Supporting Information

A designed and potentially decadentate ligand for use in lanthanide(III) catalysed biomass transformations: Targeting diastereoselective *trans*-4,5-diaminocyclopentenone derivatives.

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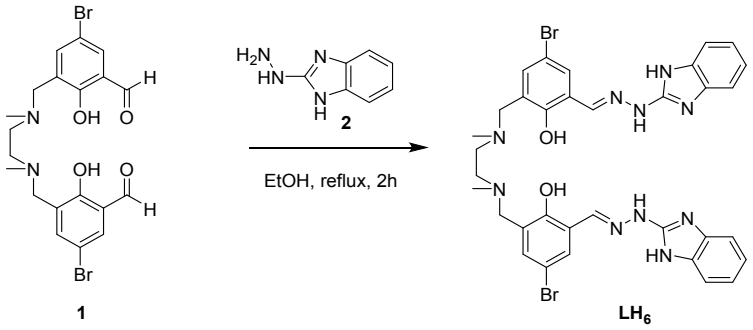
General considerations. All reagents and solvents were used as received from commercial supplies without further purification. To determine the carbon, hydrogen, nitrogen and sulfur fractions of the samples, elemental analysis was carried out using a "Vario Micro Cube" device from Perkin Elmer. Infrared spectra were recorded on a Perkin Elmer Spectrum GX FT-IR spectrometer as KBr pellets in the range 400 cm-1 to 4000 cm-1 with a resolution of 8 cm-1. The following abbreviations were used to describe the peak characteristics: br = broad, sh = shoulder, s = strong, m = medium and w = weak. NMR spectra of the compounds were measured using a Bruker Ultrashield plus 500 (500 MHz) and Varian 500 MHz spectrometer. 1H- and 13C-measurements were recorded using deuterated solvents and referenced to tetramethylsilane (TMS) as an internal standard (δ = 0 ppm). The structures were measured using single crystal X-ray diffraction (SCXRD) on area detector diffractometers: STADIVARI (Mo-Kα, λ = 0.71073 Å; Cu-Kα, λ = 1.5405 Å, detector: Dectris Pilatus 300K (detector: CMOS)) and STADIVARI (Ga-Kα, λ = 1.34143 Å, detector: Dectris Eiger2 R 4M (detector type: HPC)) (STOE). The measurements were taken at temperatures of 150 K and 180 K. The crystals were attached to the goniometer head with perfluoroether oil. Powder X-ray diffraction (PXRD) measurements were performed on an STOE STADI-P diffractometer with Cu-Kα radiation.

Preparation of *N*,*N*'-dimethyl-*N*,*N*'-ethylene-bis(5-bromo-3-(1H-benzimidazol-2-yl)hydrazineylidene)-2-hydroxybenzylamine) (LH_6)

Synthesis of the ligand **LH_6** was performed by the condensation reaction between *N*,*N*'-dimethyl-*N*,*N*'-ethylene-di(5-bromo-3-formyl-2-hydroxybenzylamine) (**1**) and 2-Hydrazino-1H-1,3-benzimidazole (**2**) under reflux in absolute ethanol for 2 hours. After completion of the reaction, yellow solid was filtered, washed with cooled ethanol and dried under reduced pressure.



Scheme1. Preparation of Schiff-base ligand **LH_6**.

Synthesis: LH_6

N,*N*'-dimethyl-*N*,*N*'-ethylene-di(5-bromo-3-formyl-2-hydroxybenzylamine (**1**) (10.91 mmol, 1.650 g) and 2-Hydrazino-1H-1,3-benzimidazole (**2**) (8.71 mmol, 1.326 g) were dissolved in absolute EtOH (100 mL). The resulting mixture was refluxed 2h. After completion of the reaction, the yellow solid was filtered, washed with cooled ethanol and dried under reduced pressure to obtain (93% yield). ^{1}H NMR (500 MHz, DMSO-d_6) = δ 11.60 (s, 4 H), 8.32 (s, 2H), 8.02 (d, J= 2.6 Hz, 2H), 7.29 (d, J = 2.6, Hz, 2H), 7.24 (t, J = 8.0 Hz, 4H), 7.01-6.95 (m, 4H), 3.74 (s, 4H), 2.66 (s, 4H), 2.23 (s, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) = δ 154.6 (CH), 151.81 (C), 148.03 (C), 154.6 (C), 153.4 (C), 131.0 (C), 126.8 (CH), 125.7 (CH), 123.0 (CH), 120.4 (CH), 110.2 (2×CH), 109.0 (CH), 27.8 (CH_2), 52.9 (CH_2), 40.6 (CH_2), KBr: 3443s, 2812s, 1650s, 1609m, 1572m, 1514s, 1459s, 1341w, 1268m, 1145m, 1021m, 741s, 491m.

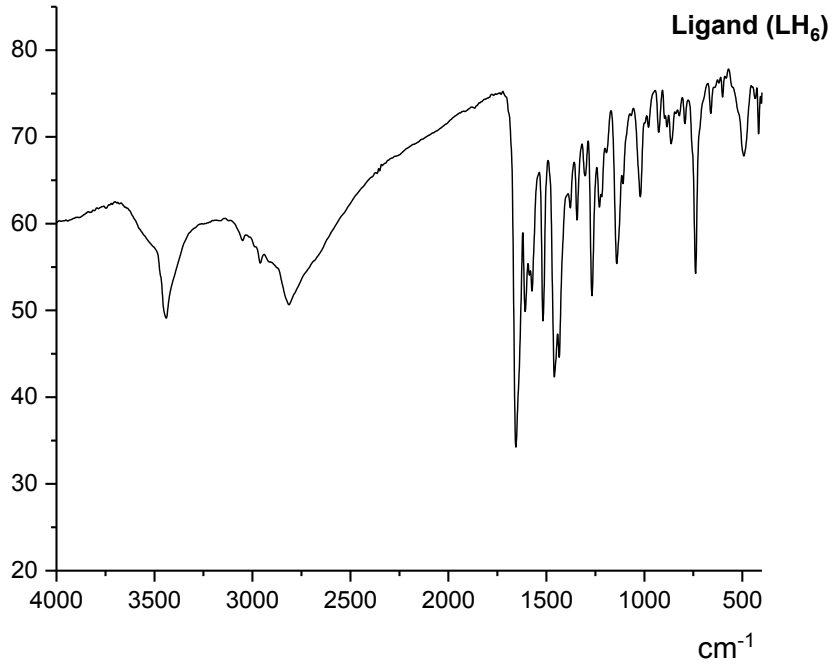
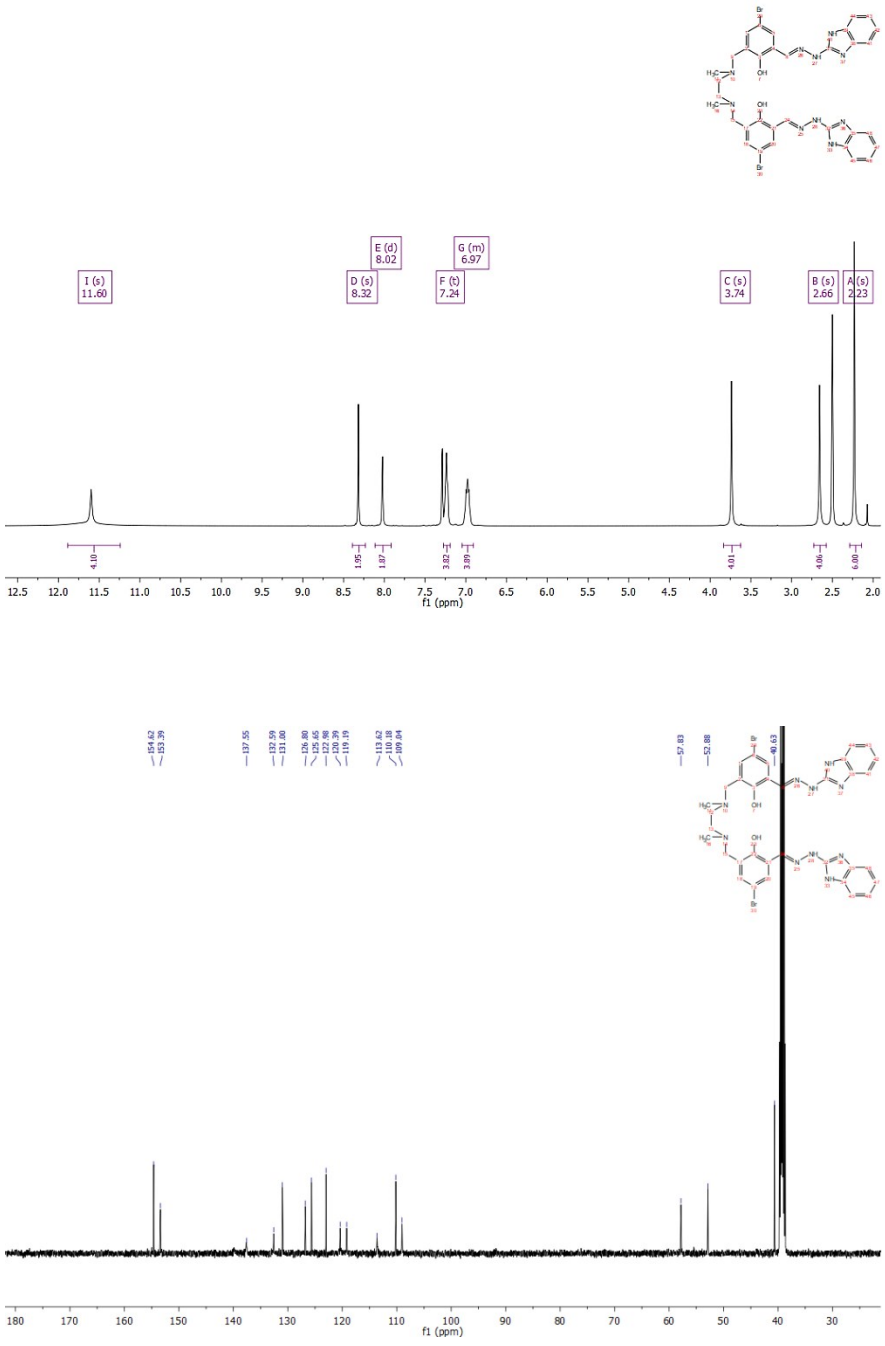


Figure S1. IR spectra of Schiff-base **LH_6** in KBr pallet.



FigureS2. NMR spectra of Schiff-base **LH_6**.

Preparation of single lanthanide complexes

General procedure: A solution of the Schiff-base ligand **LH_6** (0.1 mmol, 77.4 mg) in methanol (10 mL) was added a solution of Ln(III) (0.1 mmol) in 1:1 acetonitrile-methanol (10 mL). The resulting mixture was stirred at room temperature for 1 h. After being filtrated the pale yellow solution was left to stand at ambient temperature to allow for solvent evaporation. After 7 days, well-shaped crystals of the complex were observed. The product could be obtained in the form of powder in higher yield by extensive stirring and extending the reaction time up to 2h.

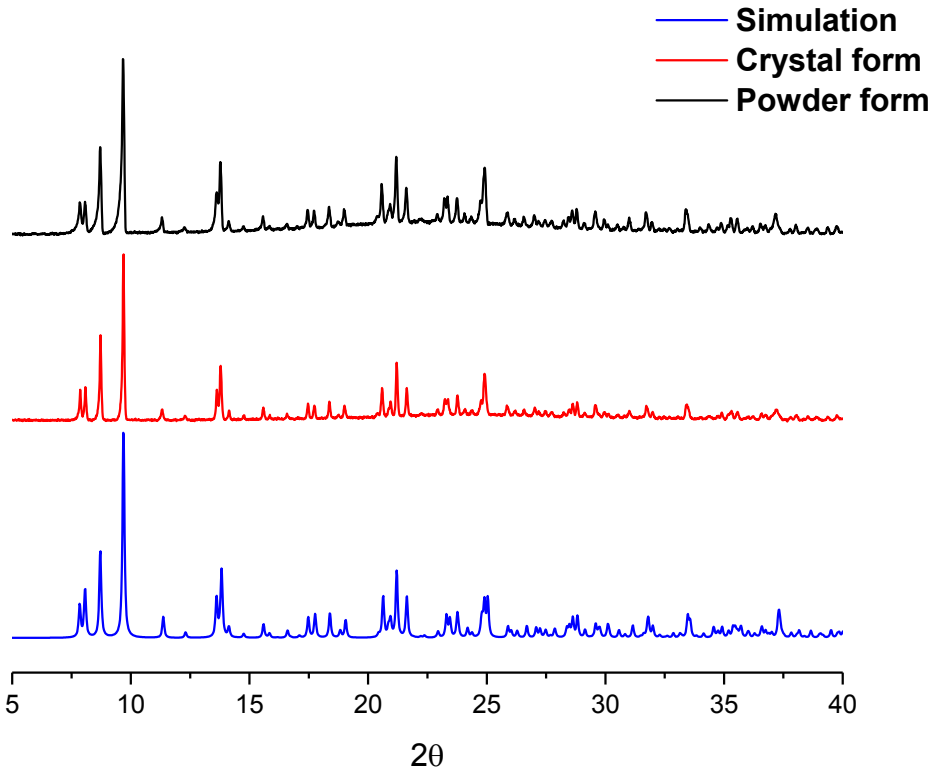
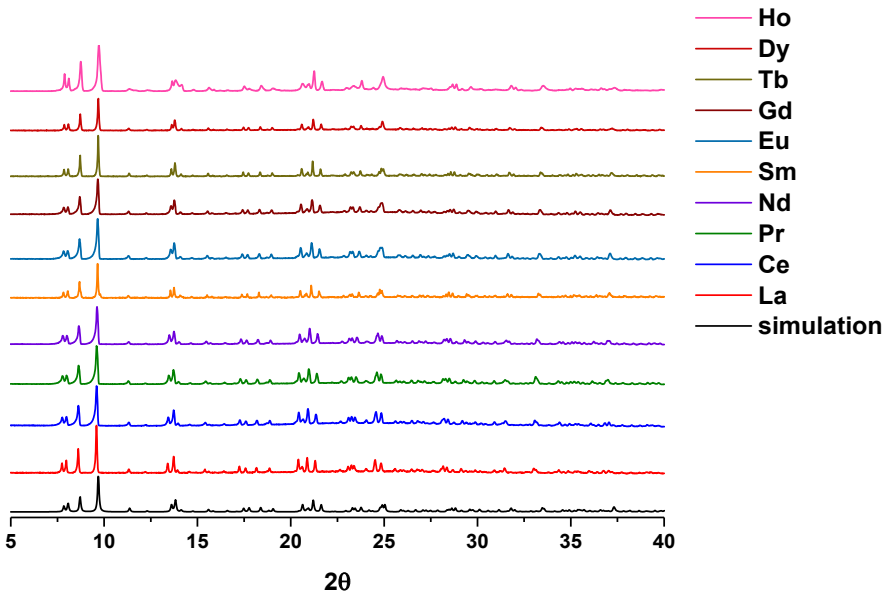


Figure S3. PXRD of measured **$C_{34}H_{34}Br_2DyN_{13}O_{11}$** Crystal and powder form compare to simulation of **$C_{34}H_{34}Br_2SmN_{13}O_{11}$**

a)



b)

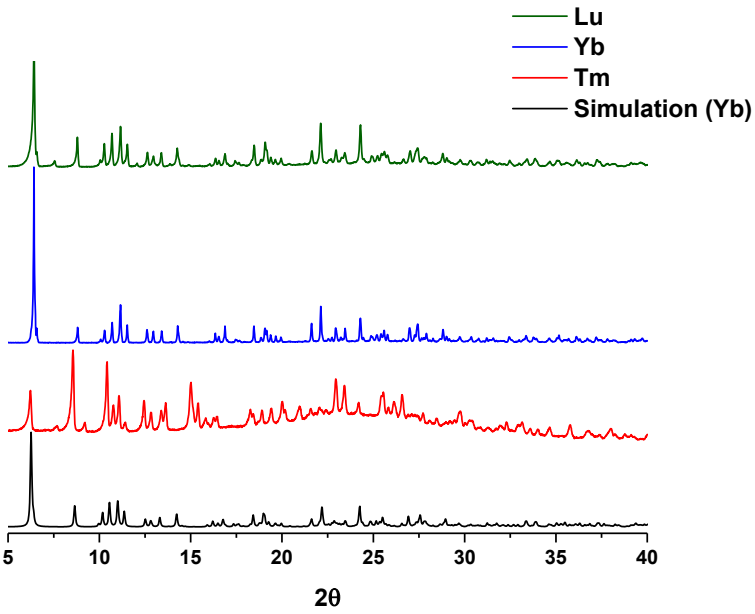


Figure S4. PXRD of measured **Ln(III)LH$_6$** and simulation, a) 10-fold coordination and b) 8-fold coordination.

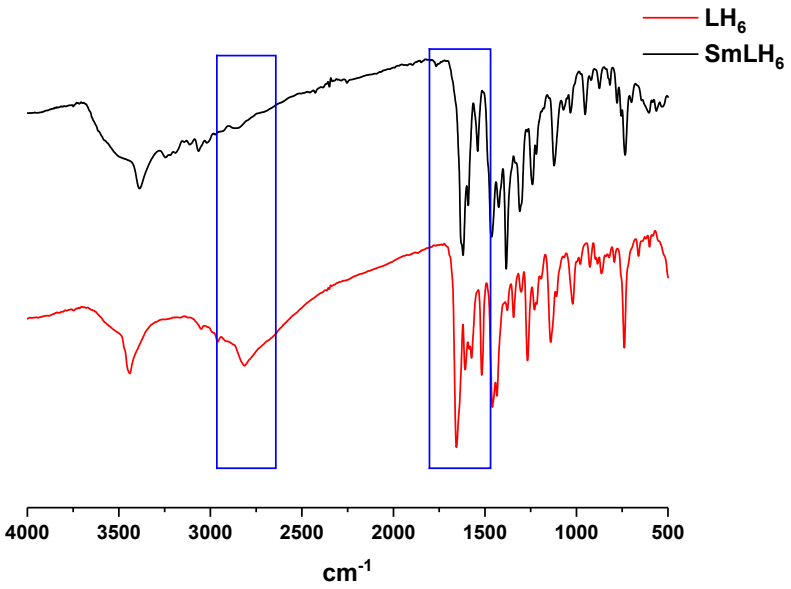


Figure S5. Comparison of IR spectra of Schiff-base **LH_6** and **$SmLH_6$** in KBr pallet.

$C_{34}H_{34}Br_2LaN_{13}O_{11}$; Yield 72% (based on $La(NO_3)_2 \bullet 6H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2LaN_{13}O_{11}$**): C, 37.14%; H, 3.12%; N, 16.65%. Found: C, 36.98%; H, 3.22%; N, 16.68%. FT-IR (cm^{-1}) KBr: 3379m, 3240w, 3062w, 1612s, 1591s, 1537m, 1462s, 1424s, 1386s, 1301s, 1238s, 1216m, 1118m, 1068w, 1033w, 947w, 872w, 736m.

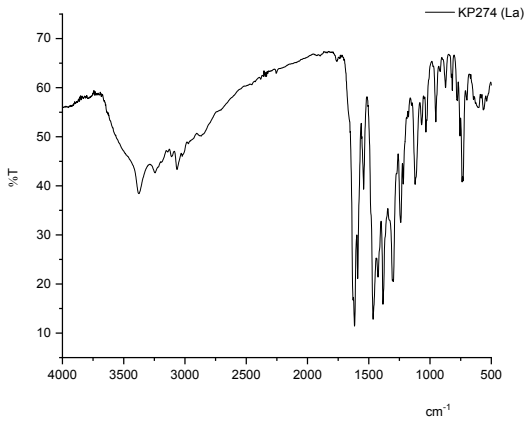


Figure S6. IR spectra of **$C_{34}H_{34}Br_2LaN_{13}O_{11}$** in KBr pallet.

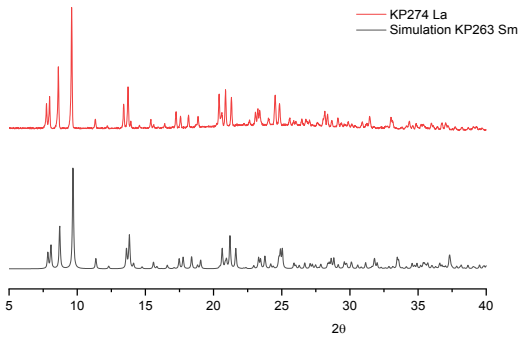


Figure S7. PXRD of measured $\mathbf{C_{34}H_{34}Br_2GdN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2CeN_{13}O_{11}}$; Yield 83% (based on $La(NO_3)_2 \bullet 6H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2LaN_{13}O_{11} \bullet H_2O}$): C, 36.51%; H, 3.24%; N, 16.28%. Found: C, 36.43%; H, 3.30%; N, 16.51%. FT-IR (cm^{-1}) KBr: 3414s, 3062w, 2962w, 1615s, 1594m, 1541w, 1461s, 1425m, 1382s, 1295m, 1243m, 1120m, 1034w, 954w, 874w, 815w, 732w.

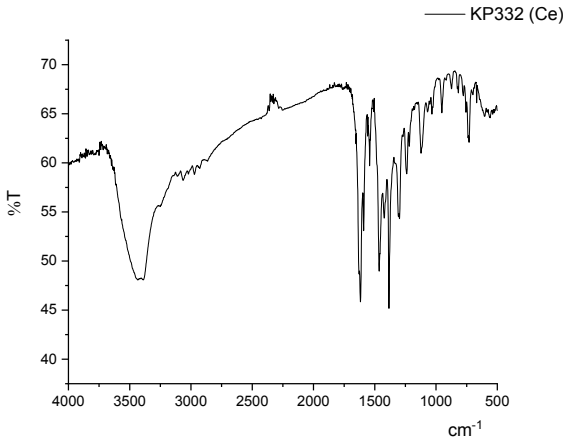


Figure S8. IR spectra of $\mathbf{C_{34}H_{34}Br_2CeN_{13}O_{11}}$ in KBr pallet.

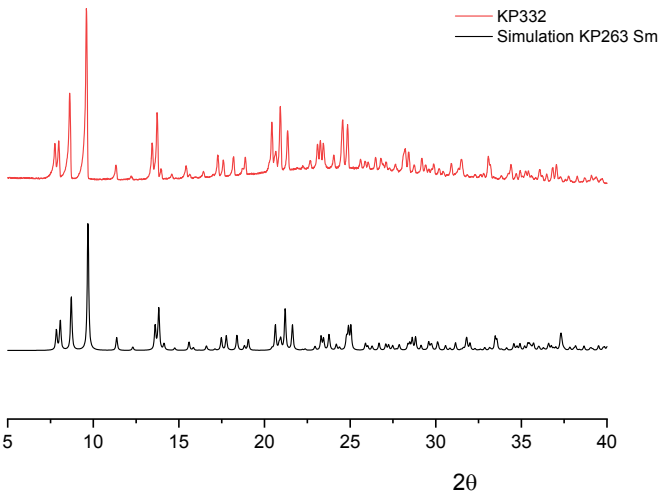


Figure S9. PXRD of measured $\mathbf{C_{34}H_{34}Br_2CeN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2PrN_{13}O_{11}}$; Yield 83% (based on $Pr(NO_3)_2 \bullet 6H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2PrN_{13}O_{11} \bullet H_2O}$): C, 36.48%; H, 3.24%; N, 16.27%. Found: C, 36.56%; H, 3.26%; N, 16.50%. FT-IR (cm^{-1}) KBr: 3389m, 3245w, 3067w, 1616s, 1587m, 1543w, 1465s, 1420s, 1388s, 1236s, 1218w, 1122m, 1069w, 1034w, 950w, 876w, 816w, 779w, 729m.

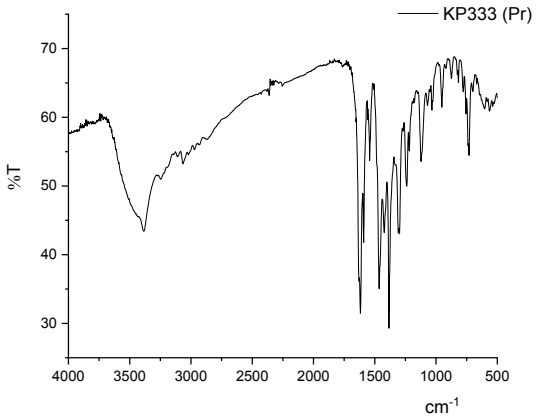


Figure S10. IR spectra of $\mathbf{C_{34}H_{34}Br_2PrN_{13}O_{11}}$ in KBr pallet.

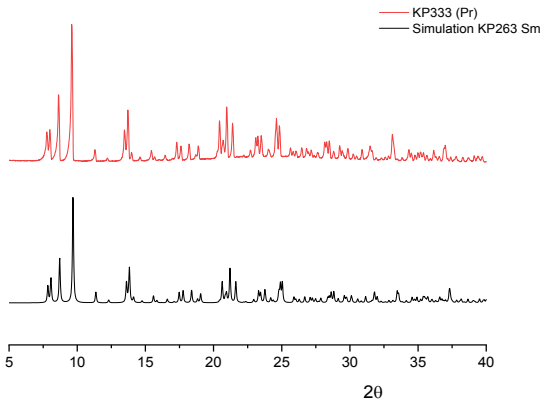


Figure S11. PXRD of measured **$C_{34}H_{34}Br_2PrN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2SmN_{13}O_{11}$**

$C_{34}H_{34}Br_2NdN_{13}O_{11}$; Yield 78% (based on $Nd(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2NdN_{13}O_{11} \bullet H_2O$**): C, 36.96%; H, 3.10%; N, 16.48%. Found: C, 36.59%; H, 3.30%; N, 16.58%. FT-IR (cm^{-1}) KBr: 3389s, 3051w, 1620s, 1538m, 1464s, 1423s, 1382s, 1301s, 1239m, 1127m, 1071w, 1035w, 954w, 871w, 815w, 733m.

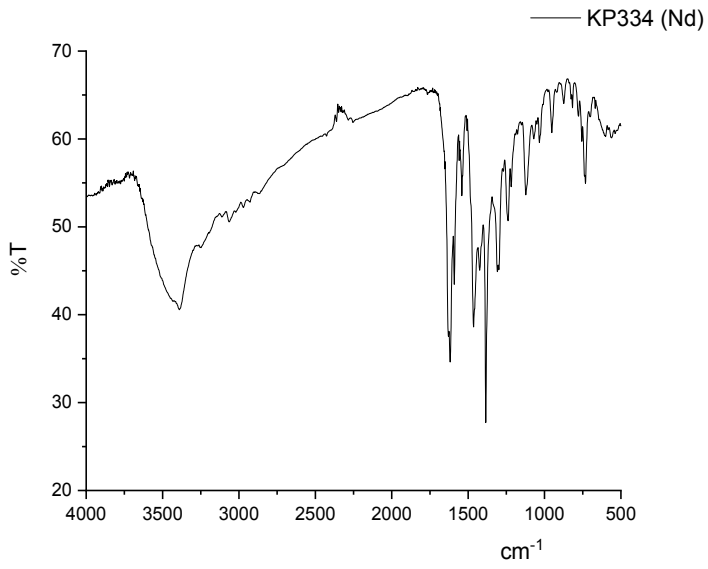


Figure S12. IR spectra of **$C_{34}H_{34}Br_2NdN_{13}O_{11}$** in KBr pallet.

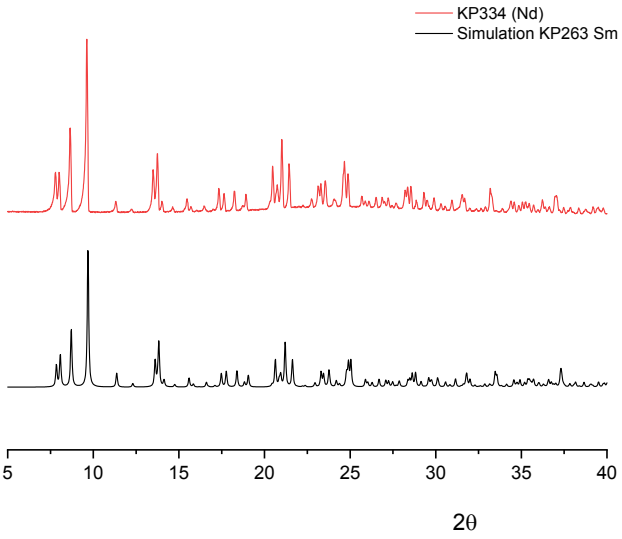


Figure S13. PXRD of measured $\mathbf{C_{34}H_{34}Br_2NdN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$; Yield 79% (based on $Sm(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11} \bullet H_2O}$): C, 36.16%; H, 3.21%; N, 16.13%. Found: C, 36.05%; H, 3.23%; N, 16.18%. FT-IR (cm^{-1}) KBr: 3391m, 1616s, 1592s, 1543m, 1460s, 1420s, 1383s, 1307s, 1241s, 1121s, 1028w, 1031w, 954w, 873w, 816w, 735m.

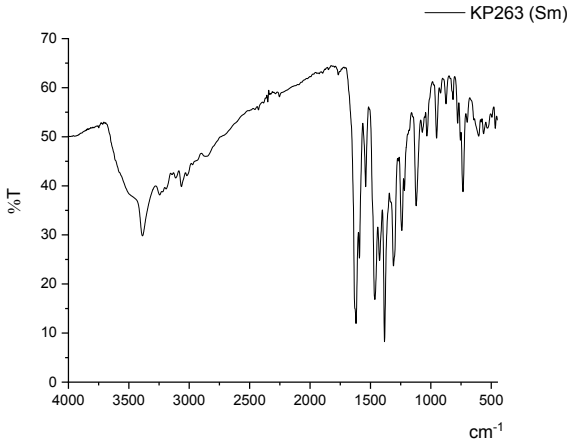


Figure S14. IR spectra of $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$ in KBr pallet.

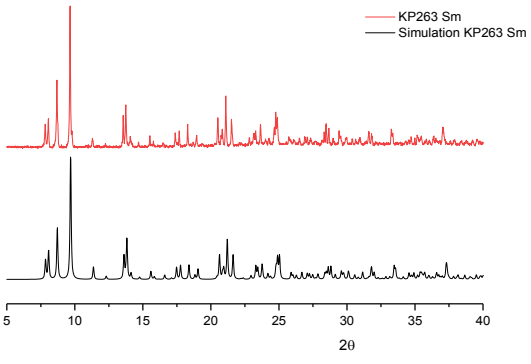


Figure S15. PXRD of measured $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2EuN_{13}O_{11}}$; Yield 82% (based on $Eu(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2EuN_{13}O_{11} \bullet H_2O}$): C, 36.12%; H, 3.21%; N, 16.11%. Found: C, 36.12%; H, 3.29%; N, 16.23%. FT-IR (cm^{-1}) KBr: 3359s, 1622m, 1592s, 1542m, 1426m, 1380s, 1306s, 1239s, 1121s, 1071w, 1031w, 953w, 874w, 814w,780w, 736m.

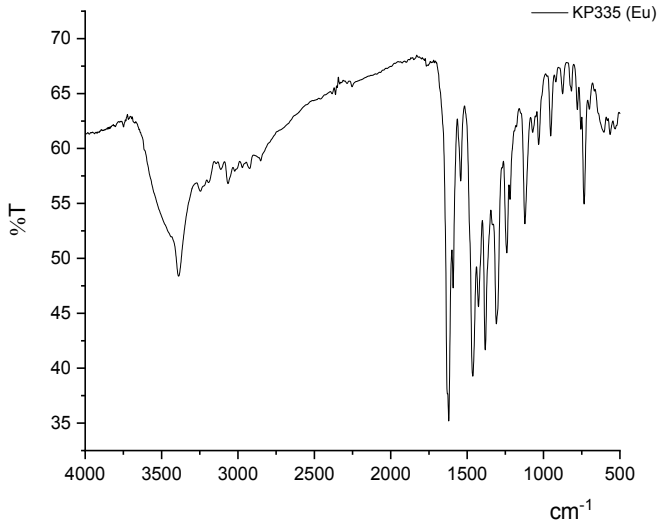


Figure S16. IR spectra of $\mathbf{C_{34}H_{34}Br_2EuN_{13}O_{11}}$ in KBr pallet.

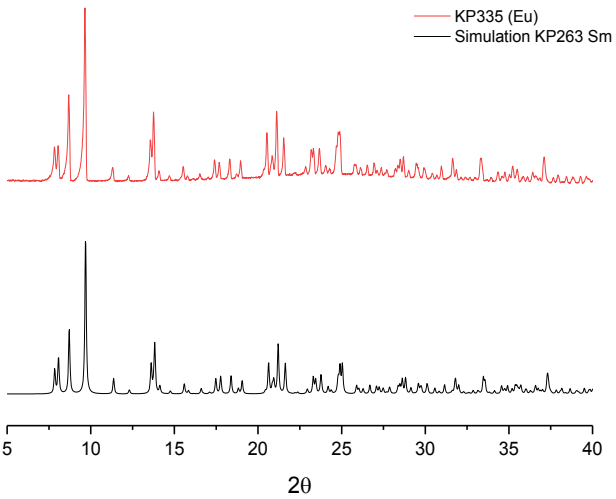


Figure S17. PXRD of measured $\mathbf{C_{34}H_{34}Br_2EuN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2GdN_{13}O_{11}}$; Yield 86% (based on $Gd(NO_3)_2 \bullet 6H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2GdN_{13}O_{11} \bullet H_2O}$): C, 35.95%; H, 3.19%; N, 16.03%. Found: C, 36.05%; H, 3.24%; N, 16.21%. FT-IR (cm^{-1}) KBr: 3391m, 1623s, 1588s, 1540m, 1463s, 1425s, 1380s, 1306s, 1238s, 1119s, 1028m, 956w, 734m.

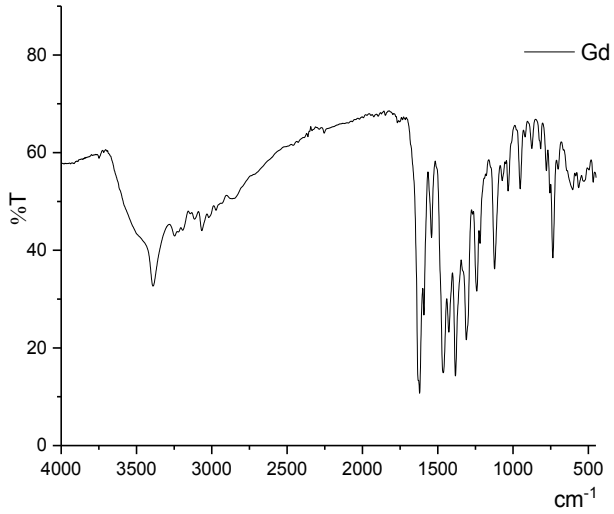


Figure S18. IR spectra of $\mathbf{C_{34}H_{34}Br_2GdN_{13}O_{11}}$ in KBr pallet.

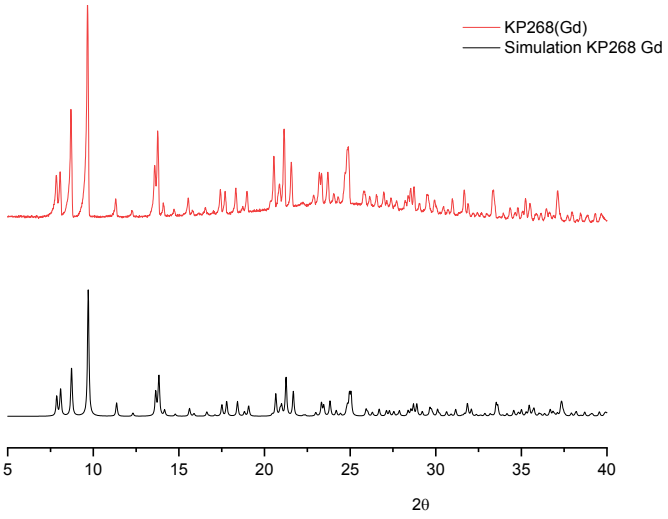


Figure S19. PXRD of measured **$C_{34}H_{34}Br_2GdN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2GdN_{13}O_{11}$**

$C_{34}H_{34}Br_2TbN_{13}O_{11}$; Yield 75% (based on $Tb(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2TbN_{13}O_{11} \bullet H_2O$**): C, 35.90%; H, 3.19%; N, 16.01%. Found: C, 35.82%; H, 3.20%; N, 16.15%. FT-IR (cm^{-1}) KBr: 3391s, 1621s, 1589m, 1543m, 1466s, 1427m, 1379s, 1308s, 1241m, 1218m, 1118m, 1028w, 1030w, 948w, 847w, 816w, 732m.

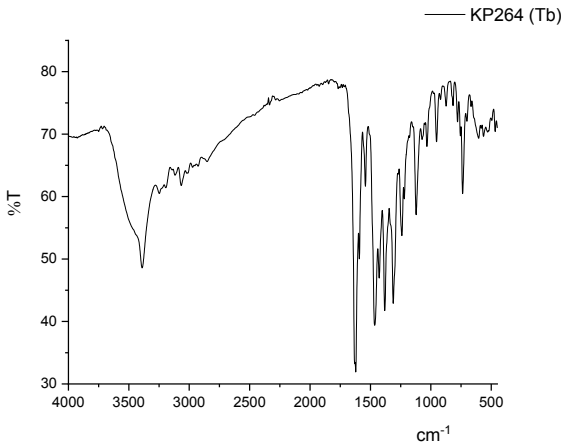


Figure S20. IR spectra of **$C_{34}H_{34}Br_2TbN_{13}O_{11}$** in KBr pallet.

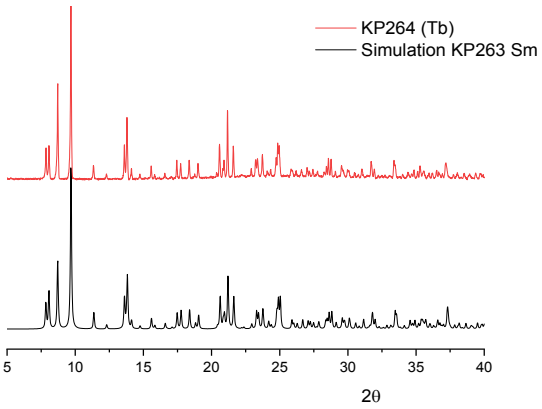


Figure S21. PXRD of measured **$C_{34}H_{34}Br_2TbN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2SmN_{13}O_{11}$**

$C_{34}H_{34}Br_2DyN_{13}O_{11}$; Yield 79% (based on $Dy(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2DyN_{13}O_{11} \bullet H_2O$**): C, 35.79%; H, 3.18%; N, 15.96%. Found: C, 35.61%; H, 3.16%; N, 15.91%. FT-IR (cm^{-1}) KBr: 3389m, 1627s, 1537m, 1468s, 1428s, 1381s, 1309s, 1244s, 1125s, 1028w, 953w, 872w, 735m.

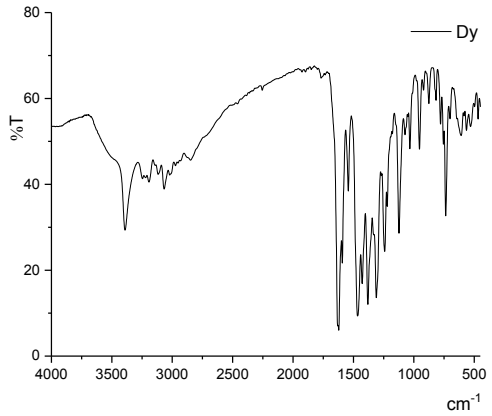


Figure S22. IR spectra of $\mathbf{C_{34}H_{34}Br_2DyN_{13}O_{11}}$ in KBr pallet.

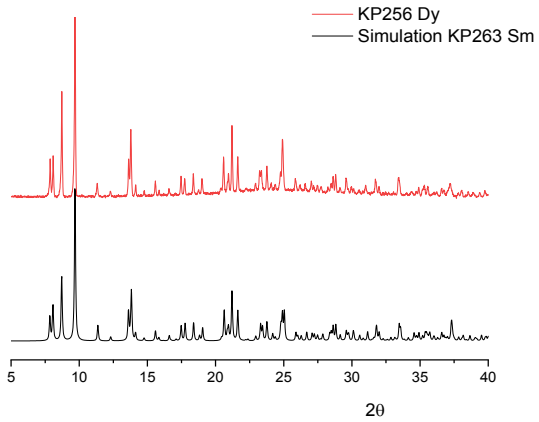


Figure S23. PXRD of measured $\mathbf{C_{34}H_{34}Br_2DyN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

$\mathbf{C_{34}H_{34}Br_2HoN_{13}O_{11}}$; Yield 84% (based on $Ho(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2HoN_{13}O_{11} \bullet H_2O}$): C, 35.71%; H, 3.17%; N, 15.92%. Found: C, 35.32%; H, 3.08%; N, 16.02%. FT-IR (cm^{-1}) KBr: 3435s, 1621s, 1589m, 1545w, 1456s, 1380m, 1298s, 1246m, 1227m, 1072w, 1029w, 1028w, 941w, 847w, 822w, 816w, 736m.

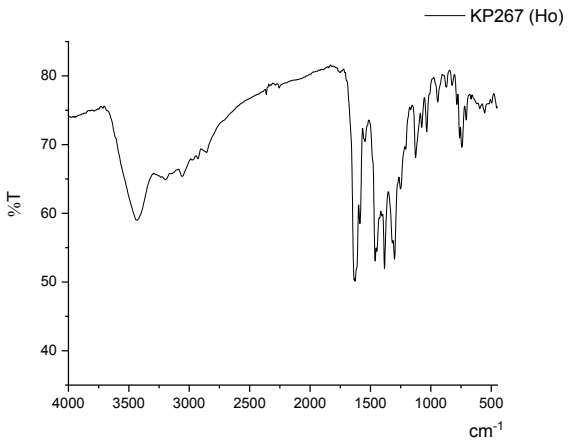


Figure S24. IR spectra of **$C_{34}H_{34}Br_2HoN_{13}O_{11}$** in KBr pallet.

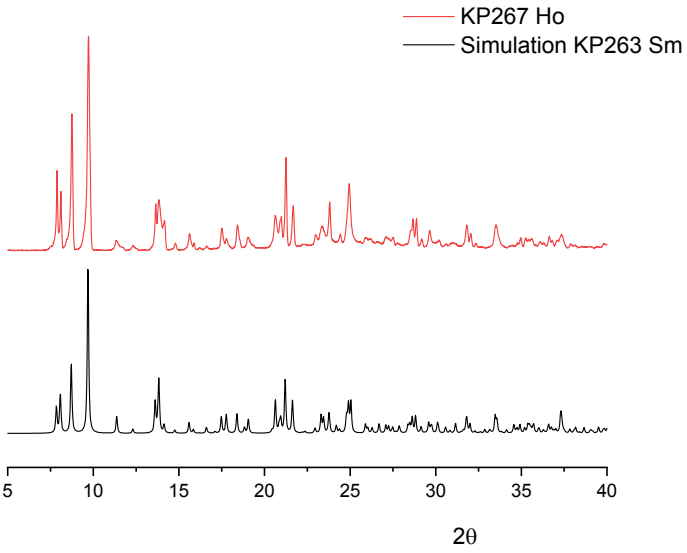


Figure S25. PXRD of measured **$C_{34}H_{34}Br_2HoN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2SmN_{13}O_{11}$**

$C_{34}H_{34}Br_2ErN_{13}O_{11}$; Yield 80% (based on $Er(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for ($C_{34}H_{34}Br_2YbN_{13}O_{11}$): C, 36.21%; H, 3.04%; N, 16.15%. Found: C, 35.61%; H, 3.16%; N, 15.91%. FT-IR (cm^{-1}) KBr: 3414s, 1617s, 1463s, 1384s, 1319s, 1241w, 1154w, 1120w, 1077w, 1035w, 948w, 812w, 744w.

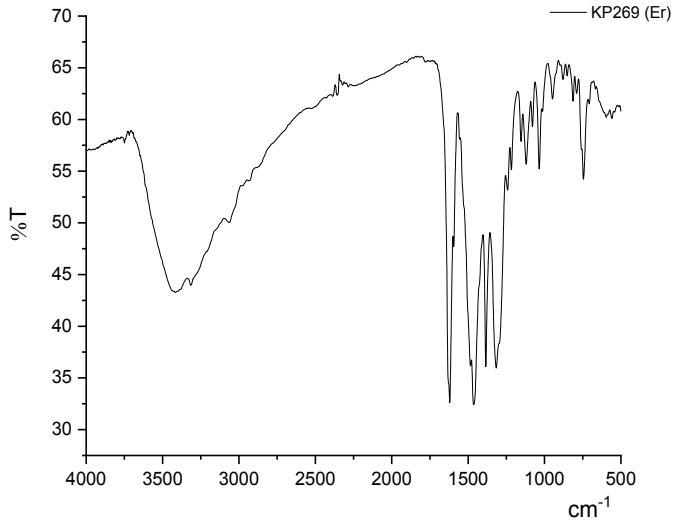


Figure S26. IR spectra of **$C_{34}H_{34}Br_2ErN_{13}O_{11}$** in KBr pallet.

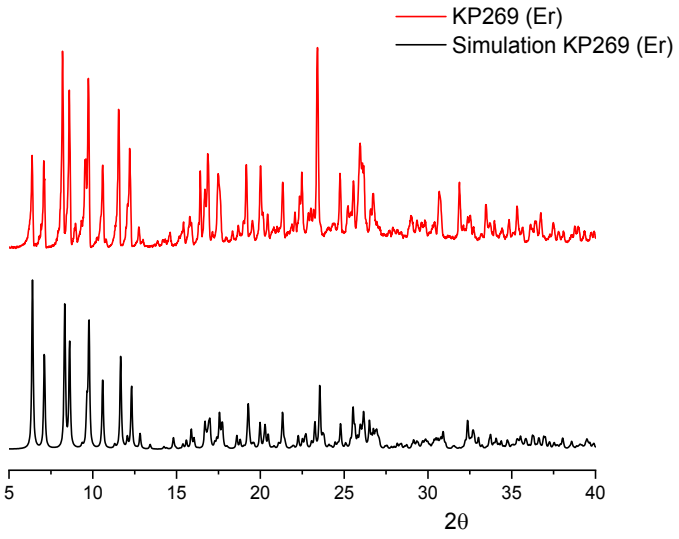


Figure S27. PXRD of measured **$C_{34}H_{34}Br_2ErN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2ErN_{13}O_{11}$**

$C_{34}H_{34}Br_2TmN_{13}O_{11}$; Yield 82% (based on $Tm(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2TmN_{13}O_{11} \bullet H_2O$**): C, 35.59%; H, 3.16%; N, 15.87%. Found: C, 35.02%; H, 3.34%; N,

15.82%. FT-IR (cm^{-1}) KBr: 3436s, 1639s, 1447s, 1381s, 1300s, 1248m, 1226m, 1077w, 1032w, 942w, 868w, 826w, 760w, 745w.

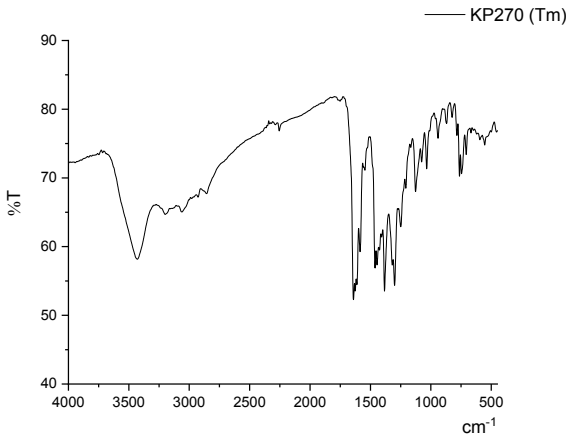


Figure S28. IR spectra of **$C_{34}H_{34}Br_2TmN_{13}O_{11}$** in KBr pallet.

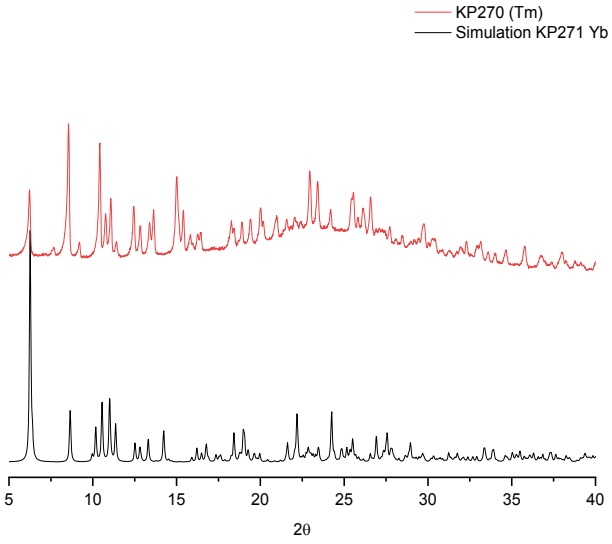


Figure S29. PXRD of measured **$C_{34}H_{34}Br_2TmN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2SmN_{13}O_{11}$**

$C_{40}H_{43}Br_2YbN_{16}O_{11}$; Yield 69% (based on $Yb(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for ($C_{34}H_{34}Br_2YbN_{13}O_{11}\bullet$**$3H_2O$**): C, 34.39%; H, 3.39%; N, 15.33%. Found: C, 34.14%; H, 3.61%; N, 15.75%. FT-IR (cm^{-1}) KBr: 3436s, 1614s, 1591s, 1533w, 1487m, 1451s, 1382s, 1321m, 1295m, 1250m, 1116w, 1073w, 1030w, 945w, 881w, 824w, 738m.

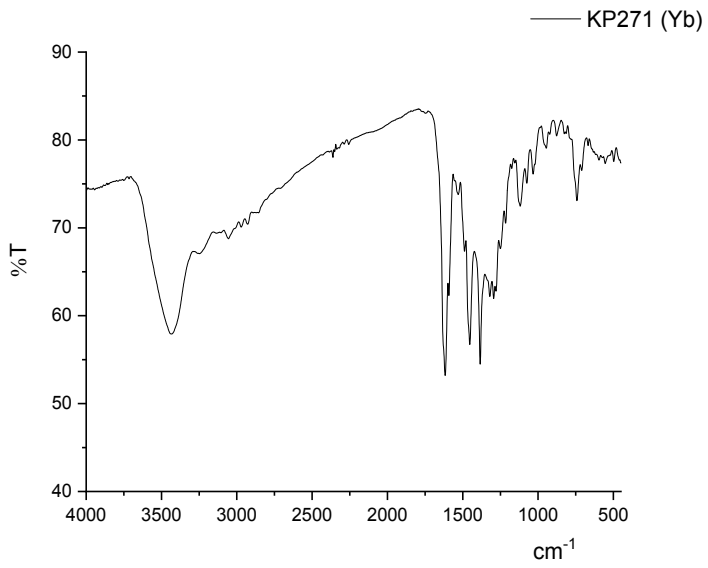


Figure S30 IR spectra of **$C_{34}H_{34}Br_2YbN_{13}O_{11}$** in KBr pallet.

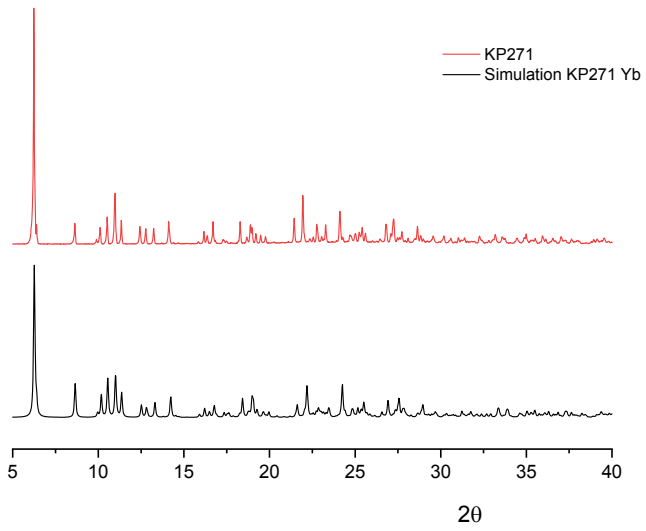


Figure S31. PXRD of measured **$C_{34}H_{34}Br_2YbN_{13}O_{11}$** and simulated **$C_{34}H_{34}Br_2YbN_{13}O_{11}$**

$C_{34}H_{34}Br_2LuN_{13}O_{11}$; Yield 77% (based on $Lu(NO_3)_2 \bullet 5H_2O$). Elemental analysis calcd for (**$C_{34}H_{34}Br_2LuN_{13}O_{11} \bullet 2H_2O$**): C, 34.86%; H, 3.27%; N, 15.54%. Found: C, 34.73%; H, 3.13%; N, 15.38%. FT-IR (cm^{-1}) KBr: 3436s, 1614s, 1591s, 1533w, 1487m, 1451s, 1382s, 1321m, 1295m, 1250m, 1116w, 1073w, 1030w, 945w, 881w, 824w, 738m.

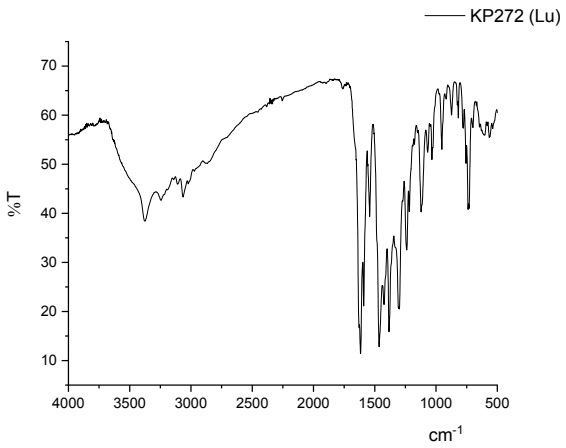


Figure S32. IR spectra of $\mathbf{C_{34}H_{34}Br_2LuN_{13}O_{11}}$ in KBr pallet.

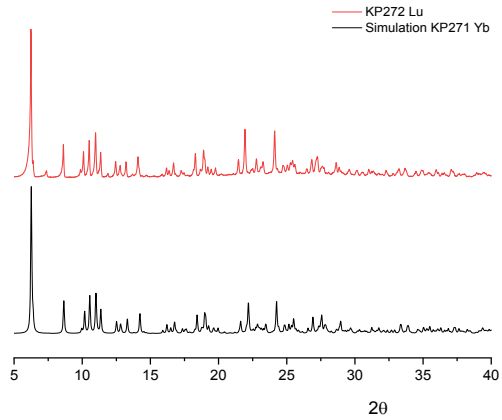


Figure S33. PXRD of measured $\mathbf{C_{34}H_{34}Br_2LuN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2YbN_{13}O_{11}}$

$C_{34}H_{34}Br_2YN_{13}O_{11}$: Yield 67% (based on $Y(NO_3)_2 \bullet 6H_2O$). Elemental analysis calcd for ($\mathbf{C_{34}H_{34}Br_2YN_{13}O_{11}}$): C, 38.91%; H, 3.27%; N, 17.35%. Found: C, 38.71%; H, 3.53%; N, 17.40%. FT-IR (cm^{-1}) KBr: 3390s, 3242w, 3056w, 1621s, 1540m, 1463s, 1429m, 1380s, 1310s, 1240s, 1118m, 1030w, 651w, 874w, 813w, 779w, 734m.

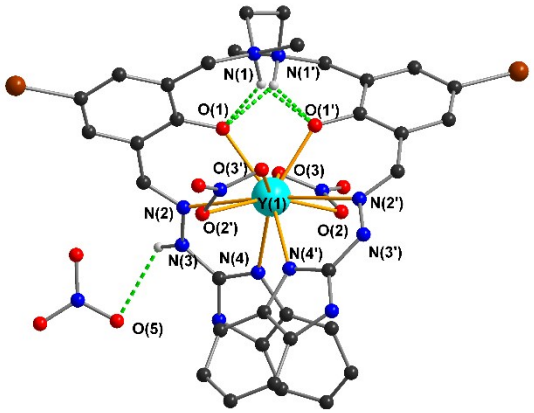


Figure S34. The structure of **YLH_6**. Colour codes for the atoms: light blue (Y), blue (N), red (O) black (C) and brow (Br). The hydrogen bond highlight in green dash line. Solvent molecules (MeCN) in lattice and H atoms are omitted for clarity.

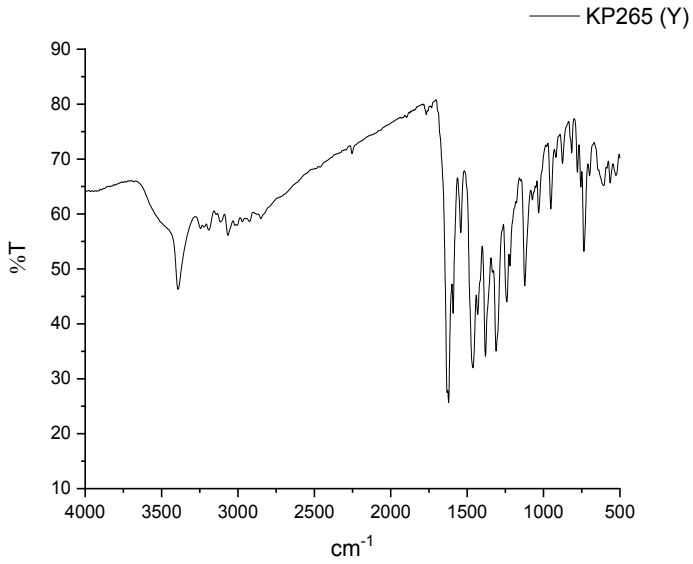


Figure S35. IR spectra of **$C_{34}H_{34}Br_2LuN_{13}O_{11}$** in KBr pallet.

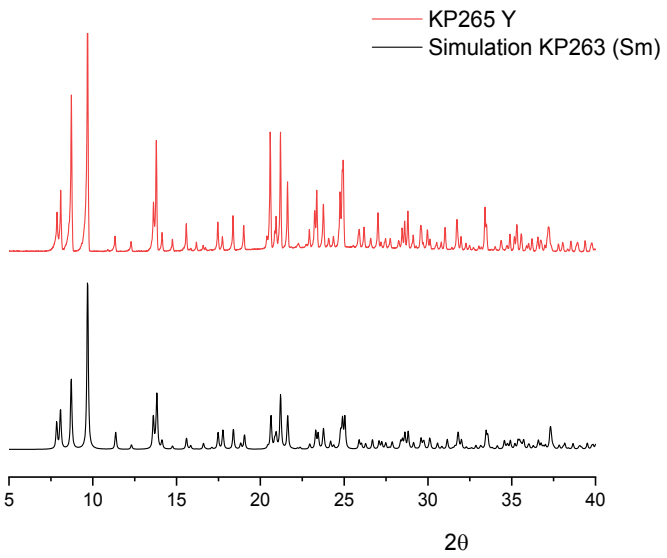


Figure S36. PXRD of measured $\mathbf{C_{34}H_{34}Br_2YN_{13}O_{11}}$ and simulated $\mathbf{C_{34}H_{34}Br_2SmN_{13}O_{11}}$

Catalytic properties study

General procedure for the synthesis of trans-4,5-dimopholino-cyclopent-2-enone (5) in MeCN: catalytic efficiency of the series of Ln(III)-complexes and Y(III)-complex. To a solution of **Ln(III)-LH$_6$** (20 mg, 1.0 mol% loading) and 200 mg 4Å molecularsive in MeCN (10 mL) were added morpholine (195 µl, 2.2 mmol) and furfural (85 µl, 1.0 mmol). The mixture was allowed to stir vigorously at room temperature for 2h. Then the reaction mixture was sampled 500 µl, filtered through celeit and washed with 5 mL of CH_2Cl_2. The solvent was evaporated under reduced pressure, and the crude product was analysed by ^{1}H NMR.

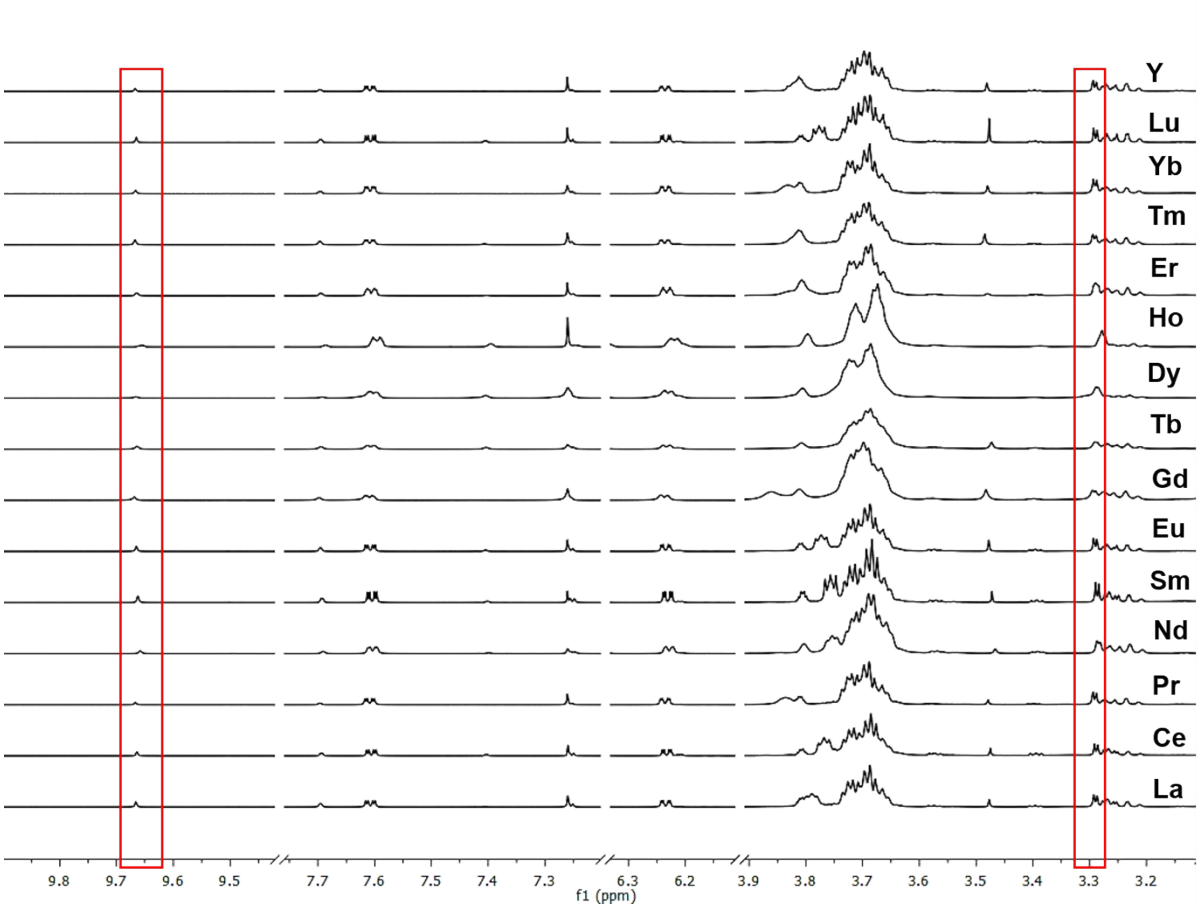


Figure S37. Time dependency experiment 1.0 mol% catalytic loading following by ^{1}H-NMR

General procedure for the synthesis of trans-4,5-dimopholino-cyclopent-2-enone (5) in MeCN time dependency experiments. To a solution of **$DyLH_6$** (0.5 mol% and 1.0 mol% loading) and 200 mg 4Å molecularsive in MeCN (10 mL) were added morpholine (195 µl, 2.2 mmol) and furfural (85 µl, 1.0 mmol). The mixture was allowed to stir vigorously at room temperature. Then the reaction mixture was sampled 500 µl, filtered through celeit and washed with 5 mL of CH_2Cl_2. The solvent was evaporated under reduced pressure, and the crude product was analysed by ^{1}H NMR.

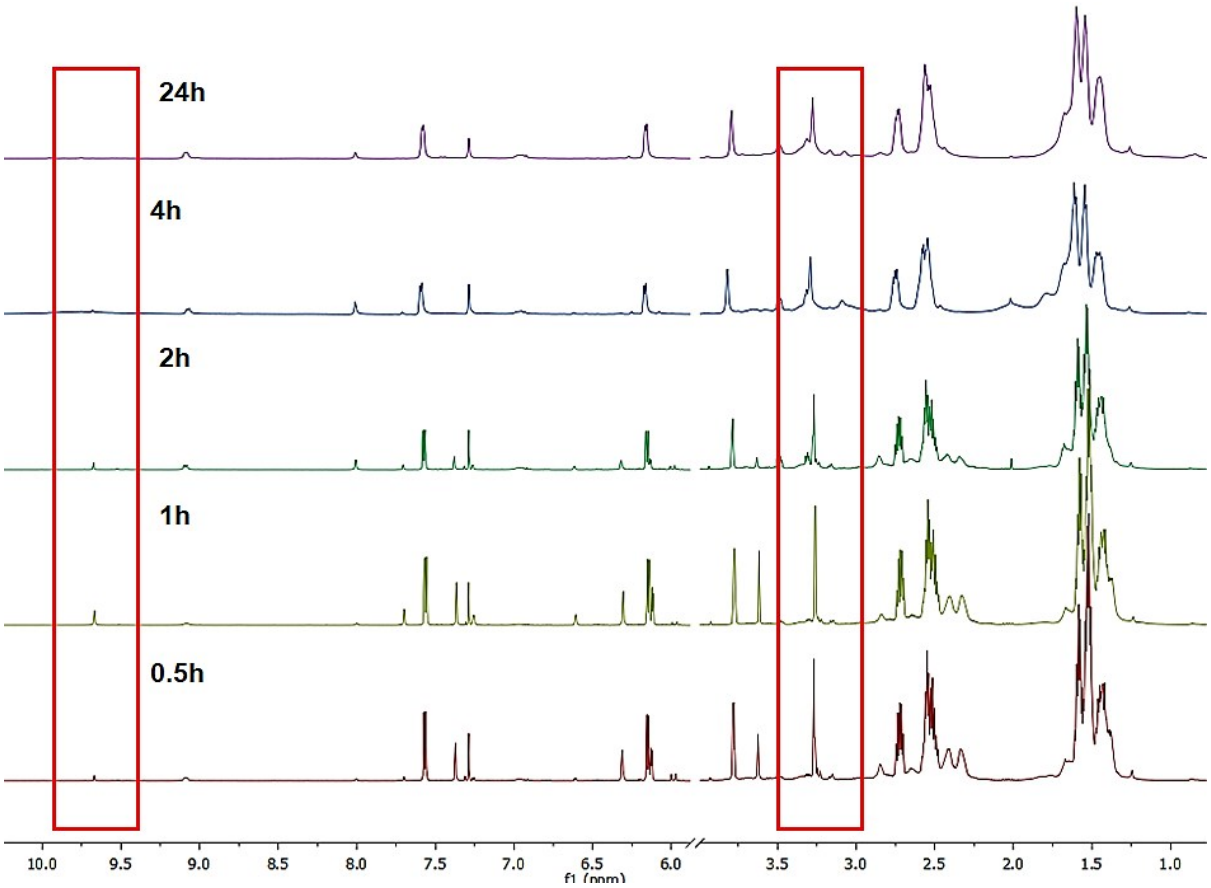


Figure S38. Time dependency experiment 0.5 mol% catalytic loading following by ^{1}H-NMR

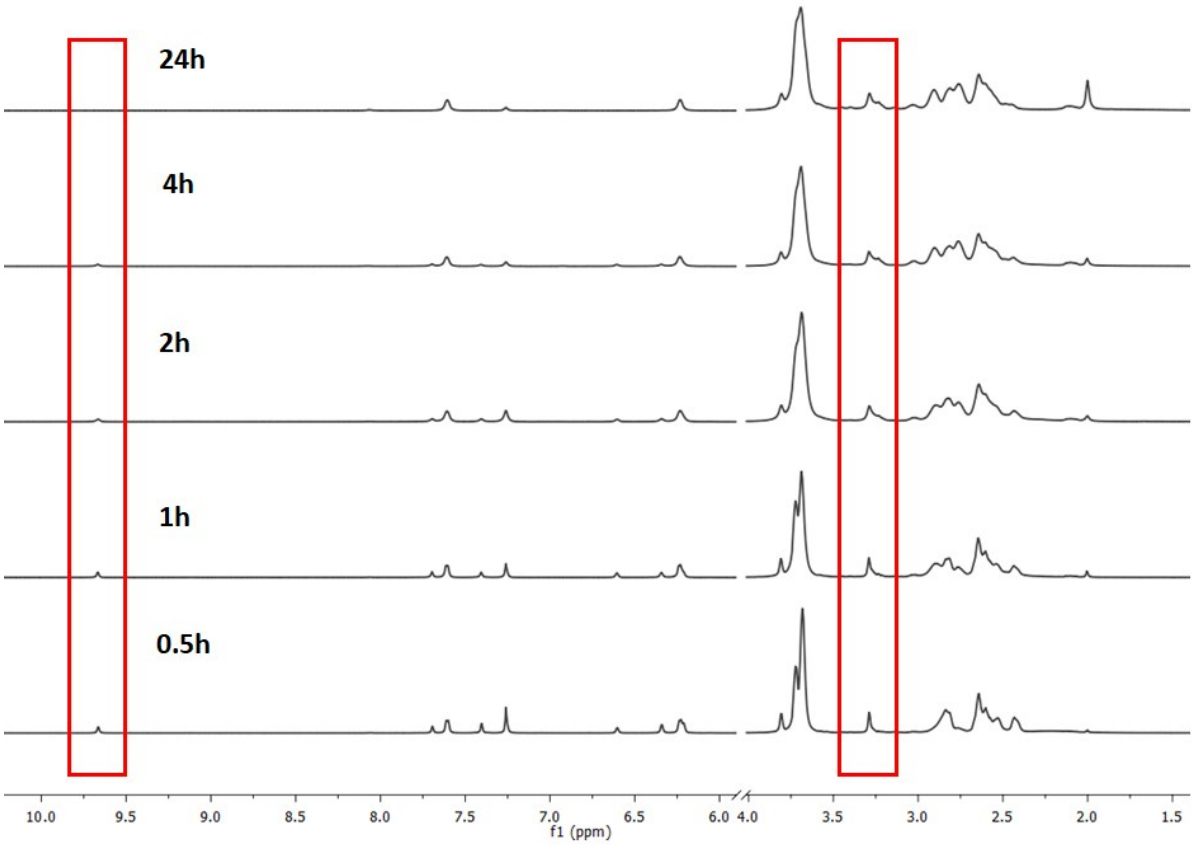
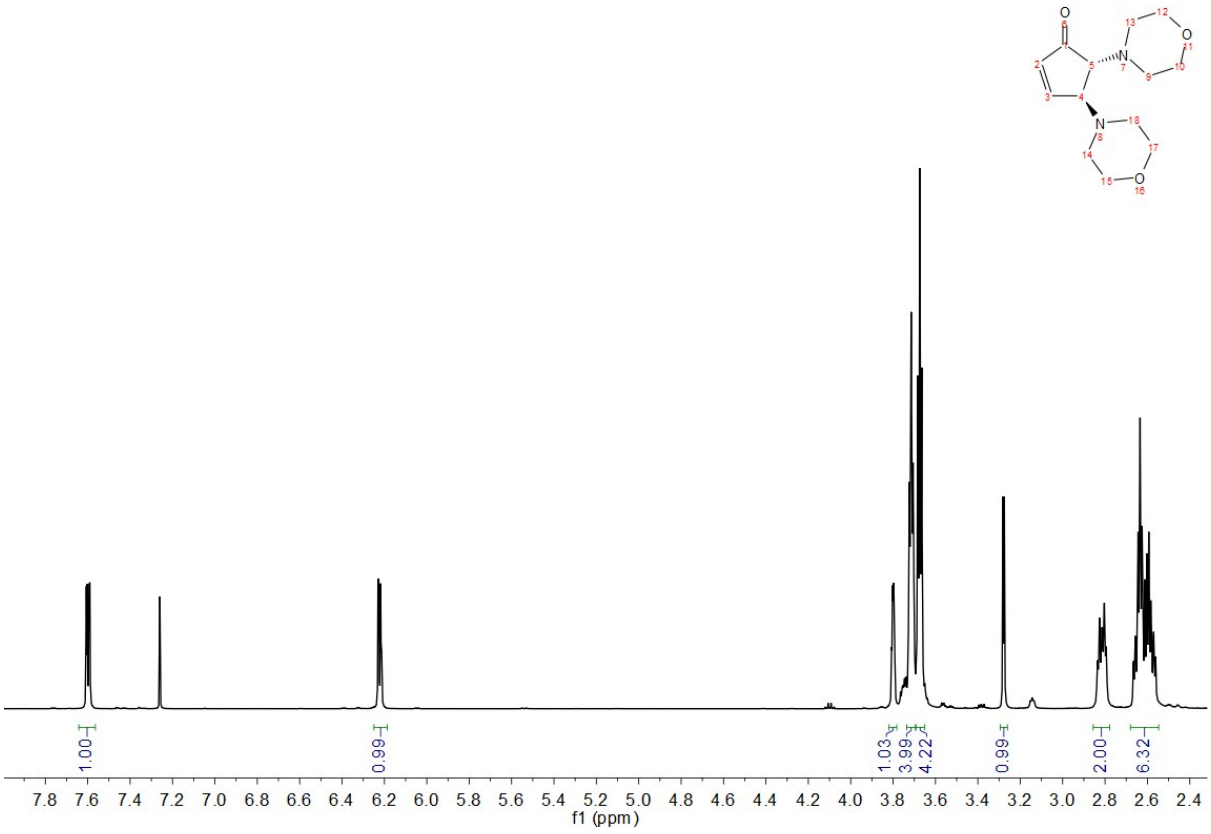


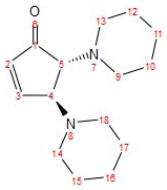
Figure S39. Time dependency experiment 1.0 mol% catalytic loading following by ^{1}H-NMR

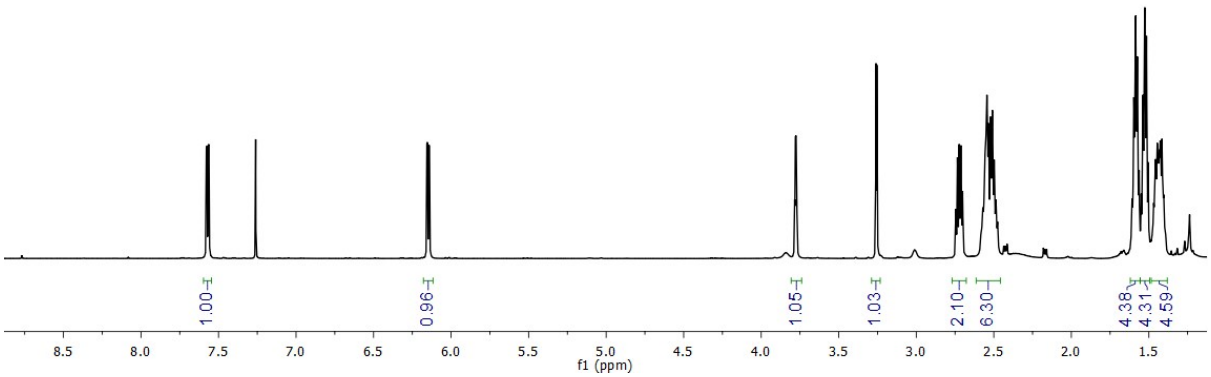
General procedure for the investigation of the efficiency of catalyst for the transformation of furfural to trans-4,5-amino-cyclopent-2-enone in MeCN. To a solution of {**Ln(III)-L4**} (1 mol%) and 200 mg 4Å molecularsieve in MeCN (10 mL) were added morpholine (195 µl, 2.2 mmol) and furfural (85 µl, 1.0 mmol). The mixture was allowed to stir vigorously at room temperature for 4 h. Then the resulting solution was filtered through celite, washed with CH_2Cl_2. The solvent was evaporated under reduced pressure, and the crude product was purifying by column chromatography to obtain colourless oil product (98% yield). ^{1}H NMR (500 MHz, $CDCl_3$) = δ 7.60 (dd, *J* = 6.2, 2.2 Hz, 1H), 8.32 (dd, *J* = 6.2, 1.8 Hz, 1H), 3.80 (q, *J* = 2.3 Hz, 1H), 3.72 (td, *J* = 4.7, 4.2, 2.1 Hz, 4H), 3.67 (t, *J* = 4.7 Hz, 4H), 3.28 (d, *J* = 3.1 Hz, 1H), 2.81 (dt, *J* = 11.5, 4.7 Hz, 2H), 2.69 – 2.54 (m, 6H).



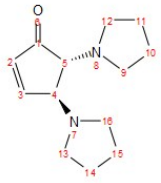
General procedure for the synthesis of trans-4,5-amino-cyclopent-2-enone in MeCN. To a solution of **$DyLH_6$** (112 mg, 1mol%) and 200 mg 4Å molecularsieve in MeCN (10 mL) were added amine (2.2 mmol) and furfural (1.0 mmol). The mixture was allowed to stir vigorously at room temperature for 4 h. Then the resulting solution was filtered through celite, washed with CH_2Cl_2. The solvent was evaporated under reduced pressure, and the crude product was purified by column chromatography.

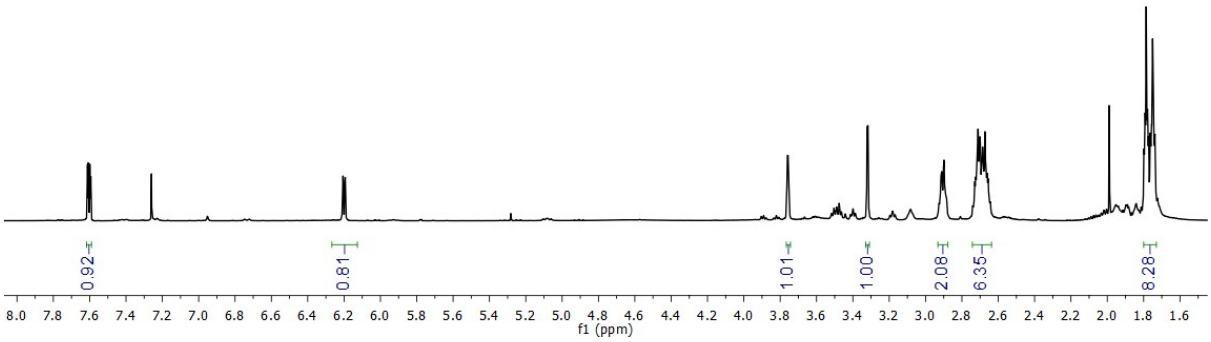
Compound 6: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 6.2, 2.2 Hz, 1H), 6.15 (dd, *J* = 6.2, 1.9 Hz, 1H), 3.78 (q, *J* = 2.3 Hz, 1H), 3.26 (d, *J* = 2.8 Hz, 1H), 2.72 (dt, *J* = 10.9, 5.3 Hz, 2H), 2.61 – 2.45 (m, 9H), 1.62 – 1.55 (m, 4H), 1.56 – 1.49 (m, 4H), 1.49 – 1.38 (m, 4H).



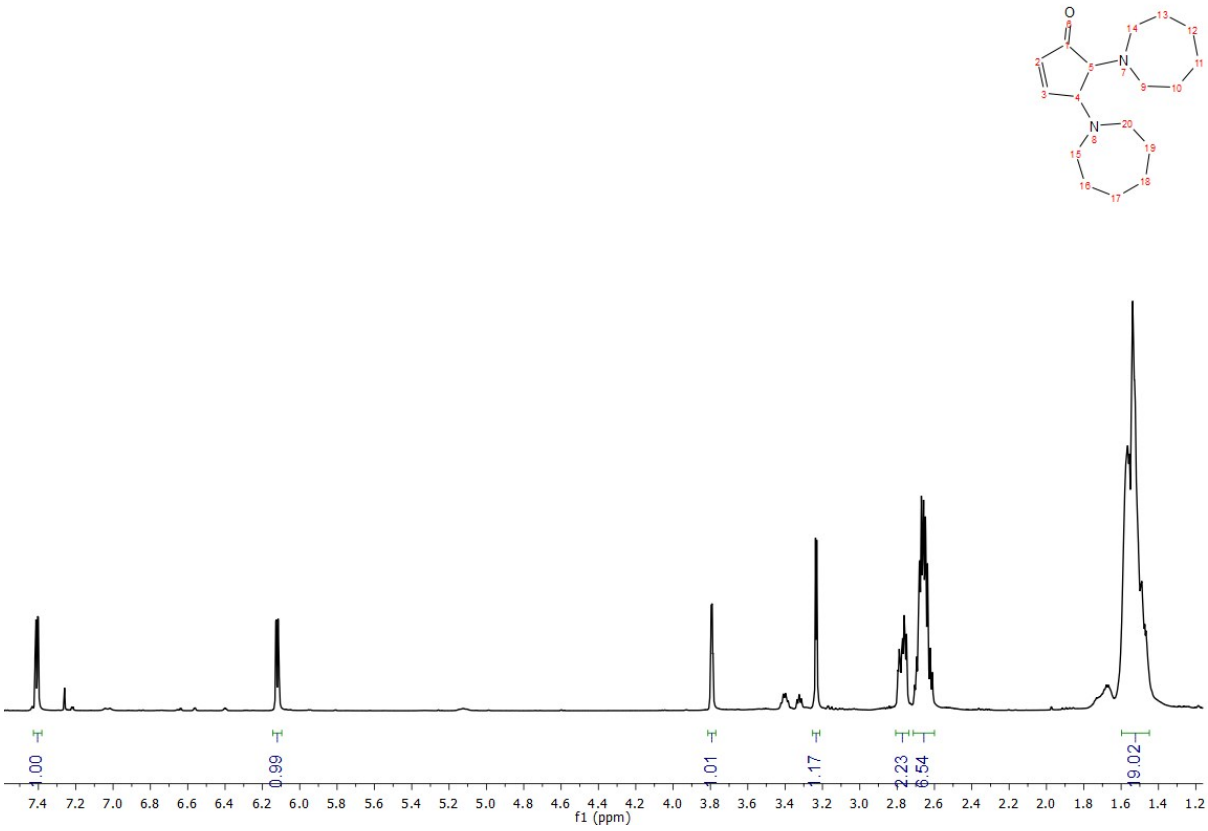


Compound 7: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 6.1, 2.2 Hz, 1H), 6.20 (dd, *J* = 6.1, 1.6 Hz, 1H), 3.76 (q, *J* = 2.2 Hz, 1H), 3.32 (d, *J* = 2.7 Hz, 1H), 2.99 – 2.85 (m, 2H), 2.76 – 2.61 (m, 6H), 1.81 – 1.70 (m, 8H).

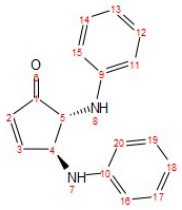


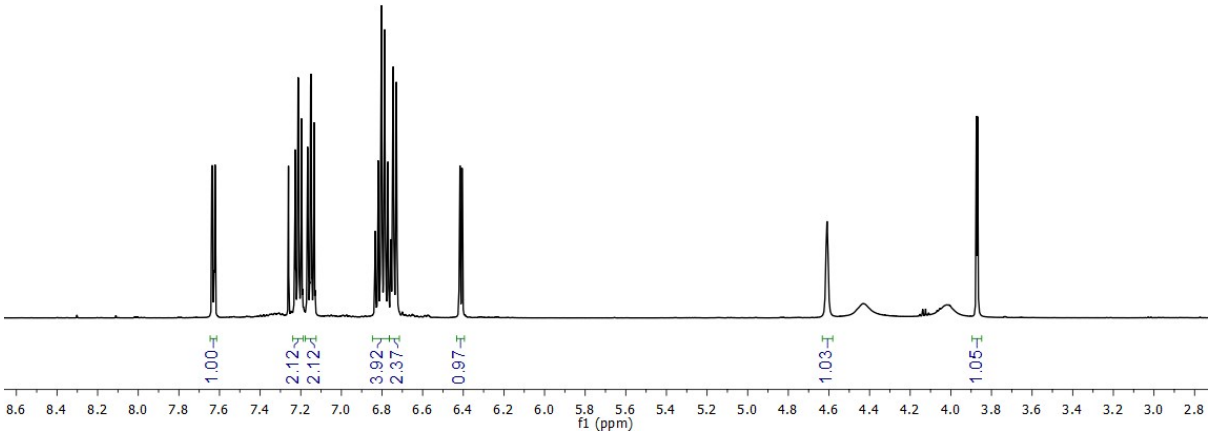


Compound 8: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 6.1, 2.0 Hz, 1H), 6.12 (dd, *J* = 6.2, 1.9 Hz, 1H), 3.79 (q, *J* = 2.3 Hz, 1H), 3.23 (d, *J* = 3.1 Hz, 1H), 2.81-2.73 (m, 2H), 2.70-2.61 (m, 6H), 1.63 – 1.43 (m, 19H).

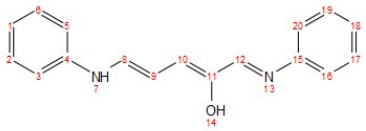


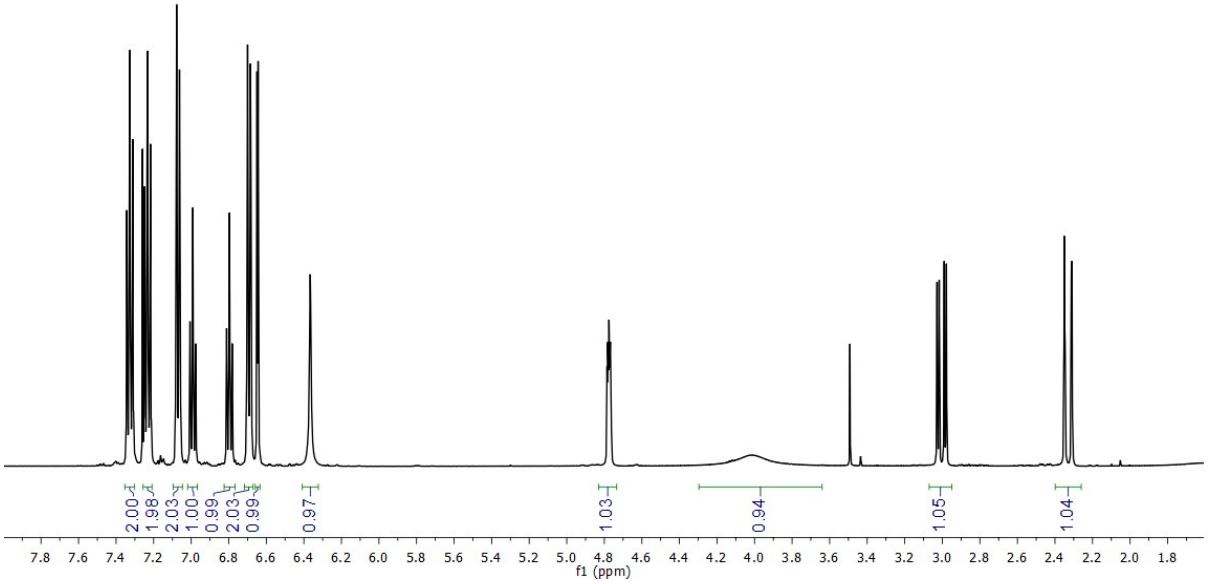
Compound 9a: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 6.0, 2.0 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.18 – 7.12 (m, 2H), 6.85 – 6.76 (m, 4H), 6.77 – 6.71 (m, 2H), 6.41 (dd, *J* = 6.0, 1.6 Hz, 1H), 4.61 (s, 1H), 3.87 (d, *J* = 2.9 Hz, 1H).



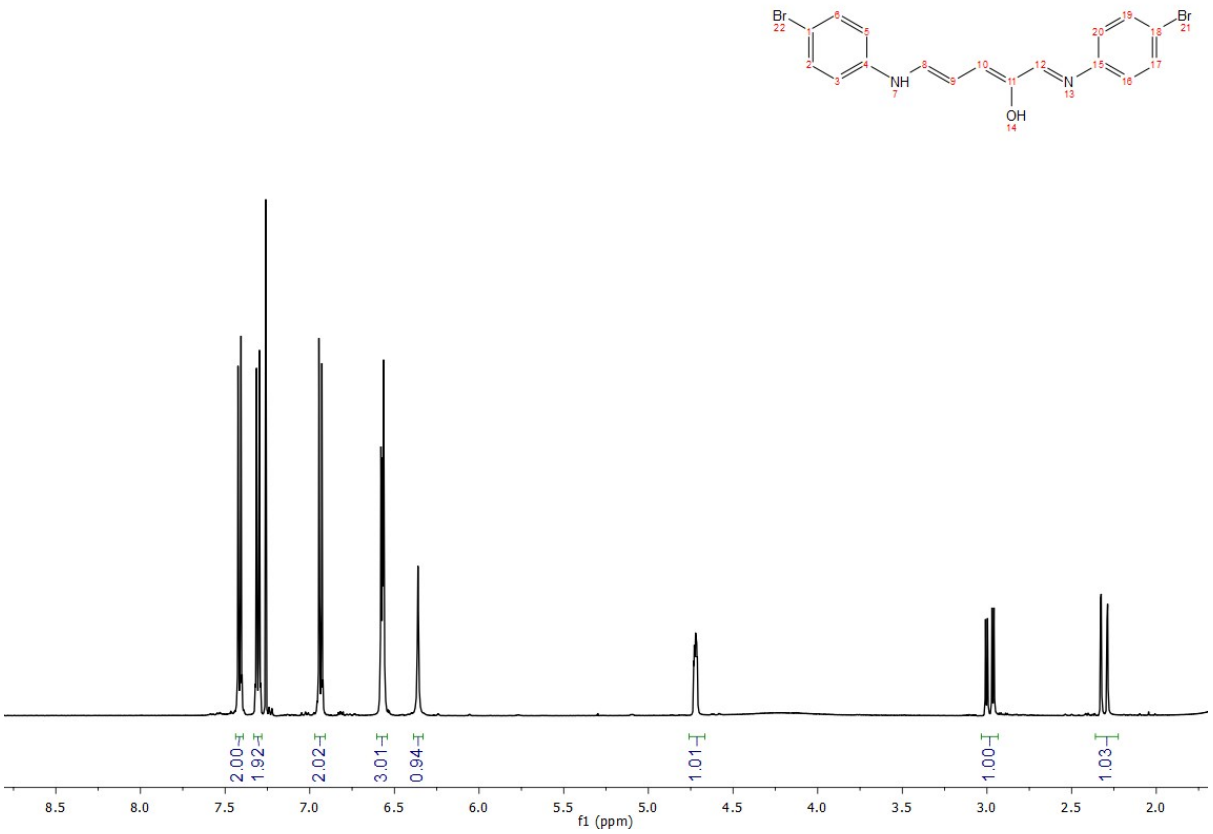


Compound 9b: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 2H), 7.26 – 7.20 (m, 2H), 7.09 – 7.05 (m, 2H), 7.02 – 6.97 (m, 1H), 6.82 – 6.77 (m, 1H), 6.72 – 6.67 (m, 2H), 6.65 (d, *J* = 3.1 Hz, 1H), 6.37 (s, 1H), 4.78 (ddd, *J* = 5.9, 3.1, 1.8 Hz, 1H), 4.01 (s, 1H), 3.00 (dd, *J* = 19.1, 5.8 Hz, 1H), 2.33 (dd, *J* = 19.1, 1.7 Hz, 1H).

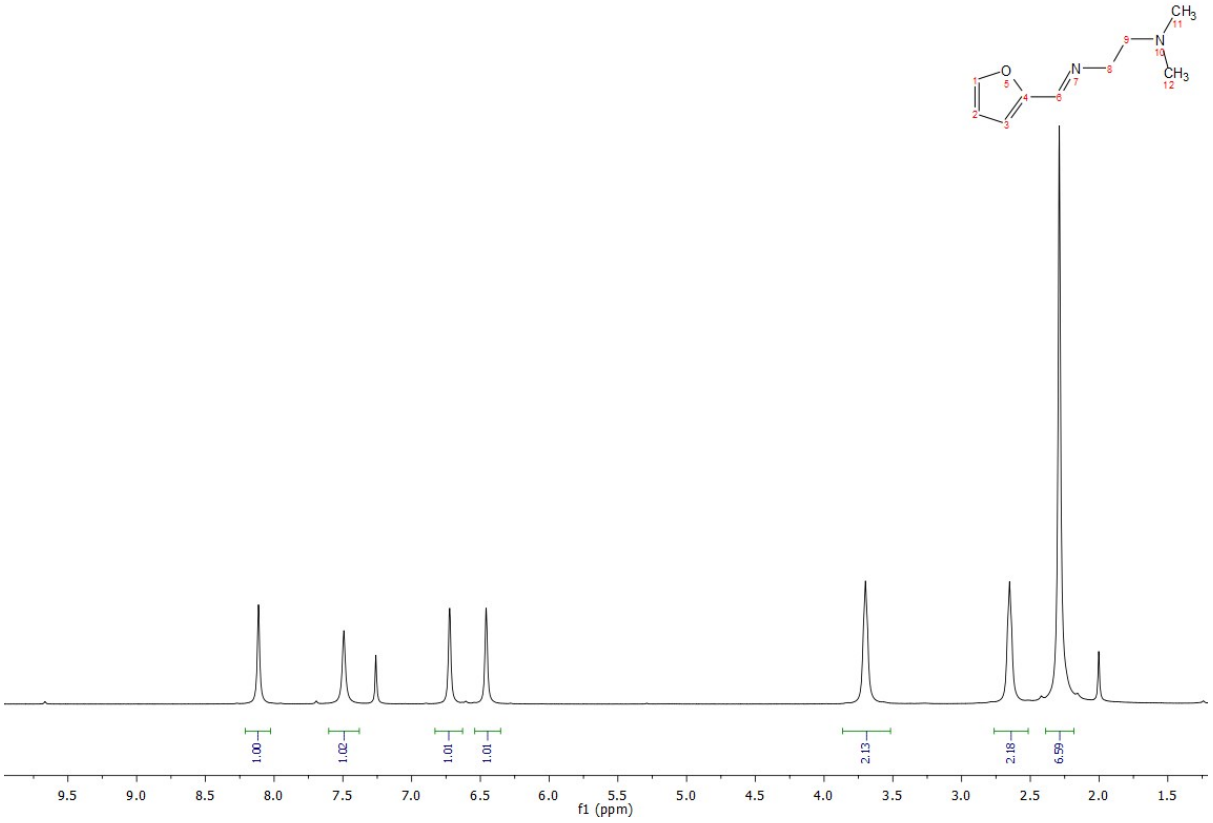




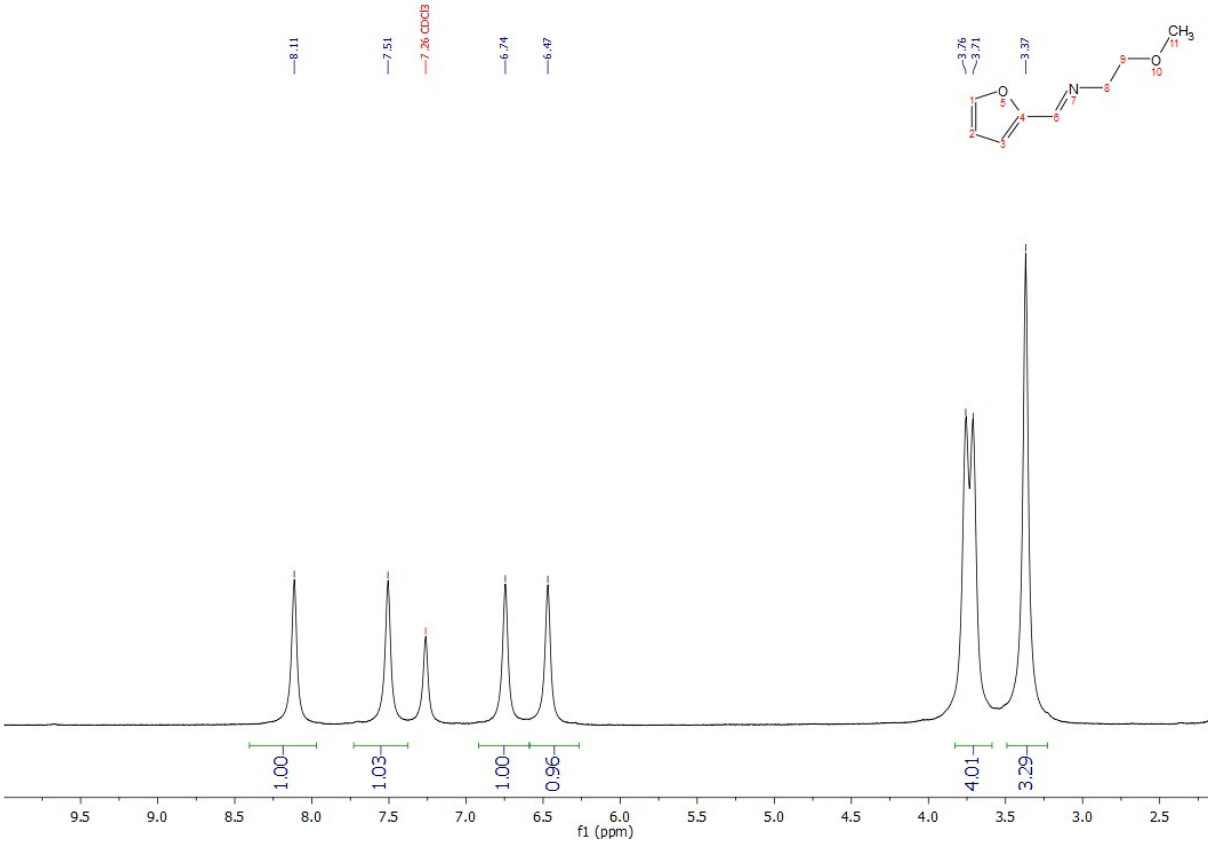
Compound 10: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 2H), 7.33 – 7.29 (m, 2H), 6.97 – 6.91 (m, 2H), 6.60 – 6.53 (m, 3H), 6.36 (s, 1H), 4.72 (ddd, *J* = 5.9, 3.2, 1.7 Hz, 1H), 2.98 (dd, *J* = 19.1, 5.9 Hz, 1H), 2.31 (dd, *J* = 19.1, 1.7 Hz, 1H).



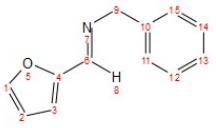
Compound 11: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.49 (s, 1H), 6.72 (s, 1H), 6.46 (s, 1H), 3.70 (t, *J* = 7.1 Hz, 2H), 2.65 (*J* = 7.1 Hz, 2H), 2.29 (s, 6H).

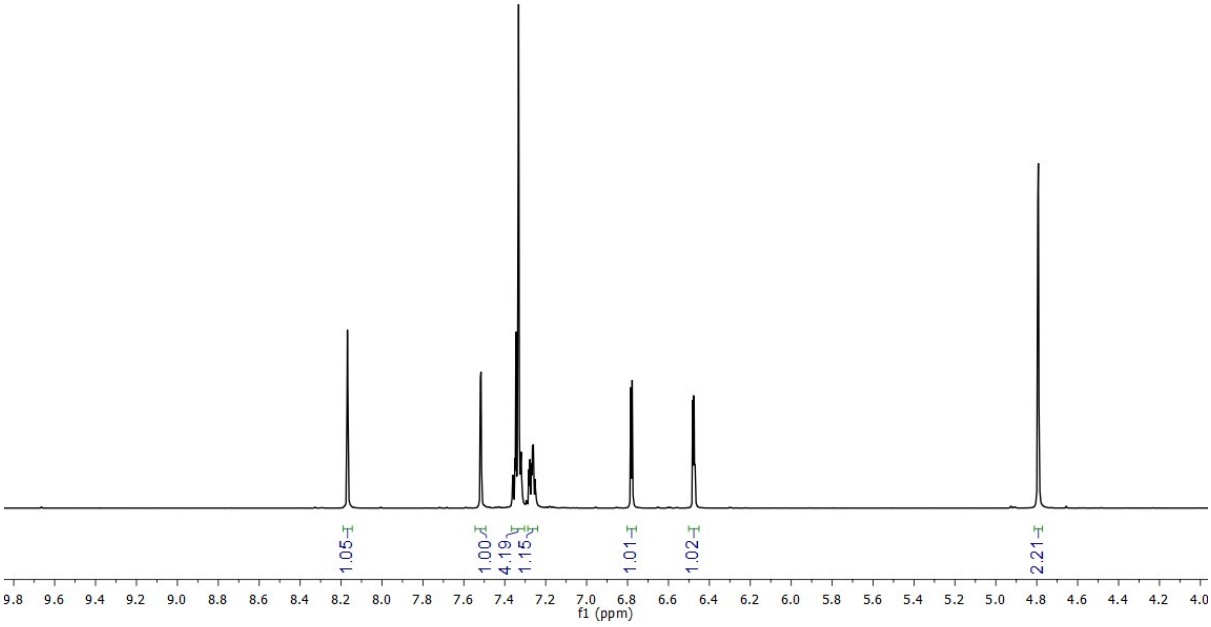


Compound 12: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.51 (s, 1H), 6.74 (s, 1H), 6.47 (s, 1H), 3.76-3.71 (m, 4H), 3.37 (s, 3H).

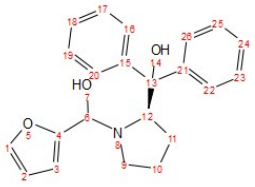


Compound 13: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (t, *J* = 1.5 Hz, 1H), 7.37-7.31 (m, 4H), 7.27 (ddd, *J* = 6.3, 4.8, 2.6 Hz, 1H), 6.78 (d, *J* = 3.4 Hz, 1H), 6.48 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.79 (d, *J* = 1.4 Hz, 2H).





Compound 14: ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.52 (d, J = 1.6 Hz, 1H), 7.44 (t, J = 6.8 Hz, 4H), 7.29 (t, J = 7.6 Hz, 2H), 7.20 (dt, J = 18.0, 7.4 Hz, 3H), 6.26 – 6.21 (m, 1H), 6.08 (d, J = 3.2 Hz, 1H), 5.71 (s, 1H), 4.42 (t, J = 6.6 Hz, 1H), 3.08 – 2.93 (m, 1H), 2.83 (dt, J = 10.7, 7.4 Hz, 1H), 1.94 – 1.82 (m, 1H), 1.70 – 1.58 (m, 1H), 1.58 – 1.45 (m, 2H).



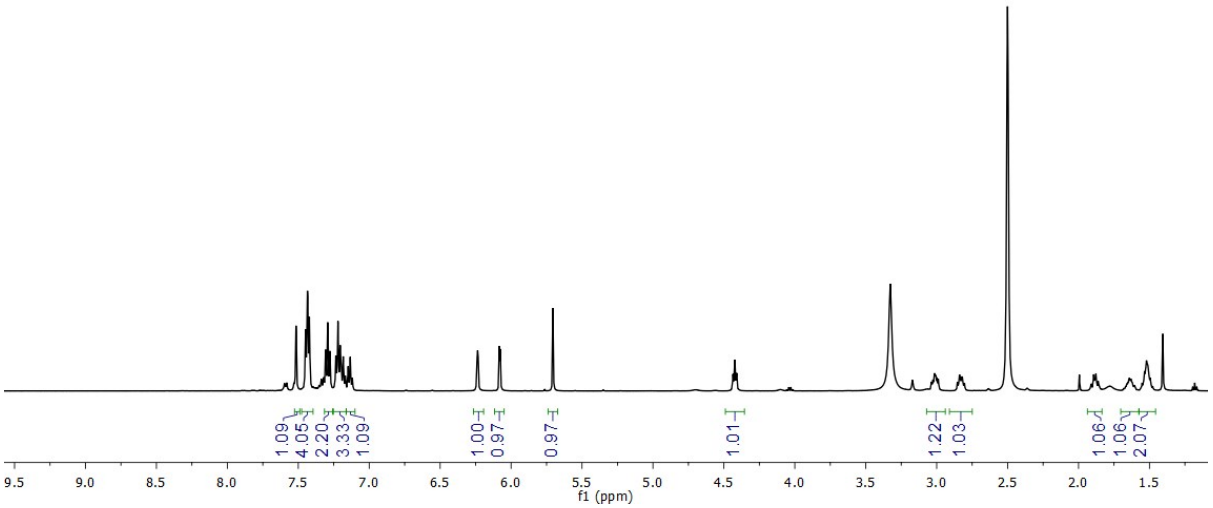


Table S1. Crystal data and structure refinement for **$SmLH_6$** and **$YbLH_6$**

Compound	**$SmLH_6$** (CCDC = 1956883)	**$YbLH_6$** (CCDC = 1939447)
Empirical formula	$C_{40}H_{43}Br_2N_{16}O_{11}Sm$	$C_{38}H_{47}Br_2N_{14}O_{14}Yb$
Formula weight	1234.07	1256.75
Temperature/K	150.15	150.15
Crystal system	hexagonal	triclinic
Space group	$P6_122$	P-1
a [Å]	13.00110(10)	10.3185(3)
b [Å]	13.00110(10)	16.0985(5)
c [Å]	46.6991(4)	16.1412(5)
α [°]	90	118.099(2)
β [°]	90	96.000(2)
γ [°]	120	92.008(2)
Volume [Å^3]	6831.56(12)	2341.39(13)
Z	6	2
ρ_{calc}g [cm^3]	1.800	1.783
μ [mm^{-1}]	8.544	6.383
F(000)	3690.0	1250.0
Crystal size [mm^3]	0.2 × 0.17 × 0.15	0.28 × 0.18 × 0.04
Radiation	GaKα (λ = 1.34143)	CuKα (λ = 1.54186)
2Θ range for data collection [°]	6.83 to 138.826	10.98 to 145.732
Index ranges	-17 ≤ h ≤ 13, -16 ≤ k ≤ 17, -46 ≤ l ≤ 63	-7 ≤ h ≤ 12, -17 ≤ k ≤ 19, -19 ≤ l ≤ 19
Reflections collected	90987	20575
Independent reflections	5066 [R_{int} = 0.0328, R_{sigma} = 0.0097]	8960 [R_{int} = 0.0486, R_{sigma} = 0.0438]
Data/restraints/parameters	6066/0/320	8960/4/632
Goodness-of-fit on F^2	1.068	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0235, wR_2 = 0.0649	R_1 = 0.0601, wR_2 = 0.1546
Final R indexes [all data]	R_1 = 0.0242, wR_2 = 0.0655	R_1 = 0.0639, wR_2 = 0.1604
Largest diff. peak/hole [e Å^{-3}]	0.49/-0.51	2.68/-2.94
Flack parameter	0.023(3)	-

Table S2. Crystal data and structure refinement for **$ErLH_6$** and **YLH_6**

Compound	**$ErLH_6$** (CCDC = 1956884)	**YLH_6** (CCDC = 1956885)
Empirical formula	$C_{34}H_{36}Br_2ErN_{13}O_{12}$	$C_{40}H_{43}Br_2N_{16}O_{11}Y$
Formula weight	1145.84	1172.63
Temperature/K	180	150.15
Crystal system	monoclinic	hexagonal
Space group	$P2_1/c$	$P6_122$
a [Å]	12.4509(3)	12.93430(10)
b [Å]	18.1610(4)	12.93430(10)
c [Å]	21.2663(6)	46.4828(6)
α [°]	90	90
β [°]	93.752(2)	90
γ [°]	90	120
Volume [Å^3]	4798.4(2)	6734.55(14)
Z	4	6
ρ_{calc}g [cm^3]	1.586	1.735
μ [mm^{-1}]	7.403	3.114
F(000)	2260.0	3522.0
Crystal size [mm^3]	0.2 × 0.04 × 0.03	0.25 × 0.24 × 0.23
Radiation	GaKα (λ = 1.34143)	GaKα (λ = 1.34143)
2Θ range for data collection [°]	5.572 to 124.992	6.866 to 124.968
Index ranges	-13 ≤ h ≤ 16, -8 ≤ k ≤ 23, -27 ≤ 1 ≤ 27	-17 ≤ h ≤ 8, -16 ≤ k ≤ 17, -59 ≤ l ≤ 61
Reflections collected	29620	69788
Independent reflections	11293 [R_{int} = 0.0258, R_{sigma} = 0.0321]	5433 [R_{int} = 0.0175, R_{sigma} = 0.0064]
Data/restraints/parameters	11293/5/555	5433/2/302
Goodness-of-fit on F^2	1.065	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0534, wR_2 = 0.1596	R_1 = 0.0266, wR_2 = 0.0758
Final R indexes [all data]	R_1 = 0.0636, wR_2 = 0.1651	R_1 = 0.0268, wR_2 = 0.0760
Largest diff. peak/hole [e Å^{-3}]	1.81/-1.06	0.77/-0.63
Flack parameter	-	-0.013(3)

SHAPE analysis

Sm(III)LH_6

Ideal structures ML10

JSPC-10 10 C2v Sphenocorona J87

SDD-10 11 D2 Staggered Dodecahedron (2:6:2)

TD-10 12 C2v Tetradecahedron (2:6:2)

HD-10 13 D4h Hexadecahedron (2:6:2) or (1:4:4:1)

Structure 1 [Sm]

Sm	7.4135	4.2802	3.8891
O	9.6182	4.3641	3.1292
O	8.5885	6.1476	4.6490
O	6.7060	4.6546	6.3412
O	7.3840	3.4802	1.4369
O	7.4633	5.6308	1.6866
O	8.6080	3.6480	6.0916
N	8.6353	1.8263	3.6234
N	5.8993	6.5653	4.1548
N	5.0587	4.2920	2.9414
N	6.2464	2.2350	4.8368

JSPC-10 Ideal structure CShM = 2.00118

Sm	M	7.4201	4.2840	3.8891
O	L3	9.5589	4.2363	3.0271
O	L8	8.4482	6.1601	4.7510
O	L9	6.5614	4.9802	6.4698
O	L2	7.5937	3.1922	1.3084
O	L7	7.4560	5.8761	2.1354
O	L4	8.8169	3.5190	5.6427

N	L1	8.4556	1.6993	3.5298
N	L10	5.6994	6.4732	4.2484
N	L6	5.3746	4.0983	2.7784
N	L5	6.2365	2.6054	4.9998

SDD-10 Ideal structure CShM = 5.20977

Sm	M	7.4201	4.2840	3.8891
O	L9	9.9058	4.2981	3.6883
O	L10	8.6751	6.4296	4.0898
O	L6	6.9787	5.0486	6.2214
O	L1	7.8615	3.5194	1.5568
O	L3	6.6309	5.6509	1.9583
O	L4	8.2093	2.9171	5.8199
N	L2	8.6507	2.1525	3.4876
N	L5	6.1895	6.4155	4.2906
N	L7	5.1552	3.8876	2.9237
N	L8	5.9444	2.5207	4.8545

TD-10 Ideal structure CShM = 4.05758

Sm	M	7.4201	4.2840	3.8891
O	L9	9.8012	4.5053	3.1302
O	L10	8.8023	6.2355	4.6480
O	L5	6.9345	5.1251	6.2024
O	L2	7.9057	3.4429	1.5758
O	L4	6.6612	5.5985	1.8913
O	L3	8.1790	2.9696	5.8869
N	L1	8.6646	2.1285	3.5736
N	L6	6.1756	6.4395	4.2046
N	L8	5.1590	3.8548	2.8902
N	L7	5.9179	2.5404	4.8880

HD-10 Ideal structure CShM = 8.27439

Sm	M	7.4201	4.2840	3.8891
O	L1	9.8713	4.2873	3.7916
O	L2	8.6486	6.4052	3.9866
O	L8	6.8932	5.1966	6.1044
O	L9	7.9470	3.3714	1.6738
O	L10	6.7243	5.4892	1.8689
O	L7	8.1159	3.0788	5.9093
N	L3	8.6428	2.1662	3.6940
N	L4	6.1974	6.4018	4.0841
N	L6	4.9689	4.2807	3.9866
N	L5	6.1916	2.1629	3.7916

Yb(III)LH_6

Ideal structures ML8

OP-8 1 D8h Octagon

HPY-8 2 C7v Heptagonal pyramid

HBPY-8 3 D6h Hexagonal bipyramid

CU-8 4 Oh Cube

SAPR-8 5 D4d Square antiprism

TDD-8 6 D2d Triangular dodecahedron

JGBF-8 7 D2d Johnson gyrobifastigium J26

JETBPY-8 8 D3h Johnson elongated triangular bipyramid J14

JBTPR-8 9 C2v Biaugmented trigonal prism J50

Structure 1 [Yb]

O		8.3225	8.3636	6.8094
O		5.7011	7.7792	7.0350
O		6.1529	10.3982	8.0181
O		4.9800	9.1604	9.3481
N		7.3920	9.1458	10.8135
N		8.8911	10.1756	8.8361
N		6.2664	6.1125	9.1689
N		8.8080	6.8426	9.5483
N		5.0351	10.2110	8.6259

OP-8 Ideal structure CShM = 33.58977

O	M	6.8388	8.6876	8.6893
O	L1	5.4983	7.2349	8.1240
O	L4	6.8661	10.7426	8.6309
O	L2	4.9703	8.6881	7.8316
N	L6	8.7073	8.6872	9.5469
N	L5	8.1793	10.1404	9.2545
N	L8	6.8115	6.6327	8.7476
N	L7	8.1408	7.2343	9.3370
N	L3	5.5368	10.1410	8.0416

HPY-8 Ideal structure CShM = 28.00755

O	M	7.0007	8.6622	8.5146
O	L2	5.5432	7.6213	7.3150
O	L4	6.7092	10.7206	7.9447
O	L1	5.5435	8.8911	10.0865
N	L6	8.5880	8.7871	9.9678
N	L5	8.0398	10.4130	9.2229
N	L8	6.5859	6.5483	8.4378
N	L7	7.9409	7.0671	9.6184

N	L3	5.5981	9.4782	7.0956

HBPY-8 Ideal structure CShM = 22.78965

O	M	6.8388	8.6876	8.6893
O	L1	6.4371	8.0036	6.6192
O	L2	7.1552	10.7519	7.9457
O	L4	4.8126	8.0281	9.3005
N	L8	7.2405	9.3717	10.7593
N	L7	8.8651	9.3472	8.0780
N	L5	6.5224	6.6234	9.4329
N	L6	8.5487	7.2830	8.8216
N	L3	5.1289	10.0923	8.5569

CU-8 Ideal structure CShM = 28.82803

O	M	6.8388	8.6876	8.6893
O	L1	6.4629	8.0413	6.6966
O	L3	7.2520	10.7755	8.6918
O	L6	5.1280	8.3015	9.8950
N	L7	7.2147	9.3340	10.6820
N	L4	8.5497	9.0738	7.4835
N	L5	6.4256	6.5998	8.6867
N	L8	8.5124	7.6322	9.4736
N	L2	5.1652	9.7430	7.9049

SAPR-8 Ideal structure CShM = 26.71759

O	M	6.8388	8.6876	8.6893
O	L1	6.5394	7.4284	6.9604
O	L2	6.4621	10.0507	7.0570
O	L6	4.7002	8.6355	8.3929

N	L8	7.6018	8.6357	10.7090
N	L3	8.5139	10.0509	8.6947
N	L5	6.2057	6.7814	9.4827
N	L4	8.5912	7.4286	8.5981
N	L7	6.0963	10.4899	9.6193

TDD-8 Ideal structure CShM = 27.15569

O	M	6.8388	8.6876	8.6893
O	L1	6.2528	7.4335	7.0399
O	L5	6.8828	9.9358	6.9352
O	L2	4.6991	8.4832	8.8156
N	L7	7.2153	8.8454	10.8034
N	L8	8.5540	9.9716	8.9037
N	L3	6.4658	6.7352	9.5172
N	L4	8.5581	7.4861	8.2028
N	L6	6.0825	10.6102	9.2962

JGBF-8 Ideal structure CShM = 23.76598

O	M	6.8388	8.6876	8.6893
O	L3	6.4237	8.1039	7.0395
O	L1	6.6111	10.6402	7.0752
O	L6	5.2244	8.1609	9.2818
N	L5	7.2539	9.2714	10.3390
N	L4	8.4532	9.2144	8.0967
N	L7	6.6514	6.1513	8.6535
N	L8	8.6808	7.2618	9.7107
N	L2	5.4119	10.6973	9.3176

JETBPY-8 Ideal structure CShM = 27.67001

O	M	6.8388	8.6876	8.6893
O	L1	5.5454	8.1904	7.6105
O	L3	6.7428	10.1501	7.7218
O	L5	5.5020	9.4567	9.5292
N	L6	7.3195	8.3006	10.3333
N	L4	8.5603	8.9939	8.5260
N	L2	7.3629	7.0342	8.4147
N	L8	9.2315	7.1656	9.7480
N	L7	4.4461	10.2097	7.6305

JBTPR-8 Ideal structure CShM = 22.49907

O	M	7.0246	8.6978	8.4541
O	L3	6.4960	7.3438	6.9805
O	L5	6.3974	10.0518	7.0196
O	L1	4.9927	8.6183	8.8407
N	L2	7.1177	8.6713	10.5217
N	L6	8.5225	10.1048	8.7006
N	L7	6.2736	6.3168	9.4786
N	L4	8.6211	7.3968	8.6615
N	L8	6.1036	10.9874	9.5460

Y(III)LH_6

Ideal structures ML10

DP-10 1 D10h Decagon

EPY-10 2 C9v Enneagonal pyramid

OBPY-10 3 D8h Octagonal bipyramid

PPR-10 4 D5h Pentagonal prism

PAPR-10 5 D5d Pentagonal antiprism

JBCCU-10 6 D4h Bicapped cube J15

JBCSAPR-10 7 D4d Bicapped square antiprism J17

JMBIC-10 8 C2v Metabidiminished icosahedron J62

JATDI-10 9 C3v Augmented tridiminished icosahedron J64

Structure 1 [Y]

O	1.0104	10.4625	10.8672
O	-1.0104	10.4625	12.3742
O	-0.6868	8.1210	13.9895
O	0.6868	8.1210	9.2519
O	1.1408	9.2457	13.7417
O	-1.1408	9.2457	9.4997
N	-2.7143	8.3843	11.8782
N	2.7143	8.3843	11.3632
N	1.1486	6.5484	12.5569
N	-1.1486	6.5484	10.6845
N	-0.2787	8.7382	8.7188

DP-10 Ideal structure CShM = 31.44118

O	M	-0.0253	8.5693	11.3569
O	L1	-1.5108	8.9577	12.9343
O	L2	-0.2944	8.8179	13.5275
O	L6	1.4601	8.1808	9.7795
O	L3	1.0247	8.5830	13.2915
O	L8	-1.0754	8.5555	9.4222
N	L10	-2.1597	8.9492	11.7386
N	L5	2.1090	8.1893	10.9752
N	L4	1.9427	8.3429	12.3166
N	L9	-1.9934	8.7956	10.3971
N	L7	0.2437	8.3206	9.1863

EPY-10 Ideal structure CShM = 20.93587

O	M	0.0610	8.7671	11.3625
O	L2	-1.7461	9.5171	12.7084
O	L3	-0.5432	8.9655	13.6505
O	L7	1.3440	8.2624	9.4290
O	L4	0.9423	8.3211	13.5221
O	L9	-1.4480	9.4735	9.6704
N	L10	-2.1034	9.7177	11.1365
N	L6	2.1741	7.8622	10.7667
N	L5	2.0155	7.8854	12.3831
N	L1	-0.8883	6.5912	11.3006
N	L8	-0.0865	8.8987	8.9960

OBPY-10 Ideal structure CShM = 22.57064

O	M	-0.0253	8.5693	11.3569
O	L2	-0.2391	10.8230	11.9463
O	L4	0.2783	8.0094	13.6079
O	L7	-0.0889	7.3715	9.3484
O	L3	0.0383	9.7670	13.3653
O	L9	-0.3912	10.5588	10.1820
N	L1	-2.3350	8.2871	11.5983
N	L10	2.2843	8.8514	11.1155
N	L5	0.3405	6.5797	12.5318
N	L6	0.1884	6.3155	10.7675
N	L8	-0.3290	9.1291	9.1059

PPR-10 Ideal structure CShM = 20.08621

O	M	-0.0253	8.5693	11.3569
O	L1	-0.5743	10.8627	11.6517
O	L7	-0.5181	8.0920	13.6323

O	L4	1.4127	8.3060	9.4832
O	L2	1.0704	9.8103	13.0619
O	L10	-1.9512	8.2146	10.0103
N	L6	-2.1628	9.1444	12.2221
N	L3	2.2985	8.2302	11.7217
N	L8	0.7100	6.5119	12.2921
N	L9	-0.1757	6.5876	10.0536
N	L5	-0.3628	9.9329	9.4399

PAPR-10 Ideal structure CShM = 19.21535

O	M	-0.0253	8.5693	11.3569
O	L1	-1.0469	10.3785	12.5370
O	L6	-0.6135	8.1615	13.6367
O	L9	0.9962	6.7600	10.1768
O	L5	1.3105	9.6530	13.0154
O	L2	-1.5090	9.9607	10.1030
N	L7	-2.3560	8.3517	11.8367
N	L4	2.3053	8.7868	10.8771
N	L10	1.4583	7.1778	12.6108
N	L8	-1.3612	7.4855	9.6984
N	L3	0.5628	8.9770	9.0771

JBCCU-10 Ideal structure CShM = 18.95343

O	M	-0.0253	8.5693	11.3569
O	L1	0.2860	10.5477	12.2559
O	L3	-0.9616	8.6266	13.3417
O	L8	0.9109	8.5119	9.3721
O	L9	1.4428	9.1029	13.9880
O	L2	-0.9303	10.1056	10.0762
N	L4	-2.1779	8.1846	11.1620

N	L7	2.1272	8.9539	11.5518
N	L5	0.8796	7.0329	12.6375
N	L6	-0.3367	6.5908	10.4578
N	L10	-1.4935	8.0357	8.7257

JBCSAPR-10 Ideal structure CShM = 19.69155

O	M	-0.0253	8.5693	11.3569
O	L1	-1.0515	10.4166	11.9587
O	L3	-0.8403	8.1487	13.3536
O	L6	0.8174	7.5637	9.5944
O	L2	1.3484	9.5586	12.7575
O	L7	-1.4269	9.0060	9.7221
N	L9	-2.9974	8.5909	11.8421
N	L10	2.9468	8.5476	10.8717
N	L4	1.2323	6.9576	12.1623
N	L5	-1.2157	6.7381	11.1169
N	L8	0.9336	10.1648	10.1897

JMBIC-10 Ideal structure CShM = 15.01810

O	M	0.1762	8.5960	11.2379
O	L10	-0.8803	10.4721	12.4344
O	L3	-0.9472	8.0550	13.3624
O	L7	1.2995	9.1368	9.1136
O	L8	1.2912	9.3563	13.2986
O	L4	-0.8752	10.3366	9.8479
N	L9	-2.2863	8.6610	11.2298
N	L5	2.6384	8.5309	11.2462
N	L6	1.2274	6.8555	12.6280
N	L2	-0.9835	6.4257	11.3495
N	L1	-0.9390	7.8358	9.1775

JATDI-10 Ideal structure CShM = 21.69634

O	M	0.0197	8.5597	11.5683
O	L7	-0.5376	10.5736	12.1959
O	L2	-0.8708	8.7526	13.5508
O	L5	0.9102	8.3669	9.5858
O	L3	1.2600	9.4797	13.1097
O	L9	-0.7537	9.8859	10.0181
N	L1	-1.2928	6.9393	12.2101
N	L4	2.1547	8.1159	11.4966
N	L8	0.7932	7.2336	13.1185
N	L6	-1.2205	7.6398	10.0268
N	L10	-0.7411	8.7148	8.0453

Er(III)LH_6

Ideal structures ML8

OP-8 1 D8h Octagon

HPY-8 2 C7v Heptagonal pyramid

HBPY-8 3 D6h Hexagonal bipyramid

CU-8 4 Oh Cube

SAPR-8 5 D4d Square antiprism

TDD-8 6 D2d Triangular dodecahedron

JGBF-8 7 D2d Johnson gyrobifastigium J26

JETBPY-8 8 D3h Johnson elongated triangular bipyramid J14

JBTPR-8 9 C2v Biaugmented trigonal prism J50

Structure 1 [Er]

Er	3.1015	6.0440	5.9832

O	3.7292	8.0262	5.3143
O	1.3616	7.4215	6.3876
O	1.5308	4.6189	7.0347
O	1.6238	5.7407	4.1554
N	3.8142	3.7611	5.4219
N	4.4297	5.8424	3.8028
N	2.8735	6.5561	8.5076
N	5.1564	5.9505	7.2452

OP-8 Ideal structure CShM = 33.58538

Er	M	3.0690	5.9957	5.9836
O	L1	4.1833	7.3443	6.8617
O	L3	1.5323	6.5703	7.0513
O	L4	1.1944	5.4484	6.1177
O	L5	1.9546	4.6471	5.1055
N	L6	3.3676	4.6358	4.6078
N	L7	4.6057	5.4211	4.9159
N	L2	2.7703	7.3556	7.3595
N	L8	4.9435	6.5430	5.8496

HPY-8 Ideal structure CShM = 22.84472

Er	M	2.9888	5.7751	6.0085
O	L1	3.7105	7.7608	5.7848
O	L2	1.0002	6.4654	5.7203
O	L3	1.5952	6.4457	7.4652
O	L8	1.9027	5.9653	4.1924
N	L6	4.8657	5.0198	5.3600
N	L7	3.6230	5.3219	4.0320
N	L4	3.2395	5.9210	8.1132
N	L5	4.6950	5.2864	7.1763

HBPY-8 Ideal structure CShM = 11.74275

Er	M	3.0690	5.9957	5.9836
O	L2	3.7275	7.8351	4.8547
O	L3	2.4044	8.0396	6.6711
O	L5	2.4105	4.1563	7.1126
O	L1	1.2411	5.8435	4.6694
N	L6	3.7335	3.9518	5.2962
N	L7	4.3920	5.7913	4.1672
N	L4	1.7459	6.2002	7.8001
N	L8	4.8969	6.1480	7.2979

CU-8 Ideal structure CShM = 7.05514

Er	M	3.0690	5.9957	5.9836
O	L1	4.3215	7.8310	5.3319
O	L2	1.7927	7.9161	6.1962
O	L7	1.8164	4.1604	6.6354
O	L3	1.1905	5.8267	4.6401
N	L8	4.3453	4.0753	5.7711
N	L4	3.7194	5.7416	3.7758
N	L6	2.4185	6.2498	8.1915
N	L5	4.9474	6.1647	7.3271

SAPR-8 Ideal structure CShM = 2.91230

Er	M	3.0690	5.9957	5.9836
O	L1	3.9314	8.1991	5.9377
O	L2	1.1727	7.4048	6.1232
O	L7	1.3961	4.6801	7.0189
O	L3	1.6508	5.3001	4.2213

N	L8	3.6849	3.7535	5.5429
N	L4	4.4095	6.0944	4.0358
N	L6	3.0088	6.7301	8.2327
N	L5	5.2976	5.8035	6.7566

TDD-8 Ideal structure CShM = 2.25784

Er	M	3.0690	5.9957	5.9836
O	L2	3.8334	8.1843	5.4695
O	L6	1.2500	7.4577	6.4227
O	L8	1.2831	4.6279	6.7444
O	L5	1.5750	5.7700	4.1518
N	L4	3.8851	3.7658	5.9717
N	L1	4.4207	5.7908	4.0420
N	L7	2.9824	6.2627	8.3416
N	L3	5.3221	6.1064	6.7254

JGBF-8 Ideal structure CShM = 12.14615

Er	M	3.0690	5.9957	5.9836
O	L3	3.5099	7.4964	5.0181
O	L1	1.3910	7.9226	6.4626
O	L5	2.6280	4.4950	6.9492
O	L4	1.5445	5.7954	4.9762
N	L8	3.2225	3.8685	4.4973
N	L7	5.1878	5.5695	4.5391
N	L2	2.4745	6.6222	8.4356
N	L6	4.5934	6.1960	6.9911

JETBPY-8 Ideal structure CShM = 23.44598

Er	M	3.0690	5.9957	5.9836

O	L1	4.4778	6.5199	5.1476
O	L4	1.6700	6.7581	6.6319
O	L6	2.7330	4.8673	7.2375
O	L3	2.3223	6.4418	4.4997
N	L5	3.3853	4.5510	5.1053
N	L7	3.9277	5.5794	3.1766
N	L8	2.2102	6.4120	8.7907
N	L2	3.8255	6.8361	7.2798

JBTPR-8 Ideal structure CShM = 2.94878

Er	M	3.1434	5.7960	6.2216
O	L1	3.5648	7.8661	5.5889
O	L7	0.8306	7.4904	6.4370
O	L4	1.3810	4.7084	6.9792
O	L2	1.9450	5.8098	4.3705
N	L6	3.6745	3.7855	5.4876
N	L8	4.7862	5.8987	3.8643
N	L3	3.0009	6.7646	8.1976
N	L5	5.2943	5.8418	6.7060