Supporting Information

Potential precursors for terminal ytterbium(II) imide complexes bearing the tris(3-tert-butyl-5-methylpyrazolyl)hydroborato ligand

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NMR Spectra

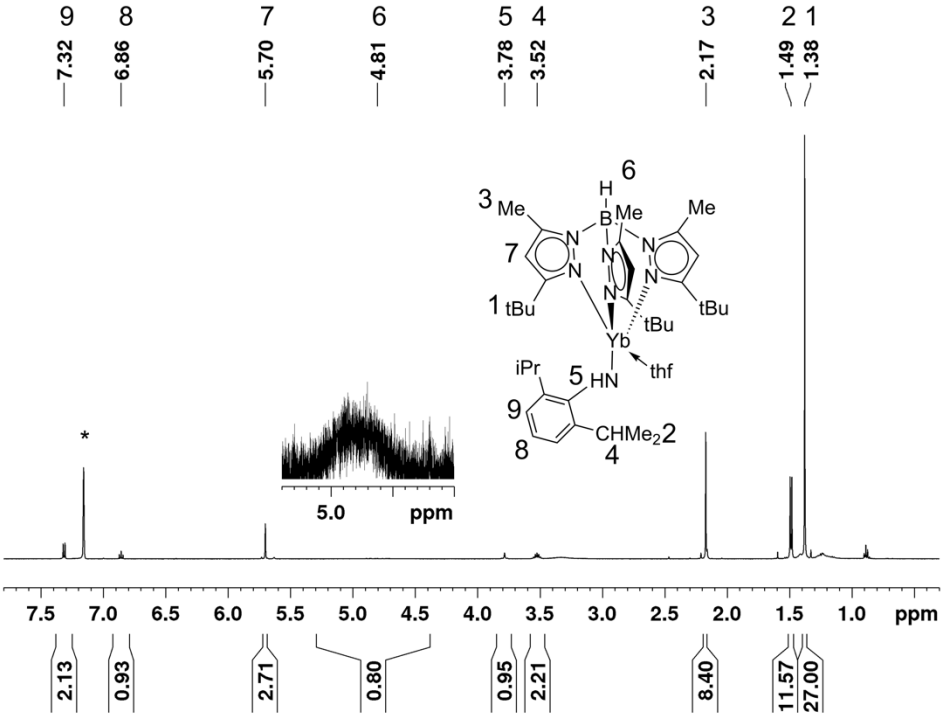

Figure S1 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(thf)$ (**1^{thf}**). Residual solvent signals are marked with *. Minor impurities are marked with #.

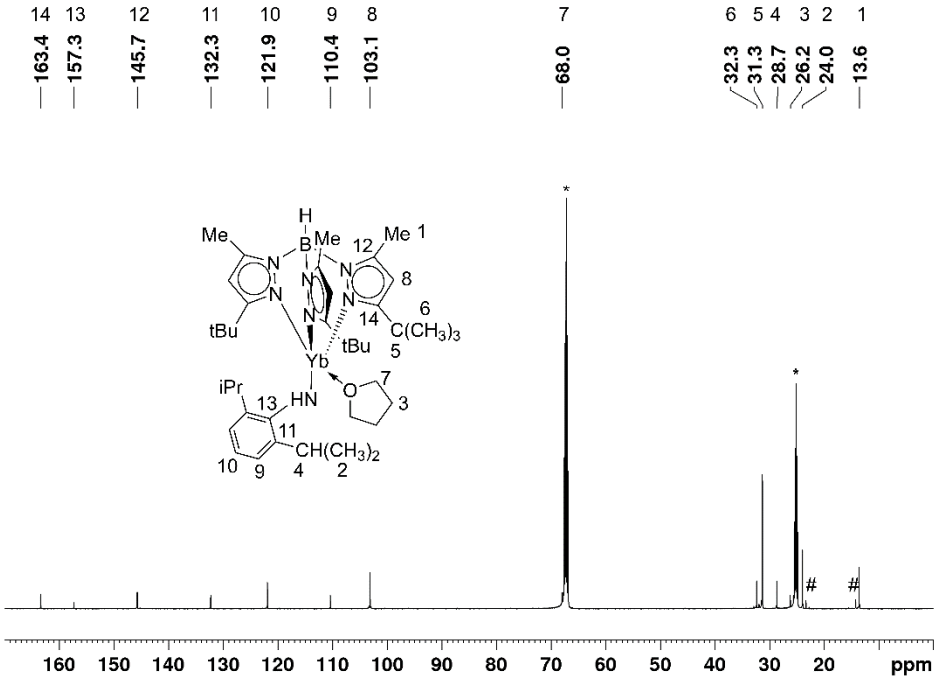

Figure S2 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, [d8]thf, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(thf)$ (**1^{thf}**). Residual solvent signals are marked with * impurities are marked with #.

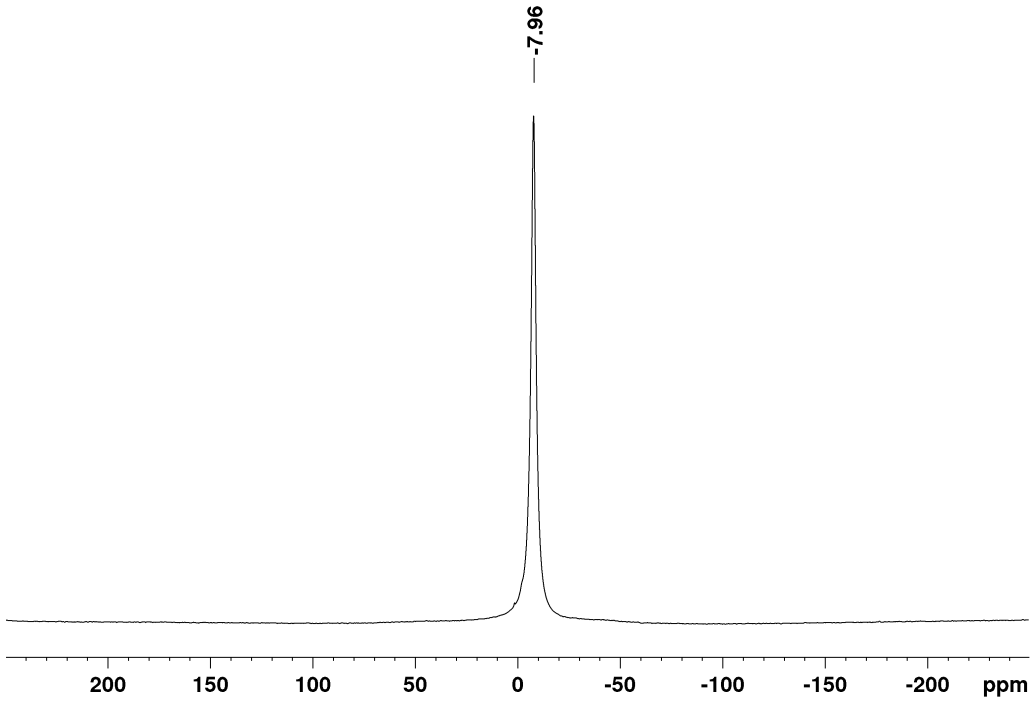

Figure S3 ^{11}B NMR spectrum (160 MHz) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(thf)$ (**1^{thf}**) in C_6D_6 at 26 °C.

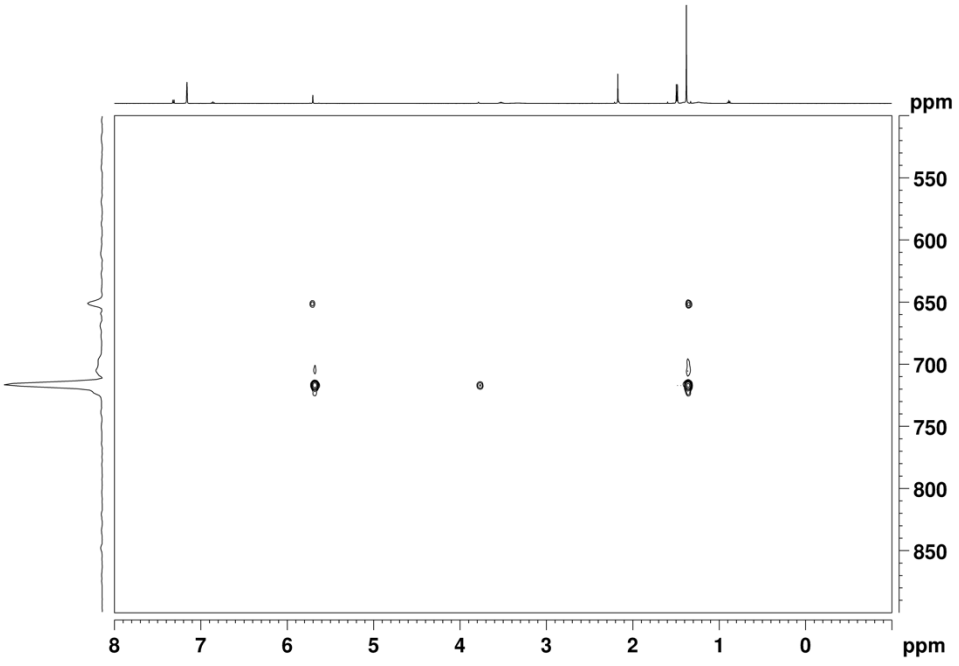

Figure S4 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(thf)$ (**1^{thf}**).

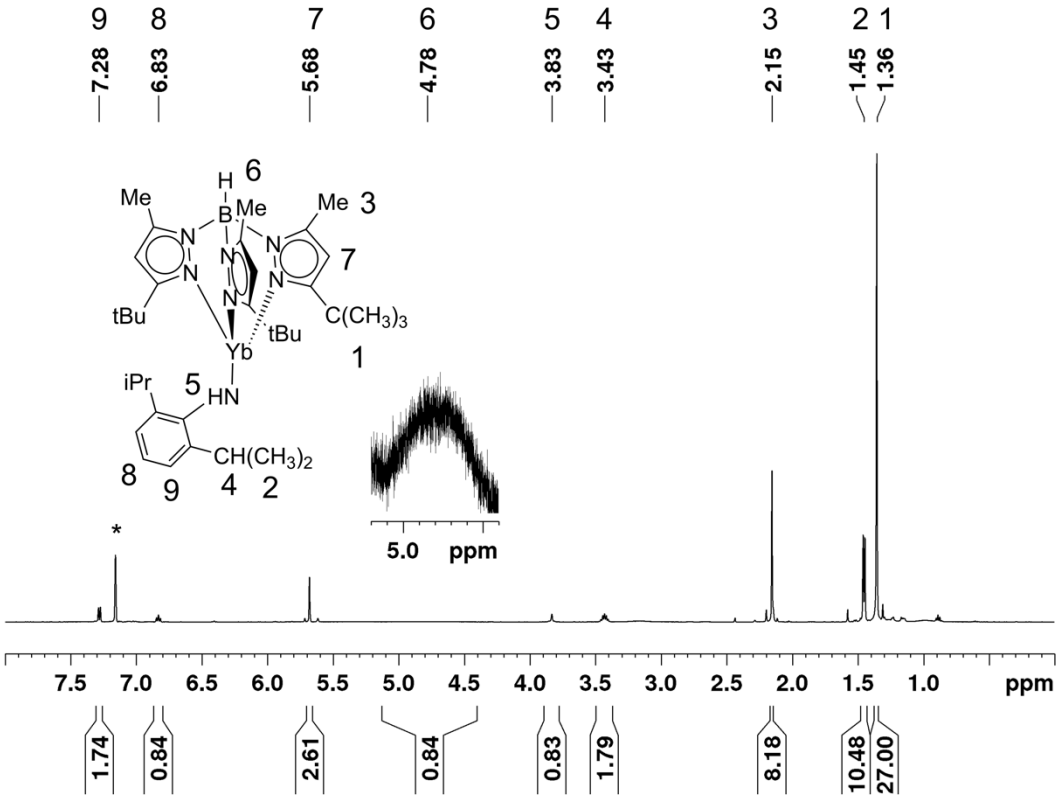

Figure S5 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})$ (**1**). Residual solvent signals are marked with *.

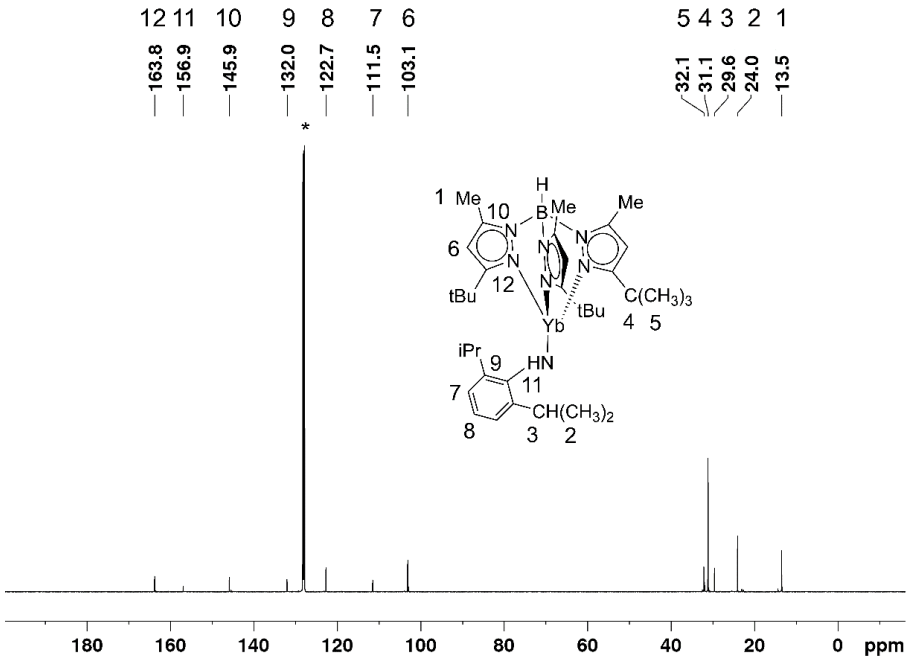

Figure S6 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})$ (**1**). Residual solvent signals are marked with *.

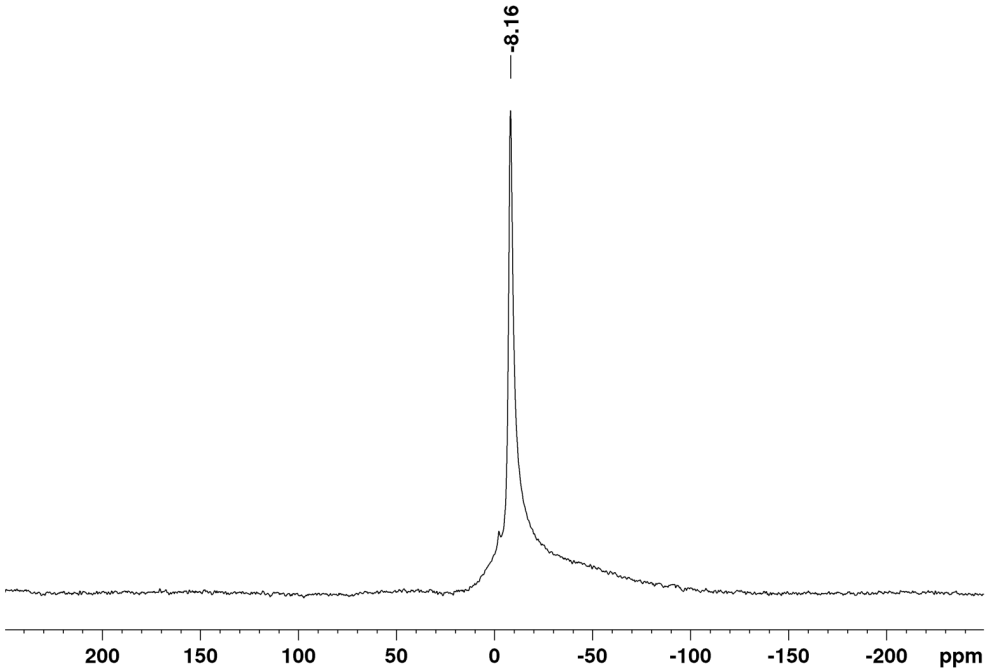

Figure S7 ^{11}B NMR spectrum (160 MHz) of a micro-scale reaction) of Tp^{tBu,Me}Yb(NHAr^{iPr}) (**1**) in C_6D_6 at 26 °C.

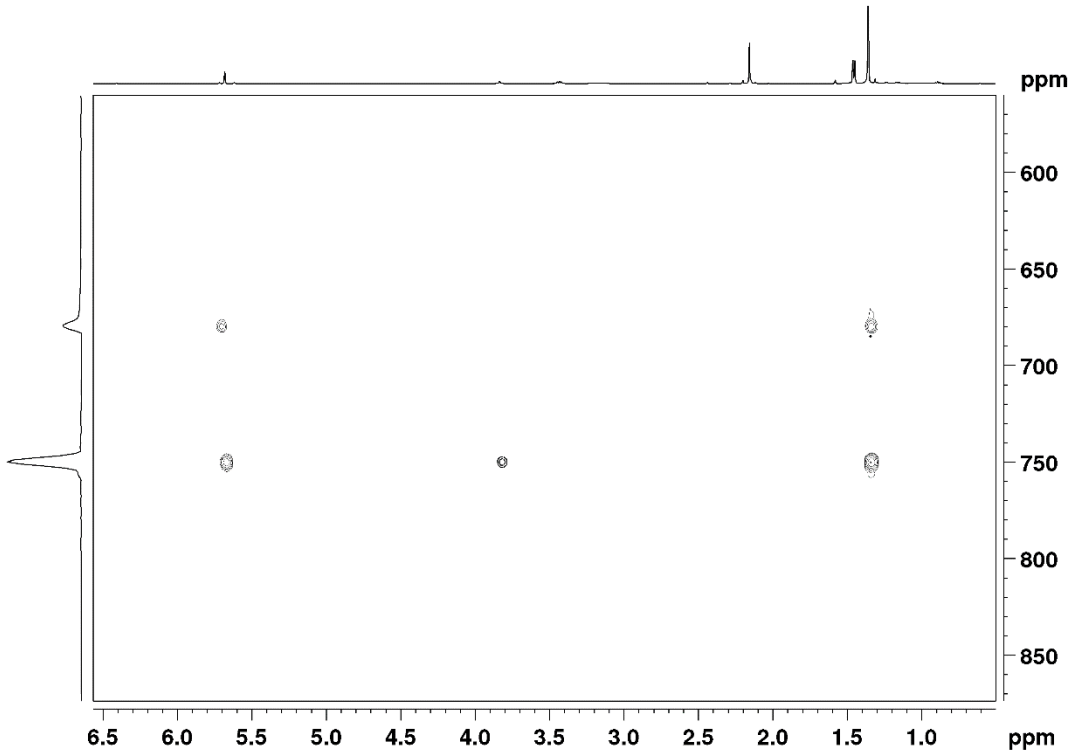

Figure S8 ^{1}H–^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz) of Tp^{tBu,Me}Yb(NHAr^{iPr}) (**1**) in C_6D_6 at 26 °C. Main product Tp^{tBu,Me}Yb(NHAr^{iPr}): signal at 750 ppm.

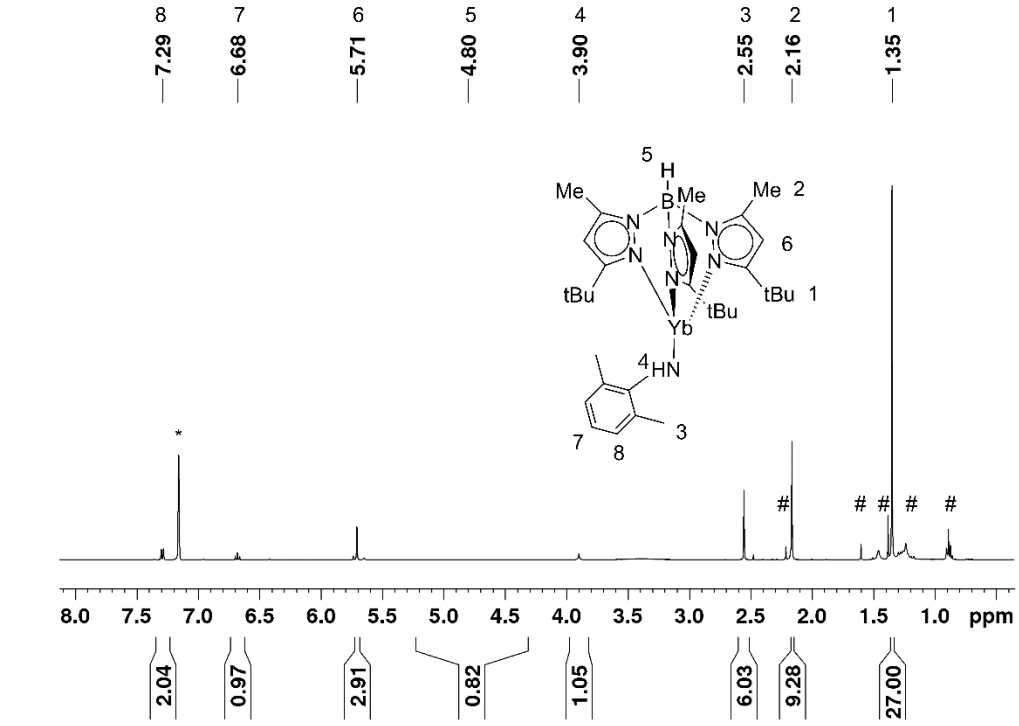

Figure S9 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{Me})$ (**2**). Residual solvent signals are marked with *. Impurities are marked with #.

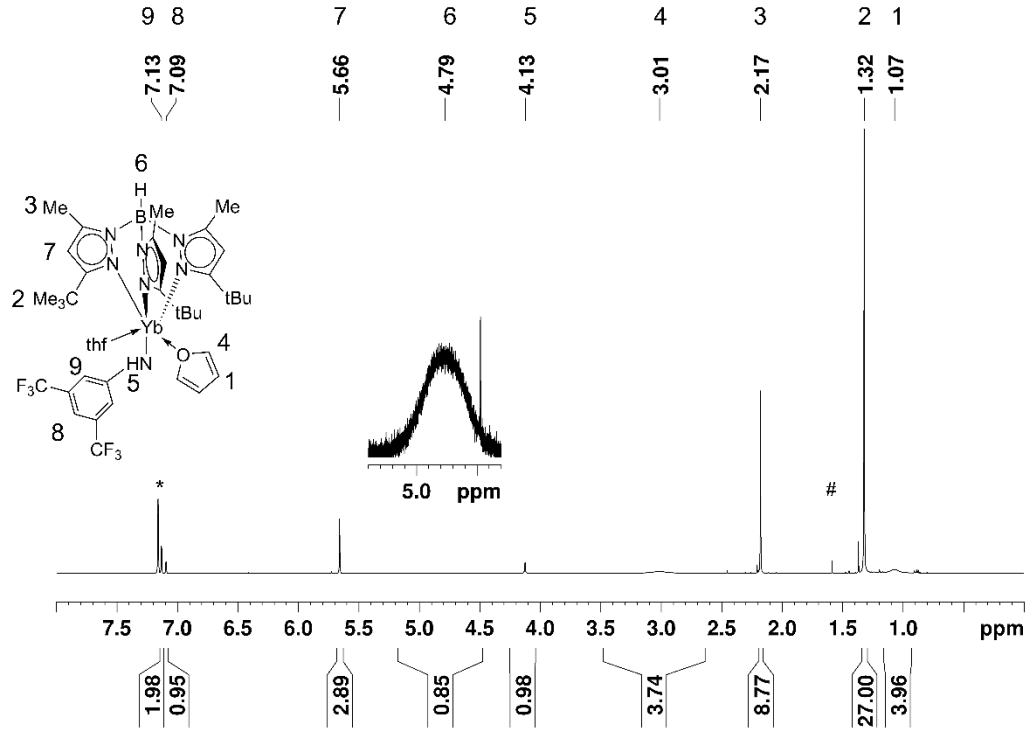

Figure S10 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ (**3^{thf}**). Residual solvent signals are marked with *. Minor impurities are marked with #.

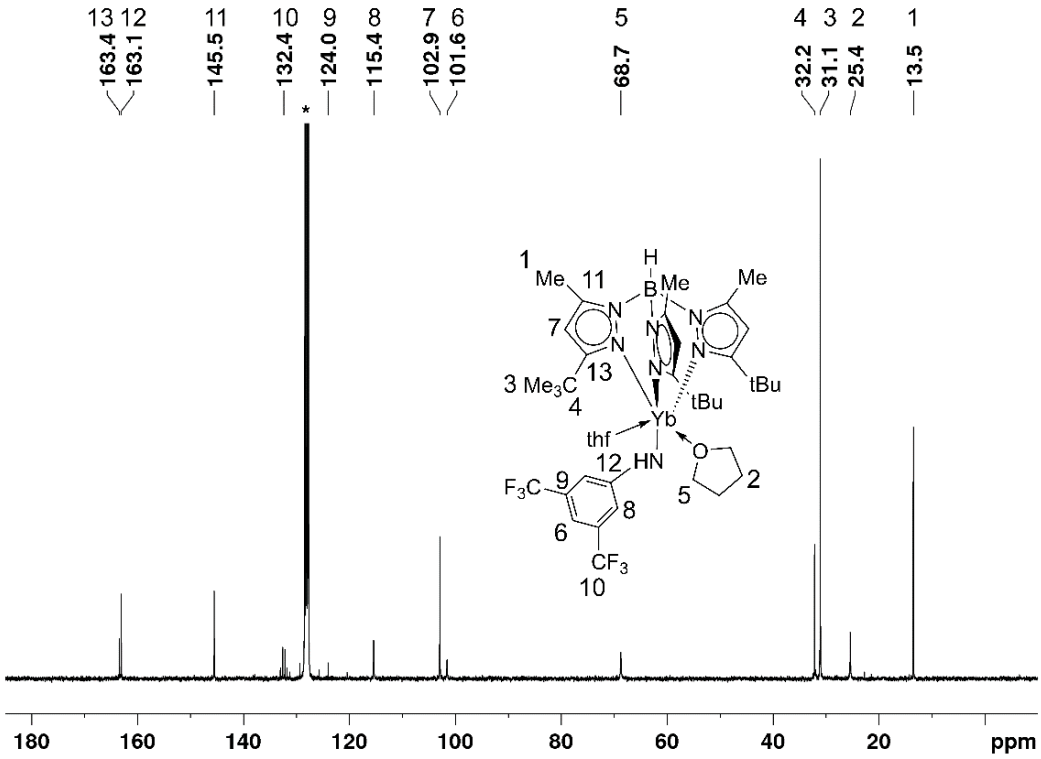

Figure S11 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ (**3^{thf}**). Residual solvent signals are marked with *.

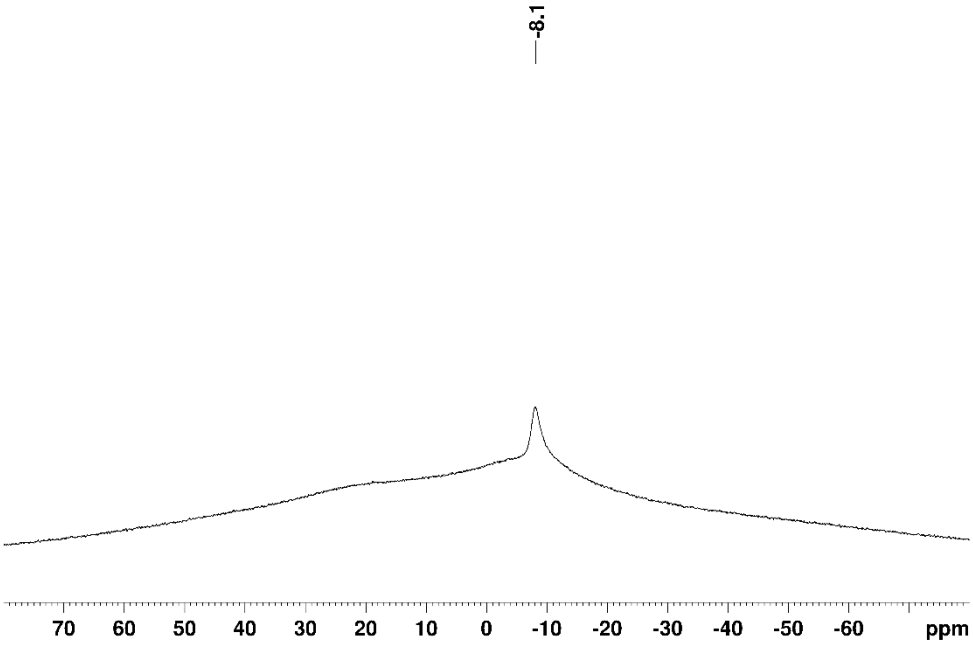

Figure S12 ^{11}B NMR spectrum (160 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ (**3^{thf}**).

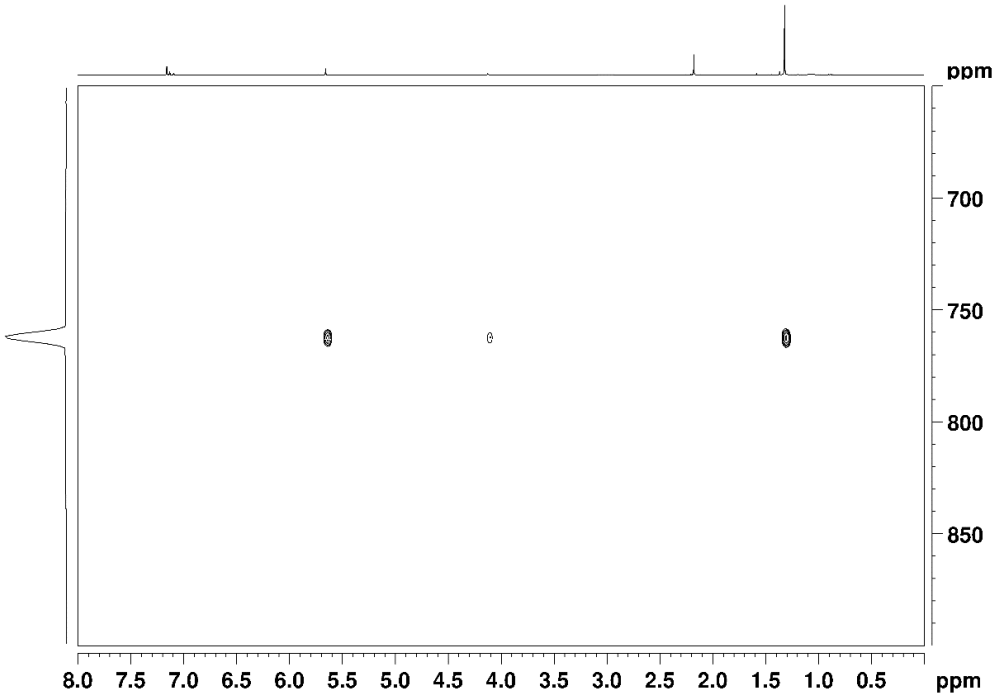

Figure S13 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ (**3**^{thf}).

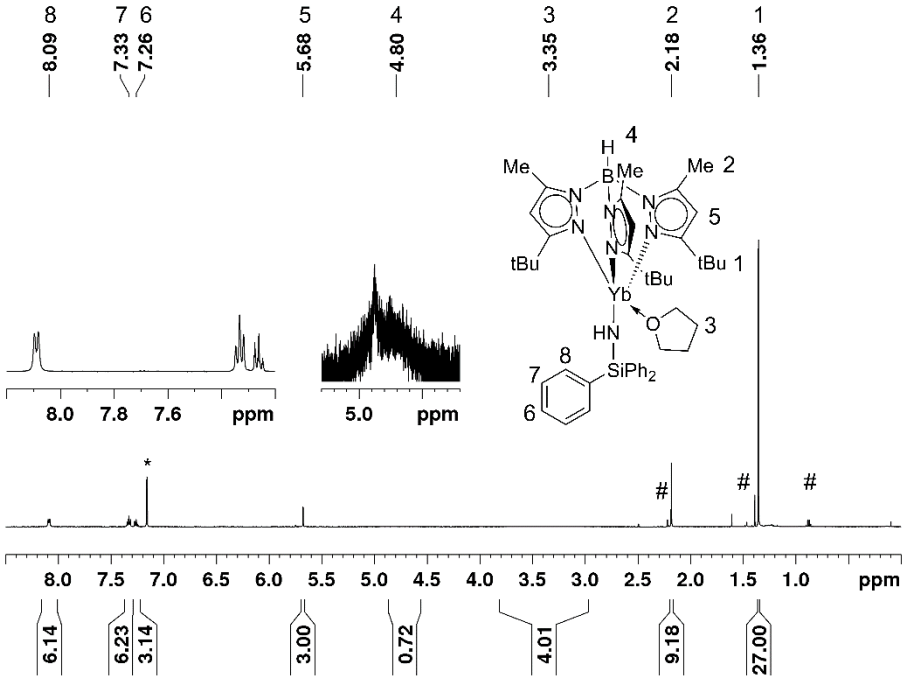

Figure S14 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ (**4**^{thf}). Residual solvent signals are marked with *, # marks minor impurities.

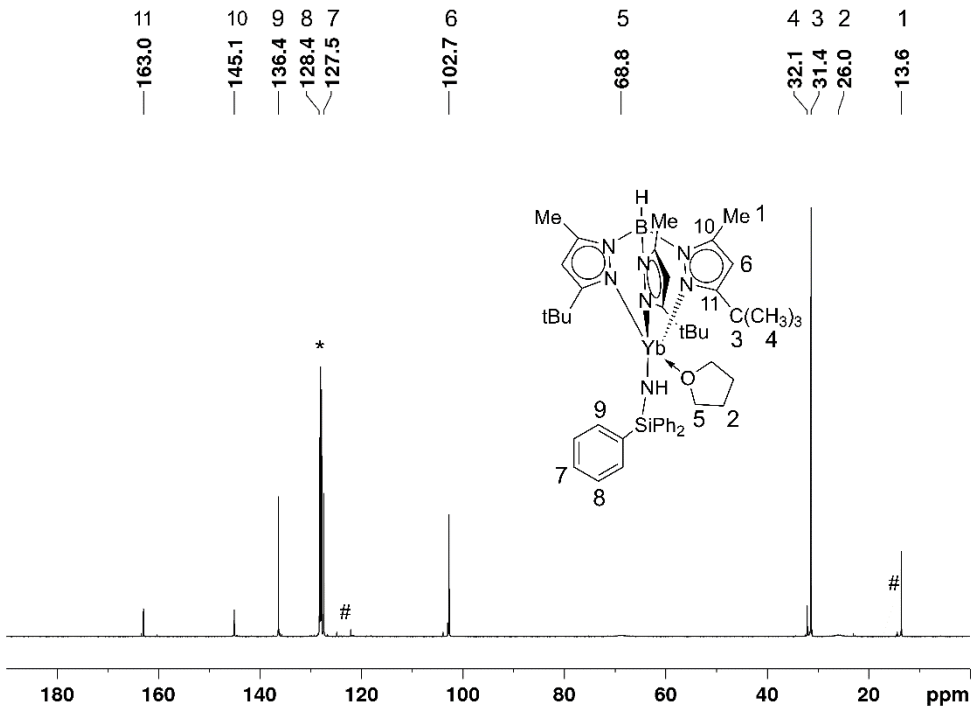

Figure S15 $^{13}C\{^{1}H\}$ UDEFT NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ (**4^{thf}**). Residual solvent signals are marked with *, minor impurities are marked with #.

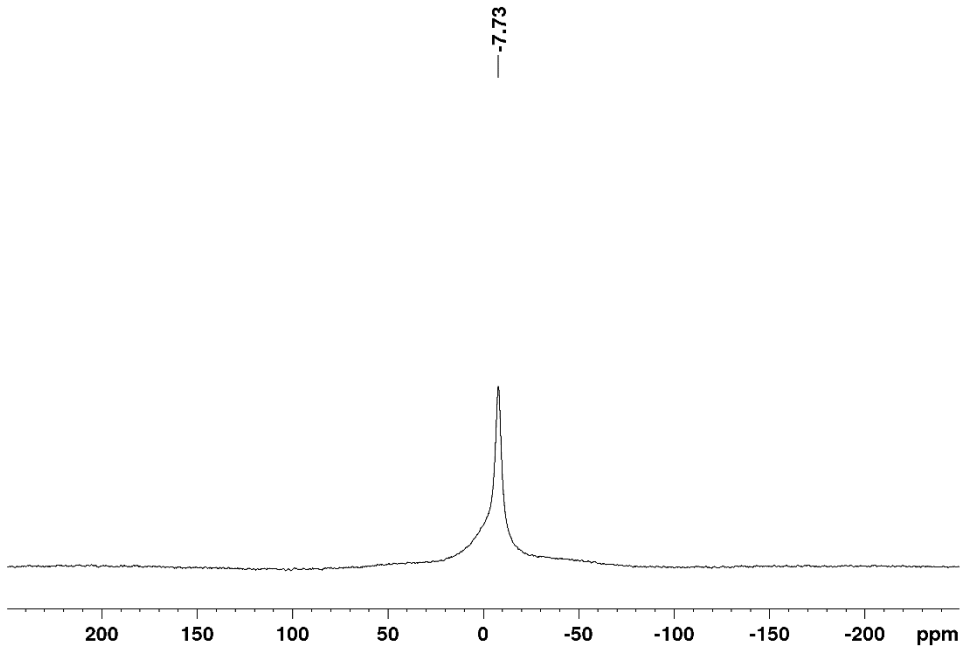

Figure S16 $^{11}B\{^{1}H\}$ NMR spectrum (160 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ (**4^{thf}**).

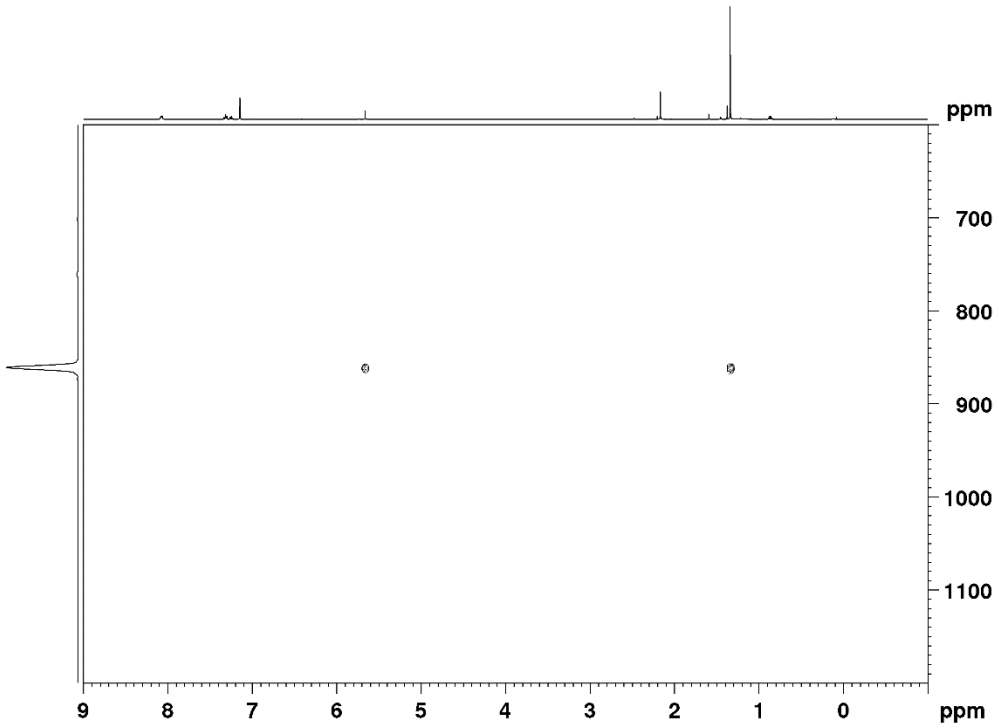

Figure S17 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz,87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ (**4**^{thf}).

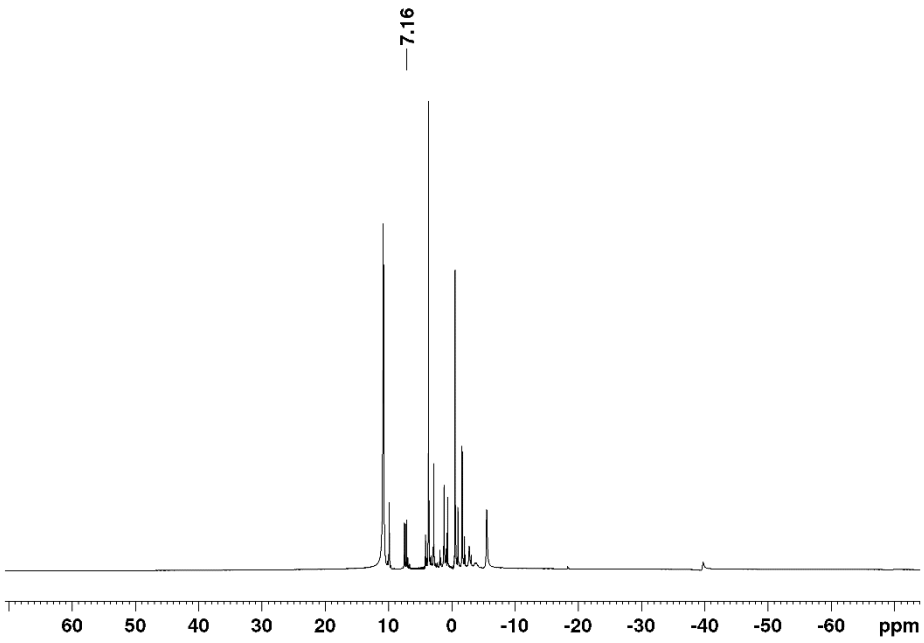

Figure S18 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Sm(NHAr^{iPr})(thf)$ (**1**^{thf,Sm})

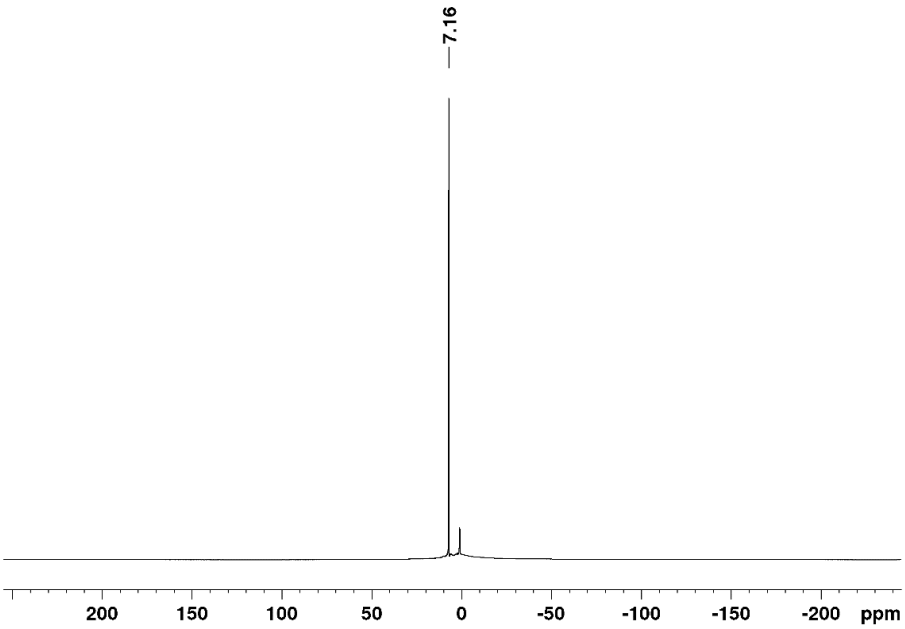

Figure S 19 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Eu(NHAr^{iPr})(thf)$ (**1^{thf,Eu}**).

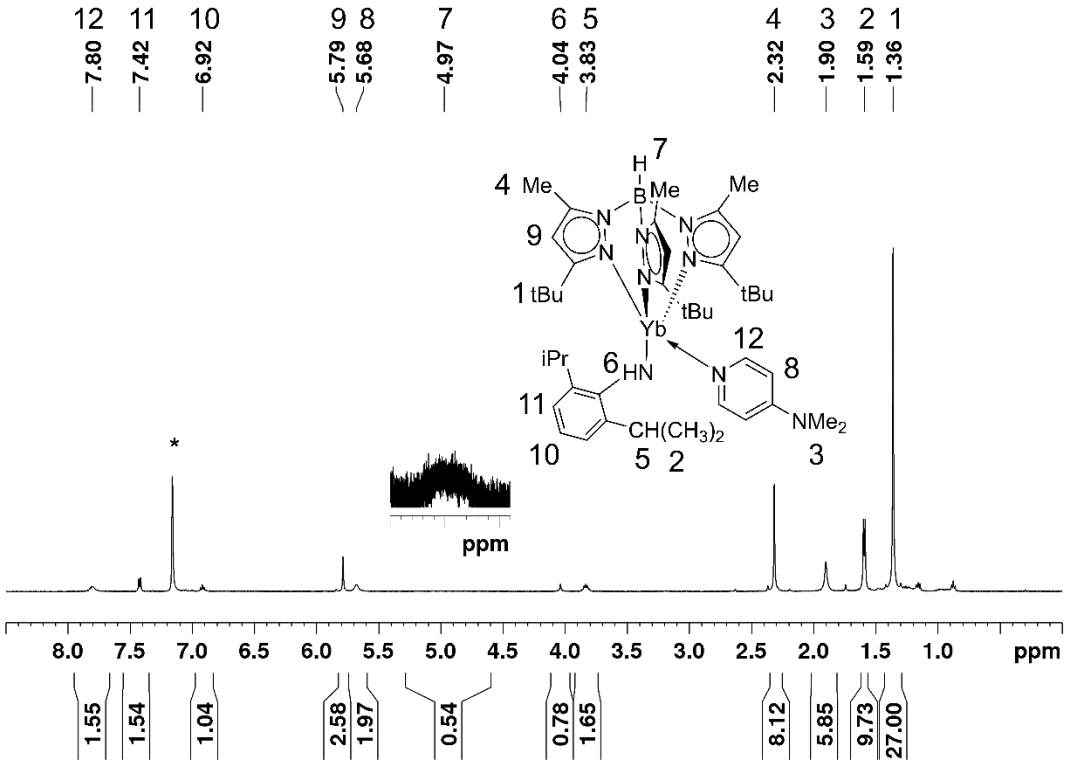

Figure S20 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(dmap)$ (**1^{dmap}**). Residual solvent signals are marked with *.

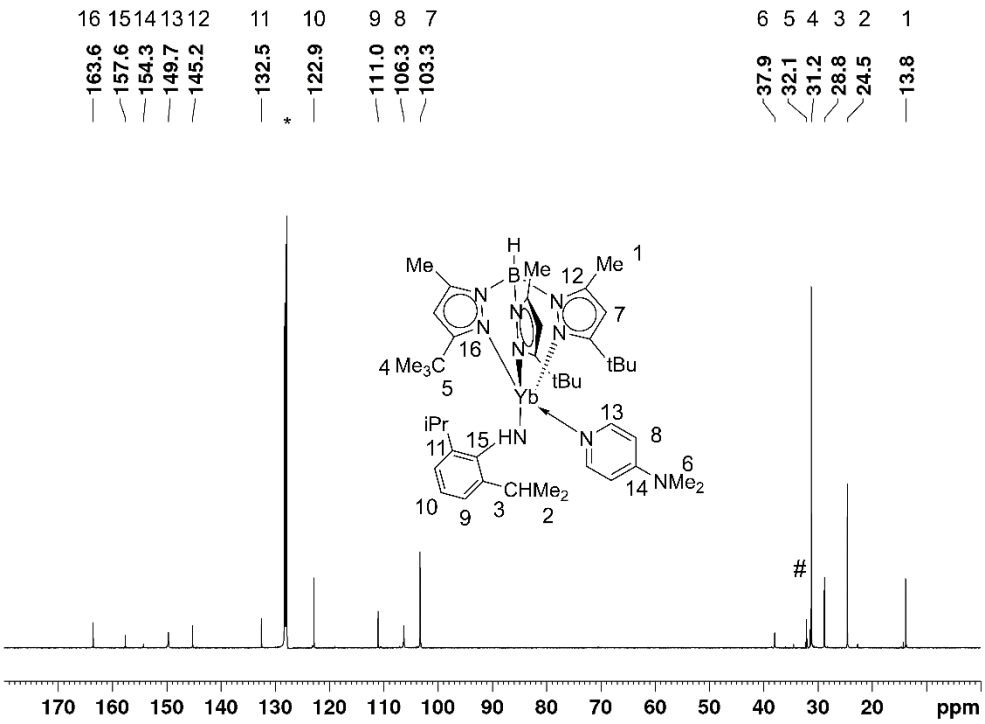

Figure S21 ^{13}C UDEFT NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})$(dmap) (**1^{dmap}**). Residual solvent signals are marked with *. Minor impurities are marked with #.

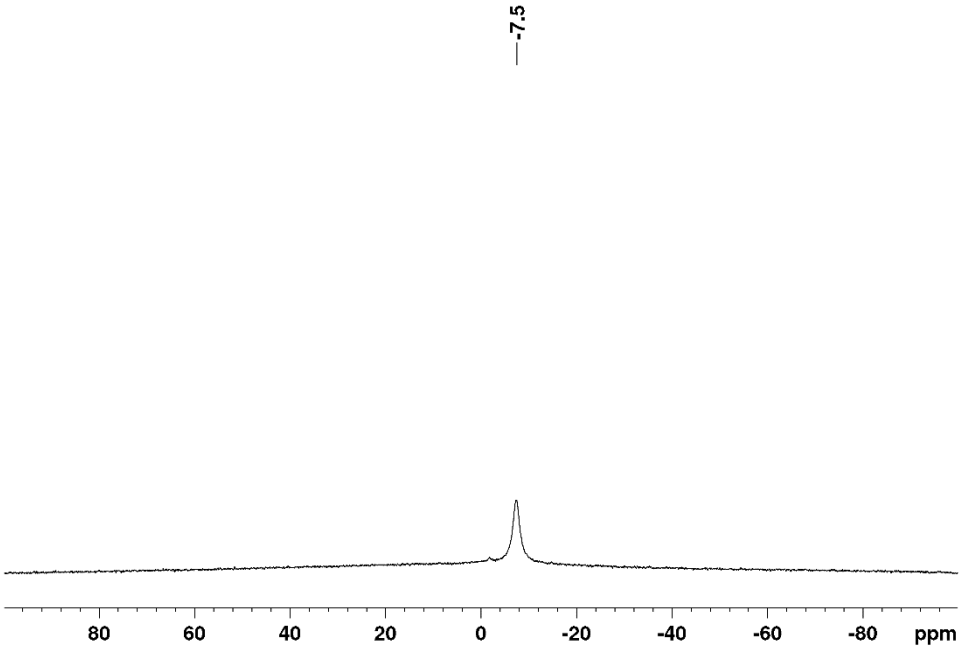

Figure S22 ^{11}B NMR spectrum (160 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})$(dmap) (**1^{dmap}**).

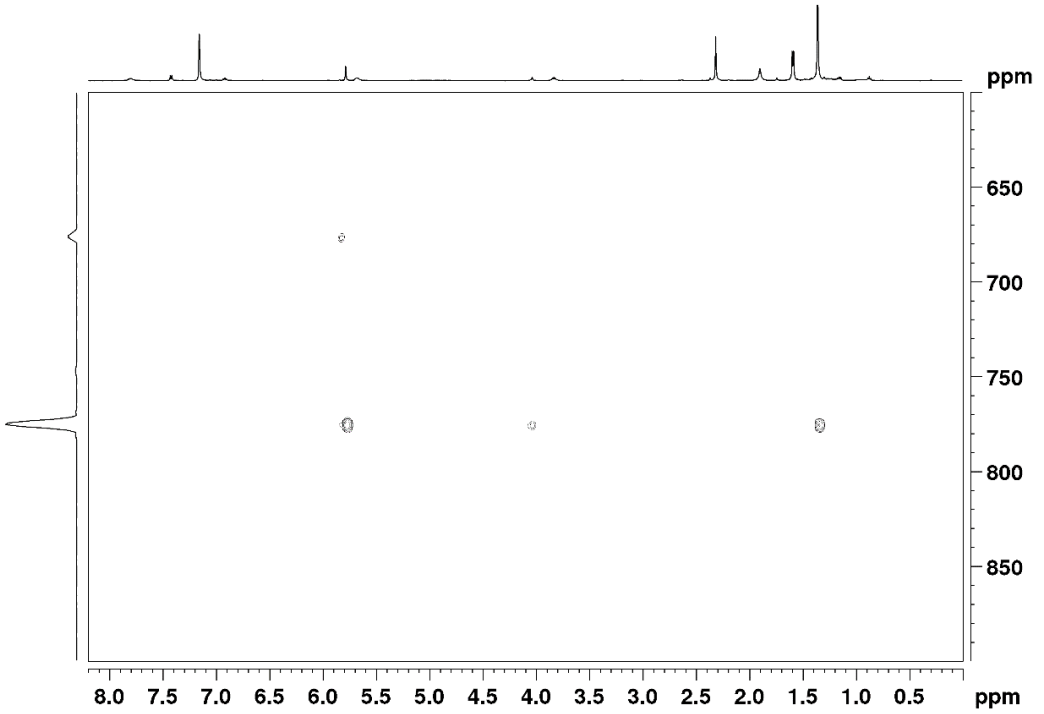

Figure S23 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})$(dmap) (**1^{dmap}**). Product signal at 776 ppm.

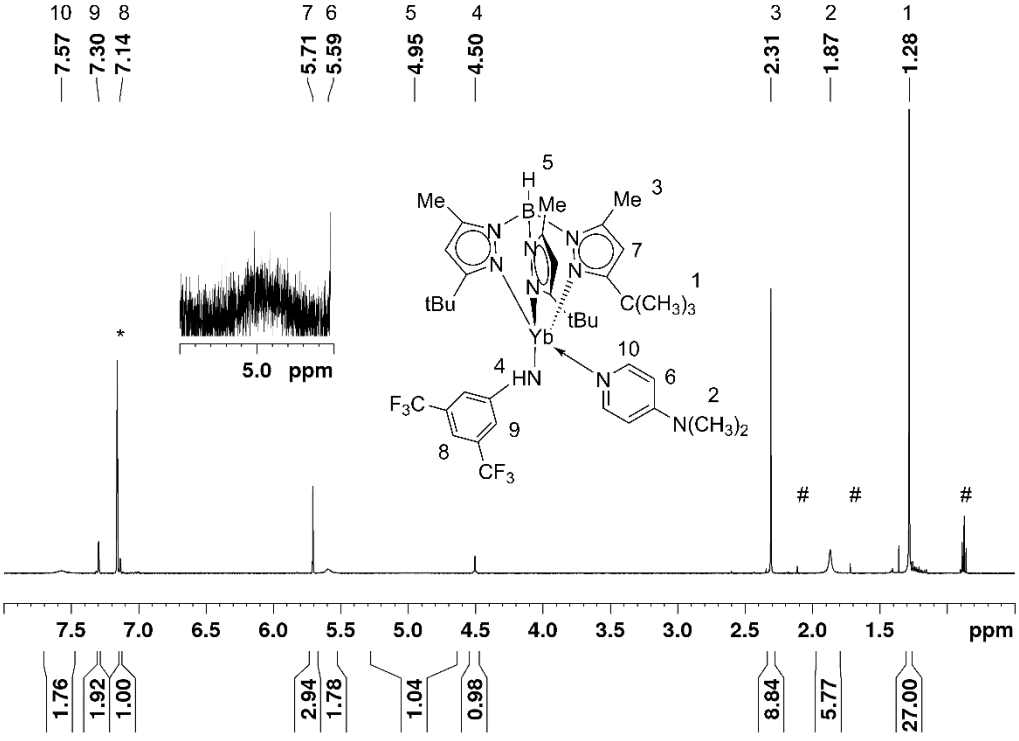

Figure S24 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})$(dmap) (**3^{dmap}**). Residual solvent signals are marked with *.

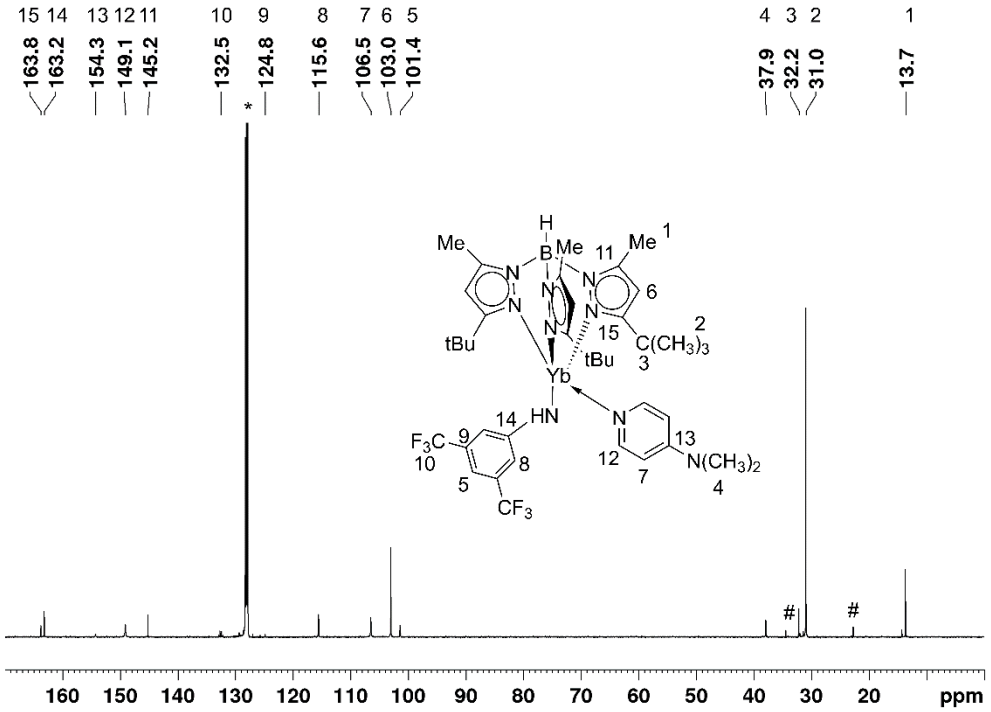

Figure S25 ^{13}C UDEFT NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})$(dmap) (**3**^{dmap}). Residual solvent signals are marked with *. Minor impurities are marked with #.

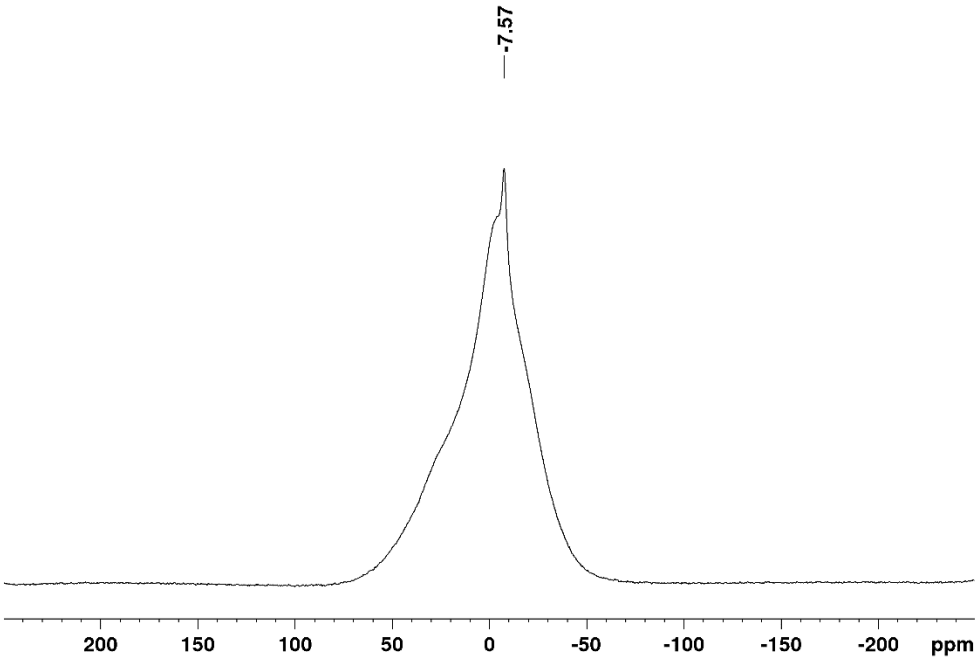

Figure S26 ^{11}B NMR spectrum (128 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})$(dmap) (**3**^{dmap}).

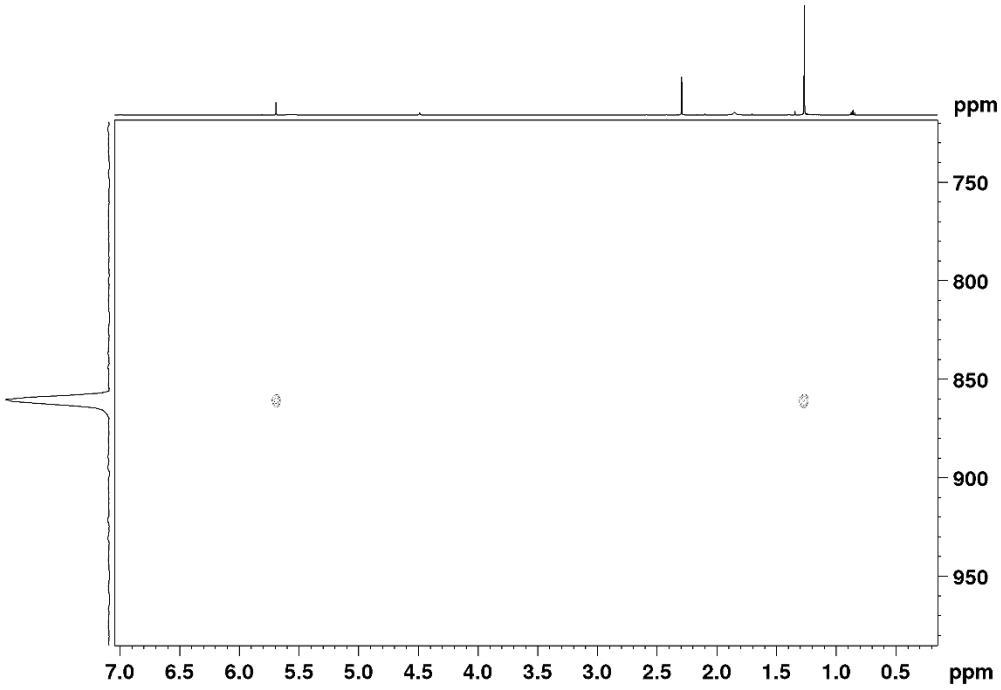

Figure S27 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(dmap)$ (**3^{dmap}**). Product signal at 862 ppm.

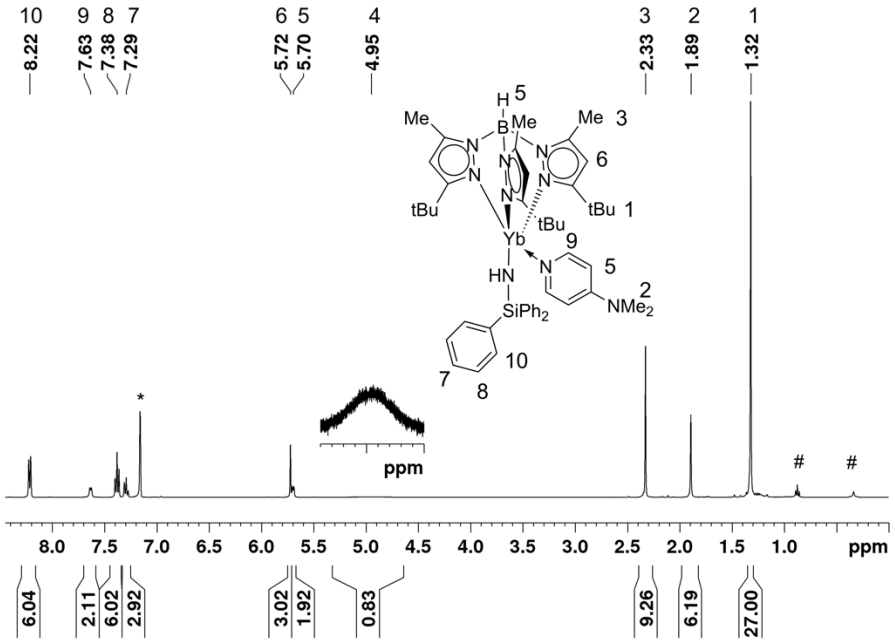

Figure S28 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4^{dmap}**). Residual solvent signals are marked with *, minor impurities are marked with #.

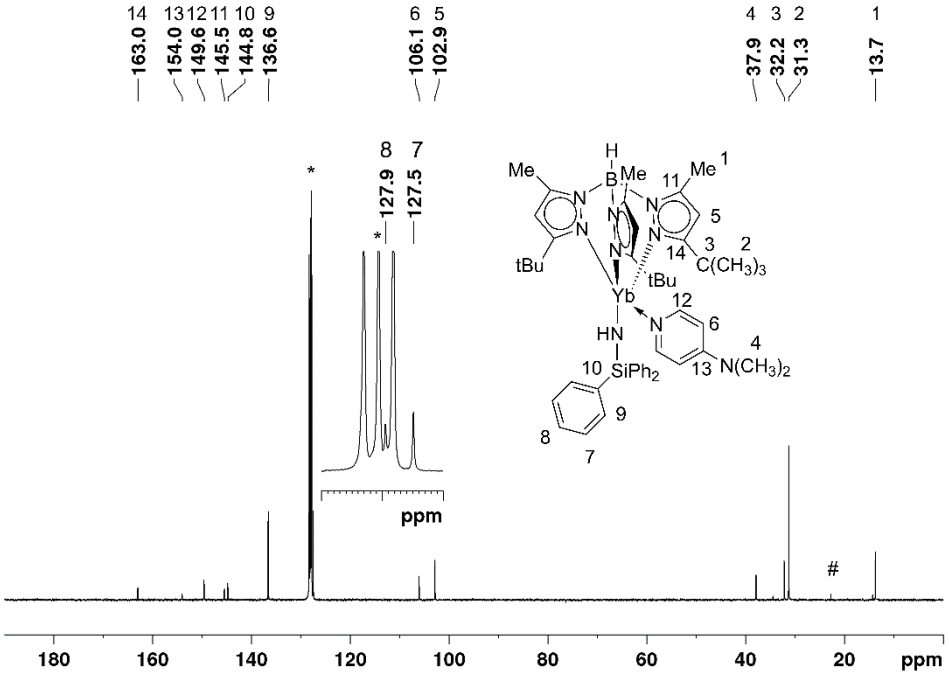

Figure S29 $^{13}C\{^{1}H\}$ UDEFT NMR spectrum (100 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4**^{dmap}). Residual solvent signals are marked with *, minor impurities are marked with #.

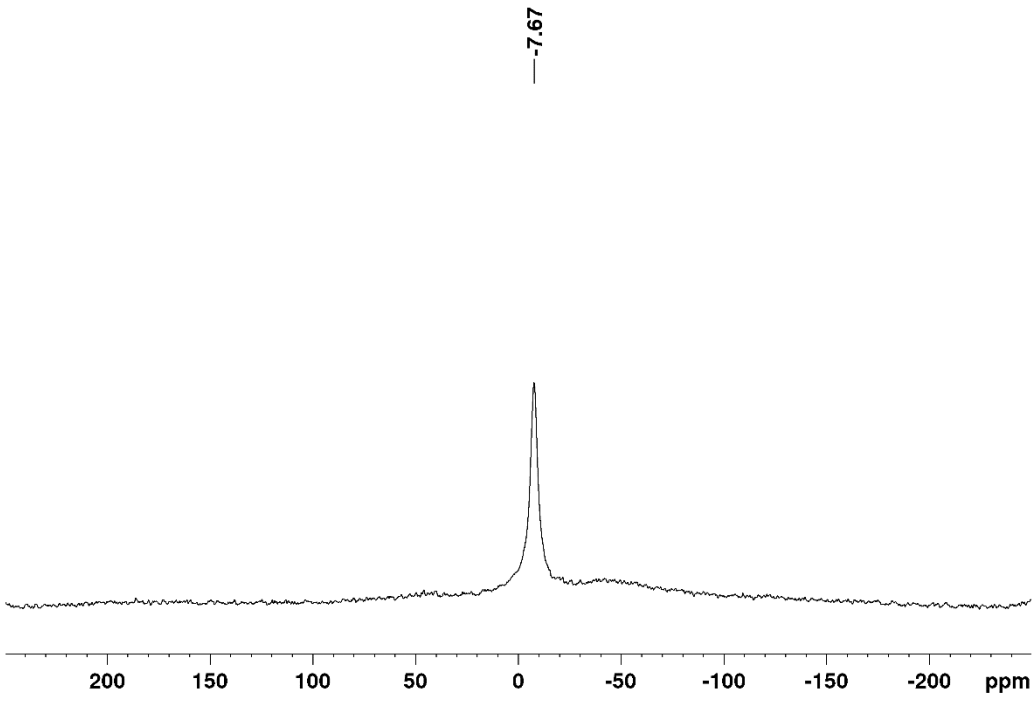

Figure S30 $^{11}B\{^{1}H\}$ NMR spectrum (96 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4**^{dmap}). Residual solvent signals are marked with *, minor impurities are marked with #.

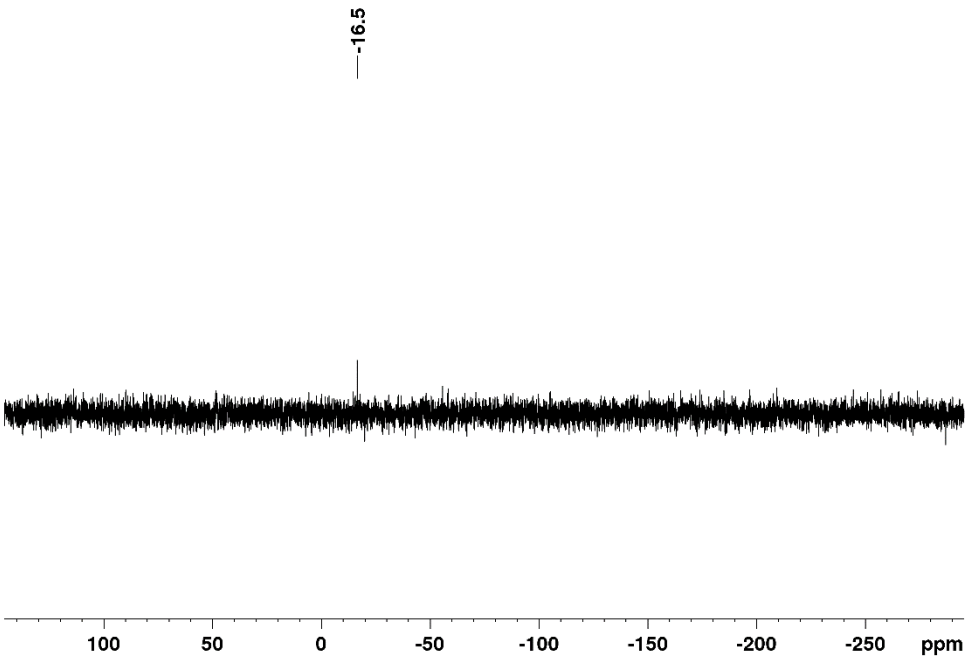

Figure S31 ^{29}Si DEPT45 NMR spectrum (60 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4^{dmap}**).

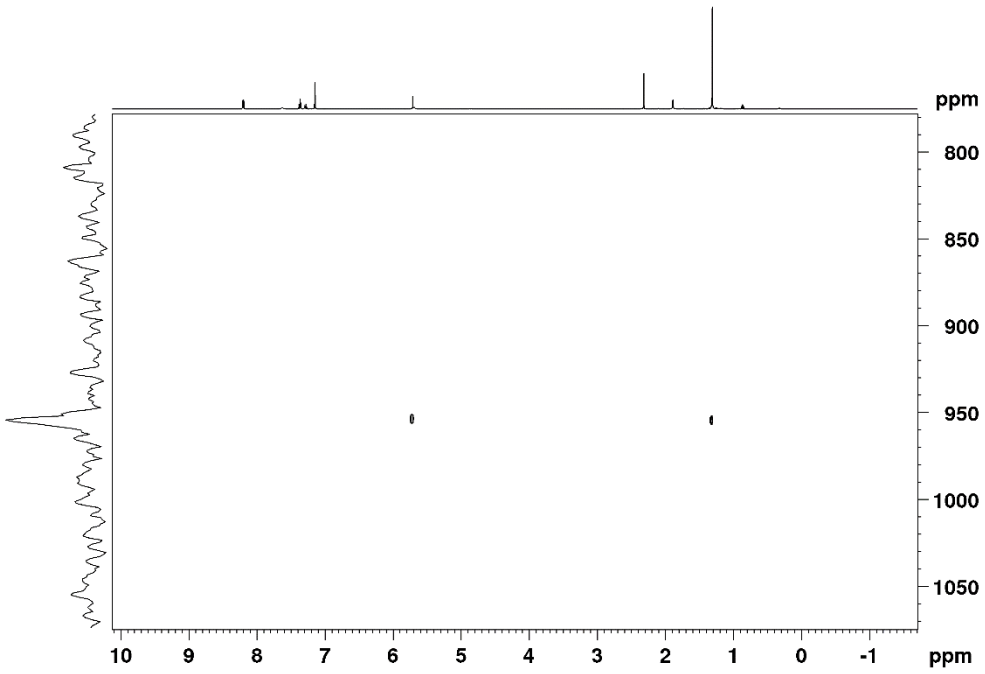

Figure S32 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4^{dmap}**). Product signal at 954 ppm

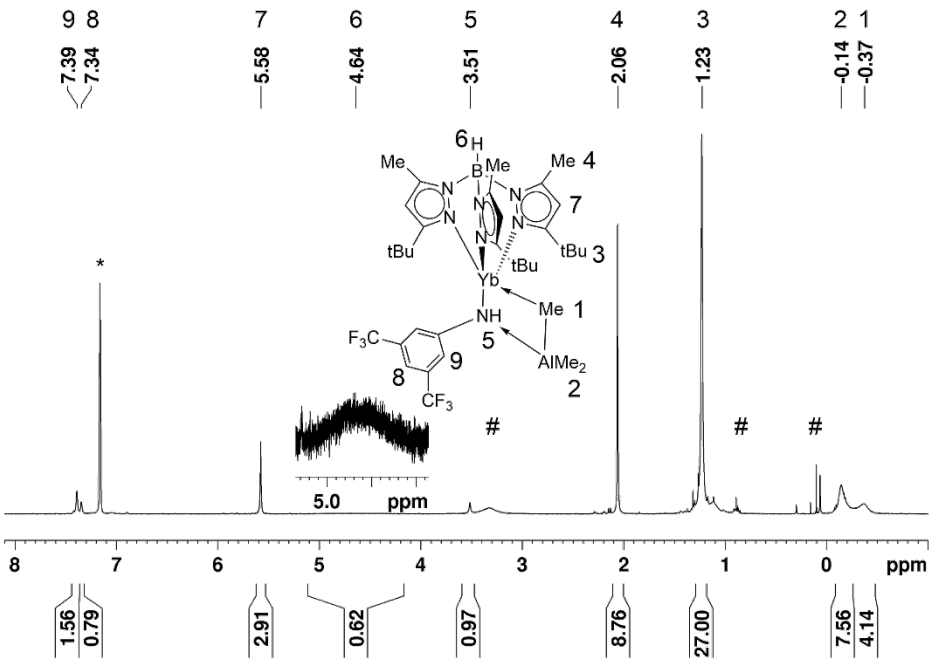

Figure S33 ^{1}H NMR spectrum (300 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(AlMe_3)$ (**6**).

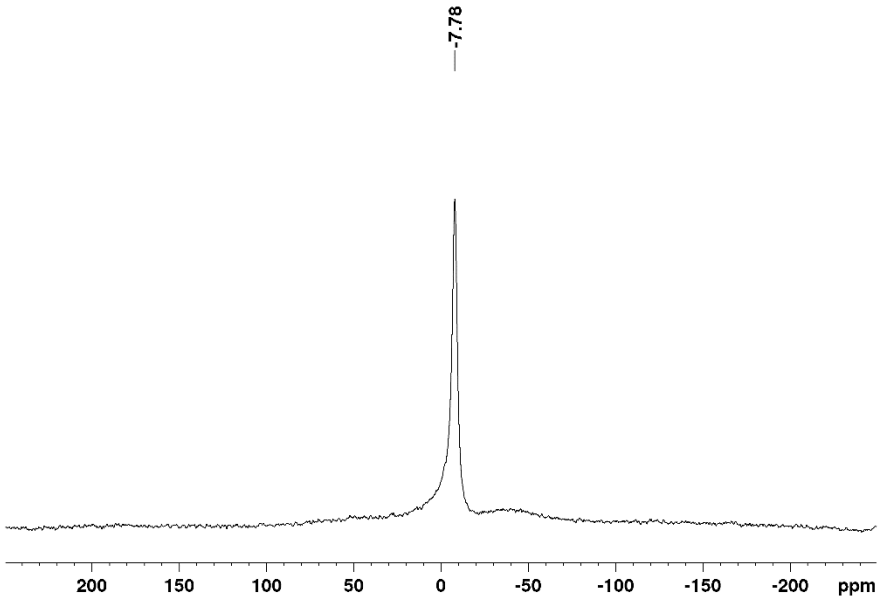

Figure S34 ^{11}B NMR spectrum (96 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(AlMe_3)$ (**6**).

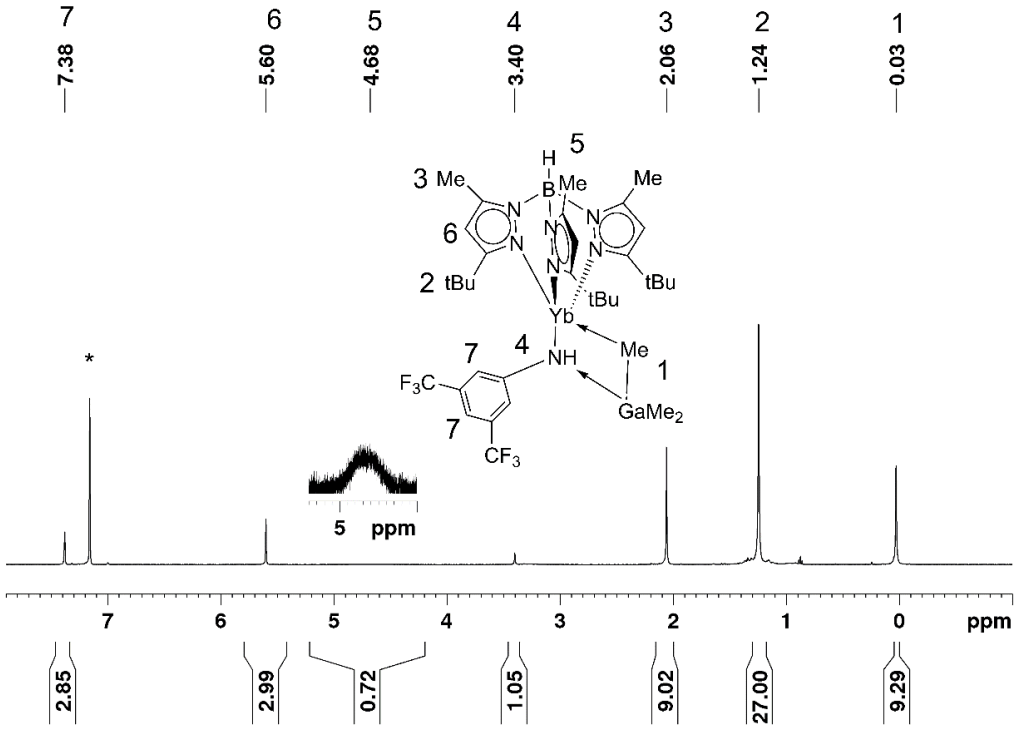

Figure S35 ^{1}H NMR spectrum (500 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**).

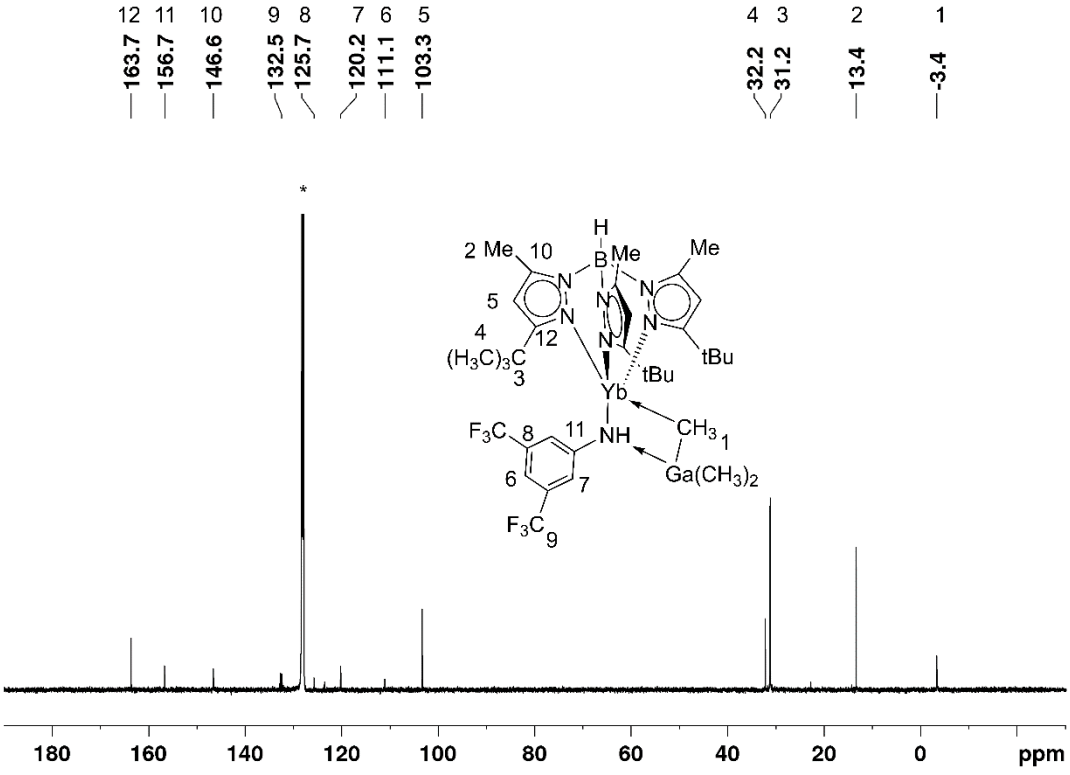

Figure S36 $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**). Residual solvent signals are marked with *

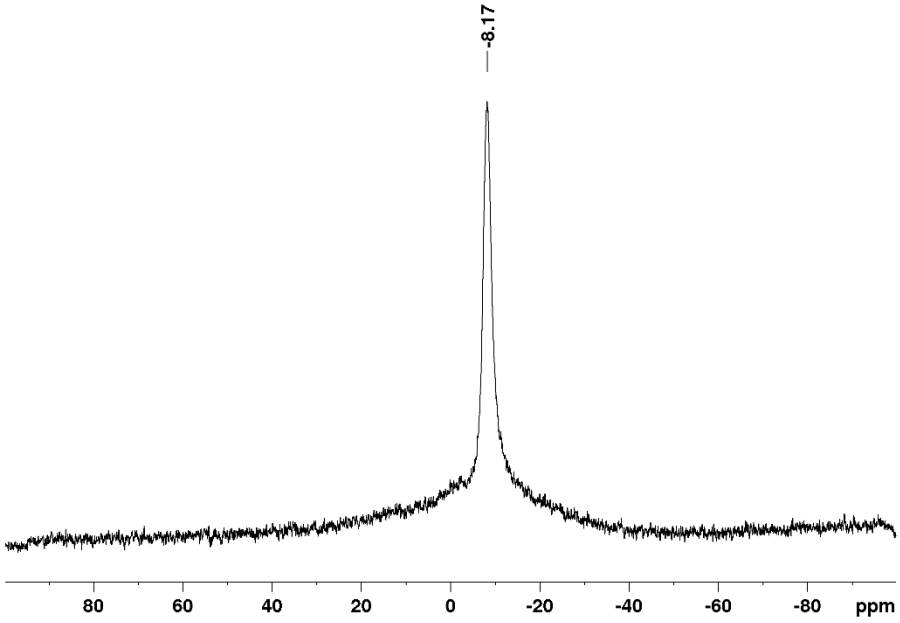

Figure S37 ^{11}B NMR spectrum (160 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**).

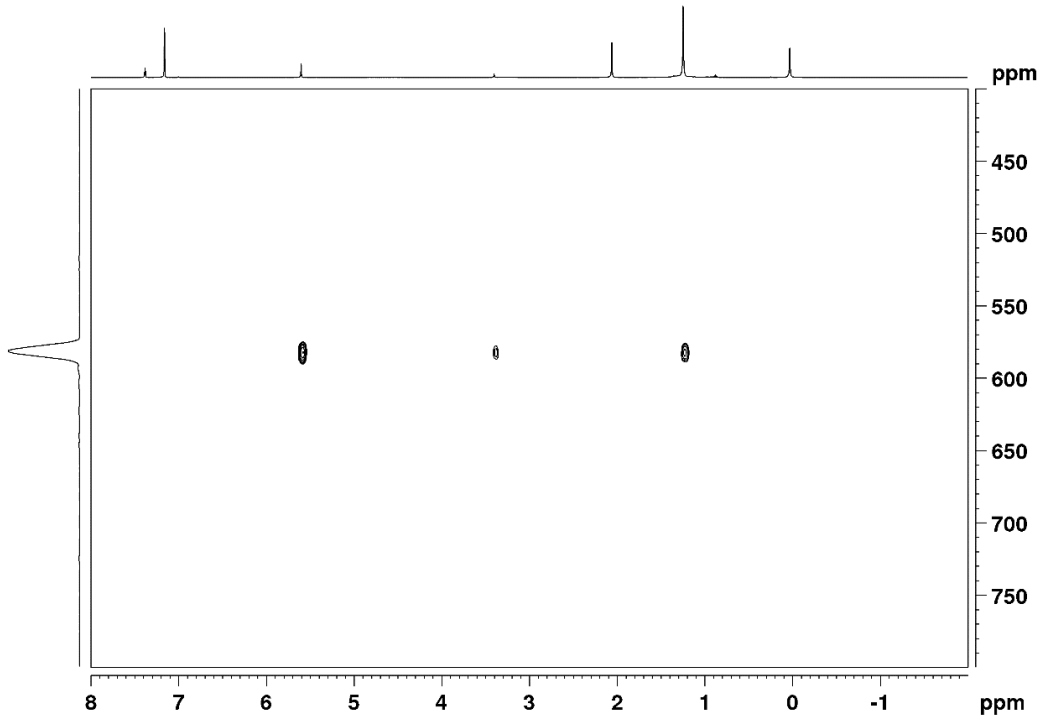

Figure S38 ^{1}H-^{171}Yb HSQC NMR spectrum (500 MHz, 87.52 MHz C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**). Product signal at 582 ppm.

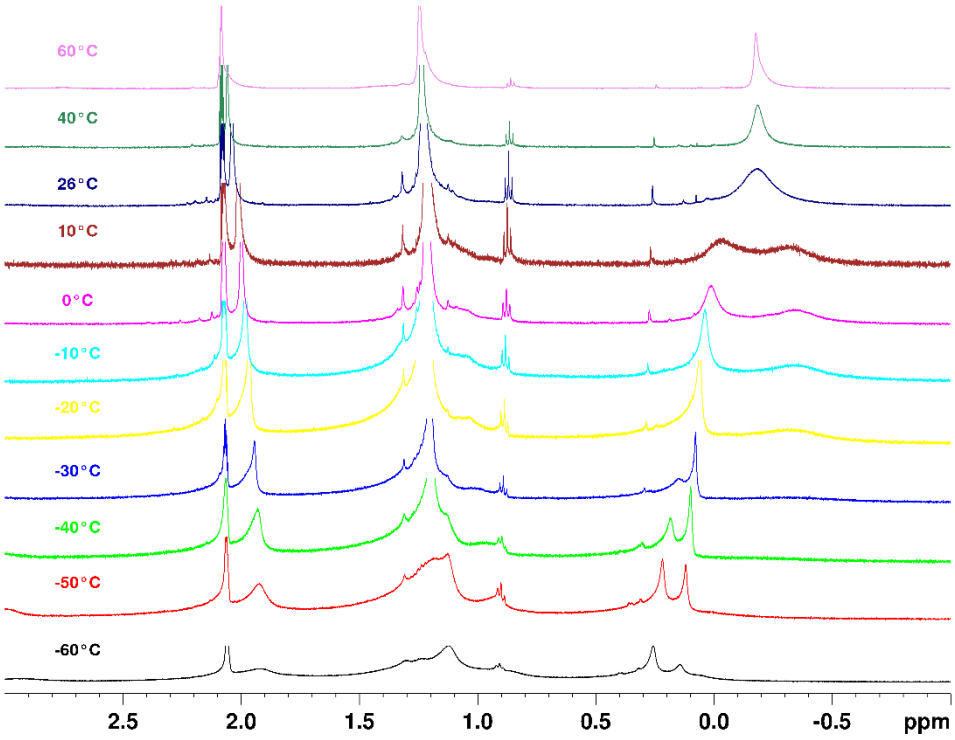

Figure S39 ^{1}H VT NMR spectra (500 MHz, toluene-d_8) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**). In the region of 0.5 to -0.5 ppm the signal splitting of the coordinated $Ga(CH_3)_3$ can be observed at low temperatures.

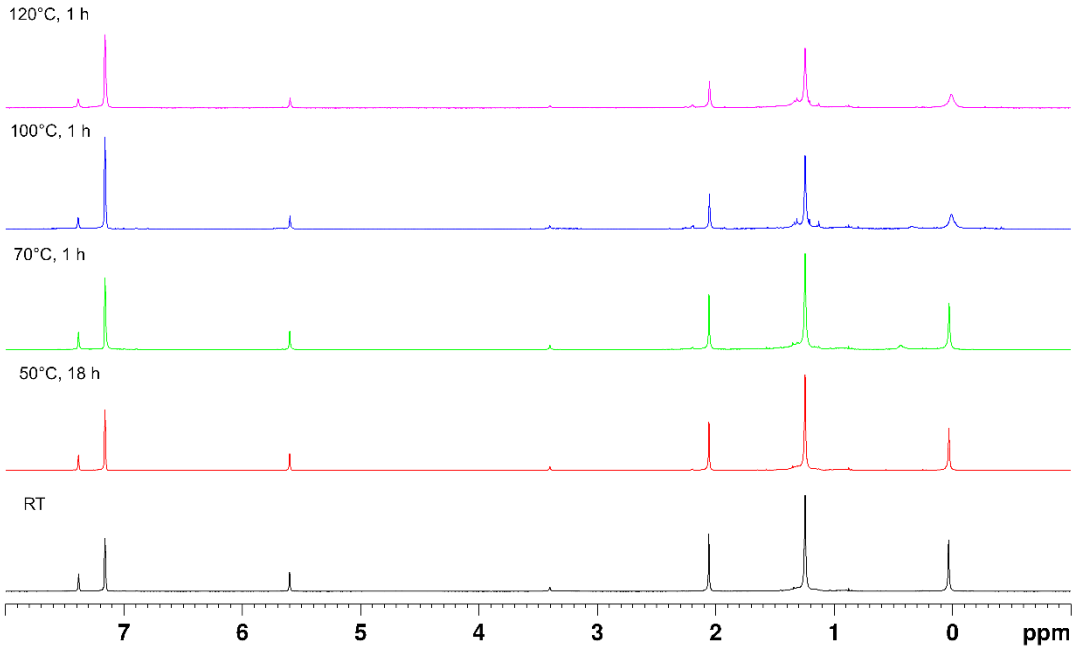

Figure S40 ^{1}H VT NMR spectra (500 MHz, C_6D_6) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**).

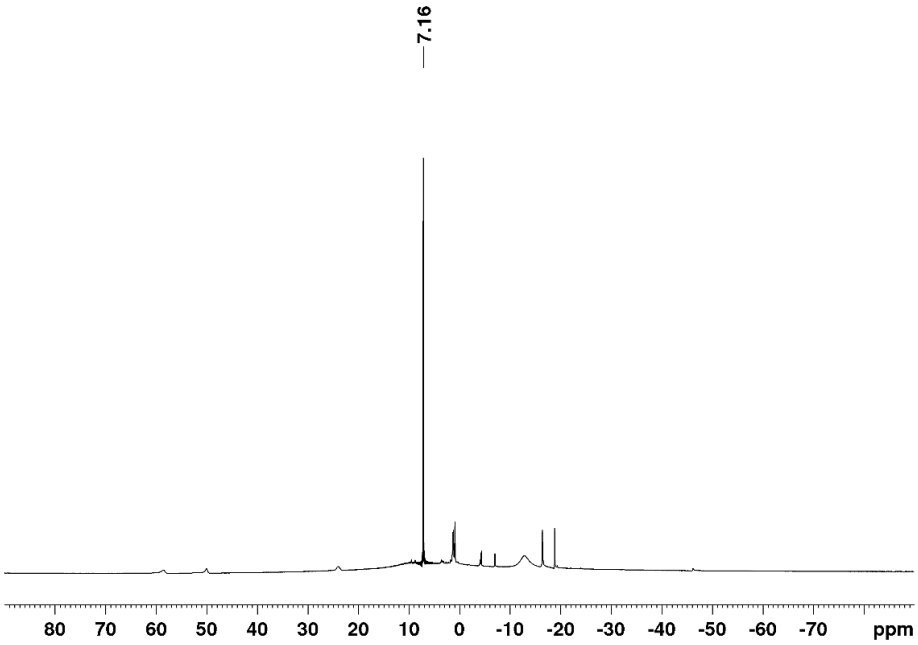

Figure S41 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(Cl)$ (**9a**).

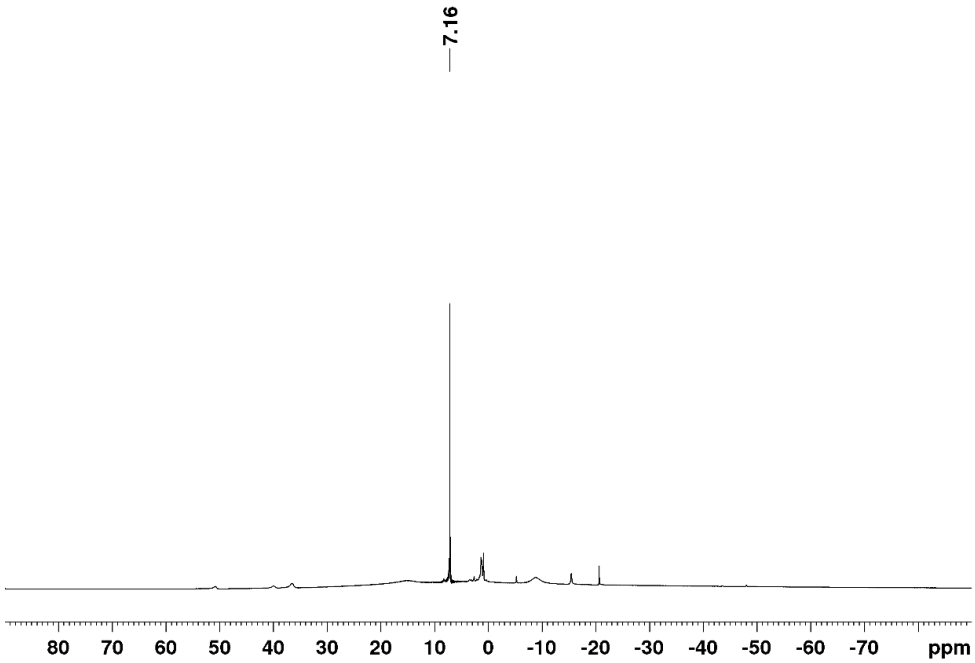

Figure S42 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{iPr})(Br)$ (**9b**).

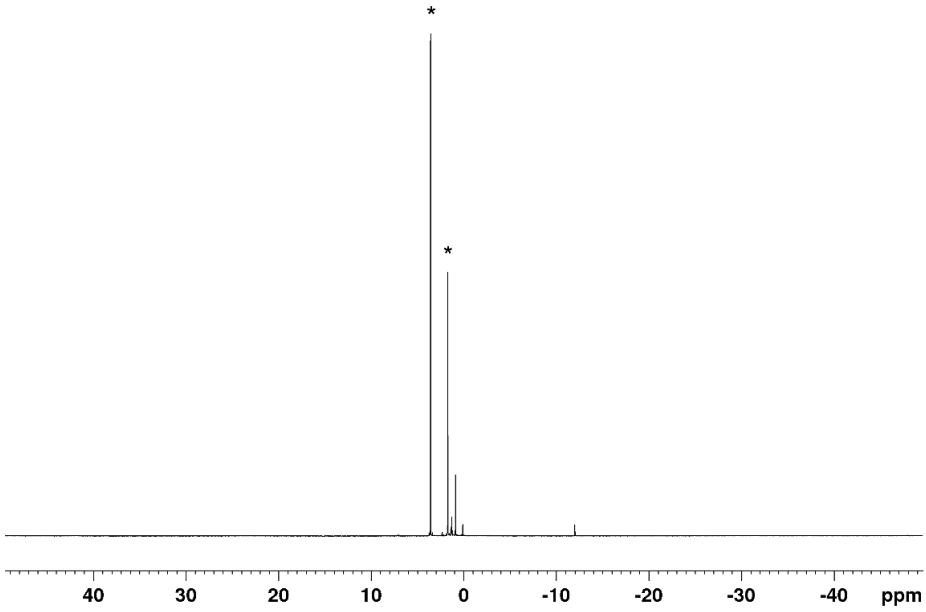

Figure S43 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(Cl)$ (**10a**).

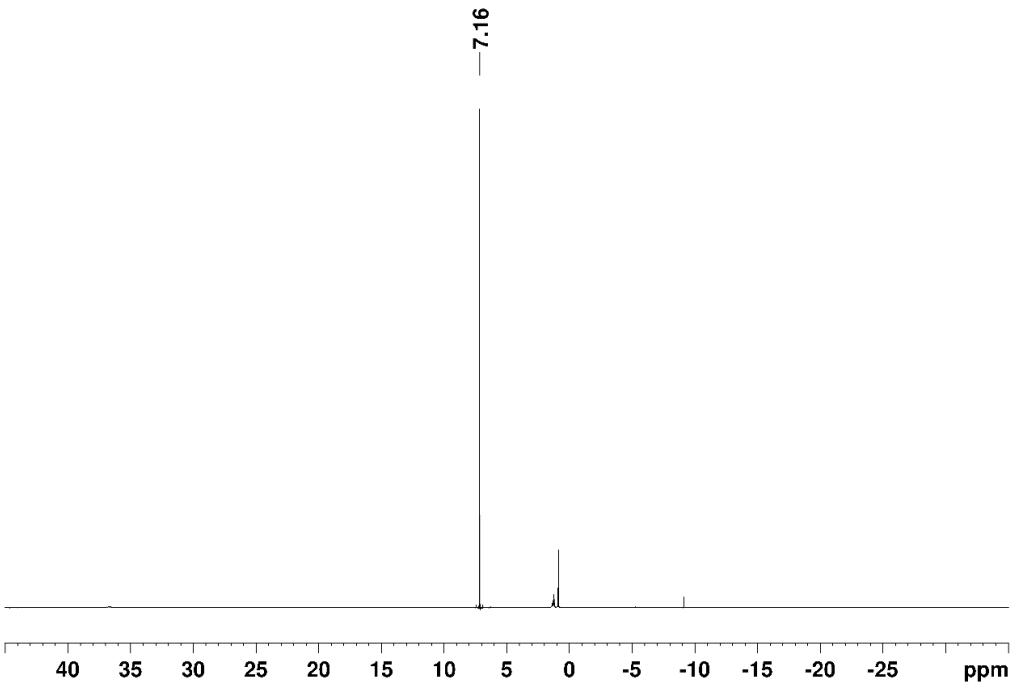

Figure S44 ^{1}H NMR spectrum (400 MHz, C_6D_6, 26 °C) of $Tp^{tBu,Me}Yb(NHAr^{CF3})(Br)$ (**10b**).

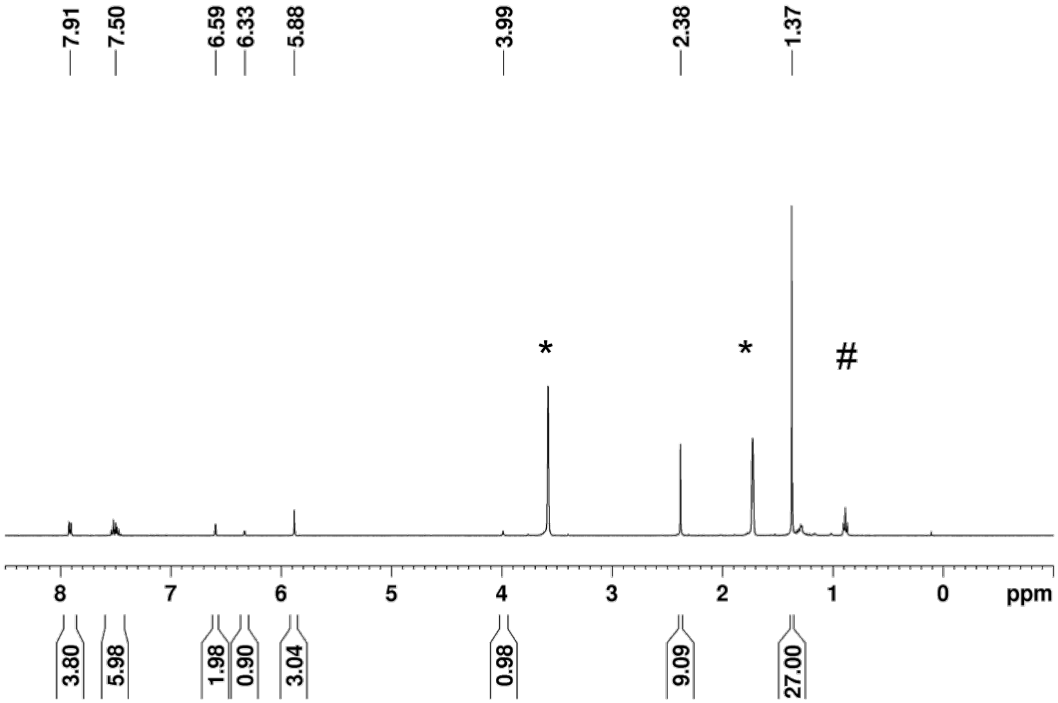

Figure S45 ^{1}H NMR spectrum (400 MHz, THF-*d*8, 26 °C) of $Tp^{tBu,Me}Yb(NHA^{CF3})(N_2Ph_2)$ (**11**). Residual solvent signals are marked with *. Minor impurities are marked with #.

Crystallographic Data

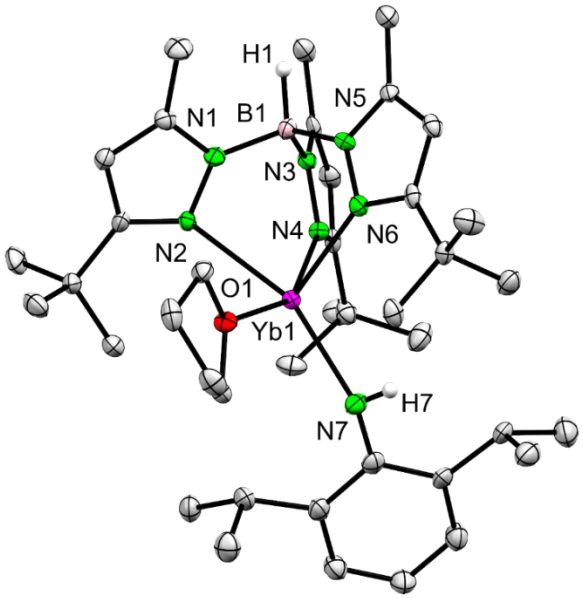

Figure S46 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{iPr})(thf)$ (**1**^{thf}). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms, lattice solvent *n*-hexane and disorder in thf are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.544(3), Yb1 – N4 2.487(3), Yb1 – N6 2.526(3), Yb1 – N7 2.353(4), Yb1 – O1 2.431(3), Yb1 – N7 – C25 147.8(3), Yb1 –N7 – H7 91(3), C25 – N7 – H7 110(3), N7 – Yb1 – O1 92.60(12).

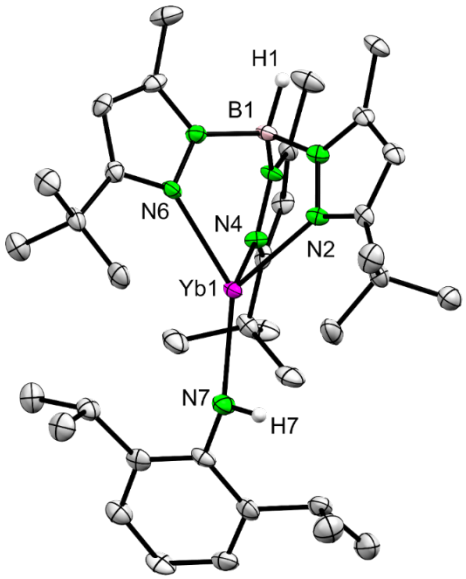

Figure S47 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{iPr})$ (**1**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorder in thf are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.428(4), Yb1 – N4 2.428(5), Yb1 – N6 2.425(4), Yb1 – N7 2.345(5), Yb1 – N7 – C25 139.1(4), Yb1 – N7 – H7 103(5), C25 – N7 – H7 105(5).

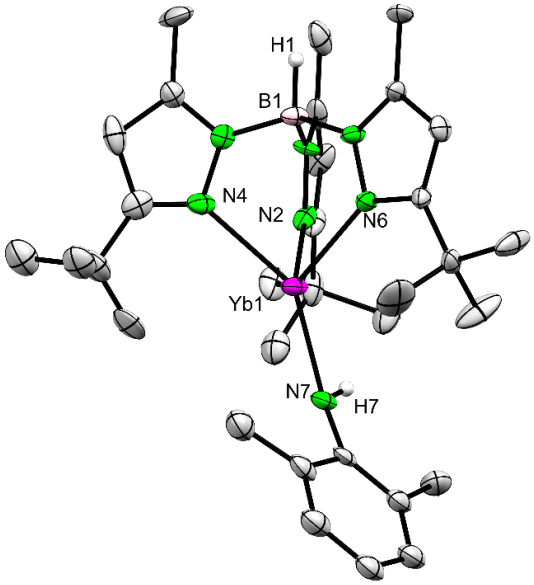

Figure S 48 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{Me})$ (**2**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorder in *t*Bu groups as well as the amid substituent are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Yb1 – N2 2.40(2), Yb1 – N4 2.457(19), Yb1 – N6 2.410(4), Yb1 – N7/7A 2.30(3)/2.29(3), Yb1 – N7 – C25 150(2), Yb1 – N7A – C25A 153(2), Yb1 – N7 – H7 77(15), Yb1 – N7A – H7A 103*, C25 – N7 – H7 118(14), C25A – N7A – H7A 103*.

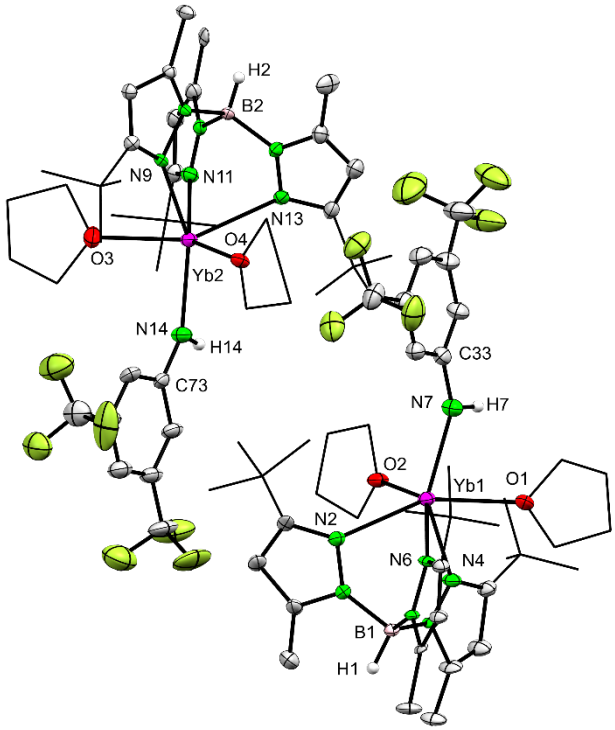

Figure S49 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ **(3^{thf})**. All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms, lattice solvent pentane and disorder in CF_3 groups are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Yb1 – N2 2.51(2), Yb1 – N4 2.55(2), Yb1 – N6 2.469(18), Yb1 – N7 2.411(12), Yb1 – N7 – C33 143.2(10), Yb1 – N7 – H7 108*, C33 – N7 – H7 108*, N7 – Yb1 – O1 78.4(5), N7 – Yb1 – O2 81.0(6), Yb2 – N9 2.599(19), Yb2 – N11 2.56(2), Yb2 – N13 2.60(2), Yb2 – N14 2.411(12), Yb2 – O3 2.50(2), Yb2 – O4 2.546(17), Yb2 – N14 – C73 145.4(10), Yb2 – N14 – H14 107*, C73 – N14 – H14 107*, N14 – Yb2 – O3 86.5(6), N14 – Yb2 – O4 83.8(5).

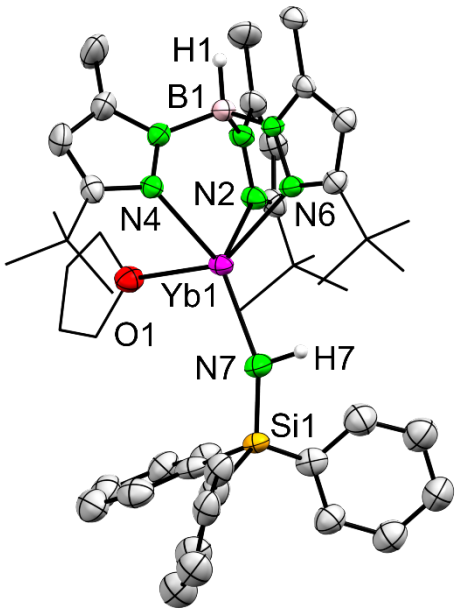

Figure S50 Crystal structure of $Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ (**4** ^{thf}). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders in phenyl, *t*Bu substituents and thf are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Yb1 – N2 2.519(2), Yb1 – N4 2.473(2), Yb1 – N6 2.450(2), Yb1 – N7/7A 2.341(3)/2.287(10), Yb1 – O1 2.4472(19), Yb1 – N7 – Si1 154.0(2), Yb1 – N7A – Si1A 153.7(6), Yb1 – N7 – H7 94(2), Si1 – N7 – H7 111(2), Si1A – N7A – H7D 92(9).

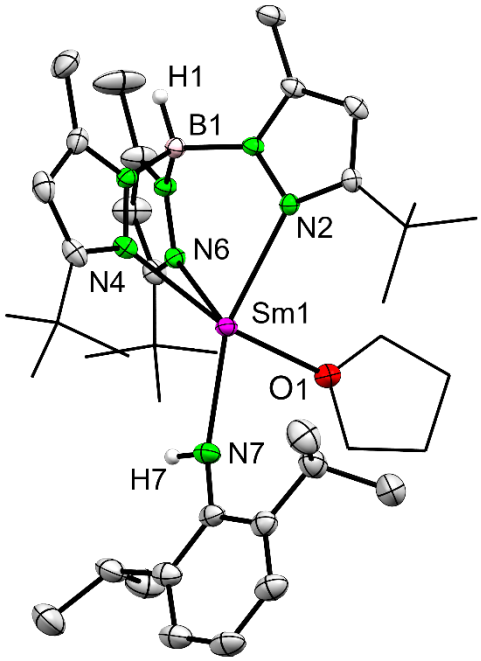

Figure S51 Crystal structure of $Tp^{tBu,Me}Sm(NHAr^{iPr})(thf)$ (**1**^{thf,Sm}). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorder in *t*Bu groups are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Sm1 – N2 2.6573(17), Sm1 – N4 2.632(2), Sm1 – N6 2.6184(17), Sm1 – N7 2.483(2), Sm1 – N7 – C25 157.46(17).

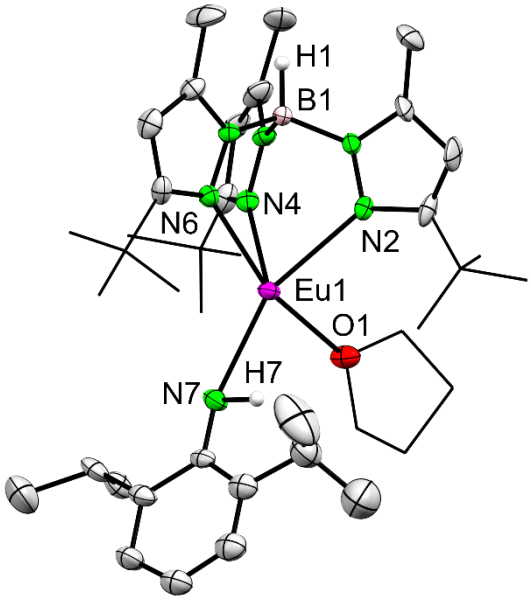

Figure S52 Crystal structure of Tp^{tBu,Me}Eu(NHAr^{iPr})(thf) (**1^{thf,Eu}**). All atoms are represented by atomic displacement ellipsoids set at 50 % probability. Hydrogen atoms and disorder in *t*Bu groups as well as the amid substituent are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Eu1 – N2 2.629(12), Eu1 – N4 2.616(12), Eu1 – N6 2.610(3), Eu1 – N7/7A 2.474(17)/2.48(3), Eu1 – N7 – C25 158.4(16), Eu1 – N7A – C25A 159(2).

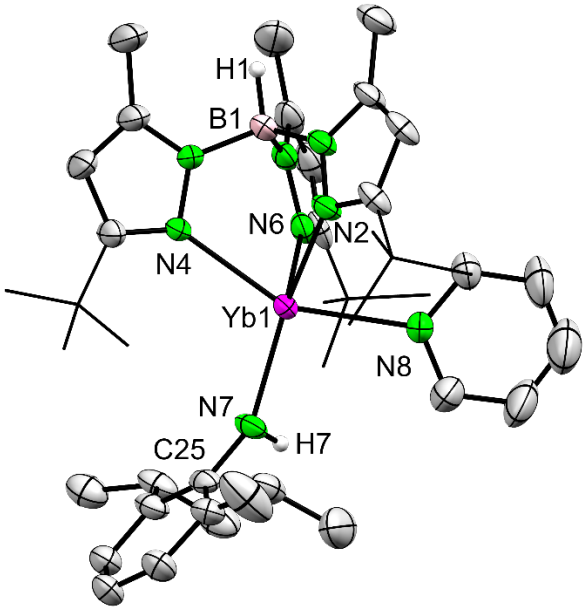

Figure S53 Crystal structure of Tp^{tBu,Me}Yb(NHAr^{iPr})(py) (**1^{py}**). All atoms are represented by atomic displacement ellipsoids set at 50 % probability. Hydrogen atoms and disorders of the *i*Pr and one *t*Bu groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.479(4), Yb1 – N4 2.508(4), Yb1 – N6 2.492(5), Yb1 – N7 2.358(4), Yb1 – N8 2.554(4), Yb1 – N7 – C30 147.6(3), Yb1 – N7 – H7 106.2, C30 – N7 – H7 106.2, N7 – Yb1 – N8 96.61(15).

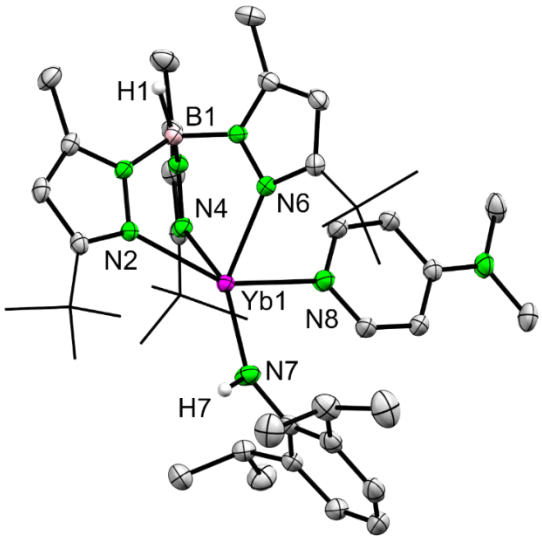

Figure S54 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{iPr})(dmap)$ (**1**^{dmap}). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorder in one *t*Bu are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Yb1 – N2 2.5105(14), Yb1 – N4 2.5294(15), Yb1 – N6 2.4535(15), Yb1 – N7 2.3443(16), Yb1 – N8 2.4896(15), Yb1 – N7 – C30 138.03(12), Yb1 – N7 – H7 125.0(13)*, C30 – N7 – H7 96.9(13)*, N7 – Yb1 – N8 97.46(5).

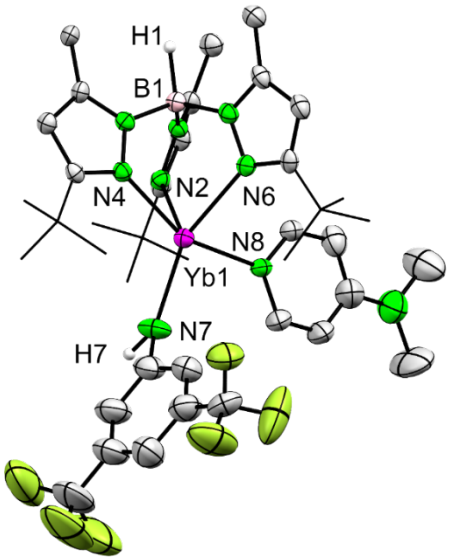

Figure S55 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(dmap)$ (**3**^{dmap}). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the CF_3 groups are omitted for clarity. Selected interatomic distances [Å] and angles [°], values marked with * were calculated with Platon: Yb1 – N2 2.461(5), Yb1 – N4 2.475(5), Yb1 – N6 2.484(5), Yb1 – N7 2.372(6), Yb1 – N8 2.486(5), Yb1 – N7 – C25 144.6(6), Yb1 – N7 – H7 84(8)*, N7 – Yb1 – N8 92.2(2).

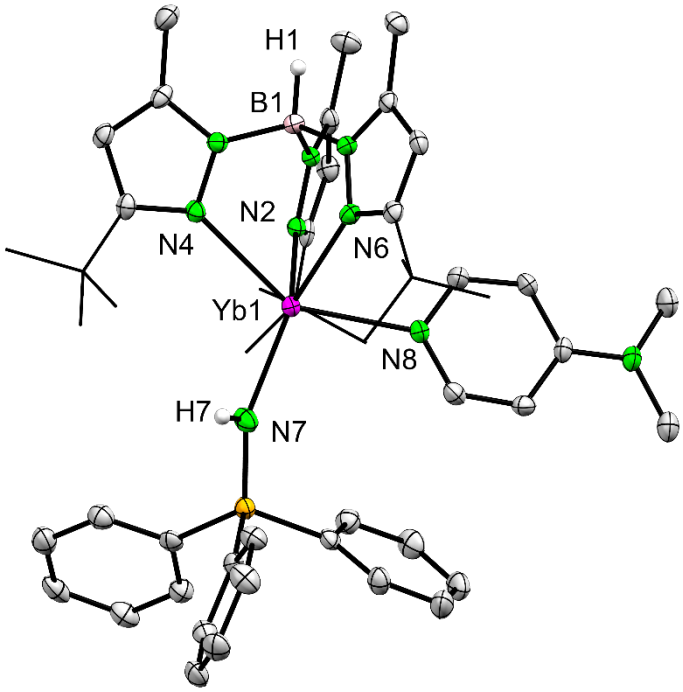

Figure S56 Crystal structure of$Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ (**4^{dmap}**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.476(3), Yb1 – N4 2.566(3), Yb1 – N6 2.460(3), Yb1 – N7 2.337(3). Yb1 – N8 2.549(3), Yb1 – N7 – Si1 149.92(18), Yb1 – N7 – H7 107(4), Si1 – N7 – H7 103(4), N7 – Yb1 – N8 103.11(10).

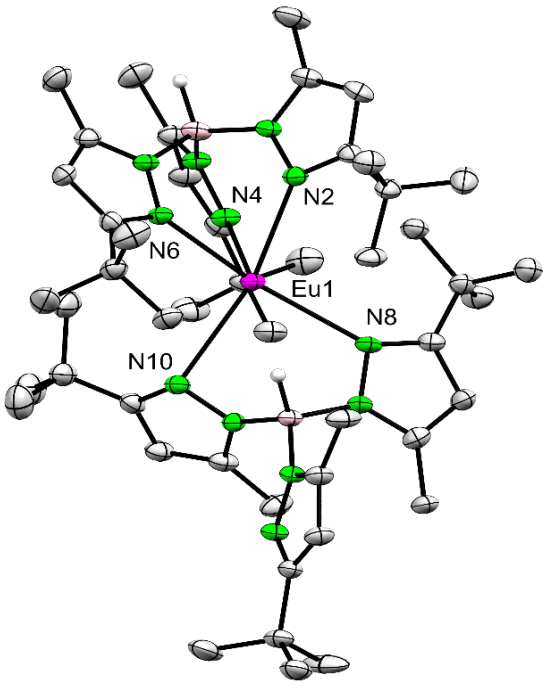

Figure S57 Crystal structure of $Eu(Tp^{tBu,Me})_2$ (**5**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the *i*Pr and one *t*Bu groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Eu1 – N2 2.618(4), Eu1 – N4 2.600(4), Eu1 – N6 2.633(4), Eu1 – N8 2.718(4), Eu1 – N10 2.710(4), B2 – Eu1 3.130(5).

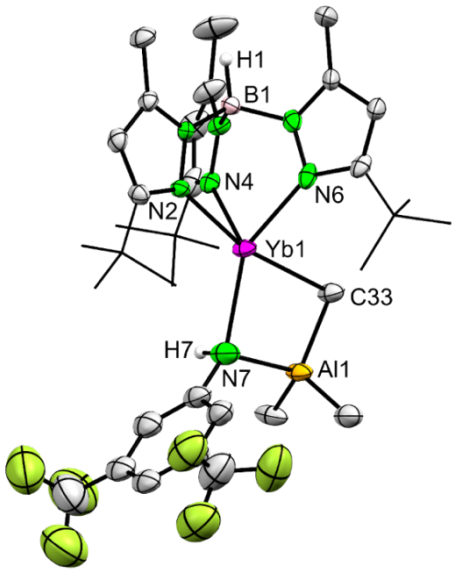

Figure S58 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(AlMe_3)$ (**6**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms, disorders of CF3 and AlMe3 groups and one disorder of one pyrazole are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.440(4), Yb1 – N4 2.422(4), Yb1 – N6 2.423(4), Yb1 – N7/N7A 2.510(9)/2.513(9), Yb1 – C33 2.810(6), Yb1 – Al1/Al1A 3.347(19)/3.43(2), Yb1 – N7/N7A – H7/H7AA 100.3/104.4, Yb1 – N7/N7A – C25/C25A, 136.0(10))/126.3(10), Yb1 – C33 – Al1/Al1A 85.4(6)/89.6(8), Yb1 – N7/N7A – Al1/Al1A 96.2(7)/98.4(9).

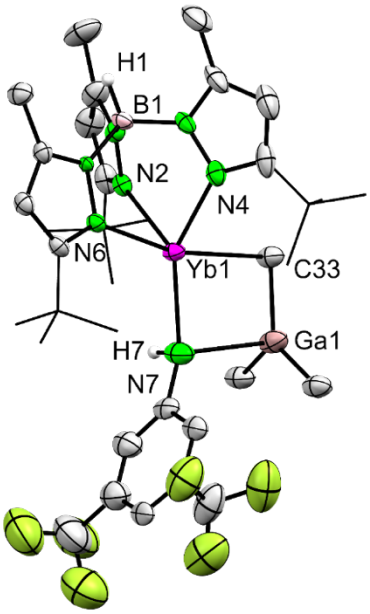

Figure S59 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ (**7**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the CF_3 and $GaMe_3$ groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.431(6), Yb1 – N4 2.425(6), Yb1 – N6 2.440(5), Yb1 – N7/N7A 2.471(14)/2.477(12), Yb1 – C33 2.868(8), Yb1 – Ga1/Ga1A 3.382(8)/3.458(11), Yb1 – N7/N7A – H7/H7A 100.1/102.9, Yb1 – N7/N7A – C25/C25A, 140.0(13)/131.6(14), Yb1 – C33 – Ga1/Ga1A 84.6(4)/88.5(4), Yb1 – N7/N7A – Ga1/Ga1A 94.9(6)/97.8(6).

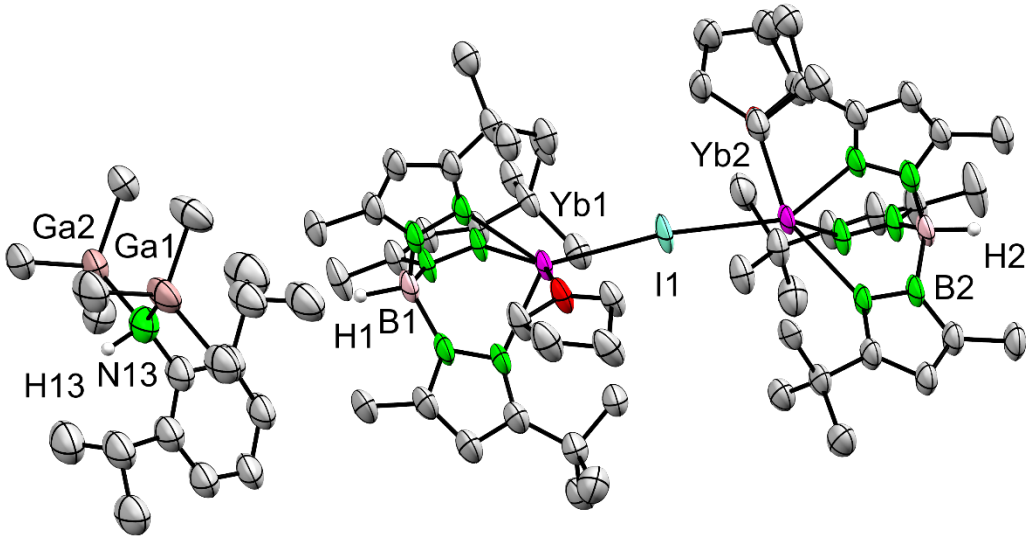

Figure S60 Crystal structure of $[(Tp^{tBu,Me})_2Yb_2I][NHAr^{iPr}(GaMe_3)_2]$ (**8**). Due to bad crystallization properties only a connectivity was obtained.

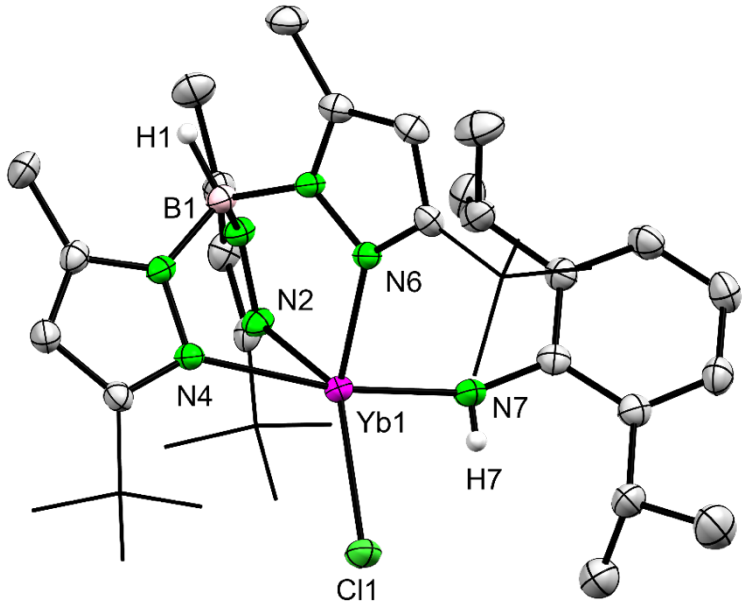

Figure S61 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{iPr})(Cl)$ (**9a**). All atoms are represented by atomic displacement ellipsoids set at 50 % probability. Hydrogen atoms and disorders of the CF_3 groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.326(2), Yb1 – N4 2.476(2), Yb1 – N6 2.303(2), Yb1 – N7 2.160(2), Yb1 – Cl1 2.5152(11), Yb1 – N7 – C25 156.08(19), Cl1 – Yb1 – N7 87.23(7).

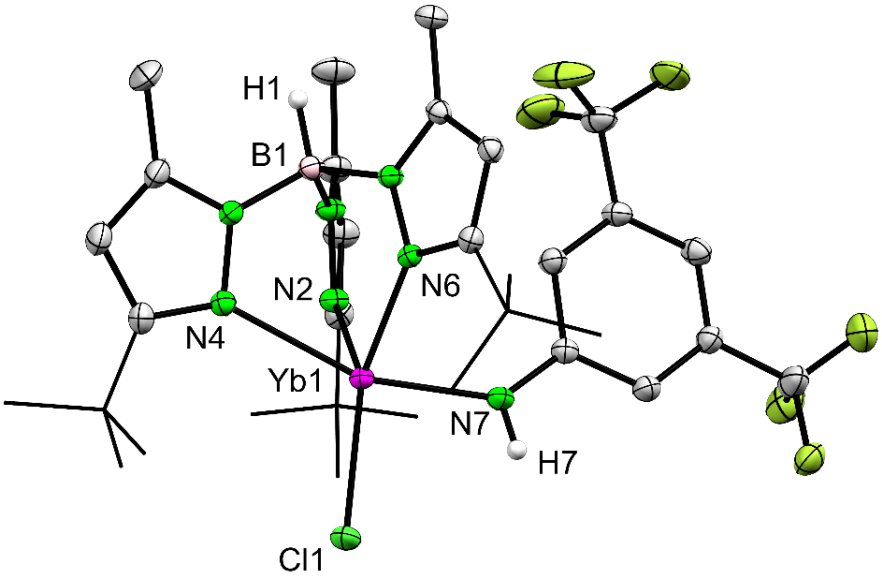

Figure S62 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(Cl)$ (**10a**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the CF_3 groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.3155(14), Yb1 – N4 2.4249(13), Yb1 – N6 2.3315(13), Yb1 – N7 2.2131(14), Yb1 – Cl1 2.5217(4), Yb1 – N7 – C25 137.42(11), Cl1 – Yb1 – N7 91.71(4).

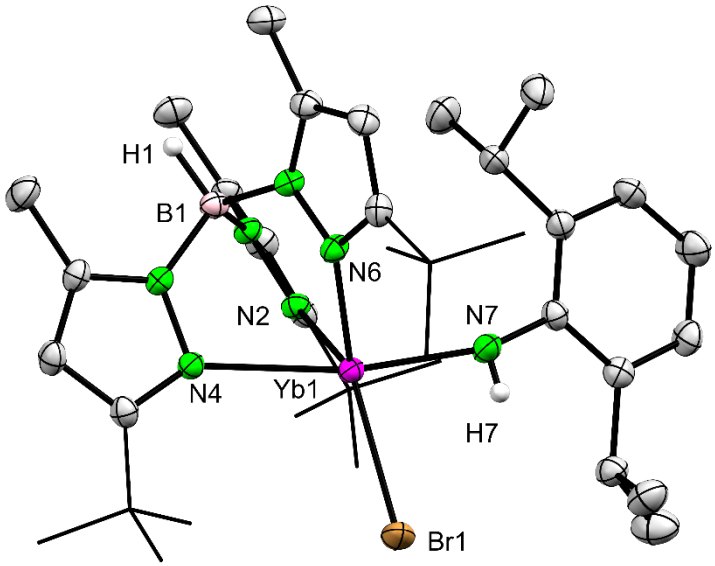

Figure S63 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{iPr})(Br)$ (**9b**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.331(2), Yb1 – N4 2.485(2), Yb1 – N6 2.305(2), Yb1 – N7 2.162(2), Yb1 – Br1 2.6947(13), Yb1 – N7 – C25 155.52(16), Br1 – Yb1 – N7 87.00(7).

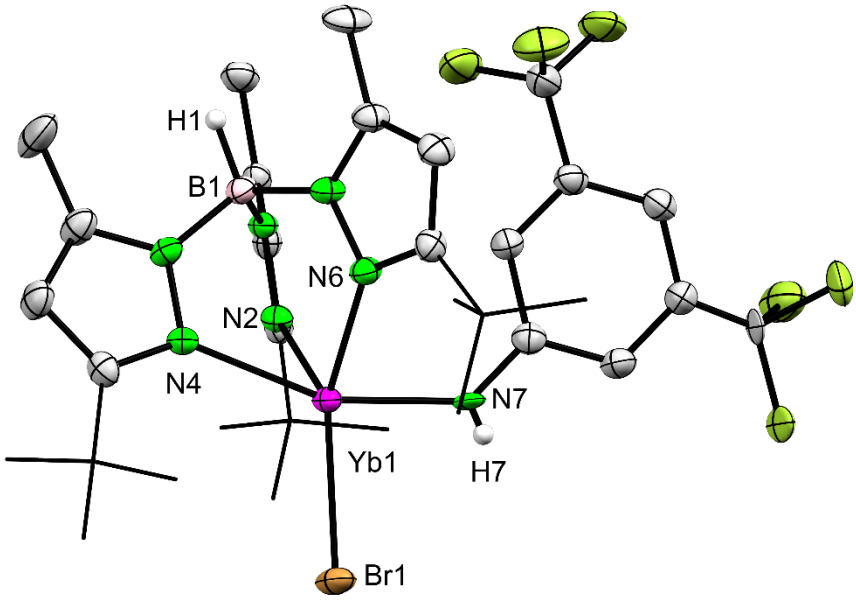

Figure S64 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(Br)$ (**10b**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of one CF_3 group are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.419 (3), Yb1 – N4 2.321(3), Yb1 – N6 2.307(3), Yb1 – N7 2.253(3), Yb1 – Br1 2.6760(4), Yb1 – N7 – C25 136.6(2), Br1 – Yb1 – N7 91. 40(6).

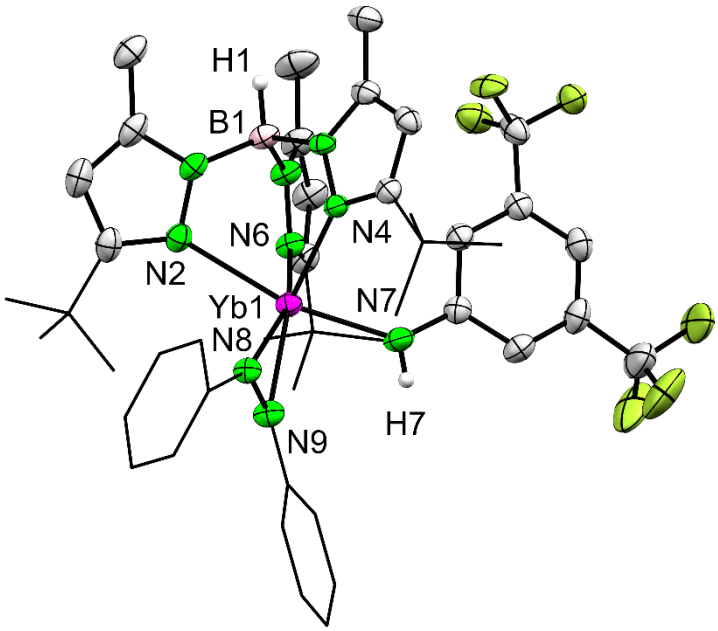

Figure S65 Crystal structure of $Tp^{tBu,Me}Yb(NHAr^{CF3})(N_2Ph_2)$ (**11**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the *i*Pr and one *t*Bu groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb – N2 2.449(2), Yb1 – N4 2.378(2), Yb1 – N6 2.360(2), Yb1 – N7 2.233(3), Yb1 – N8 2.274(2), Yb1 – N9 2.229(2), Yb1 – N7 –C25 136.0(2), Yb1 – N7 – H7 115(3), N7 – Yb1 – N8 107.80(9), N7 – Yb1 – N9 86.78(10).

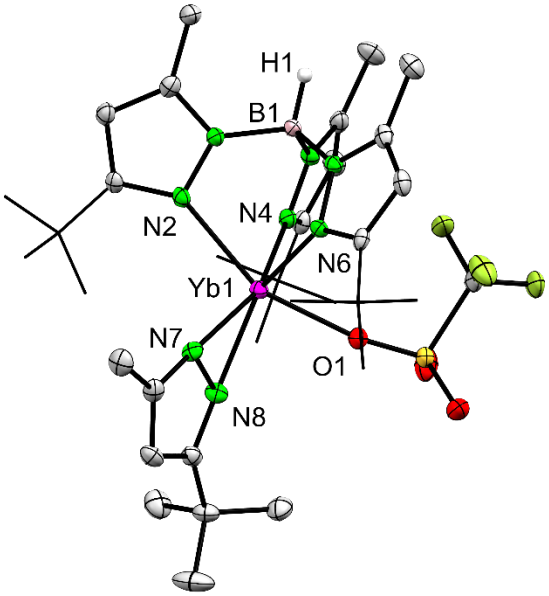

Figure S66 Crystal structure of $Tp^{tBu,Me}Yb(pz^{tBu,Me})(OTf)$ (**12**). All atoms are represented by atomic displacement ellipsoids set at 50% probability. Hydrogen atoms and disorders of the *i*Pr and one *t*Bu groups are omitted for clarity. Selected interatomic distances [Å] and angles [°]: Yb1 – N2 2.380(3), Yb1 – N4 2.345(3), Yb1 – N6 2.366(3), Yb1 – N7 2.272(3), Yb1 – N8 2.230(3), Yb1 – O1 2.216(3).

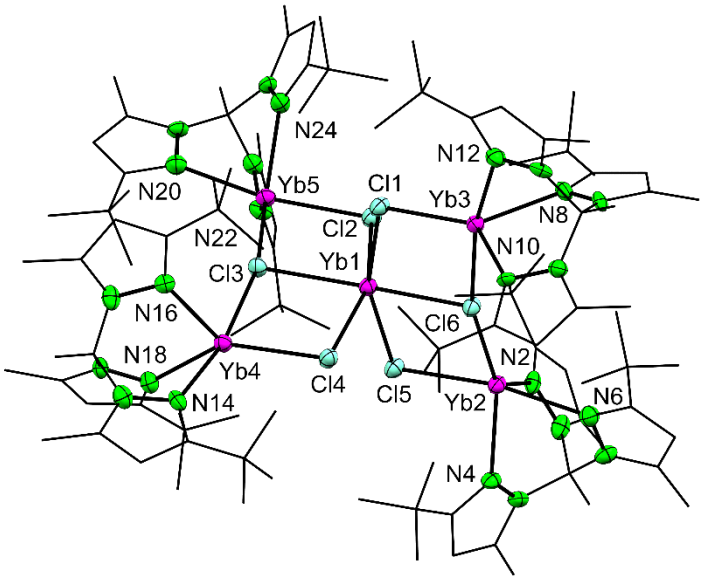

Figure S67 Crystal structure of $(Tp^{tBu,Me})_4Yb_6Cl_6$ (**13**). Due to bad crystallization properties only a connectivity was obtained.

Table **S1** Crystallographic data of compounds **1**^{thf}, **1** and **2**

Compound[a]	Tp^{tBu,Me}Yb(NHAr^{iPr})(thf) **1**^{thf}	Tp^{tBu,Me}Yb(NHAr^{iPr}) **1**	Tp^{tBu,Me}Yb(NHAr^{Me}) **2**
Molecular formula	$C_{43}H_{73}BN_7OYb$	$C_{36}H_{58}BN_7Yb$	$C_{32}H_{50}BN_7Yb$
CCDC No.	2248528	2248521	2248522
M [g/mol]	887.93	772.74	716.64
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.156 x 0.134 x 0.090	0.246 x 0.134 x 0.072	0.460 x 0.094 x 0.065
Crystal description	orange needle	red needle	orange needle
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	C2/c	$P2_1/n$	$Pca2_1$
a [Å]	21.1160(14)	9.5488(4)	19.726(2)
b [Å]	13.3578(9)	23.9283(11)	10.5723(12)
c [Å]	32.769(2)	16.2362(7)	16.2311(19)
α [°]	90	90	90
β [°]	101.5050(10)	93.3820(10)	90
γ [°]	90	90	90
V [³]	9057.2(11)	3384.9(7)	3384.9(7)
Z	8	4	4
ρ [mg/m³]	1.302	1.386	1.406
μ [mm^{-1}]	2.104	2.559	2.794
F (000)	3704	1592	1464
θ range [°]	2.099 to 28.700	2.116 to 29.227	2.065 to 30.403
Indices	-28<=h<=28	-12<=h<=11	-26<=h<=28
	-18<=k<=18	-20<=k<=32	-13<=k<=15
	-44<=l<=43	-22<=l<=22	-23<=l<=23
Number of reflexes	91652	30426	33340
Unique reflexes	11676	9592	10155
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0446, wR2 = 0.0984	R1 = 0.0512, wR2 = 0.1024	R1 = 0.0360, wR2 = 0.0756
R1[a]/wR2[a] (all)	R1 = 0.0542, wR2 = 0.1014	R1 = 0.0926, wR2 = 0.1196	R1 = 0.0580, wR2 = 0.0872
GOF [c]	1.256	1.001	1.024

[c]GOF = $[\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compounds **3**^{thf}, **4**^{thf} and **1**^{thf,Sm}

Compound[a]	$Tp^{tBu,Me}Yb(NHAr^{CF3})(thf)_2$ **3**^{thf}	$Tp^{tBu,Me}Yb(NHSiPh_3)(thf)$ **4**^{thf}	$Tp^{tBu,Me}Sm(NHAr^{iPr})(thf)$ **1**^{thf,Sm}
Molecular formula	$C_{43}H_{67}BF_6N_7O_2Yb$	$C_{46}H_{64}BN_7OSiYb$	$C_{40}H_{66}BN_7OSm$
CCDC No.	2248537	2248530	2248529
M [g/mol]	1011.88	942.98	822.15
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.244 x 0.062 x 0.049	0.226 x 0.225 x 0.205	0.193 x 0.140 x 0.117
Crystal description	red needle	red block	green block
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P1	C2/c	$P2_1/c$
a [Å]	11.6419(9)	41.2689(13)	9.9313(5)
b [Å]	12.1357(10)	11.6943(4)	16.9639(8)
c [Å]	17.4345(14)	19.9784(7)	24.6920(12)
α [°]	100.123(3)	90	90
β [°]	107.912(3)	90.4350(10)	93.4090(10)
γ [°]	90.396(3)	90	90
V [^{3}]	2302.4(3)	9641.5(6)	4152.6(4)
Z	2	8	4
ρ [mg/m^3]	1.460	1.299	1.313
μ [mm^{-1}]	2.098	2.004	1.452
F (000)	1038	3888	1720
θ range [°]	1.249 to 26.505	1.810 to 28.308	2.043 to 30.519
Indices	-14<=h<=14	-54<=h<=43	-14<=h<=14
	-15<=k<=15	-15<=k<=15	-24<=k<=24
	-21<=l<=21	-26<=l<=26	-35<=l<=35
Number of reflexes	54467	64839	75787
Unique reflexes	18830	11912	12666
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0526, wR2 = 0.1091	R1 = 0.0289, wR2 = 0.0649	R1 = 0.0328, wR2 = 0.0767
R1[a]/wR2[a] (all)	R1 = 0.0837, wR2 = 0.1253	R1 = 0.0369, wR2 = 0.0682	R1 = 0.0486, wR2 = 0.0851
GOF [c]	1.067	1.030	1.028

[c]GOF = $[\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compounds $\mathbf{1}^{thf,Eu}$, $\mathbf{1}^{py}$ and $\mathbf{1}^{dmap}$

Compound[a]	$Tp^{tBu,Me}Eu(NHAr^{iPr})(thf)$ $\mathbf{1}^{thf,Eu}$	$Tp^{tBu,Me}Yb(NHAr^{iPr})(py)$ $\mathbf{1}^{py}$	$Tp^{tBu,Me}Yb(NHAr^{iPr})(dmap)$ $\mathbf{1}^{dmap}$
Molecular formula	$C_{40}H_{66}BEuN_7O$	$C_{41}H_{63}BN_8Yb$	$C_{43}H_{68}BN_9Yb$
CCDC No.	2248540	2248527	2248526
M [g/mol]	823.76	851.84	894.91
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.190 x 0.088 x 0.033	0.253 x 0.057 x 0.044	0.400 x 0.179 x 0.146
Crystal description	yellow needle	black needle	red block
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1$	$P2_1/c$	$P2_1/n$
a [Å]	9.934(6)	11.854(7)	11.1230(7)
b [Å]	16.980(10)	21.460(14)	21.4324(13)
c [Å]	12.308(8)	19.117(11)	18.9230(11)
α [°]	90	90	90
β [°]	93.396(16)	96.938(10)	97.5190(10)
γ [°]	90	90	90
V [3]	2073(2)	4827(5)	4472.3(5)
Z	2	4	4
ρ [mg/m³]	1.320	1.172	1.329
μ [mm⁻¹]	1.551	1.970	2.130
F (000)	862	1760	1856
θ range [°]	1.657 to 30.507	1.731 to 27.102	2.171 to 30.534
Indices	-14<=h<=14	-15<=h<=13	-15<=h<=15
	-24<=k<=24	-27<=k<=27	-30<=k<=30
	-15<=l<=17	-21<=l<=24	-24<=l<=26
Number of reflexes	55048	51249	81723
Unique reflexes	12637	10647	13646
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0305, wR2 = 0.0635	R1 = 0.0517, wR2 = 0.1168	R1 = 0.0238, wR2 = 0.0559
R1[a]/wR2[a] (all)	R1 = 0.0378, wR2 = 0.0675	R1 = 0.0818, wR2 = 0.1313	R1 = 0.0306, wR2 = 0.0586
GOF [c]	1.041	0.961	1.044

[c]GOF = $[\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compounds **3**^{dmap}, **4**^{dmap} and **5**

Compound[a]	$Tp^{tBu,Me}Yb(NHAr^{CF3})(dmap)$ **3**^{dmap}	$Tp^{tBu,Me}Yb(NHSiPh_3)(dmap)$ **4**^{dmap}	$Eu(Tp^{tBu,Me})_2$ **5**
Molecular formula	$C_{39}H_{54}BF_6N_9Yb$	$C_{63}H_{82}BN_9SiYb$	$C_{48}H_{80}B_2EuN_{12}\cdot 1/2C_5H_{12}$
CCDC No.	2248541	2248531	2248536
M [g/mol]	946.76	1177.31	1034.89
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.113 x 0.062 x 0.039	0.402 x 0.079 x 0.065	0.321 x 0.129 x 0.047
Crystal description	orange plate	yellow block	yellow block
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/c$	$P2_1/n$
a [Å]	12.013(10)	11.3413(10)	12.110(9)
b [Å]	12.377(10)	19.1966(18)	25.76(2)
c [Å]	16.032(14)	27.315(3)	17.757(12)
α [°]	85.204(12)	90	90
β [°]	87.406(10)	90.707(2)	92.761(12)
γ [°]	64.265(12)	90	90
V [^{3}]	2140(3)	5946.4(9)	5534(7)
Z	2	8	4
ρ [mg/m^3]	1.470	1.315	1.242
μ [mm^{-1}]	2.250	1.639	1.177
F (000)	960	2448	2184
θ range [°]	1.275 to 28.517	1.297 to 26.418	1.394 to 28.386
Indices	-16<=h<=16	-14<=h<=14	-16<=h<=16
	-16<=k<=16	-23<=k<=24	-34<=k<=34
	-21<=l<=21	-33<=l<=34	-23<=l<=23
Number of reflexes	81932	73316	82682
Unique reflexes	10733	12169	13753
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0531, wR2 = 0.1264	R1 = 0.0360, wR2 = 0.0753	R1 = 0.0511, wR2 = 0.1076
R1[a]/wR2[a] (all)	R1 = 0.0799, wR2 = 0.1439	R1 = 0.0583, wR2 = 0.0846	R1 = 0.0972, wR2 = 0.1274
GOF [c]	1.016	1.007	1.011

[c]$GOF = [\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compounds **6**, **7** and **8**

Compound[a]	$Tp^{tBu,Me}Yb(NHAr^{CF3})(AlMe_3)$ **6**	$Tp^{tBu,Me}Yb(NHAr^{CF3})(GaMe_3)$ **7**	$[(Tp^{tBu,Me})_2Yb_2I][NHAr^{iPr}(GaMe_3)_2]$ **8***
Molecular formula	$C_{35}H_{53}AlBF_6N_7Yb$	$C_{35}H_{53}GaBF_6N_7Yb$	$C_{95}H_{156}B_2Ga_2IN_{13}O_2Yb$
CCDC No.	2248523	2248525	2248534
M [g/mol]	896.67	939.41	2146.36
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.142 x 0.139 x 0.098	0.198 x 0.123 x 0.057	0.248 x 0.058 x 0.037
Crystal description	Yellow needle	Yellow needle	yellow needle
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a [Å]	9.6523(8)	9.6012(8)	17.520(15)
b [Å]	17.0921(15)	17.1131(14)	30.61(3)
c [Å]	25.098(2)	25.200(2)	19.717(18)
α [°]	90	90	90
β [°]	90.5840(10)	90.868(3)	103.34(3)
γ [°]	90	90	90
V [3]	4140.4(6)	4140.0(6)	10291(16)
Z	4	4	4
ρ [mg/m³]	1.438	1.507	1.385
μ [mm⁻¹]	2.340	2.955	2.669
F (000)	1816	1888	4392
θ range [°]	1.623 to 26.369	1.438 to 28.474	1.194 to 27.679
Indices	-12<=h<=12	-12<=h<=10	-22<=h<=22
	-21<=k<=21	-22<=k<=22	-35<=k<=35
	-31<=l<=31	-33<=l<=32	-20<=l<=20
Number of reflexes	55710	73872	124709
Unique reflexes	8434	10363	17261
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0443, wR2 = 0.0997	R1 = 0.0656, wR2 = 0.1500	R1 = 0.0806, wR2 = 0.1817
R1[a]/wR2[a] (all)	R1 = 0.0608, wR2 = 0.1096	R1 = 0.0981, wR2 = 0.1674	R1 = 0.1963, wR2 = 0.2386
GOF [c]	1.035	1.055	1.008

[c]$GOF = [\Sigma w(F_o^2 - F_c^2)^2 / (n_o - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$, $F_o > 4\sigma(F_o)$. [b]$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2 / \Sigma[w(F_o^2)^2]\}^{1/2}$; * only connectivity obtained.

Table **S1** continued Crystallographic data of compounds **9a**, **10a** and **9b**

Compound[a]	$Tp^{tBu,Me}Yb(NHAr^{iPr})(Cl)$ **9a**	$Tp^{tBu,Me}Yb(NHAr^{CF3})(Cl)$ **10a**	$Tp^{tBu,Me}Yb(NHAr^{iPr})(Br)$ **9b**
Molecular formula	$C_{36}H_{58}BClN_7Yb$	$C_{32}H_{44}BClF_6N_7Yb$	$C_{36}H_{58}BBrN_7Yb$
CCDC No.	2248524	2248533	2248532
M [g/mol]	808.19	860.04	852.65
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal dimensions [mm]	0.119 x 0.113 x 0.094	0.154 x 0.128 x 0.125	0.179 x 0.119 x 0.105
Crystal description	intense blue needle	purple needle	turquoise needle
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$
a [Å]	11.645(6)	11.6245(3)	11.675(8)
b [Å]	18.016(10)	16.0723(4)	18.213(13)
c [Å]	18.923(10)	20.2693(5)	18.789(13)
α [°]	90	90	90
β [°]	98.925(10)	104.3460(10)	98.165(19)
γ [°]	90	90	90
V [3]	3922(4)	3668.87(16)	3955(5)
Z	4	4	4
ρ [mg/m³]	1.369	1.557	1.432
μ [mm⁻¹]	2.486	2.685	3.408
F (000)	1660	1724	1732
θ range [°]	1.570 to 28.336	1.637 to 30.539	1.565 to 30.544
Indices	-15<=h<=15	-16<=h<=15	-16<=h<=16
	-24<=k<=24	-22<=k<=22	-26<=k<=26
	-25<=l<=25	-28<=l<=24	-26<=l<=26
Number of reflexes	61775	79290	202113
Unique reflexes	9777	11225	12111
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0257, wR2 = 0.0536	R1 = 0.0201, wR2 = 0.0473	R1 = 0.0257, wR2 = 0.0570
R1[a]/wR2[a] (all)	R1 = 0.0360, wR2 = 0.0580	R1 = 0.0236, wR2 = 0.0490	R1 = 0.0345, wR2 = 0.0612
GOF [c]	1.022	1.048	1.069

[c]$GOF = [\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compounds **10b**, **11** and **12**

Compound[a]	$Tp^{tBu,Me}Yb(NHAr^{CF3})(Br)$ **10b**	$Tp^{tBu,Me}Yb(NHAr^{CF3})(N_2Ph_2)$ **11**	$Tp^{tBu,Me}Yb(pz^{tBu,Me})(OTf)$ **12**
Molecular formula	$C_{32}H_{44}BBrF_6N_7Yb$	$C_{44}H_{54}BF_6N_9Yb$	$C_{33}H_{53}BF_3N_8O_3SYb$
CCDC No.	2248539	2248535	2248520
M [g/mol]	904.50	1006.81	882.74
Temperature [K]	100(2)	100(2)	100(2)
Wavelength [Å]	0.71073	0.71073	0.710703
Crystal dimensions [mm]	0.142 x 0.120 x 0.116	0.251 x 0.091 x 0.089	2.461
Crystal description	deep blue needle	yellow needle	light green plate
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
a [Å]	11.7019(11)	10.2802(4)	10.572(12)
b [Å]	16.1670(15)	12.5250(5)	11.769(13)
c [Å]	20.2544(19)	18.7909(8)	17.94(2)
α [°]	90	94.0850(10)	87.201(18)
β [°]	104.1270(10)	94.0530(10)	83.321(18)
γ [°]	90	111.3230(10)	63.69(3)
V [³]	3715.9(6)	2235.98(16)	1988(4)
Z	4	2	2
ρ [mg/m³]	1.617	1.495	1.475
μ [mm^{-1}]	3.654	2.158	2.461
F (000)	1796	1020	898
θ range [°]	1.631 to 27.102	1.755 to 28.310	1.143 to 26.341
Indices	-15<=h<=15	-13<=h<=13	-13<=h<=13
	-20<=k<=20	-16<=k<=16	-14<=k<=14
	-25<=l<=25	-25<=l<=25	0<=l<=22
Number of reflexes	53047	52910	8088
Unique reflexes	8187	11115	8088
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0283, wR2 = 0.0559	R1 = 0.0319, wR2 = 0.0709	R1 = 0.0261, wR2 = 0.0587
R1[a]/wR2[a] (all)	R1 = 0.0459, wR2 = 0.0622	R1 = 0.0410, wR2 = 0.0749	R1 = 0.0296, wR2 = 0.0604
GOF [c]	1.029	1.038	1.069

[c]$GOF = [\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$.

Table **S1** continued Crystallographic data of compound **13**

Compound[a]	$(Tp^{tBu,Me})_4Yb_5Cl_6$ **13***
Molecular formula	$C_{108}H_{188}B_4Cl_4N_{24}Yb_5$
CCDC No.	2248538
M [g/mol]	2943.95
Temperature [K]	97(2)
Wavelength [Å]	0.71073
Crystal dimensions [mm]	0.136 x 0.056 x 0.047
Crystal description	green-yellow plate
Crystal system	Monoclinic
Space group	C2/c
a [Å]	46.844(2)
b [Å]	19.2663(8)
c [Å]	28.8401(13)
α [°]	90
β [°]	96.973(2)
γ [°]	90
V [³]	25836.1(19)
Z	8
ρ [mg/m³]	1.514
μ [mm^{-1}]	3.760
F (000)	11808
θ range [°]	1.144 to 26.404
Indices	-58<=h<=58
	-24<=k<=24
	-36<=l<=36
Number of reflexes	256180
Unique reflexes	26462
R1[a]/wR2[b] (I < 2σ)	R1 = 0.0537, wR2 = 0.0875
R1[a]/wR2[a] (all)	R1 = 0.1168, wR2 = 0.1428
GOF [c]	0.999

[c]GOF = $[\Sigma w(F_0^2 - F_c^2)^2 / (n_0 - n_p)]^{1/2}$. [a]$R_1 = \Sigma(||F_0| - |F_c||) / \Sigma|F_0|$, $F_0 > 4\sigma(F_0)$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)^2 / \Sigma[w(F_0^2)^2]\}^{1/2}$; * only connectivity obtained.