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Supporting information for article:

Isomorphous rare-earth tris[bis(2,6-diisopropylphenyl) phosphate] complexes and their catalytic properties in 1,3-diene polymerization and in inhibited oxidation of polydimethylsiloxane

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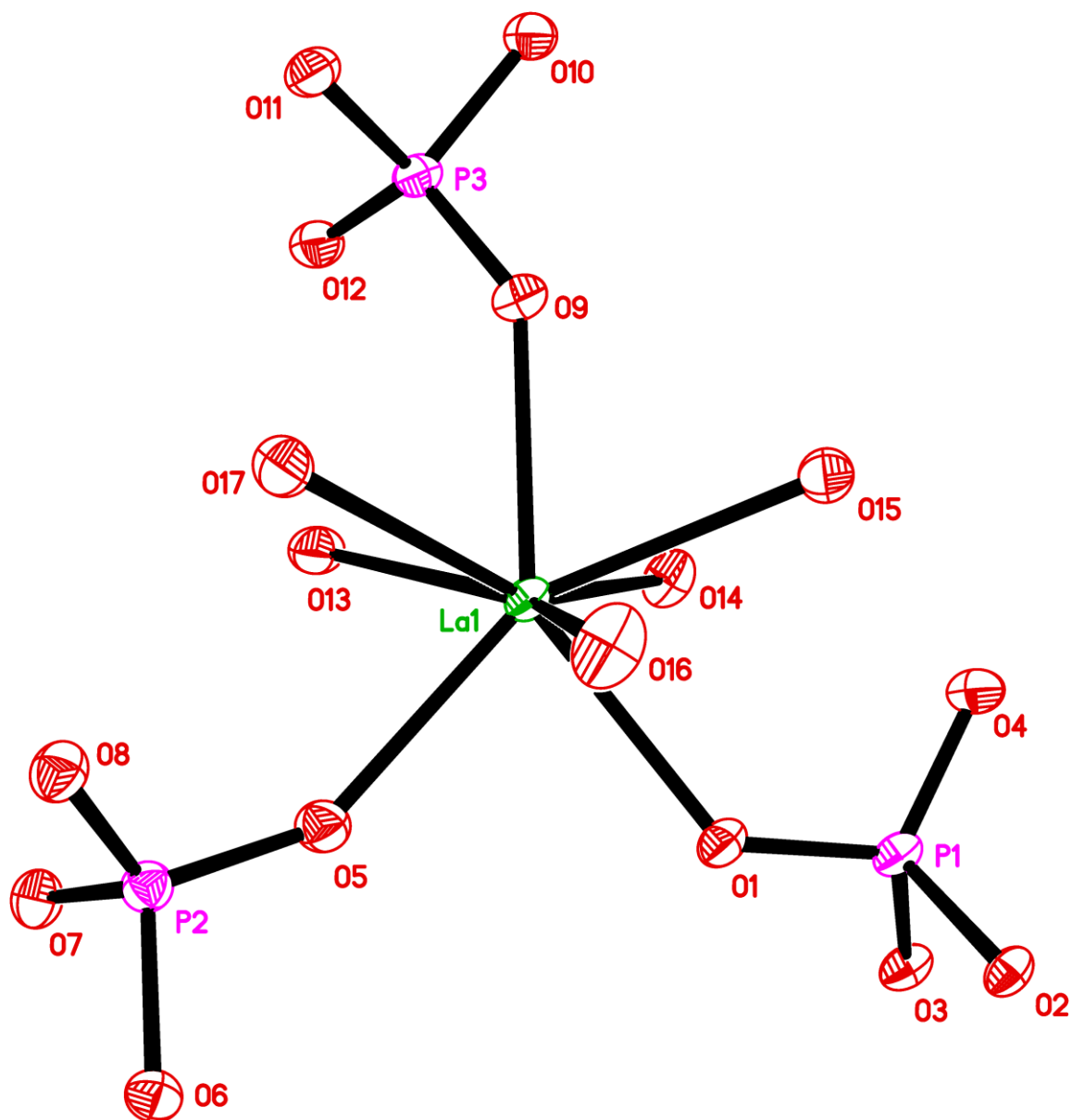


Figure S1 Environments about Ln and P atoms in $[\text{Ln}(\text{C}_{24}\text{H}_{34}\text{O}_4\text{P})_3(\text{CH}_4\text{O})_5]\cdot\text{CH}_3\text{OH}$, using (1) (Ln=La) as an example.

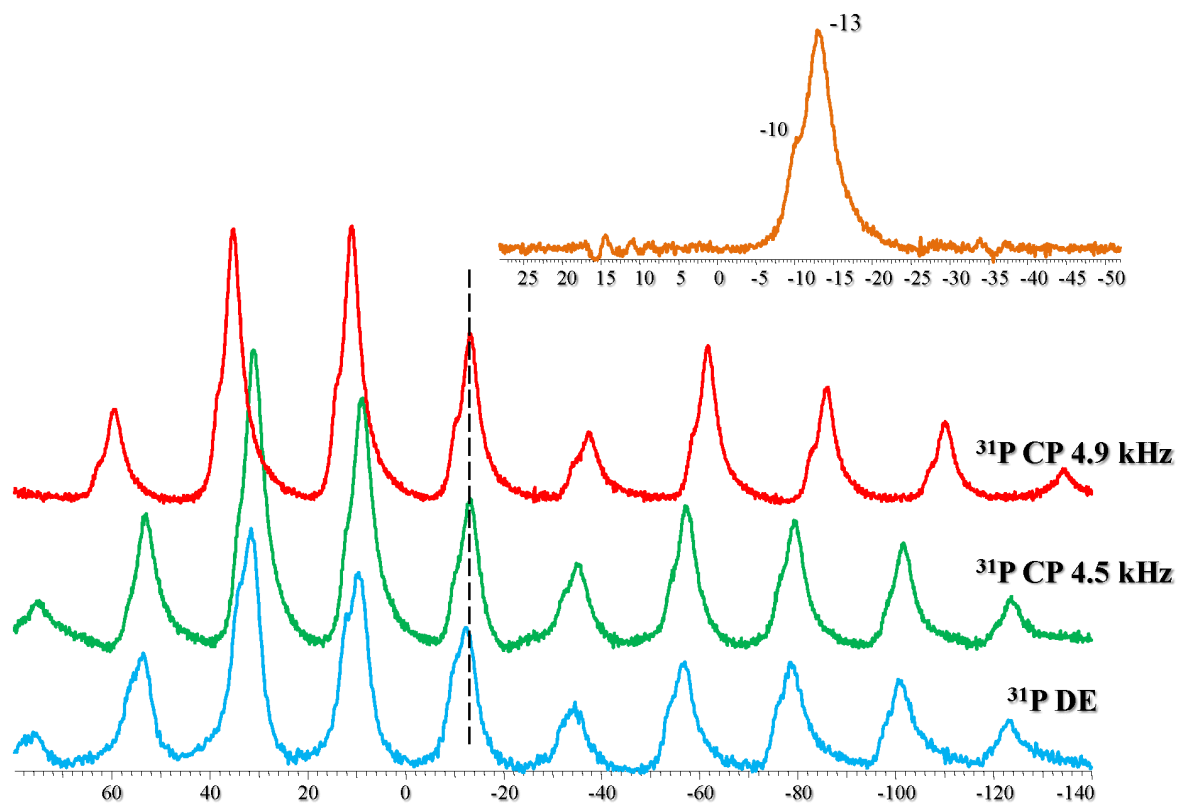


Figure S2 ^{31}P CP MAS NMR spectra of $[\text{La}(\text{C}_{24}\text{H}_{34}\text{O}_4\text{P})_3(\text{CH}_4\text{O})_5]\cdot\text{CH}_3\text{OH}$, (**1**), at different rotation frequencies demonstrate signals that correspond to two symmetrically non-equivalent phosphorous centers.

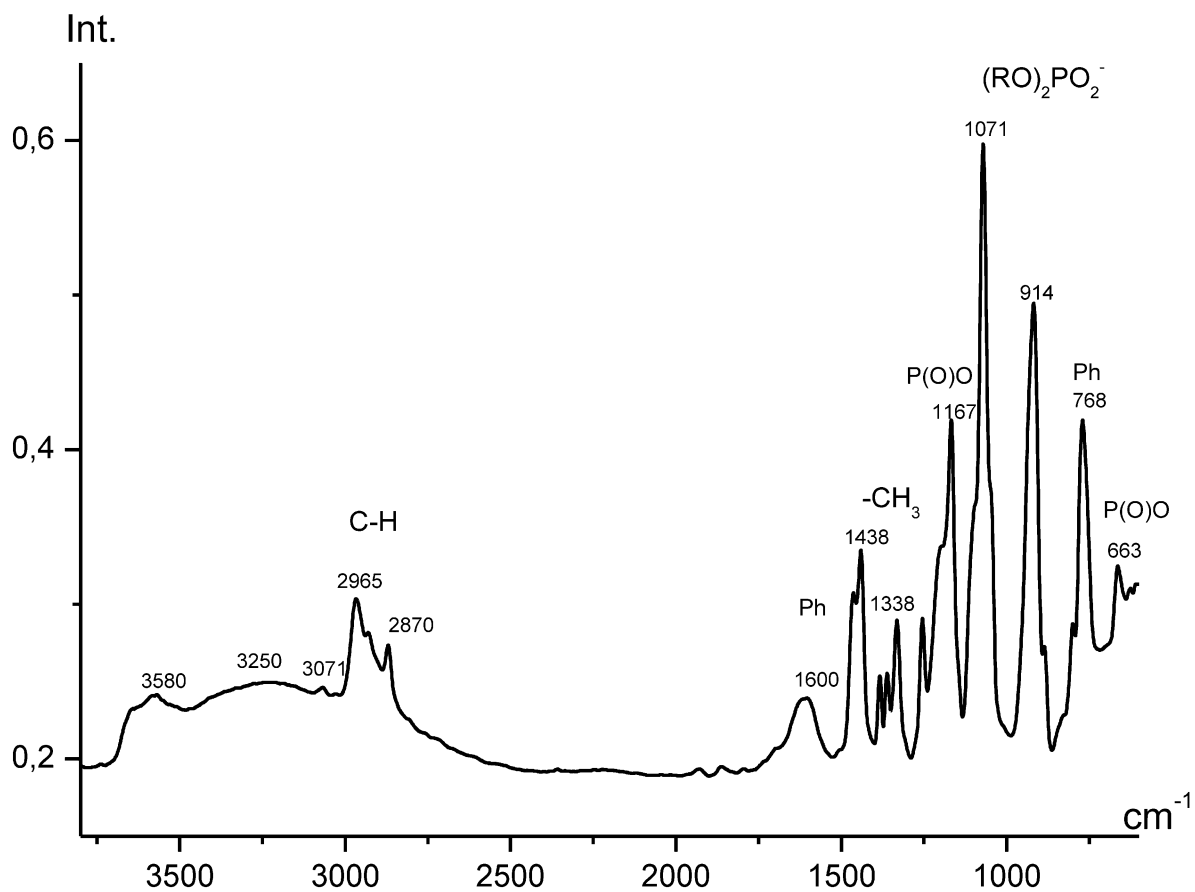


Figure S3 ATR-FT-IR spectrum for $[\text{Ce}(\text{C}_{24}\text{H}_{34}\text{O}_4\text{P})_3(\text{CH}_4\text{O})_5] \cdot \text{CH}_3\text{OH}$, (**2**).

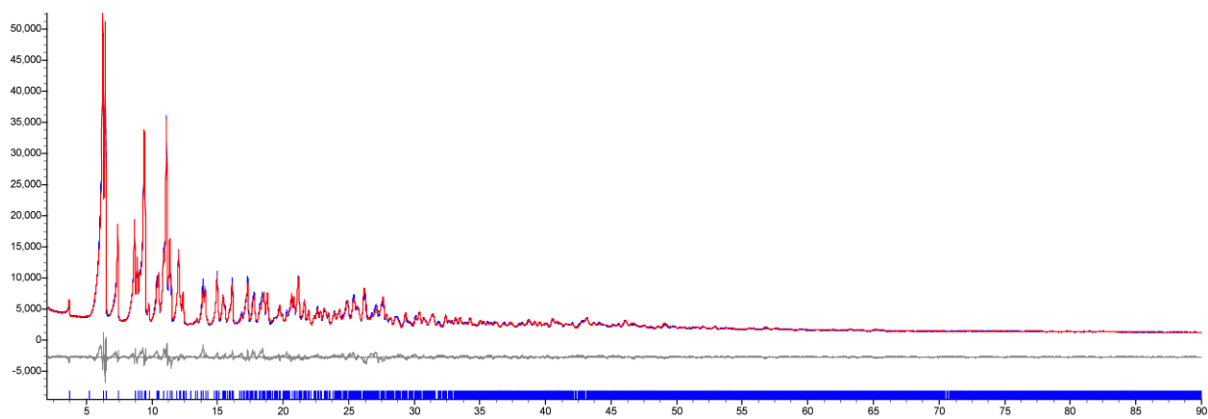


Figure S4 The experimental (blue line), calculated (red line), and difference (grey line) powder XRD patterns of **(1)** (Ln=La). The unit cell parameters found by the Rietveld method at room temperature: $a = 23.8015(8)\text{\AA}$, $b = 10.6296(3)\text{\AA}$, $c = 34.0486(14)\text{\AA}$, $\beta = 91.889(2)^\circ$, $V = 8609.6(5)\text{\AA}^3$.

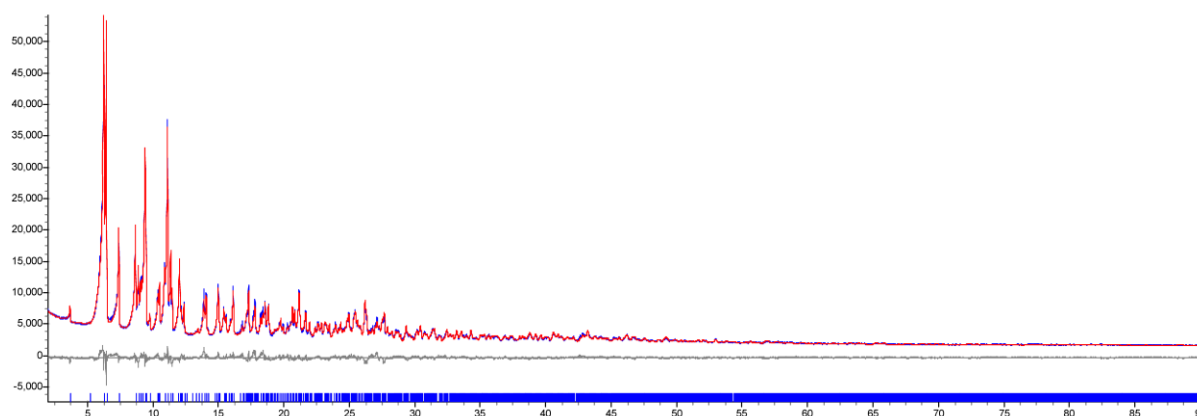


Figure S5 The experimental (blue line), calculated (red line), and difference (grey line) powder XRD patterns of **(2)** (Ln=Ce). The unit cell parameters found by the Rietveld method at room temperature: $a = 23.7395(5)\text{\AA}$, $b = 10.6163(2)\text{\AA}$, $c = 33.9902(9)\text{\AA}$, $\beta = 91.8523(16)^\circ$, $V = 8561.9(3)\text{\AA}^3$.

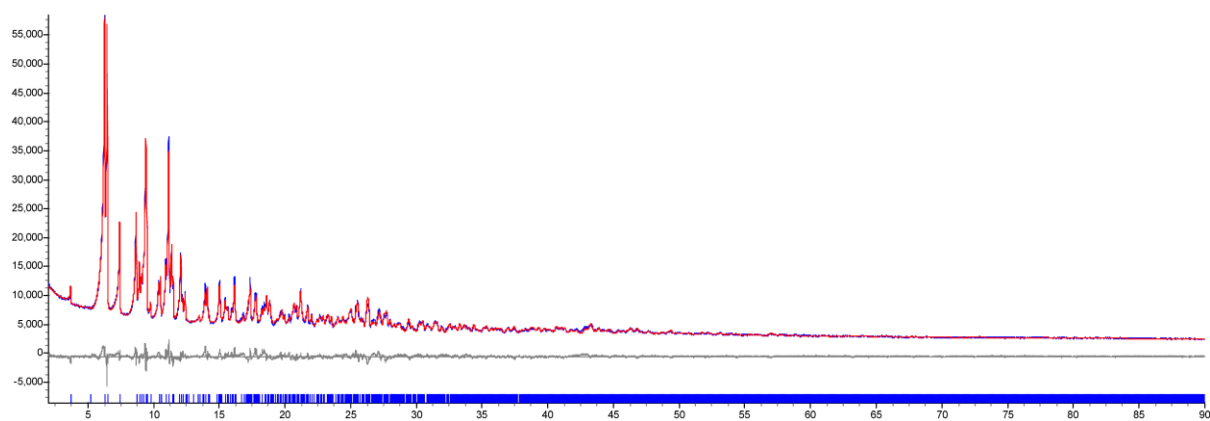


Figure S6 The experimental (blue line), calculated (red line), and difference (grey line) powder XRD patterns of (**3**) (Ln=Nd). The unit cell parameters found by the Rietveld method at room temperature: $a = 23.6788(8)\text{\AA}$, $b = 10.6196(3)\text{\AA}$, $c = 33.8903(14)\text{\AA}$, $\beta = 91.862(2)^\circ$, $V = 8517.5(5)\text{\AA}^3$.

Table S1 Weight loss (g) in pyrolysis of PDMS-50 in the presence of additive (2) or (3) and without a rare-earth complex.

The starting mass of PDMS-50 was 2.000g. Thermal destruction experiments were carried out at T=573K.

| Entry | Additive | Time | | | | | | |
|-------|------------------|------|------|------|------|------|------|------|
| | | 1h | 2h | 3h | 5h | 8h | 9h | 10h |
| 1* | Blank experiment | 0.03 | 0.07 | 0.11 | 0.18 | 0.24 | 0.27 | n/d |
| 2* | 0.1% (3), Ln=Nd | 0.04 | 0.08 | 0.12 | 0.17 | n/d | 0.28 | n/d |
| 3** | 0.1% (2), Ln=Ce | 0.02 | 0.03 | 0.04 | 0.06 | n/d | 0.09 | 0.10 |

*Abrupt increase in viscosity and formation of some precipitate after 1h. PDMS-50 was fully solidified after 5h. **No precipitate, low viscosity, clear liquid even after 10h.