Supplementary Information

Coordination of Ln$^{3+}$ in Ortho-tetramethyl Substituted Cucurbituril Supramolecular Assemblies Formed in the Presence of Cadmium Nitrate: Potential Applications for Isolation of Heavier Lanthanides

Jia-Jia Zhou, Xin Yu, Ying-Chun Zhao, Xin Xiao, Yun-Qian Zhang, Sai-Feng Xue, Zhu Tao, Jing-Xin Liu,* and Qian-Jiang Zhu*

a Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China
b College of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan 243002, China.
SI-Figure 1 (a) ITC profile of o-TMeQ[6] with Ce(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -8.903$ kJ mol$^{-1}$, $T\Delta S^0 = 28.145$ kJ mol$^{-1}$; (b) ITC profile of o-TMeQ[6] with Eu(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -5.861$ kJ mol$^{-1}$, $T\Delta S^0 = 28.363$ kJ mol$^{-1}$; (c) ITC profile of o-TMeQ[6] with Yb(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -7.912$ kJ mol$^{-1}$, $T\Delta S^0 = 24.863$ kJ mol$^{-1}$; (d) ITC profile of o-TMeQ[6]+Cd(NO$_3$)$_2$ with Ce(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -6.824$ kJ mol$^{-1}$, $T\Delta S^0 = 28.232$ kJ mol$^{-1}$; (e) ITC profile of o-TMeQ[6]+Cd(NO$_3$)$_2$ with Eu(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -5.621$ kJ mol$^{-1}$, $T\Delta S^0 = 30.411$ kJ mol$^{-1}$; (f) ITC profile of o-TMeQ[6]+Cd(NO$_3$)$_2$ with Yb(NO$_3$)$_3$ at 298.15 K: $\Delta H^0 = -7.048$ kJ mol$^{-1}$, $T\Delta S^0 = 26.595$ kJ mol$^{-1}$. 
SI-Figure 2  the electron spectroscopies of o-TMeQ[6]/NO$_3^-$ systems with 1:1 ratio of La:Yb, Ce:Yb, Pr:Yb and corresponding crystals with a general yields

The yield of 60% ~ 66%

The yield of 80% ~ 85%

The yield of 83% ~ 88%
SI-Figure 3  the electron spectroscopy of $o$-TMeQ[6]/NO$_3^-$ systems with 1:1 ratios of light : heavy lanthanides
SI-Figure 4  the electron spectroscopy of \( o\text{-TMeQ}[6]/\text{NO}_3^- \) systems with 10:1, 5:1, 1:1, 1:5 and 1:10 ratios of Eu:Yb
SI-Figure 5 Powder X-ray diffraction (PXRD) of the representative crystals from the two isomorphic groups respectively
SI-Figure 6 DTA (left) and TG (right) curves of the representative crystals from the two isomorphous groups with a comparison $\alpha$-TMeQ[6] in N$_2$ respectively.
SI-Figure 7  FT-IR spectra of the representative crystals from the two isomorphous groups with a comparison of $\alpha$-TMeQ[6] powders respectively.