

Electronic Supplementary Information (ESI)

Host-guest complexation of HMeQ[7] with alkyldiammonium ions and alkyldiamines: A comparative study

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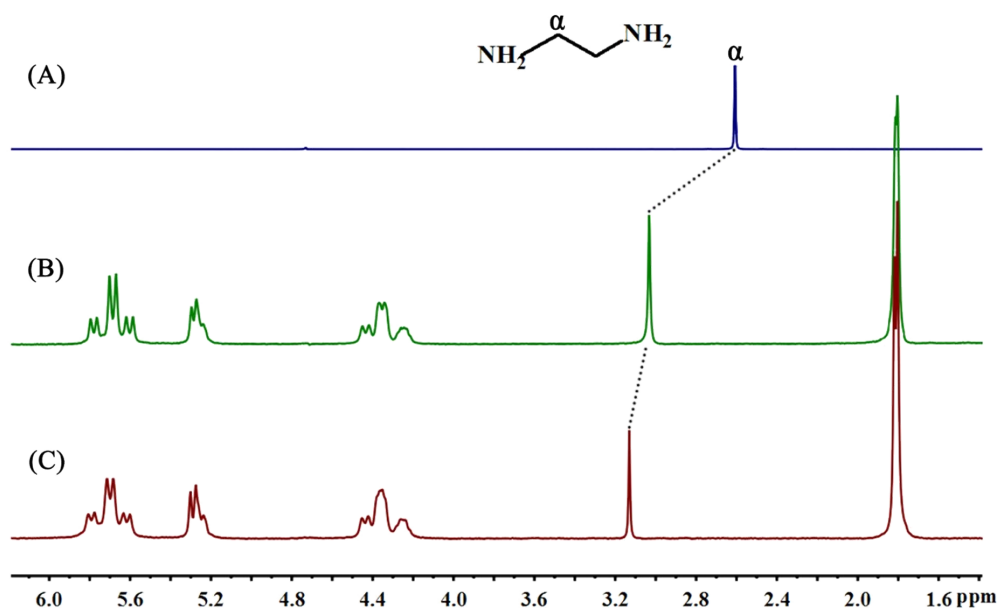


Figure S1. ¹H NMR spectra (400 MHz, D₂O) of guest **1** (A) in the absence and in the presence of (B) 0.75 and (C) 1.63 equiv of HMeQ[7] in D₂O at 20 °C.

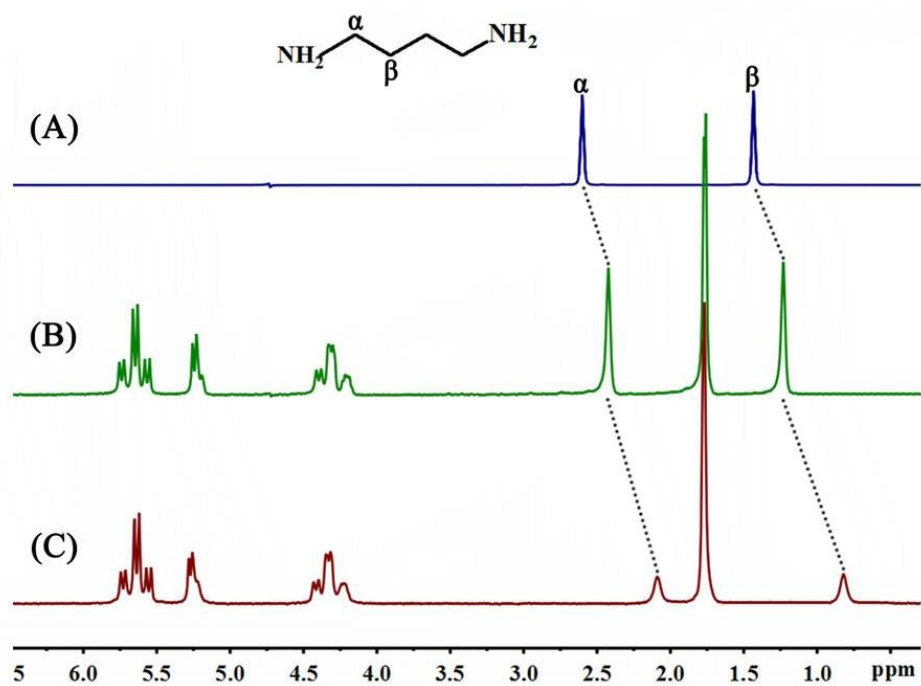


Figure S2. ¹H NMR spectra (400 MHz, D₂O) of guest **2** (A) in the absence and in the presence of (B) 0.34 and (C) 1.12 equiv of HMeQ[7] in D₂O at 20 °C.

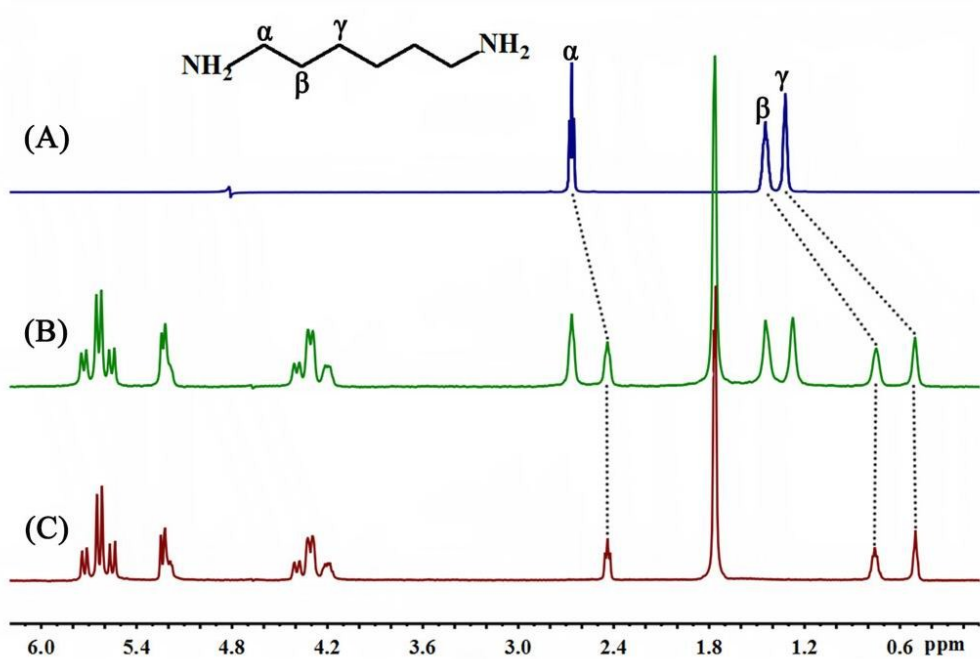


Figure S3. ¹H NMR spectra (400 MHz, D₂O) of guest **3** (A) in the absence and in the presence of (B) 0.40 and (C) 1.13 equiv of HMeQ[7] in D₂O at 20 °C.

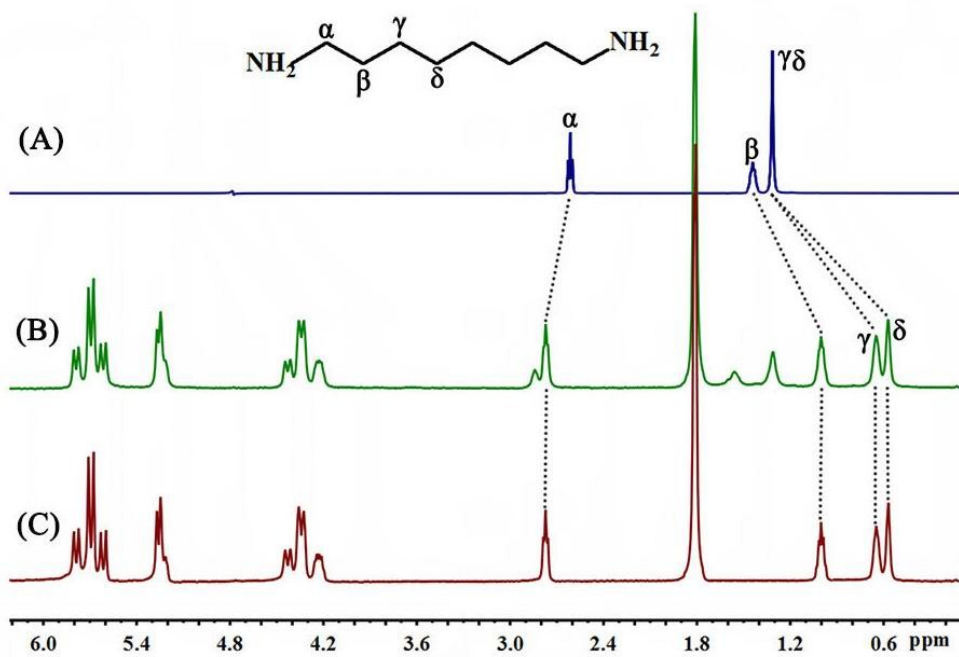


Figure S4. ^1H NMR spectra (400 MHz, D_2O) of guest 4 (A) in the absence and in the presence of (B) 0.79 and (C) 1.13 equiv of HMeQ[7] in D_2O at 20 $^\circ\text{C}$.

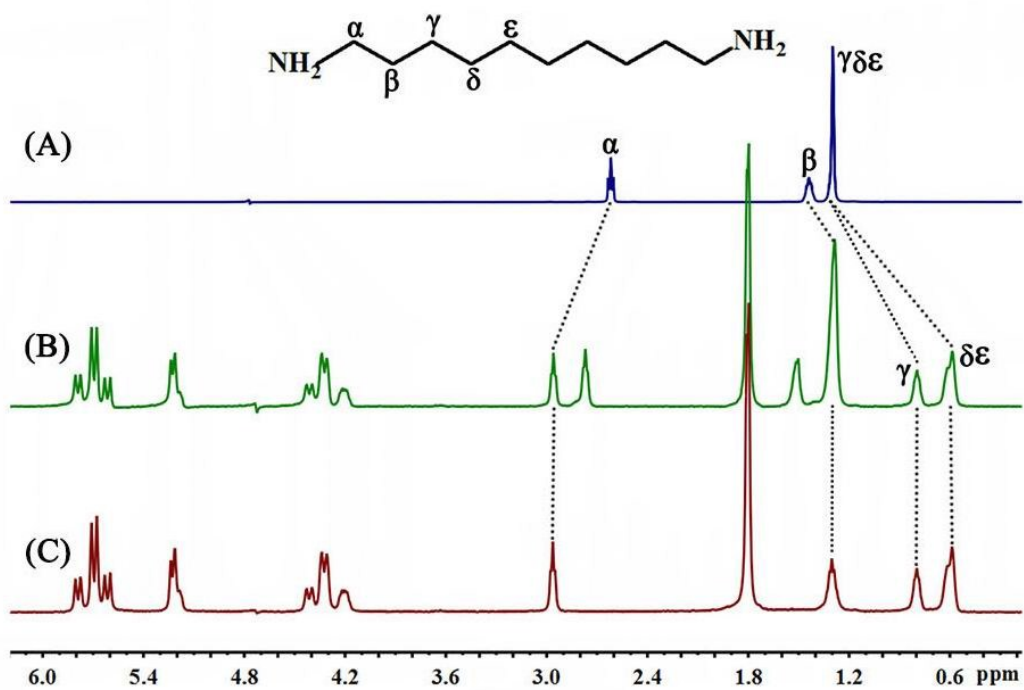
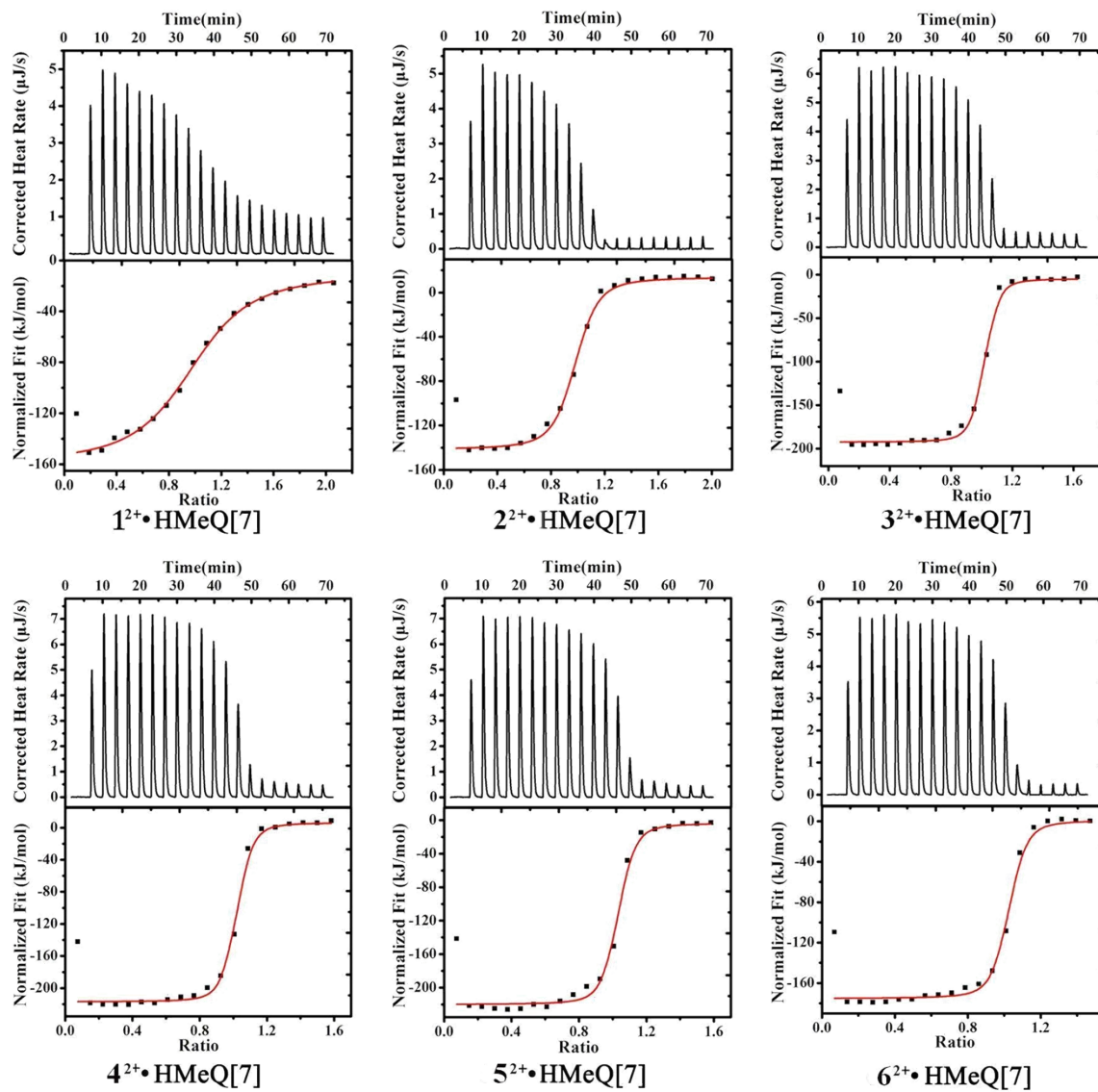


Figure S5. ^1H NMR spectra (400 MHz, D_2O) of guest **5** (A) in the absence and in the presence of (B) 0.42 and (C) 1.02 equiv of HMeQ[7] in D_2O at 20 $^\circ\text{C}$.

(a)



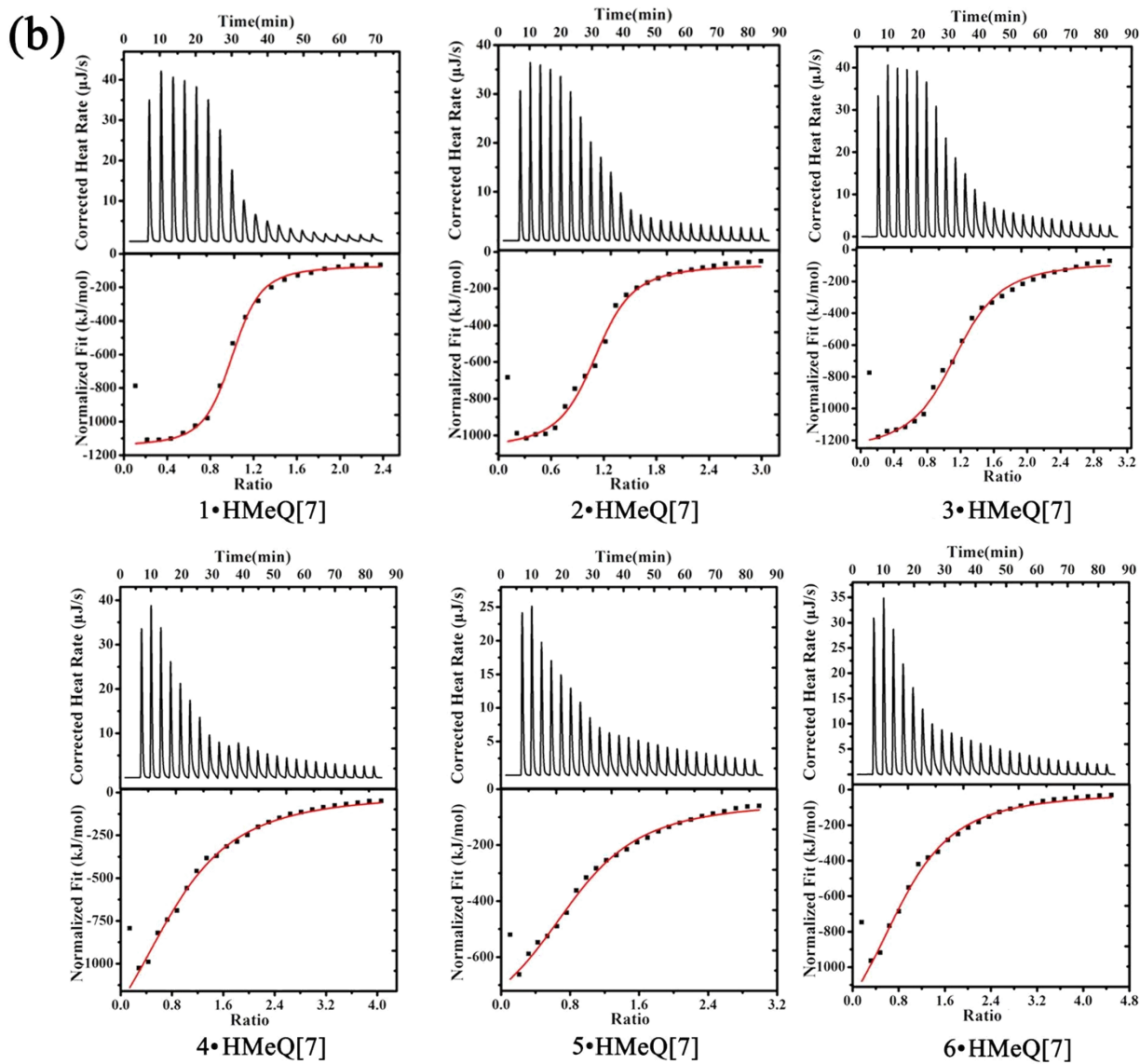


Figure S6. Isothermal titration calorimetry (ITC) binding curves for (a) HMeQ[7] - alkyldiammonium and (b) HMeQ[7]-alkyldiamine complexes.

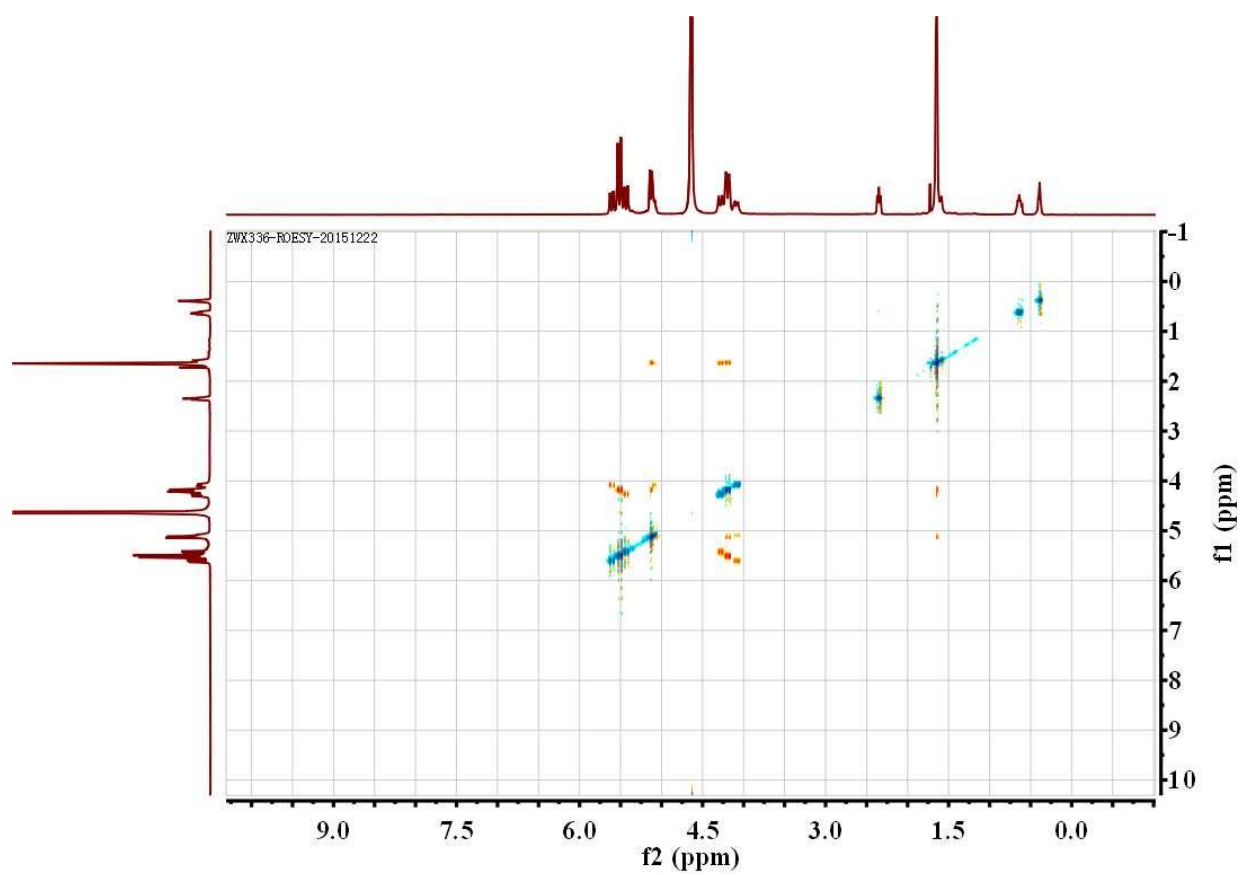


Figure S7. NOESY NMR spectrum (400 MHz, D₂O) of HMeQ[7] with guest 3²⁺.

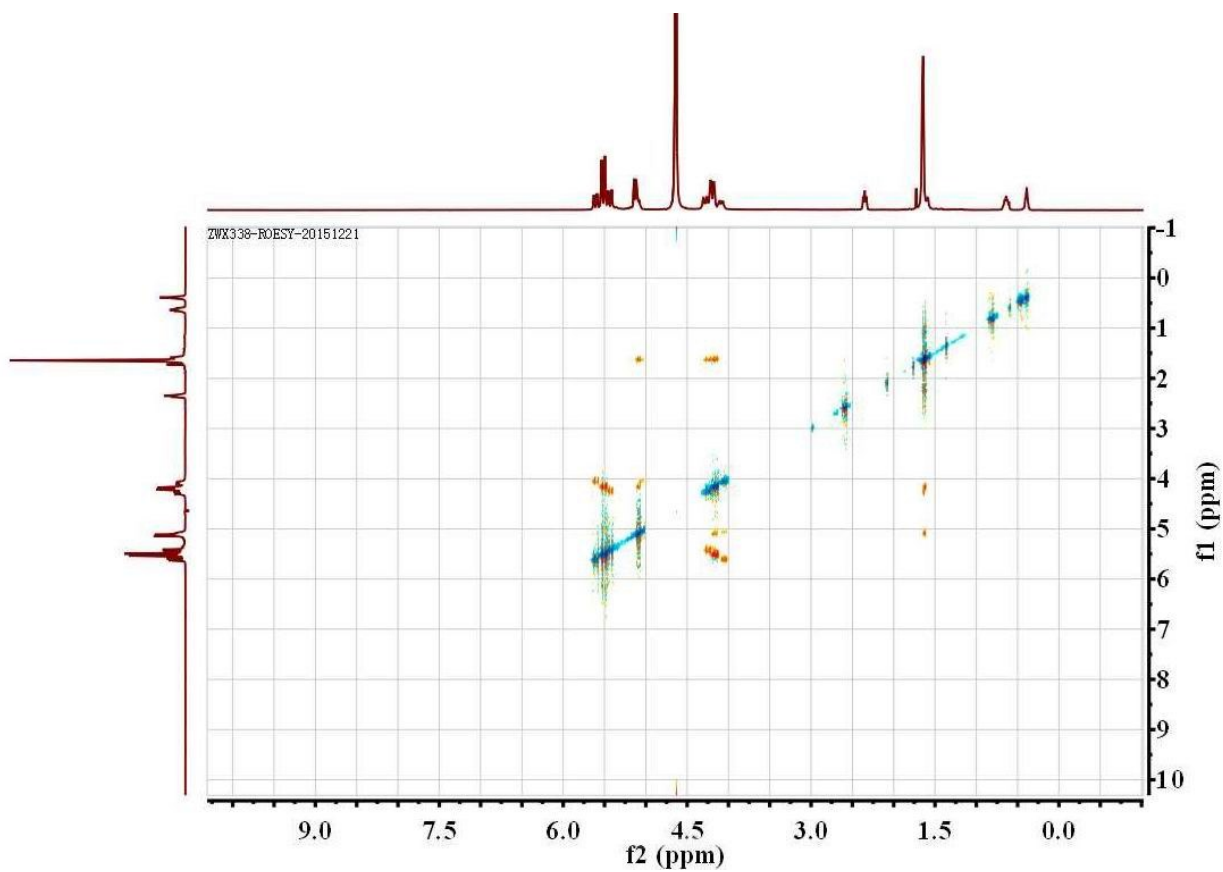


Figure S8. NOESY NMR spectrum (400 MHz, D₂O) of HMeQ[7] with guest 3²⁺.