Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

In situ Synthesis of Lanthanide Complexes Supported by a Ferrocene Diamide Ligand: Extension to Redox-Active Lanthanide Ions

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X-Ray Crystallography Data S2

(NN^{TBS})CeI(THF)$_2$

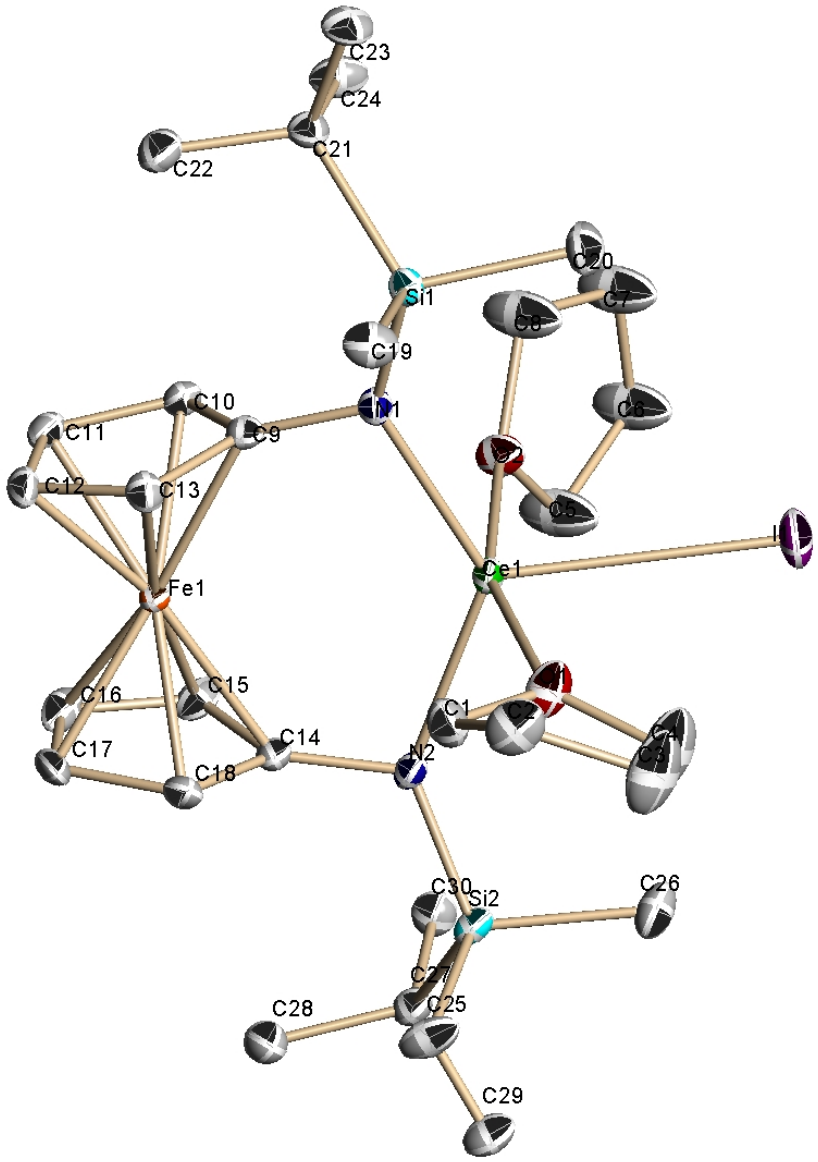

Figure S1. Thermal-ellipsoid (50% probability) representation of one of the two crystallographically independent molecules of (NN^{TBS})CeI(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{30}H_{54}IFeCeO_2N_2Si_2$; M_r = 853.80; triclinic; space group P-1; *a* = 11.347(3) Å; *b* = 11.360(3) Å; *c* = 16.303(7) Å; α = 99.150(5)°; β = 93.557(5) °; γ = 118.858(3)°; V = 1793.7(11) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 2.612 mm^{-1}; d_{calc} = 1.581 g·cm^{-3}; 25177 reflections collected; 10133 unique (R_{int} = 0.0242); giving R_1 = 0.0330 for 8971 data with [I>2σ(I)] and R_1 = 0.0380, wR_2 = 0.0790 for all 10133 data. Residual electron density (e$^-$·Å^{-3}) max/min: 1.85/-1.86.

[(NN^{TBS})Pr(THF)(μ-I)]$_2$

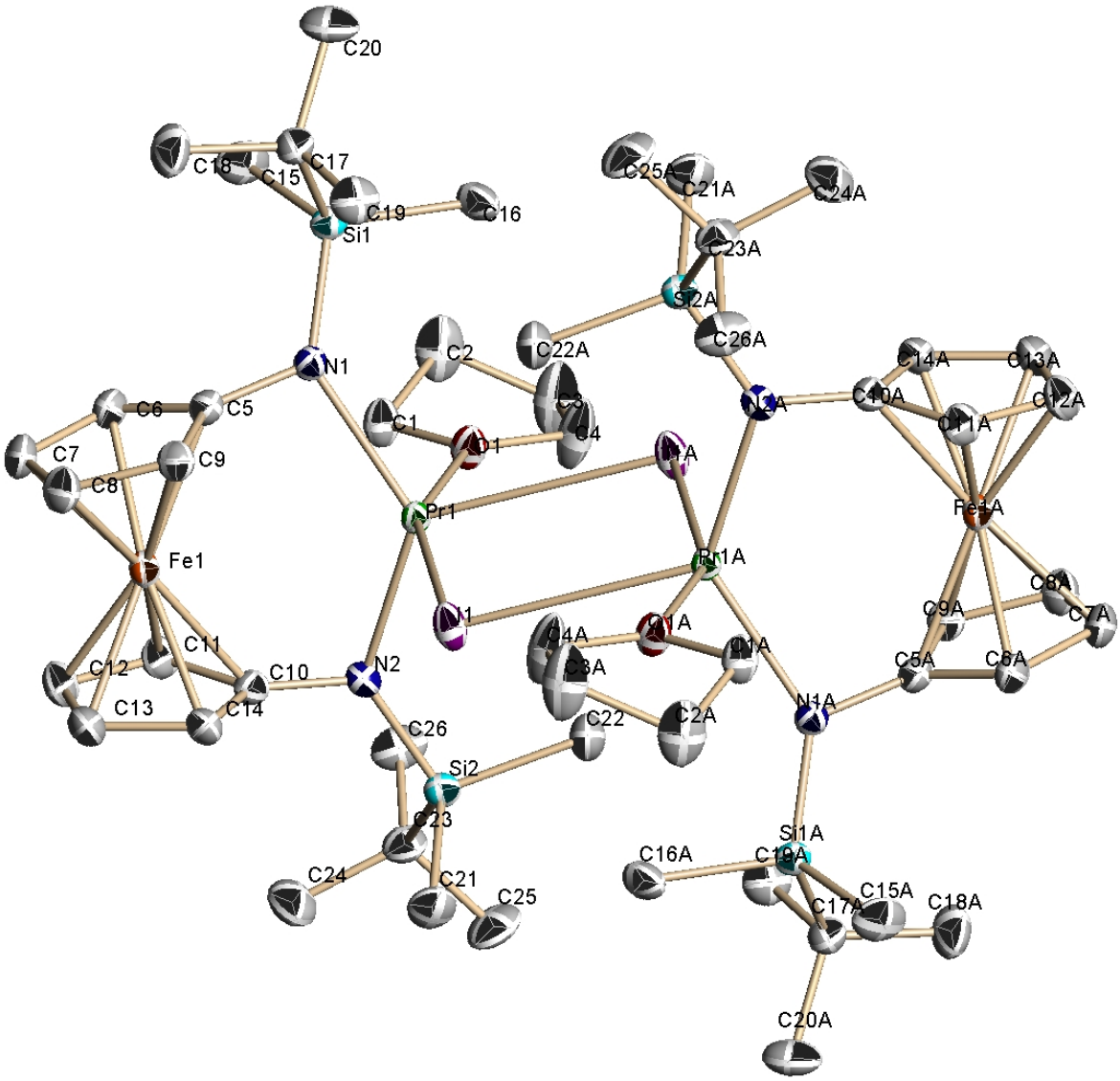

Figure S2. Thermal-ellipsoid (50% probability) representation of [(NN^{TBS})Pr(THF)(μ-I)]$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{52}H_{92}Fe_2I_2N_4O_2Si_4Pr_2$; M_r = 1564.98; monoclinic; space group P21/n; *a* = 14.879(4) Å; *b* = 13.738(4) Å; *c* = 15.468(4) Å; α = 90°; β = 91.074(3)°; γ = 90°; V = 3161.3(15) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 3.054 mm^{-1}; d_{calc} = 1.644 g·cm^{-3}; 43971 reflections collected; 9270 unique (R_{int} = 0.0283); giving R_1 = 0.0226 for 8022 data with [I>2σ(I)] and R_1 = 0.0299, wR_2 = 0.0520 for all 9270 data. Residual electron density (e$^-$·Å^{-3}) max/min: 0.78/-0.70.

(NN^{TBS})SmI(THF)$_2$

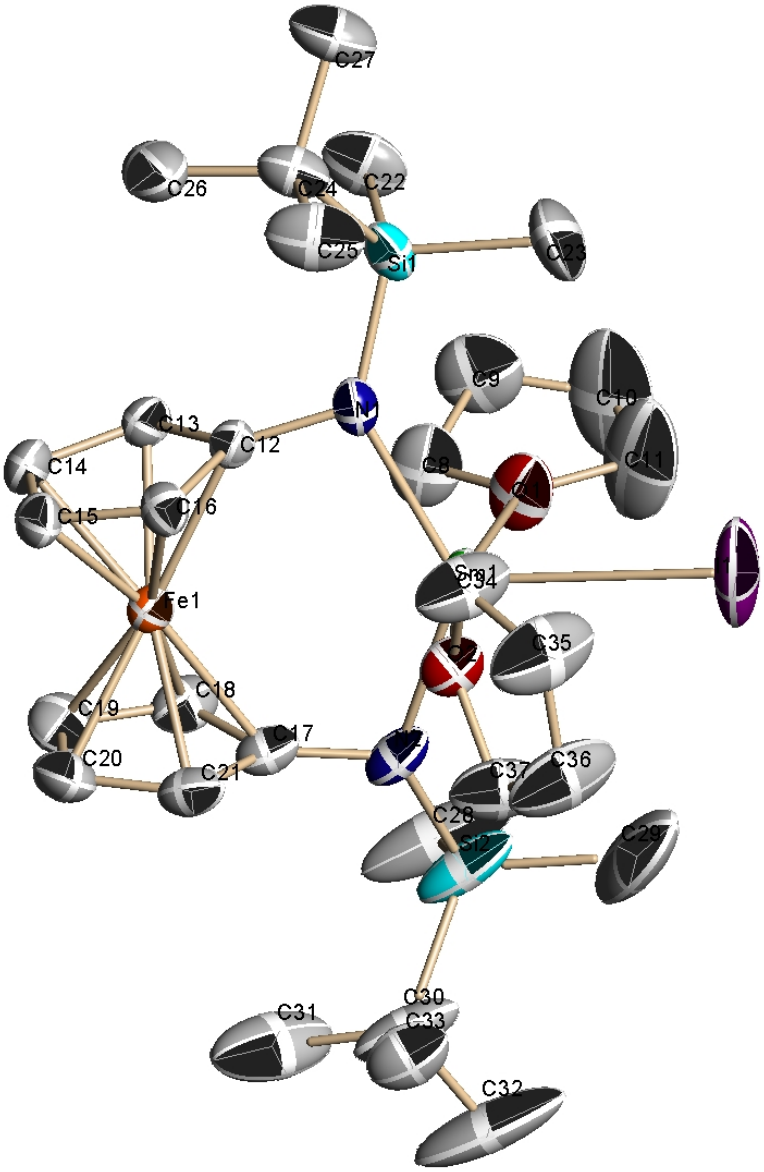

Figure S3. Thermal-ellipsoid (50% probability) representation of (NN^{TBS})SmI(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{60}H_{108}Fe_2I_2N_4O_2Si_4Sm_2$; M_r = 1728.06; triclinic; space group P-1; a = 11.2530(13) Å; b = 11.6706(13) Å; c = 16.3205(19) Å; α = 101.063(1)°; β = 92.506(1)°; γ = 118.408(1)°; V = 1827.5(4) Å^3; Z = 1; T = 100(2) K; λ = 0.71073 Å; μ = 2.925 mm^{-1}; d_{calc} = 1.570 g·cm^{-3}; 25436 reflections collected; 10243 unique (R_{int} = 0.0175); giving R_1 = 0.0371 for 8822 data with [I>2σ(I)] and R_1 = 0.0443, wR_2 = 0.0854 for all 10243 data. Residual electron density (e$^-$·Å^{-3}) max/min: 1.62/-2.95.

(NN^{TBS})TbI(THF)$_2$

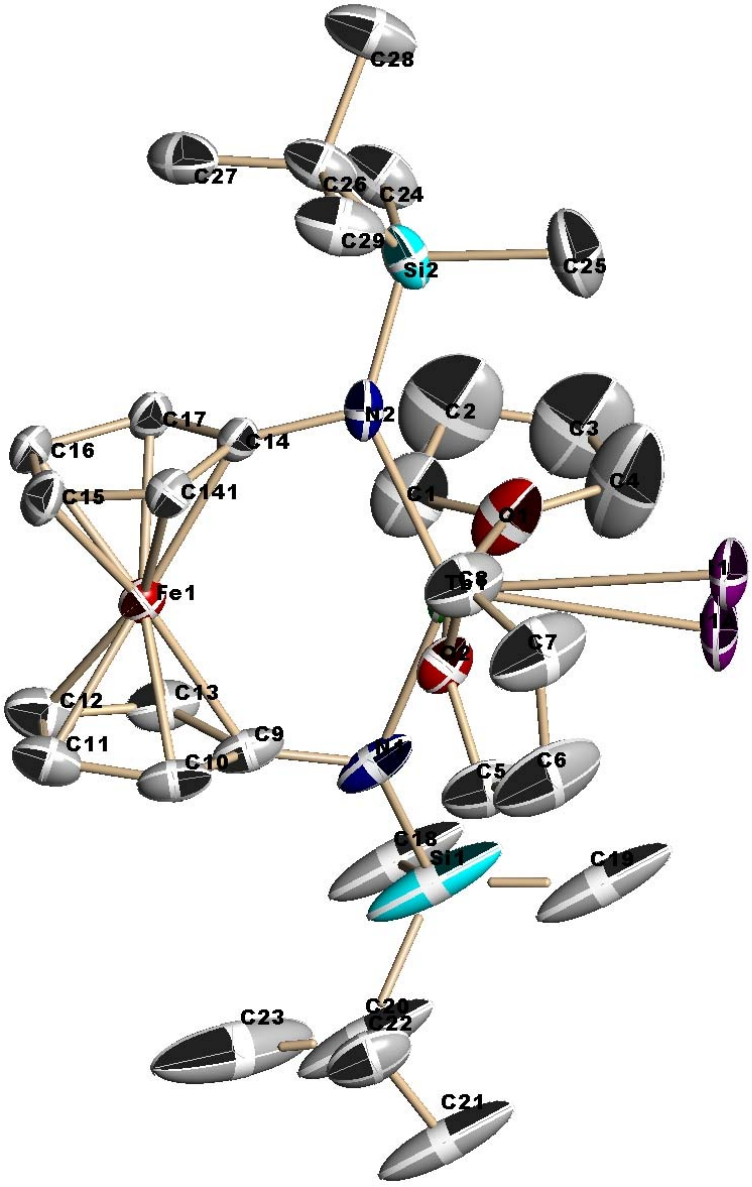

Figure S4. Thermal-ellipsoid (50% probability) representation of (NN^{TBS})TbI(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{30}H_{54}IFeTbO_2N_2Si_2$; M_r = 872.60; triclinic; space group P-1; *a* = 11.130(4) Å; *b* = 11.608(5) Å; *c* = 16.122(9) Å; α = 101.564(6)°; β = 91.881(6)°; γ = 118.404(4)°; V = 1775.0(14) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 3.349 mm^{-1}; d_{calc} = 1.633 g·cm^{-3}; 24683 reflections collected; 9991 unique (R_{int} = 0.0309); giving R_1 = 0.0589 for 7766 data with [I>2σ(I)] and R_1 = 0.0791, wR_2 = 0.1467 for all 9991 data. Residual electron density (e$^-$·Å^{-3}) max/min: 3.07/-5.08.

(NN^{TBS})TmI(THF)$_2$

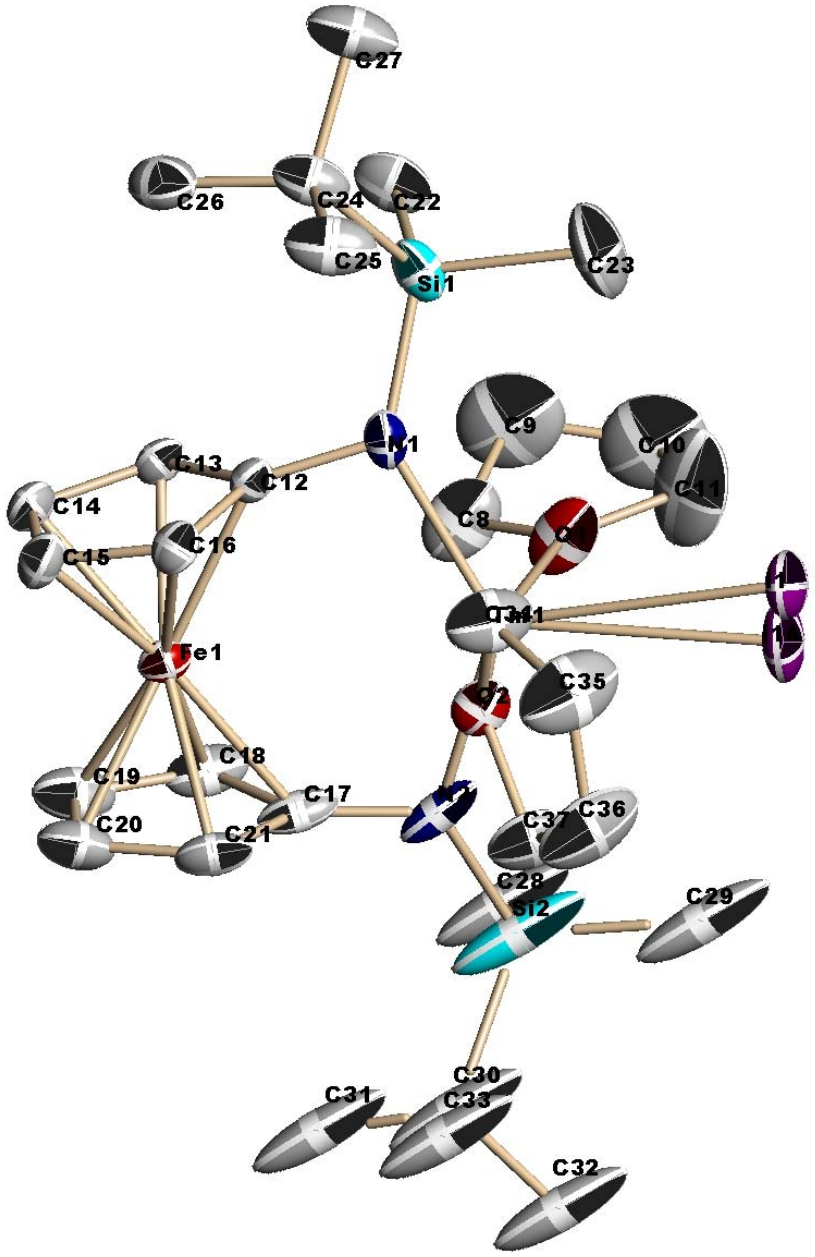

Figure S5. Thermal-ellipsoid (50% probability) representation of (NN^{TBS})TmI(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{30}H_{54}IFeTmO_2N_2Si_2$; M_r = 882.61; triclinic; space group P-1; a = 11.140(3) Å; b = 11.605(3) Å; c = 16.073(7) Å; α = 101.474(5)°; β = 92.374(5)°; γ = 118.292(3)°; V = 1770.9(10) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 3.865 mm^{-1}; d_{calc} = 1.655 g·cm^{-3}; 24486 reflections collected; 9915 unique (R_{int} = 0.0242); giving R_1 = 0.0609 for 8240 data with [I>2σ(I)] and R_1 = 0.0741, wR_2 = 0.1399 for all 9915 data. Residual electron density (e$^-$·Å^{-3}) max/min: 3.95/-6.27.

(NN^{TBS})YbI(THF)$_2$

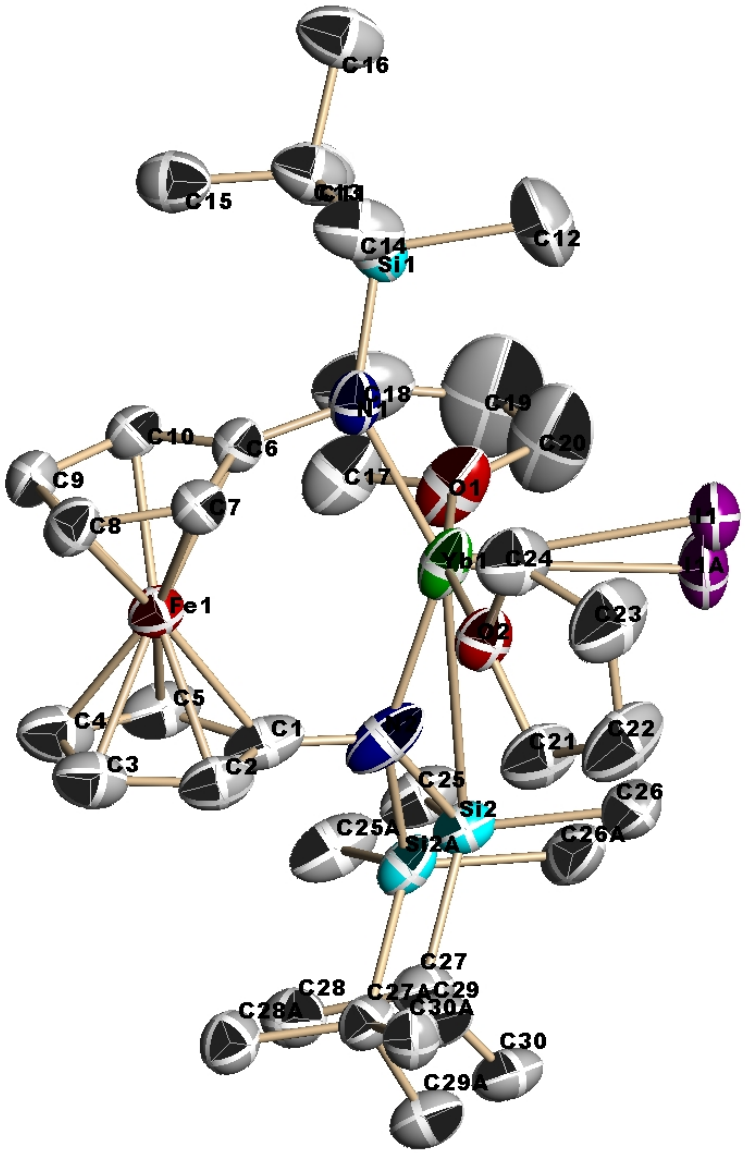

Figure S6. Thermal-ellipsoid (50% probability) representation of (NN^{TBS})YbI(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{30}H_{54}IFeYbO_2N_2Si_2$; M_r = 886.72; triclinic; space group P-1; *a* = 11.5979(17) Å; *b* = 11.6945(17) Å; *c* = 16.109(2) Å; α = 76.069(2)°; β = 78.510(2)°; γ = 56.888(2)°; V = 1770.1(4) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 4.002 mm^{-1}; d_{calc} = 1.664 g·cm^{-3}; 15984 reflections collected; crystal was a two component twin and refined, BASF was 0.48. B-level alert PLAT_ALERT_1_B and 4_B should be ignored as data was not merged due to twinning. C19 and C18 are THF carbons with some disorder; giving R_1 = 0.0420 for 13789 data with [I>2σ(I)] and R_1 = 0.0478, wR_2 = 0.1074 for all 15982 data. Residual electron density (e$^-$·Å^{-3}) max/min: 3.24/-4.73.

[K(toluene)][(NN^{TBS})$_2$Yb]

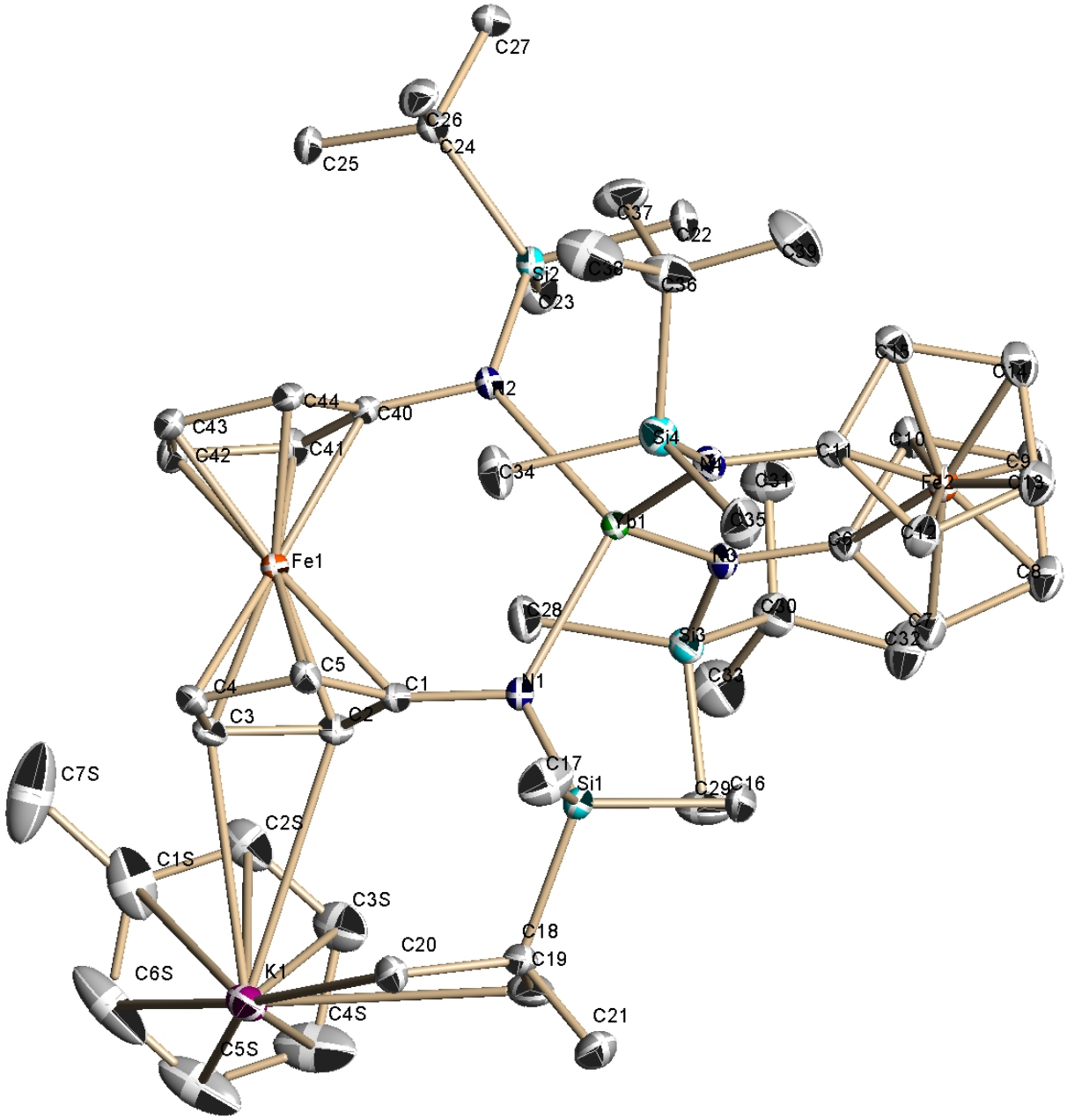

Figure S7. Thermal-ellipsoid (50% probability) representation of [K(toluene)][(NN^{TBS})$_2$Yb]. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{51}H_{84}KFe_2YbN_4Si_4$; M_r = 1189.42; orthorhombic; space group P212121; *a* = 13.541(2) Å; *b* = 19.611(3) Å; *c* = 20.563(3) Å; V = 5460.6(15) Å^3; Z = 4; T = 100(2) K; λ = 0.71073 Å; μ = 2.424 mm^{-1}; d_{calc} = 1.447 g·cm^{-3}; 76900 reflections collected; 16119 unique (R_{int} = 0.0417); giving R_1 = 0.0298 for 14904 data with [I>2σ(I)] and R_1 = 0.0310, wR_2 = 0.0761 for all 16119 data. Residual electron density (e$^-$·Å^{-3}) max/min: 2.56/-1.45.

(NN^{TBS})YbCl(THF)$_2$

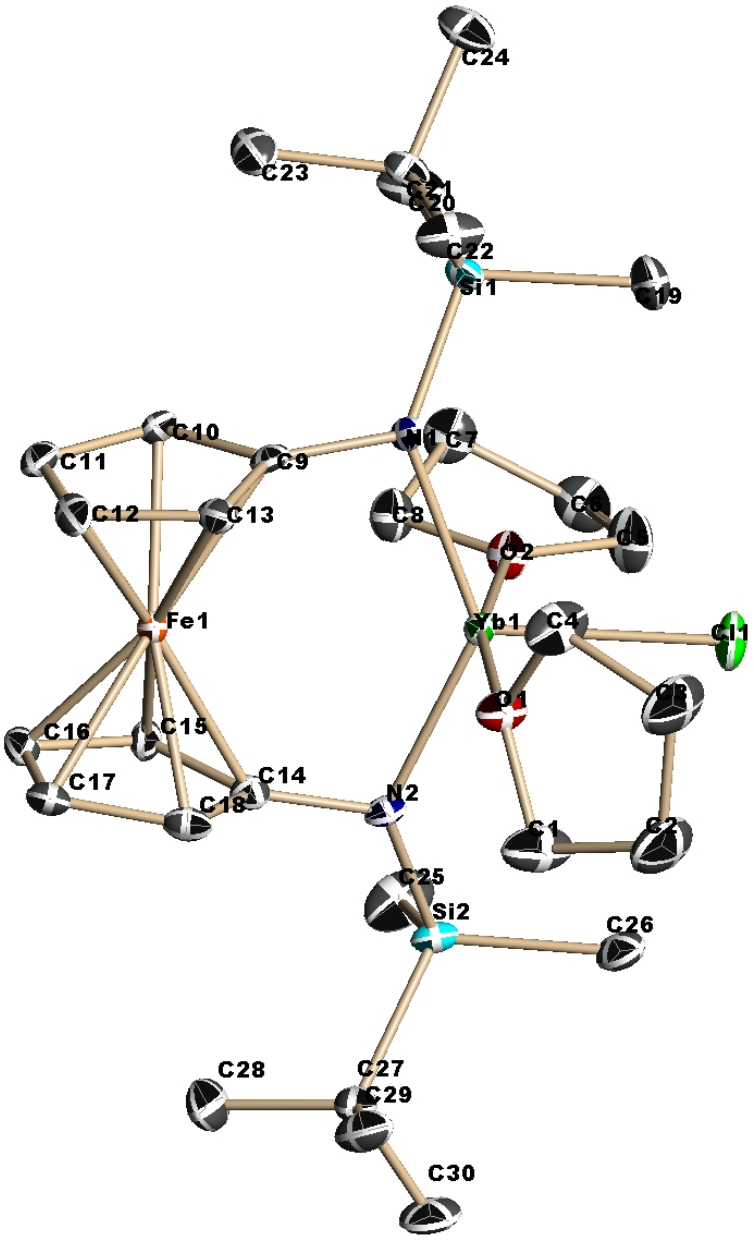

Figure S8. Thermal-ellipsoid (50% probability) representation of (NN^{TBS})YbCl(THF)$_2$. Hydrogen atoms were omitted for clarity.

Crystal data for $C_{30}H_{54}ClFeYbO_2N_2Si_2$; M_r = 795.27; triclinic; space group P-1; *a* = 10.605(4) Å; *b* = 11.350(4) Å; *c* = 16.204(6) Å; α = 100.677(4)°; β = 94.486(4)°; γ = 114.277(4)°; V = 1721.0(10) Å^3; Z = 2; T = 100(2) K; λ = 0.71073 Å; μ = 3.297 mm^{-1}; d_{calc} = 1.535 g·cm^{-3}; 22731 reflections collected; 6916 unique (R_{int} = 0.0309); giving R_1 = 0.0347 for 6277 data with [I>2σ(I)] and R_1 = 0.0380, wR_2 = 0.0945 for all 6916 data. Residual electron density (e$^-$·Å^{-3}) max/min: 3.03/-1.01.