Electronic Supplementary Material (ESI) for CrystEngComm.

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

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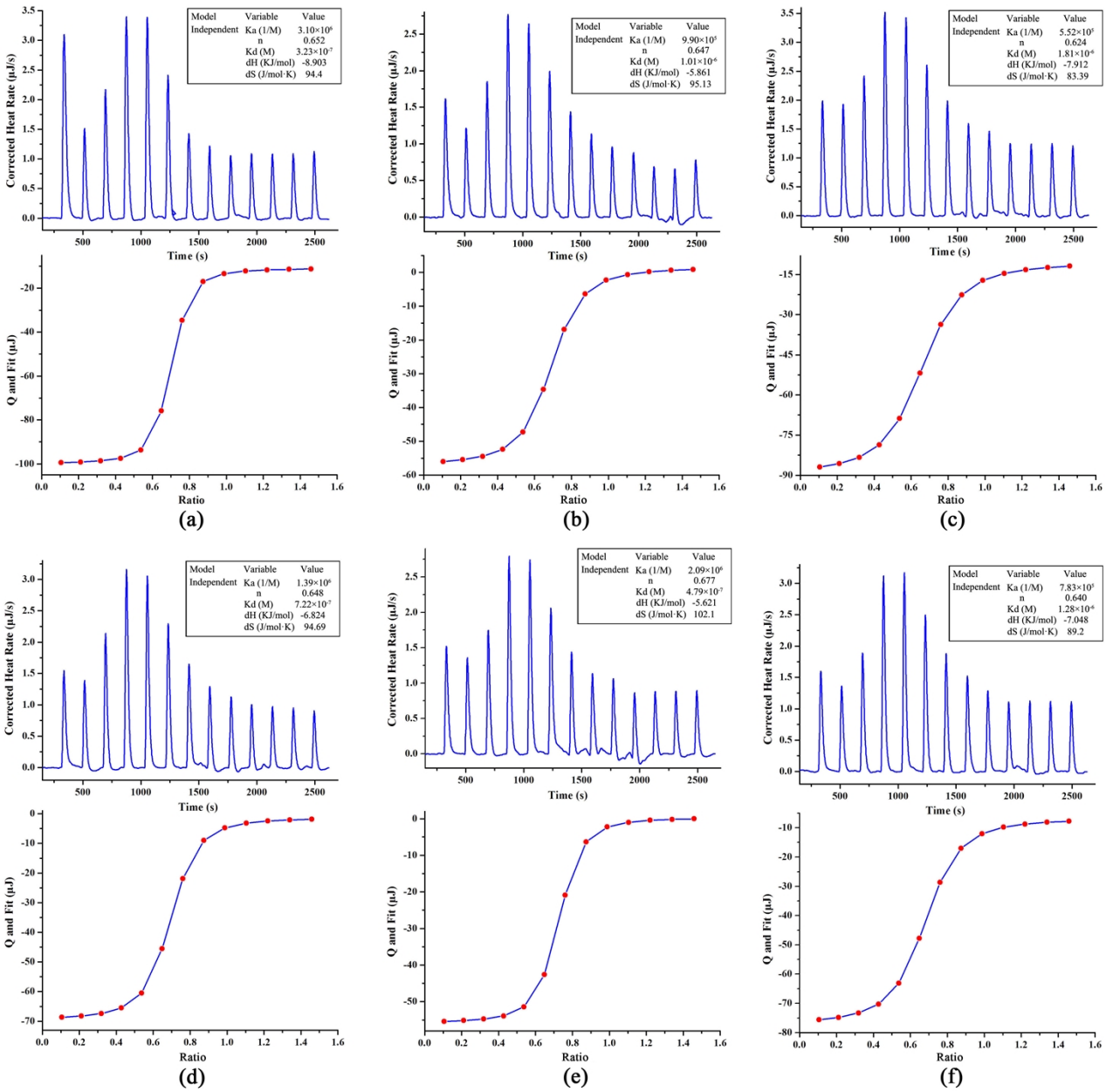
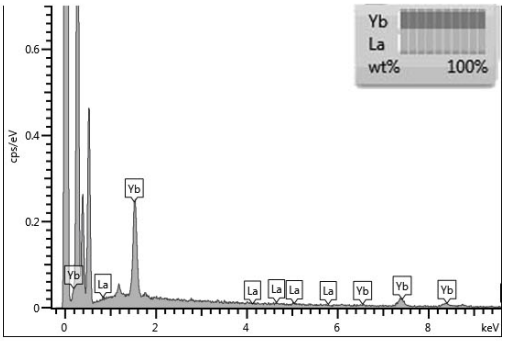


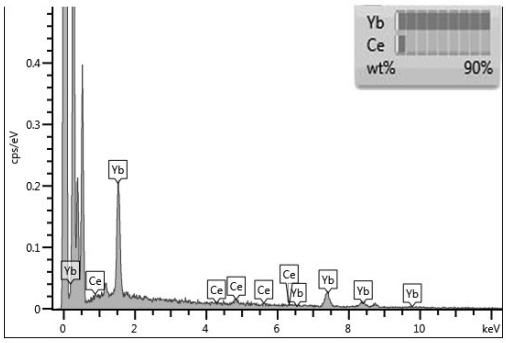
SI-Figure 1 (a) ITC profile of *o*-TMeQ[6] with $Ce(NO_3)_3$ at 298.15 K: ΔH^o = -8.903 kJ mol^{-1}, $T\Delta S^o$ = 28.145 kJ mol^{-1}; (b) ITC profile of *o*-TMeQ[6] with $Eu(NO_3)_3$ at 298.15 K: ΔH^o = -5.861 kJ mol^{-1}, $T\Delta S^o$ = 28.363 kJ mol^{-1}; (c) ITC profile of *o*-TMeQ[6] with $Yb(NO_3)_3$ at 298.15 K: ΔH^o = -7.912 kJ mol^{-1}, $T\Delta S^o$ = 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: ΔH^o = -6.824 kJ mol^{-1}, $T\Delta S^o$ = 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: ΔH^o = -5.621 kJ mol^{-1}, $T\Delta S^o$ = 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: ΔH^o = -7.048 kJ mol^{-1}, $T\Delta S^o$ = 26.595 kJ mol^{-1}.

o-TMeQ[6]+$Cd(NO_3)_2$+$La(NO_3)_3$,$Yb(NO_3)_3$ (1:1)

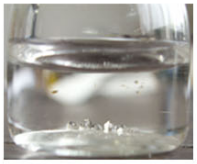


The yield of 60% ~ 66%

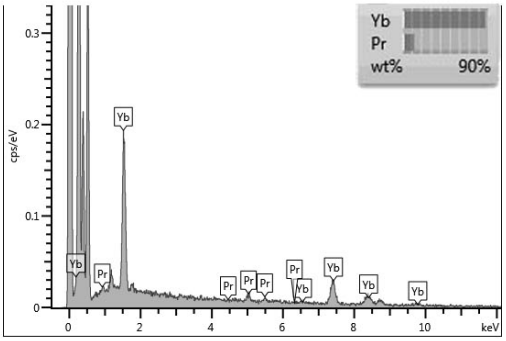
o-TMeQ[6]+$Cd(NO_3)_2$+$Ce(NO_3)_3$,$Yb(NO_3)_3$ (1:1)



The yield of 80% ~ 85%

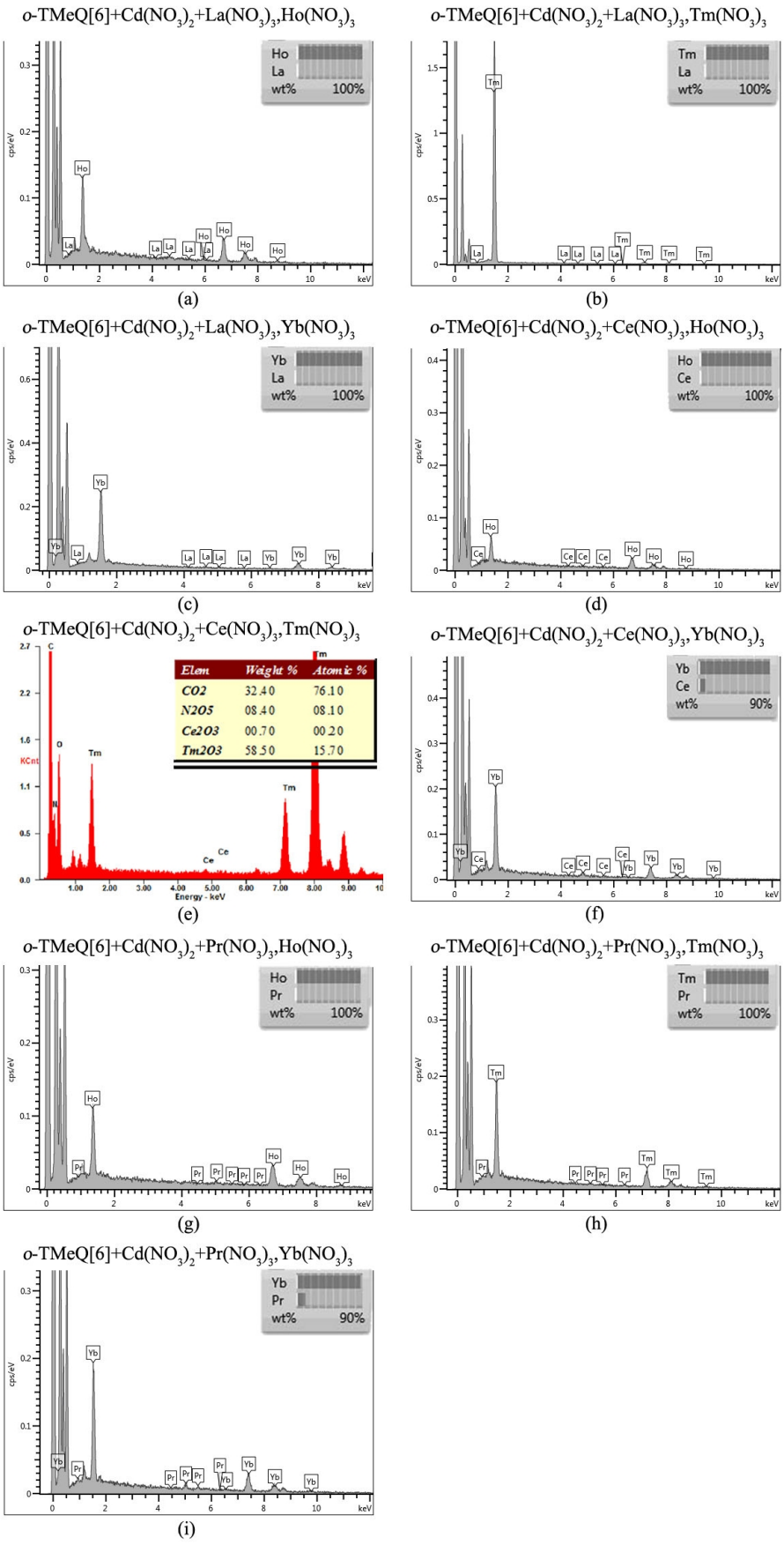


o-TMeQ[6]+$Cd(NO_3)_2$+$Pr(NO_3)_3$,$Yb(NO_3)_3$ (1:1)

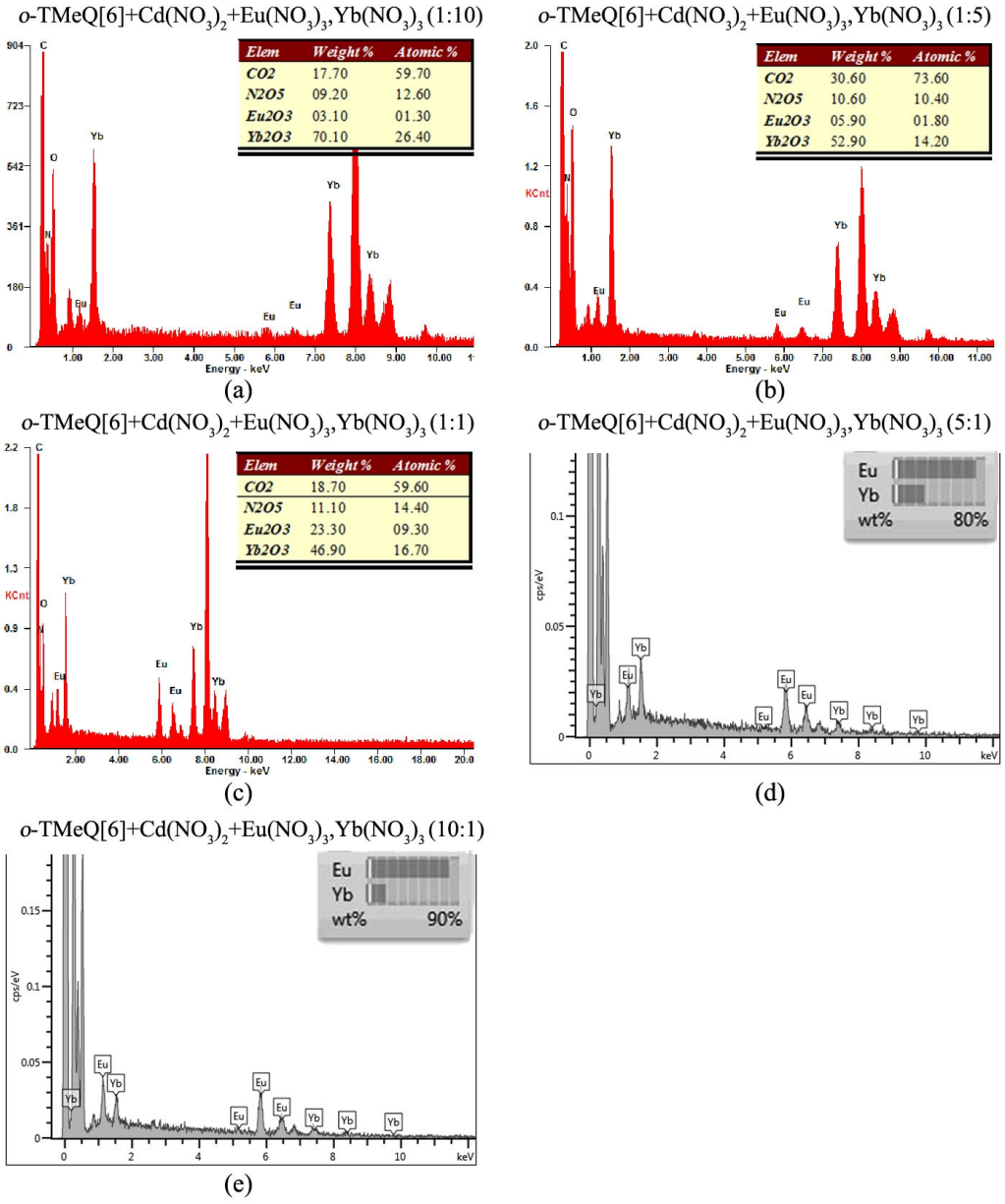


The yield of 83% ~ 88%

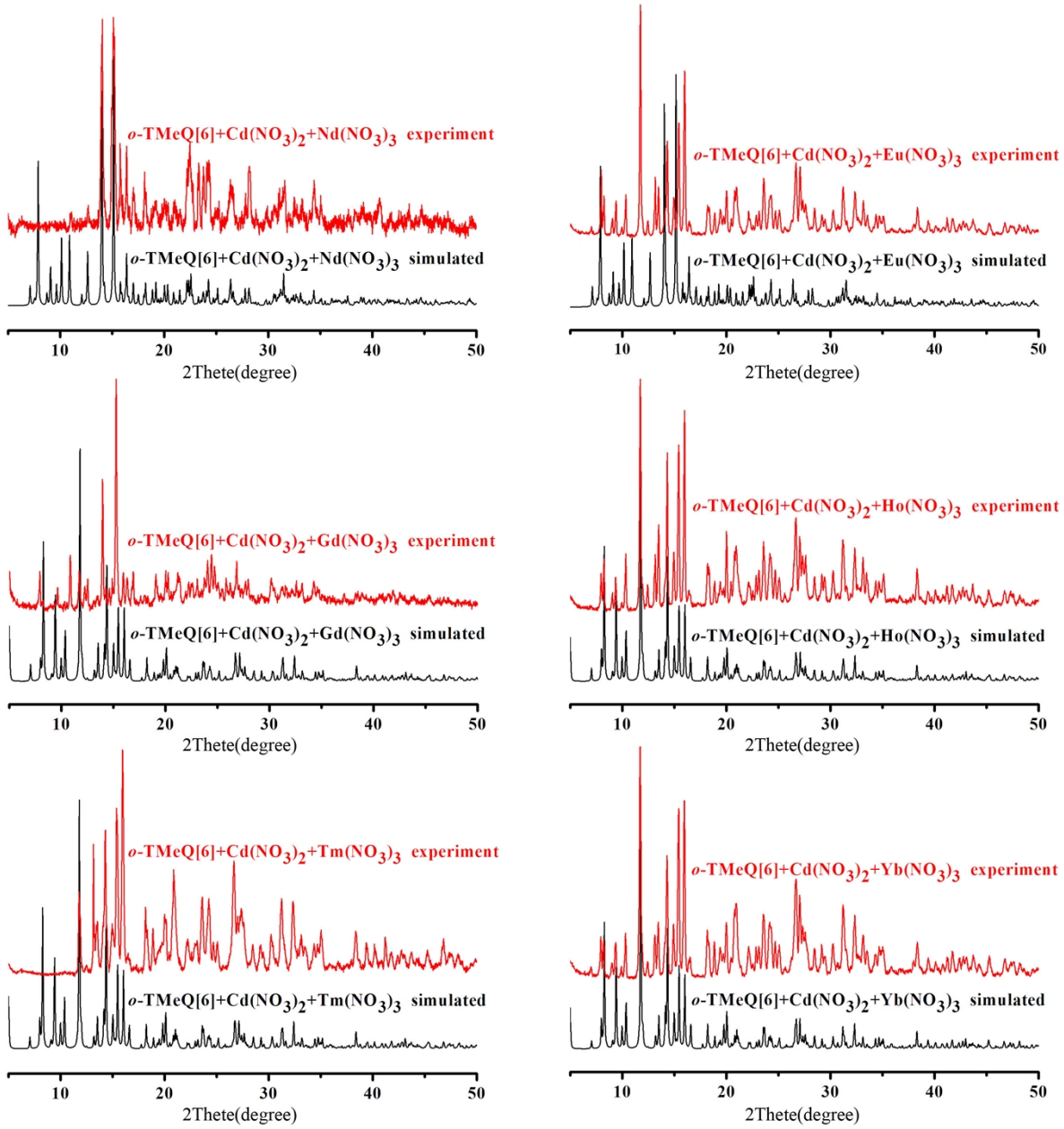
SI-Figure 2 the electron spectroscopies of *o*-TMeQ[6]/NO_3^- systems with 1:1 ratio of La:Yb、Ce:Yb、Pr:Yb and corresponding crystals with a general yields



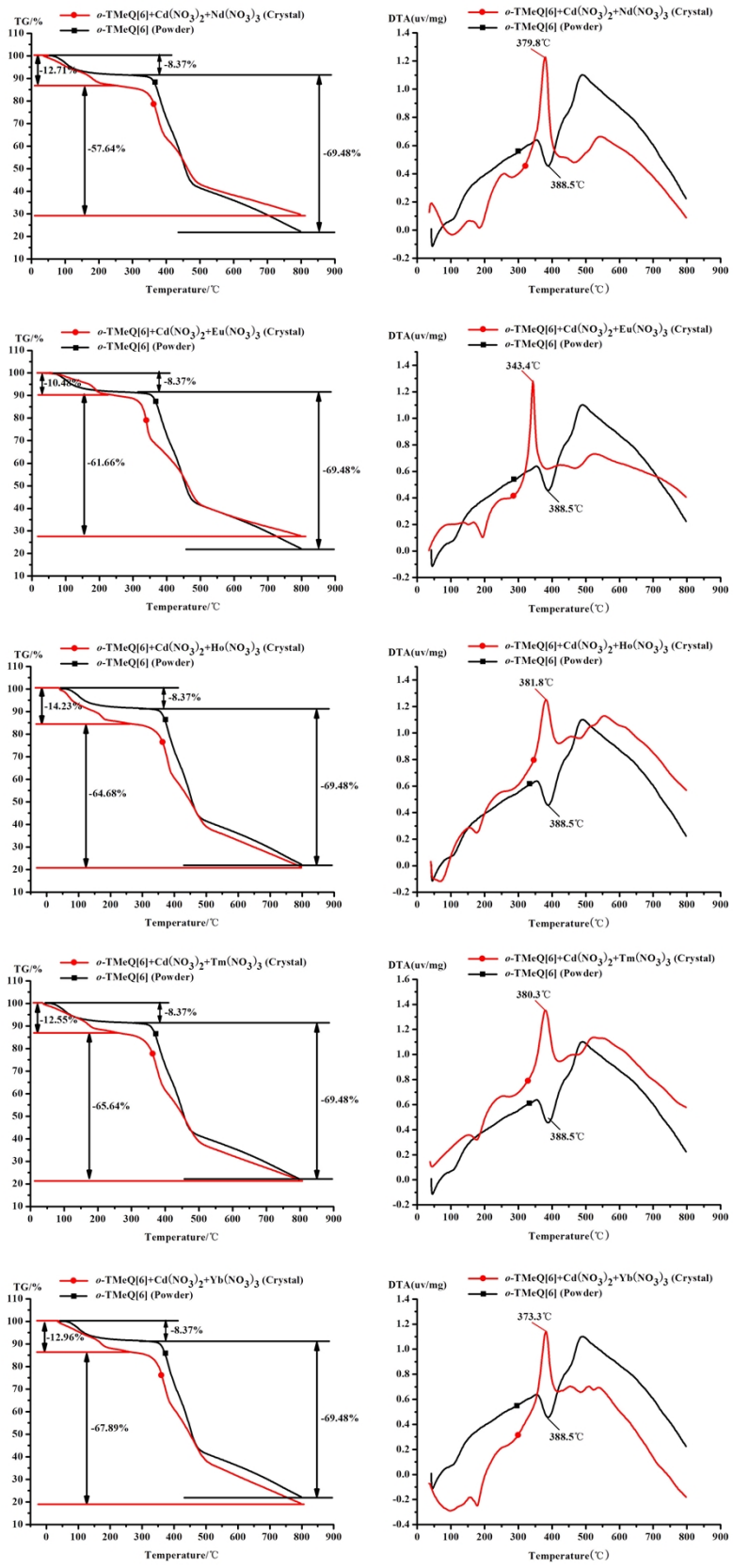
SI-Figure 3 the electron spectroscopy of *o*-TMeQ[6]/NO_3^- systems with 1:1 ratios of light : heavy lanthanides



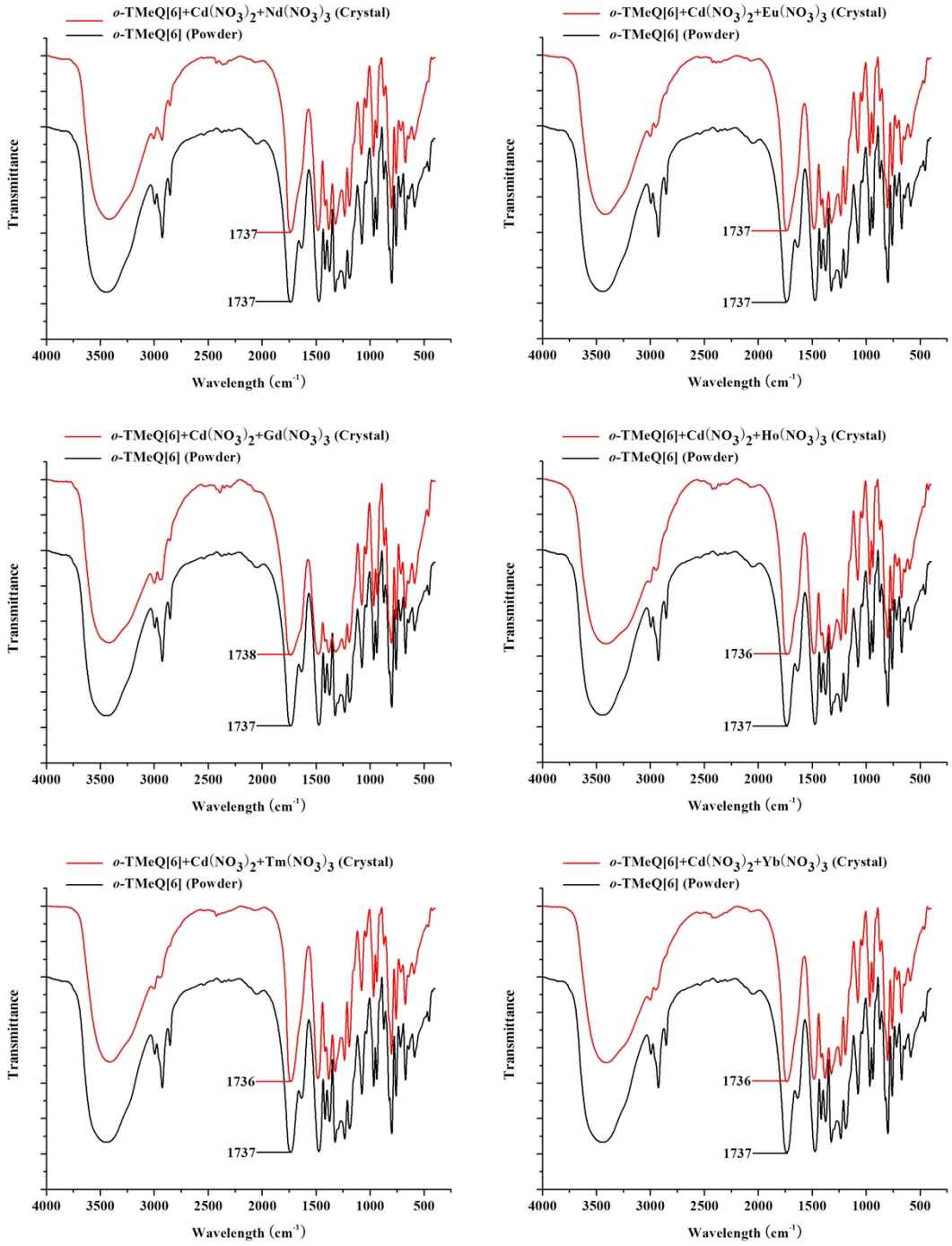
SI-Figure 4 the electron spectroscopy of *o*-TMeQ[6]/NO_3^- systems with 10:1，5:1，1:1，1:5 and 1:10 ratios of Eu:Yb



SI-Figure 5 Powder X-ray diffraction (PXRD) of the representative crystals from the two isomorphous groups respectively



SI-Figure 6 DTA (left) and TG (right) curves of the representative crystals from the two isomorphous groups with a comparison *o*-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 *o*-TMeQ[6] powders respectively.