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Effects of cucurbituril size on the binding of a lutidine guest

Jan Svec,[a] Vladimir Sindelar*[a,b] and Angel E. Kaifer*[c]

[a] *Department of Chemistry, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic*
[b] *Centre for Toxic Compounds in the Environment, Masaryk University, Kamenice 3, 625 00 Brno, Czech Republic. Fax: (+420)549-49-2443; Tel: (+420)549-49-8142; E-mail: sindelar@chemi.muni.cz*
[c] *Center for Supramolecular Science and Department of Chemistry, University of Miami, Coral Gables, FL 33124-0431, USA. Fax: 1-305-284-4571; Tel: 1-305-284-3468; E-mail: akaifer@miami.edu*

ELECTRONIC SUPPLEMENTARY INFORMATION

Methods

NMR spectra were recorded using a Bruker Avance 300 spectrometer operating at frequencies of 300.13 MHz (^{1}H) at 298 K. pD values were obtained using H_2O-calibrated pH-meter after conversion.[1]

NMR experiments

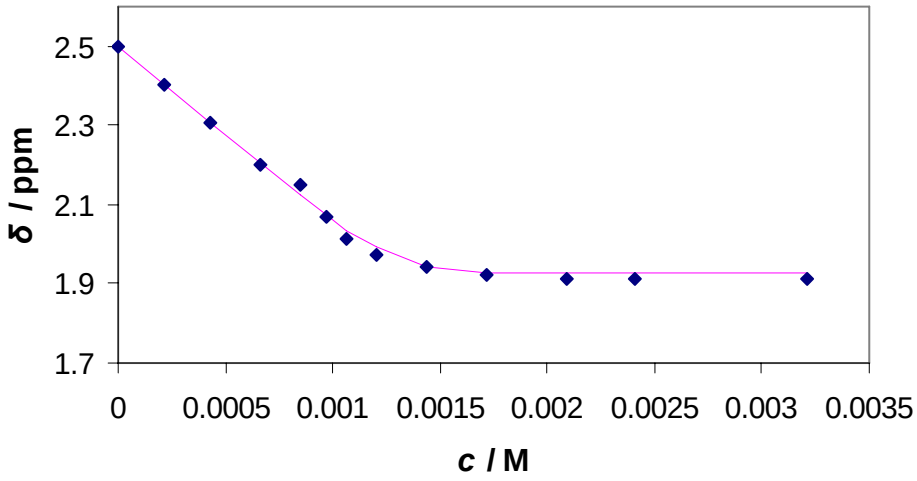

Figure S1. ^{1}H NMR (300 MHz) titration curve of **1**$^+$ with **CB7** in 0.02 M NaCl-D_2O, pD 3. Line shows best fit of the experimental data to the 1:1 binding model.

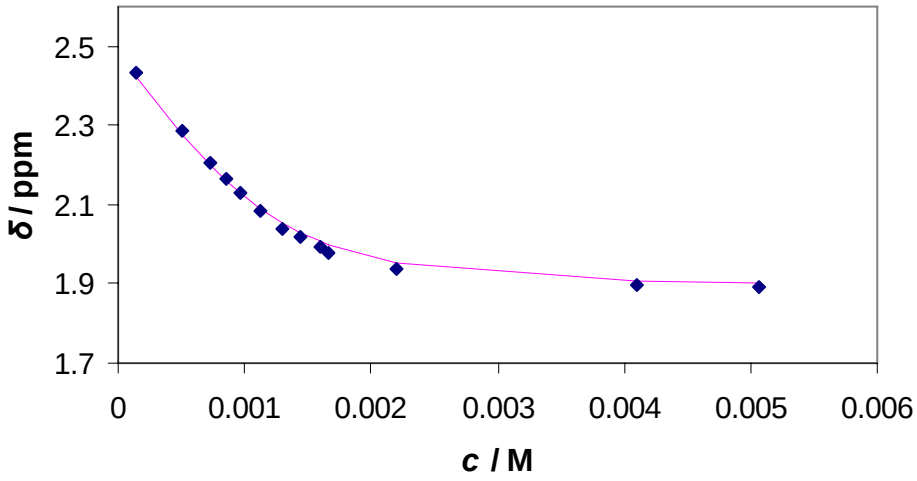

Figure S2. ^{1}H NMR (300 MHz) titration curve of **1**$^+$ with **CB7** in 0.02 M NaCl-D_2O, pD 9. Line shows best fit of the experimental data to the 1:1 binding model.

[1] A. Krezel, W. Bal, *J. Inorg. Biochem.*, 2004, **98**, 161.

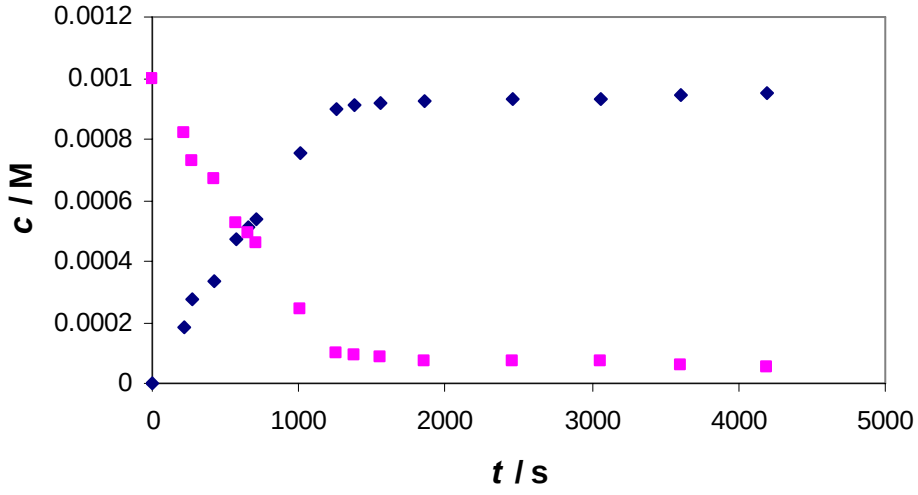

Figure S3. Kinetic traces, recorded at 293 K and pD 9, for the NMR signal intensity changes obtained upon addition of 1.1 equiv of **CB6** to the solution of 1 equiv of $\mathbf{1}^+$ and 1.1 equiv of **CB6**.

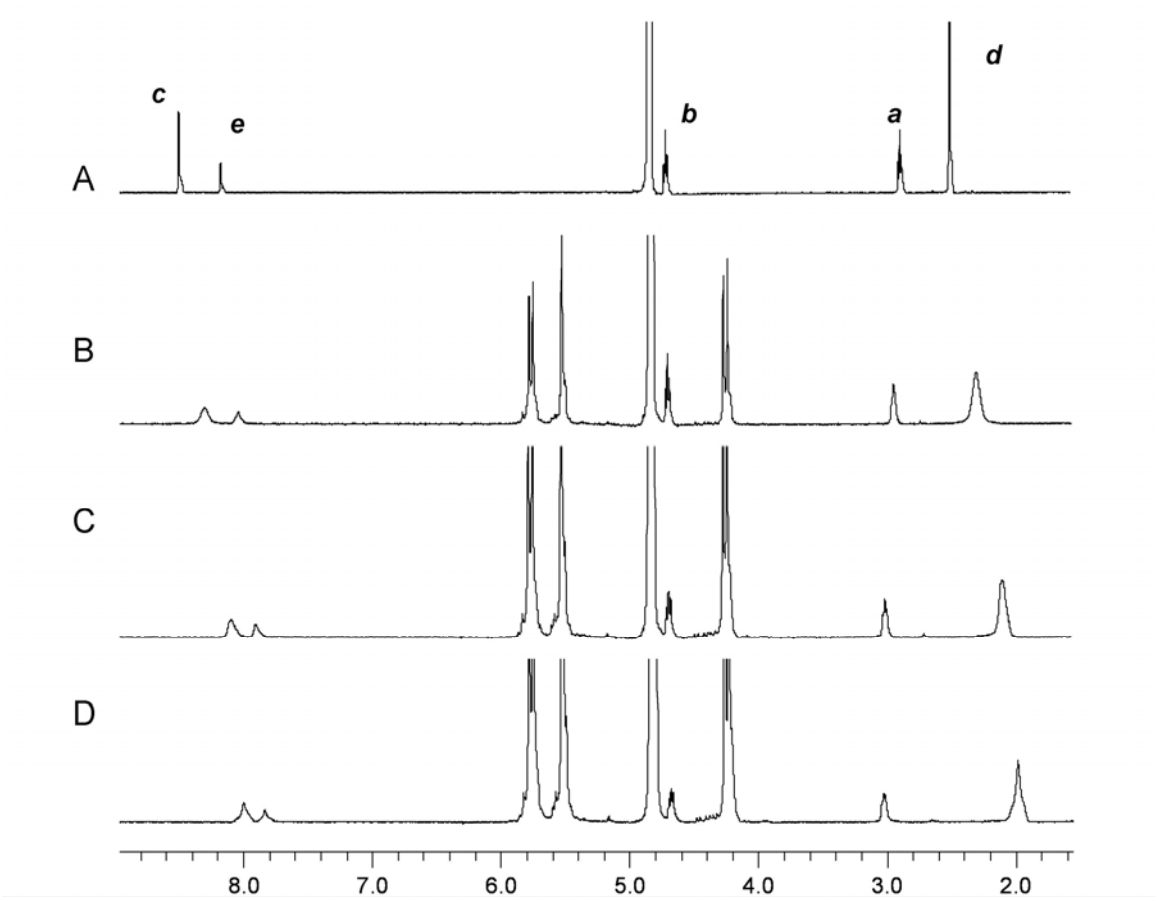

Figure S4. ^{1}H NMR spectra (300 MHz, 0.02 M NaCl – D_2O, pD 11) of $\mathbf{1}^+$ in the absence (A) and in the presence of 0.5 equiv (B), 1.2 equiv (C), and 1.9 equiv (D) of **CB7**.

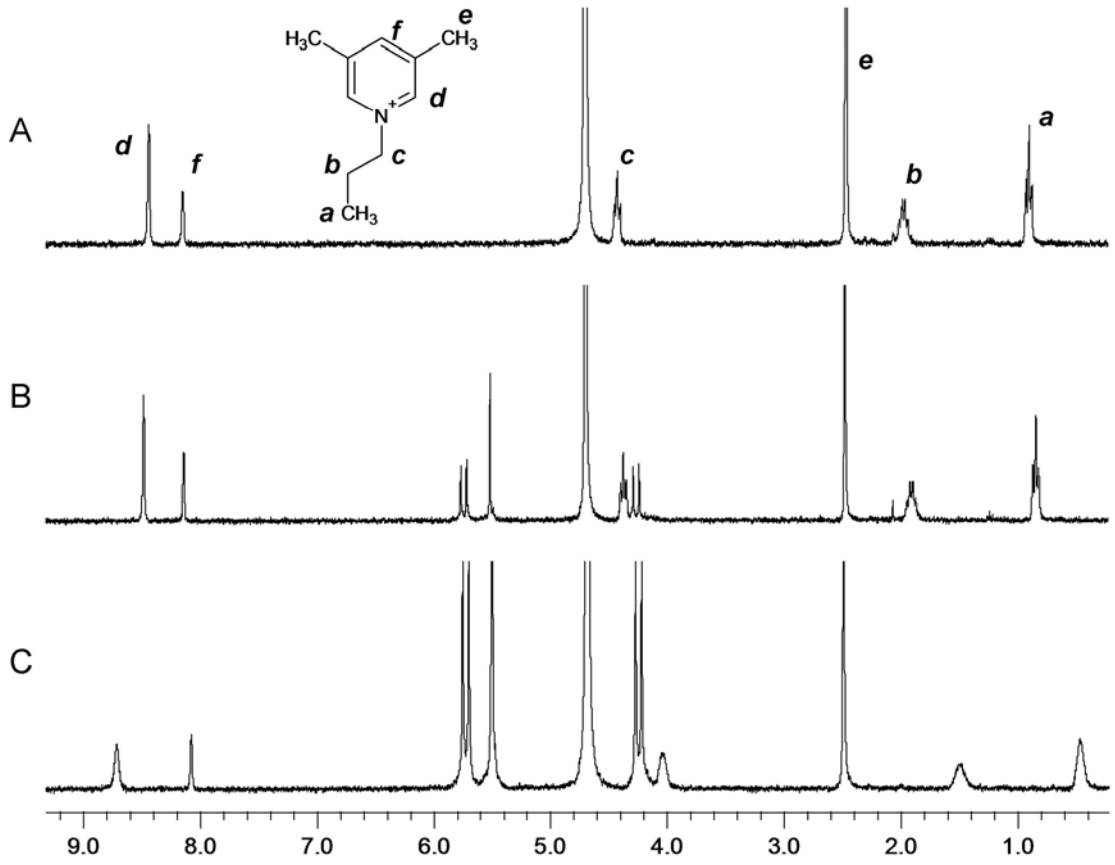

Figure S5. ^{1}H NMR spectra (300 MHz, 0.02 M NaCl – D_2O, pD 3) of comparative lutidine guest in the absence (A) and in the presence of 0.2 equiv (B) and 0.7 equiv (C) of **CB6**.