

Supplementary Information

Adducts of Aqua Complexes of Ln³⁺ with hexanohydroxyhexanomethylcucurbit[6]uril: Potential Application in the Isolation of Heavy Lanthanides

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EXPERIMENTAL SECTION

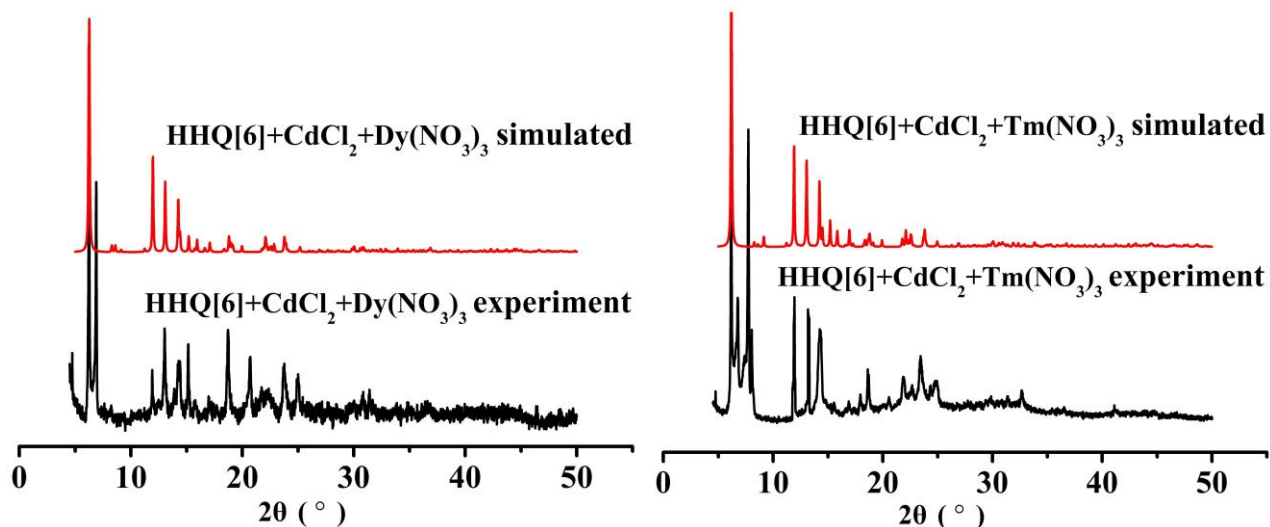
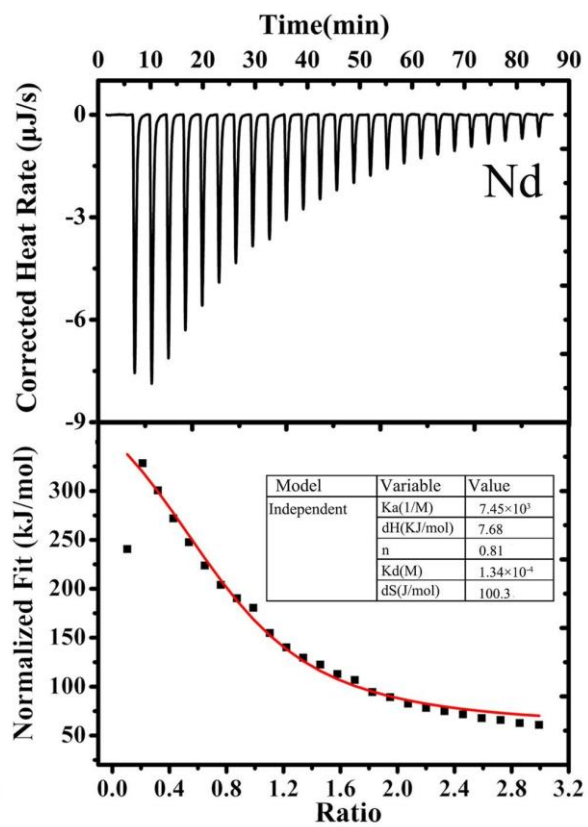
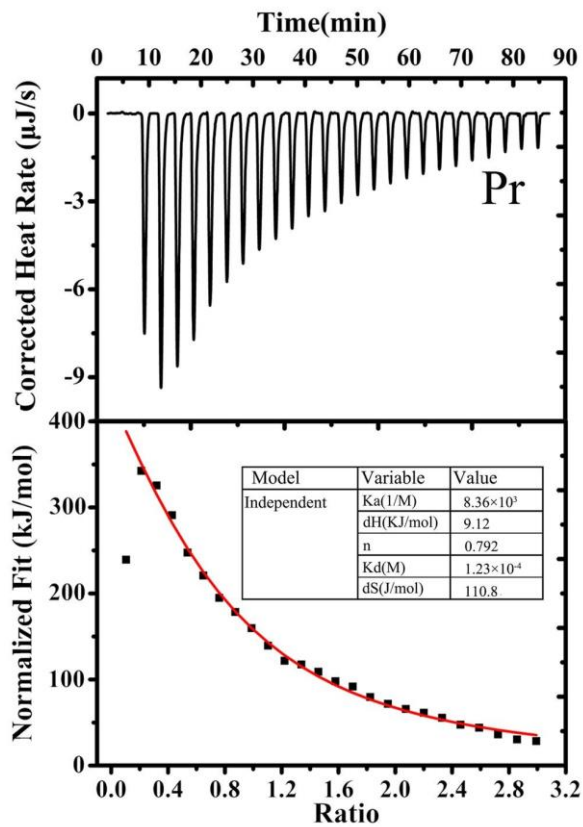
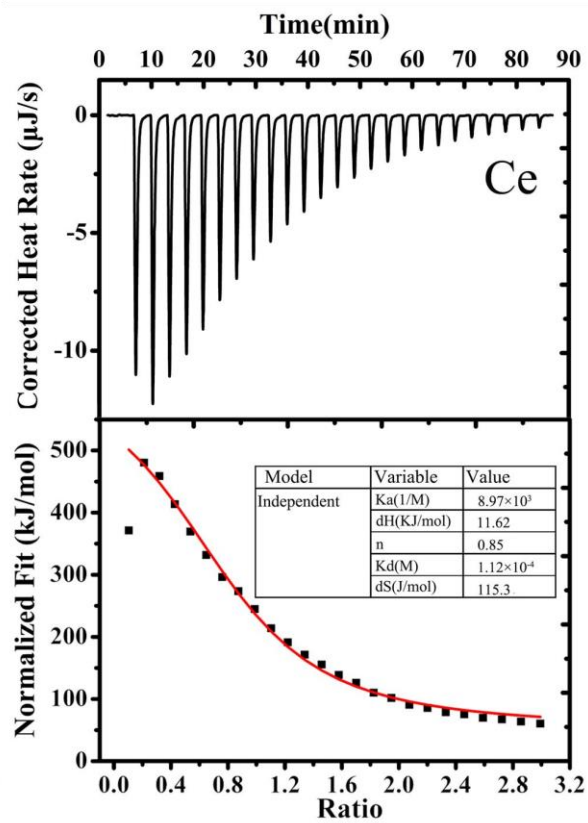
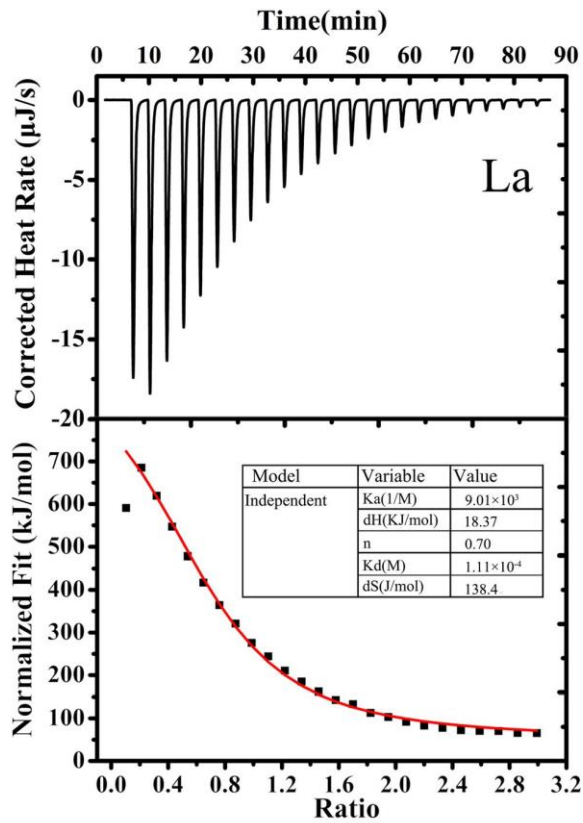
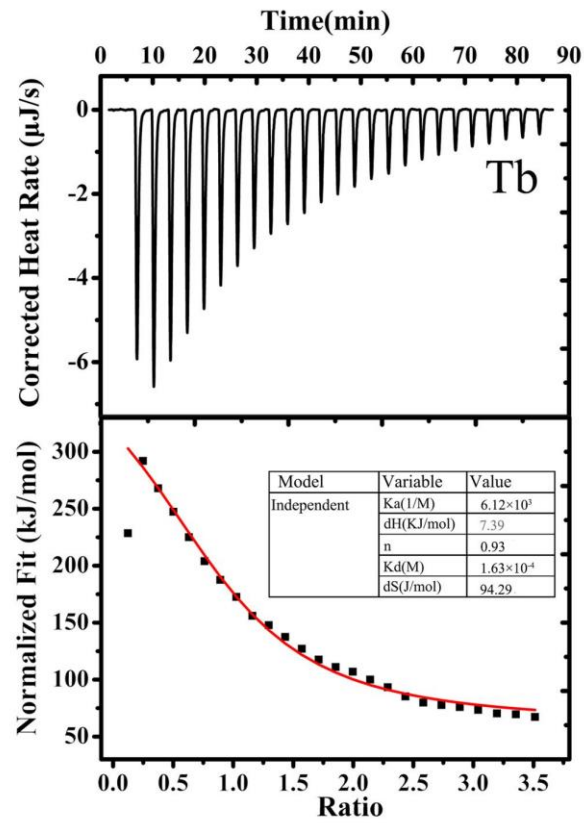
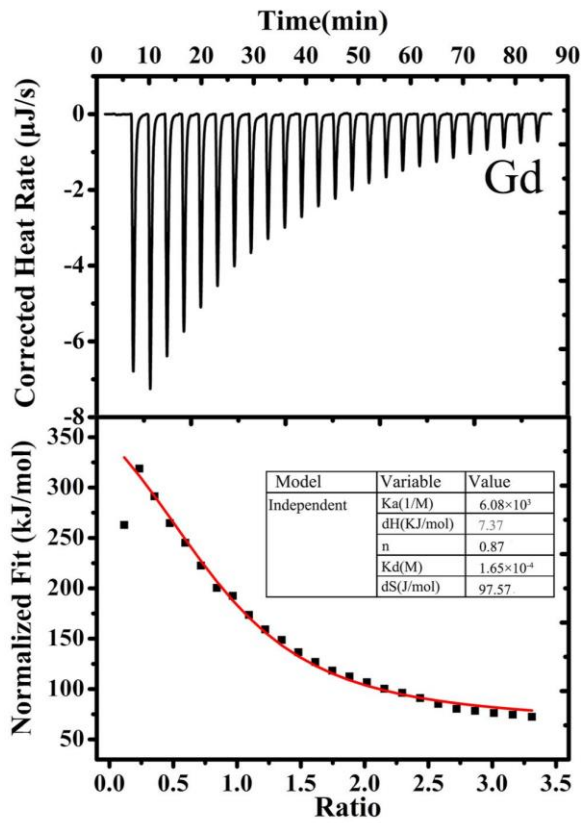
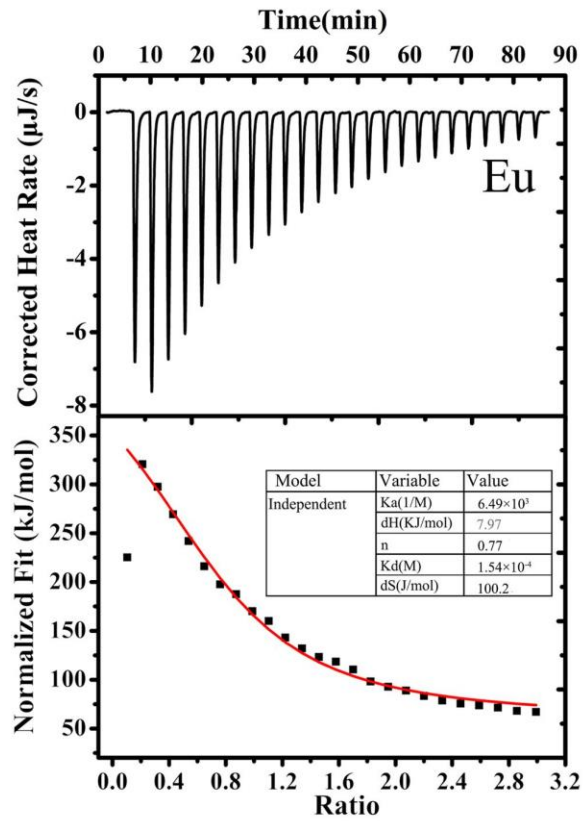
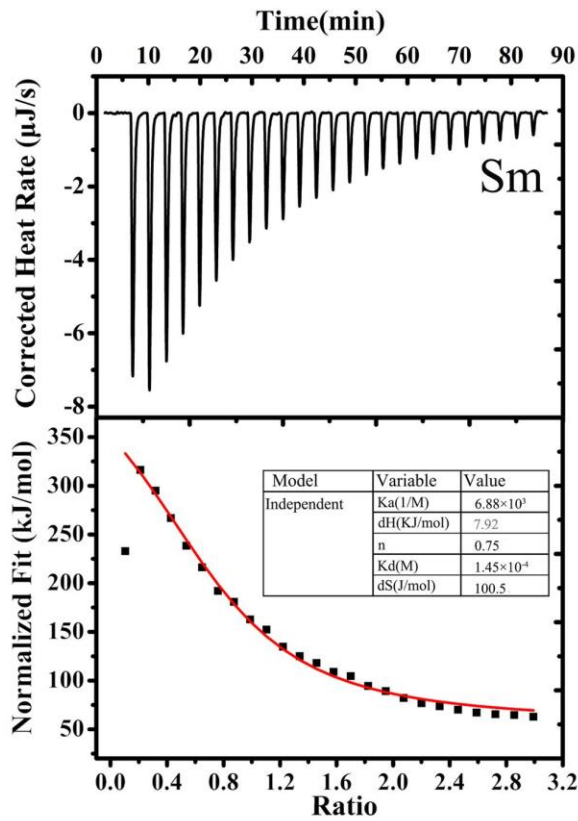
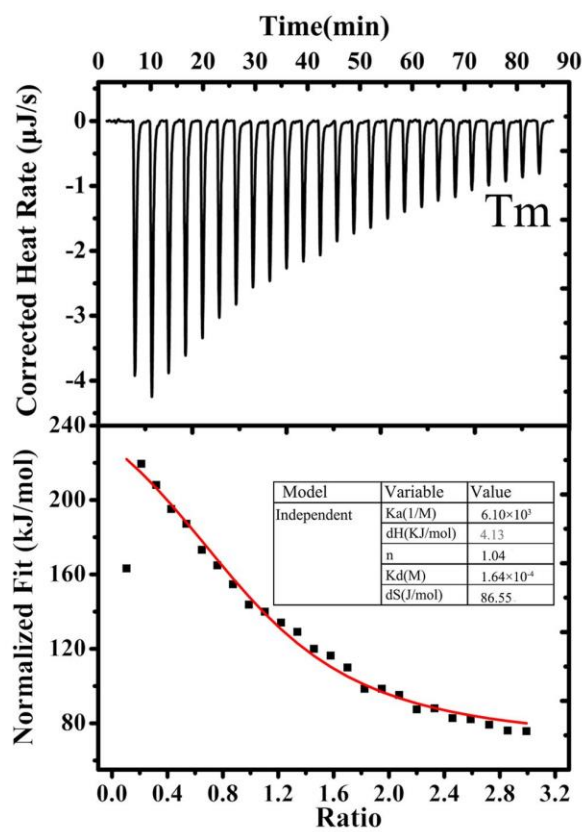
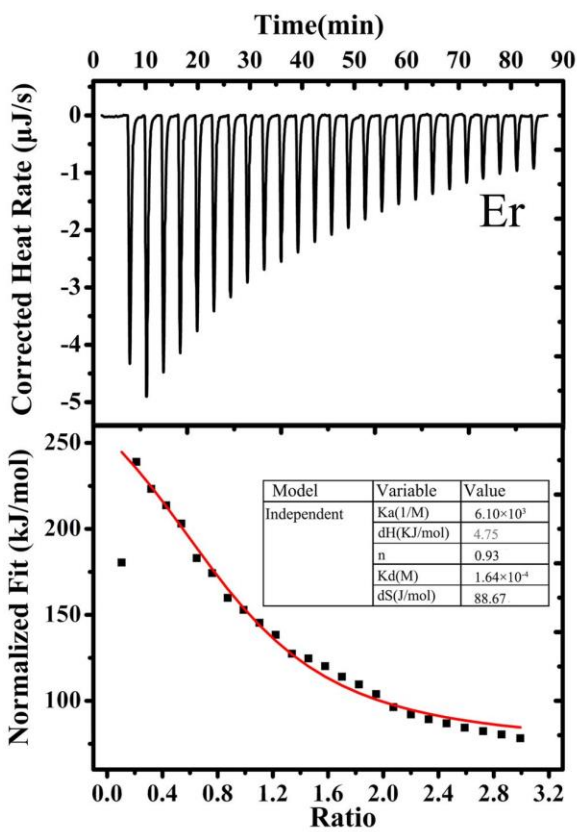
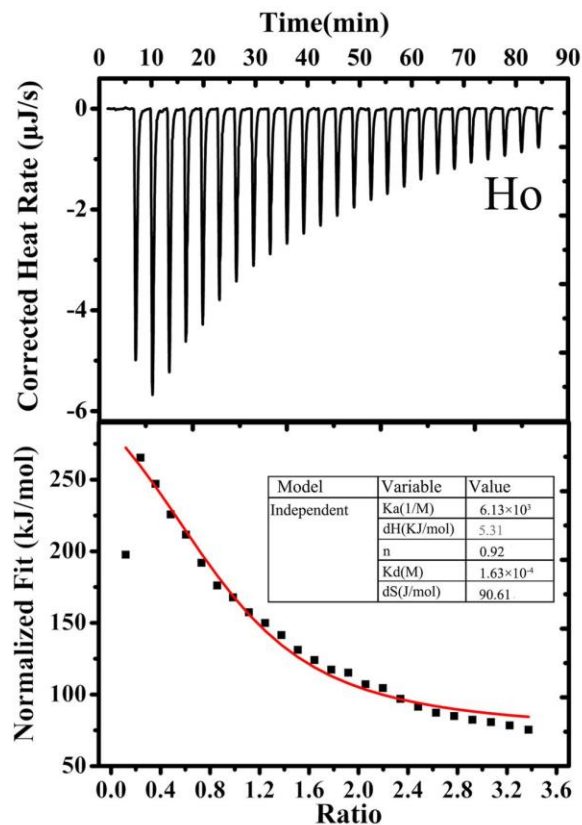
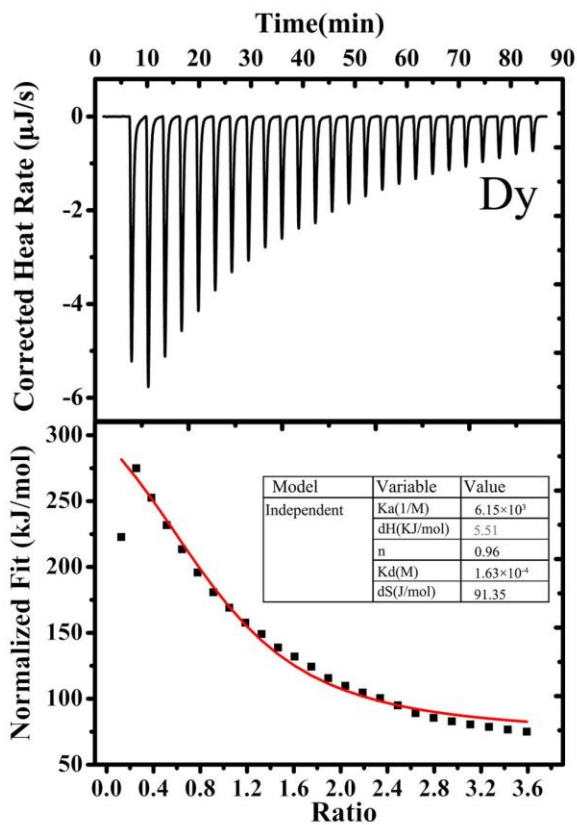


Figure S1 Powder X-ray diffraction (PXRD) of the four coordination complexes from the isomorphous group, respectively

Isothermal titration calorimetry: Microcalorimetric experiments were performed using an isothermal titration calorimeter Nano ITC 2G (TA, USA) at 293.15 K. Each experiment consisted of 25 consecutive injections (10 μ L) of a solution of (Ln(NO₃)₃·5 or 6H₂O respectively: 5×10^{-3} M) into the microcalorimetric reaction cell (1 mL) charged with a solution of HHQ[6] (5×10^{-4} M). The heat of reaction was corrected for the heat of dilution of the guest solution, determined in the separate experiments. All solutions were degassed prior to titration experiment by sonication. Computer simulations (curve fitting) were performed using the Nano ITC analyze software.







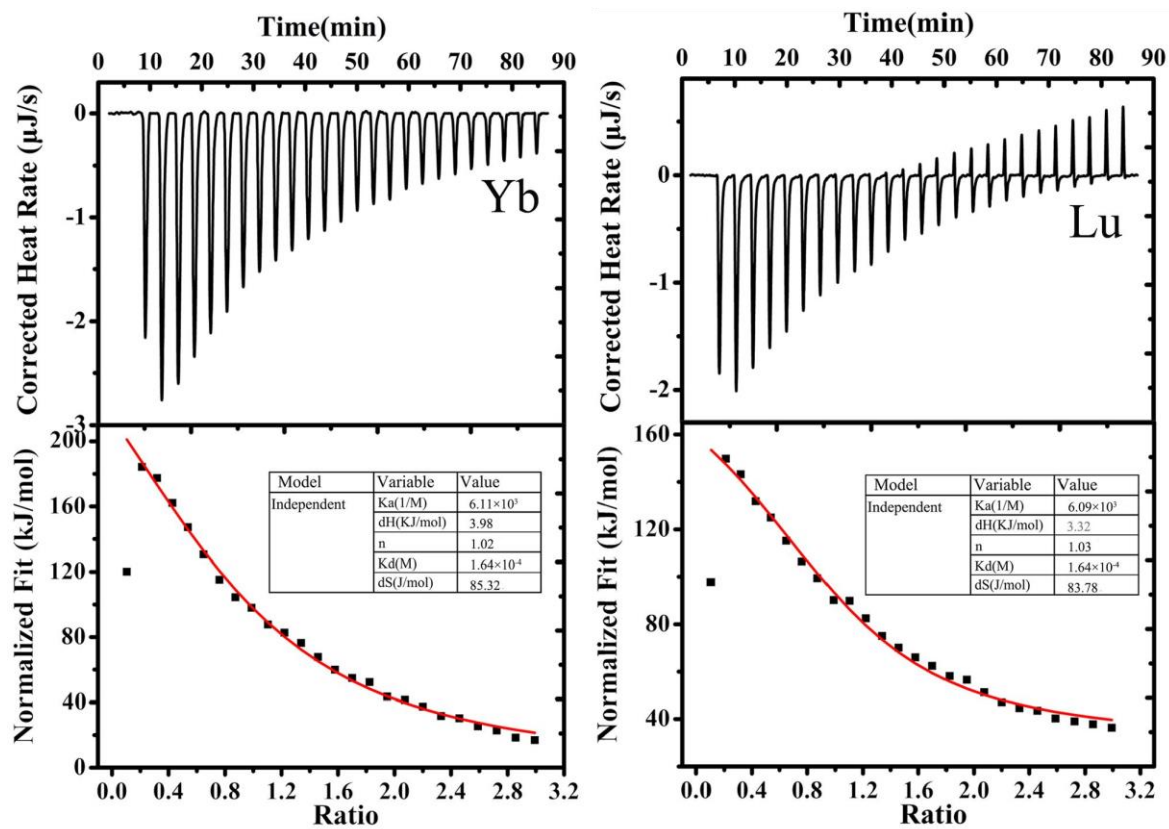
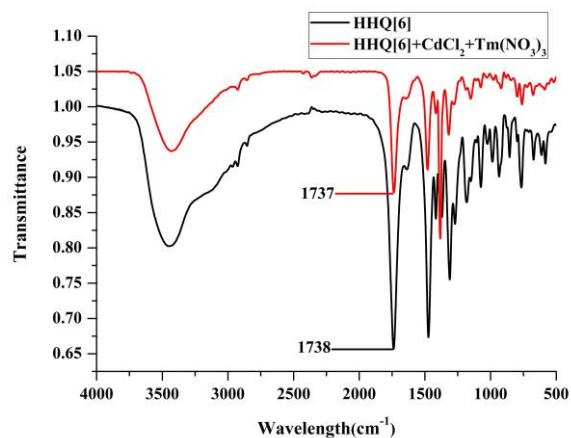
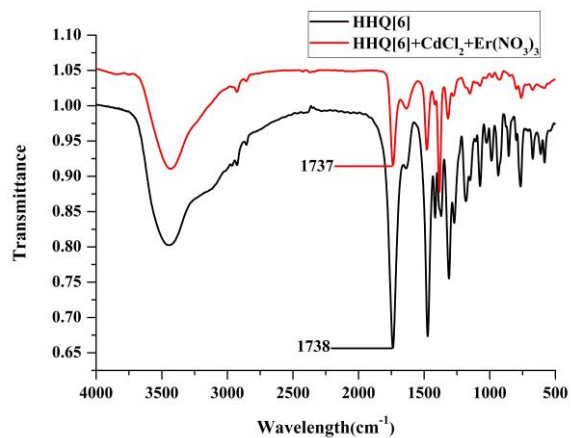
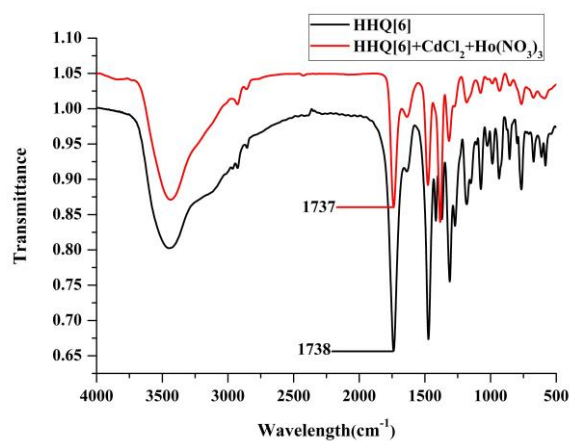
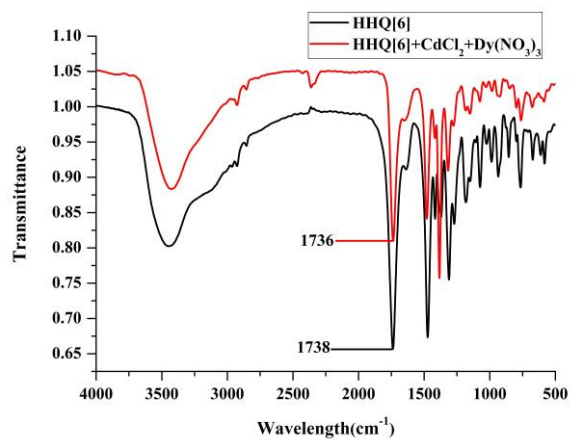
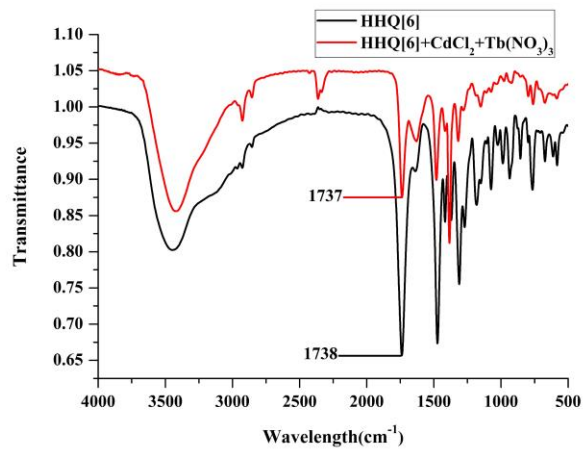
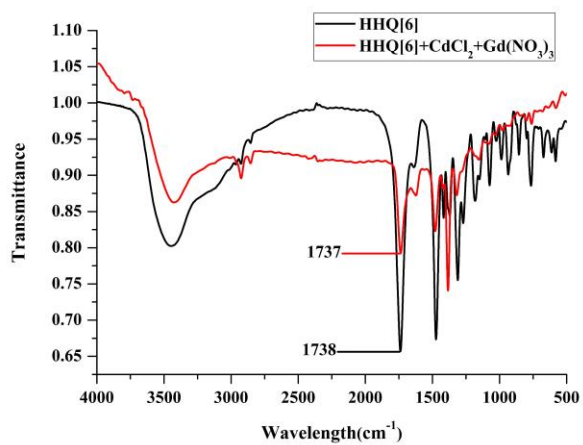


Figure S2 Isothermal titration calorimetry profiles of HHQ[6] with $\text{Ln}(\text{NO}_3)_3$ at 293.15 K: Ln = (a) La; (b) Ce; (c) Pr; (d) Nd; (e) Sm; (f) Eu; (g) Gd; (h) Tb; (i) Dy; (j) Ho; (k) Er; (l) Tm; (m) Yb; (n) Lu.



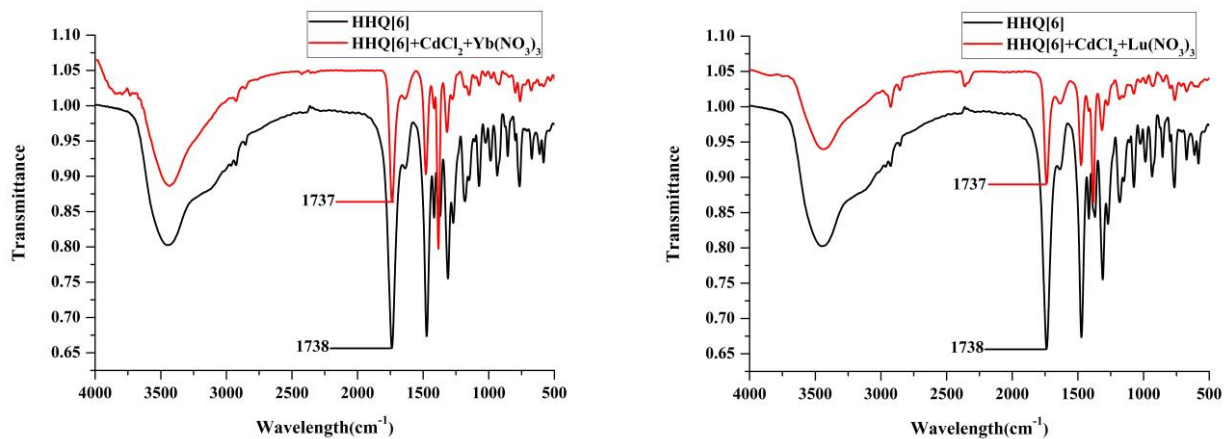


Figure S3 FT-IR spectra of compounds 1~8 with a comparison of HHQ[6] powders respectively.

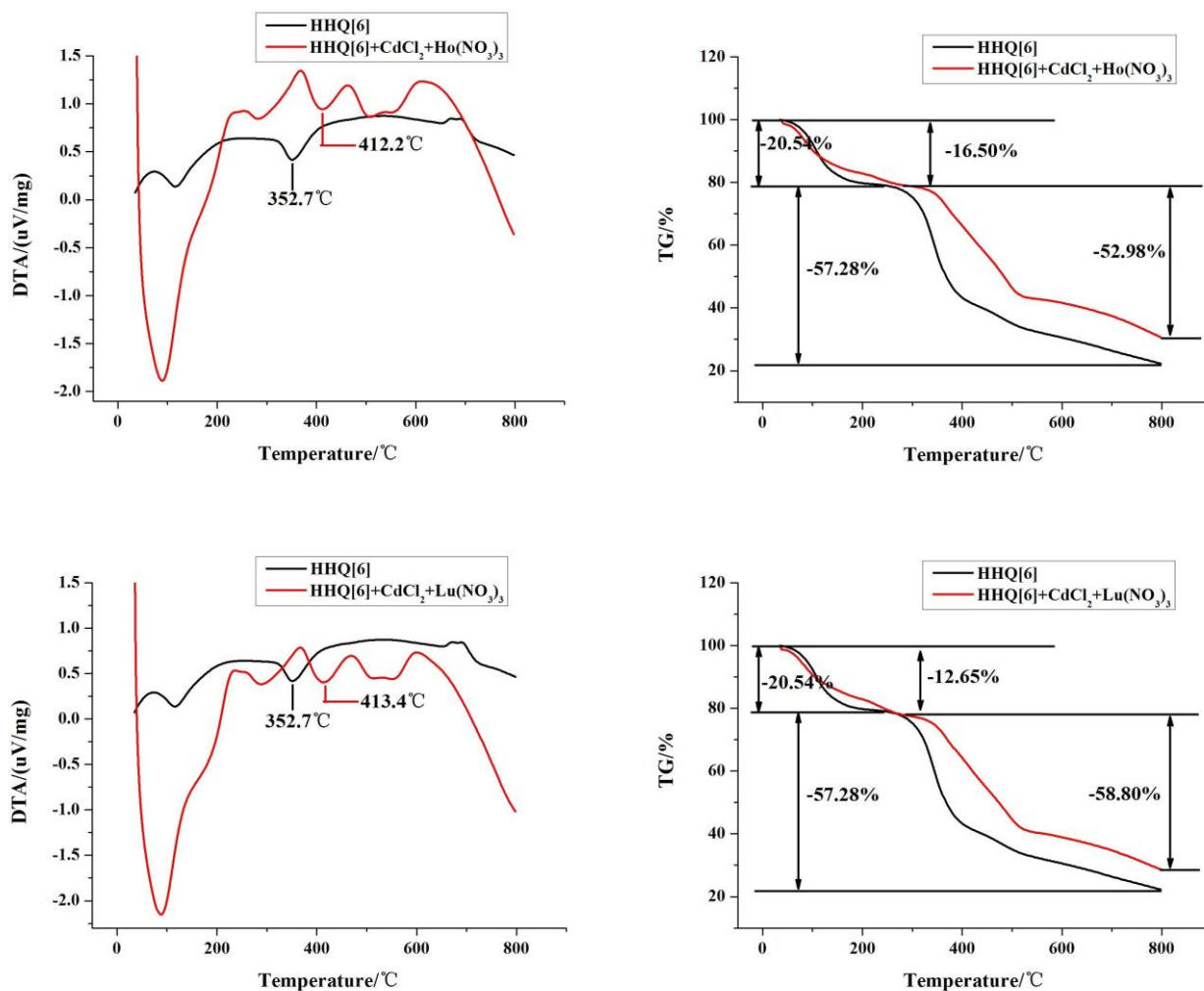
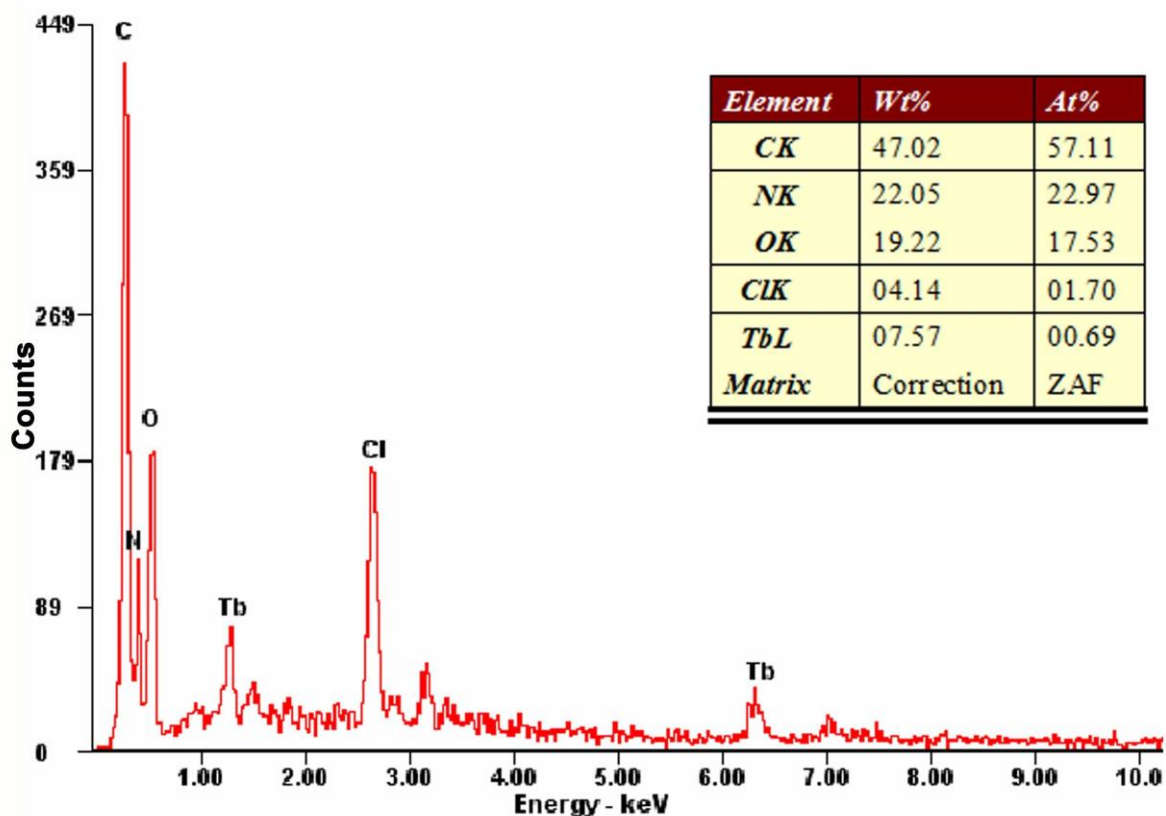
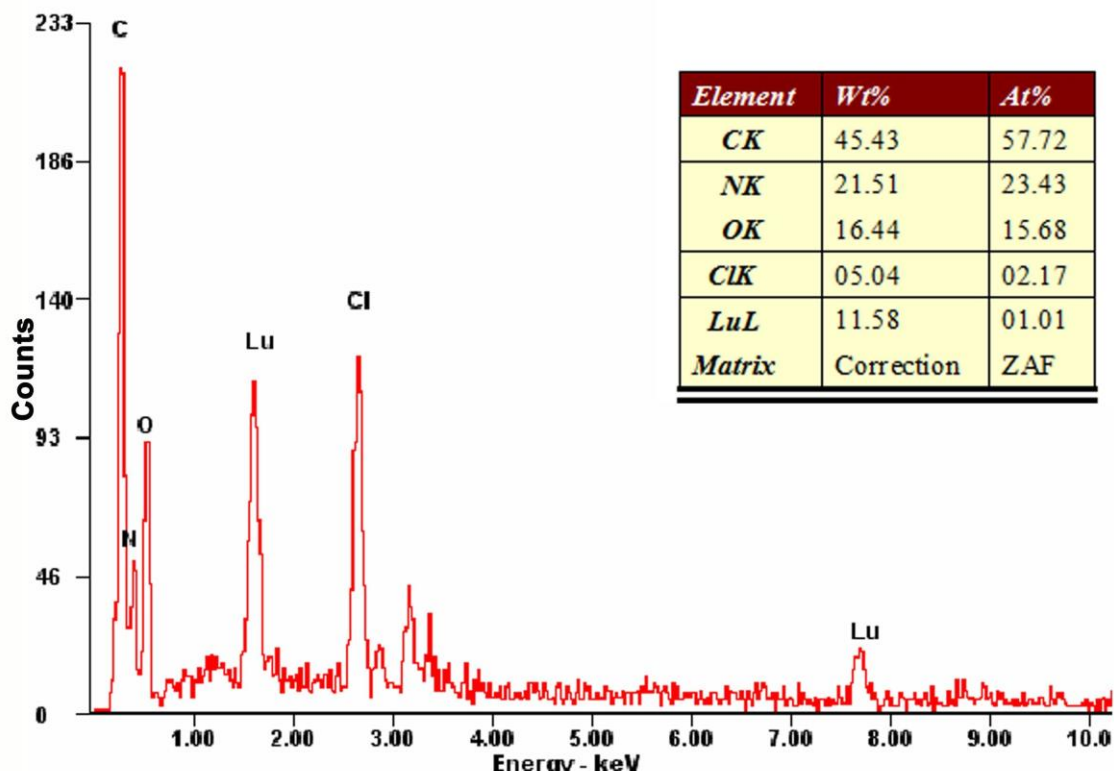


Figure S4 DTA (left) and TG (right) curves of compounds 4 , 8 with a comparison HHQ[6] in N₂ respectively



<i>Element</i>	<i>Wt%</i>	<i>At%</i>
<i>CK</i>	47.02	57.11
<i>NK</i>	22.05	22.97
<i>OK</i>	19.22	17.53
<i>ClK</i>	04.14	01.70
<i>TbL</i>	07.57	00.69
<i>Matrix</i>	Correction	ZAF

HHQ[6]+CdCl₂+La(NO₃)₃,Tb(NO₃)₃(1:1)



<i>Element</i>	<i>Wt%</i>	<i>At%</i>
<i>CK</i>	45.43	57.72
<i>NK</i>	21.51	23.43
<i>OK</i>	16.44	15.68
<i>ClK</i>	05.04	02.17
<i>LuL</i>	11.58	01.01
<i>Matrix</i>	Correction	ZAF

HHQ[6]+CdCl₂+La(NO₃)₃,Lu(NO₃)₃(1:1)

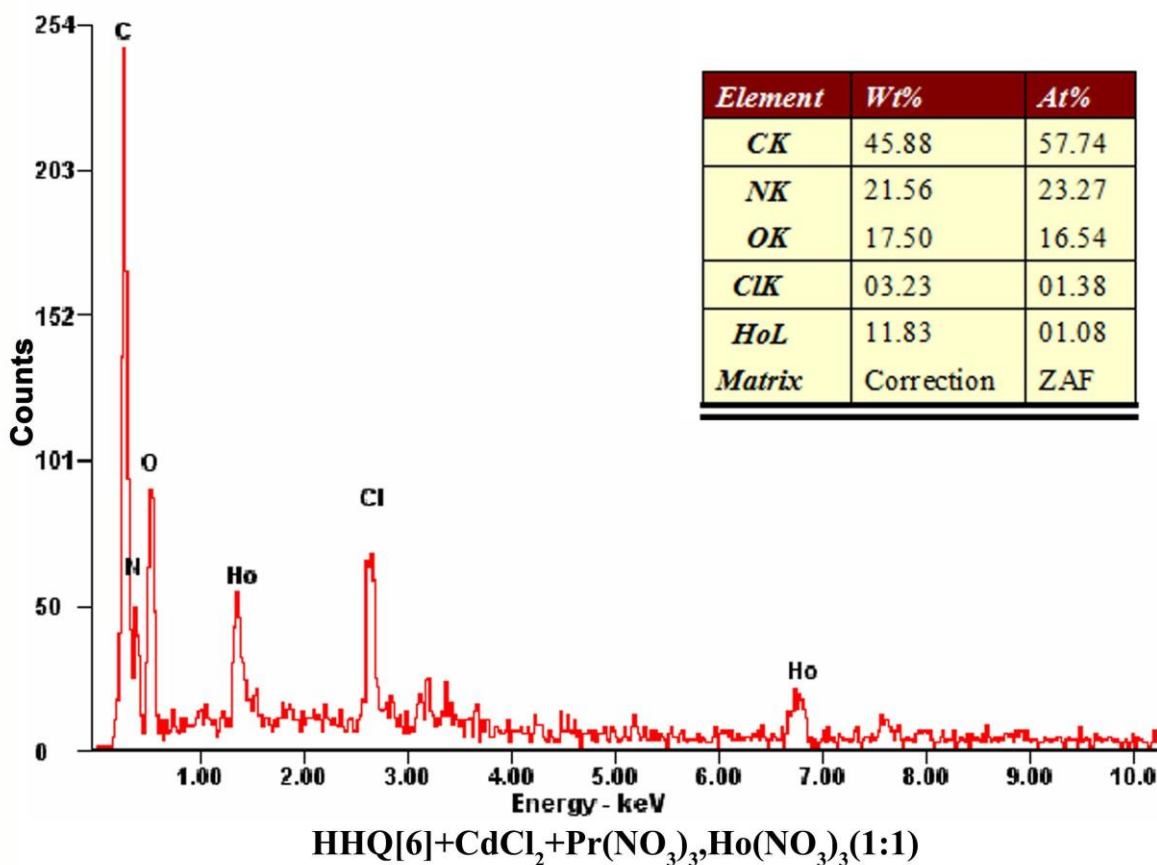
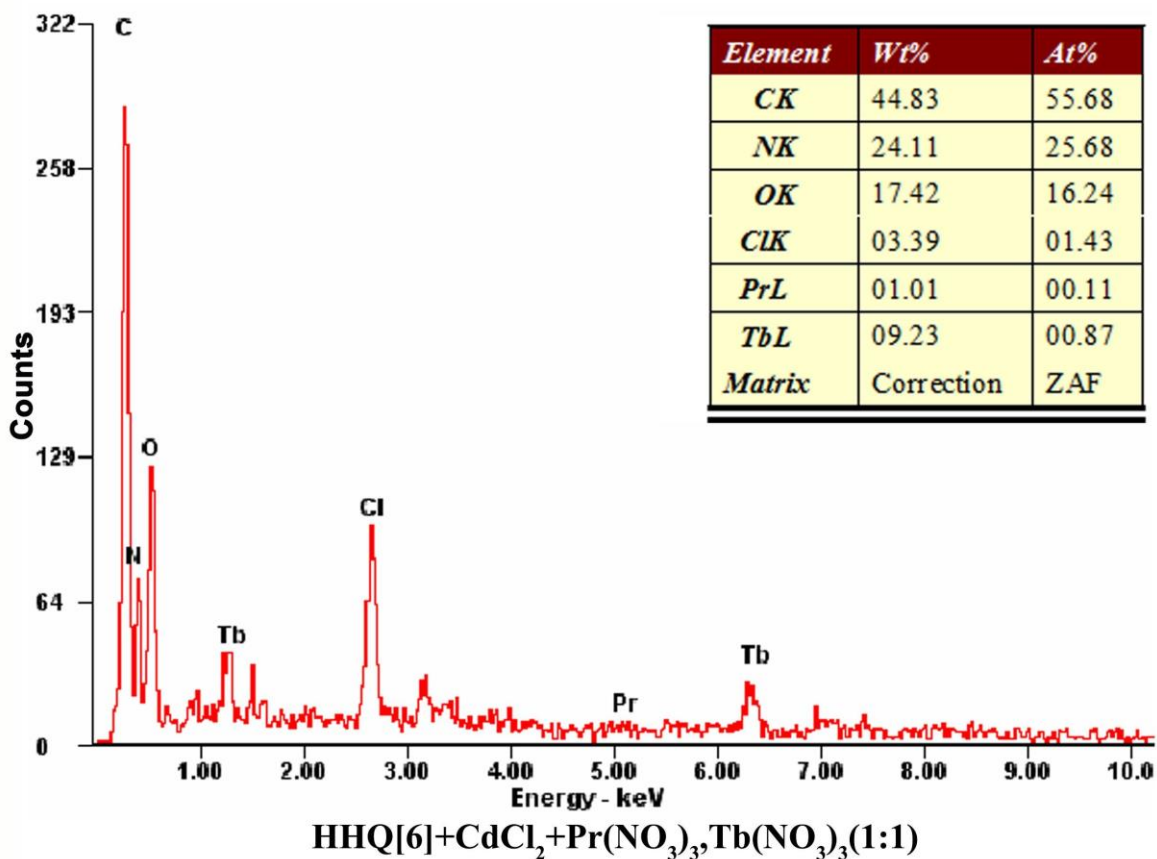


Figure S5 Electron spectroscopies of the representative products isolated from $\text{Ln}^{3+}_{\text{light}}-\text{Ln}^{3+}_{\text{heavy}}-\text{CdCl}_2$ systems mixtures with 1:1 $\text{Ln}^{3+}_{\text{light}}:\text{Ln}^{3+}_{\text{heavy}}$ ratios

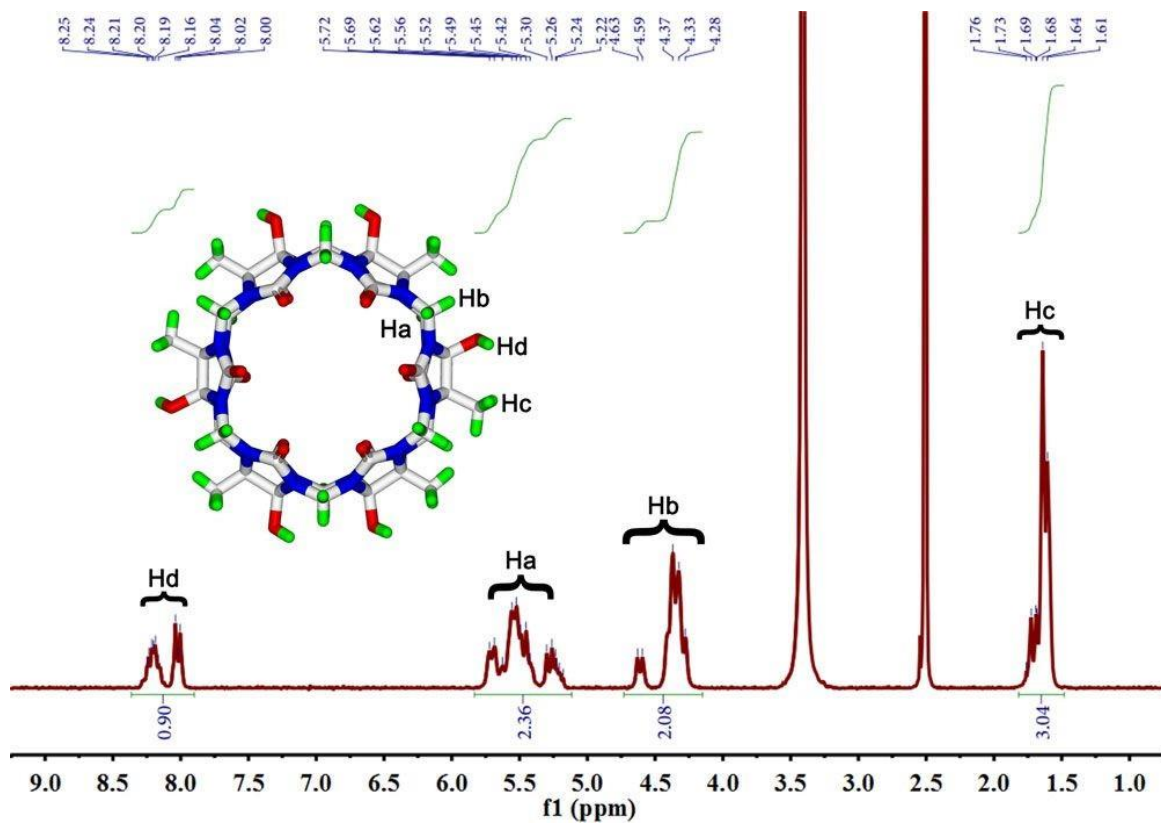


Figure S6 ^1H NMR spectra of HHQ[6] in DMSO- d_6