Supplementary Information (SI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2026

Supplementary Information (SI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2026

Reactivity of homodinuclear rare-earth metal complexes with an indol-2-yl based pincer ligand toward nitrogen- and oxygen-containing compounds

Jianwu Wen,[a§] Fuxiang Chai,[a§] Yonghu Bao,[a] Mengxin Tao,[a] Zeming Huang,[b] Xiancui Zhu,*[a] Qingbing Yuan,[a] and Shaowu Wang,*[b,c]

Table of Contents

1. ^{1}H, $^{13}C\{^{1}H\}$, $^{11}B\{^{1}H\}$ & $^{31}P\{^{1}H\}$ NMR spectra of complexes 2
2. OLEX 2 drawing of complexes.....15
3. Tables of crystal data and structure refinement 28

[a.] *Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials, College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, Anhui (P.R. China).*
[b.] *Anhui Laboratory of Clean Catalytic Engineering, Anhui Laboratory of Functional Coordinated Complexes for Materials Chemistry and Application, College of Chemical and Environmental Engineering, Anhui Polytechnic University, Wuhu 241000, Anhui (P.R. China). *E-mail: wsw@ahpu.edu.cn.*
[c.] *State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032 (P.R. China).*

1. ^{1}H, ^{13}C{^{1}H}, ^{11}B{^{1}H} & ^{31}P{^{1}H} NMR spectra of complexes

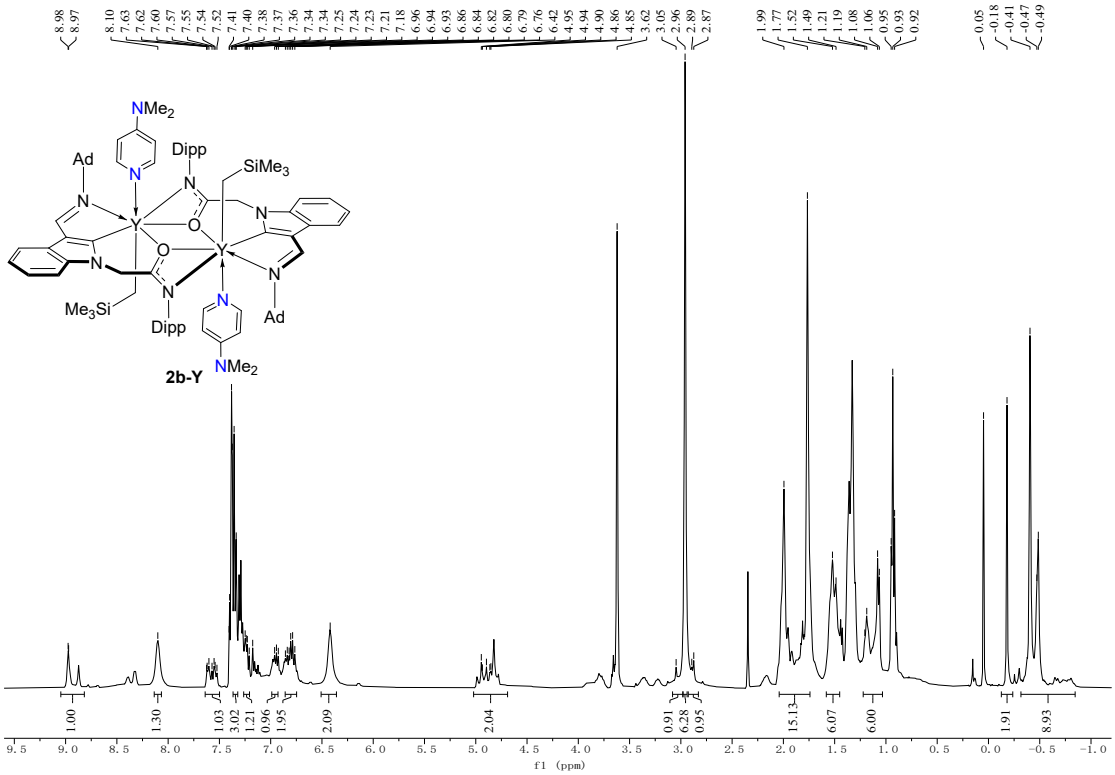

Figure S1. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **2b-Y**.

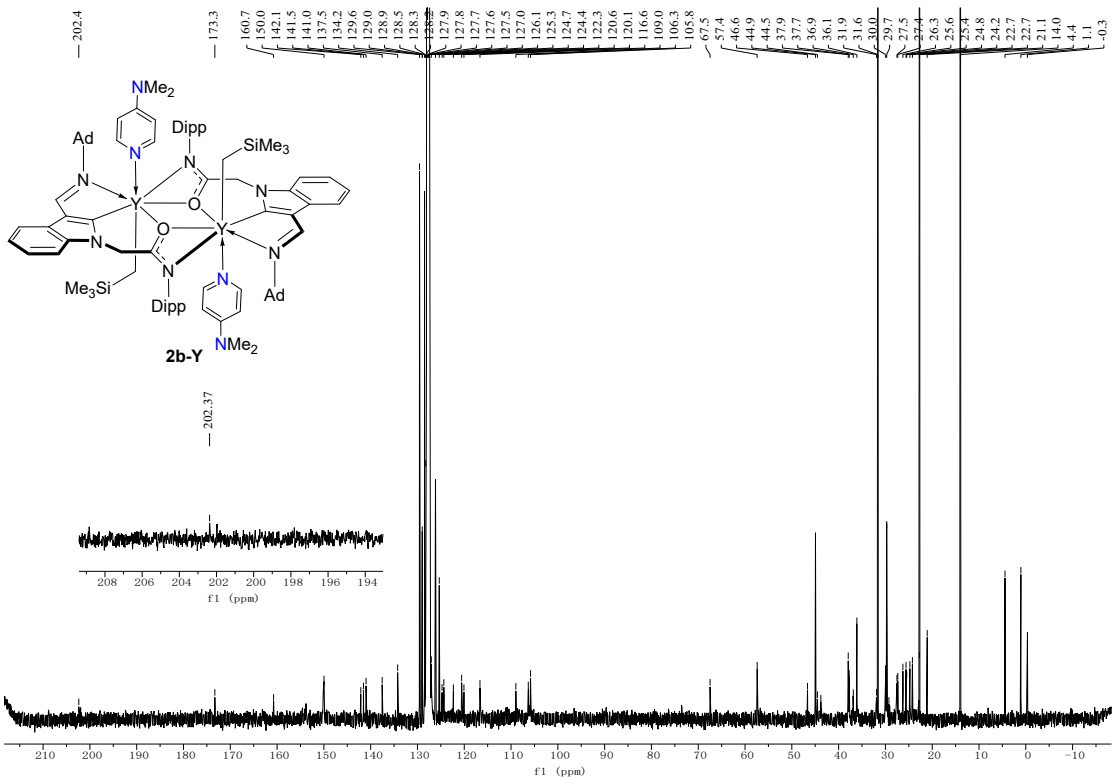

Figure S2. ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K) spectrum of **2b-Y**.

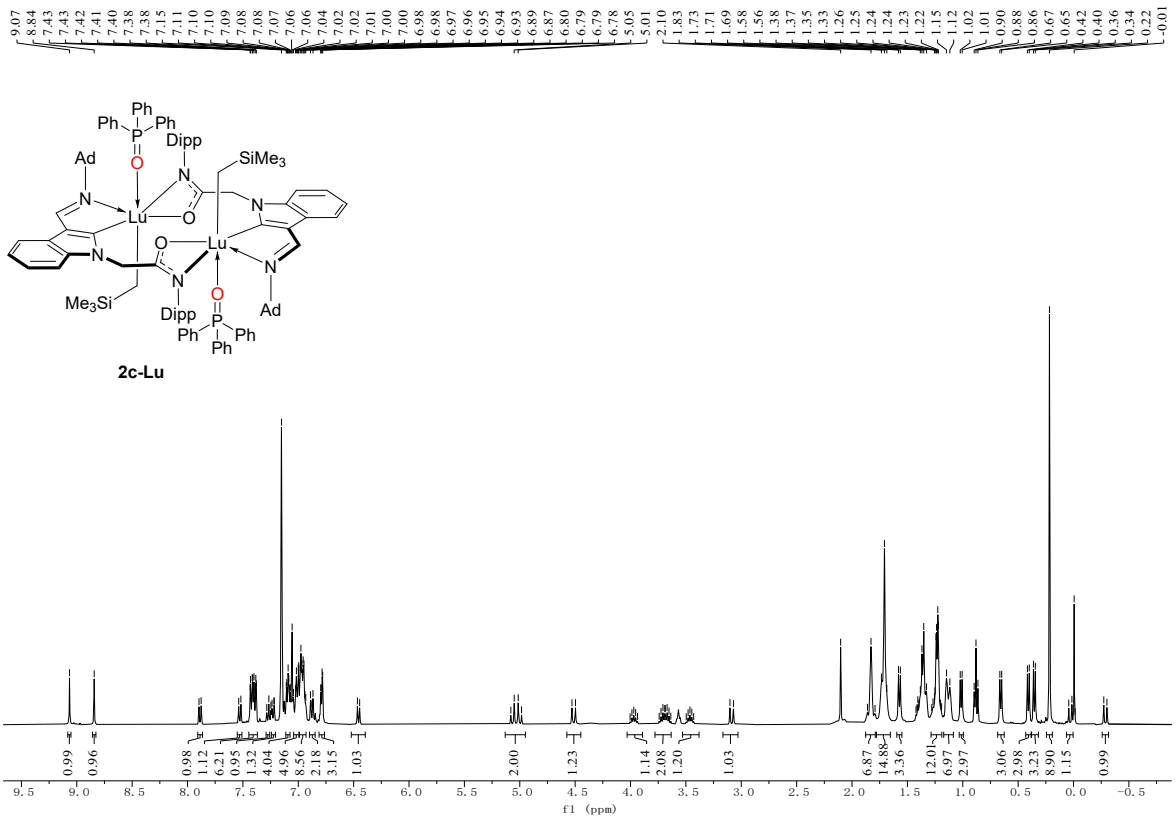

Figure S3. ^{1}H NMR (400 MHz, C_6D_6, 298 K) spectrum of **2c-Lu**.

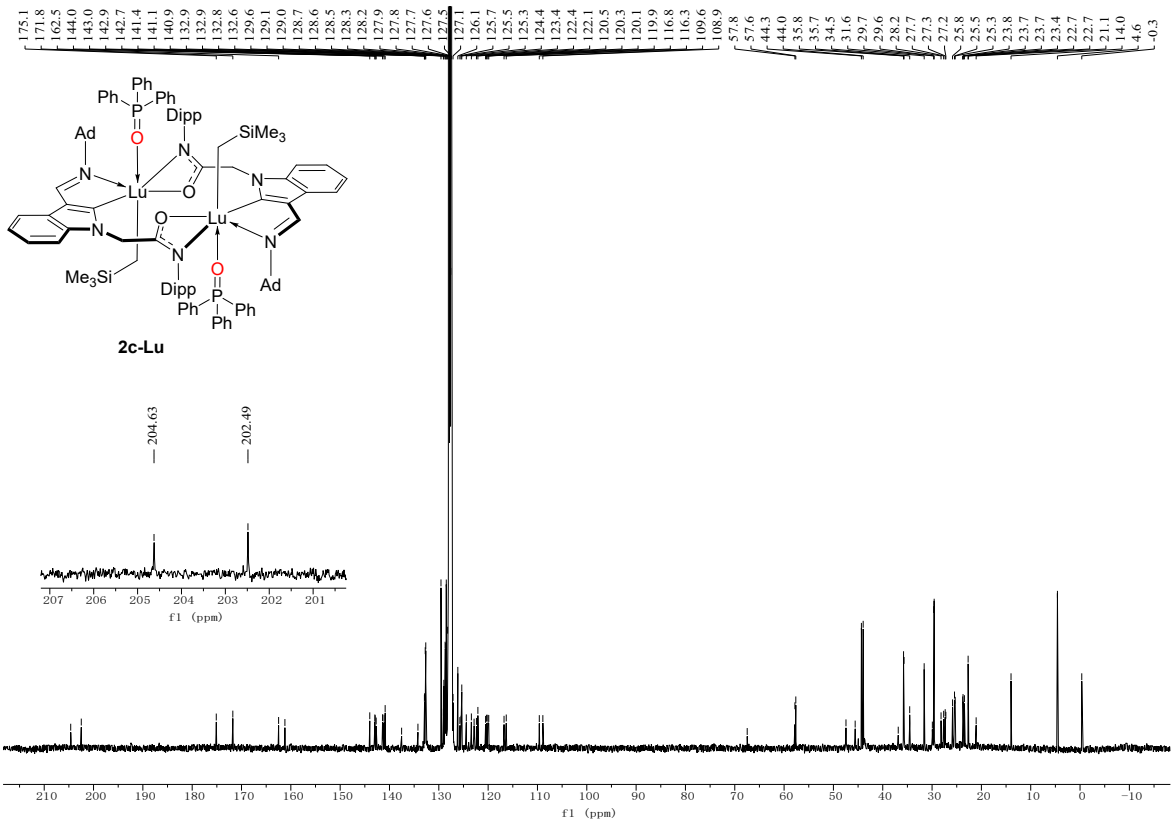

Figure S4. ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K) spectrum of **2c-Lu**.

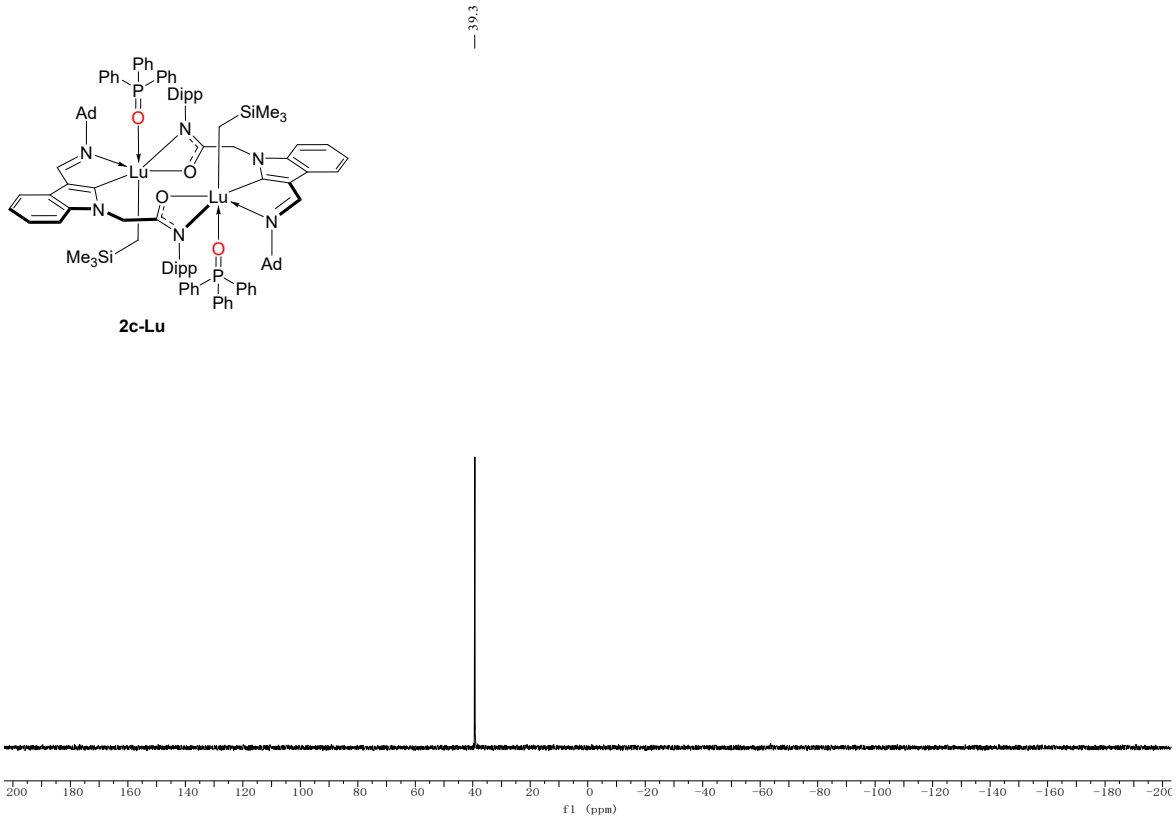

Figure S5. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 298 K) spectrum of complex **2c-Lu**.

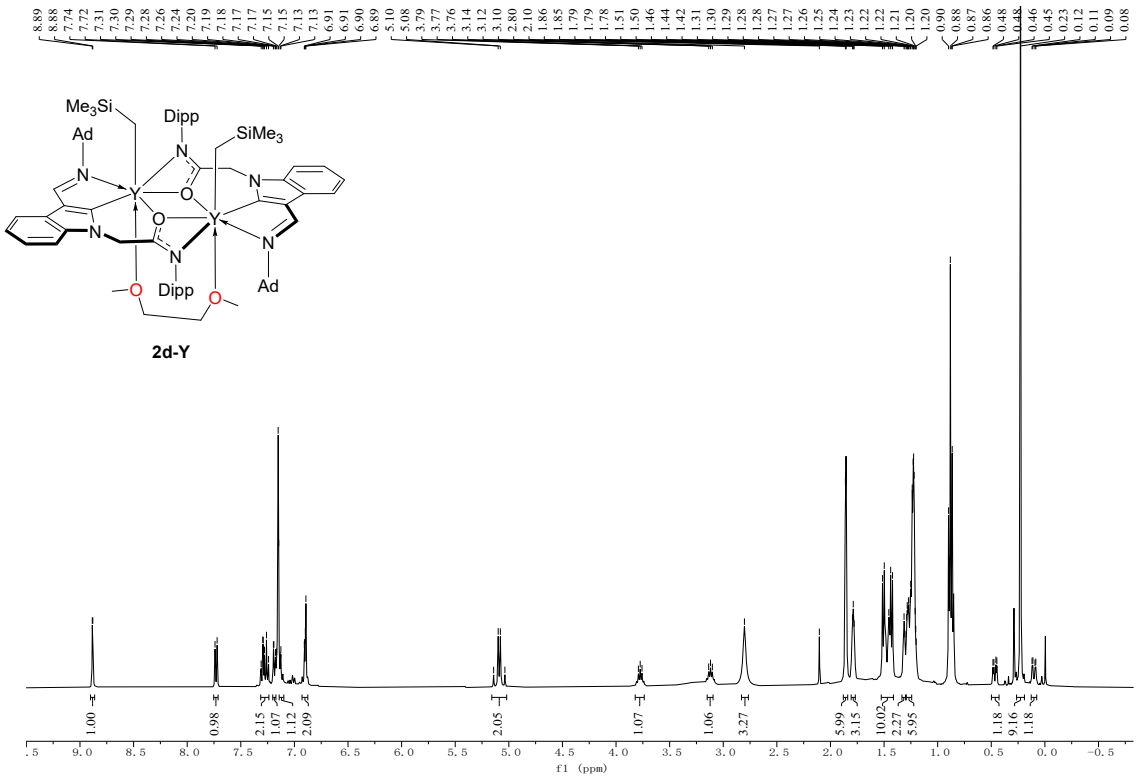

Figure S6. ^{1}H NMR (400 MHz, C_6D_6, 298 K) spectrum of **2d-Y**.

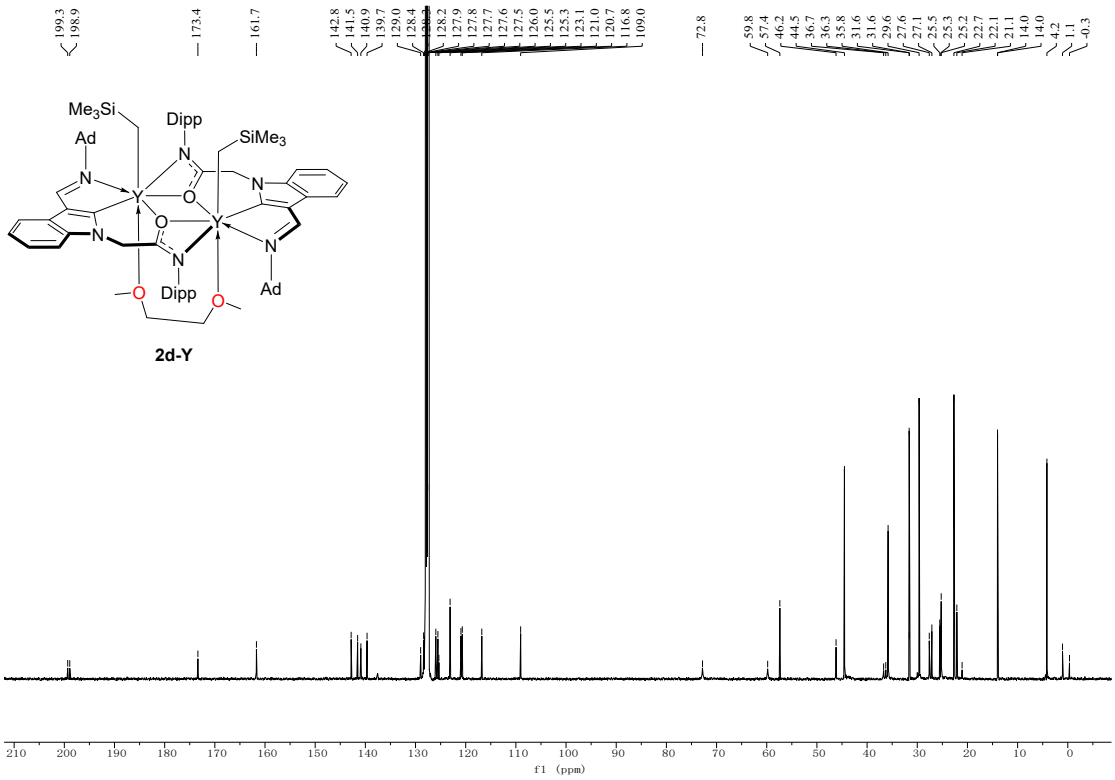

Figure S7. $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6, 298 K) spectrum of **2d-Y**.

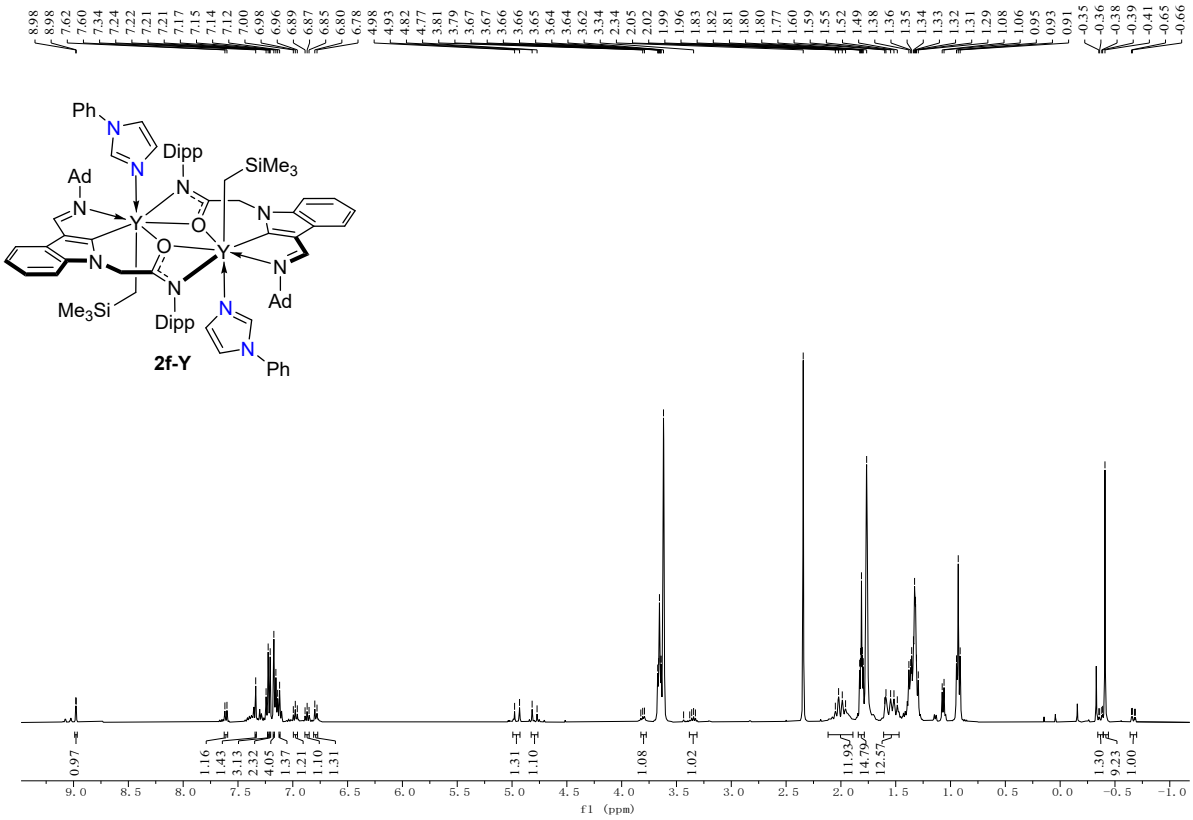

Figure S8. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **2f-Y**.

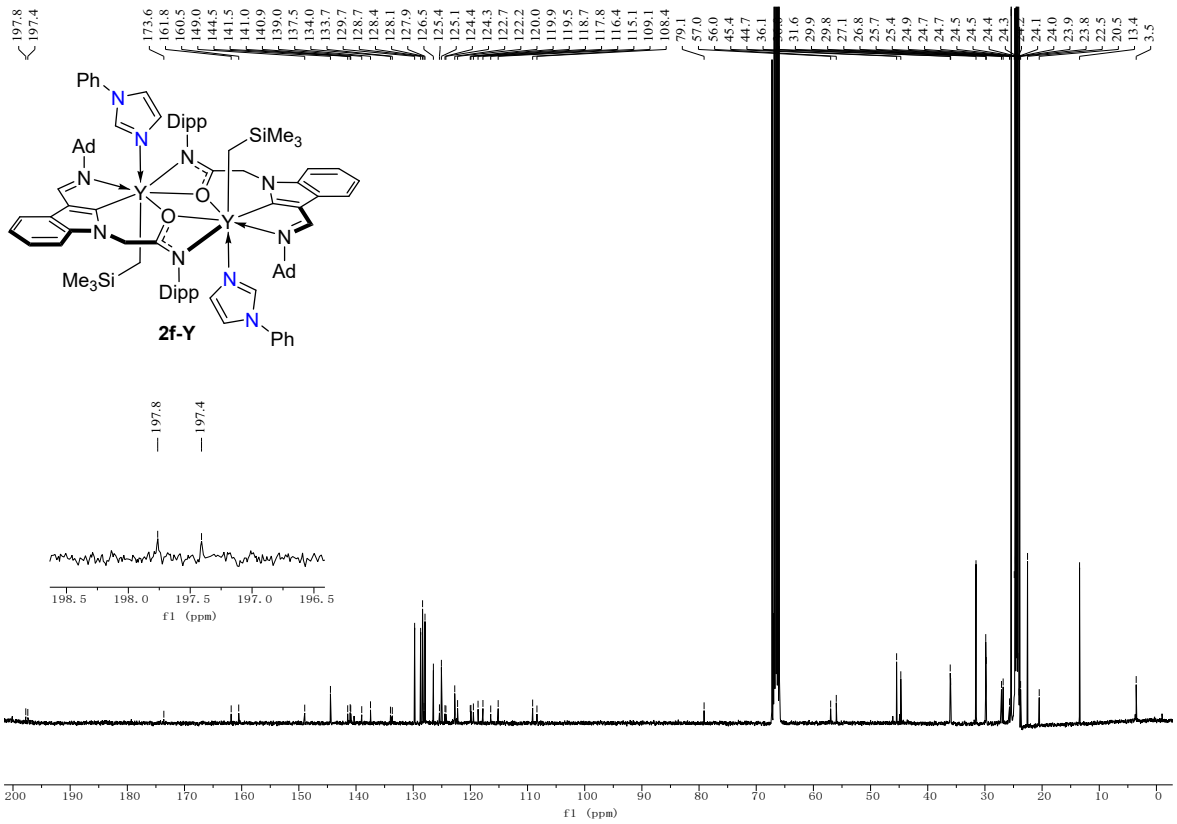

Figure S9. $^{13}C\{^{1}H\}$ NMR (100 MHz, THF-d_8, 298 K) spectrum of **2f-Y**.

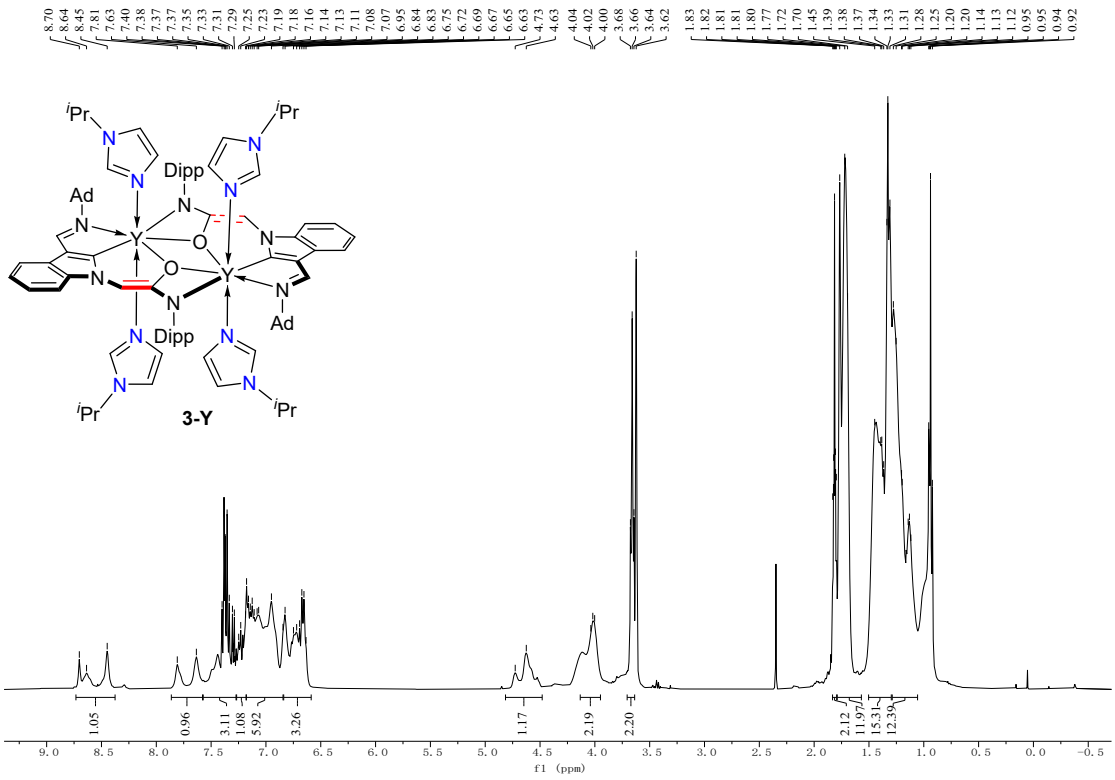

Figure S10. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **3-Y**.

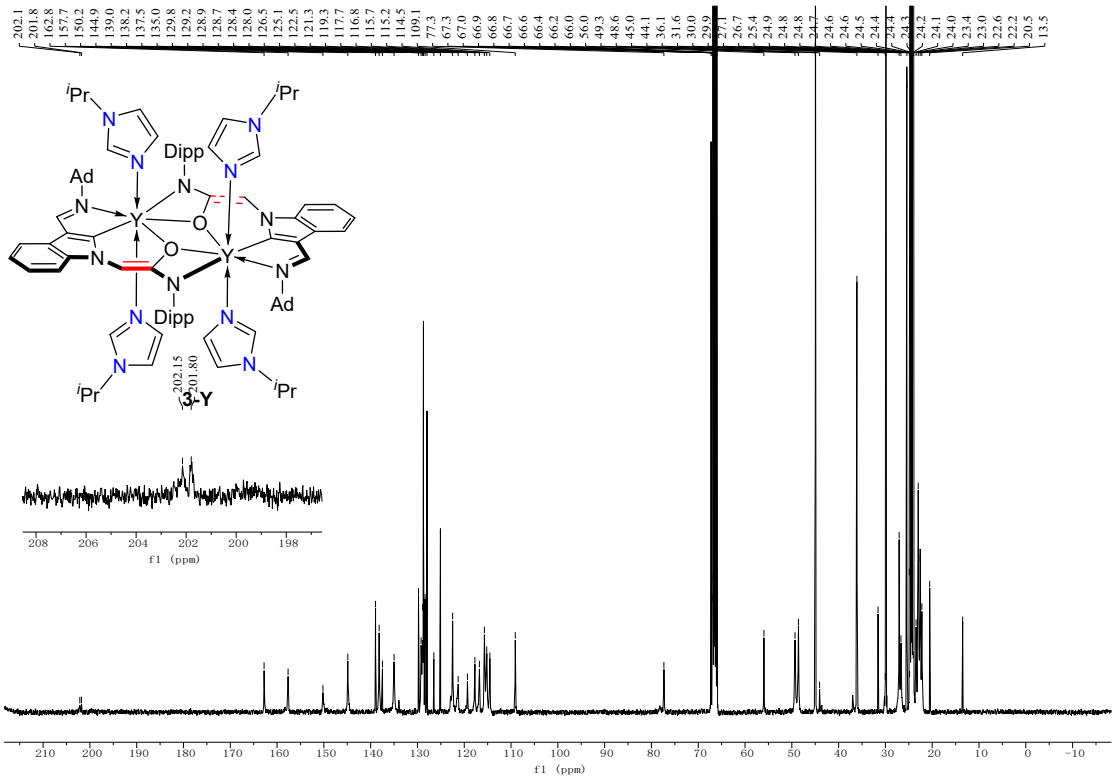

Figure S11. $^{13}C\{^{1}H\}$ NMR (100 MHz, THF-d_8, 298 K) spectrum of **3-Y**.

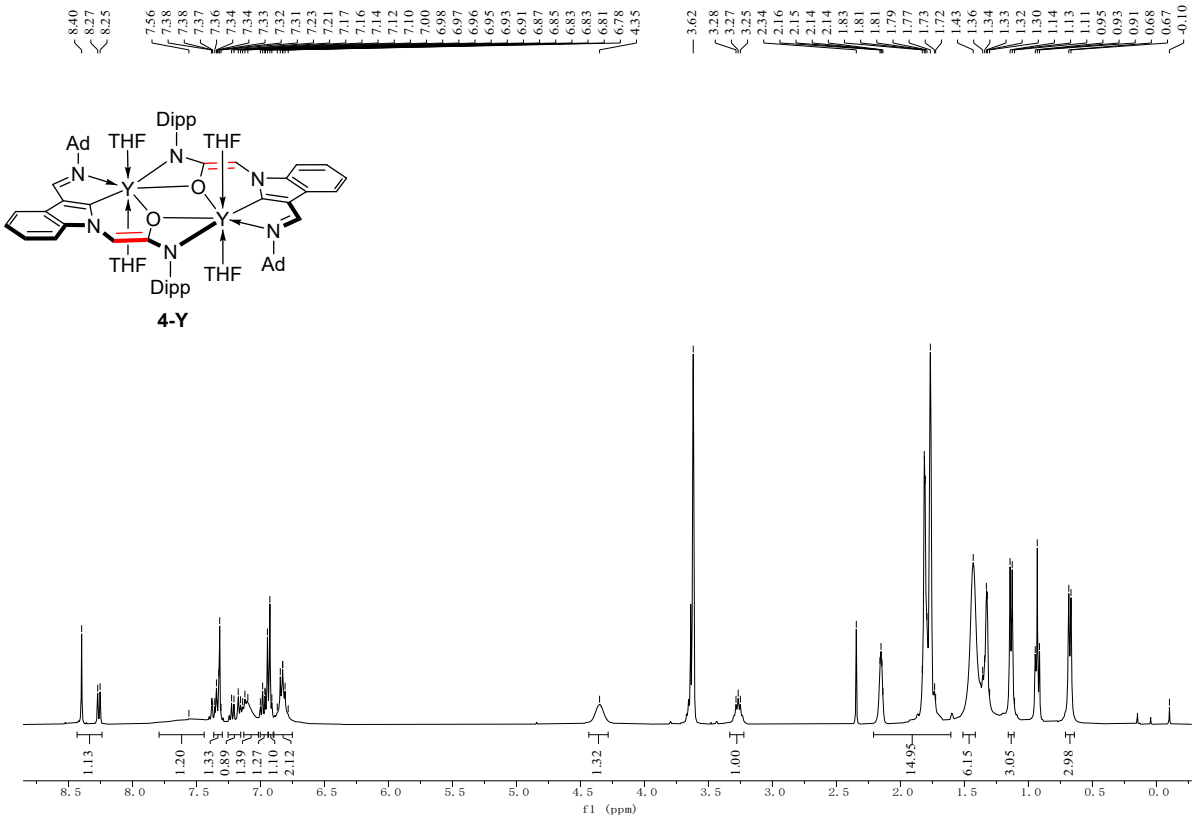

Figure S12. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **4-Y.**

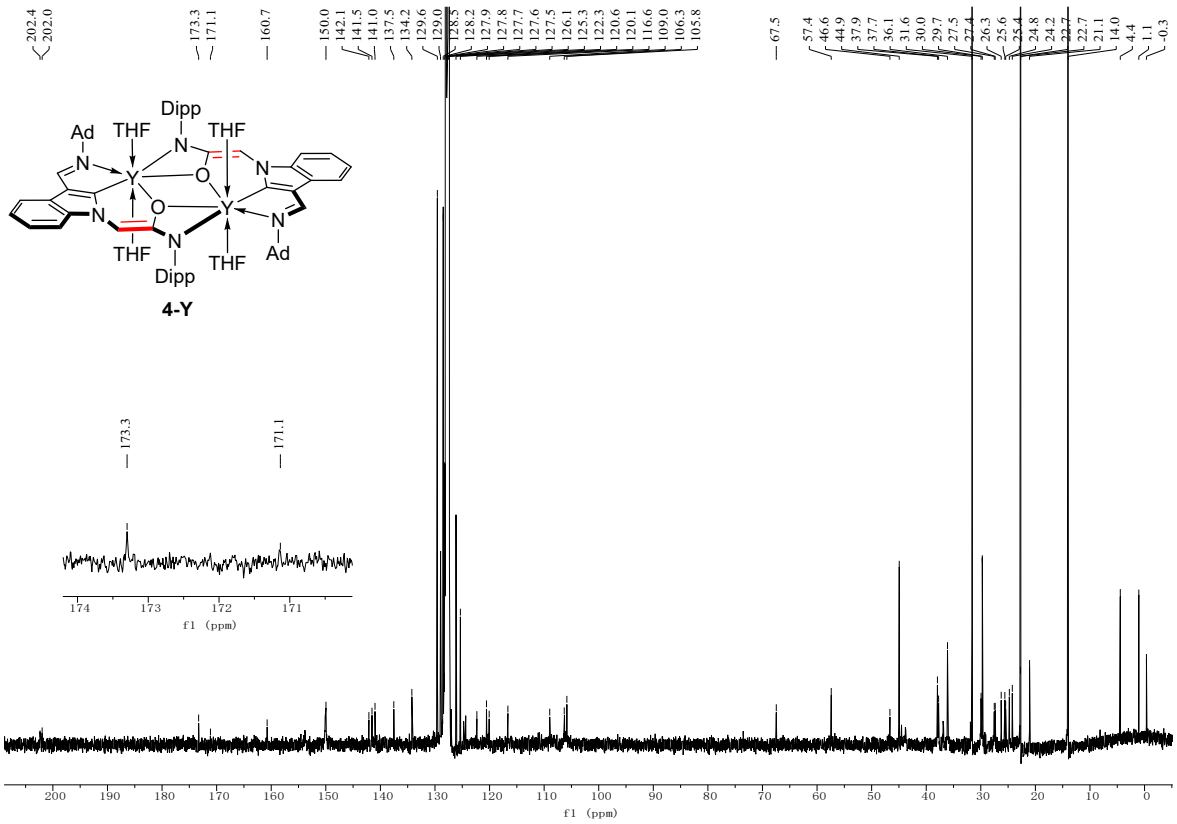

Figure S13. $^{13}C\{^{1}H\}$ NMR (100 MHz, THF-d_8, 298 K) spectrum of **4-Y.**

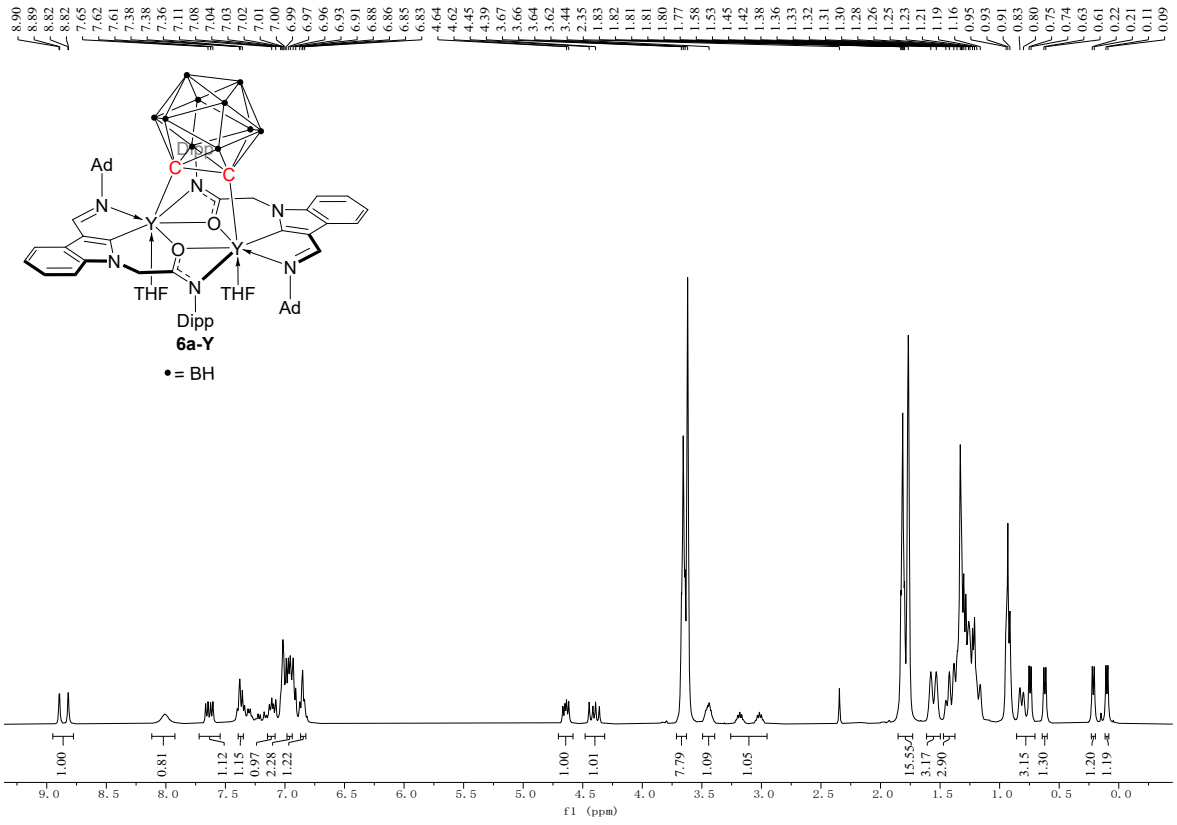

Figure S14. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **6a-Y.**

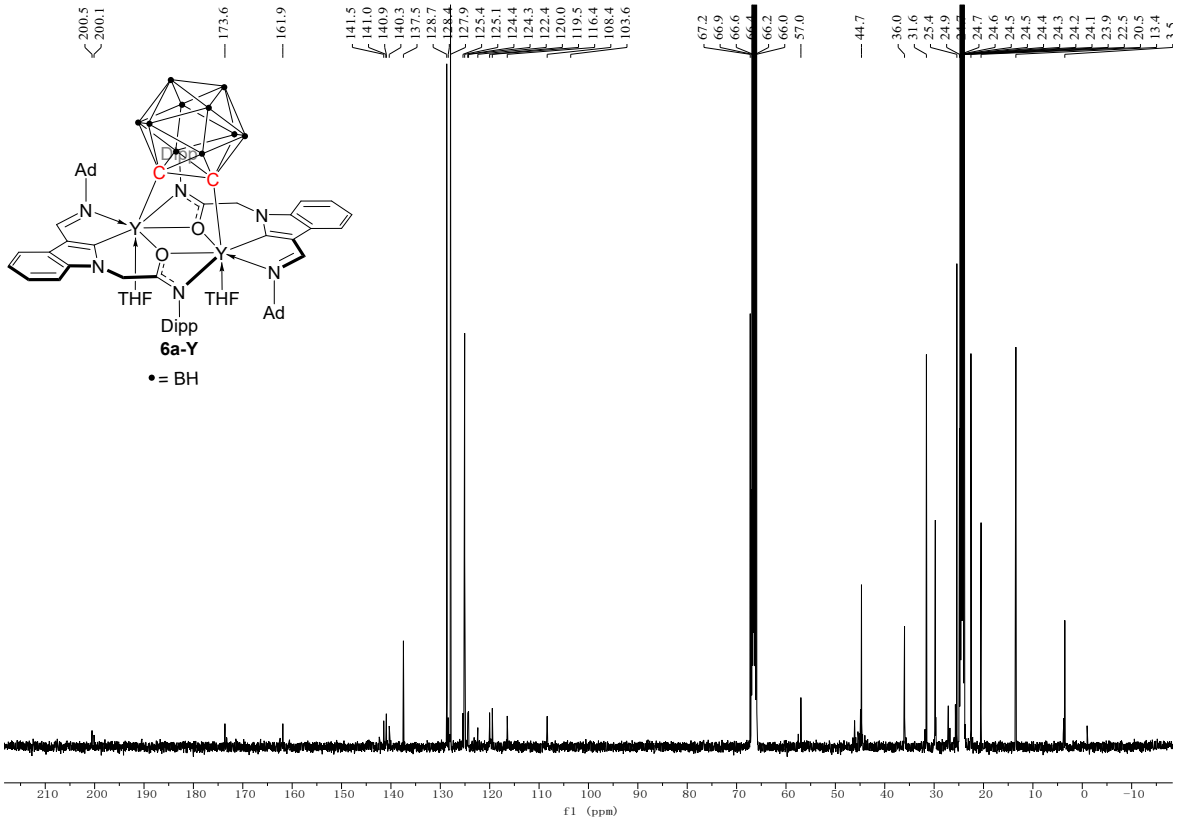

Figure S15. $^{13}C\{^{1}H\}$ NMR (100 MHz, THF-d_8, 298 K) spectrum of **6a-Y**.

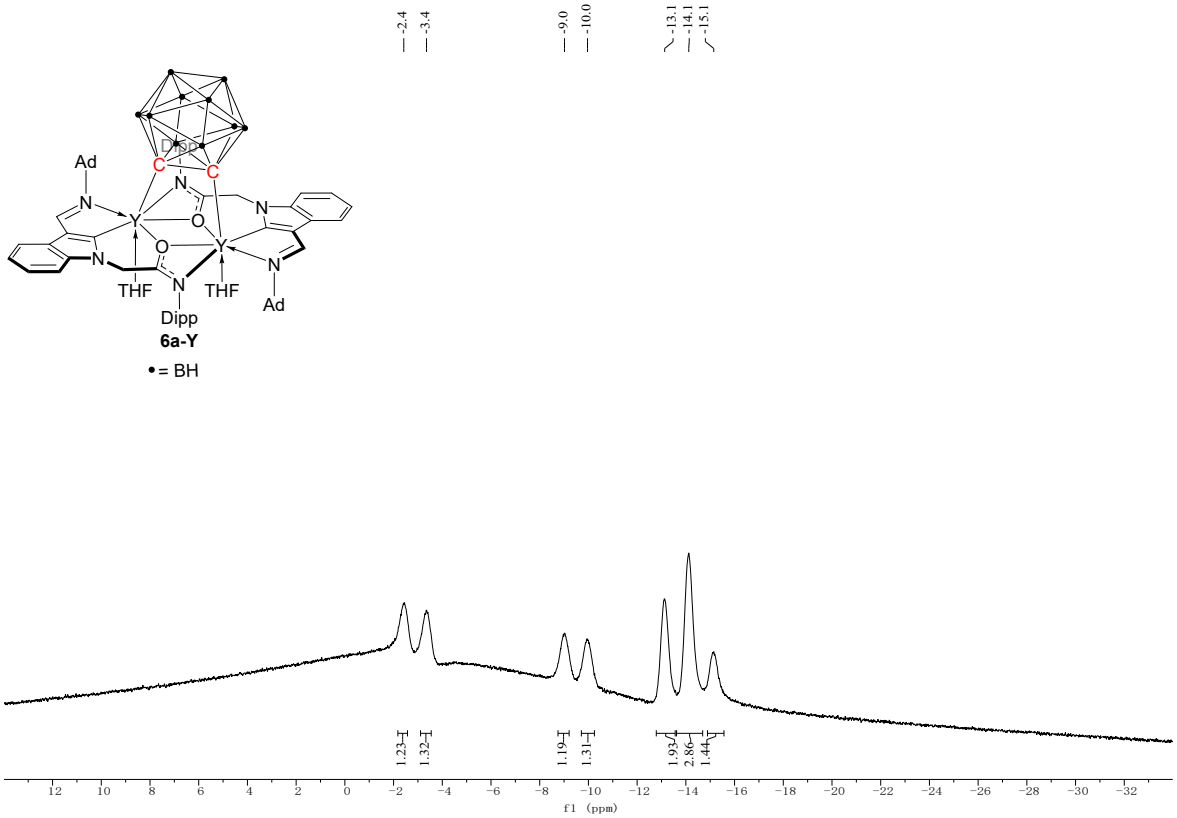

Figure S16. $^{11}B\{^{1}H\}$ NMR (128 MHz, THF-d_8, 298 K) spectrum of **6a-Y**.

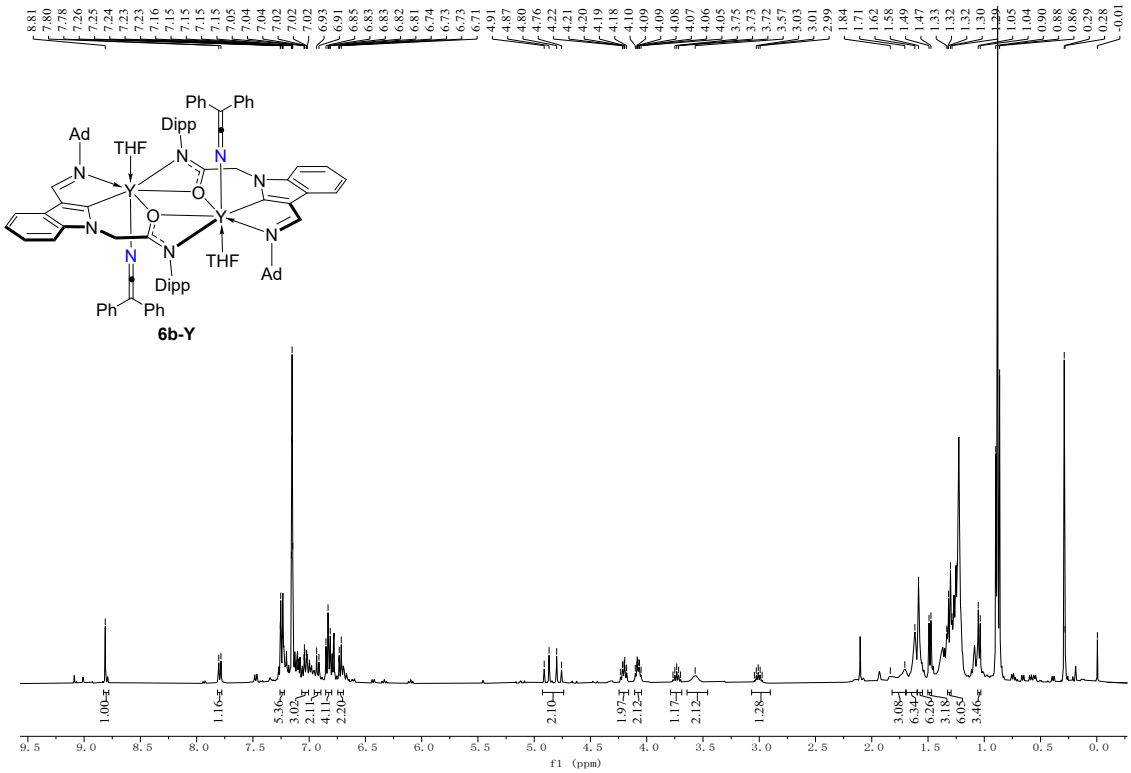

Figure S17. ^{1}H NMR (400 MHz, C_6D_6, 298 K) spectrum of **6b-Y**.

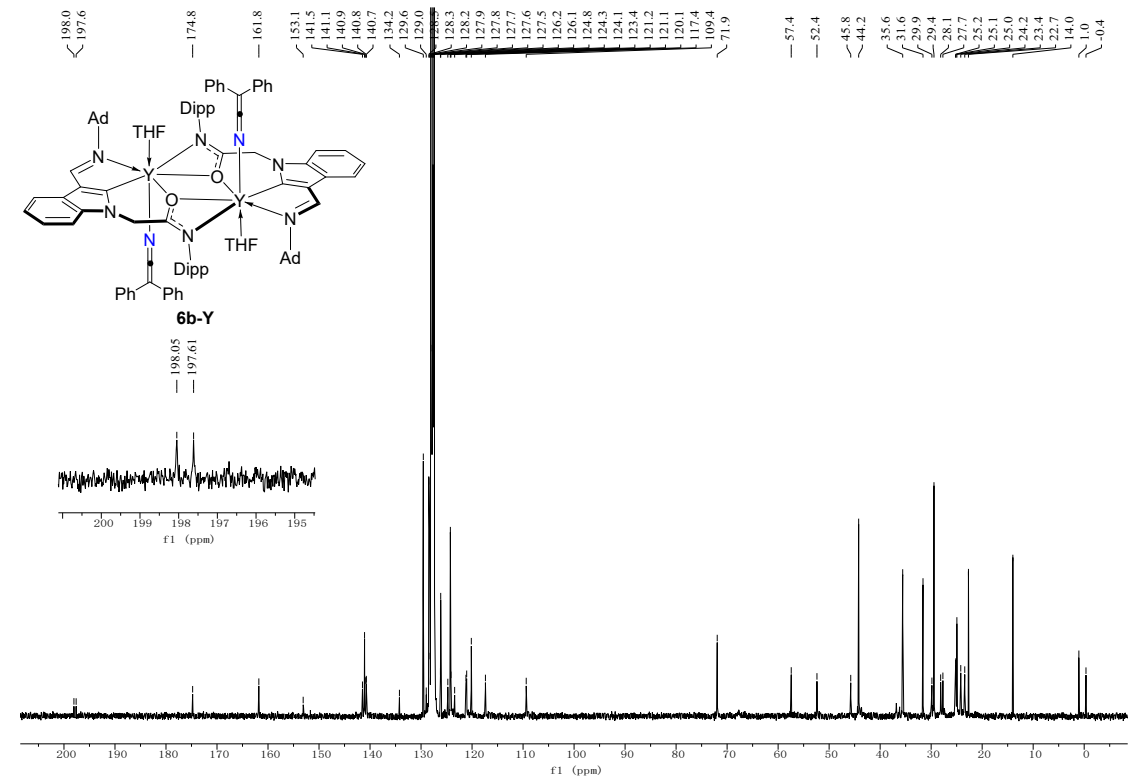

Figure S18. $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6, 298 K) spectrum of **6b-Y**.

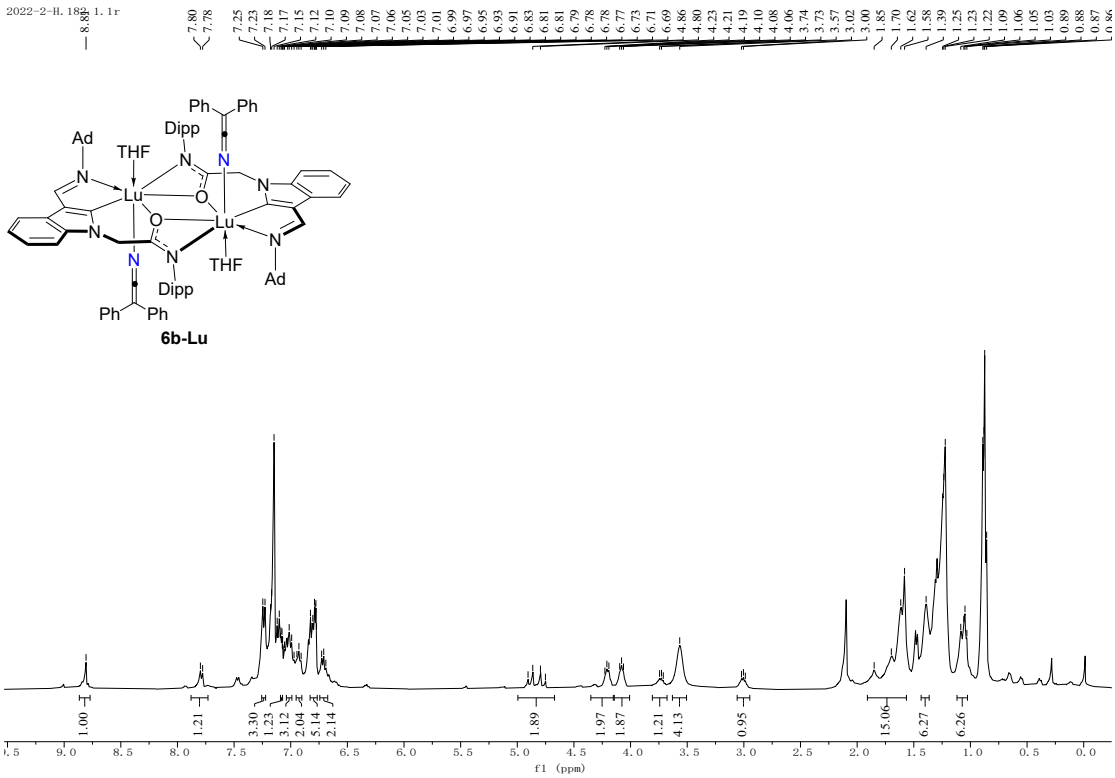

Figure S19. ^{1}H NMR (400 MHz, C_6D_6, 298 K) spectrum of **6b-Lu**.

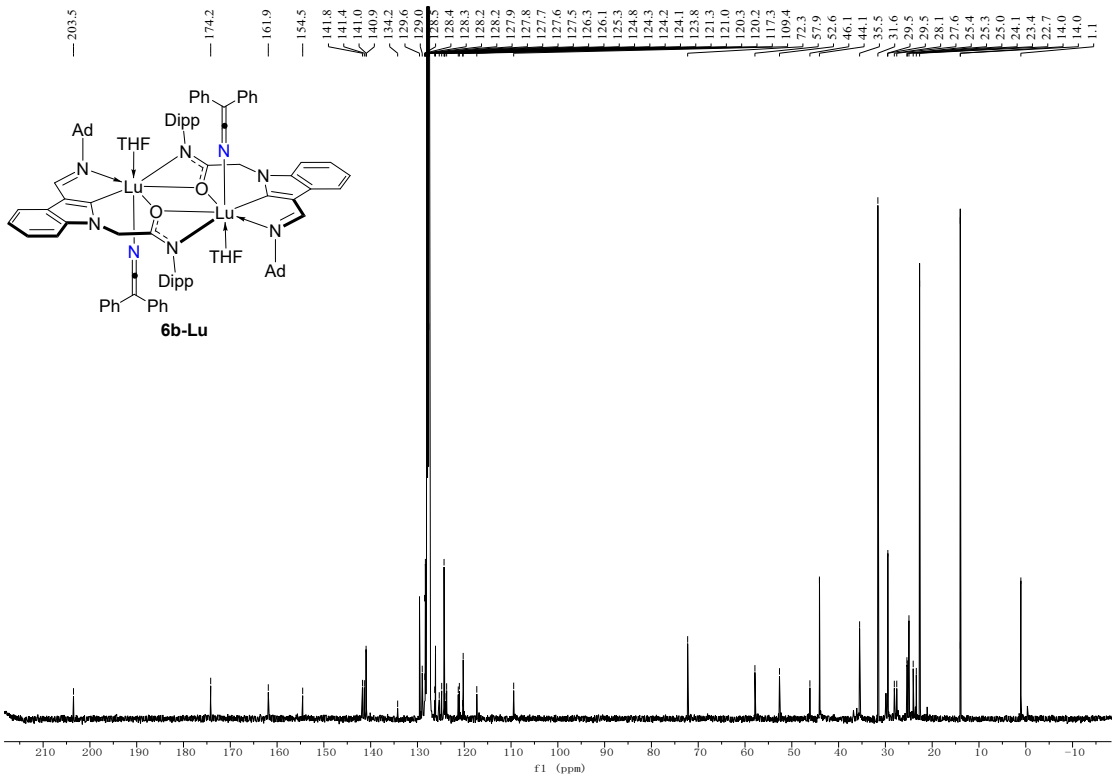

Figure S20. $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6, 298 K) spectrum of **6b-Lu**.

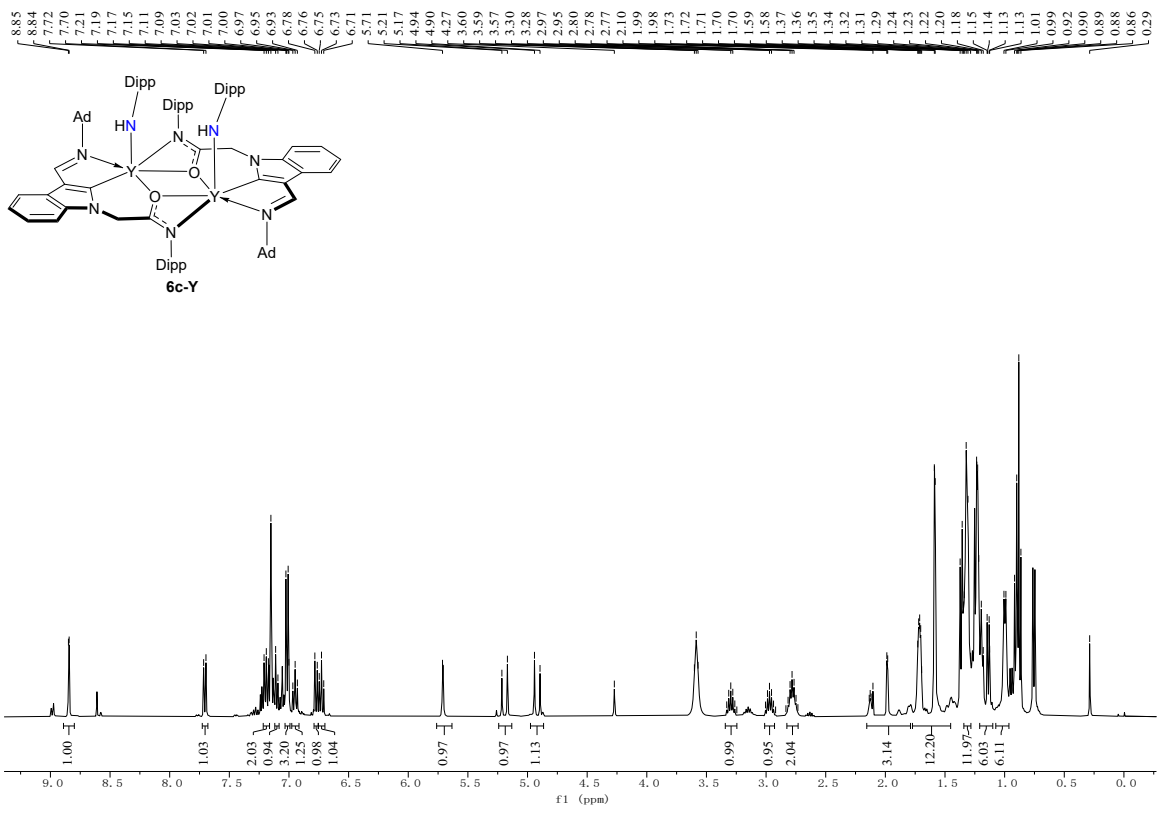

Figure S21. ^{1}H NMR (400 MHz, C_6D_6, 298 K) spectrum of **6c-Y**.

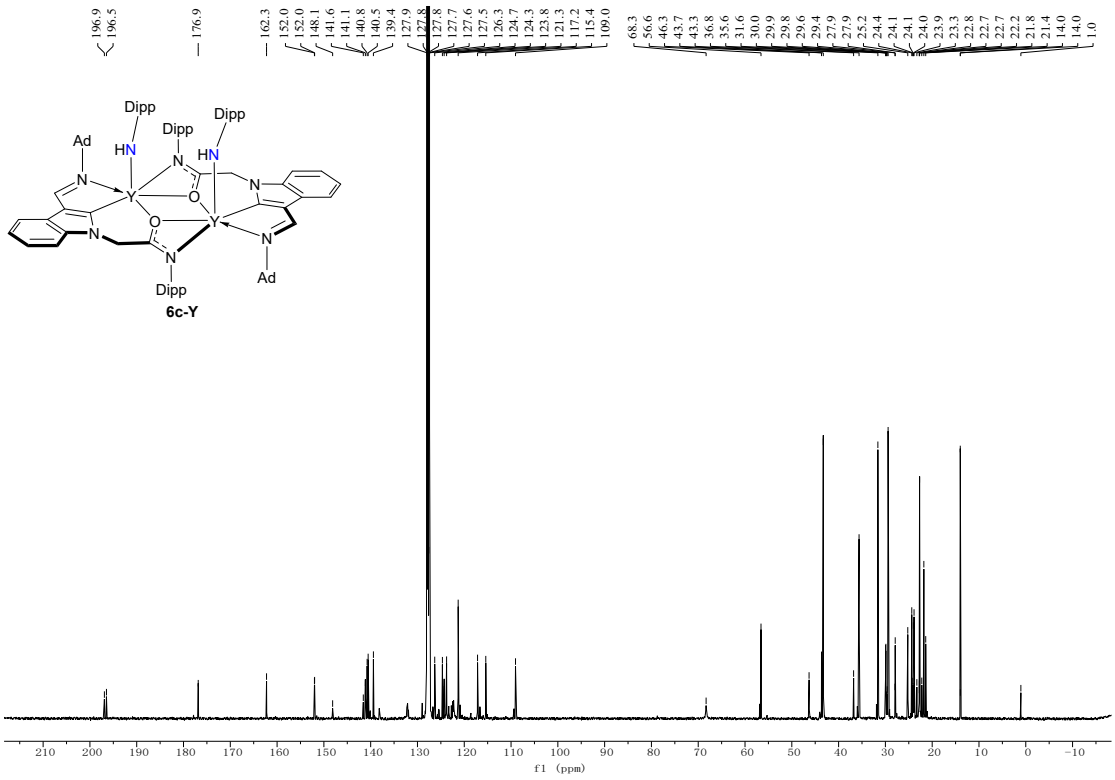

Figure S22. $^{13}C\{^{1}H\}$ NMR (100 MHz, C_6D_6, 298 K) spectrum of **6c-Y.**

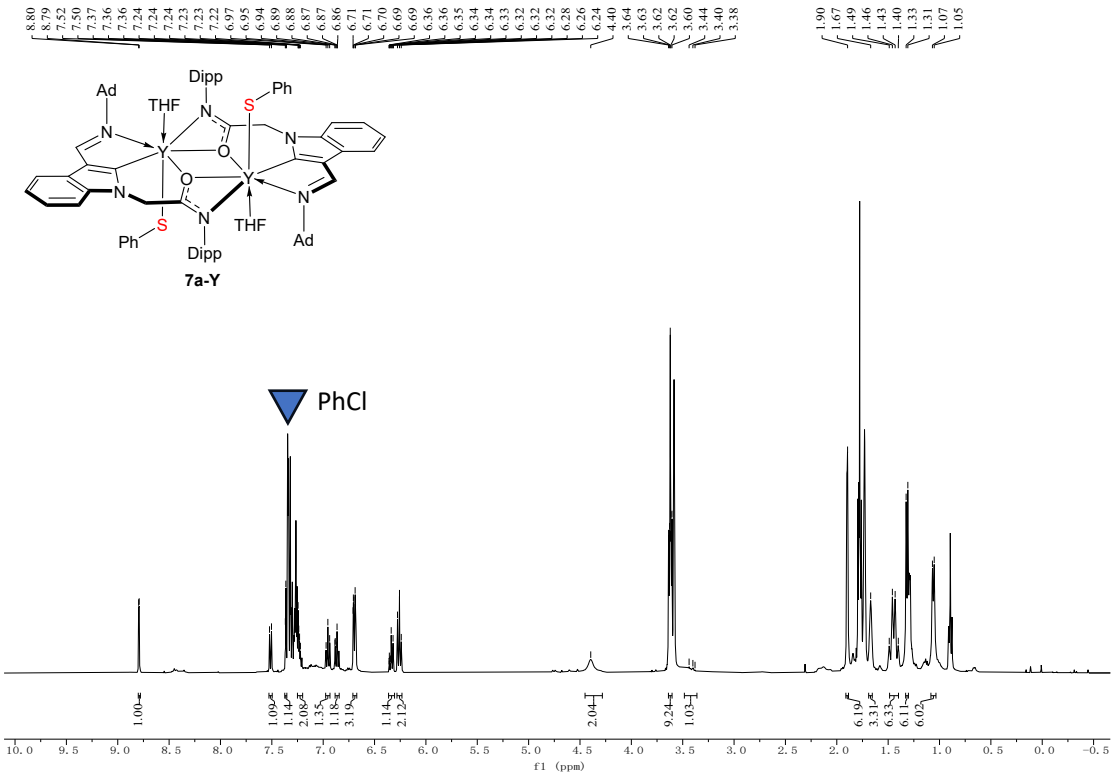

Figure S23. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **7a-Y.**

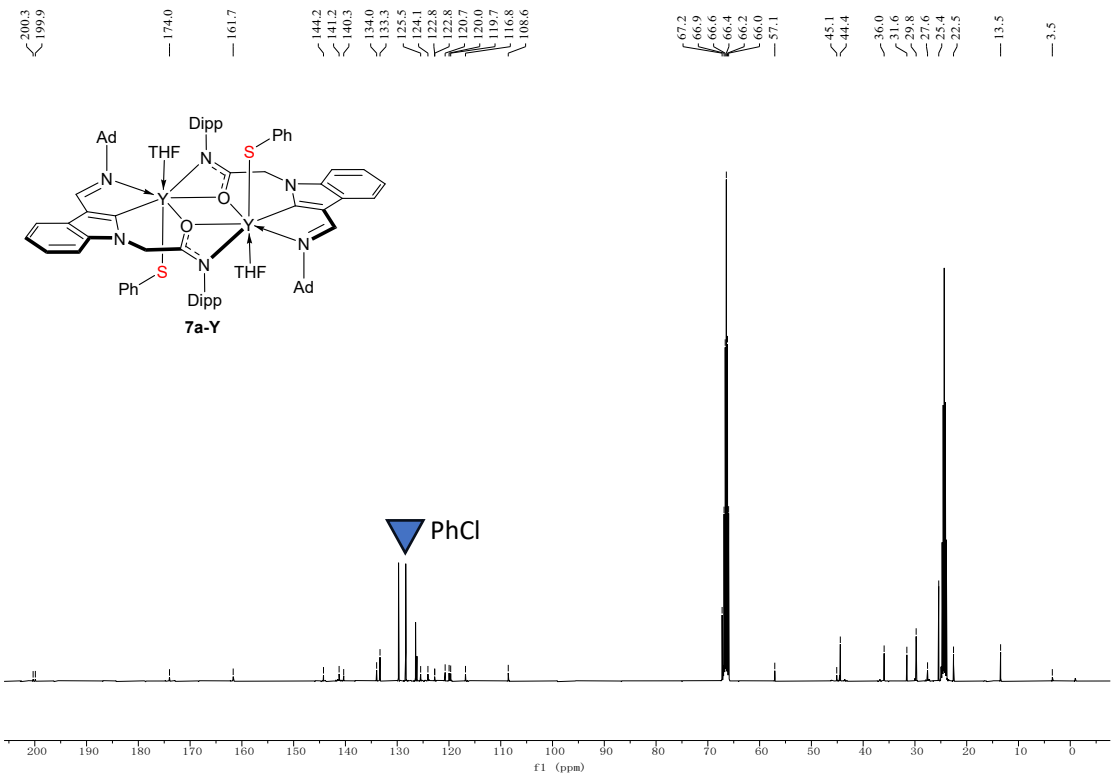

Figure S24. ^{13}C{^{1}H} NMR (400 MHz, THF-d_8, 298 K) spectrum of **7a-Y.**

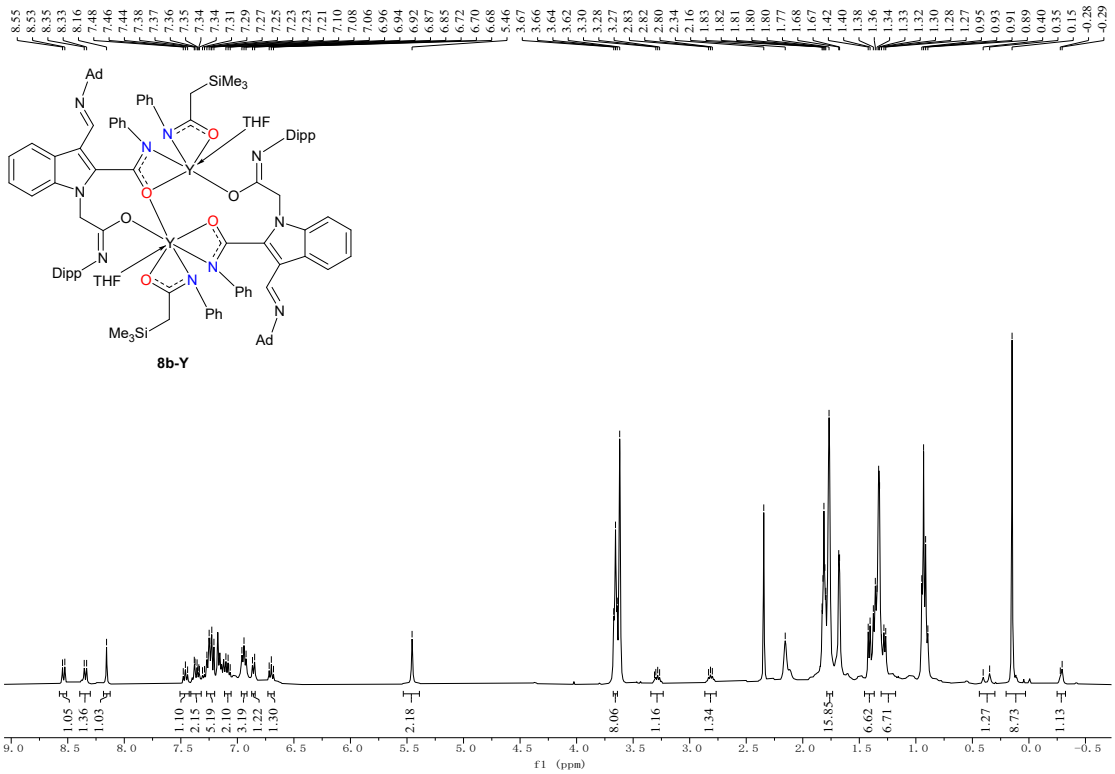

Figure S25. ^{1}H NMR (400 MHz, THF-d_8, 298 K) spectrum of **8b-Y**.

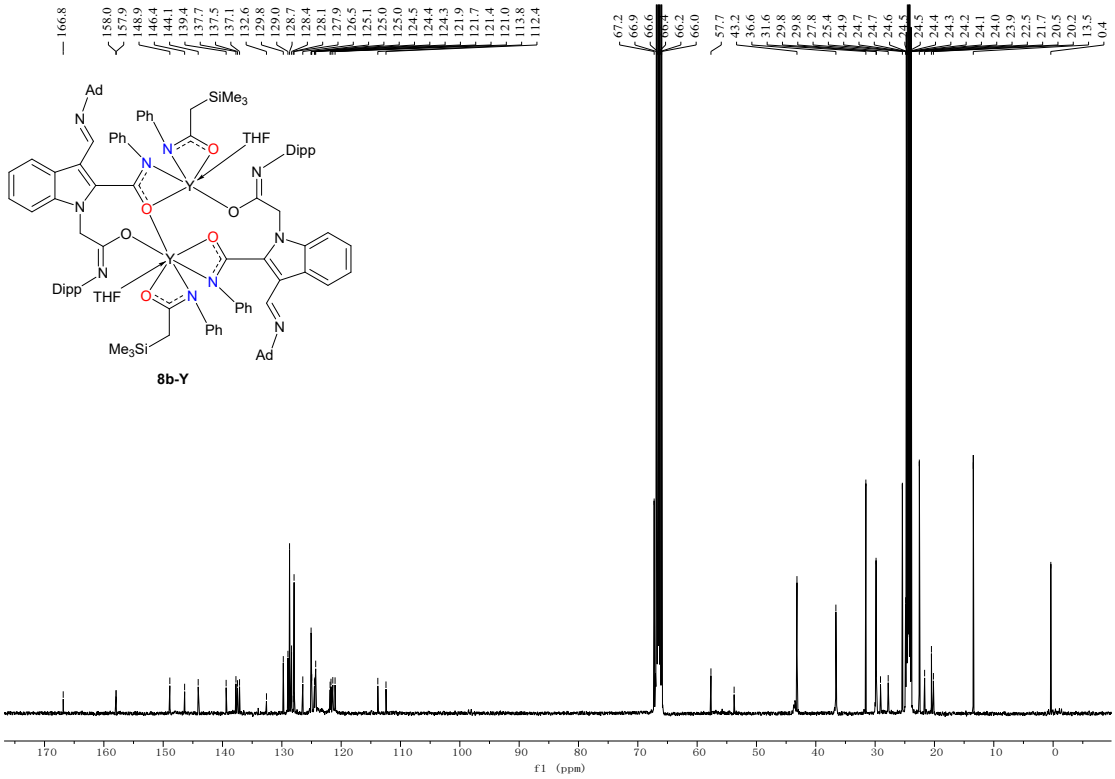

Figure S26. ^{13}C{^{1}H} NMR (100 MHz, THF-d_8, 298 K) spectrum of **8b-Y**.

2. OLEX 2 drawing of complexes

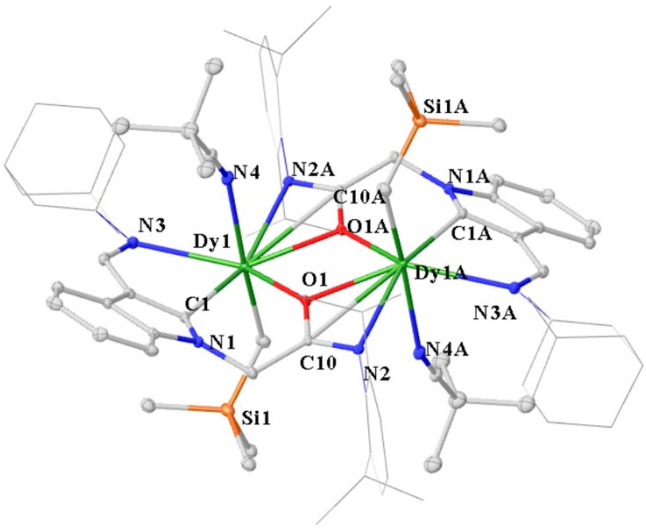

Figure S27: OLEX 2 drawing of **2a-Dy** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1A 2.372(4), Dy1-O1 2.373(4), Dy1-N2A 2.661(5), Dy1-C10A 2.941(7), Dy1-N3 2.597(5), Dy1-N4 2.568(7), Dy1-C1, 2.403(7), Dy1-C34 2.405(9), O1-C10 1.311(8), N2-C10 1.290(8), O1A-Dy1-O1 64.7(3), O1A-Dy1-C10A 25.84(18), N3-Dy1-N2A 98.93(17), N2A-Dy1-C10A 26.02(17), C1-Dy1-N3 68.3(2), O1-Dy1-C1 70.9(2), N4-Dy1-N2A 80.3(2), N4-Dy1-C10A 81.5(2), N4-Dy1-N3 77.5(2), O1A-Dy1-N4 82.4(2), O1-Dy1-N4 83.3(2), C1-Dy1-N4 82.9(2), C34-Dy1-N4 172.1(5), O1A-Dy1-C34 94.5(3), O1-Dy1-C34 102.1(3), C34-Dy1-N2A 95.4(7), C34-Dy1-C10A 91.7(6), C34-Dy1-N3 109.9(6), C34-Dy1-C1 102.3(6), N2-C10-O1 116.7(6).

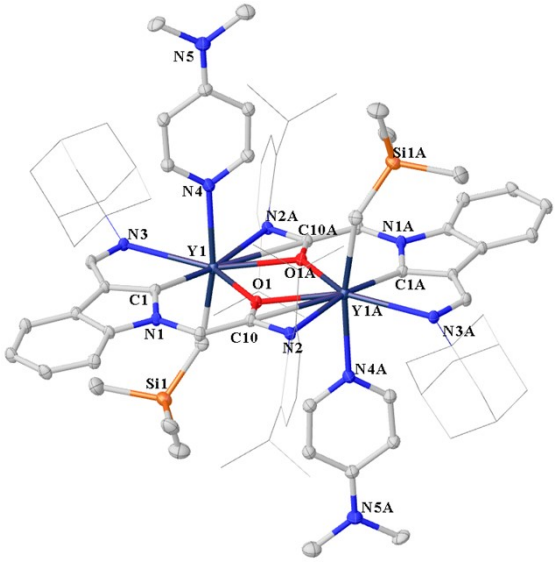

Figure S28: OLEX 2 drawing of **2b-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.329(4), Y1-O1A 2.399(4), Y1-N3 2.591(5), Y1-N2A 2.672(5), Y1-N4 2.483(6), Y1-C1 2.391(6), Y1-C10A 2.955(6), Y1-C34 2.422(7), O1-C10 1.310(7), N2-C10 1.286(8), O1-Y1-O1A 64.75(16), O1A-Y1-C10A 25.76(16), N2A-Y1-C10A 25.81(16), N3-Y1-N2A 103.42(17), C1-Y1-N3 68.02(19), O1-Y1-C1 71.90(18), O1A-Y1-N4 88.86(15), N4-Y1-N3 80.90(16), N4-Y1-N2A 88.17(16), C1-Y1-N4 84.24(19), N4-Y1-C10A 90.22(17), O1-Y1-N4 93.26(15), C34-Y1-N3 87.6(2), C34-Y1-N2A

92.1(2), C34-Y1-N4 168.2(2), O1A-Y1-C34 100.6(2), C1-Y1-C34 94.0 (2), O1-Y1-C34 97.1(2), C34-Y1-C10A 95.0(2), N2-C10-O1 116.9(6).

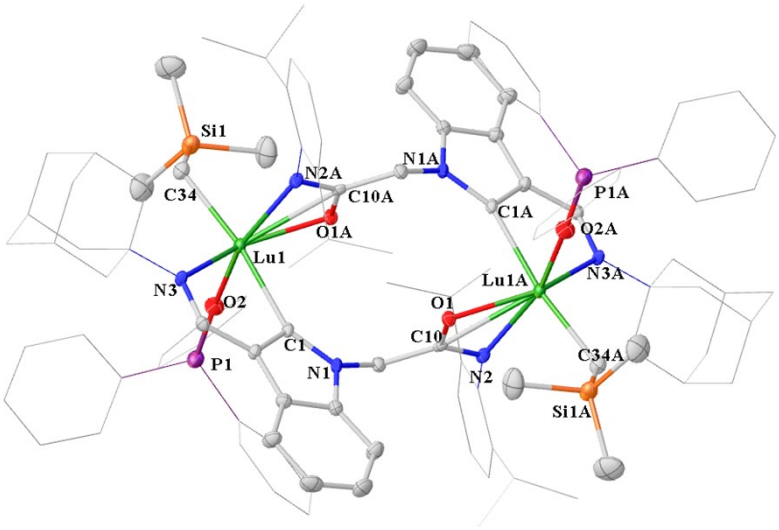

Figure S29: OLEX 2 drawing of **2c-Lu** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl, Phenyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Lu1-O1A 2.243(5), Lu1-O2 2.201(6), Lu1-N2A 2.380(7), Lu1-N3 2.455(6), Lu1-C10A 2.685(8), Lu1-C1 2.434(8), Lu1-C34 2.418(8), P1-O2 1.516(6), N2-C10 1.318(9), O1-C10 1.283(9), O1A-Lu1-N3 142.4(2), O1A-Lu1-C10A 28.4(2), O1A-Lu1-C1 85.1(2), O1A-Lu1-C34, 101.4(3), O2-Lu1-O1A 104.4(2), O1A-Lu1-N2A 57.5(2), O1-C10-N2 117.9(7), O2-Lu1-N2A 161.9(2), O2-Lu1-N3 102.6(2), O2-Lu1-C10A 132.5(2), O2-Lu1-C1 84.4(2), O2-Lu1-C34 88.5(3), N2A-Lu1-N3 93.0(2), N2A-Lu1-C10A 29.4(2), N2A-Lu1-C1 91.8(2), N2A-Lu1-C34 96.4(3), N3-Lu1-C10A 117.8(2), O2-P1-C38 108.4(11), C34-Lu1-C10A 103.0(3), C1-Lu1-C10A 85.4(2).

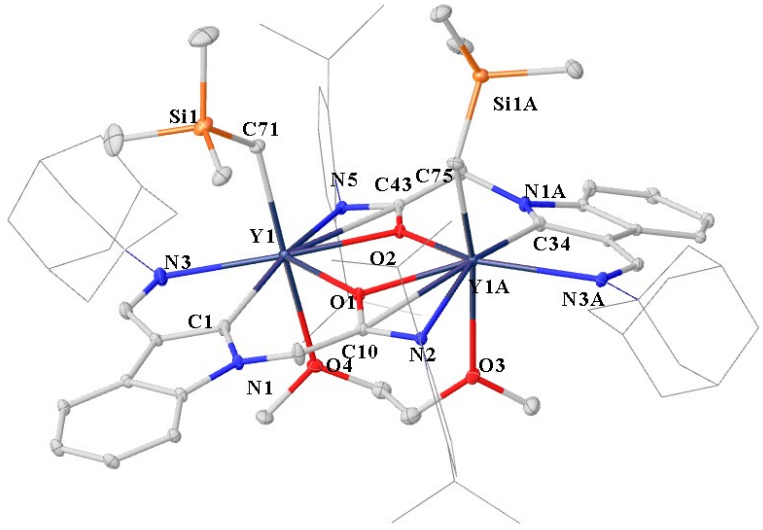

Figure S30: OLEX 2 drawing of **2d-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O2 2.364(3), Y1-O1 2.349(3), Y1-O4 2.536(3), Y1-N5 2.636(3), Y1-N3 2.604(4), Y1-C1 2.392(5), Y1-C71 2.366(5), O1-C10 1.307(5), N2-C10 1.286(6), O2-Y1-O4 82.78(11), O2-Y1-N3 153.24(11), O2-Y1-C1 134.60(15), O2-Y1-C71 95.45(15), O1-Y1-O2 64.56(10), O1-Y1-O4 83.89(11), O1-Y1-C1 71.03(15), O1-Y1-C71 99.69(16), O4-Y1-N5 80.32(11), O4-Y1-N3 86.89(12), N3-Y1-N5 101.92(12), C1-Y1-O4 83.68(15), C1-Y1-N3 67.98(15), C71-Y1-O4 174.91(16), C71-Y1-N5 94.82(16).

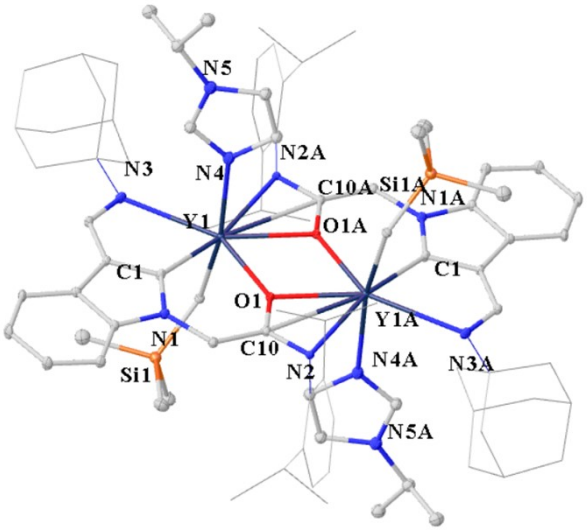

Figure S31: OLEX 2 drawing of **2e-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.346(3), Y1-O1A 2.346(3), Y1-N3 2.663(4), Y1-N2A 2.662(4), Y1-N4 2.496(5), Y1-C10A 2.953(5), Y1-C1 2.403(5), O1-C10 1.319(5), N2-C10 1.288(6), Y1-C40 2.421(5), O1-Y1-O1A 66.05(13), O1-Y1-C1 71.60(14), O1A-Y1-C10A 25.91(11), N2A-Y1-C10A 25.85(12), N3-Y1-N2A 102.32(12), C1-Y1-N3 67.84(15), N4-Y1-N3 84.8(15), N4-Y1-N2A 80.8(14), O1A-Y1-N4 82.6(15), O1-Y1-N4 94.9(15), C1-Y1-N4 90.5(16), N4-Y1-C10A 87.79(15),

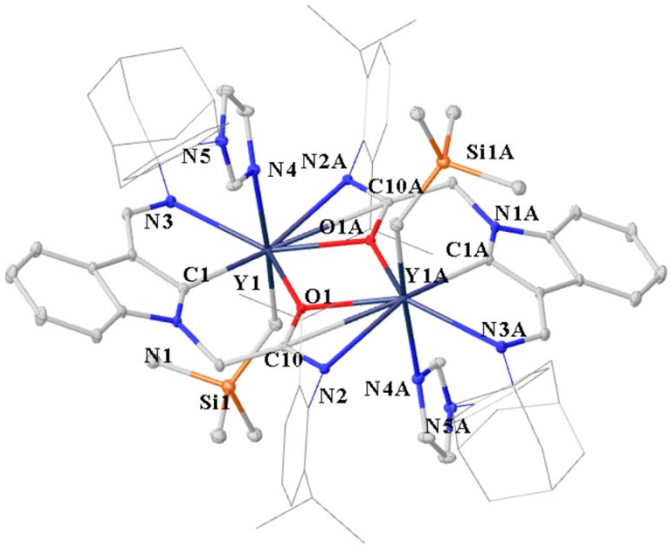

Figure S32: OLEX 2 drawing of **2f-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.372(3), Y1-O1 2.362(3), Y1-N2A 2.688(3), Y1-N3 2.590(4) Y1-N4 2.558(4), Y1-C1 2.397(4), Y1-C10A 2.959(4), Y1-C34 2.409(5), O1-C10 1.313(5), N2-C10 1.300(5), O1-Y1-O1A 65.80(10), O1-Y1-C1 71.06(12), C1-Y1-N3 68.59(13), N4-Y1-N2A 88.82(12), O1-Y1-N4 83.78(11), C1-Y1-N4 79.27(14), C34-Y1-C1 98.99(16), , N4-Y1-N3 79.06(12), N4-Y1-C10A 87.61(12).

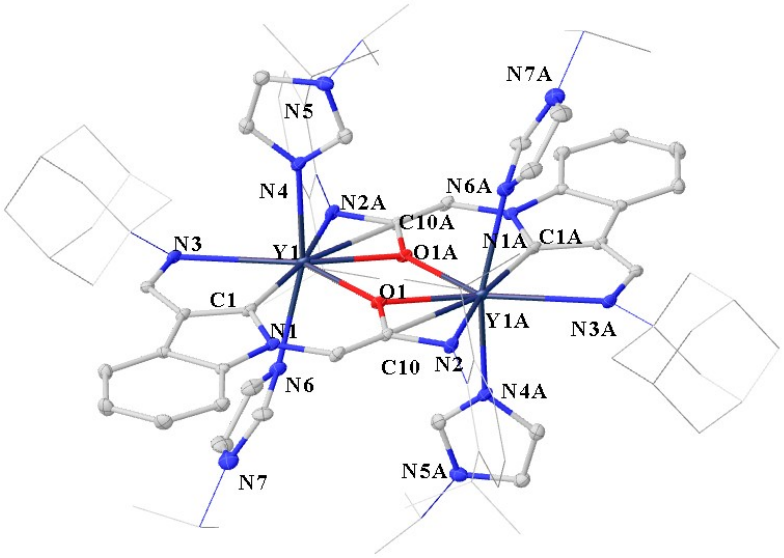

Figure S33: OLEX 2 drawing of **3-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl, Isopropyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.254(4), Y1-O1 2.309(4), Y1-N3 2.643(5), Y1-N2A 2.461(5), Y1-N4 2.435(6), Y1-N6 2.458(6), Y1-C1 2.414(7), Y1-C10A 2.861(8), O1-C10 1.349(8), N2-C10 1.385(8), O1A-Y1-O1 65.39(18), O1A-Y1-C10A 27.44(16), N2A-Y1-C10A 28.94(17), N2A-Y1-N3 100.10(18), C1-Y1-N3 67.5(2), O1-Y1-C1 70.92(19), N4-Y1-N3 92.68(17), N4-Y1-N2A 96.00(19), N4-Y1-N6 166.1(2), N6-Y1-N3 83.06(15), N6-Y1-C10A 100.44(17), N4-Y1-C10A 92.57(16), O1-Y1-N4 90.21(15), O1A-Y1-N4 88.78(14), O1A-Y1-N6 100.45(16), O1-Y1-N6 84.18(17), C1-Y1-N4 86.6(2), C1-Y1-N6 79.5(2).

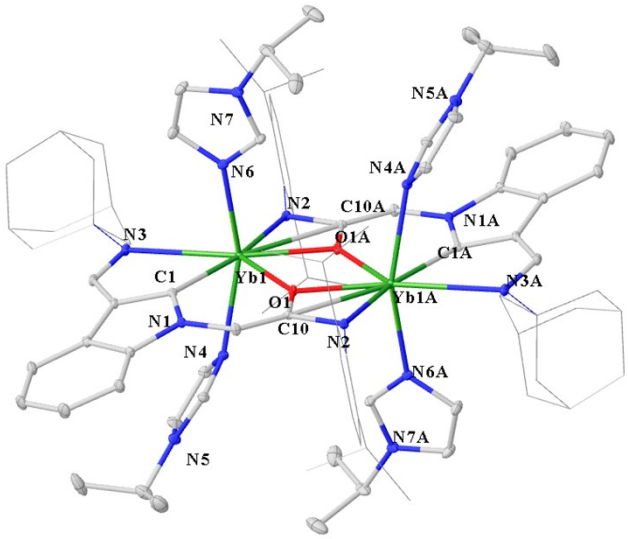

Figure S34: OLEX 2 drawing of **3-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.241(3), Yb1-O1A 2.248(3), Yb1-N2A 2.415(4), Yb1-N3 2.711(4), Yb1-N4 2.447(5), Yb1-N6 2.394(5), Yb1-C1 2.385(5), Yb1-C10A 2.838(5), O1-C10 1.355(5), N2-C10 1.380(6), O1-Yb1-O1A 63.72(14), O1A-Yb1-C10A 27.95(12), N2A-Yb1-C10A 29.06(13), N2A-Yb1-N3 99.95(14), C1-Yb1-N3 66.47(16), O1-Yb1-C1 72.76(15), N4-Yb1-Yb11 96.29(10), N4-Yb1-N3 78.91(14), N4-Yb1-C10A 100.31(15), N6-Yb1-N2A 97.29(16), N6-Yb1-N3 86.68(15), N6-Yb1-N4 160.77(16), O1-Yb1-N4 90.37(14), O1A-Yb1-N4 100.34(14), O1-Yb1-N6 92.30(15), C1-Yb1-N4 79.18(17), C1-Yb1-N6 83.43(17), O1A-Yb1-N6 97.91(15), N6-Yb1-C10A 98.65(15).

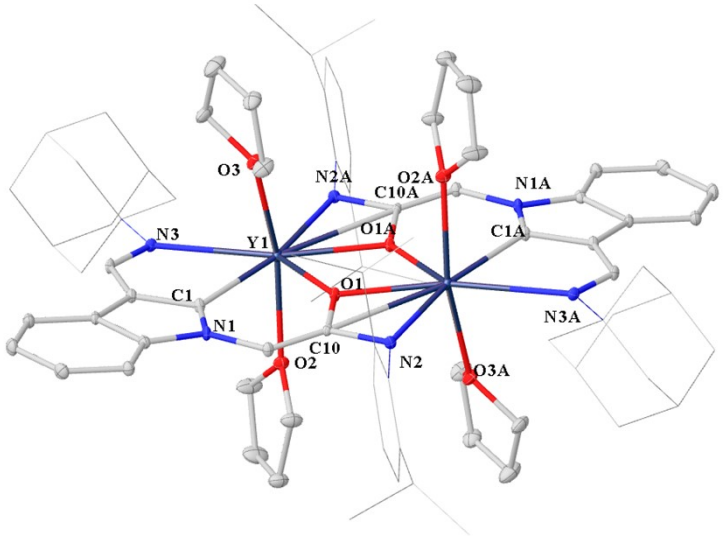

Figure S35: OLEX 2 drawing of **4-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.262(4), Y1-O1A 2.279(4), Y1-O2 2.386(4), Y1-O3 2.371(4), Y1-N3 2.661(5), Y1-N2A 2.442(4), Y1-C10A 2.868(6), Y1-C1 2.404(6), O1-C10 1.356(6), N2-C10 1.386(7), N2A-Y1-N3 101.04(15), C1-Y1-N3 66.95(18), O1-Y1-C1 71.42(17), O1-Y1-O2 84.86(14), O2-Y1-O3 164.23(16), O2-Y1-N3 85.97(15), O2-Y1-N2A 98.18(16), O2-Y1-C1 80.36(19), O1A-Y1-O2 98.11(14), O3-Y1-N3 89.19(15), O3-Y1-C1 83.94(18), O1A-Y1-O3 92.09(14).

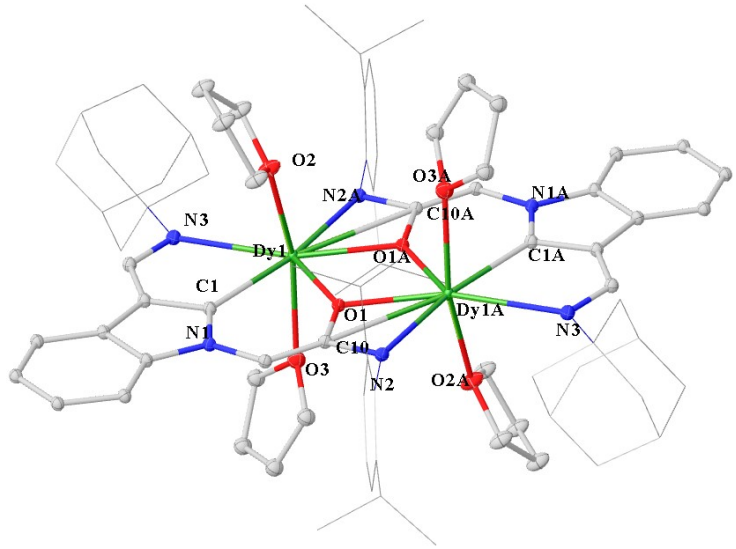

Figure S36: OLEX 2 drawing of **4-Dy** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Dy1-O1 2.270(3), Dy1-O1A 2.295(3), Dy1-N2A 2.426(4), Dy1-N3 2.688(4), Dy1-O3 2.422(5), Dy1-C10A 2.874(5), Dy1-O2 2.392(5), Dy1-C1 2.414(6), O1-C10 1.353(6), N2-C10 1.373(7), O1-Dy1-O1A 64.24(14), C1-Dy1-N3 66.66(18), O1-Dy1-C1 71.12(16), O1A-Dy1-C10A 27.54(13), N2A-Dy1-N3 101.97(15), N2A-Dy1-C10A 28.46(14), O1-C10-N2 109.0(4), O1-Dyl-O3 87.43(16), C1-Dy1-O3 82.1(2), O1A-Dy1-O3 95.70(16), O3-Dy1-N2A 98.54(17), O3-Dy1-N3 89.19(16), O3-Dy1-C10A 98.11(17), O2-Dy1-N2A 97.25(17), O2-Dy1-N3 85.95(17), O1-Dy1-O2 86.04(16).

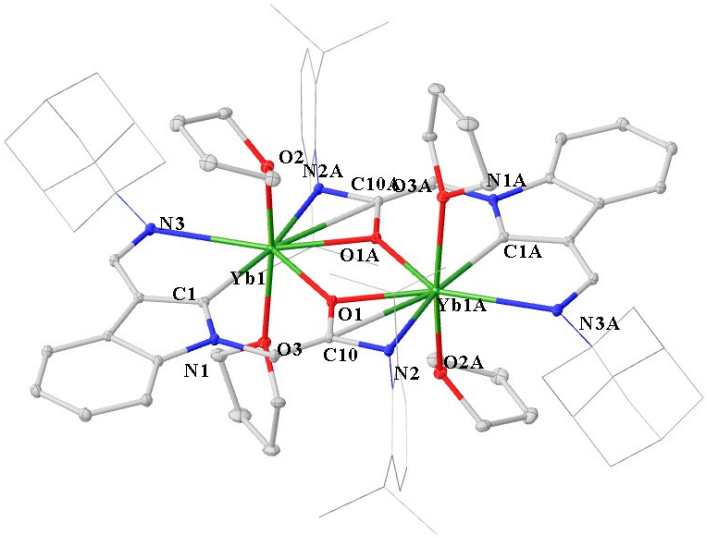

Figure S37: OLEX 2 drawing of **4-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1A 2.2363(19), Yb1-O1 2.2421(18), Yb1-N2A 2.399(2), Yb1-O3 2.337(2), Yb1-N3 2.676(5), Yb1-O2 2.337(2), Yb1-C1 2.389(5), Yb1-C10A 2.821(3), O1-C10 1.354(3), N2-C10 1.366(4), O1A-Yb1-O1 63.58(8), O1A-Yb1-C10A 28.14(7), N2A-Yb1-C10A 28.93(8), N2A-Yb1-N3 100.50(12), C1-Yb1-N3 66.83(16), O1-Yb1-C1 72.00(13), O1-Yb1-O3 87.54(8), O2-Yb1-O3 167.20(9), O3-Yb1-N3 86.0(3), O3-Yb1-C1 78.0(2), O1A-Yb1-O3 94.29(9).

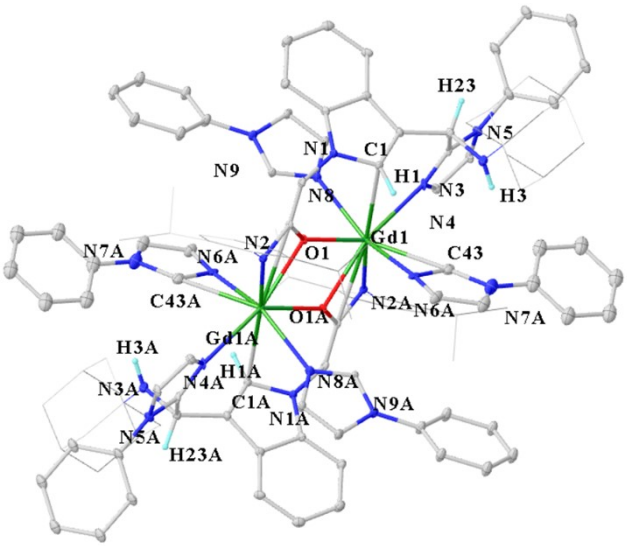

Figure S38: OLEX 2 drawing of **5-Gd** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms(except for C1, C23 and N3), all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Gd1-O1 2.298(6), Gd1-O1A 2.335(7), Gd1-N2A 2.363(8), Gd1-N4 2.556(8), Gd1-N8 2.507(8), Gd1-C1 3.035(11), Gd1-C43A 2.557(10), Gd1-N6A 2.502(8), O1-C10 1.376(11), N2-C10 1.372(12) , O1-Gd1-O1A 67.0(3), O1-Gd1-N2A 119.4(2), O1A-Gd1-N2A 57.2(2), O1A-Gd1-N4 150.3(3), O1-Gd1-N4 140.2(3), O1A-Gd1-N8 107.3(2), O1-Gd1-N8 78.8(2), O1-Gd1-C1 69.3(3), O1A-Gd1-C1 132.7(3), N2A-Gd1-N4 93.2(3), N2A-Gd1-N8 96.0(2), N2A-Gd1-C1 170.0(2), N4-Gd1-C1 77.0(3).

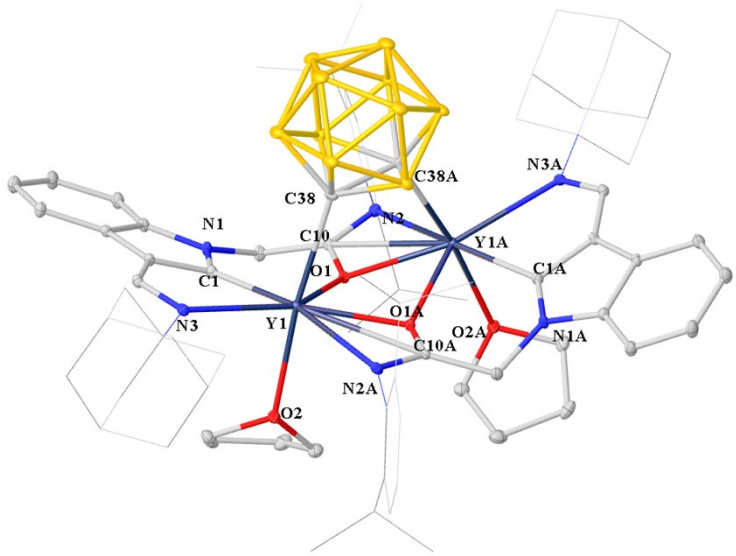

Figure S39: OLEX 2 drawing of **6a-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1 2.374(3), Y1-O1A 2.343(3), Y1-O2 2.426(3), Y1-N2A 2.689(4), Y1-N3 2.561(4), Y1-C10A 2.939(5), Y1-C1 2.393(5), Y1-C38 2.479(5), O1-C10 1.320(5), N2-C10 1.294(5), C38-C38A 1.752(9), O1A-Y1-O1 64.20(12), O1A-Y1-O2 89.97(11), O1-Y1-O2 90.83(12), O1A-Y1-N2A 51.97(10), O1-Y1-N2A 115.82(10), O2-Y1-C38 173.91(13), N2A-Y1-C10A 26.11(11), N3-Y1-N2A 104.05(12), N3-Y1-C10A 130.10(13), C1-Y1-O2 86.16(15), C1-Y1-N3 68.87(14), C1-Y1-C38 97.48(17), C38-Y1-N3 98.60(13), C38-Y1-C10A 87.25(15), N1-C1-Y1 137.1(3).

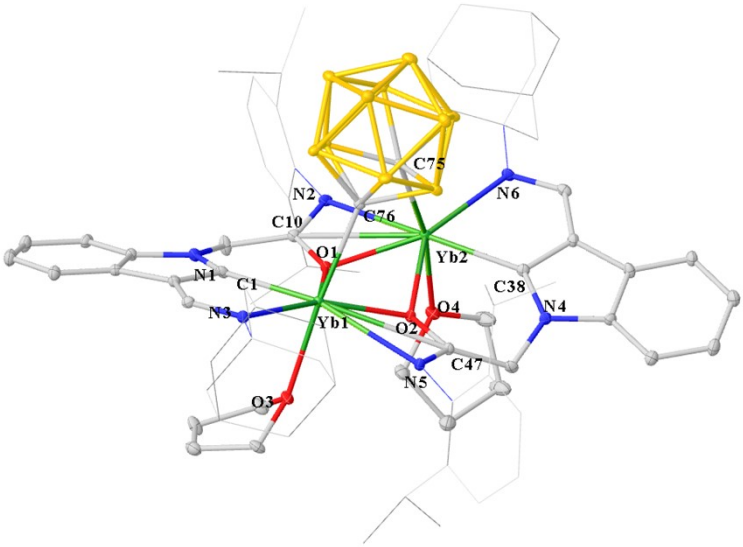

Figure S40: OLEX 2 drawing of **6a-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-O2 2.285(5), Yb1-O1 2.344(5), Yb1-O3 2.367(6), Yb1-N5 2.754(7), Yb1-N3 2.496(7), Yb1-C1 2.331(9), Yb1-C76 2.405(9), O1-C10 1.319(10), N2-C10 1.290(11), C75-C76 1.775(12), O2-Yb1-O1 64.44(19), O1-Yb1-C76 86.4(3), O3-Yb1-N5 85.2(2), O3-Yb1-N3 87.3(2), O3-Yb1-C76 172.9(3), C1-Yb1-O1 71.4(3) , C1-Yb1-O3 82.9(3), C1-Yb1-N5 165.5(2), C1-Yb1-N3 70.2(3), C1-Yb1-C76 99.5(3), C76-Yb1-N5 93.3(3), C76-Yb1-N3 99.8(3), O2-Yb2-N2 116.0(2), O1-Yb2-N2 52.1(2), N2-C10-O1 116.7(8), N2-C10-C9 123.7(8).

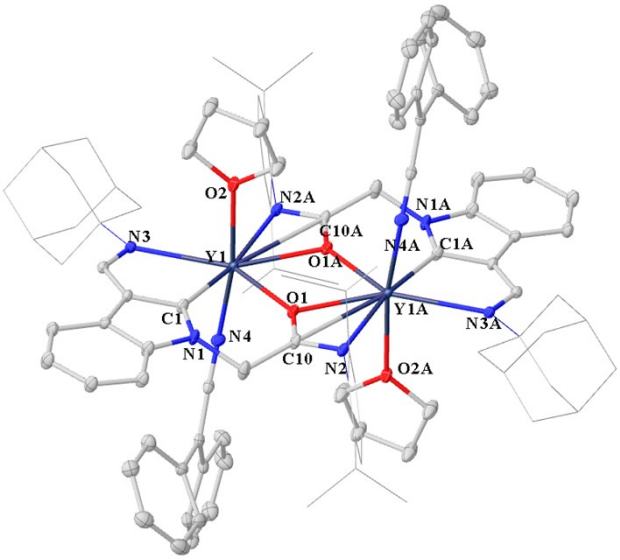

Figure S41: OLEX 2 drawing of **6b-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.402(7), Y1-O1 2.346(6), Y1-O2 2.364(6), Y1-N3 2.569(6), Y1-N2A 2.605(9), Y1-N4 2.285(9), Y1-C1 2.401(9), O1-C10 1.306(10), N2-C10 1.282(10), N4–C34 1.180(11), O1-Y1-O1A 64.2(3), O1A-Y1-C10A 29.2(4), N2A-Y1-C10A 26.7(3), N3-Y1-N2A 105.0(2), C1-Y1-N3 68.0(3), O1-Y1-C1 71.4(3), O2-Y1-O1A 82.0(3), N2-C10-O1 116.6(7), O2-Y1-N3 83.6(2), O2-Y1-N2A 83.6(3), O2-Y1-C10A 91.8(8), O2-Y1-C1 91.2(2), N4-Y1-O1A 105.1(3), N4-Y1-O1 91.9(3), N4-Y1-O2 170.2(2), N4-Y1-N3 87.2(2), N4-Y1-N2A 95.4(3), N4-Y1-C10A 91.5(8), N4-Y1-C1 88.6(3) , O1-Y1-O2 97.3(3).

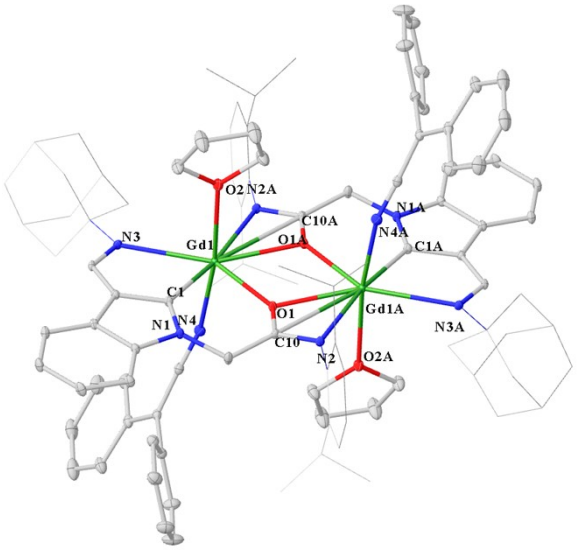

Figure S42: OLEX 2 drawing of **6b-Gd** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Gd1-O1A 2.425(3), Gd1-O1 2.364(3), Gd1-O2 2.420(3), Gd1-N3 2.575(3), Gd1-N2A 2.670(6), Gd1-C1 2.411(4), Gd1-N4 2.314(4), Gd1-C10A 2.974(5), N2-C10 1.287(6), O1-C10 1.314(6), N4-C38 1.174(6), O1-Gd1-O1A 64.31(11), O1A-Gd1-C10A 25.68(11), N2A-Gd1-C10A 25.64(12), N3-Gd1-N2A 106.27(13), C1-Gd1-N3 67.72(13), O1-Gd1-C1 71.01(12), O2-Gd1-O1A 83.28(11), O1-Gd1-O2 94.17(11), C1-Gd1-O2 88.10(14), O2-Gd1-N3 85.19(11), O2-Gd1-N2A 85.7(6), O2-Gd1-C10A 86.7(10), N4-Gd1-O1 93.71(13), N4-Gd1-O1A 102.84(13), N4-Gd1-O2 171.59(13).

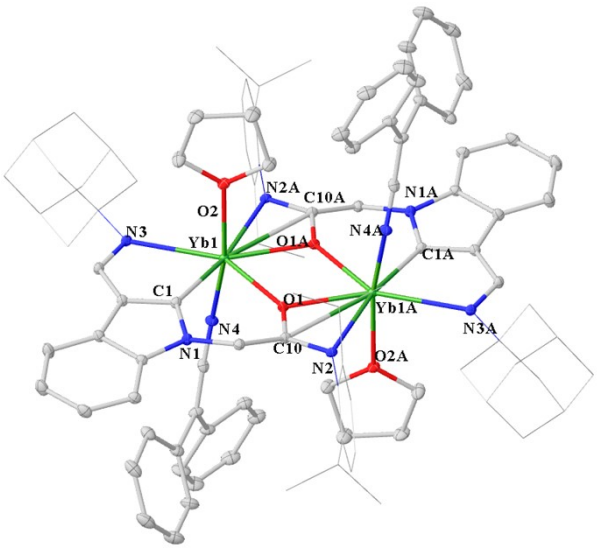

Figure S43: OLEX 2 drawing of **6b-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1A 2.341(2), Yb1-O1 2.3190(19), Yb1-O2 2.355(2), Yb1-N2A 2.577(2), Yb1-N4 2.216(3), Yb1-N3 2.532(11), Yb1-C10A 2.885(3), Yb1-C1 2.353(10), O1-C10 1.311(3), N2-C10 1.277(4) O1A-Yb1-C10A 26.55(7), N2A-Yb1-C10A 26.29(8), N3-Yb1-N2A 102.6(3), C1-Yb1-N3 69.3(4), O1-Yb1-C1 72.2(3), O2-Yb1-O1A 88.30(9), O2-Yb1-N2A 84.95(9), O2-Yb1-N3 86.1(5), O2-Yb1-C10A 87.51(10), O2-Yb1-C1 92.68(19), O1-Yb1-O2 96.70(8), N4-Yb1-O1A 98.53(10), N4-Yb1-O1 95.75(10), N4-Yb1-O2 167.48(11) , N4-Yb1-N2A 90.82(10), N4-Yb1-N3 83.3(5), N4-Yb1-C1 89.83(19).

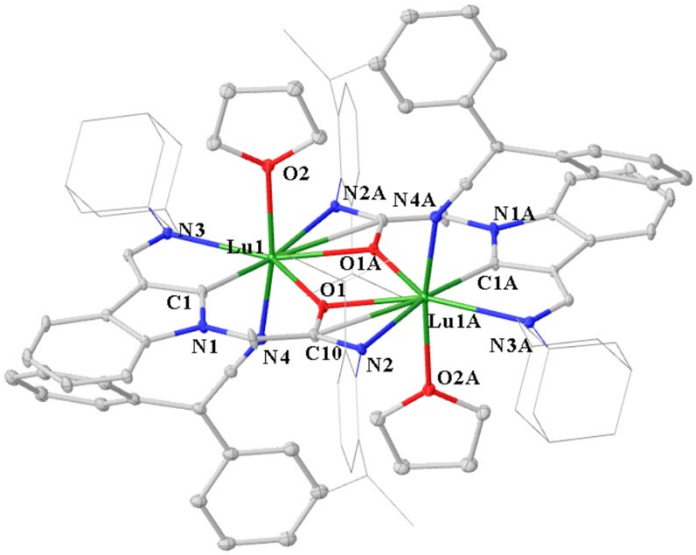

Figure S44: OLEX 2 drawing of **6b-Lu** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Lu1-O1A 2.359(8), Lu1-O1 2.335(6), Lu1-O2 2.337(3), Lu1-N2A 2.617(10), Lu1-N3 2.559(3), Lu1-N4 2.234(7), Lu1-C1 2.348(6), O1-C10 1.339(8), N2-C10 1.306(7), O1A-Lu1-O1 65.8(3) N3-Lu1-N2A 100.97(18), C1-Lu1-N3 69.7(2), O1-Lu1-C1 72.2(2), O1-Lu1-O2 98.3(5), O1A-Lu1-O2 85.4(5), O2-Lu1-N2A 84.8(4), O2-Lu1-N3 85.21(12), C1-Lu1-O2 84.9(2), N4-Lu1-N3 83.5(7), N4-Lu1-C1 95.8(6).

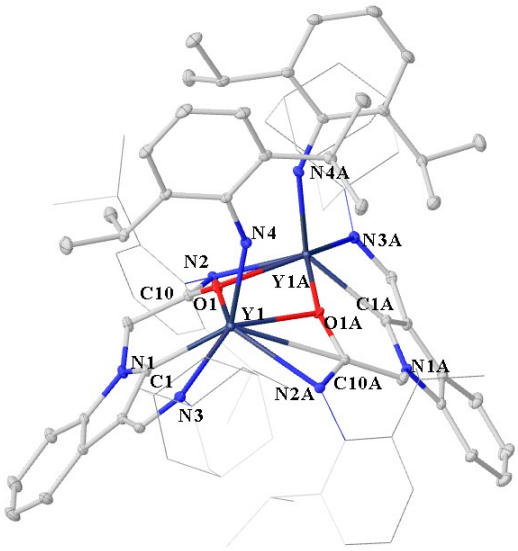

Figure S45: OLEX 2 drawing of **6c-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.3819(17), Y1-O1 2.3390(18), Y1-N2A 2.473(2), Y1-N3 2.558(2), Y1-N4 2.180(2), Y1-C1 2.392(3), O1-C10 1.297(3), N2-C10 1.295(3), O1-Y1-O1A 65.16(8), O1-Y1-C1 71.37(8), N3-Y1-N2A 88.72(7), C1-Y1-N3 68.26(8), N4-Y1-N2A 109.82(8), O1-Y1-N4 95.96(8), C1-Y1-N4 133.41(9), O1A-Y1-N4 89.49(7), N4-Y1-N3 109.67(8).

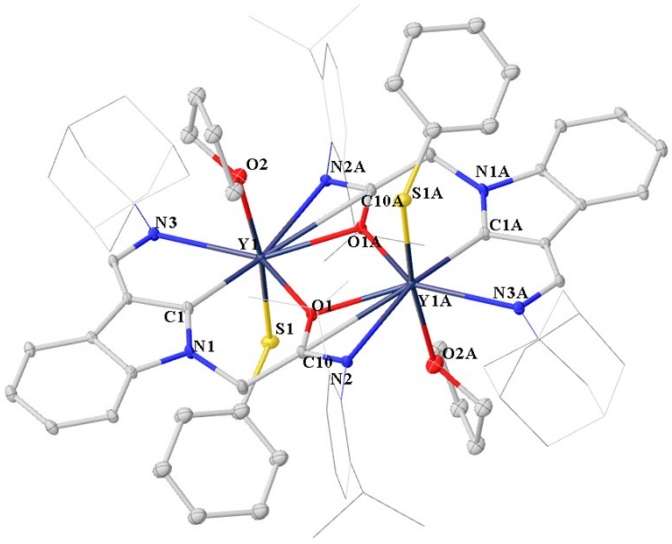

Figure S46: OLEX 2 drawing of **7a-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-S1 2.6998(17), Y1-O1 2.347(5), Y1-O1A 2.342(9), Y1-O2 2.392(4), Y1-N2A 2.615(11), Y1-N3 2.560(6), Y1-C1 2.389(7), O1-C10 1.311(7), N2-C10 1.303(8), S1-Y1-C1 102.3(6), O1A-Y1-S1 99.2(5), O2-Y1-S1 169.77(10), N2A-Y1-S1 90.1(4), N3-Y1-S1 91.0(4), O1-Y1-S1 101.2(5), C1-Y1-S1 102.3(6), N2A-Y1-S1 90.1(4).

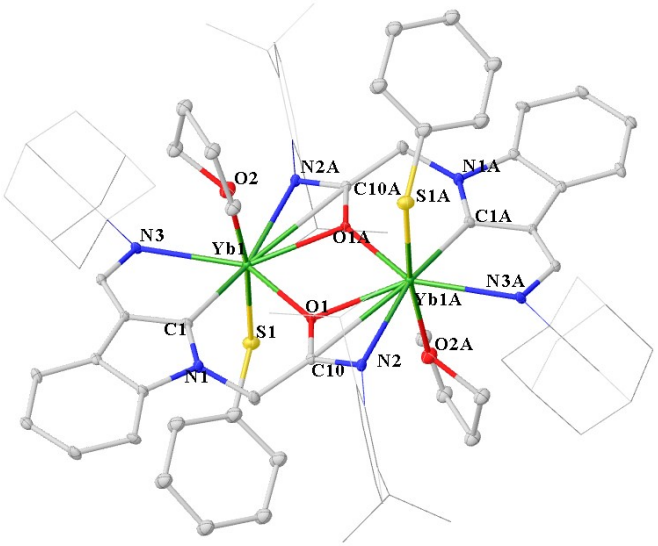

Figure S47: OLEX 2 drawing of **7a-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-S1 2.659(4), Yb1-O1 2.323(7), Yb1-O1A 2.352(7), Yb1-O2 2.371(9), Yb1-N2A 2.602(9), Yb1-N3 2.539(10), Yb1-C10A 2.918(11), Yb1-C1 2.340(11), O1-C10 1.312(13), N2-C10 1.283(14), O1-Yb1-O1A 64.8(3), O1A-Yb1-C10A 26.1(3), N2A-Yb1-C10A 26.1(3), N3-Yb1-N2A 101.4(3), C1-Yb1-N3 68.8(4), S1-Yb1-C10A 99.0(3), O1-Yb1-S1 96.3(2), O2-Yb1-S1 169.6(2), N3-Yb1-S1 89.5(3), C1-Yb1-S1 97.5(3).

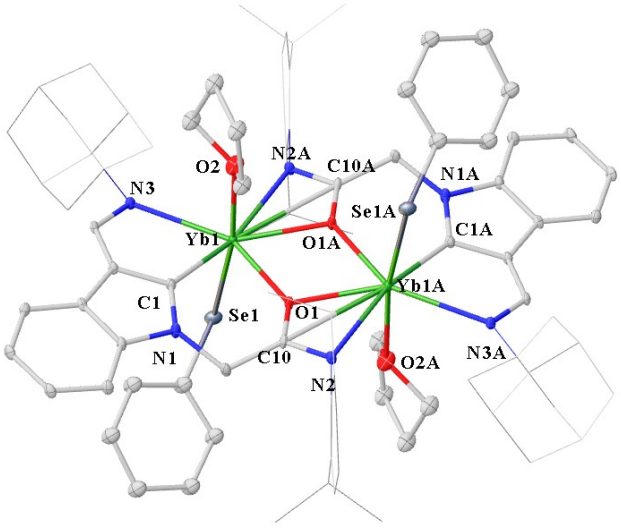

Figure S48: OLEX 2 drawing of **7b-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-Se1 2.801(2), Yb1-O1 2.322(9), Yb1-O1A 2.369(11), Yb1-O2 2.344(11), Yb1-N3 2.538(10), Yb1-N2A 2.640(11), Yb1-C1 2.320(12), O1-C10 1.321(14), N2-C10 1.285(14), O1-Yb1-Se1 91.7(5), O2-Yb1-Se1 169.0(6), N3-Yb1-Se1 88.7(5), N2A-Yb1-Se1 94.6(4), C1-Yb1-Se1 91.3(4), O1A-Yb1-Se1 108.3(5), C1-Yb1-N3 68.9(4), O1-Yb1-C1 73.3(4), O2-Yb1-N3 81.2(8), C1-Yb1-O2 89.1(5), O1-Yb1-O2 98.9(8), O1A-Yb1-O2 79.0(7).

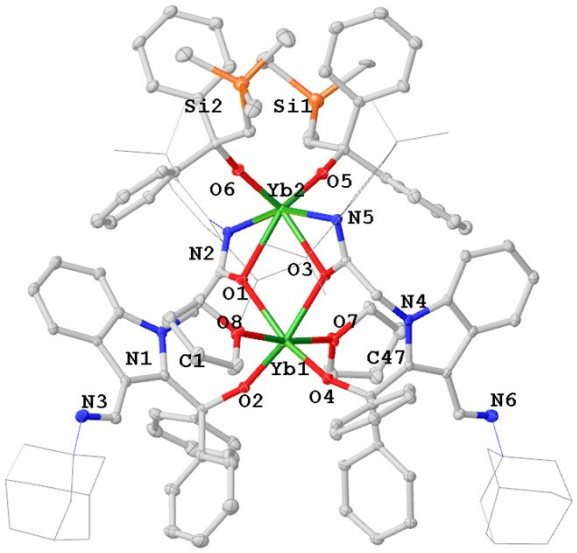

Figure S49: OLEX 2 drawing of **8a-Yb** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Yb1-O1 2.286(7), Yb1-O2 2.059(7), Yb1-O3 2.276(7), Yb1-O4 2.053(7), Yb1-O7 2.351(8), Yb1-O8 2.353(8), Yb2-O1 2.390(7), Yb2-O3 2.398(7), Yb2-O5 2.023(8), Yb2-O6 2.036(8), Yb2-N2 2.649(9), Yb2-N5 2.683(9), O1-C10 1.312(12), N2-C10 1.297(14), O3-C56 1.297(11), N5-C56 1.297(12), O1-Er1-O3 70.8(2), O1-Er1-O7 80.2(8), O2-Er1-O1 92.2(3), O2-Er1-O3 156.3(3), O3-Yb1-O7 79.3(3), O3-Yb1-O8 94.6(3), O2-Yb1-O4 106.9(2), O2-Yb1-O7 87.7(3), O2-Yb1-O8 96.9(3), O3-Yb2-N5 51.4(2), O5-Yb2-O6 114.5(2), O5-Yb2-N2 89.5(3), O6-Yb2-N5 90.6(3), N5-C56-O3 116.4(10).

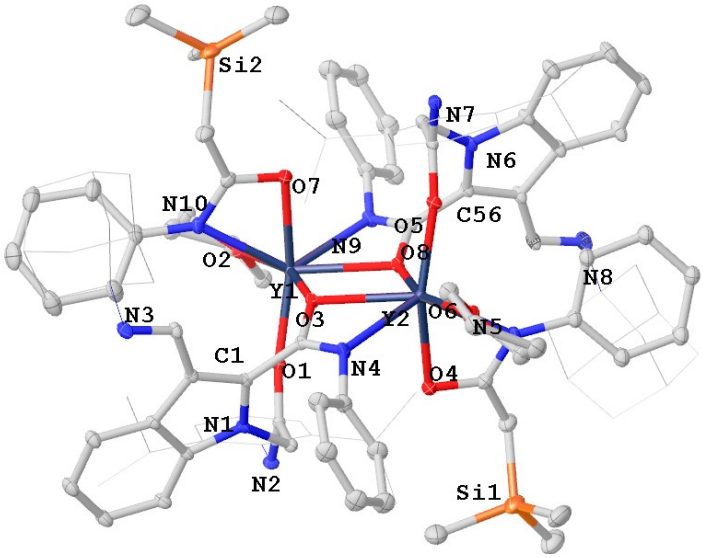

Figure S50: OLEX 2 drawing of **8b-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms, all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O8 2.431(3), Y1-O1 2.141(3), Y1-O3 2.322(3), Y1-O7 2.300(3), Y1-N10 2.402(4), Y1-O2 2.356(3), Y1-N9 2.486(4), O1-C10 1.309(5), N2-C10 1.281(6), O4-C51 1.296(6), N5-C51 1.330(7), O8-Y1-N9 52.88(12), O7-Y1-N9 82.05(14), O7-Y1-N10 55.95(14), O1-Y1-N10 111.33(14), O1-Y1-O3 86.47(12), O3-Y1-O8 67.70(10), N9-C89-O8 116.5(5).

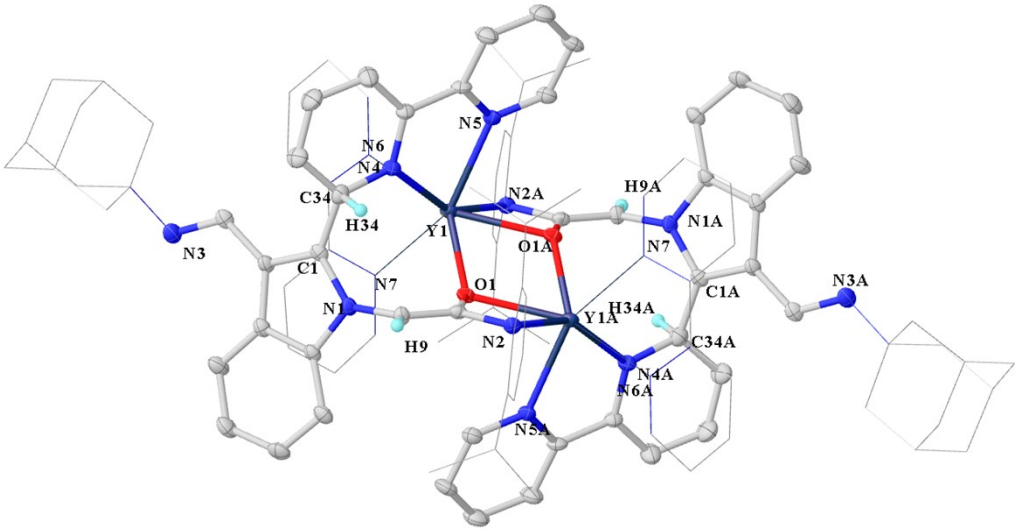

Figure S51: OLEX 2 drawing of **9-Y** with thermal ellipsoids drawn at the 10% probability level. All the hydrogen atoms(except for C9 and C34), all the atoms belong to the minor disordered parts and all the solvent molecules were omitted and the Adamantyl and Dipp groups for clarity. Selected bond lengths (Å) and angles (°): Y1-O1A 2.362(5), Y1-O1 2.227(5), Y1-N5 2.446(7), Y1-N2A 2.367(6), Y1-N7 2.479(7), Y1-N6 2.507(7), Y1-N4 2.433(7), Y1-C1 3.5845(4), Y1-C10A 2.844(9), O1-C10 1.367(9), N2-C10 1.356(9), C1-C34 1.482(11), O1-Y1-O1A 70.5(2), O1A-Y1-N5 80.1(2), O1-Y1-N5 116.75(19), O1A-Y1-N2A 56.71(19), O1-Y1-N2A 113.5(2), O1A-Y1-N7 119.5(2), O1-Y1-N7-83.9(2), O1A-Y1-N6 141.5(2), O1-Y1-N6-143.0(2), O1-Y1-N4 90.9(2), O1A-Y1-N4 129.3(2), N5-Y1-N4 66.7(2), N5-Y1-C10A 83.5(2), N2A-Y1-N5 92.4(2), N4-Y1-N7 104.0(2), N4-Y1-N6 79.0(2) , N4-Y1-C10A 148.5(2).

3. Tables of crystal data and structure refinement

Table S1. Crystal data and structure refinement for **2a**-**2f**.

	2a-Dy	**2b-Y**	**2c-Lu**	**2d-Y**	**2e-Y**	**2f-Y**
Formula	$C_{90}H_{134}Dy_2N_8O_2Si_2$	$C_{211}H_{280}N_{20}O_4Si_4Y_4$	$C_{117}H_{138}Lu_2N_6O_4P_2Si_2$	$C_{78}H_{110}N_6O_4Si_2Y_2$	$C_{98}H_{130}Cl_2N_{10}O_2SiY_2$	$C_{205}H_{256}N_{20}O_4Si_4Y_4$
FW	1741.285	3628.53	2160.39	1429.71	1785.01	3532.28
T (K)	293.15	293.15	293.15	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P2_1/c$
a (Å)	13.894(2)	16.328(2)	13.270(2)	15.5034(11)	13.8518(14)	13.9386(12)
b (Å)	16.106(2)	18.979(3)	14.812(3)	20.4486(14)	16.4987(16)	19.2482(17)
c (Å)	20.287(3)	20.337(3)	15.684(3)	26.0592(18)	23.322(2)	20.3638(18)
α (deg)	90	89.856 (2)	107.330(2)	90	80.5588(14)	90
β (deg)	93.565(2)	69.3928(19)	104.832(2)	105.7370(10)	75.9193(15)	109.7720(10)
γ (deg)	90	67.5264(18)	102.616(2)	90	71.7886(14)	90
V (Å^3)	4530.9(12)	5387.1(13)	2695.7(8)	7951.7(10)	4888.3(14)	5141.4(8)
Z	2	1	1	4	2	1
ρ_{calc} (g·cm^{-3})	1.276	1.118	1.331	1.194	1.213	1.141
μ (mm^{-1})	1.711	1.143	1.926	1.531	1.311	1.196
F (000)	1813.3	1930.0	1114.0	3032.0	1888.0	1870.0
θ range (deg)	2.14 to 28.37	1.082 to 22.044	1.449 to 24.779	1.285 to 22.986	1.305 to 24.784	1.499 to 25.077
Reflections collected	11003	40113	24865	64660	35183	49693
Independent reflections	10998	13252	9191	11048	16657	9121
R_{int}	0.0000	0.0813	0.0778	0.1183	0.0596	0.0956
Data / restraints / parameters	10998 / 1509 / 828	13252 / 2555 / 1365	9191 / 1177 / 887	11048 / 964 / 1109	16657 / 2770 / 1684	9121/ 2017 / 963
Goodness-of-fit on F^2	0.968	1.029	1.017	1.017	1.024	1.025
R1, *w*R2 [$I>=2\sigma(I)$]	0.0770, 0.2060	0.0638, 0.1619	0.0571, 0.0980	0.0507, 0.0921	0.0652, 0.1603	0.0564, 0.1343
R1, *w*R2 (all data)	0.1425, 0.2406	0.1245, 0.1932	0.0980, 0.1433	0.1075, 0.1121	0.1277, 0.1895	0.1140, 0.1614
Largest diff. peak and hole e.Å^{-3}	2.67, -1.36	0.55, -0.40	1.07, -1.13	0.42, -0.36	0.60, -0.48	0.41, -0.38

Table S2. Crystal data and structure refinement for **3**-**4**.

	3-Y	**3-Yb**	**4-Y**	**4-Dy**	**4-Yb**
Formula	$C_{102.88}H_{130.72}N_{14}O_2Y_2$	$C_{90}H_{116}N_{14}O_2Yb_2$	$C_{96}H_{124}N_6O_6Y_2$	$C_{94}H_{118}Cl_2Dy_2N_6O_6$	$C_{94}H_{118}Cl_2N_6O_6Yb_2$
FW	1773.31	1772.04	1635.82	1823.84	1844.92
T (K)	293.15	293.15	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	*P*$\bar{1}$	$P2_1/c$	$P2_1/c$	$P2_1/c$	*P*$\bar{1}$
a (Å)	14.003(2)	11.1364(10)	11.2935(17)	15.8687(8)	11.5500(7)
b (Å)	17.783(3)	14.3255(12)	20.388(3)	13.0193(7)	11.6597(7)
c (Å)	22.446(4)	27.014(2)	19.294(3)	22.0001(10)	16.8044(9)
α (deg)	111.9838(19)	90	90	90	95.7650(10)
β (deg)	90.766(2)	100.1613(12)	102.707(2)	104.730(2)	96.8490(10)
γ (deg)	106.259(2)	90	90	90	98.5150(10)
V (Å^3)	4931.8(13)	4242.1(6)	4333.6(11)	4395.8(4)	2206.0(2)
Z	2	2	2	2	1
ρ_{calc} (g·cm^{-3})	1.194	1.387	1.254	1.378	1.389
μ (mm^{-1})	1.225	2.246	1.389	1.803	2.222
F (000)	1880.0	1820.0	1736.0	1876.0	946.0
θ range (deg)	0.987 to 20.826	1.532 to 27.995	1.472 to 21.836	2.566to 27.535	1.779 to 28.791
Reflections collected	31074	36886	29960	129853	26576
Independent reflections	10184	9976	5135	10118	10513
R_{int}	0.0922	0.0627	0.0929	0.1301	0.0263
Data / restraints / parameters	10184 / 1346 / 1347	9976 / 727 / 637	5135 / 912 / 722	10118 / 963 / 720	10513 / 1761 / 902
Goodness-of-fit on F^2	1.006	1.033	1.018	1.090	1.053
R1, wR2 [I>=2σ(I)]	0.0581, 0.1305	0.0457, 0.0959	0.0536, 0.1224	0.0502, 0.0908	0.0298, 0.0734
R1, wR2 (all data)	0.1111, 0.1519	0.0773, 0.1058	0.0943, 0.1443	0.1017, 0.1144	0.0375, 0.0765
Largest diff. peak and hole e.Å^{-3}	0.46, -0.39	1.79, -0.72	0.34, -0.34	1.80, -0.92	0.98, -0.73

Table S3. Crystal data and structure refinement for **5-6a**.

	5-Gd	**6a-Y**	**6a-Yb**
Formula	$C_{148}Gd_2H_{156}N_{18}O_2$	$C_{45}H_{60}B_5N_3O_2Y$	$C_{90}H_{120}\ B_{10}N_6O_4Yb_2$
FW	2533.40	817.92	1804.09
T (K)	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*ī	*C2/c*	$P2_1/c$
a (Å)	12.403(4)	36.948(5)	17.6489(11)
b (Å)	16.355(5)	12.4060(15)	26.5767(14)
c (Å)	17.761(6)	21.4689(17)	21.5698(12)
α (deg)	71.152(3)	90	90
β (deg)	69.794(3)	114.410(6)	112.927(2)
γ (deg)	75.184(3)	90	90
V (Å^3)	3157.5(17)	8961.2(18)	9318.1(9)
Z	1	8	4
ρ_{calc} (g·cm^{-3})	1.332	1.213	1.286
μ (mm^{-1})	1.103	1.340	2.044
F (000)	1314.0	3448.0	3696.0
θ range (deg)	1.265 to 22.464	2.985 to 25	2.771 to 25
Reflections collected	22847	25218	54714
Independent reflections	8195	7680	16347
R_{int}	0.0864	0.0914	0.0951
Data / restraints / parameters	8195 / 1382 / 972	7680 / 90 / 1.012 498	16347 / 1322 / 1226
Goodness-of-fit on F2	1.040	1.012	1.044
R1, wR2 [I>=2σ(I)]	0.0727, 0.1832	0.0706, 0.1857	0.0575, 0.1274
R1, wR2 (all data)	0.1044, 0.2031	0.1278, 0.2275	0.1072, 0.1556
Largest diff. peak and hole e.Å^{-3}	1.50, -1.19	1.28, -0.58	2.53, -1.20

Table S4. Crystal data and structure refinement for **6b-6c**.

	6b-Y	**6b-Gd**	**6b-Yb**	**6b-Lu**	**6c-Y**
Formula	$C_{210}H_{233}ClN_{16}O_8Y_4$	$C_{102}H_{114}Gd_2N_8O_4$	$C_{116}H_{144}N_8O_6Yb_2$	$C_{108}H_{115}ClLu_2N_8O_4$	$C_{96}H_{128}N_8O_2Y_2$
FW	3500.20	1830.51	2092.562	1974.46	1603.88
T (K)	293.15	293.15	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	*P2₁/c*	*P2₁/c*	*P2₁/c*	*P*$\bar{1}$	*C2/c*
a (Å)	11.2380(14)	15.1436(8)	13.0075(7)	13.2763(8)	23.3363(17)
b (Å)	19.856(2)	13.3787(8)	14.8286(9)	13.3771(8)	18.0958(13)
c (Å)	21.857(3)	22.0380(12)	15.8738(9)	15.0490(9)	23.817(2)
α (deg)	90	90	114.4286(11)	96.1636(7)	90
β (deg)	98.1121(18)	97.5563(8)	107.878(1)	108.0725(7)	115.9220(10)
γ (deg)	90	90	90.1070(12)	108.4906(7)	90
V (Å^3)	4828.4(10)	4426.2(4)	2623.6(3)	2346.1(2)	9037.6(10)
Z	1	2	1	1	4
ρ_{calc} (g·cm^{-3})	1.204	1.373	1.324	1.398	1.178
μ (mm^{-1})	1.264	1.542	1.829	2.177	1.327
F (000)	1842.0	1884.0	1084.6	1010.0	3416.0
θ range (deg)	1.392 to 21.918	1.356 to 27.476	2.56 to 31.81	1.462 to 28.774	1.486 to 27.492
Reflections collected	34578	51059	73939	28324	52308
Independent reflections	5843	10121	16314	11171	10316
R_{int}	0.0846	0.0719	0.0240	0.0365	0.0642
Data / restraints / parameters	5843 / 1915 / 1057	10121 / 1440 / 904	16314 / 1264 / 934	11171 / 1967 / 1065	10316 / 39 / 526
Goodness-of-fit on F^2	1.023	1.018	1.057	1.029	1.005
R1, wR2 [I>=2σ(I)]	0.0736, 0.1990	0.0421, 0.0846	0.0364, 0.0991	0.0410, 0.0983	0.0436, 0.0970
R1, wR2 (all data)	0.1192, 0.2334	0.0844, 0.0993	0.0447, 0.1047	0.0572, 0.1052	0.0935, 0.1141
Largest diff. peak and hole e.Å^{-3}	0.79, -0.49	0.69, -0.38	1.04, -0.60	1.59, -0.59	0.39, -0.31

Table S5. Crystal data and structure refinement for **7a-7b**.

	7a-Y	**7a-Yb**	**7b-Yb**
Formula	$C_{98}H_{114}Cl_2N_6O_4S_2Y_2$	$C_{98}H_{114}Cl_2N_6O_4S_2Yb_2$	$C_{98}H_{114}Cl_2N_6O_4Se_2Yb_2$
FW	1752.79	1921.05	2014.85
T (K)	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	15.8156(12)	15.844(5)	15.755(3)
b (Å)	13.3389(10)	13.313(4)	13.423(2)
c (Å)	21.6468(17)	21.688(6)	21.611(4)
α (deg)	90	90	90
β (deg)	97.5740(11)	97.393(4)	97.254(3)
γ (deg)	90	90	90
V (Å^3)	4526.8(6)	4536(2)	4533.7(13)
Z	2	2	2
ρ_{calc} (g·cm^{-3})	1.286	1.406	1.476
μ (mm^{-1})	1.434	2.207	2.965
F (000)	1840.0	1964.0	2036.0
θ range (deg)	1.299 to 27.592	1.296 to 24.8	1.303 to 23.407
Reflections collected	52252	30555	36844
Independent reflections	10445	7774	6511
R_{int}	0.1051	0.1053	0.1352
Data / restraints / parameters	10445 / 1994 / 1012	7774 / 1451 / 878	6511 / 2062 / 1021
Goodness-of-fit on F^2	1.022	1.046	1.021
R1, wR2 [I>=2σ(I)]	0.0651, 0.1519	0.0733, 0.1792	0.0636, 0.1449
R1, wR2 (all data)	0.1556, 0.1896	0.1278, 0.2076	0.1222, 0.1787
Largest diff. peak and hole e.Å^{-3}	0.56, -0.58	2.09, -1.59	1.17, -1.45

Table S6. Crystal data and structure refinement for **8a-9**.

	8a-Yb	**8b-Y**	**9-Y**
Formula	$C_{144}H_{171}N_6O_8Si_2Yb_2$	$C_{122.04}H_{149.76}N_{10}O_8Si_2Y_2$	$C_{120}H_{124}N_{14}O_2Y_2$
FW	2516.12	2118.75	1972.14
T (K)	293.15	293.15	293.15
λ (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*$\bar{1}$	$P2_1/n$	$P2_1/c$
a (Å)	14.0244(6)	17.4148(13)	13.425(2)
b (Å)	21.3042(9)	28.557(2)	23.520(4)
c (Å)	24.2316(10)	23.4190(17)	16.835(3)
α (deg)	107.2910(10)	90	90
β (deg)	97.8820(10)	92.4319(12)	98.277(2)
γ (deg)	100.3630(10)	90	90
V (Å^3)	6658.4(5)	11636.1(15)	5260.7(14)
Z	2	4	2
ρ_{calc} (g·cm^{-3})	1.255	1.209	1.245
μ (mm^{-1})	1.471	1.072	1.156
F (000)	2618.0	4488.0	2072.0
θ range (deg)	1.905 to 25.212	1.125 to 23.377	1.498 to 20.862
Reflections collected	23906	98083	33691
Independent reflections	23906	16848	5516
R_{int}	0.0628	0.1217	0.1263
Data / restraints / parameters	23906 / 2281 / 1868	16848 / 2435 / 1746	5516 / 1066 / 804
Goodness-of-fit on F^2	1.040	1.024	1.020
R1, wR2 [I>=2σ(I)]	0.0599, 0.1292	0.0612, 0.1343	0.0677, 0.1507
R1, wR2 (all data)	0.1013, 0.1528	0.1272, 0.1606	0.1276, 0.1810
Largest diff. peak and hole e.Å^{-3}	2.65, -0.83	0.47, -0.27	0.39, -0.33