

## Electronic supplementary information for:

# Rare-earth complexes supported by an ansa-bis(amidinate) ligand with a rigid *o*-phenylene linker: synthesis, structure, and catalytic activity for polymerization of cyclic esters

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### Supporting Information

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## I Crystallographic data of the complexes

**Table S1** Crystallographic data and structure refinement for complexes **2, 3**

| Crustal date                                     | <b>2</b>  | <b>3</b>  |
|--|---|---|
| Empirical formula                                | C <sub>38</sub> H <sub>58</sub> N <sub>5</sub> OSi <sub>2</sub> Y | C <sub>38</sub> H <sub>58</sub> ErN <sub>5</sub> OSi <sub>2</sub> |
| Formula weight                                   | 745.98  | 824.33  |
| Crystal system,                                  | Orthorhombic  | Orthorhombic  |
| Space group                                      | Ama2  | Ama2  |
| a (Å)  | 18.4951(17)   | 18.4980(12)   |
| b (Å)  | 21.577(2)   | 21.5082(17)   |
| c (Å)  | 10.5804(10)   | 10.6134(7)  |
| α (°)  | 90.00   | 90.00   |
| β (°)  | 90.00   | 90.00   |
| γ (°)  | 90.00   | 90.00   |
| V (Å <sup>3</sup> )                              | 4222.3(7)   | 4222.6(5)   |
| T (K)  | 293(2)  | 293(2)  |
| D <sub>calc</sub> (g cm <sup>-3</sup> )          | 1.174   | 1.297   |
| μ (mm <sup>-1</sup> )                            | 1.471   | 2.077   |
| Z  | 4   | 4   |
| F(0 0 0)   | 1584  | 1700  |
| Reflections collected/unique                     | 23319/4981  | 23830/4983  |
| R (int)  | 0.0513  | 0.0262  |
| Completeness to θ (%)                            | 99.8  | 99.7  |
| λ (Mo Kα radiation) (Å)                          | 0.71073   | 0.71073   |
| θ Range (°)                                      | 1.89- 27.56   | 1.89 to 27.54   |
| GOF  | 1.020   | 1.016   |
| R <sub>1</sub> , wR <sub>2</sub> [I > 2σ (I)]    | 0.0469, 0.1059  | 0.0218, 0.0490  |
| R <sub>1</sub> , wR <sub>2</sub> (all data)      | 0.0832, 0.1236  | 0.0278, 0.0511  |
| Largest diff. peak and hole (e Å <sup>-3</sup> ) | 0.305 and -0.344  | 0.501 and -0.307  |

**Table S2** Crystallographic data and structure refinement for complexes **4, 5**

| Crustal date      | <b>4</b>  | <b>5</b>  |
|-------------------|---|---|
| Empirical formula | C <sub>84</sub> H <sub>96</sub> N <sub>12</sub> La <sub>2</sub> | C <sub>84</sub> H <sub>96</sub> N <sub>12</sub> Nd <sub>2</sub> |
| Formula weight    | 1551.54   | 1562.20   |
| Crystal system,   | Monoclinic  | Monoclinic  |
| Space group       | P2 <sub>1</sub> /n  | P2 <sub>1</sub> /c  |
| a (Å)             | 13.0485(12)   | 12.9980(5)  |
| b (Å)             | 19.6899(18)   | 19.4421(7)  |
| c (Å)             | 31.006(3)   | 31.006(3)   |
| α (°)             | 90.00   | 90.00   |
| β (°)             | 91.50   | 112.1490(10)°   |
| γ (°)             | 90.00   | 90.00   |

|   |                 |                  |
|---|-----------------|------------------|
| V (Å <sup>3</sup> )                                 | 7963.5(13)      | 7761.2(5)        |
| T (K)   | 293(2)          | 293(2)           |
| D <sub>calc</sub> (g cm <sup>-3</sup> )             | 1.294           | 1.337            |
| μ (mm <sup>-1</sup> )                               | 1.108           | 1.374            |
| Z   | 4               | 4                |
| F(0 0 0)  | 3192            | 3216             |
| Reflections<br>collected/unique                     | 79888/14535     | 69681/17852      |
| R (int)   | 0.0586          | 0.0929           |
| Completeness to θ (%)                               | 99.7            | 99.9             |
| λ (Mo Kα radiation) (Å)                             | 0.71073         | 0.71073          |
| θ Range (°)   | 1.225- 25.344   | 2.197-27.554     |
| GOF   | 1.092           | 1.029            |
| R <sub>1</sub> , wR <sub>2</sub> [I > 2σ (I)]       | 0.0582, 0.1246  | 0.0535, 0.1301   |
| R <sub>1</sub> , wR <sub>2</sub> (all data)         | 0.0873, 0.1378  | 0.0801, 0.1452   |
| Largest diff. peak and<br>hole (e Å <sup>-3</sup> ) | 1.339 and 1.065 | 2.279 and -1.729 |

## II Copies of <sup>1</sup>H NMR, <sup>13</sup>C NMR Spectra of the complex **2**

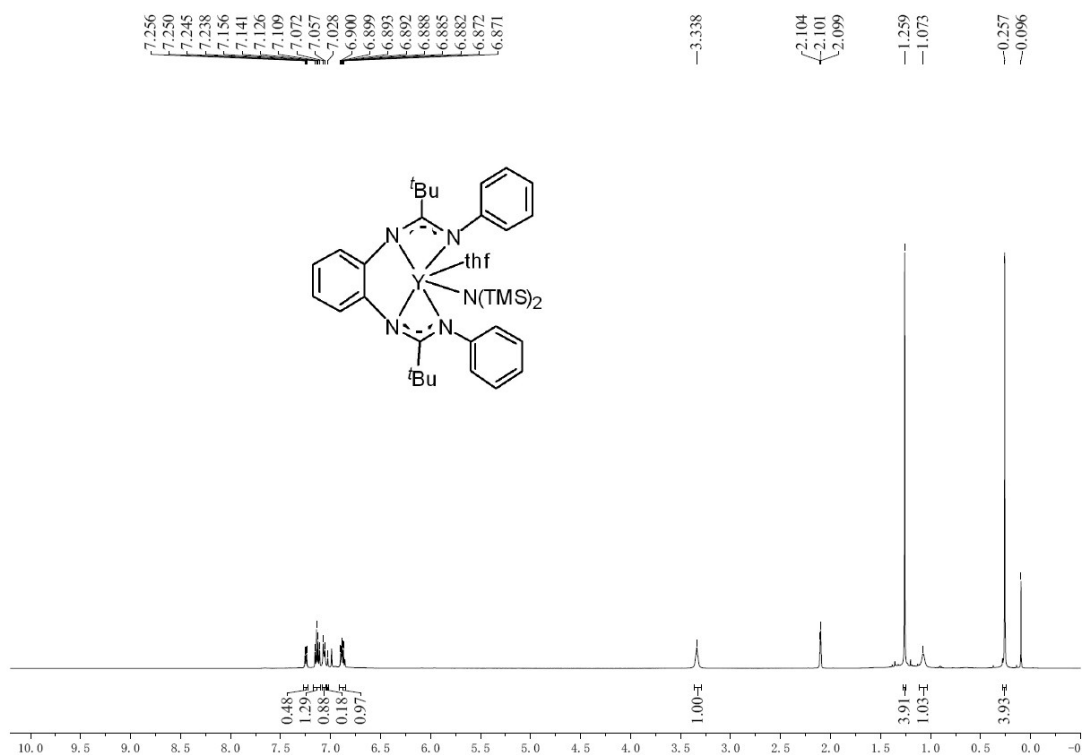


Figure S1. <sup>1</sup>H NMR spectrum (500 MHz, C<sub>7</sub>D<sub>8</sub>, 298 K) of the complex **2**

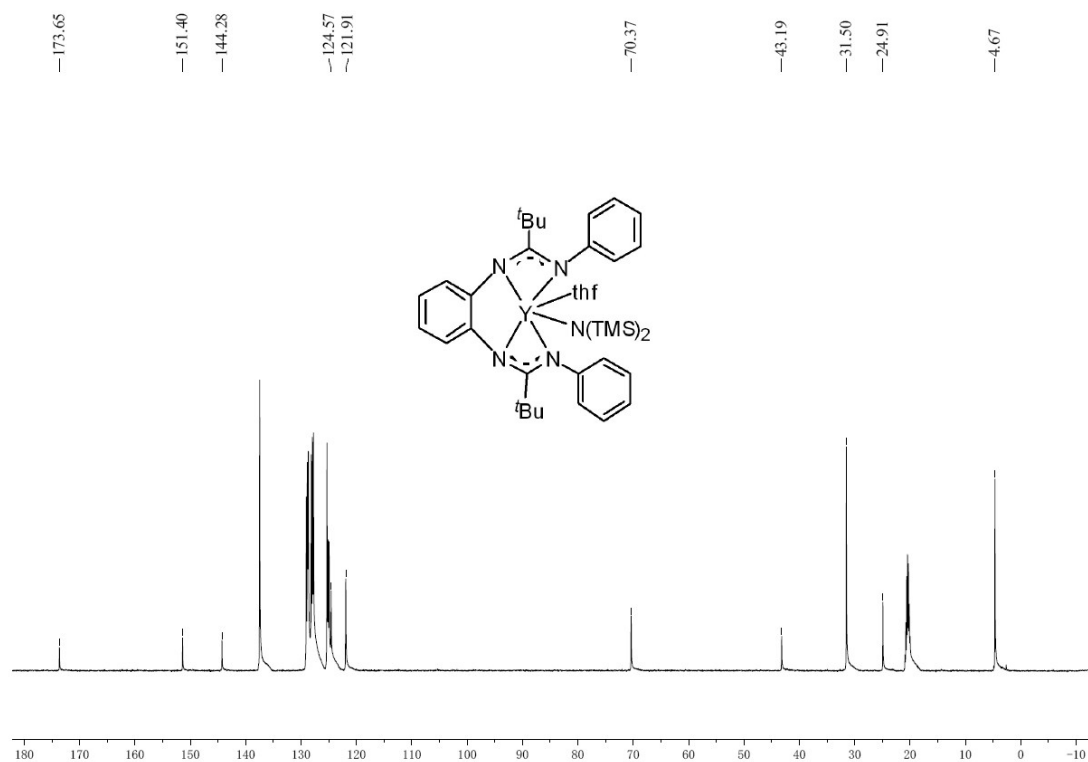


Figure S2. <sup>13</sup>C NMR spectrum (125 MHz, C<sub>7</sub>D<sub>8</sub>, 298 K) of the complex **2**

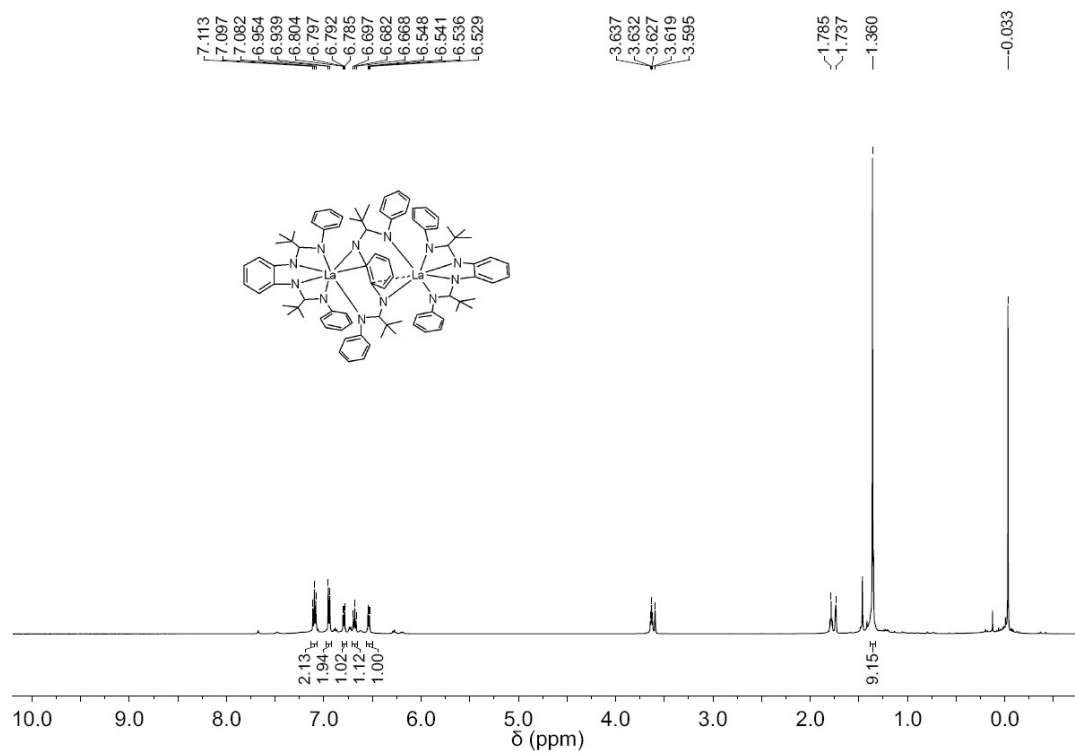


Figure S3. <sup>1</sup>H NMR spectrum (500 MHz, C<sub>4</sub>D<sub>8</sub>O, 298 K) of the complex **4**

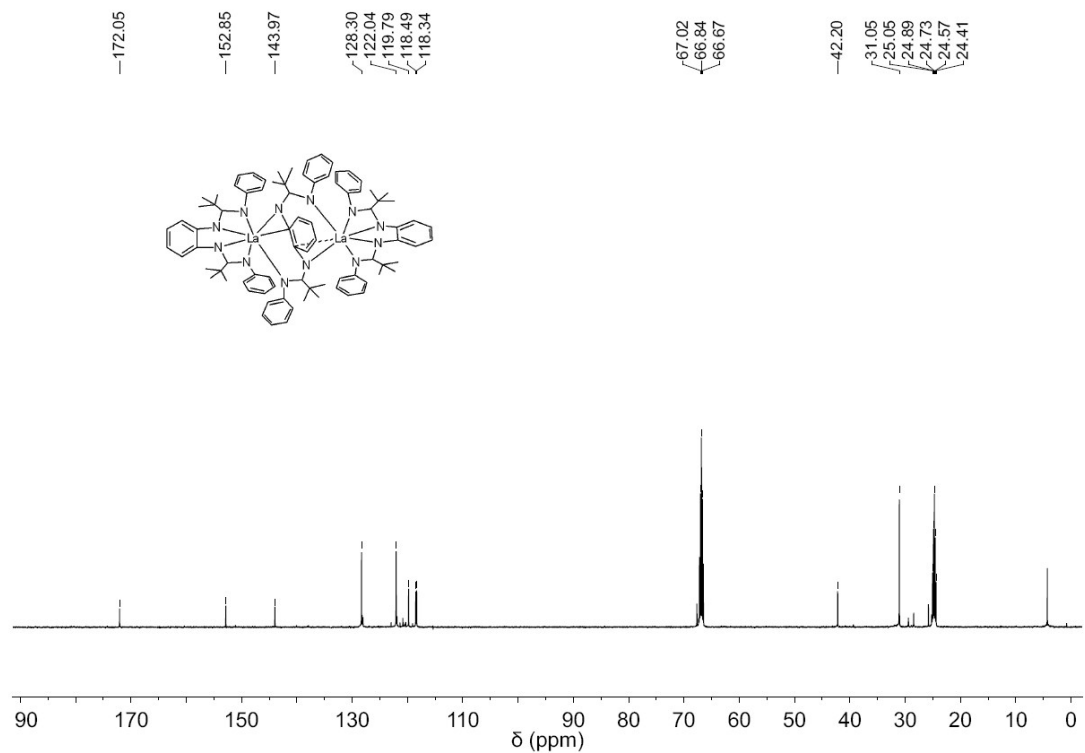


Figure S4.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{C}_4\text{D}_8\text{O}$ , 298 K) of the complex 4

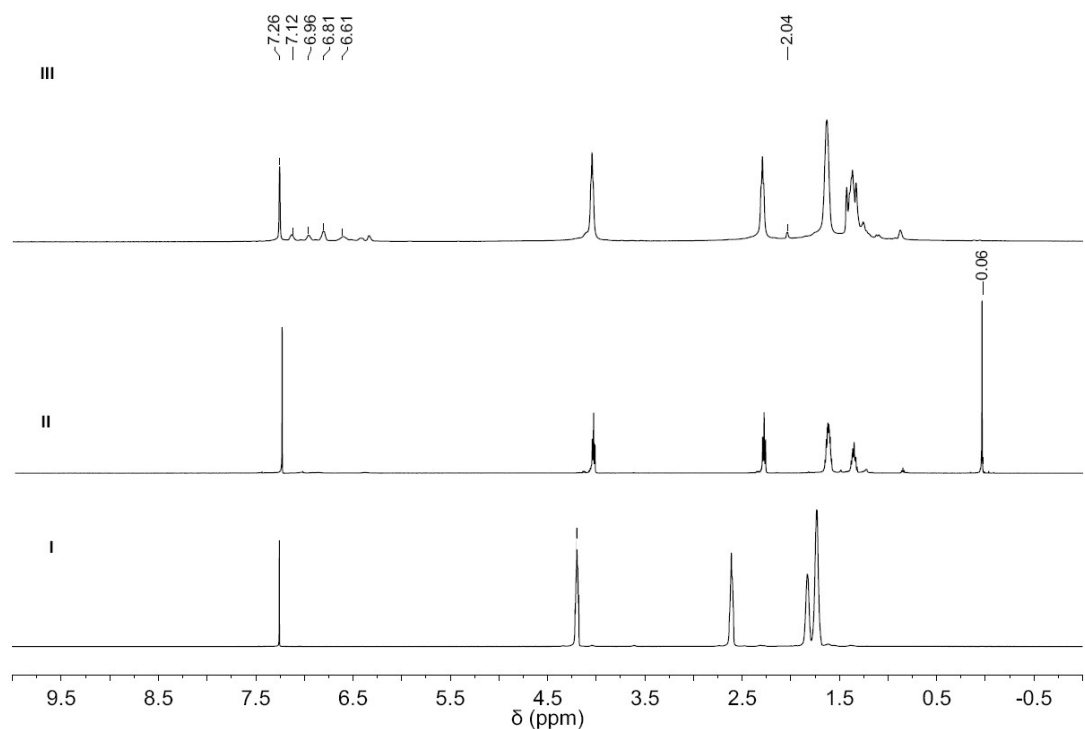


Figure S5.  $^1\text{H}$  NMR spectra ( $\text{CDCl}_3$  without TMS, 500 MHz) of (I)  $\epsilon\text{-CL}$ ; (II) the oligomer of  $\epsilon\text{-CL}$  obtained using complex **2** as initiator ( $[\epsilon\text{-CL}]/[\mathbf{2}] = 20$ , in toluene, room temperature; (III) the oligomer of  $\epsilon\text{-CL}$  obtained using complex **4** as initiator ( $[\epsilon\text{-CL}]/[\mathbf{4}] = 20$ , in toluene, room temperature).

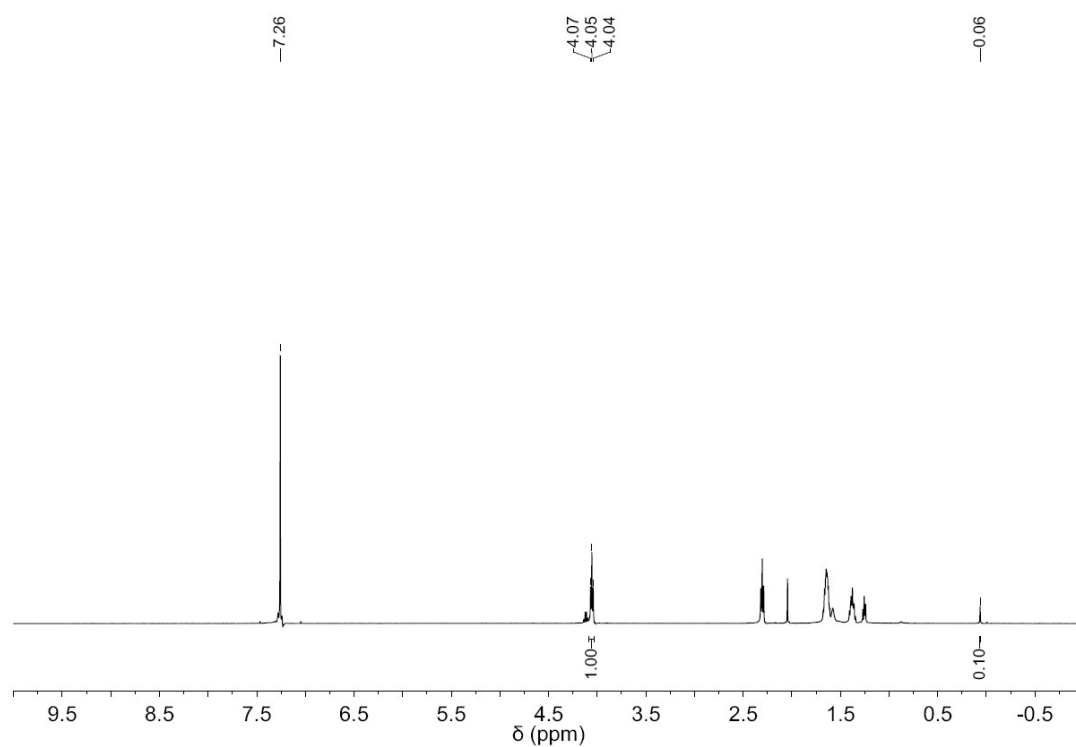


Figure S6. <sup>1</sup>H NMR spectra (CDCl<sub>3</sub> without TMS, 500 MHz) of ε-CL under [ε-CL]/[**2**] = 100:1. From the NMR spectrum, it was found that integral ratio of CH<sub>2</sub> : N(SiMe<sub>3</sub>)<sub>2</sub> = 10:1, the number of H atoms of CH<sub>2</sub> : N(SiMe<sub>3</sub>)<sub>2</sub> = 1:9, the calculated molecular weight is 10260 g.mol<sup>-1</sup>. The theoretical value may be 11400 g.mol<sup>-1</sup>. So, the calculated molecular weight is in good agreement with the theoretical value.