Supporting Information

1,2-Addition and Cycloaddition Reactions of Niobium Bis(imido) and Oxo Imido Complexes

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A. Crystallographic Data

Table S1. Crystallographic data for compounds **1**, **3a · HMDSO**, **4** and **5**.

Compound	**1**	**3a · HMDSO**	**4**	**5**
Empirical formula	$C_{37}H_{61}N_4Nb$	$C_{49}H_{85}N_4NbOSi_3$	$C_{43}H_{72}BN_4NbO_2$	$C_{42}H_{71}N_4NbO_2Si$
Formula weight (amu)	654.80	923.38	780.76	785.02
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Space group	$P2_1/c$	P-1	P-1	$P2_1/n$
a (Å)	13.322(5)	10.6684(3)	9.897(2)	10.650(1)
b (Å)	12.754(5)	12.8523(4)	11.357(2)	24.638(2)
c (Å)	21.266(5)	21.1721(7)	21.303(4)	16.578(1)
α (°)	90	101.451(2)	90.045(6)	90
β (°)	91.766(5)	103.695(1)	101.926(5)	97.111(3)
γ (°)	90	103.100(1)	113.572(6)	90
V (Å^3)	3612(2)	2647.7(1)	2138.1(8)	4316.8(5)
Z	4	2	2	4
ρ_{calcd} (g/cm^3)	1.204	1.158	1.213	1.208
μ (mm^{-1})	0.362	0.331	0.320	0.344
F_{000} (e$^-$)	1408	996	840	1688
Crystal size (mm^3)	.20 x .20 x .12	.13 x .07 x .05	.08 x .06 x .05	.08 x .05 x .05
Theta min / max (˚)	1.529 / 25.496	1.688 / 25.483	0.981 / 25.379	1.488 / 25.428
Reflections collected	70529	46576	18471	9146
R_{int}	0.0615	0.0709	0.0456	0.0361
T_{max} / T_{min}	0.7452 / 0.6810	0.7452 / 0.6936	0.7452 / 0.6836	0.7452 / 0.7031
Data / restr. / param.	6652 / 0 / 436	9696 / 0 / 557	7562 / 6 / 479	9146 / 0 / 477
GoF	1.090	1.026	1.052	1.119
R_1 / wR_2 ($I>2\sigma(I)$)	0.0660 / 0.1485	0.0476 / 0.0880	0.0758 / 0.2054	0.0336 / 0.0948
R_1 / wR_2 (all data)	0.0694 / 0.1500	0.0771 / 0.0995	0.0843 / 0.2190	0.0396 / 0.0995
Flack parameter	-	-	-	-
Res. peak / hole (e$^-$/Å^3)	1.210 / -1.496	1.117 / -0.912	1.800 / -0.707	0.630 / -0.421
τ_5[1]	0.02	0.00	0.28	0.02
CSD number	2004310	2004311	2004312	2004313

[1] A. W. Addison, T. N. Rao, J. Reedijk, J. van Rijn, G. C. Verschoor. *J. Am. Chem. Soc., Dalton Trans.,* 1984, 1349-1356.

Table S2. Crystallographic data for compounds **6**, **7**, **8**, and **9**.

Compound	**6**	**7**	**8**	**9**
Empirical formula	$C_{44}H_{72}BN_4NbO_4$	$C_{43}H_{69}N_4Nb$	$C_{56}H_{75}N_4SNb$	$C_{51}H_{69}N_4NbO$
Formula weight (amu)	824.77	734.93	929.17	847.01
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Space group	*P*n	*P*bca	*P*-1	$P2_1/c$
a (Å)	12.5350(5)	19.517(2)	13.4066(4)	24.1458(11)
b (Å)	17.4460(8)	18.796(2)	13.5108(4)	15.8759(7)
c (Å)	20.5667(8)	22.580(3)	14.4569(4)	24.2007(11)
α (°)	90	90	101.7150(10)	90
β (°)	96.552(2)	90	96.702(2)	101.813(2)
γ (°)	90	90	90.848(2)	90
V ($Å^3$)	4468.3(3)	8283(2)	2544.57(13)	9081.5(7)
Z	4	8	2	8
ρ_{calcd} (g/cm^3)	1.226	1.179	1.213	1.239
μ (mm^{-1})	0.313	0.323	0.317	0.306
F_{000} (e^-)	1768	3168	992	3616
Crystal size (mm^3)	.10 x .06 x .06	.12 x .08 x .08	.08 x .06 x .05	.20 x .16 x .16
Theta min / max (˚)	1.167 / 25.392	1.754 / 25.407	1.449 / 25.426	1.544 / 25.441
Reflections collected	8187	7601	57967	123296
R_{int}	0.0538	0.0696	0.0478	0.0400
T_{max} / T_{min}	0.7452 / 0.7242	0.7452 / 0.7100	0.745 / 0.705	0.953 / 0.941
Data / restr. / param.	8187 / 2 / 1013	7601 / 0 / 450	9328 / 0 / 575	16641 / 0 / 1059
GoF	1.031	1.051	1.055	1.052
R_1 / wR_2 ($I>2\sigma(I)$)	0.0384 / 0.0778	0.0447 / 0.0918	0.0329 / 0.0753	0.0395 / 0.1044
R_1 / wR_2 (all data)	0.0519 / 0.0847	0.0559 / 0.0970	0.0416 / 0.0799	0.0531 / 0.1145
Flack parameter	0.08(3)	-	-	-
Res. peak / hole ($e^-/Å^3$)	0.62 / -0.36	1.03 / -1.25	0.47 / -0.37	1.391 / -0.509
τ_5	0.03	0.21	0.89 (τ_4)[2]	0.09 (avg)
CSD number	2004314	2004315	2004316	2004177

[2] A. Okuniewski, D. Rosiak, J. Chojnacki and B. Becker, *Polyhedron*, 2015, **90**, 47–57.

Table S3. Crystallographic data for compounds **10**, **11 · C_7H_8**, **12 · Et_2O**, and **13 · 2 HMDSO**.

Compound	**10**	**11 · C_7H_8**	**12 · Et_2O**	**13 · 2 HMDSO**
Empirical formula	$C_{66}H_{100}N_6Nb_2S_2$	$C_{85}H_{126}N_8Nb_2O_8$	$C_{50}H_{77}N_4NbO_3$	$C_{48}H_{76}N_3NbO_4Si_2$
Formula weight (amu)	1227.45	1573.75	875.06	908.2
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Space group	*C*2/c	*P*2$_1$/c	*C*c	*P*-1
a (Å)	22.292(5)	17.141(2)	18.1386(6)	13.3294(12)
b (Å)	14.181(5)	25.100(3)	13.7454(5)	15.6578(14)
c (Å)	22.910(5)	22.772(3)	19.8912(7)	24.934(2)
α (°)	90.000(5)	90	90	76.581(4)
β (°)	117.461(5)	111.348(5)	106.288(1)	81.666(4)
γ (°)	90.000(5)	90	90	83.559(4)
V (Å^3)	6426(3)	9125(2)	4760.3(3)	4991.7(8)
Z	4	4	4	4
ρ_{calcd} (g/cm^3)	1.269	1.146	1.221	1.208
μ (mm^{-1})	0.465	0.304	0.297	0.332
F_{000} (e$^-$)	2608	3352	1880	1944
Crystal size (mm^3)	.70 x .40 x .10	.06 x .06 x .04	.12 x .08 x .05	.14 x .12 x .10
Theta min / max (˚)	1.767 / 25.380	1.257 / 25.415	1.888 / 25.370	1.341 / 25.499
Reflections collected	70667	71870	27774	85486
R_{int}	0.0312	0.0901	0.0524	0.1465
T_{max} / T_{min}	0.7452 / 0.7023	0.7452 / 0.6712	0.7452 / 0.7071	0.7452 / 0.6683
Data / restr. / param.	5882 / 0 / 356	16734 / 0 / 961	7825 / 2 / 542	18439 / 0 / 1079
GoF	1.045	1.022	1.048	1.002
R_1 / wR_2 (I>2σ(I))	0.0228 / 0.0586	0.0494 / 0.1038	0.0325 / 0.0770	0.0603 / 0.1587
R_1 / wR_2 (all data)	0.0244 / 0.0598	0.0901 / 0.1179	0.0347 / 0.0784	0.0849 / 0.1698
Flack parameter	-	-	-0.04(2)	-
Res. peak / hole (e$^-$/Å^3)	0.600 / -0.315	0.650 / -0.570	0.623 / -0.372	1.731 / -1.010
τ_5	-	-	0.20	-
CSD number	2004133	2004175	2004134	2004135

Table S4. Crystallographic data for compounds **15 · Et_2O**, **16 · ½ C_6H_6**, **18**, and **20 · Et_2O**.

Compound	**15 · Et_2O**	**16 · ½ C_6H_6**	**18**	**20 · Et_2O**
Empirical formula	$C_{91}H_{131}N_7Nb_2O_3$	$C_{51}H_{71}N_5NbO$	$C_{54}H_{79}N_4NbO_2Si$	$C_{68}H_{77}BF_{15}N_4NbO_3$
Formula weight (amu)	1556.84	863.03	937.21	1387.05
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Space group	$P2_1/n$	P-1	$P2_1/n$	$P2_1/c$
a (Å)	17.639(1)	11.665(1)	12.629(2)	22.223(2)
b (Å)	20.811(1)	12.637(1)	21.336(4)	24.338(2)
c (Å)	25.088(2)	17.247(1)	19.715(4)	24.561(2)
α (°)	90	81.664(2)	90	90
β (°)	100.667(1)	85.819(3)	92.431(4)	91.576(3)
γ (°)	90	68.744(2)	90	90
V (Å^3)	9050(1)	2343.6(2)	5307(2)	13279(2)
Z	4	2	4	8
ρ_{calcd} (g/cm^3)	1.143	1.223	1.173	1.388
μ (mm^{-1})	0.302	0.298	0.290	0.272
F_{000} (e$^-$)	3328	922	2008	5744
Crystal size (mm^3)	.18 x .12 x .10	.16 x .12 x .12	.12 x .10 x .08	.14 x .06 x .04
Theta min / max (˚)	1.280 / 25.359	1.194 / 25.469	1.407 / 25.389	1.507 / 25.427
Reflections collected	83162	31429	59328	63281
R_{int}	0.0546	0.0396	0.0530	0.1107
T_{max} / T_{min}	0.7452 / 0.6621	0.7452 / 0.7049	0.7452 / 0.6620	0.7452 / 0.5545
Data / restr. / param.	16411 / 3 / 958	8583 / 0 / 539	9689 / 0 / 578	24250 / 0 / 1695
GoF	1.069	1.065	1.043	0.969
R_1 / wR_2 (I>2σ(I))	0.0445 / 0.1130	0.0288 / 0.0716	0.0453 / 0.1023	0.0688 / 0.1694
R_1 / wR_2 (all data)	0.0639 / 0.1237	0.0312 / 0.0732	0.0576 / 0.1082	0.1239 / 0.1923
Flack parameter	-	-	-	-
Res. peak / hole (e$^-$/Å^3)	1.39 / -0.92	0.624 / -0.337	0.914 / -0.257	0.941 / -1.599
τ_5	-	0.18	0.03	-
CSD number	2004176	2004136	2004137	2004138

Table S5. Selected bond lengths (Å) and angles (°) for compound **1**.

Bond or Angle	**1**
Nb – N(1)	2.211(4)
Nb – N(2)	2.266(4)
Nb – N(3)	1.738(6)
Nb – N(4)	1.955(7)
Nb – H(1)	1.76(6)
N(1) – Nb – H(1)	148(2)
N(2) – Nb – N(4)	147.4(2)
N(1) – Nb – N(3)	103.5(2)
Nb – N(3) – C(30)	176.8(5)
Nb – N(4) – C(34)	127.5(4)

Table S6. Selected bond lengths (Å) and angles (°) for compounds **3a · HMDSO** and **4**.

Bond or Angle	**3a · HMDSO**	**4**
Nb – N(1)	2.262(3)	2.168(6)
Nb – N(2)	2.228(3)	2.292(7)
Nb – N(3)	1.750(3)	1.783(6)
Nb – N(4)	2.017(3)	2.068(6)
Nb – H(1)	1.75(3)	1.97(7)
N(n) – Nb – H(1)	149(1) (n = 2)	128(2) (n = 1)
N(1) – Nb – N(4)	149.2(1)	126.5(2)
N(1) – Nb – N(3)	103.1(1)	103.07(8)
Nb – N(3) – C(30)	173.5(2)	163.1(5)
Nb – N(4) – C(34)	116.4(2)	129.2(5)
Nb – N(4) – X(1)	121.3(1) (X = Si)	110.0(5) (X = B)

Table S7. Selected bond lengths (Å) and angles (°) for compounds **5** and **6**.

Bond or Angle	**5**	**6**
Nb – N(1)	2.289(2)	2.192(4)
Nb – N(2)	2.282(2)	2.276(4)
Nb – N(3)	1.757(2)	1.746(4)
Nb – N(4)	2.016(2)	2.035(5)
Nb – O	2.041(2)	2.068(4)
N(1) – Nb – O	154.55(8)	154.8(2)
N(2) – Nb – N(4)	155.78(8)	152.7(2)
N(1) – Nb – N(3)	98.00(9)	98.6(2)
Nb – N(3) – C(30)	173.6(2)	175.0(4)
Nb – N(4) – C(34)	118.1(2)	113.7(3)
Nb – N(4) – X(1)	117.7(1) (X = Si)	127.6(4) (X = B)
Nb – O – C	167.2(2)	127.8(4)

Table S8. Selected bond lengths (Å) and angles (°) for compounds **7** and **8**.

Bond or Angle	**7**	**8**
Nb – N(1)	2.291(2)	2.065(2)
Nb – N(2)	2.204(2)	–
Nb – N(3)	1.783(2)	1.748(2)
Nb – N(4)	1.959(3)	1.972(2)
Nb – X	2.199(3) (X = C(38))	2.414(1) (X = S(1))
C(38) – C(39)	1.210(4)	–
N(2) – Nb – X	146.7(1) (X = C(38))	117.21(5) (X = S(1))
N(1) – Nb – N(4)	159.2(1)	115.28(7)
N(1) – Nb – N(3)	99.3(1)	103.71(7)
Nb – N(3) – C(30)	172.0(2)	172.3(2)
Nb – N(4) – C(34)	137.6(2)	139.5(2)
Nb – C(38) – C(39)	168.3(3)	–
C(38) – C(39) – C(40)	179.1(3)	–
N(3) – Nb – S(1)	–	92.92(6)
N(4) – Nb – S(1)	–	116.60(5)
Nb – S(1) – C(38)	–	121.63(6)

Table S9. Selected bond lengths (Å) and angles (°) for compound **9**.

Bond or Angle	**9**
Nb – N(1)	2.1271(17)
Nb – N(2)	2.1718(17)
Nb – N(3)	1.7777(17)
Nb – N(4)	2.0353(17)
Nb – O(1)	2.0910(15)
C(38) – N(4)	1.429(3)
C(38) – O(1)	1.351(3)
C(38) – C(39)	1.365(3)
N(1) – Nb – O(1)	118.65(6)
N(2) – Nb – N(4)	142.06(7)
N(1) – Nb – N(3)	102.20(7)
Nb – N(3) – C(30)	171.52(14)
Nb – N(4) – C(38)	91.00(12)

Table S10. Selected bond lengths (Å) and angles (°) for compounds **10** and **11 · C_7H_8**.

Bond or Angle	**10**	**11 · C_7H_8**
Nb – N(1)	2.238(2)	2.193(3)
Nb – N(2)	2.204(1)	2.183(2)
Nb – N(3)	1.760(1)	1.749(3)
Nb – X	2.385(1) (X = S(1))	2.104(2) (X = O(1))
Nb – X	2.419(1) (X = S(1a))	2.322(2) (X = O(2))
Nb – O(7)	–	2.049(2)
N(1) – Nb – X	155.12(4) (X = S(1))	163.0(1) (X = O(1))
N(2) – Nb – X	145.30(4) (X = S(1a))	163.5(1) (X = O(7))
N(1) – Nb – N(3)	97.73(6)	–
Nb – N(3) – C(30)	173.0(1)	172.1(2)
N(3) – Nb – O(2)	–	157.4(1)
Nb – O(1) – C(34)	–	95.7(2)
Nb – O(7) – C(74)	–	131.6(2)

Table S11. Selected bond lengths (Å) and angles (°) for compounds **12 · Et_2O** and **13 · 2 HMDSO**.

Bond or Angle	**12 · Et_2O**	**13 · 2 HMDSO**
Nb – N(1)	2.2097(3)	2.199(3)
Nb – N(2)	2.211(3)	2.125(3)
Nb – N(3)	1.789(3)	1.787(3)
Nb – N(4)	2.071(3)	–
Nb – O(1)	2.070(3)	2.085(2)
Nb – O(2)	–	2.290(2)
Nb – O(7)	–	2.072(2)
C(46) – N(4)	1.391(5)	–
C(46) – O(1)	1.345(5)	–
C(46) – O(2)	1.205(5)	–
N(1) – Nb – O(n)	129.0(1) (n = 1)	165.7(1) (n = 6)
N(2) – Nb – X	140.0(1) (X = N(4))	151.4(1) (X = O(2))
X – Nb – N(3)	104.9(1) (X = N(1))	166.9(1) (X = O(2))
Nb – N(3) – C(30)	174.2(3)	173.0(3)
Nb – N(4) – C(41)	146.2(3)	–
Nb – O(1) – C(42)	–	93.6(2)
Nb – O(6) – C(84)	–	126.0(2)

Table S12. Selected bond lengths (Å) and angles (°) for compounds **15 · Et_2O** and **16 · ½ C_6H_6**.

Bond or Angle	**15 · Et_2O**	**16 · ½ C_6H_6**
Nb(1) – N(1)	2.221(2)	2.299(1)
Nb(1) – N(2)	2.217(2)	2.186(1)
Nb(1) – N(3)	1.800(3)	1.816(1)
Nb(1) – N(4)	–	2.263(1)
Nb(1) – O(1)	1.938(2)	1.750(1)
Nb(1) – O(2)	1.949(2)	–
Nb(2) – N(4)	2.100(3)	–
Nb(2) – N(6)	1.777(3)	–
Nb(2) – N(7)	2.413(2)	–
Nb(2) – O(1)	1.980(2)	–
Nb(2) – O(2)	1.969(2)	–
N(1) – Nb(1) – O(1)	146.8(1)	143.72(5)
N(2) – Nb(1) – N(4)	–	154.70(5)
N(1) – Nb(1) – N(3)	101.1(1)	103.89(6)
Nb – N(3) – C(30)	173.2(2)	156.1(1)
N(2) – Nb(1) – O(2)	141.4(1)	–
Nb(1) – O(1) – Nb(2)	100.5(1)	–
N(4) – Nb(2) – O(1)	145.3(1)	–
N(7) – Nb(2) – O(2)	148.0(1)	–
N(6) – Nb(2) – N(4)	101.7(10	–
Nb(2) – N(6) – C(71)	170.3(2)	–

Table S13. Selected bond lengths (Å) and angles (°) for compounds **18** and **20 · Et_2O**.

Bond or Angle	**18**	**20 · Et_2O**
Nb – N(1)	2.191(2)	2.076(4)
Nb – N(2)	2.218(2)	2.193(4)
Nb – N(3)	1.772(2)	1.758(4)
Nb – N(4)	–	2.126(4)
Nb – O(1)	1.925(2)	2.134(4)
Nb – O(2)	1.937(2)	–
C(46) – N(4)	–	1.325(6)
C(46) – O(1)	–	1.302(6)
C(46) – O(2)	–	1.293(6)
N(1) – Nb – O(n)	150.1(1) (n = 2)	134.8(1) (n = 1)
N(2) – Nb – O(1)	148.5(1)	–
N(1) – Nb – N(3)	100.0(1)	103.7(2)
N(2) – Nb – N(4)	–	140.5(2)
Nb – N(3) – C(30)	172.9(2)	174.0(4)
Nb – O(1) – Si	154.2(1)	–
Nb – O(2) – C(50)	164.4(2)	–
Nb – N(4) – C(42)	–	144.2(3)

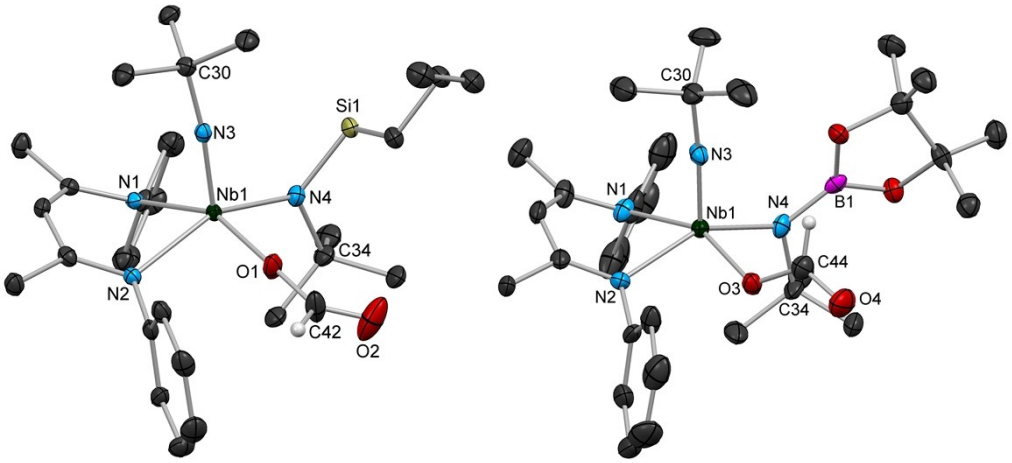

Figure S1. Crystal structures of **5** (left) and **6** (right) with 50% probability thermal ellipsoids. Selected H atoms, aryl ^{i}Pr groups, and second crystallographically inequivalent molecule of **6** are excluded.

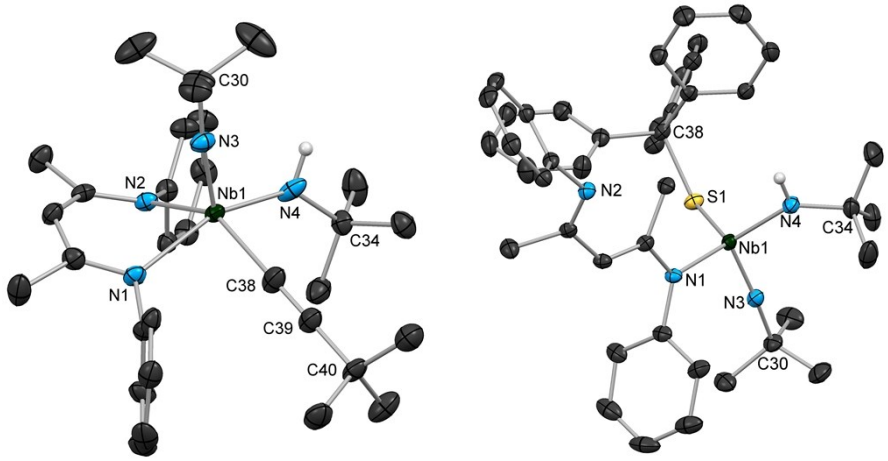

Figure S2. Crystal structures of **7** (left) and **8** (right) with 50% probability thermal ellipsoids. Selected H atoms and aryl ^{i}Pr groups are excluded.

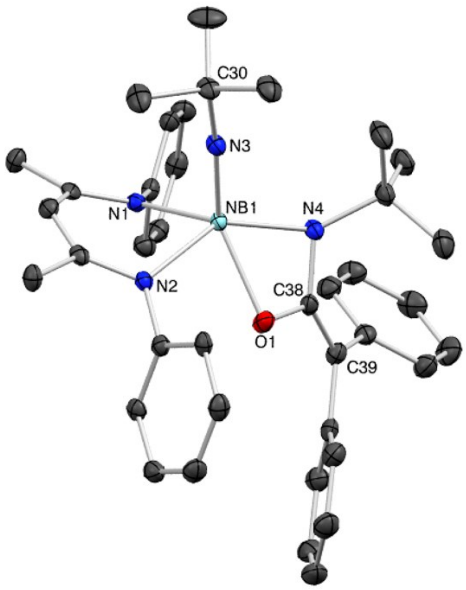

Figure S3. Crystal structure of **9** with 50% probability thermal ellipsoids. H atoms and aryl ^{i}Pr groups are excluded.

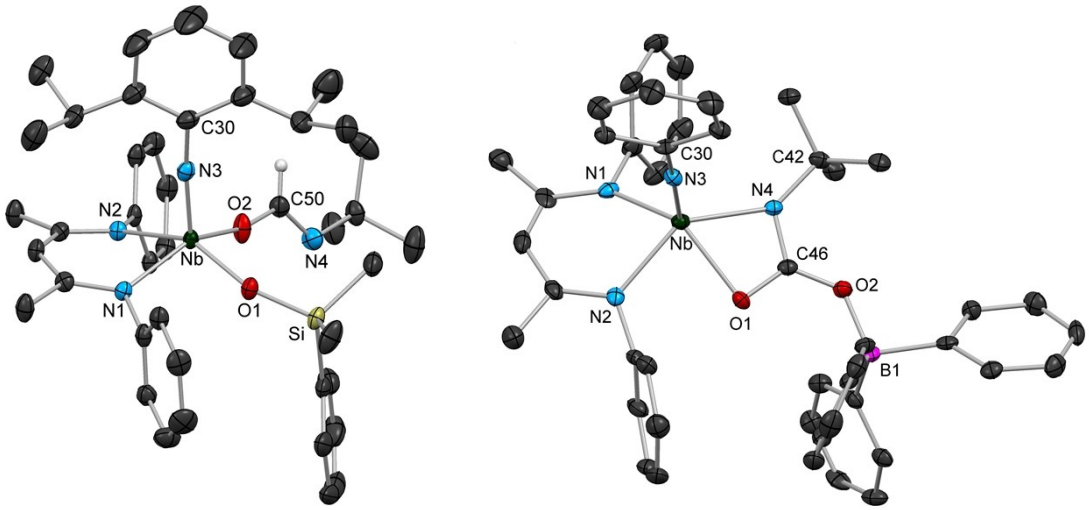

Figure S4. Crystal structures of **18** (left) and **20** (right) with 50% probability thermal ellipsoids. H atoms, selected aryl ^{i}Pr groups, aryl fluorine atoms, lattice solvent, and a second crystallographically inequivalent molecule of **20** are excluded.

B. NMR Spectral Data

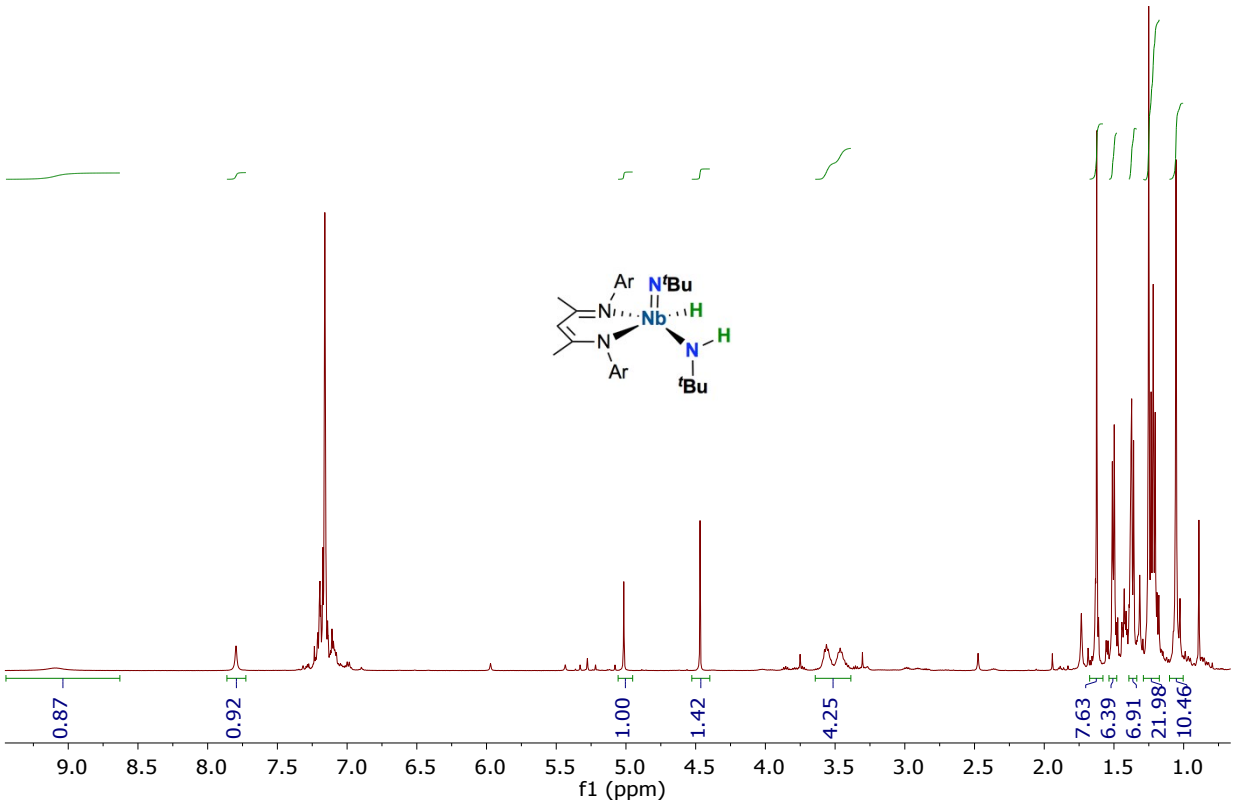

Figure S5. ^{1}H NMR Spectrum of **1** in C_6D_6 (500 MHz, 293K).

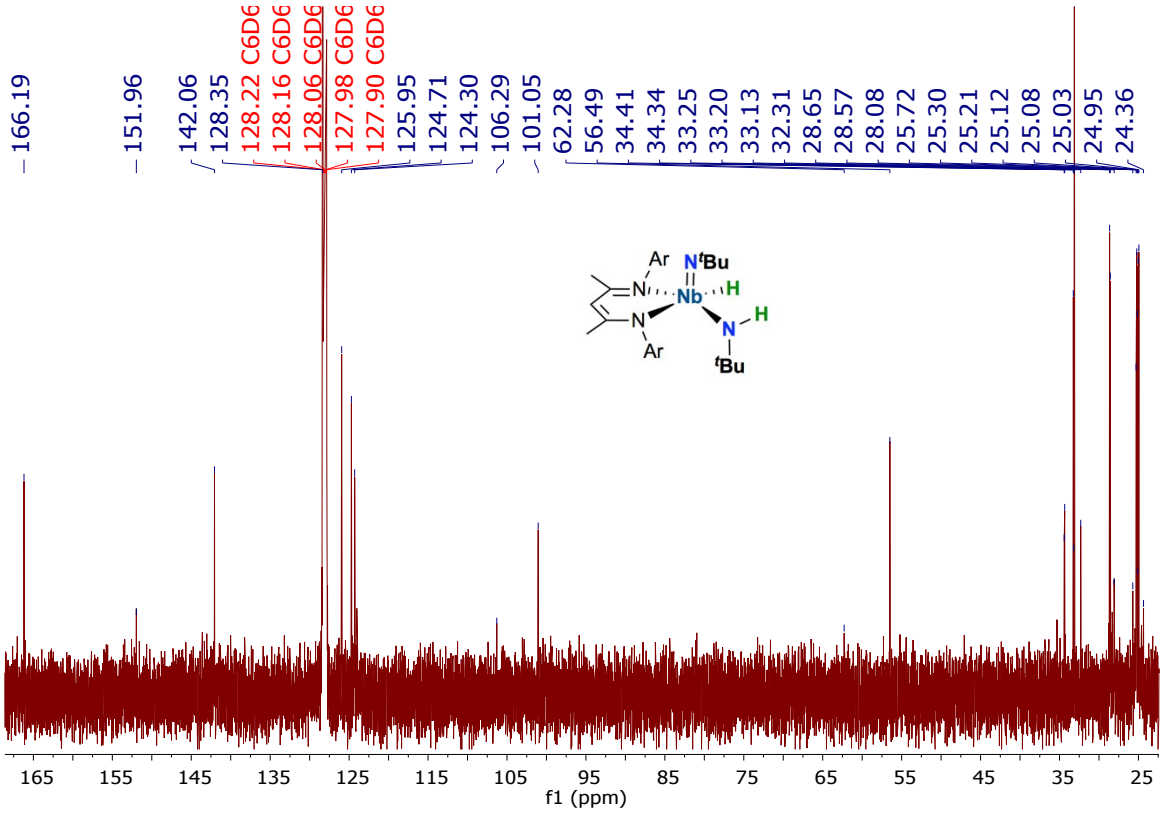

Figure S6. ^{13}C NMR Spectrum of **1** in C_6D_6 (151 MHz, 293K).

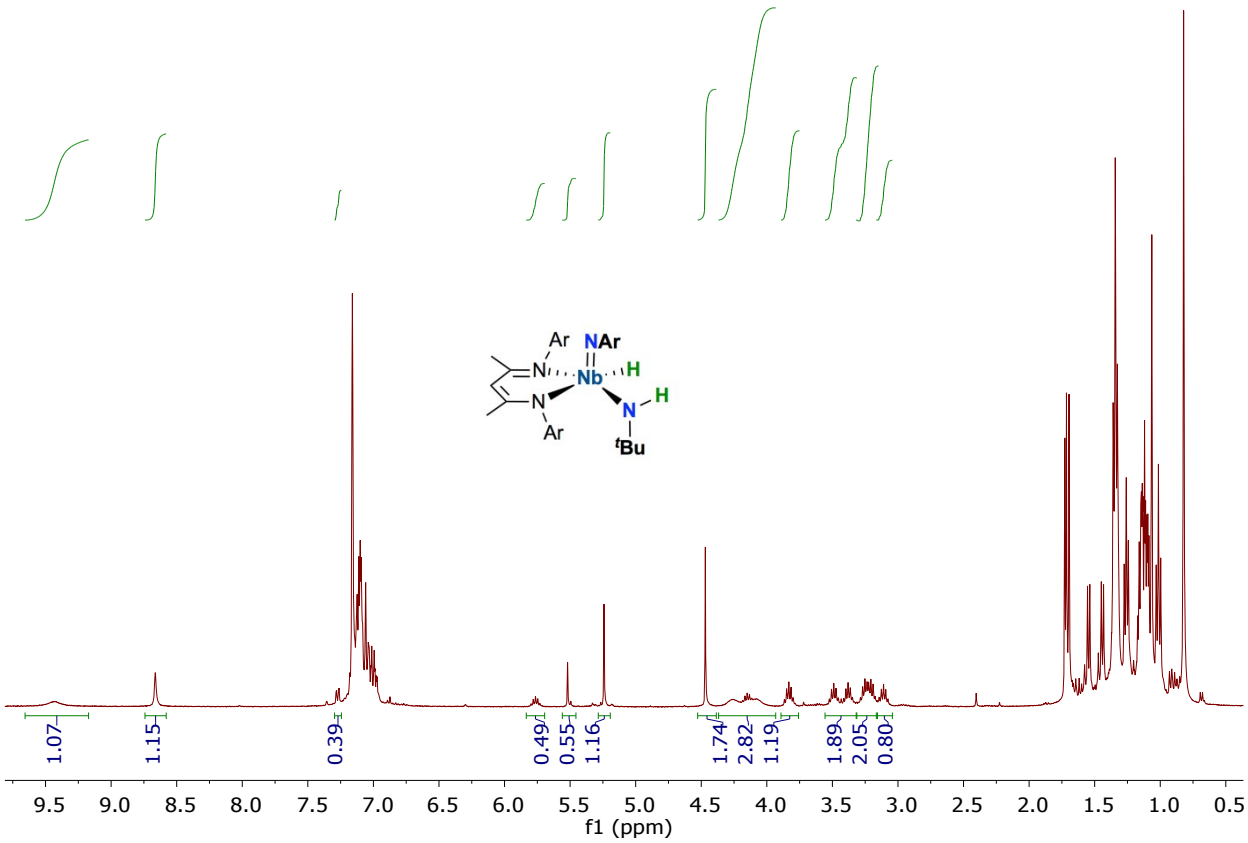

Figure S7. ^{1}H NMR Spectrum of **2** in C_6D_6 (400 MHz, 293K).

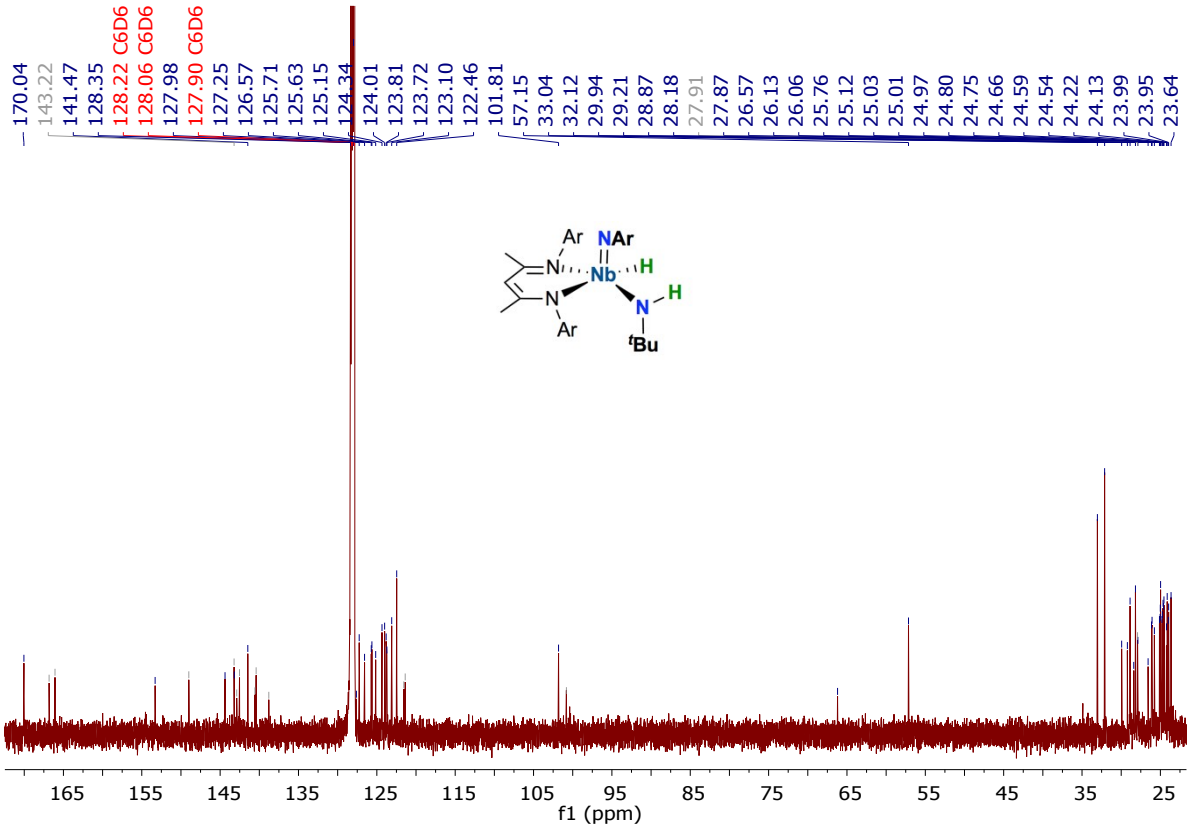

Figure S8. ^{13}C NMR Spectrum of **2** in C_6D_6 (151 MHz, 293K).

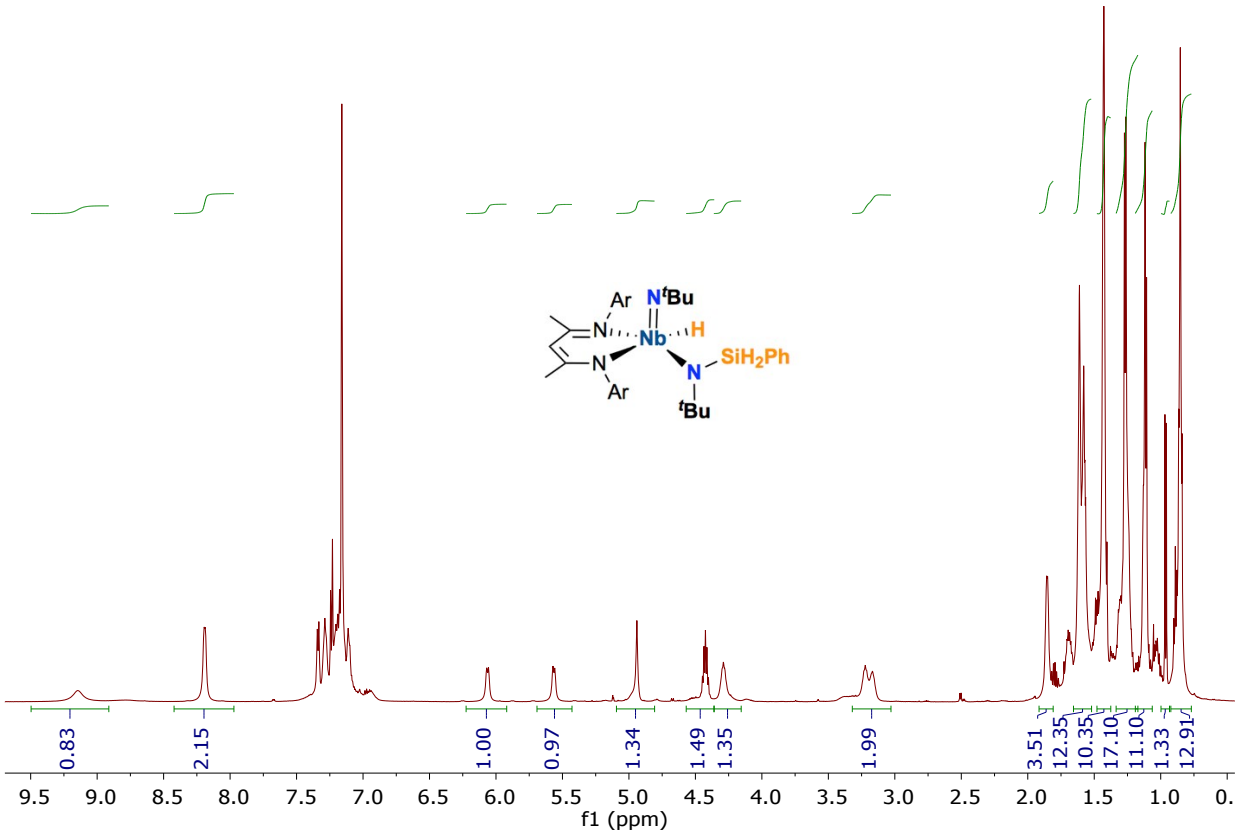

Figure S9. ^{1}H NMR Spectrum of **3a** in C_6D_6 (600 MHz, 293K).

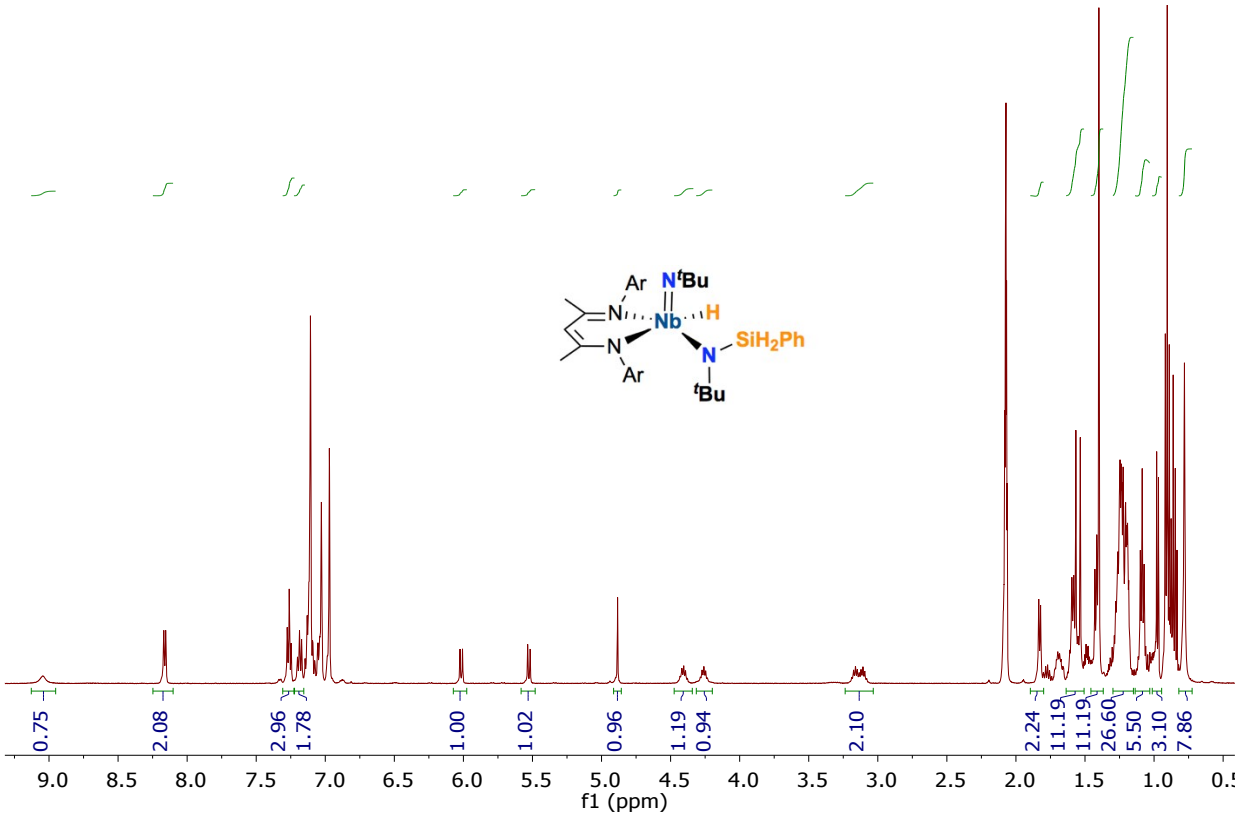

Figure S10. ^{1}H NMR Spectrum of **3a** in C_7D_8 (500 MHz, 253 K).

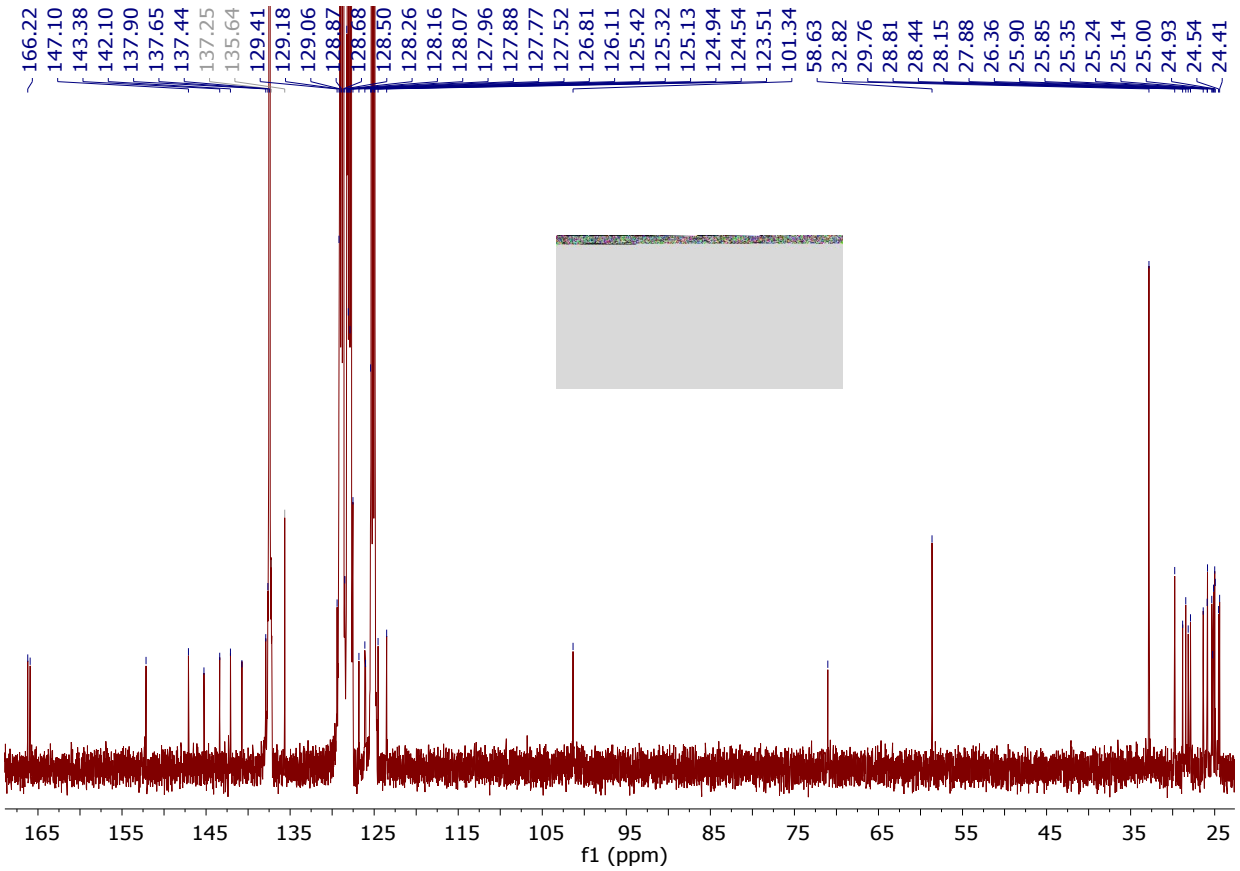

Figure S11. ^{13}C NMR Spectrum of **3a** in C_7D_8 (126 MHz 253 K).

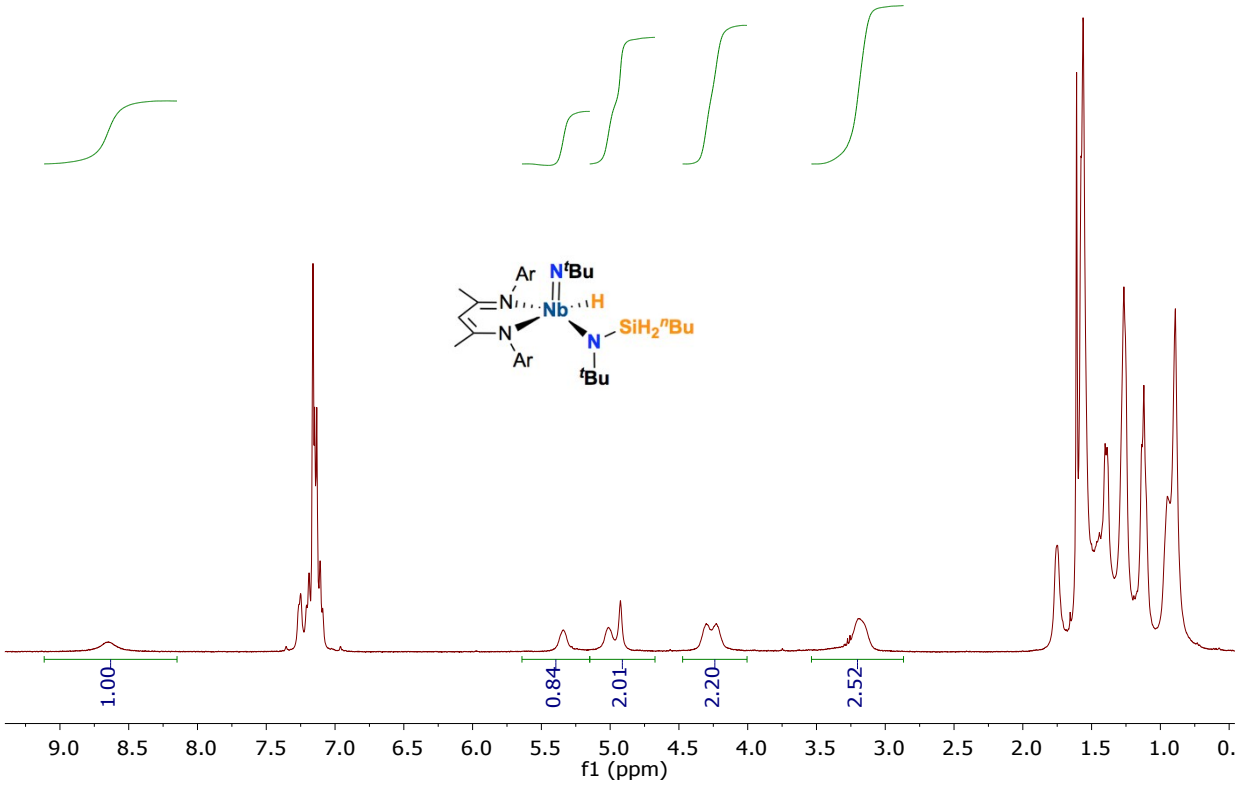

Figure S12. ^{1}H NMR Spectrum of **3b** in C_6D_6 (600 MHz, 293K).

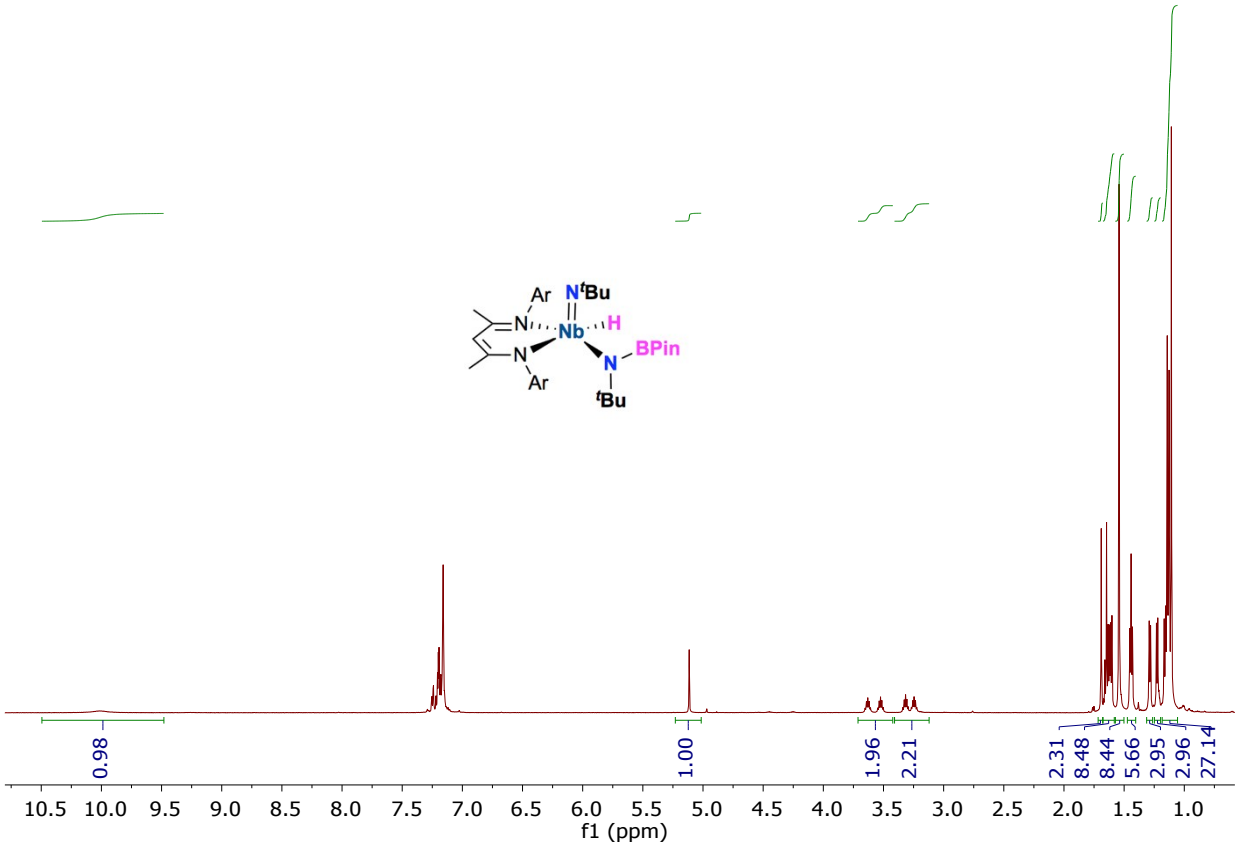

Figure S13. ^{1}H NMR Spectrum of **4** in C_6D_6 (600 MHz, 293K).

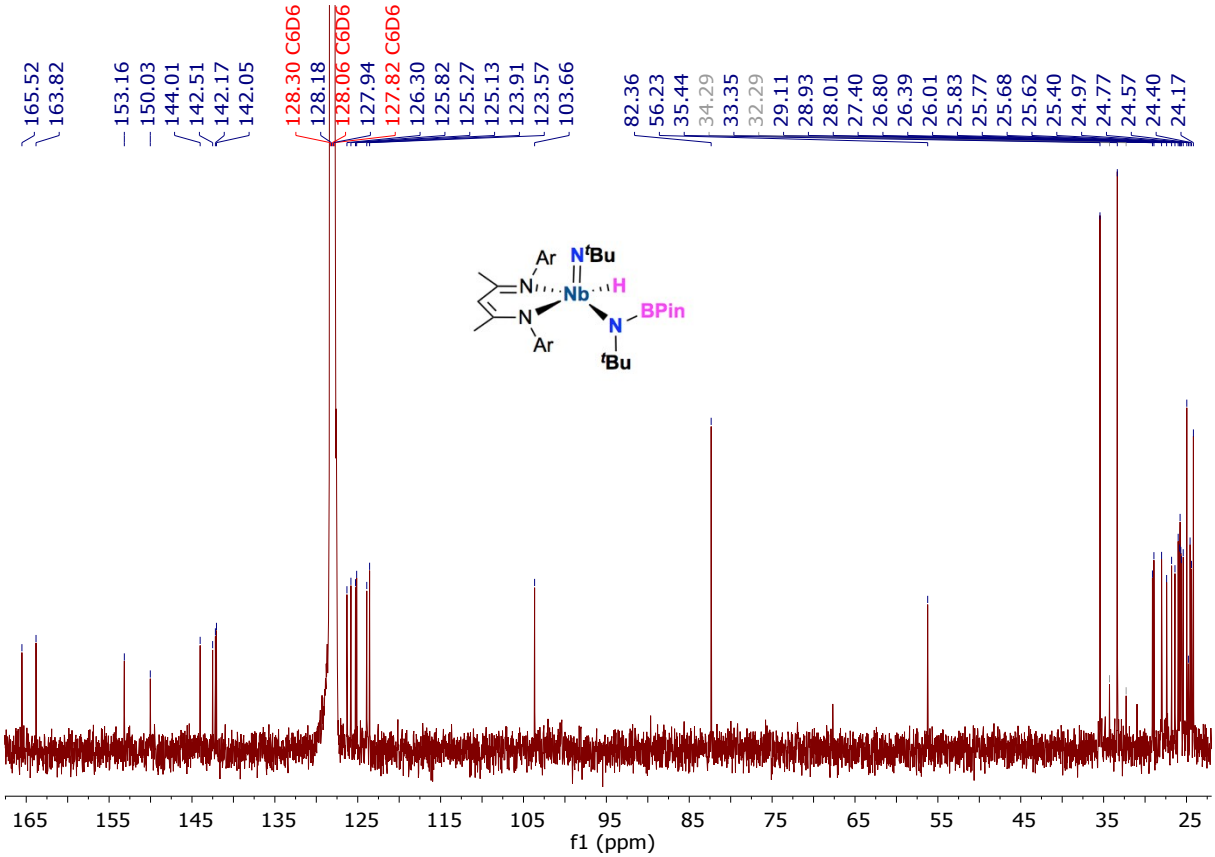

Figure S14. ^{13}C NMR Spectrum of **4** in C_6D_6 (101 MHz, 293K).

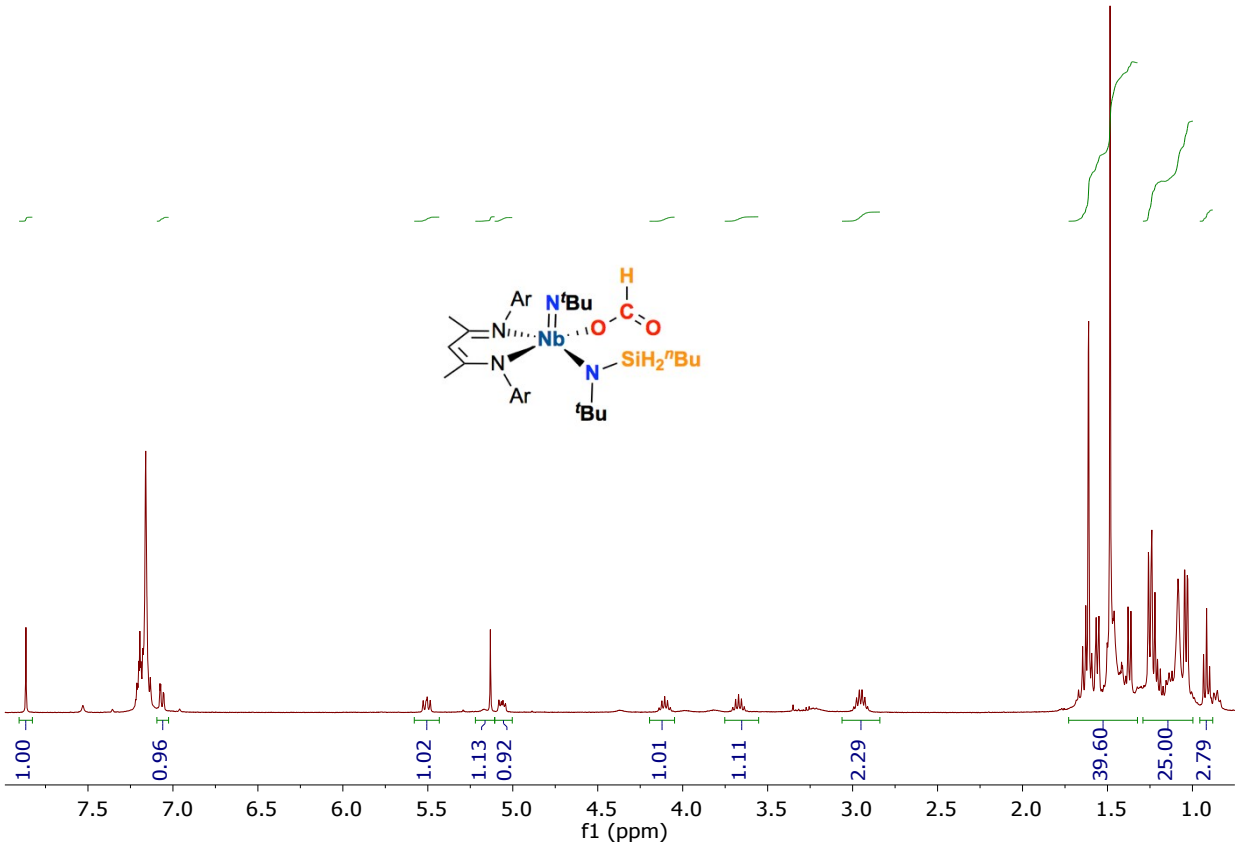

Figure S15. ^{1}H NMR Spectrum of **5** in C_6D_6 (400 MHz, 293K).

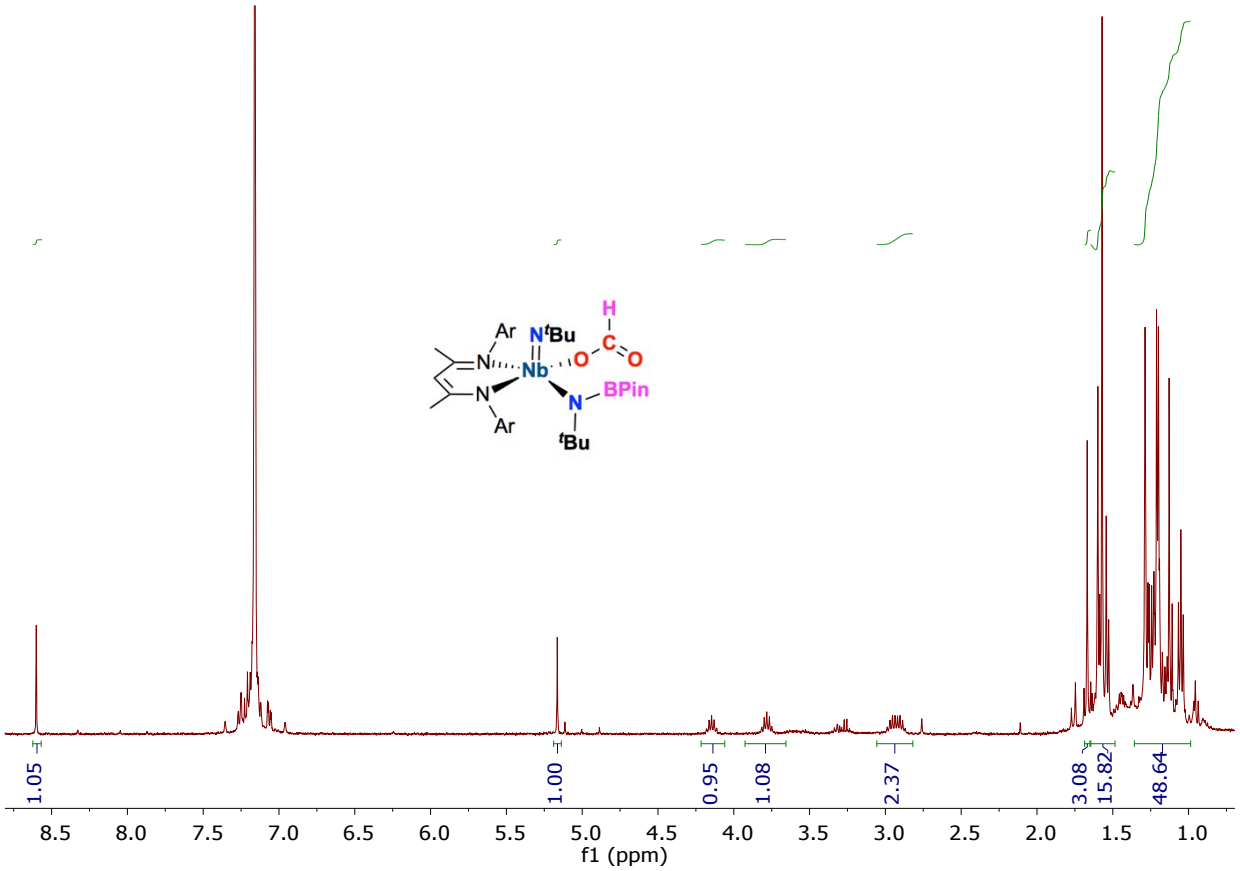

Figure S16. ^{1}H NMR Spectrum of **6** in C_6D_6 (400 MHz, 293K).

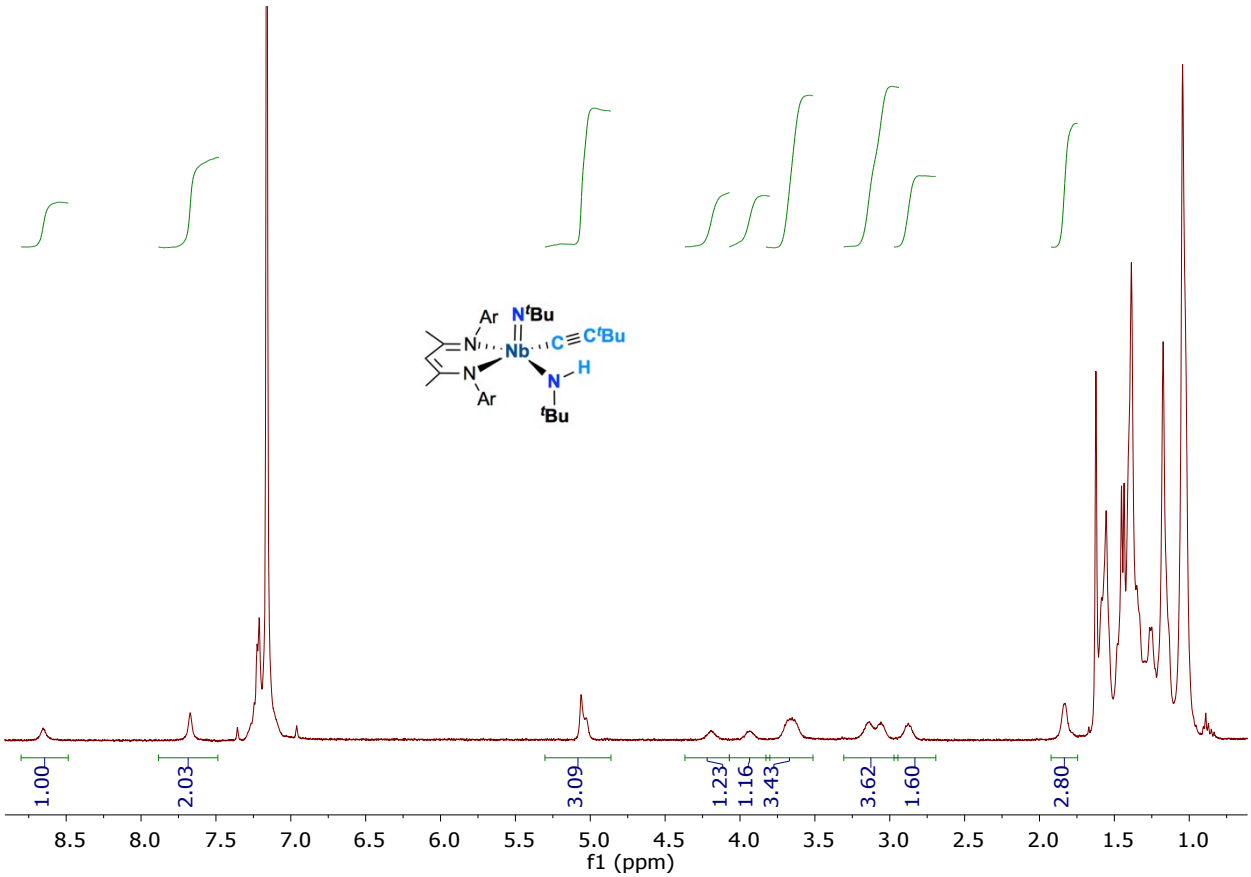

Figure S17. ^{1}H NMR Spectrum of **7** in C_6D_6 (600 MHz, 293K).

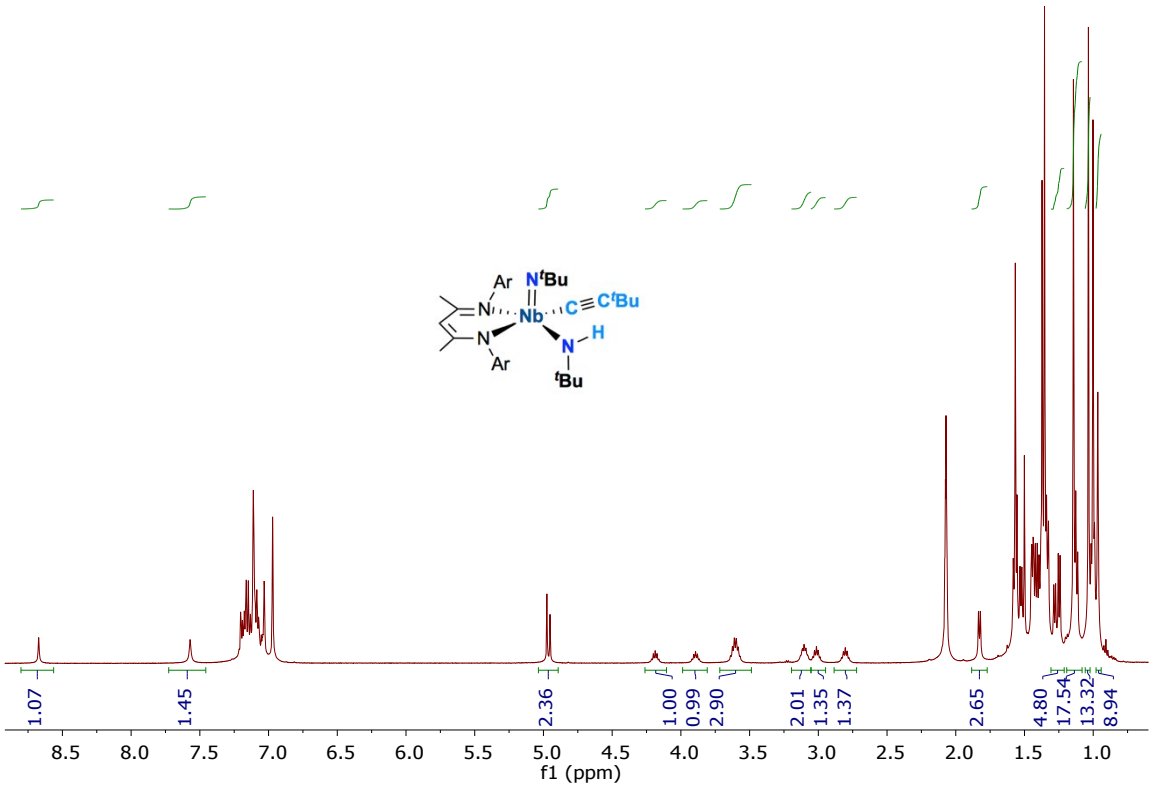

Figure S18. ^{1}H NMR Spectrum of **7** in C_7D_8 (500 MHz, 253 K).

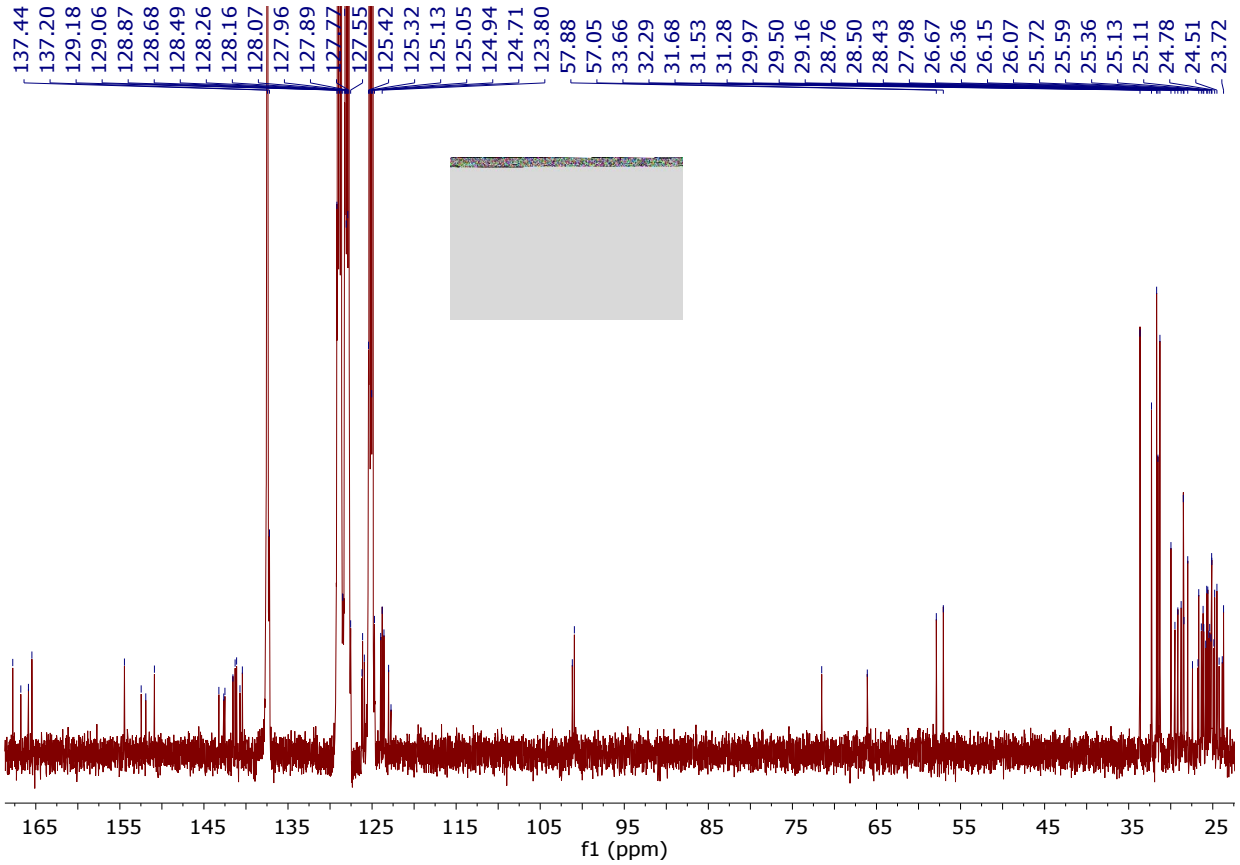

Figure S19. ^{13}C NMR Spectrum of **7** in C_7D_8 (126 MHz, 253 K).

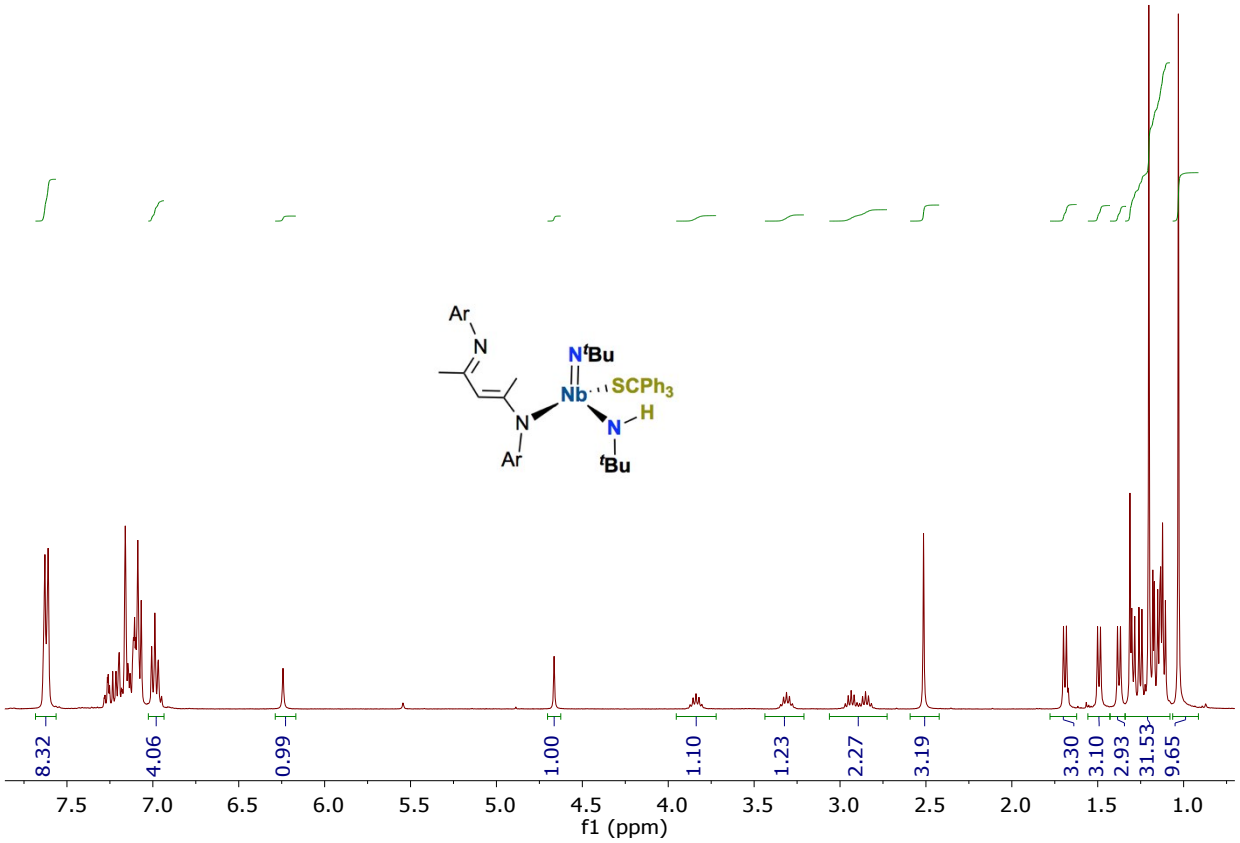

Figure S20. ^{1}H NMR Spectrum of **8** in C_6D_6 (400 MHz, 293K).

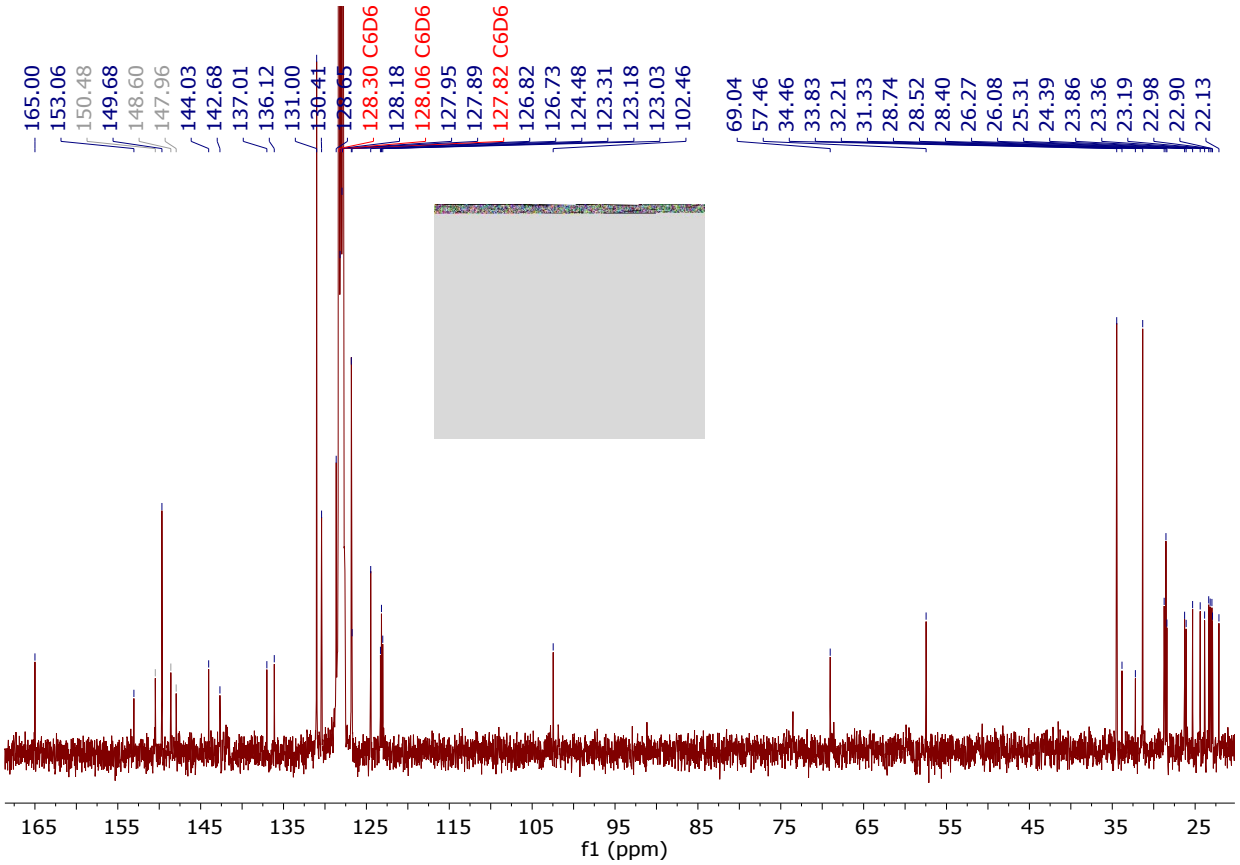

Figure S21. ^{13}C NMR Spectrum of **8** in C_6D_6 (151 MHz, 293K).

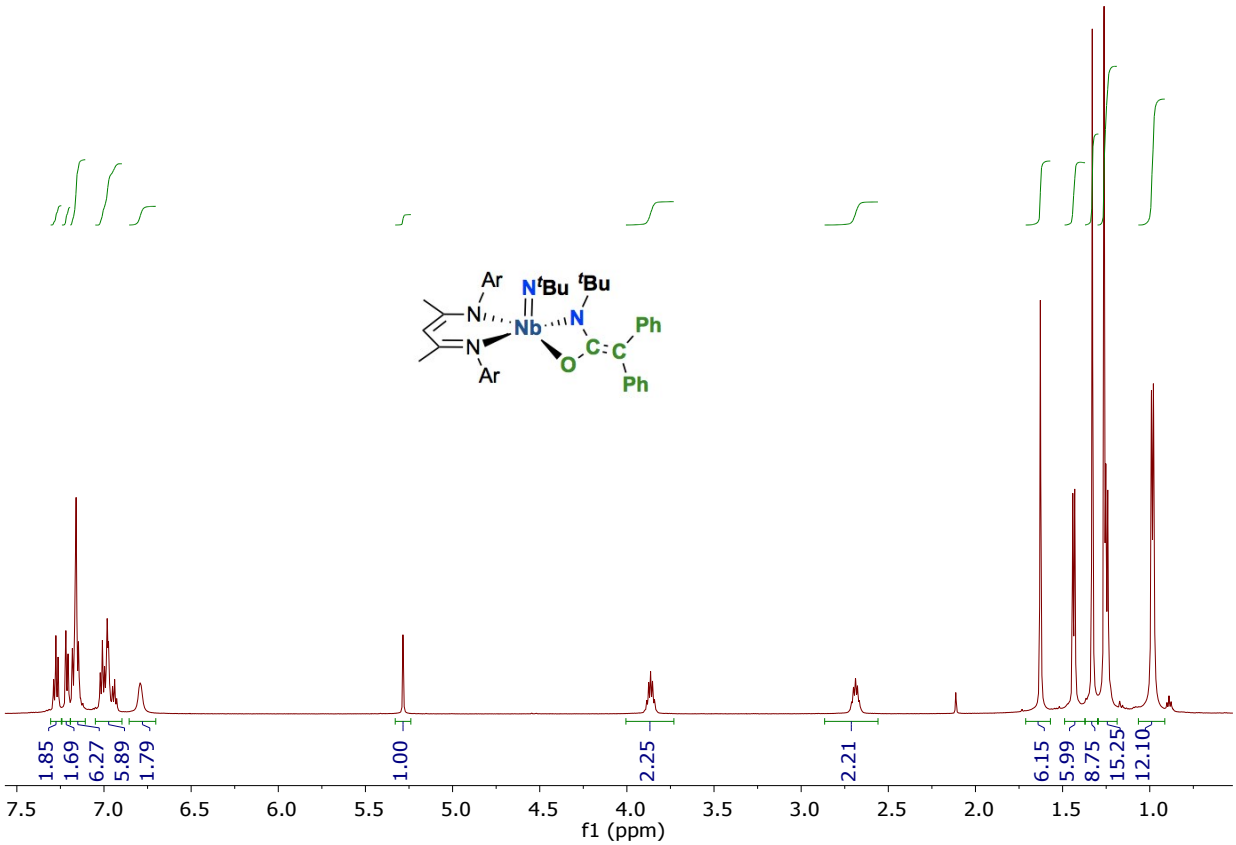

Figure S22. ^{1}H NMR Spectrum of **9** in C_6D_6 (600 MHz, 293K).

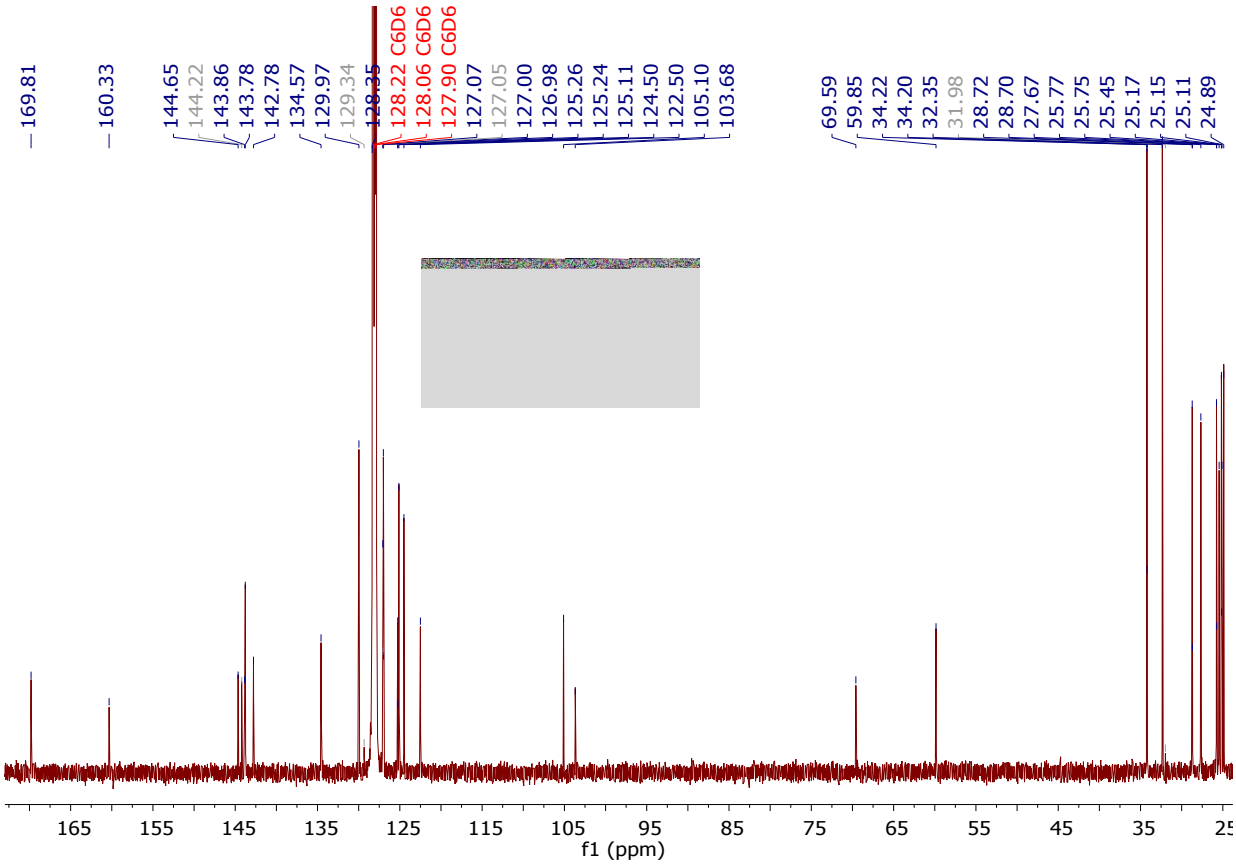

Figure S23. ^{13}C NMR Spectrum of **9** in C_6D_6 (151 MHz, 293K).

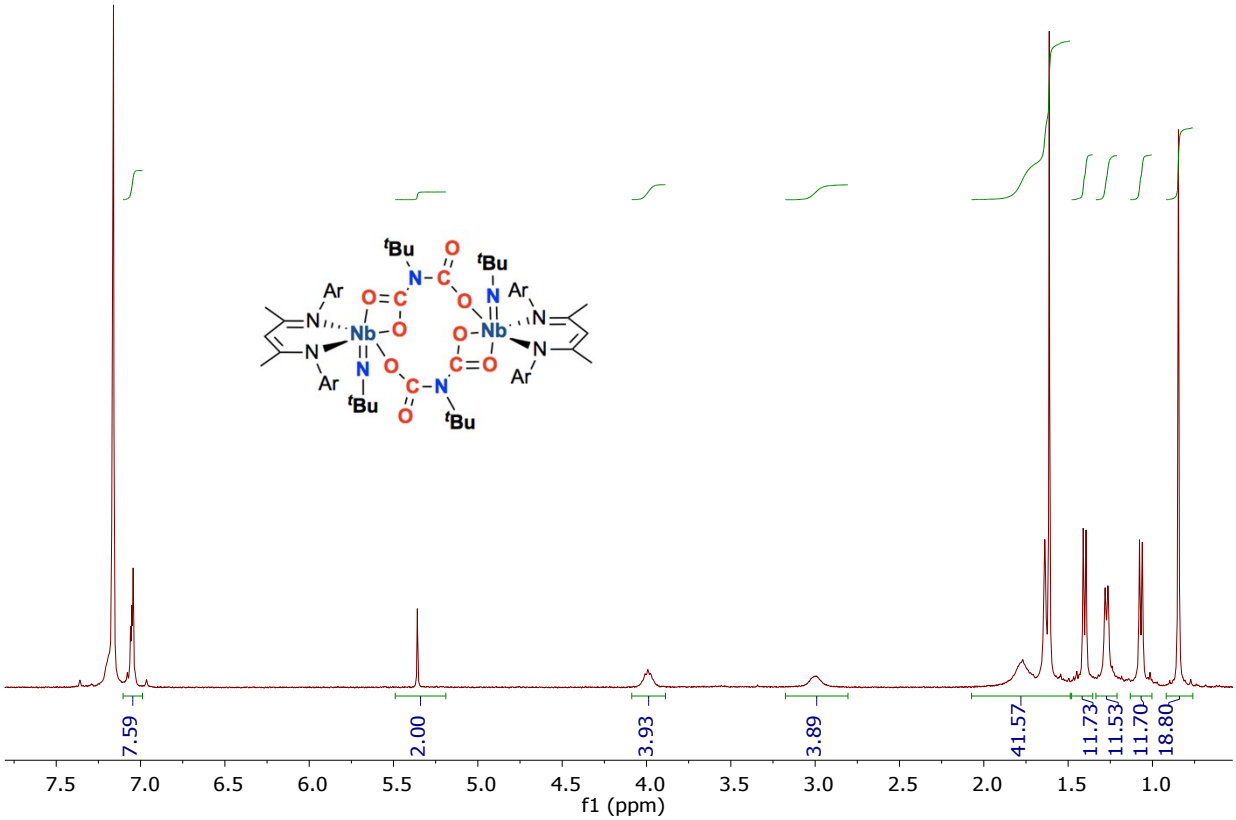

Figure S24. ^{1}H NMR Spectrum of **11** in C_6D_6 (400 MHz, 293K).

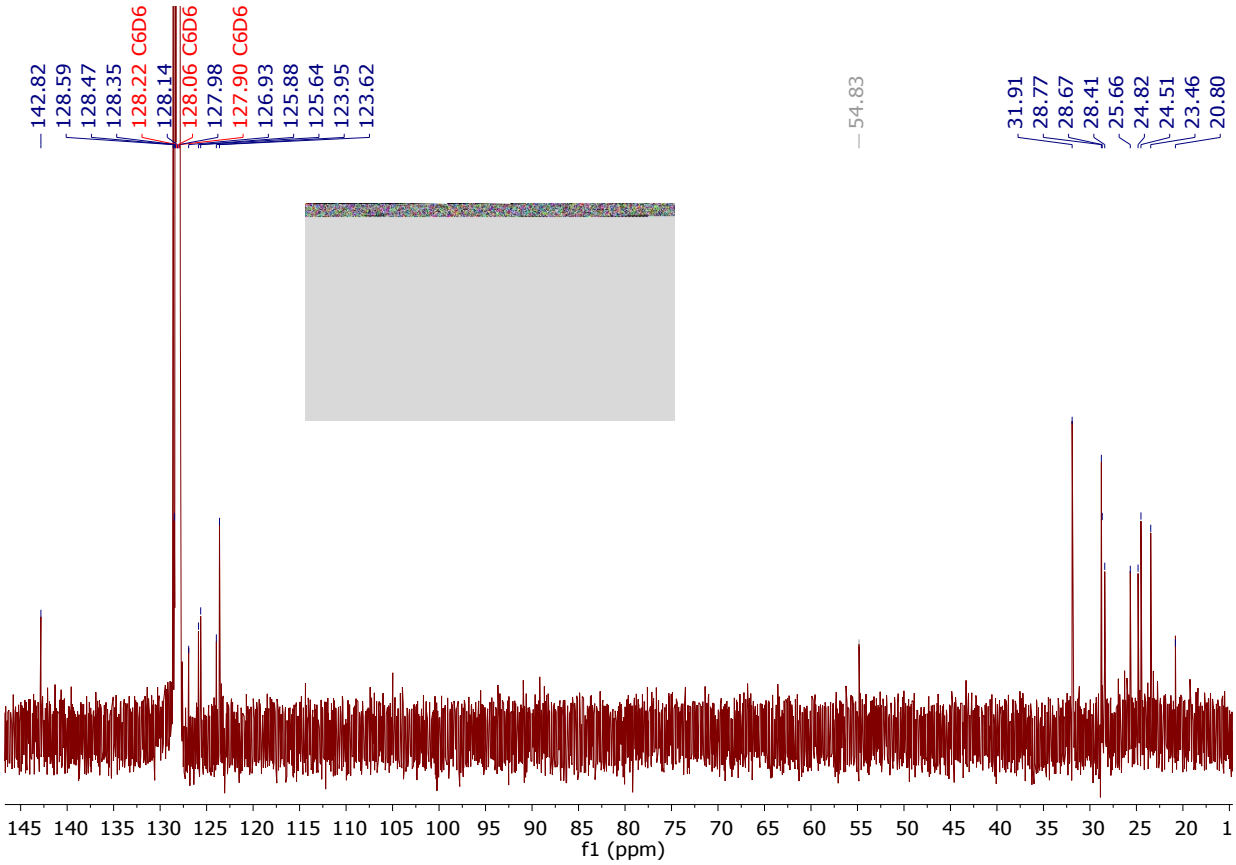

Figure S25. ^{13}C NMR Spectrum of **11** in C_6D_6 (101 MHz, 293K).

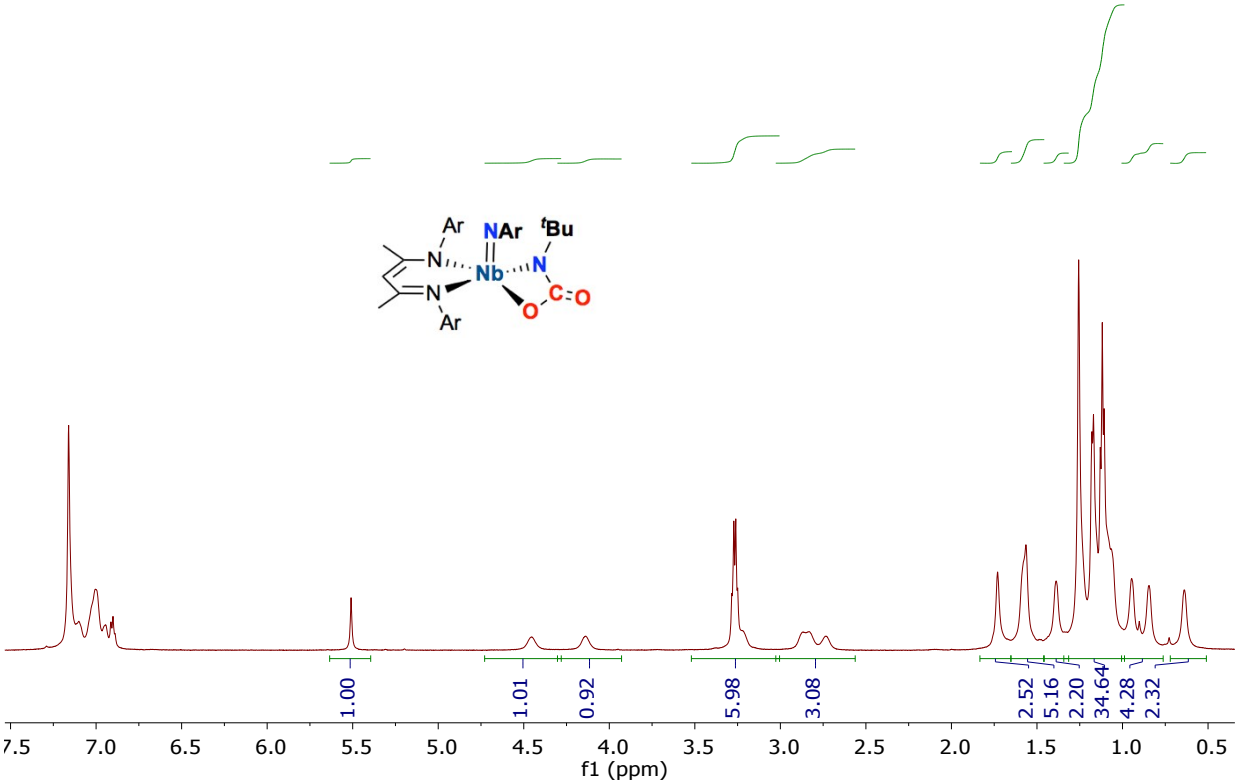

Figure S26. ^{1}H NMR Spectrum of **12** in C_6D_6 (600 MHz, 293K).

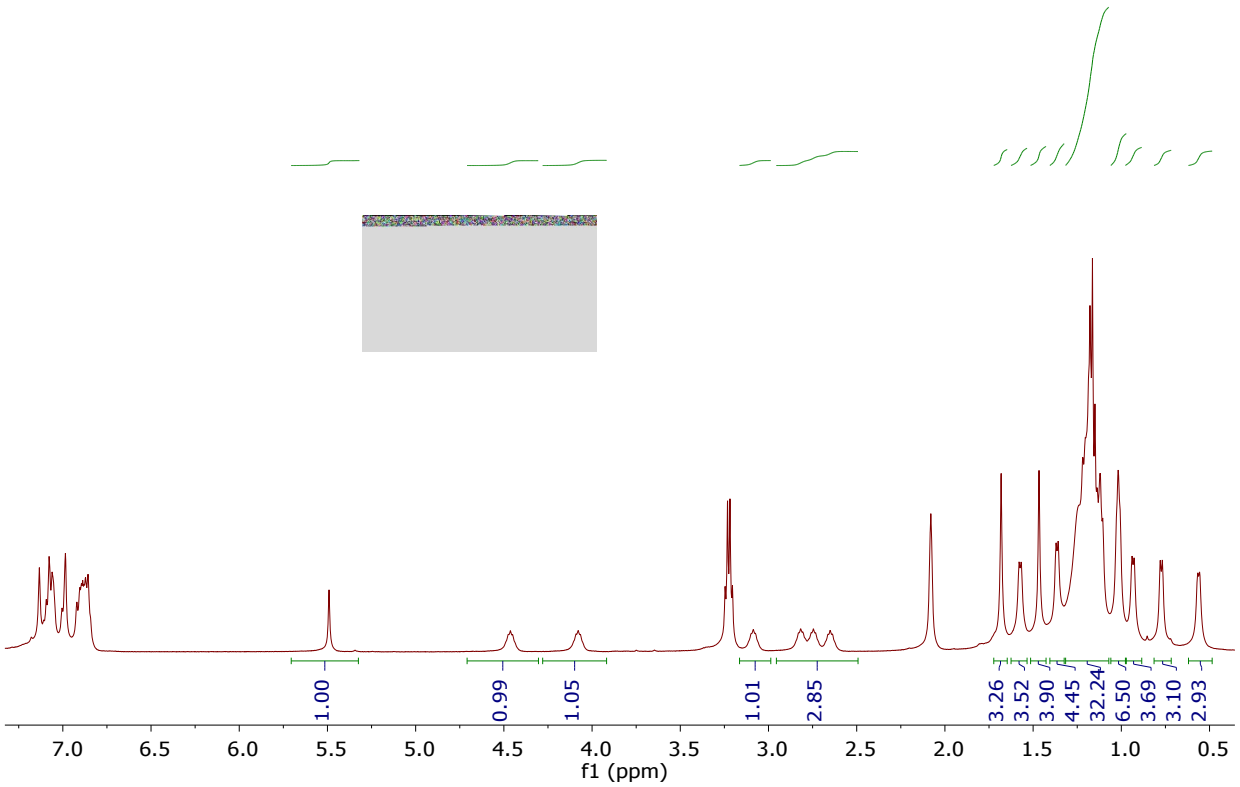

Figure S27. ^{1}H NMR Spectrum of **12** in C_7D_8 (500 MHz, 233K).

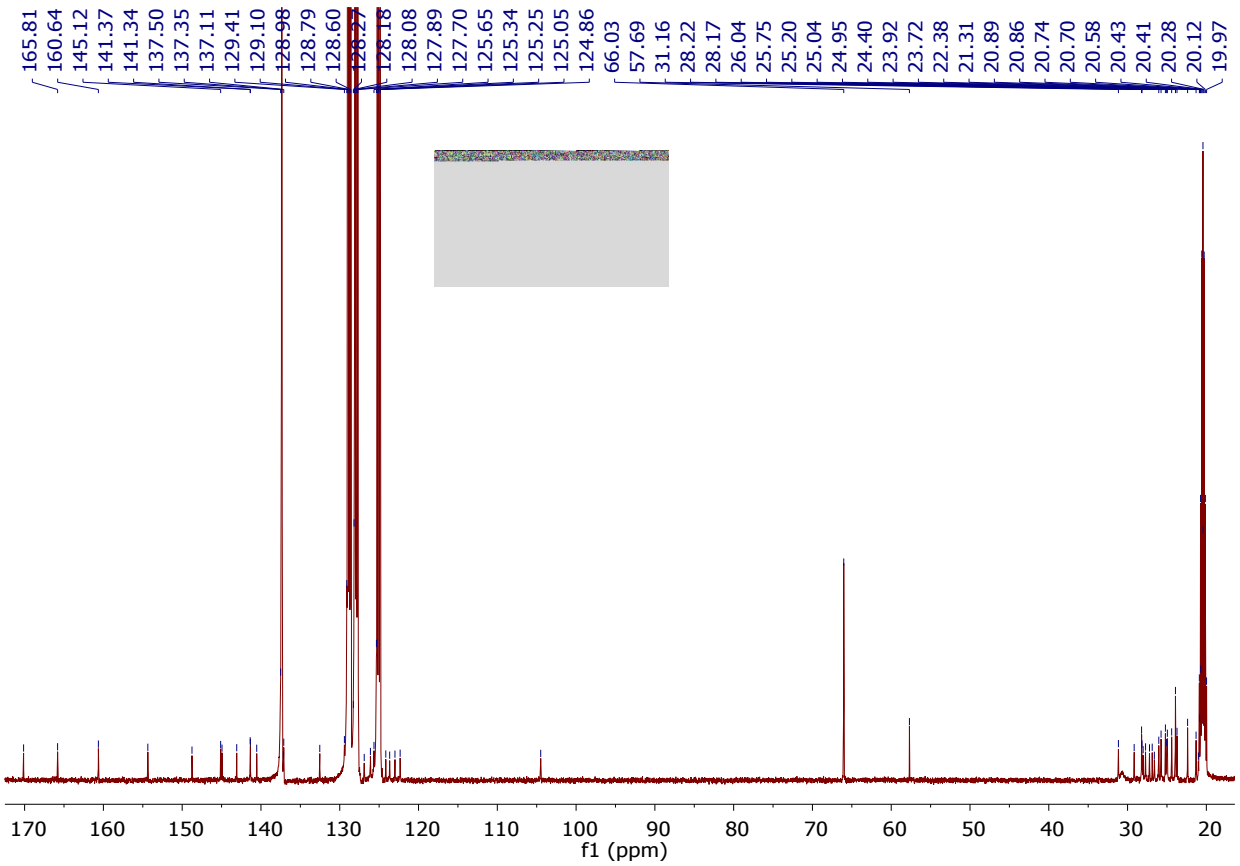

Figure S28. ^{13}C NMR Spectrum of **12** in C_7D_8 (126 MHz, 233 K).

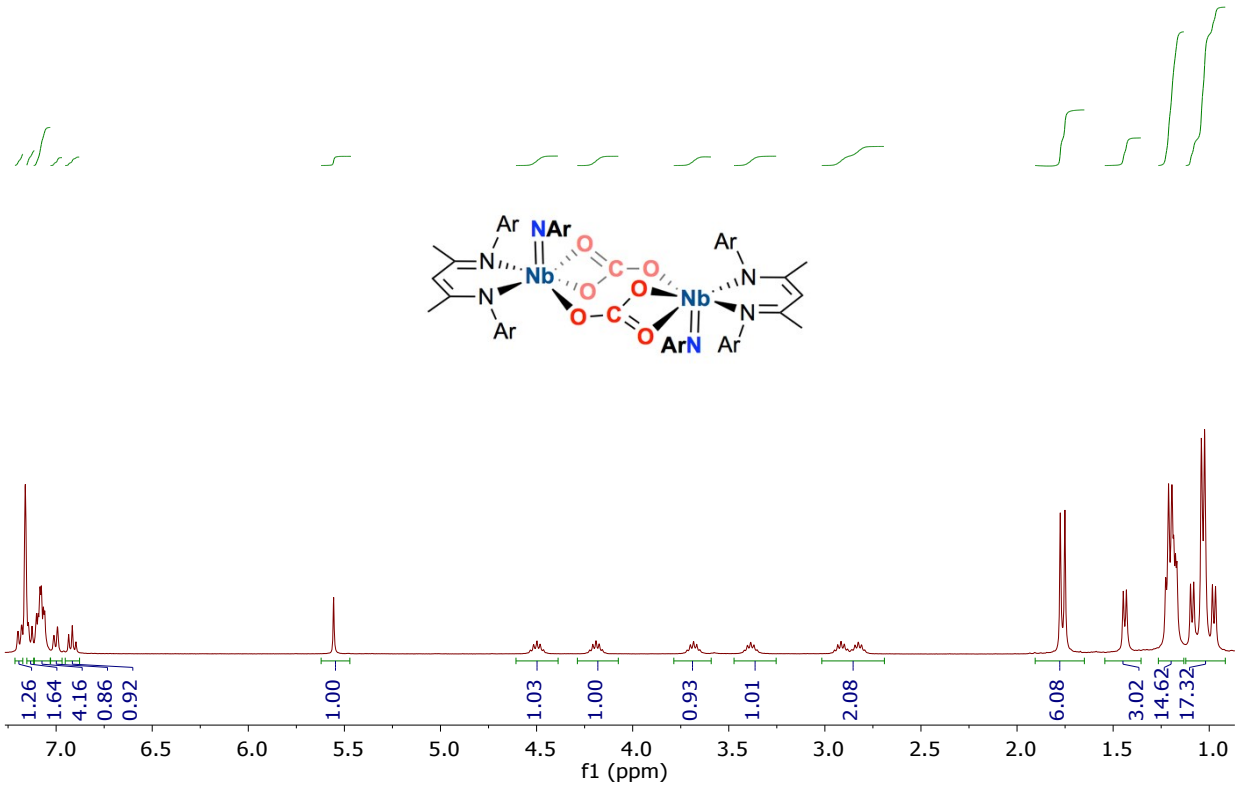

Figure S29. ^{1}H NMR Spectrum of **13** in C_6D_6 (400 MHz, 293K).

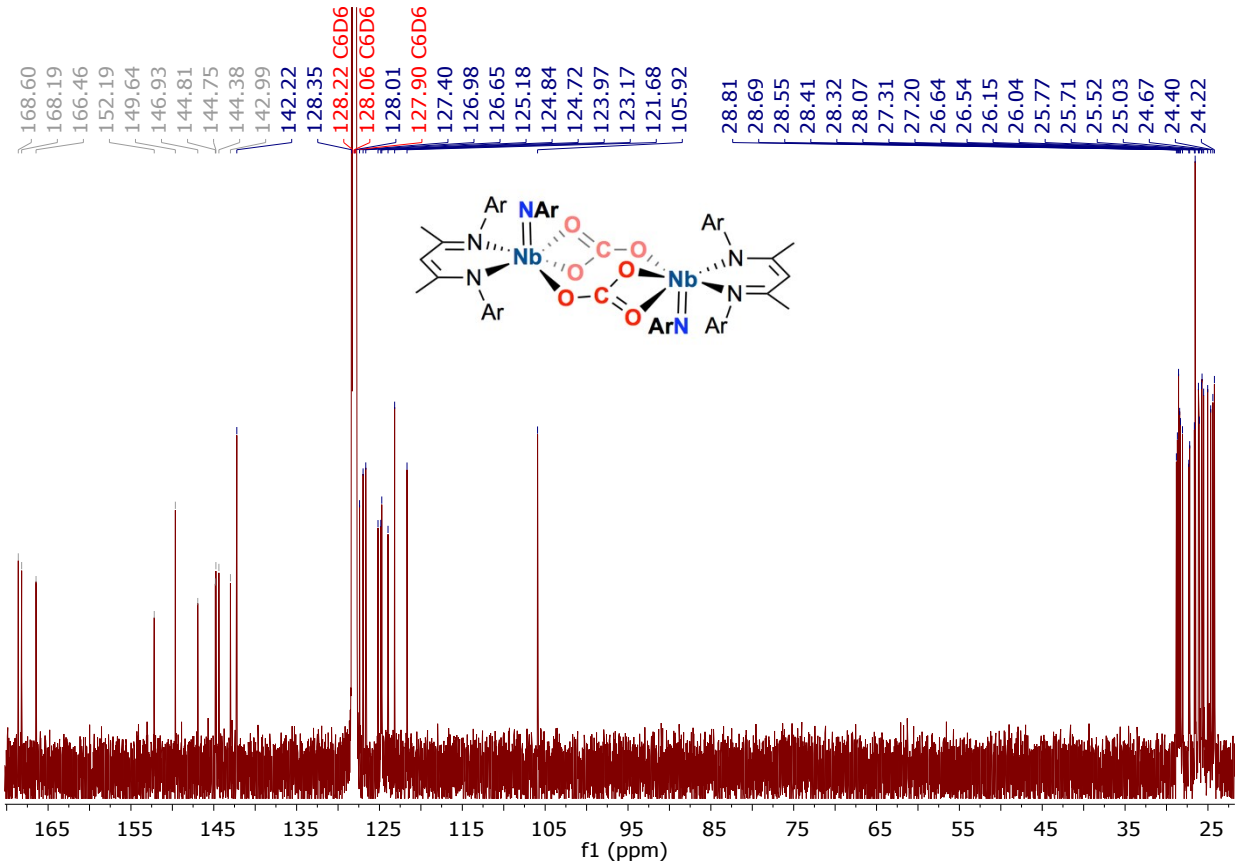

Figure S30. ^{13}C NMR Spectrum of **13** in C_6D_6 (151 MHz, 293K).

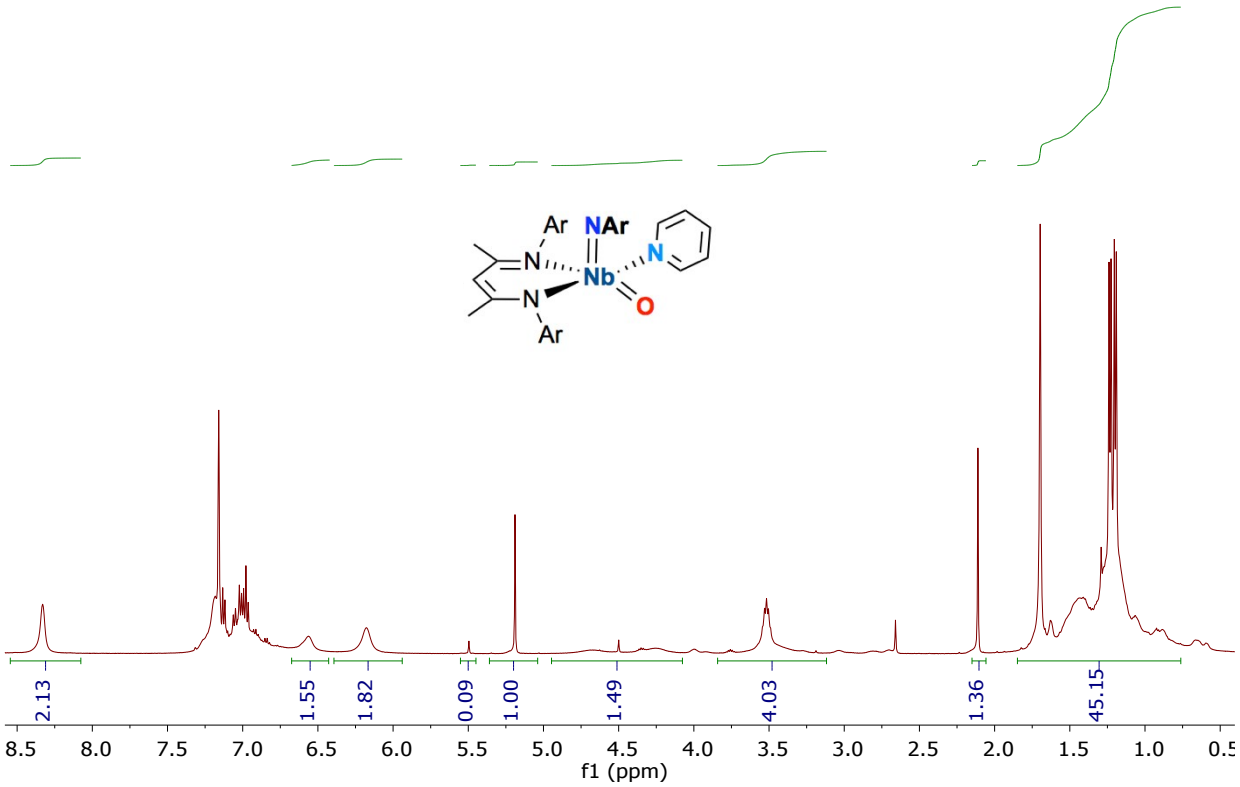

Figure S31. ^{1}H NMR Spectrum of **14** in C_6D_6 (600 MHz, 293K).

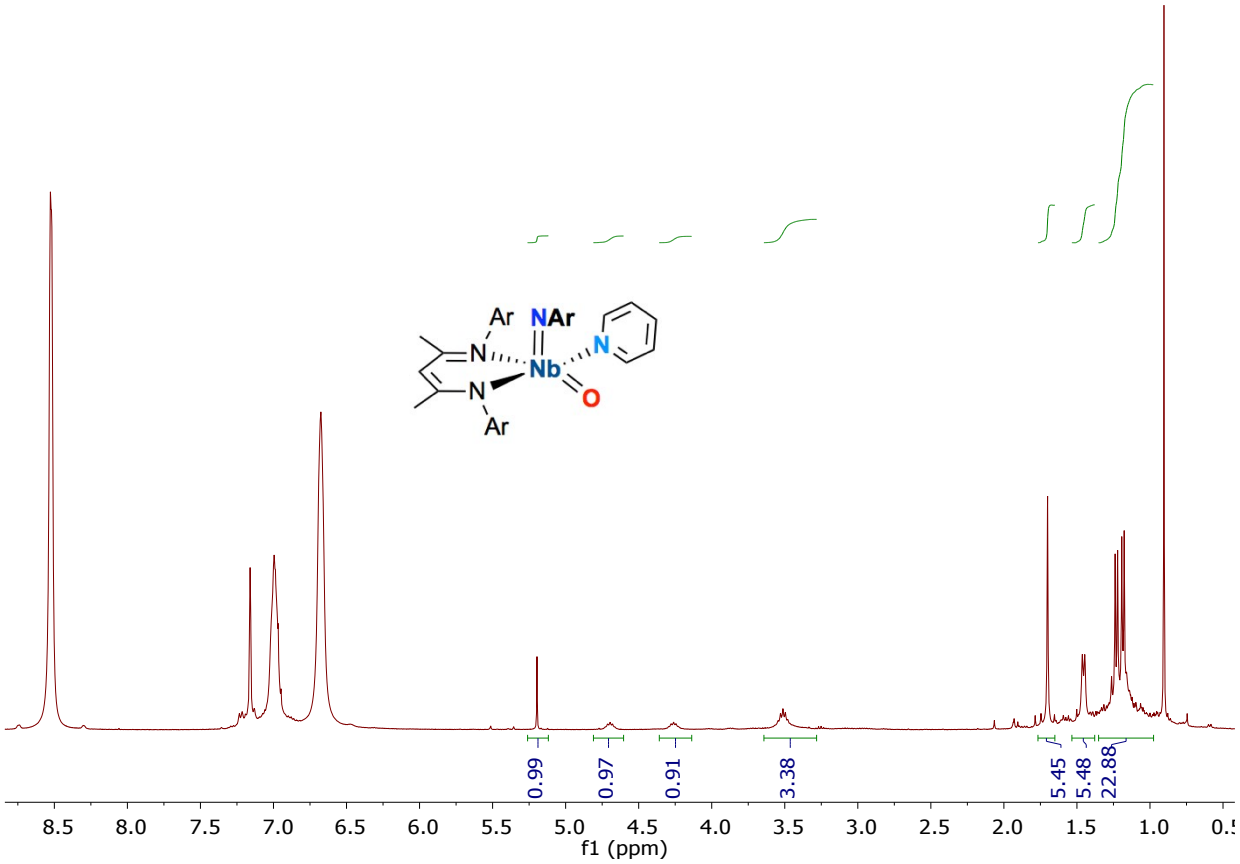

Figure S32. ^{1}H NMR Spectrum of **14** in C_6D_6/Pyridine (600 MHz, 293K).

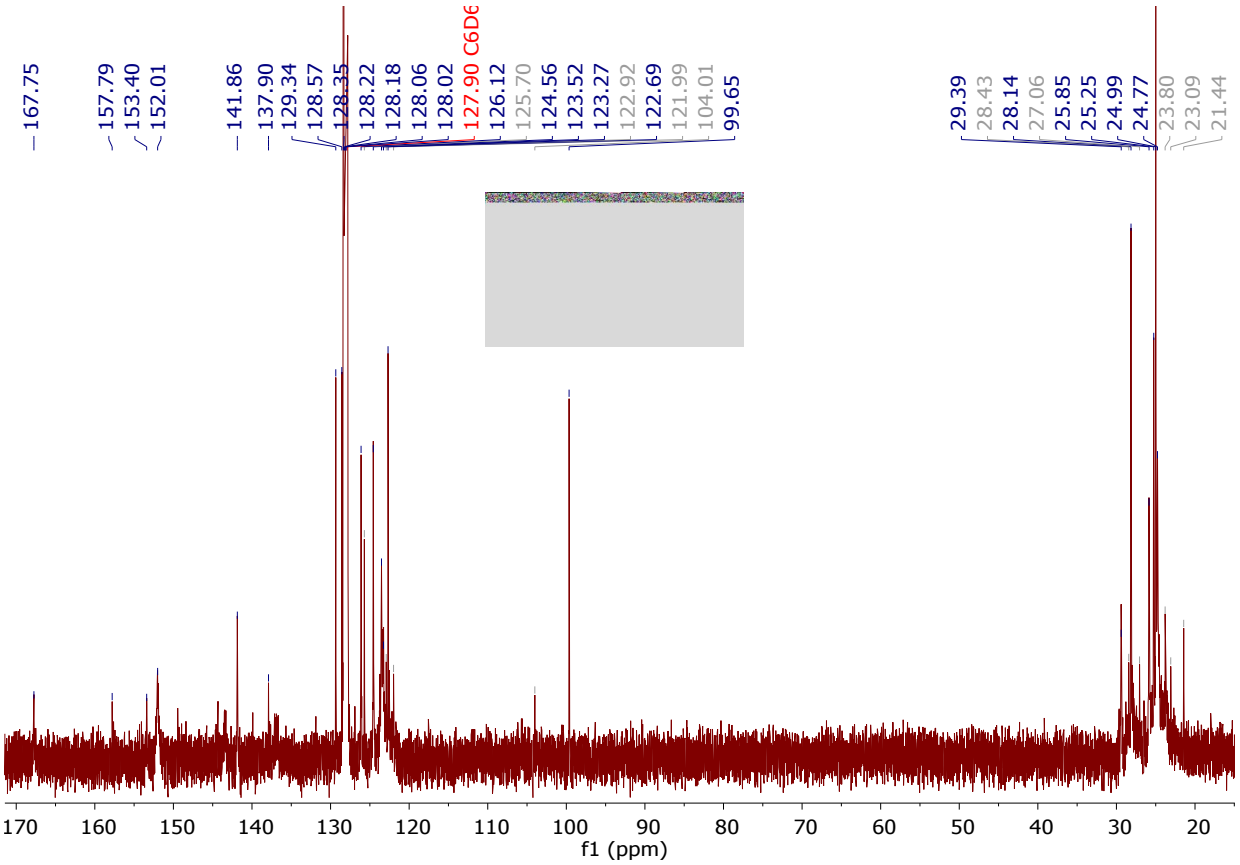

Figure S33. ^{13}C NMR Spectrum of **14** in C_6D_6 (151 MHz, 293K).

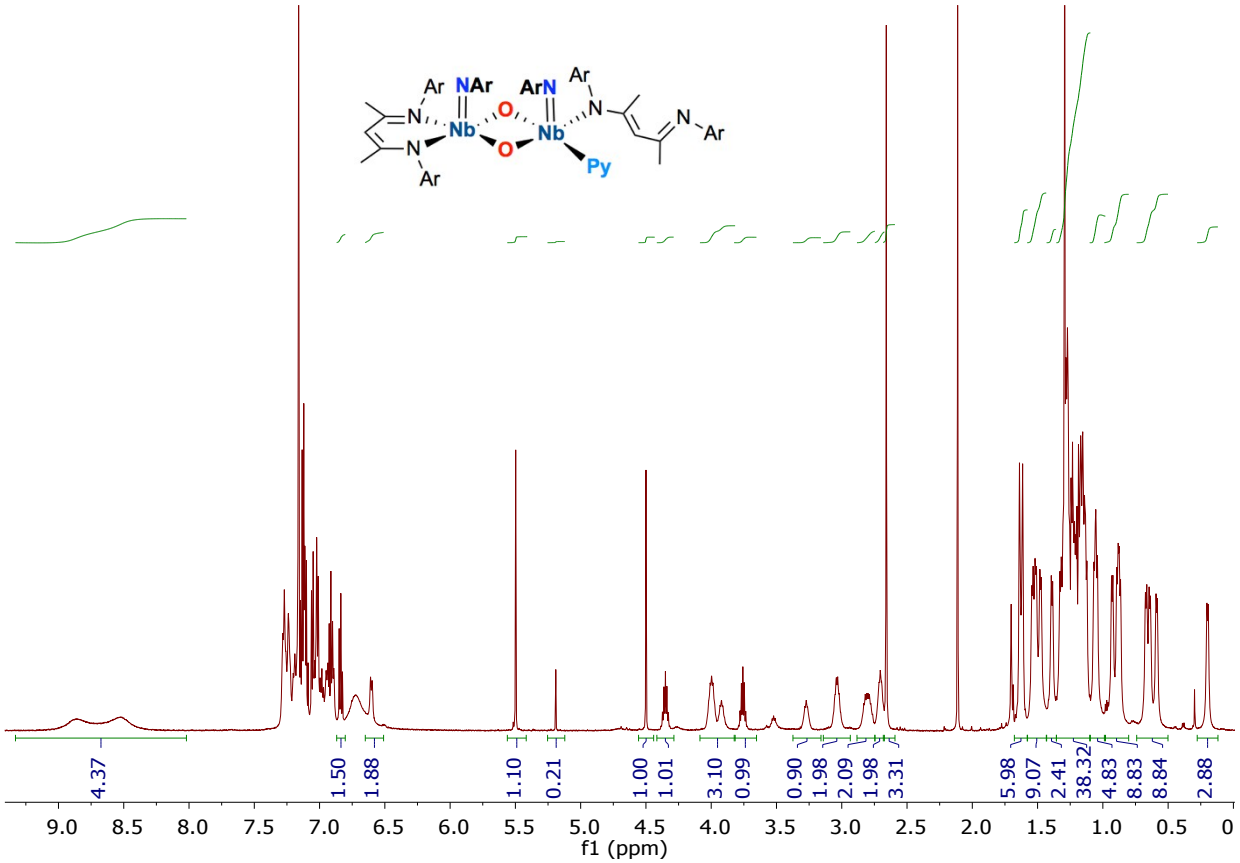

Figure S34. ^{1}H NMR Spectrum of **15** in C_6D_6 (600 MHz, 293K).

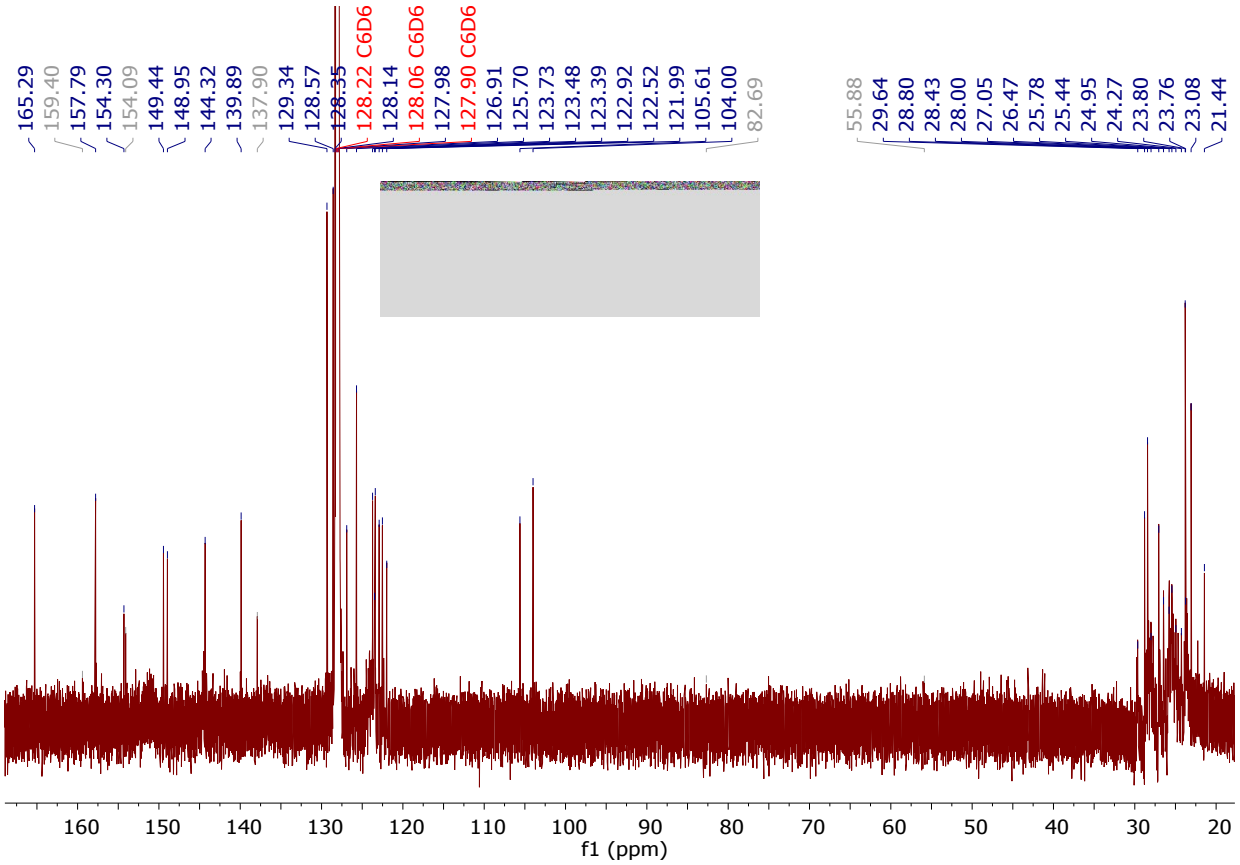

Figure S35. ^{13}C NMR Spectrum of **15** in C_6D_6 (151 MHz, 293K).

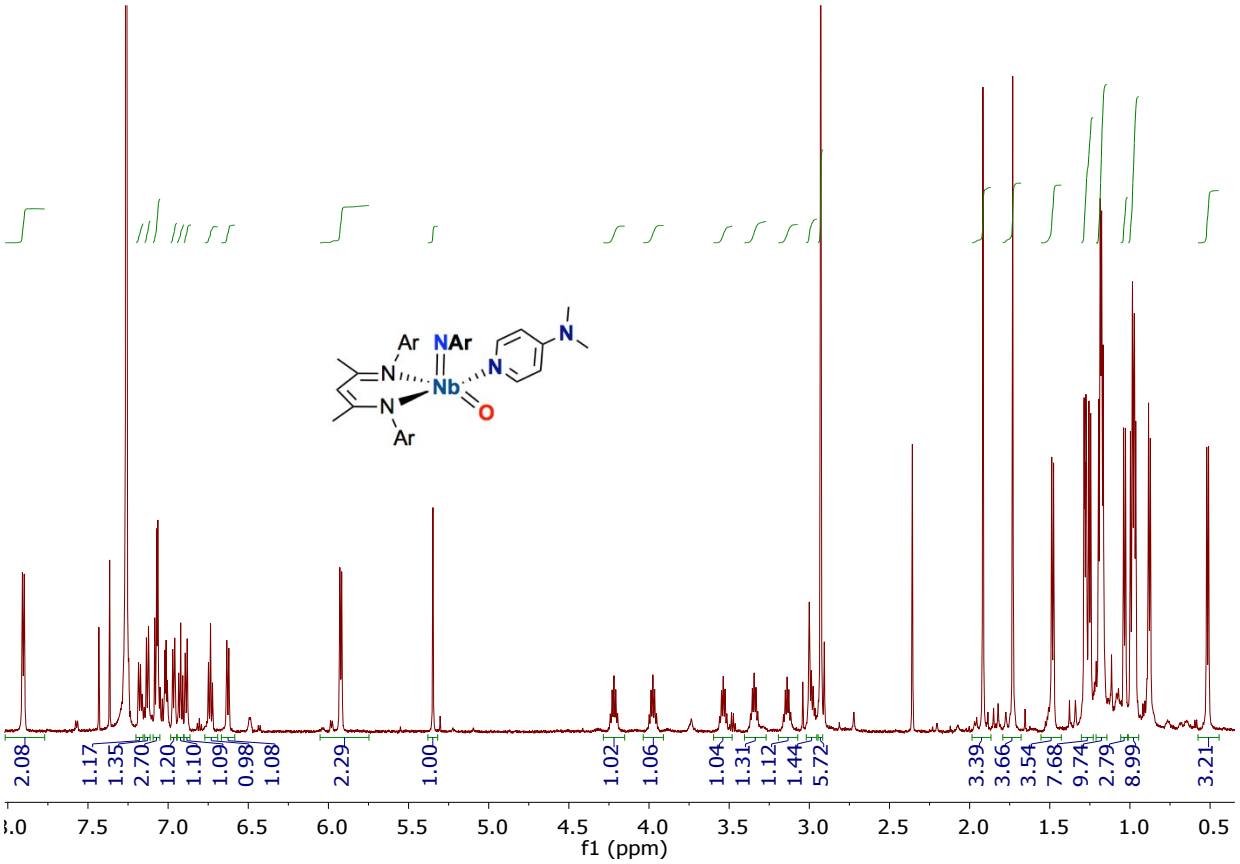

Figure S36. ^{1}H NMR Spectrum of **16** in $CDCl_3$ (600 MHz, 293K).

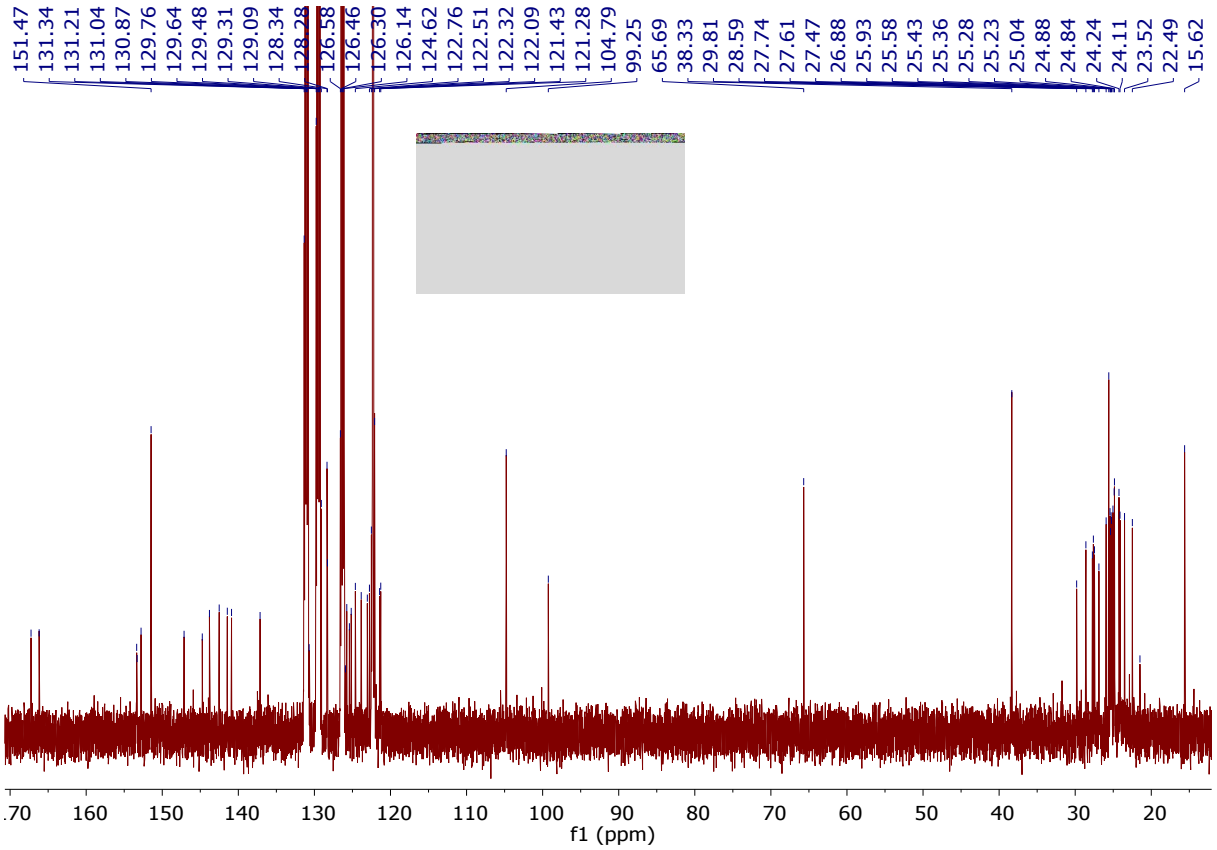

Figure S37. ^{13}C NMR Spectrum of **16** in C_6D_5Br (151 MHz, 293K).

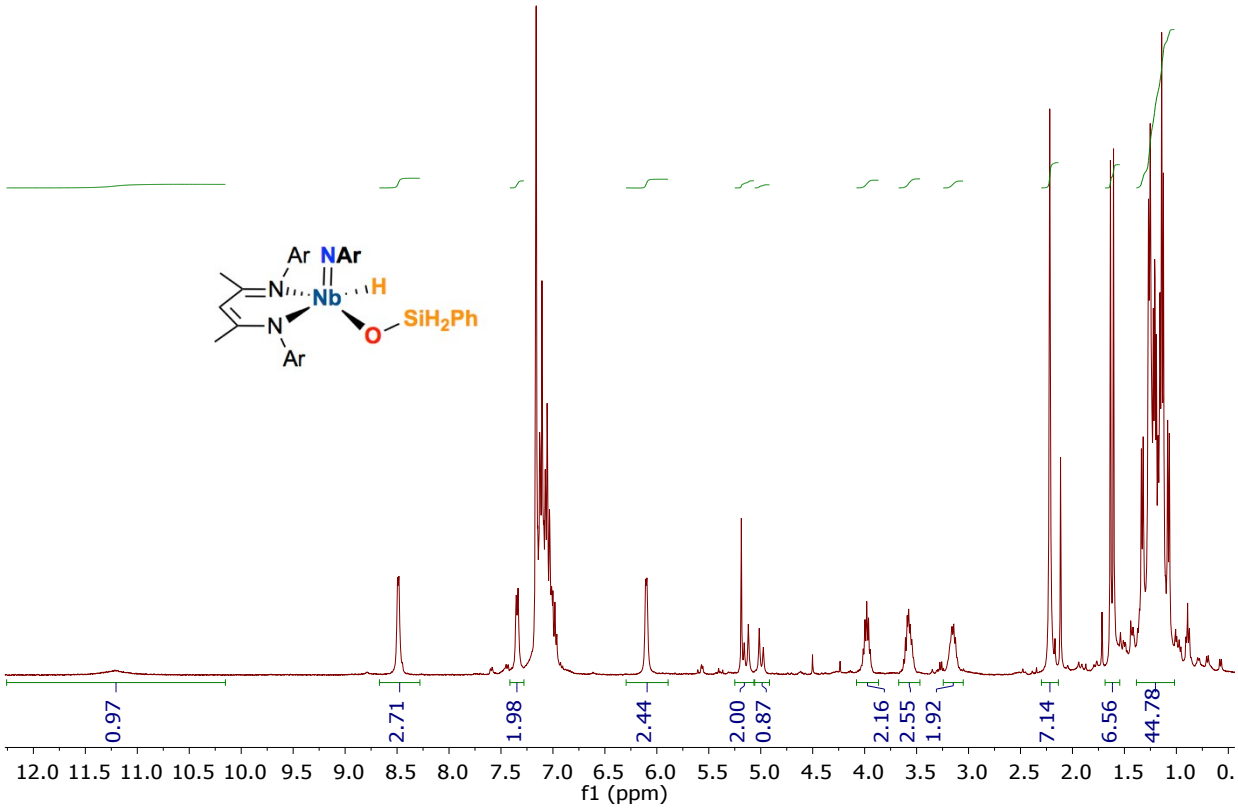

Figure S38. ^{1}H NMR Spectrum of **17a** in C_6D_6 (400 MHz, 293K).

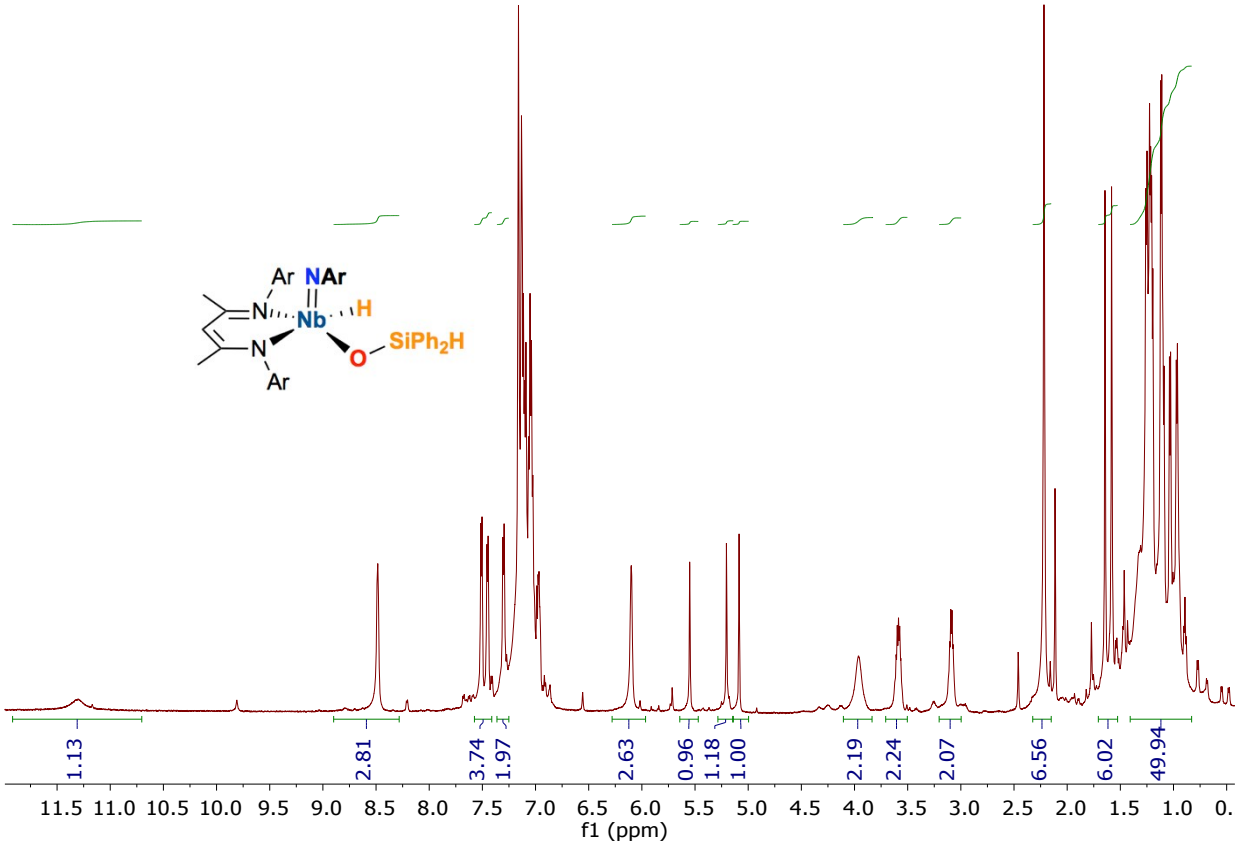

Figure S39. ^{1}H NMR Spectrum of **17b** in C_6D_6 (600 MHz, 293K).

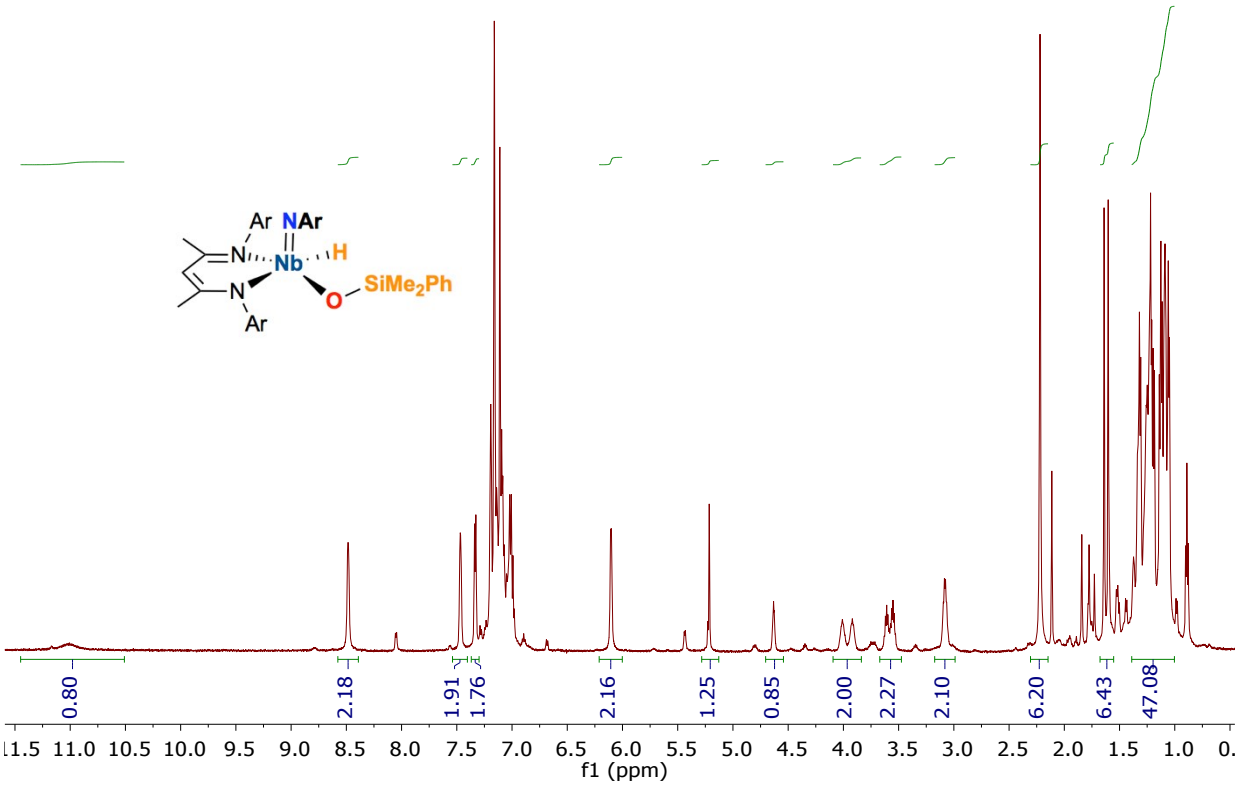

Figure S40. ^{1}H NMR Spectrum of **17c** in C_6D_6 (600 MHz, 293K).

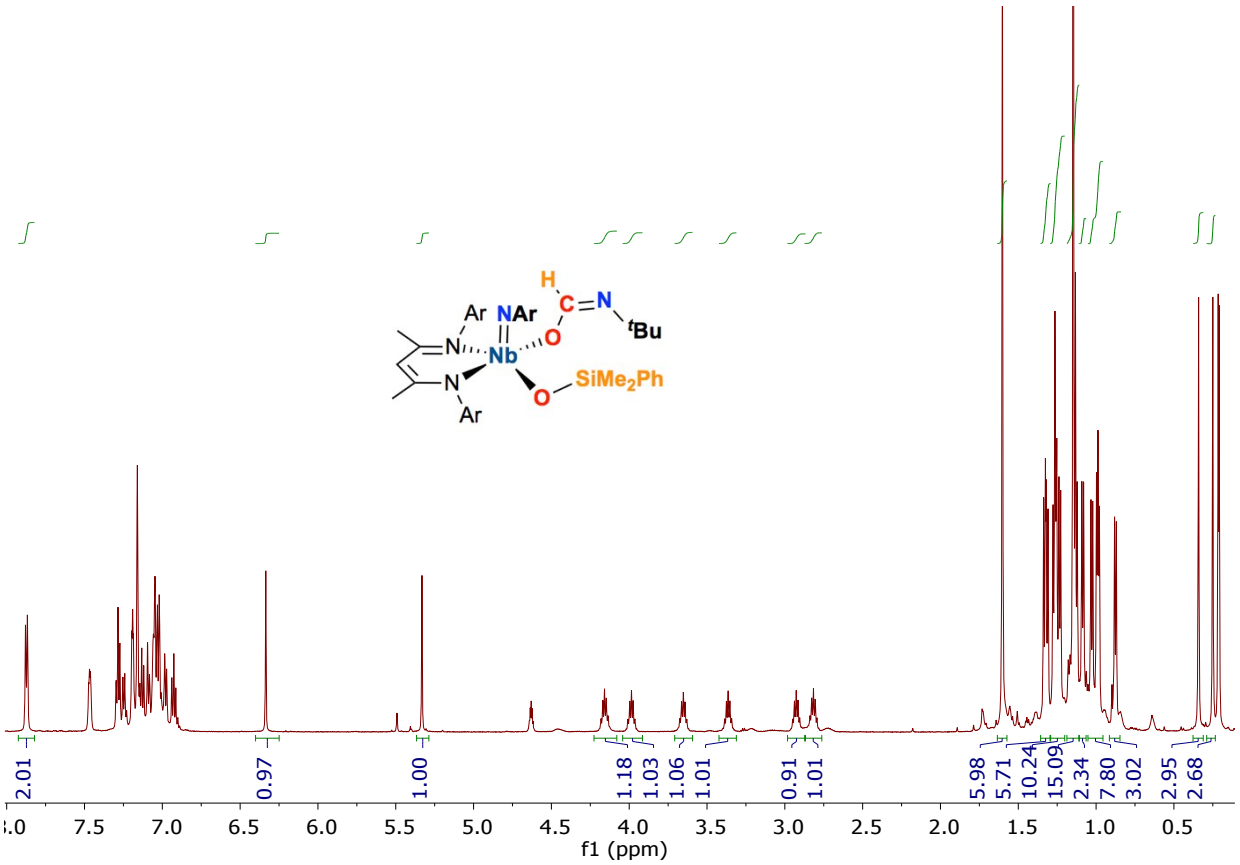

Figure S41. ^{1}H NMR Spectrum of **18** in C_6D_6 (600 MHz, 293K).

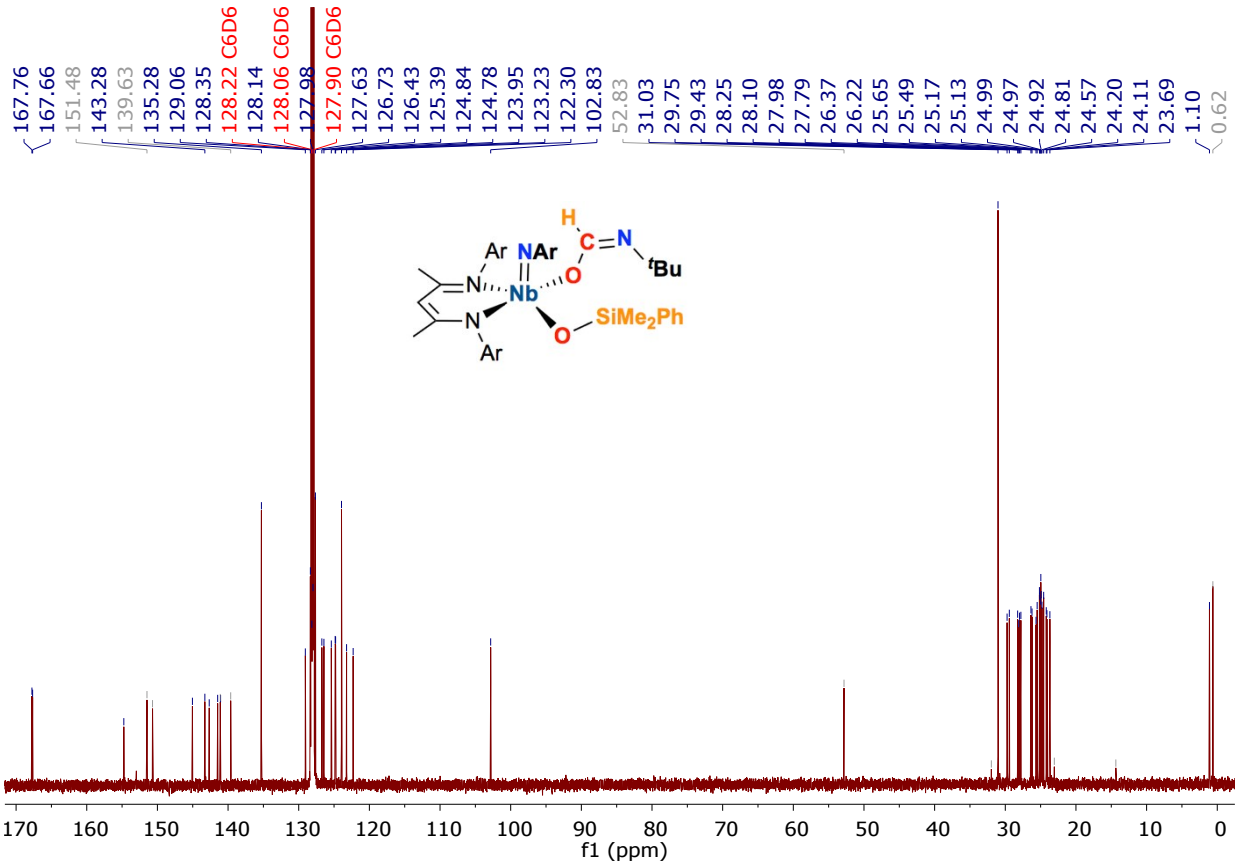

Figure S42. ^{13}C NMR Spectrum of **18** in C_6D_6 (151 MHz, 293K).

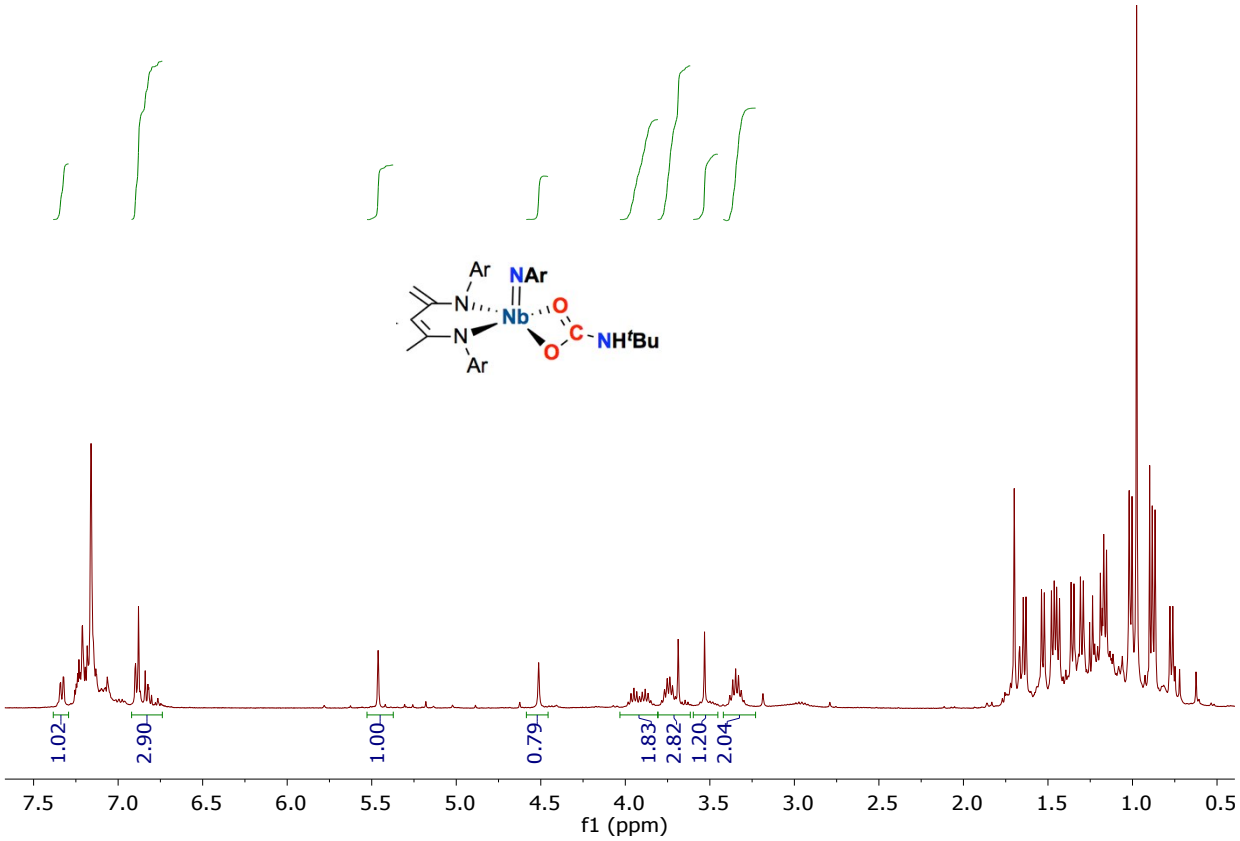

Figure S43. ^{1}H NMR Spectrum of **19** in C_6D_6 (400 MHz, 293K).

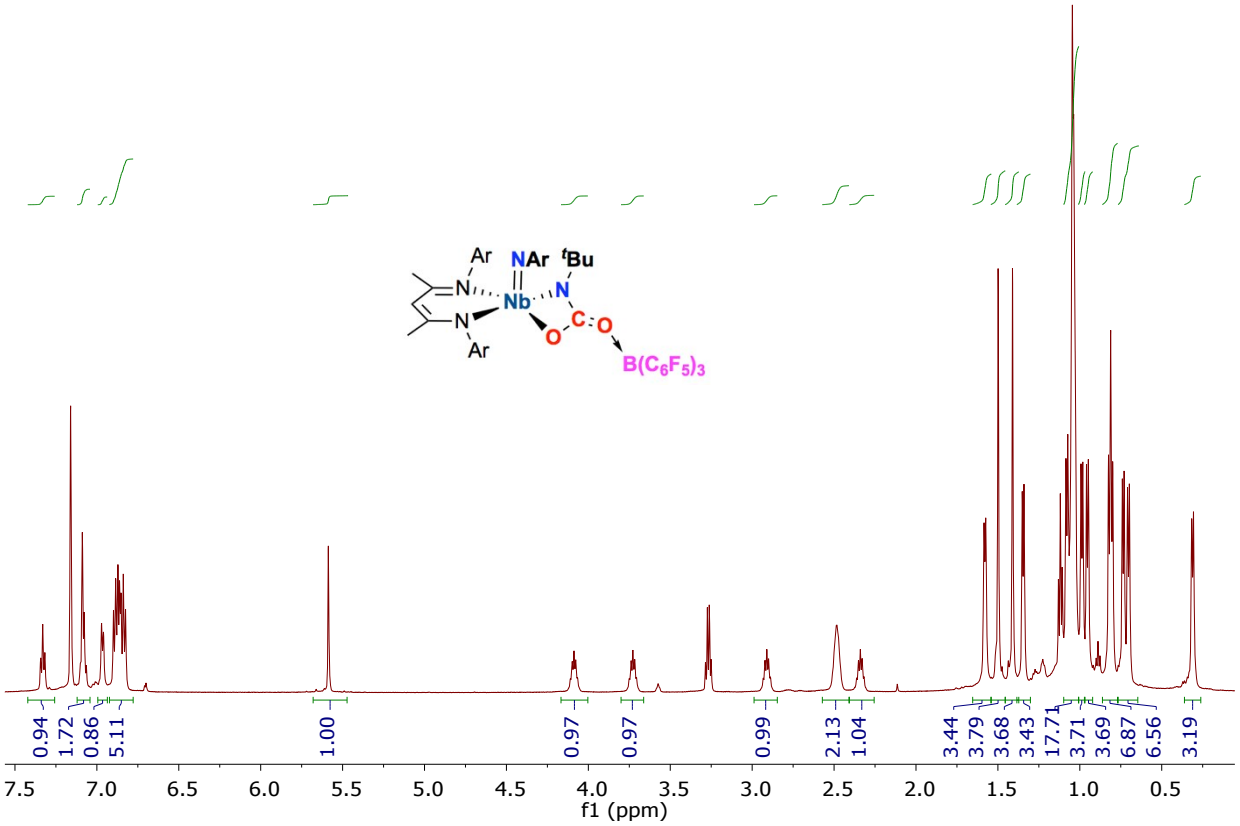

Figure S44. ^{1}H NMR Spectrum of **20** in C_6D_6 (600 MHz, 293K).

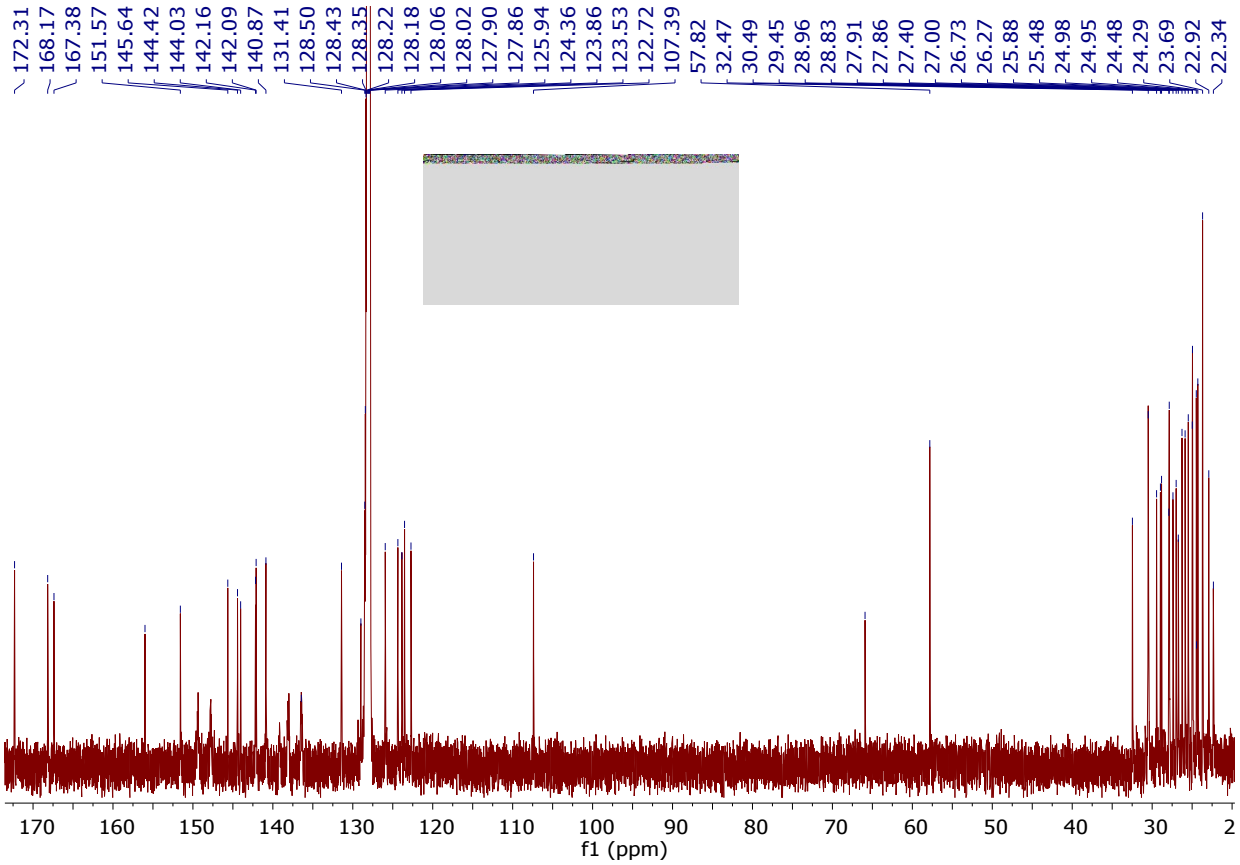

Figure S45. ^{13}C NMR Spectrum of **20** in C_6D_6 (151 MHz, 293K).