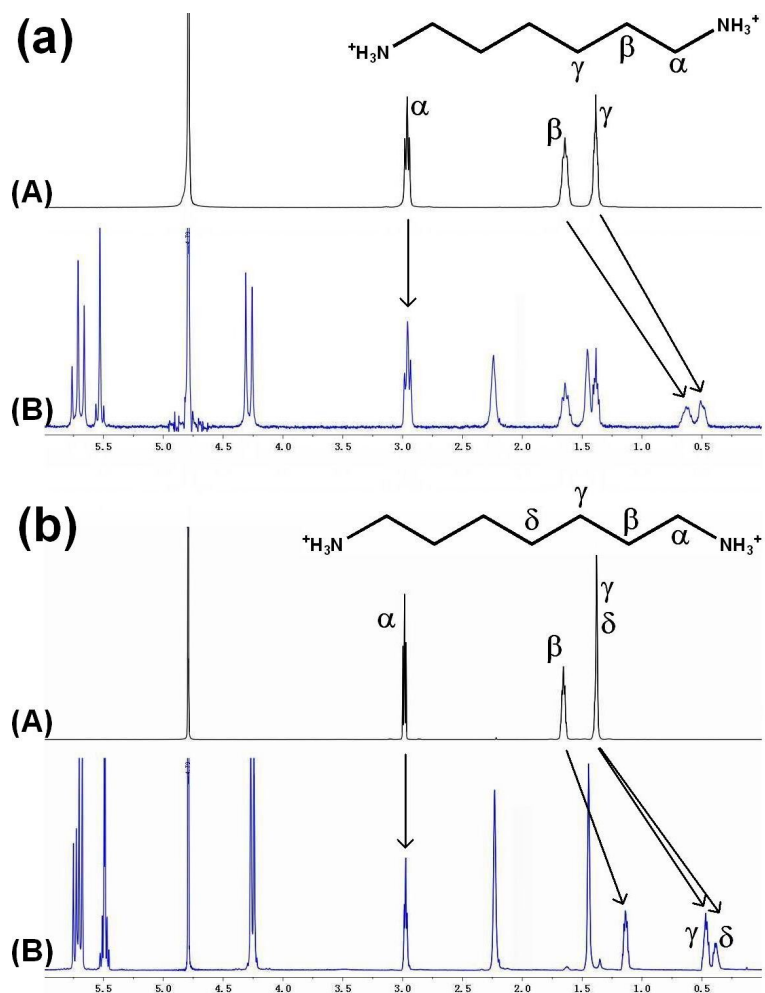


Figure S3 (a) ^1H NMR spectra (400 MHz, D_2O) of guest **7** in the absence (A) and in the presence of 0.42 (B) equiv of $\text{Cy2Q}[6]$; (b) ^1H NMR spectra (400 MHz, D_2O) of guest **7** in the absence (A) and in the presence of 0.46 (B) equiv of $\text{Cy6Q}[6]$.

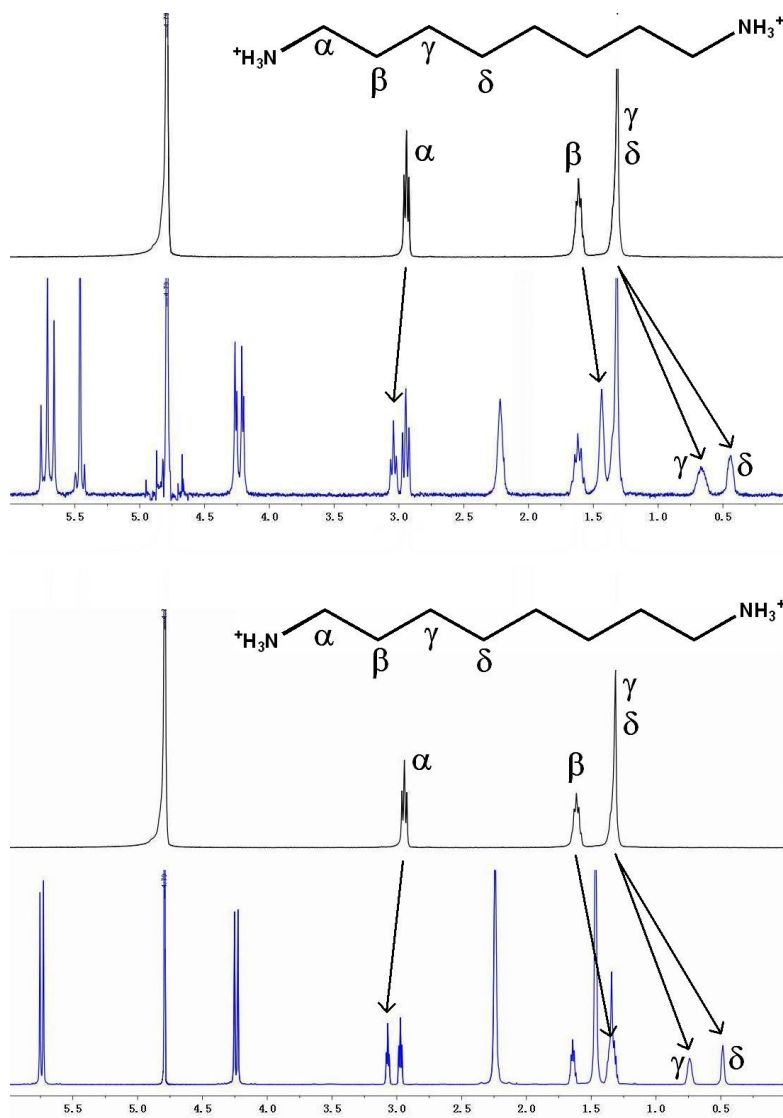


Figure S4. Isothermal titration calorimetry (ITC) binding curves for (a) Cy2Q[6]-alkyldiammonium and (b) Cy6Q[6]-alkyldiammonium complexes.

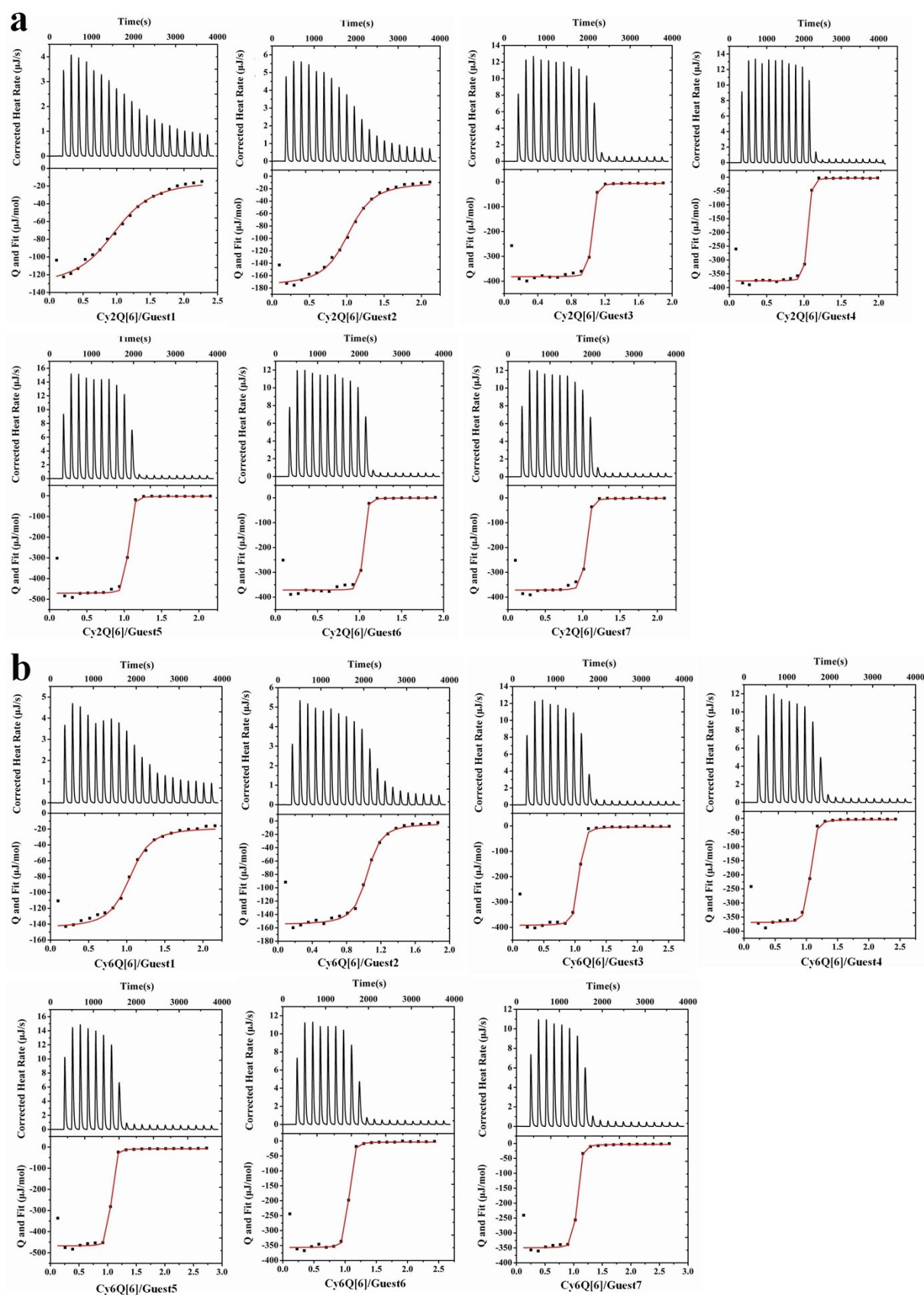


Figure S5 Electrostatic surface potentials calculated for Cy2Q[6] (left) and Cy6Q[6] (right).

