

Supplementary Material

Preparation and Structures of Rare Earth 3-Benzoylpropanoates and 3-Phenylpropanoates

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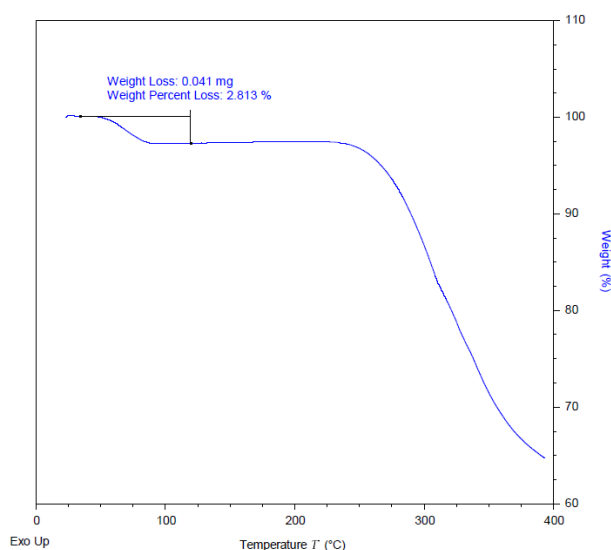


Fig. S1. TGA plot of bulk La(bp)₃ sampled for microanalysis.

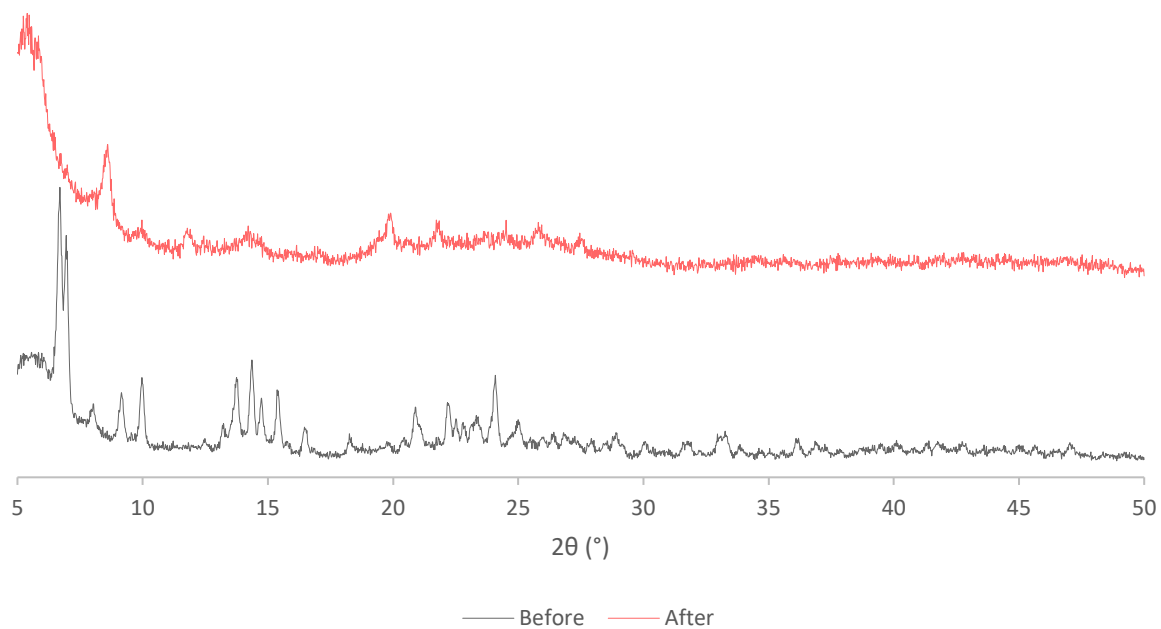


Fig. S2. Powder XRD of bulk $\text{La}(\text{bp})_3$ before and after heating.

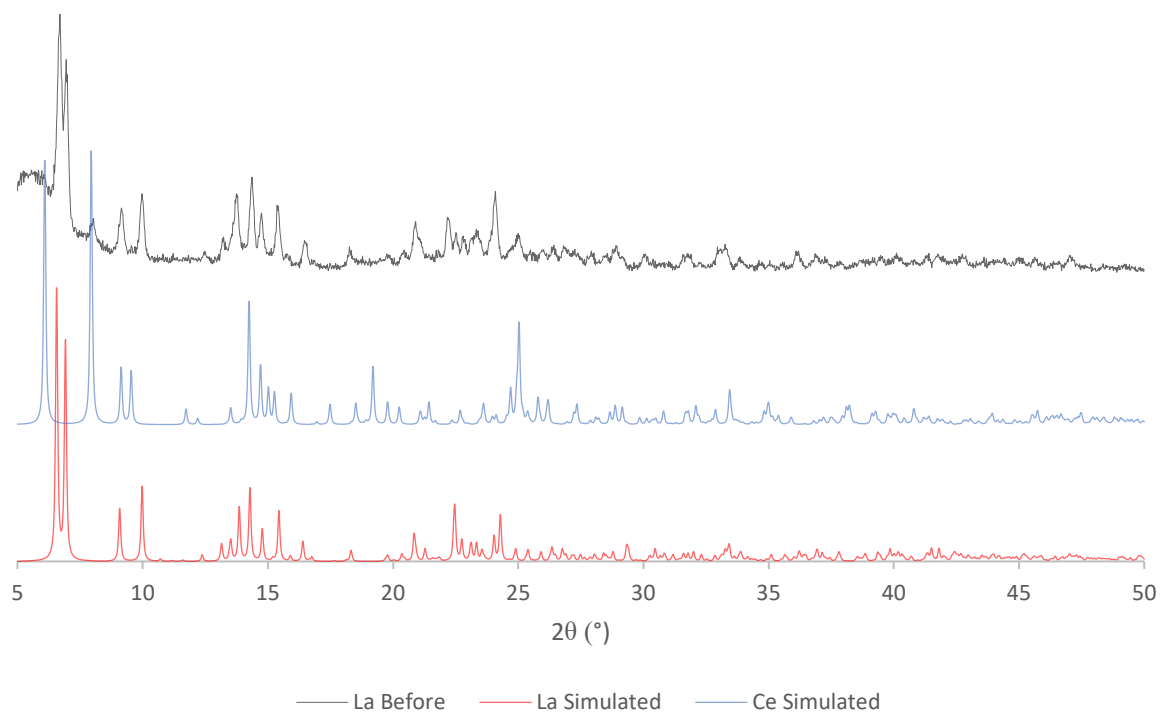


Fig. S3. Powder XRD of bulk $\text{La}(\text{bp})_3$ before heating, simulated $[\text{La}(\text{bp})_3(\text{H}_2\text{O})_2] \cdot \frac{1}{3}\text{H}_2\text{O}$ and simulated $[\text{Ce}(\text{bp})_3(\text{H}_2\text{O})]$. Simulated patterns generated from single crystal data.

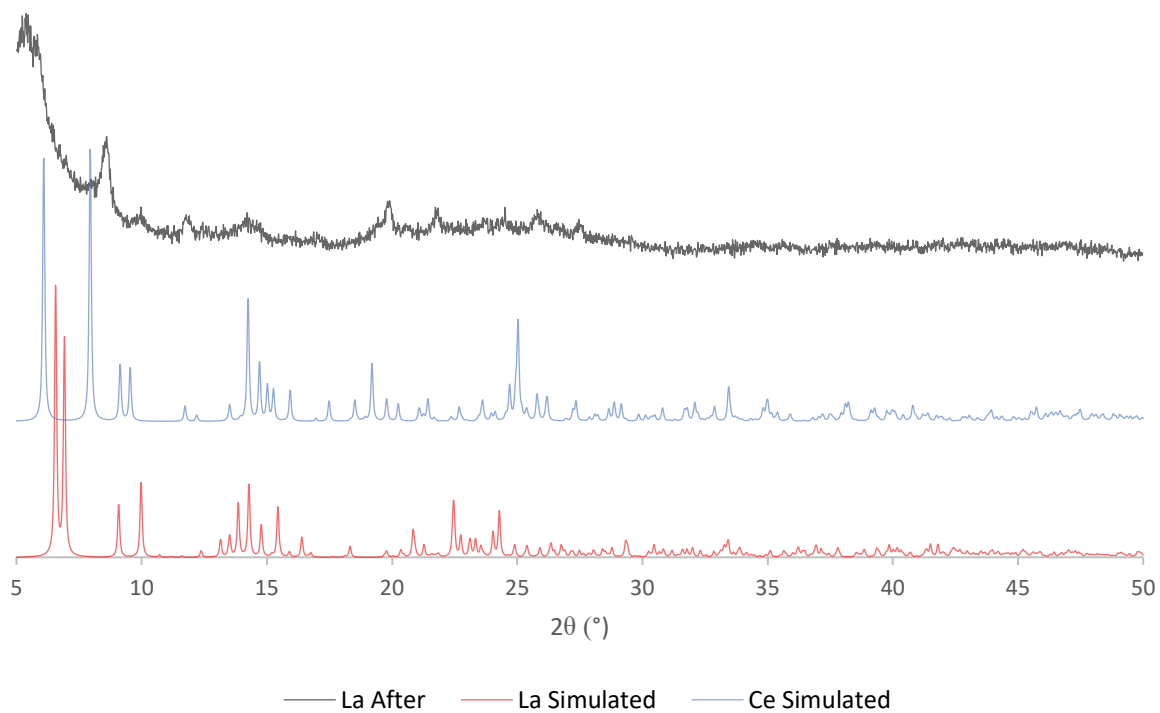


Fig. S4. Powder XRD of bulk $\text{La}(\text{bp})_3$ after heating, simulated $[\text{La}(\text{bp})_3(\text{H}_2\text{O})_2] \cdot \frac{1}{3}\text{H}_2\text{O}$ and simulated $[\text{Ce}(\text{bp})_3(\text{H}_2\text{O})]$. Simulated patterns generated from single crystal data.

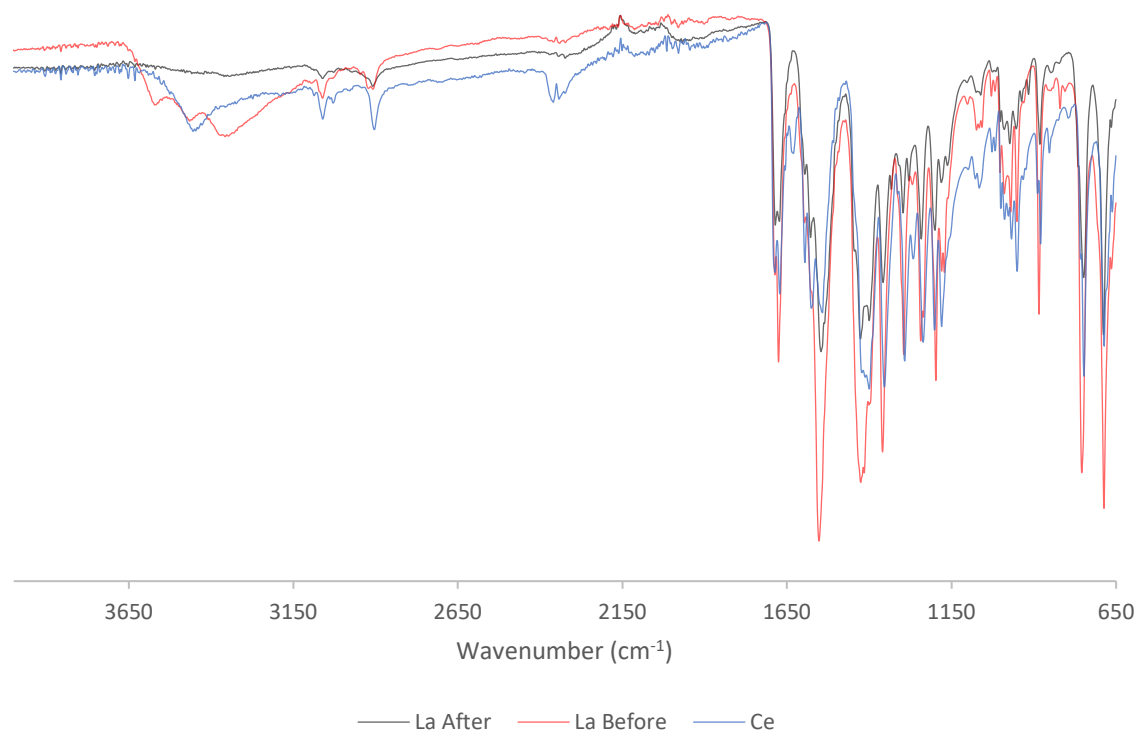


Fig. S5. ATR-IR of bulk $\text{La}(\text{bp})_3$ before heating, after heating and $[\text{Ce}(\text{bp})_3(\text{H}_2\text{O})]$.

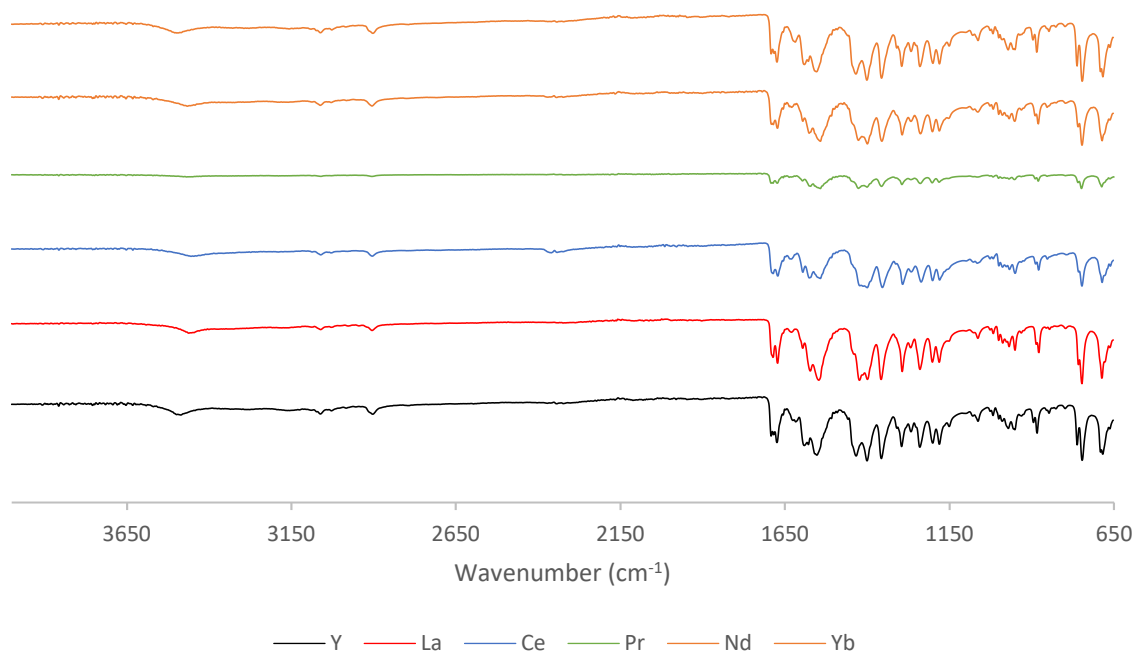


Fig. S6. ATR-IR of $[\text{RE}(\text{bp})_3(\text{H}_2\text{O})_n]$ complexes (RE = La, $n = 2$; RE = Y, Ce, Pr, Nd, Yb, $n = 1$).

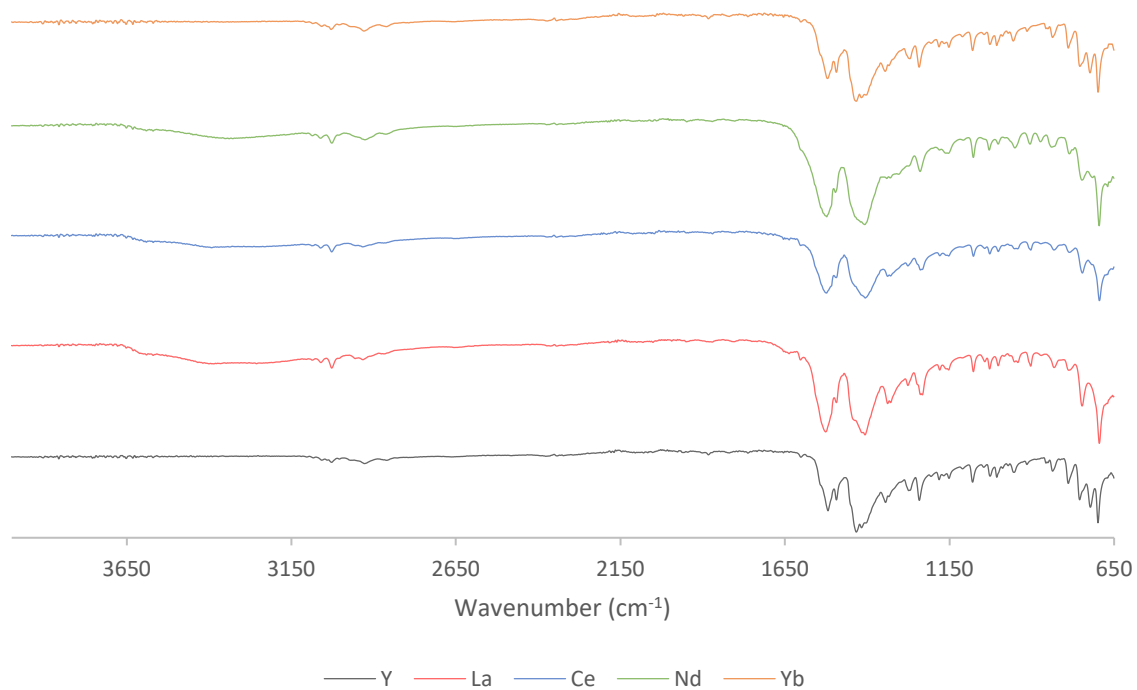


Fig. S7. ATR-IR of $[\text{RE}(\text{pp})_3]$ (RE = Y, Yb) and $[\text{Ln}(\text{pp})_3] \cdot n\text{H}_2\text{O}$ (Ln = La, $n = 0.5$; Ln = Ce, $n = 1$; Ln = Nd, $n = 3$)

$[\text{La}(\text{mbp})_3(\text{H}_2\text{O})_2] \cdot 3\text{H}_2\text{O}$ Crystal and Structure Refinement Data:

$C_{33}H_{43}LaO_{14}$, M 802.58, triclinic, space group $P\bar{1}$ (No. 2), a 8.6610(17), b 9.941(2), c 21.902(4) Å, α 80.81(3)°, β 87.61°, γ 66.27(3)°, V 1703.6(7) Å³, Z 2, λ 0.71073 Å, T 100(2) K, μ 1.322 mm⁻¹, $2\theta_{max}$ 51.364°, 24936 reflections collected, 6450 unique (R_{int} 0.1146), N_o 6062, 444 parameters, R_1 ($I > 2\sigma(I)$) 0.0865, wR_2 (all data) 0.2118, GoF 1.098, $\Delta\rho_{min/max}$ -4.33/5.72 e⁻ Å⁻³.

Table S1. Selected bond distances (Å) for [La(mbp)₃(H₂O)₂] \cdot 3H₂O

Atoms	La(mbp) ₃
M-O(1)	2.470(7)
M-O(2) ⁱ	2.586(7)
M-O(4)	2.462(7)
M-O(4) ⁱ	2.765(7)
M-O(5) ⁱ	2.628(7)
M-O(7)	2.535(7)
M-O(7) ⁱⁱ	2.678(7)
M-O(8) ⁱⁱ	2.624(7)
M-O(10)	2.600(7)
M-O(11)	2.655(6)

ⁱ Symmetry operator: 1-x,1-y,1-z

ⁱⁱ Symmetry operator: -x,1-y,1-z