

Supporting Information

A Niobium Pentafulvene Ethylene Complex: Synthesis, Properties and Reaction Pathways

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Supplementary Synthesis and Experiments

Extraction of 2: The crude, dried reaction mixture of **2** was brought into a glovebox, ground and mixed with an equal volume of industrially washed, vigorously dried sand. The mixture was placed in an extraction apparatus (**Photography S1**), transferred out, and continuously extracted by refluxing dry *n*-pentane. The sand is used to disperse the material and to inhibit blockage of the extraction frit.



Photography S1: Schematic extraction apparatus with solvent flask (bottom), cooler (top), and vapor bypass (right).

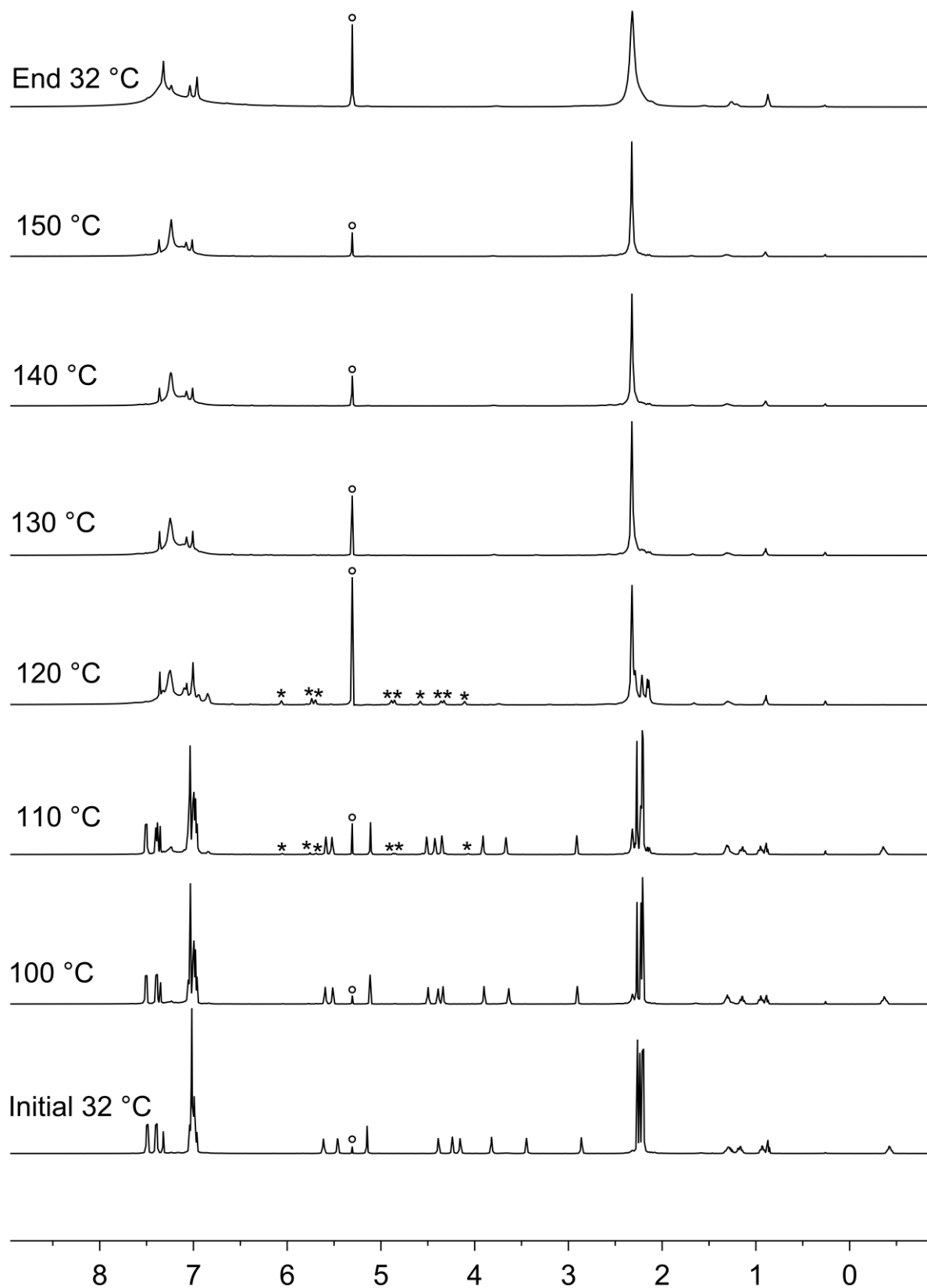
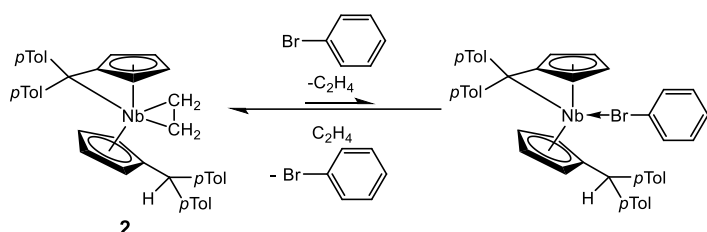


Figure S1: Variable temperature ^1H NMR spectra (500 MHz, $\text{C}_6\text{H}_5\text{Br}$) of a sample of **2**. ° = ethylene, * = possible intermediate species.

Variable Temperature NMR of 2: Measuring ^1H NMR spectra of **2** in toluene- d_8 at increasing temperatures did not show any significant change even upon heating to 100 °C. No liberation of ethylene could be detected. Changing the solvent to bromobenzene- d_5 and gradually heating from 100 °C to 150°C, recording spectra in 10 K intervals (**Figure S1**), a clear liberation of ethylene started at 110 °C (consistent to detected decomposition of **2** in solid state (110 °C)). A second set of signals briefly appears retaining the symmetry of **2** (eight signals for Cp'/fulvene protons, one for $\text{C}_{\text{exo}}\text{H}$) still being detectable at 120 °C while **2** decomposed fully. Minimal amounts of ethylene can already be observed in the initial ^1H NMR spectrum in bromobenzene, but not in benzene, THF or toluene. This finding combined with the appearance of a second set of signals leads us to propose the equilibrium formulated in **Scheme S1**. Purposefully removing the ethylene from the reaction mixture as well as repeating the reaction under multiple conditions to yield the proposed adduct or a subsequent oxidative addition product were unsuccessful.



Scheme S1: Proposed equilibrium of **2** in bromobenzene.

Synthesis of 2,6-Xylidene- d_2 : 5 ml of 2,6-xylidene, 20 ml D_2O and a drop of concentrated $\text{DCI}/\text{D}_2\text{O}$ were stirred to emulsify the mixture as good as possible. The exchange was monitored by ^1H NMR of the organic phase, exchanging the aqueous phase for a fresh one, if no further deuteration was detected. Upon achieving satisfactory deuteration, the phases were separated, the organic phase was distilled from molecular sieves and stored over molecular sieve until use. Yield: 3.2 ml (64%) Deuteration: 96% (N-D, see **Figure S2**).

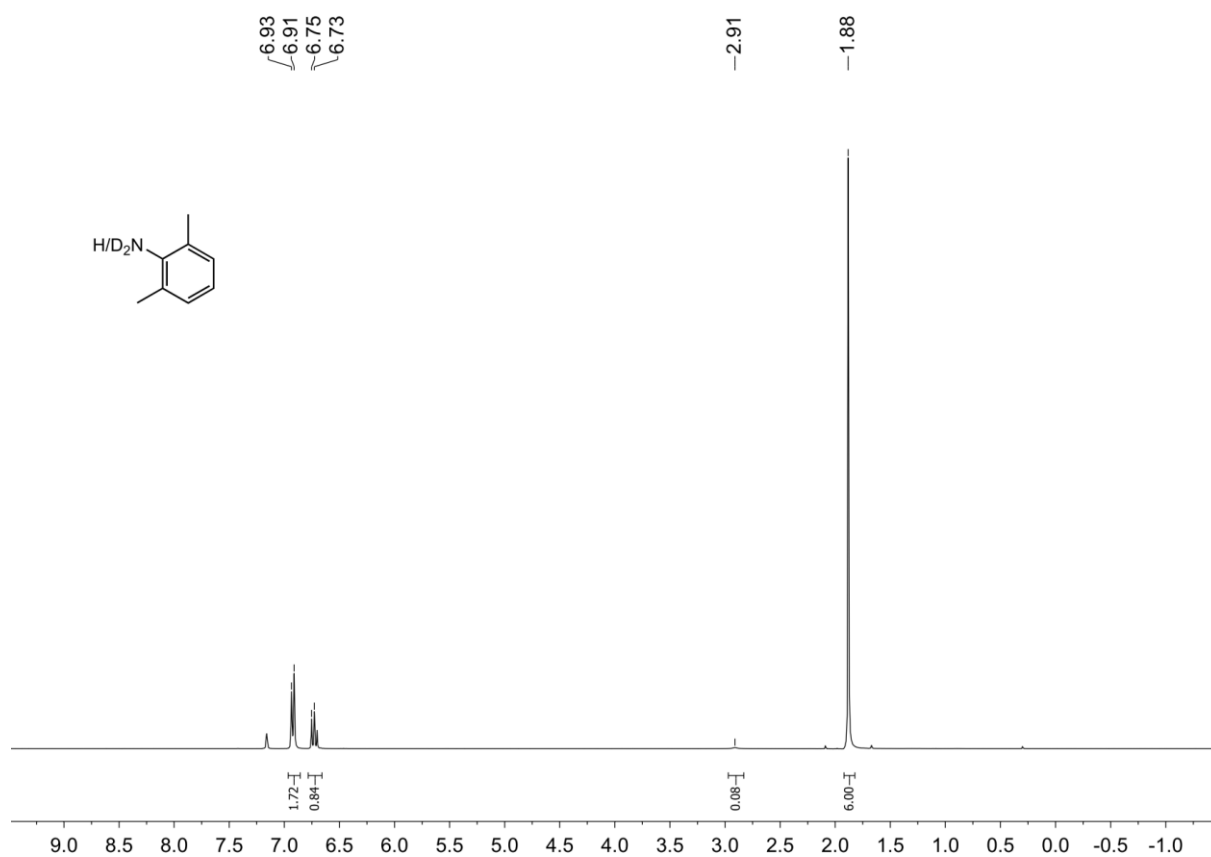


Figure S2: ¹H NMR spectrum of 2,6-xylidene-d₂ (300 MHz, C₆D₆, 294 K).

Synthesis of 4-d₂: Analog to the synthesis of **4**, ethylene complex **2** was reacted with 2,6-Xylidene-d₂ to give **4-d₂**. The product was dissolved in C₆D₆ or C₆H₆ and ¹H or ²H NMR spectra were recorded.

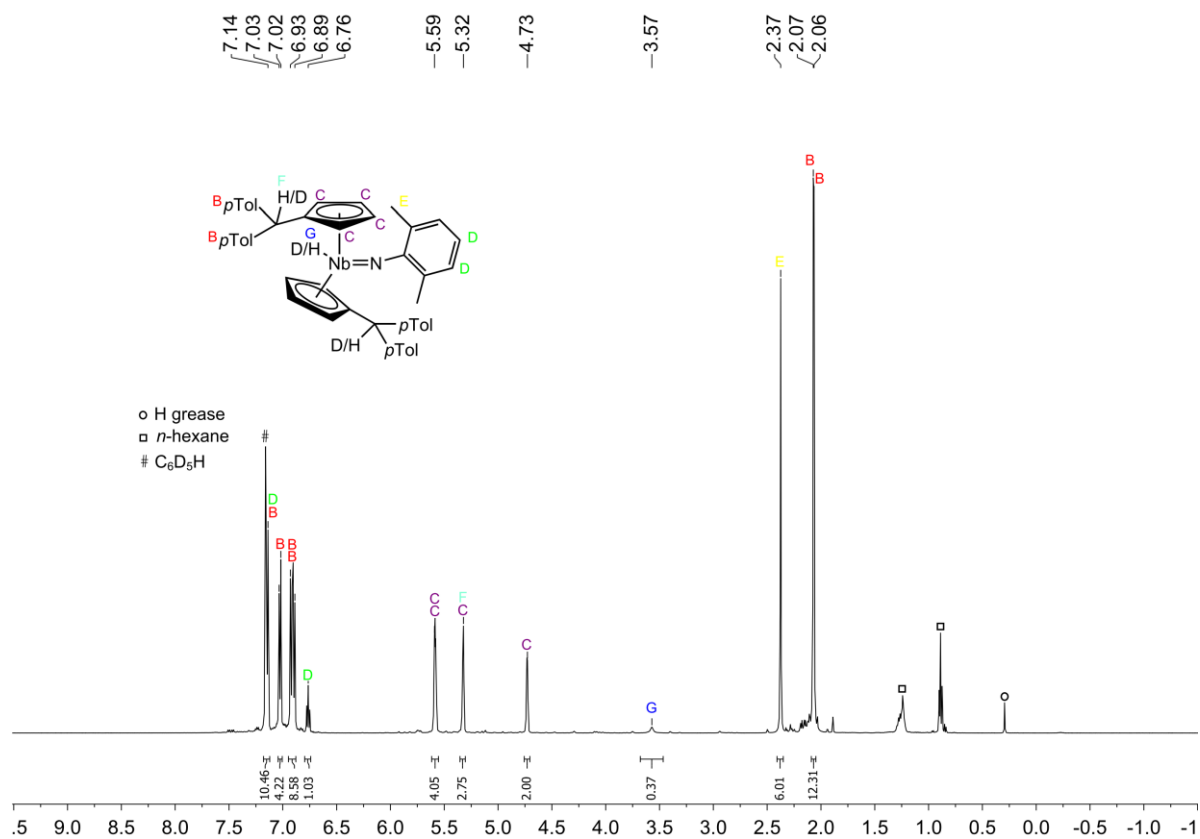


Figure S3: ¹H NMR spectra of **4-d₂** (500 MHz, C₆D₆, 305 K).

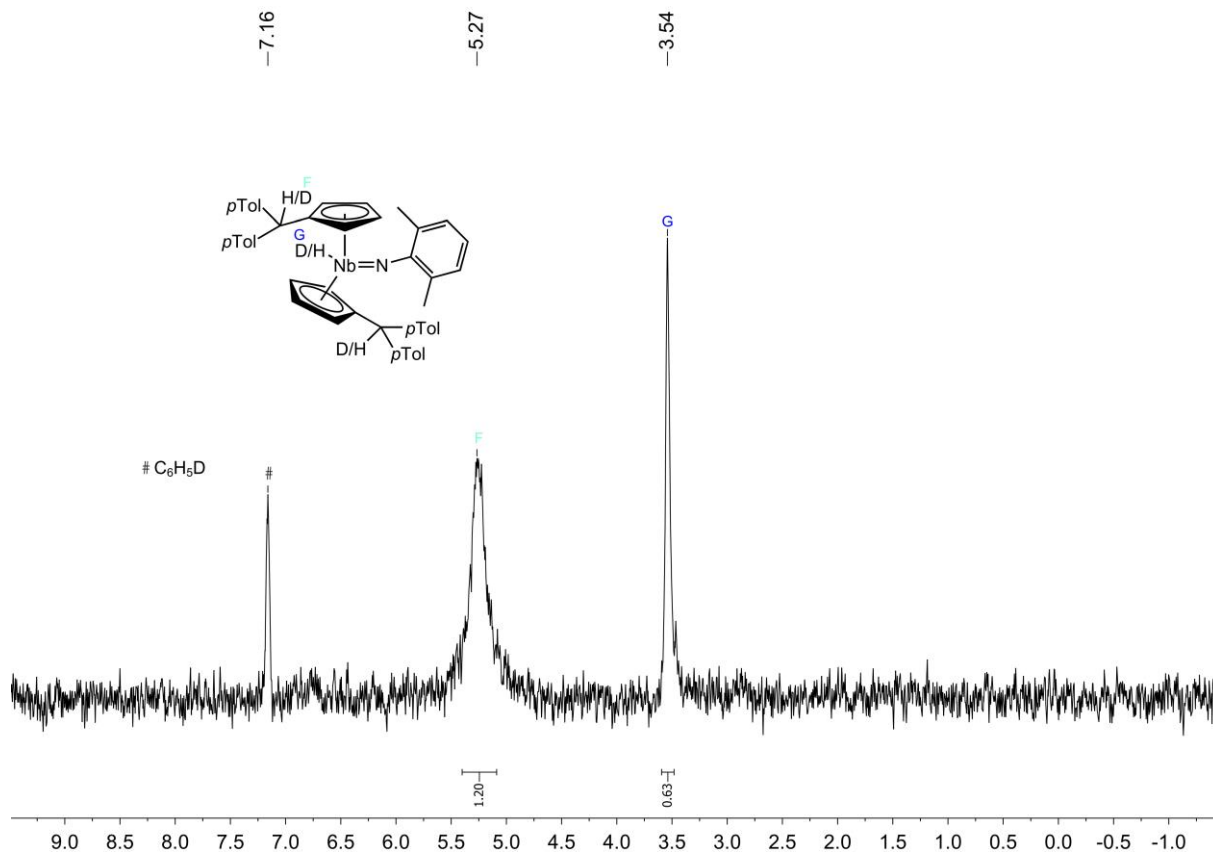


Figure S4: ²H NMR spectra of **4-d₂** (77 MHz, C₆H₆, 305 K).

Synthesis of 5 with deuterium labelled amines: The reaction of **2** with *N*-methylaniline was repeated with *N-d-N*-methylaniline and *N*-(methyl- d_3)-aniline. 60 mg of **2** (0.092 mmol) and 3 equivalents (0.282 mmol) of the respected amine was dissolved in 3 mL of toluene and stirred for four days at 60 °C. The solvent and excess amine were removed as best as possible by drying in high vacuum at 60 °C. Without further purification the residues were dissolved in C_6D_6 or C_6H_6 and 1H or 2H NMR spectra were recorded.

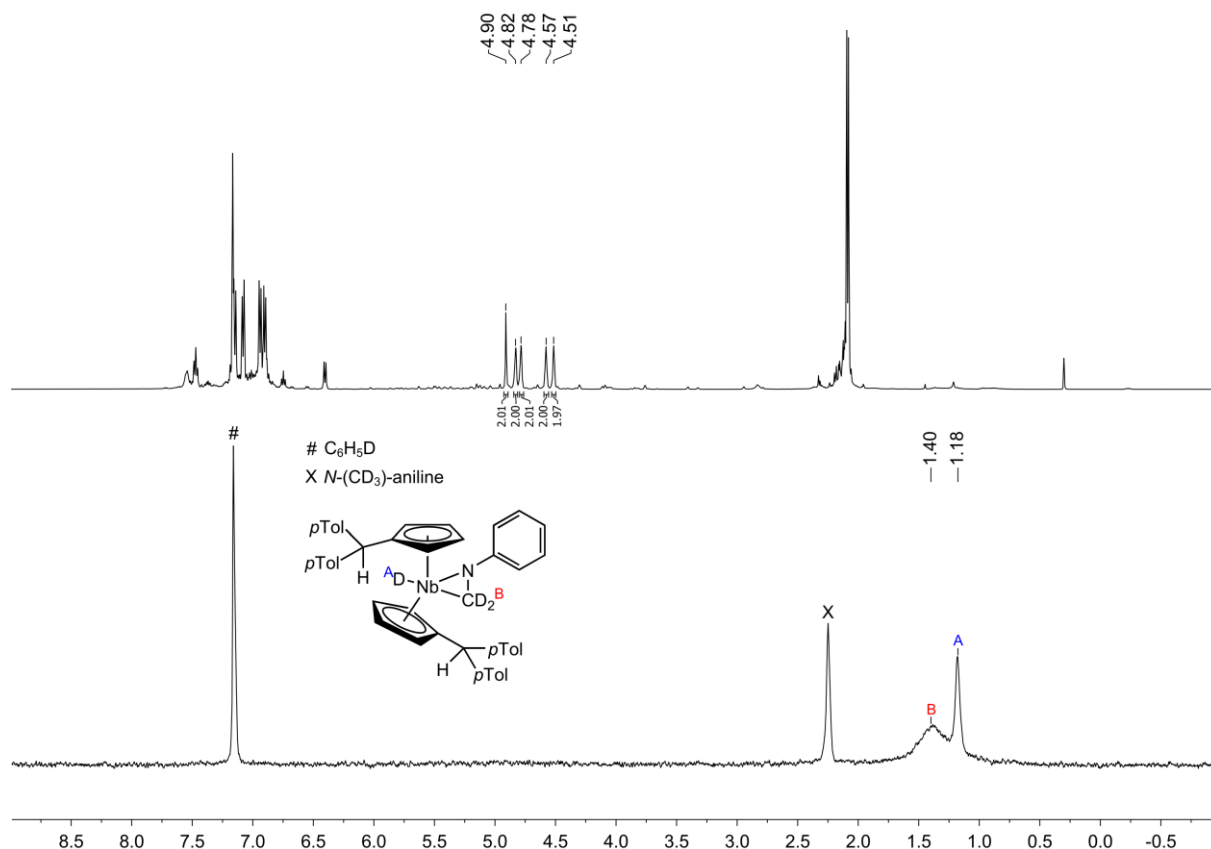


Figure S5: 1H NMR spectrum (500 MHz, C_6D_6 , 305 K, top) and 2H NMR spectrum (77 MHz, C_6H_6 , 305 K, bottom) of the product of **2** and *N*-(methyl- d_3)-aniline.

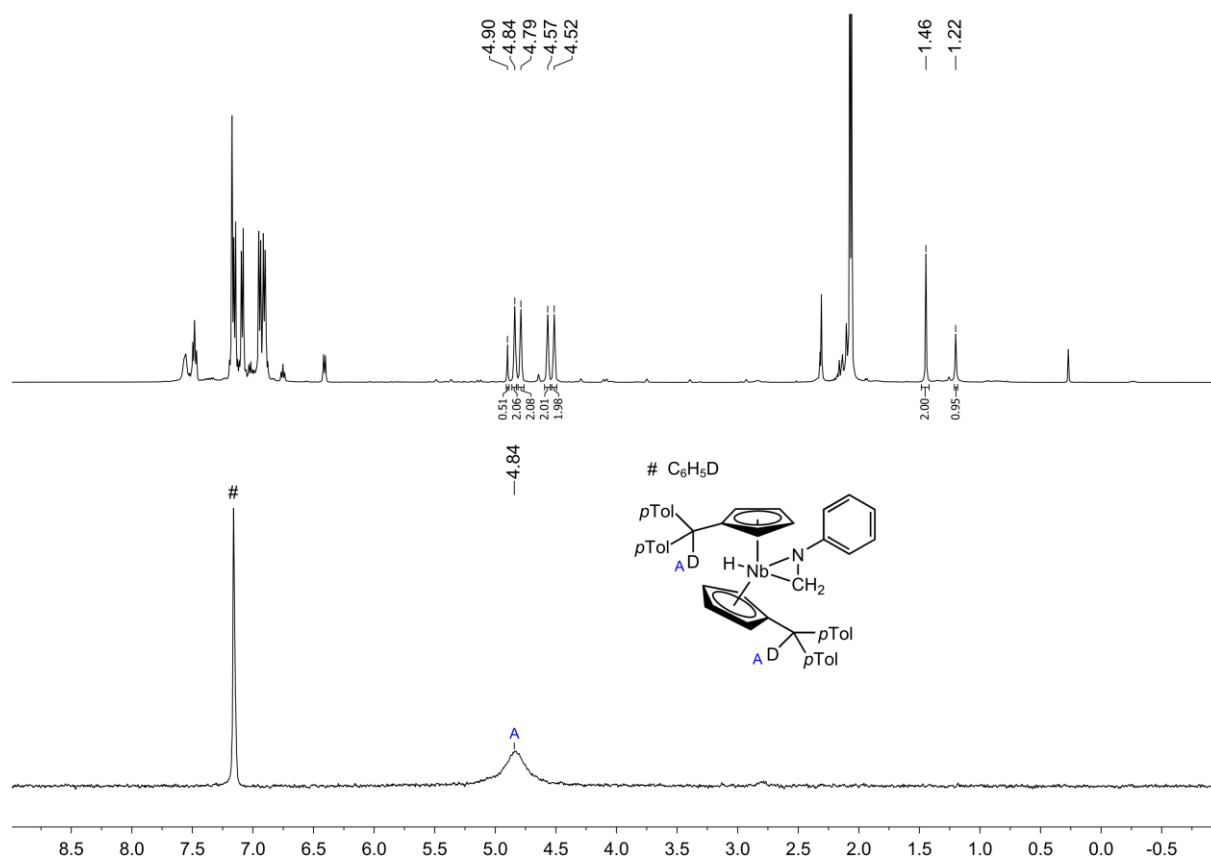
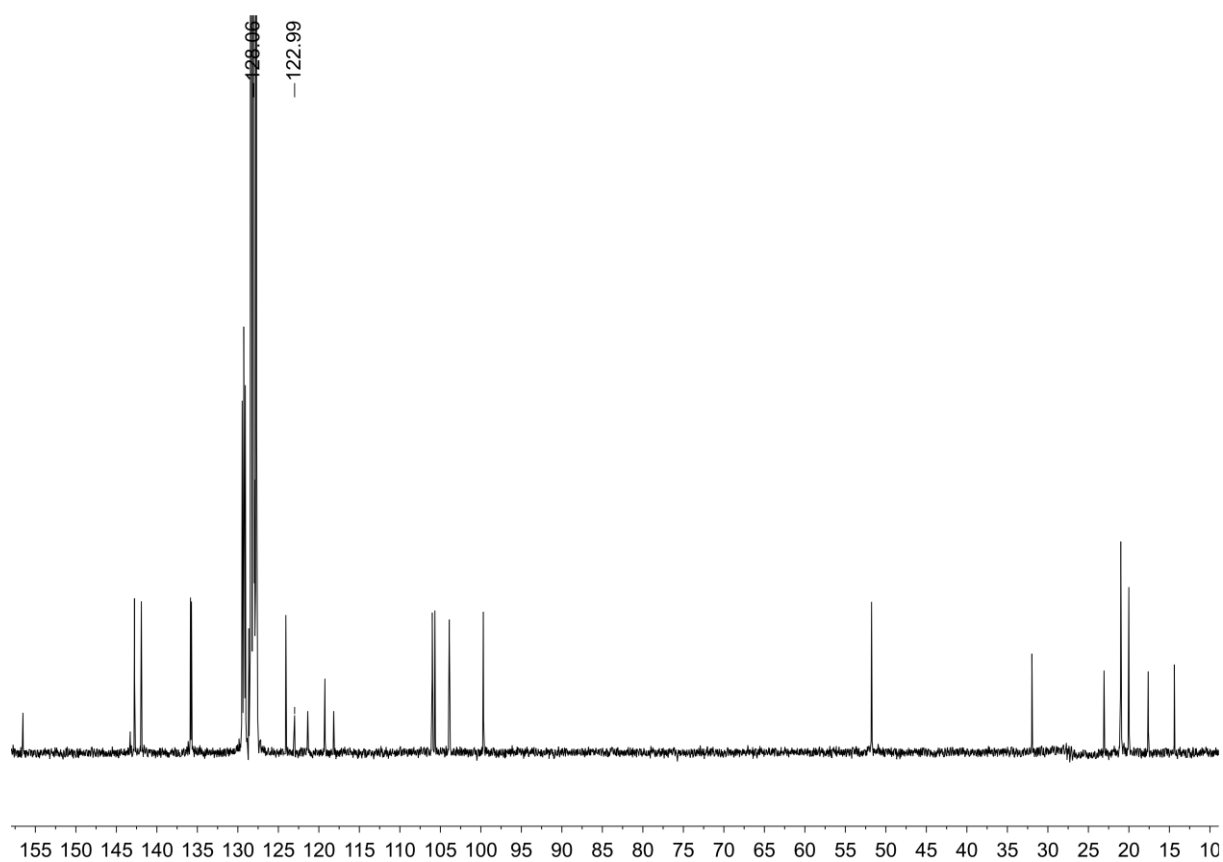
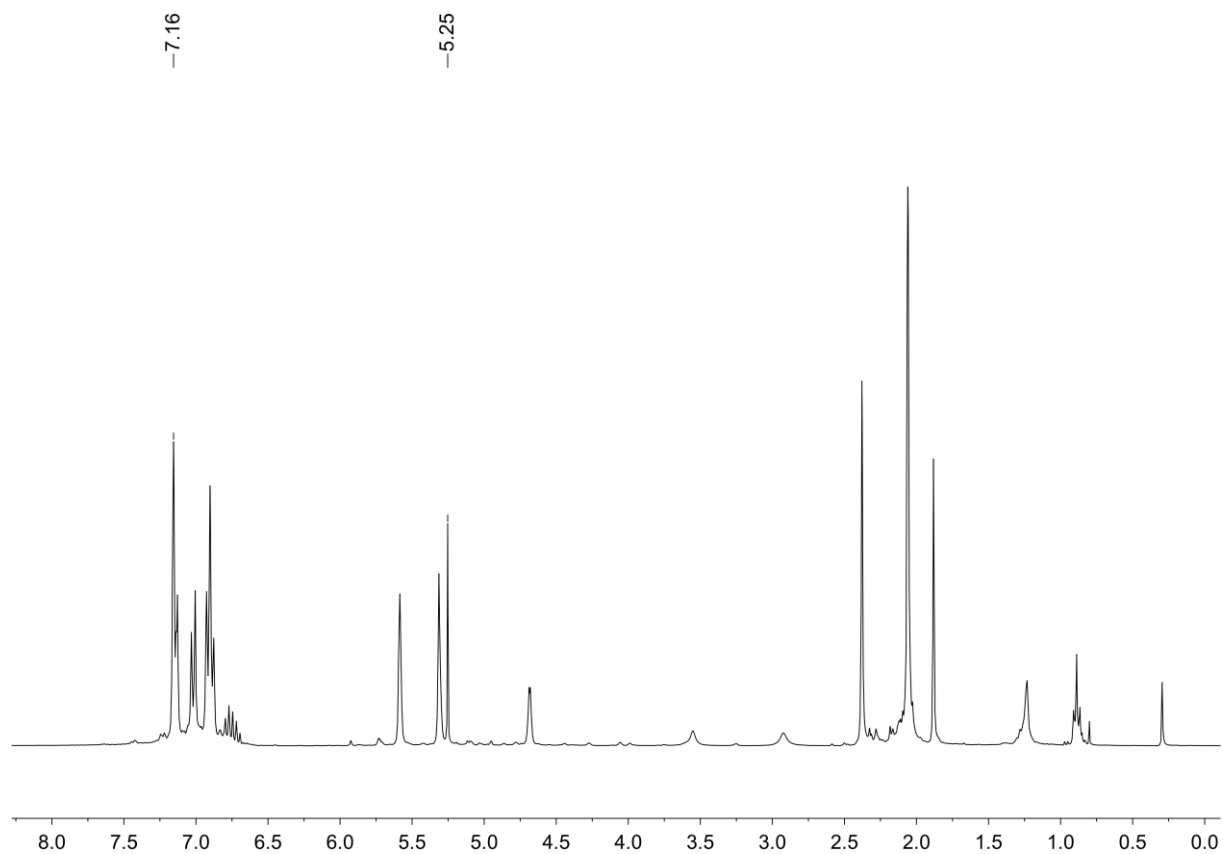


Figure S6: ^1H NMR spectrum (500 MHz, C_6D_6 , 305 K, top) and ^2H NMR spectrum (77 MHz, C_6H_6 , 305 K, bottom) of the product of **2** and *N-d-N*-methylaniline.

Ethylene liberation: To prove the liberation of ethylene in the formation of **4** and **5**, the reactions were repeated in an J. Young NMR tube. A small portion of **2** (approx. 80 mg) was dissolved in C_6D_6 and mixed with a slight excess of the respected amine (**4**: 2,6-xylylidine; **5**: *N*-methylaniline). The mixtures were heated to 60°C for two days and shaken occasionally. The resulting NMR spectra are shown in **Figures S7-S9** for **4** and **Figures S10-S12** for **5**. By ^1H and ^{13}C NMR chemical shift comparison, the liberation of ethylene is proven.¹



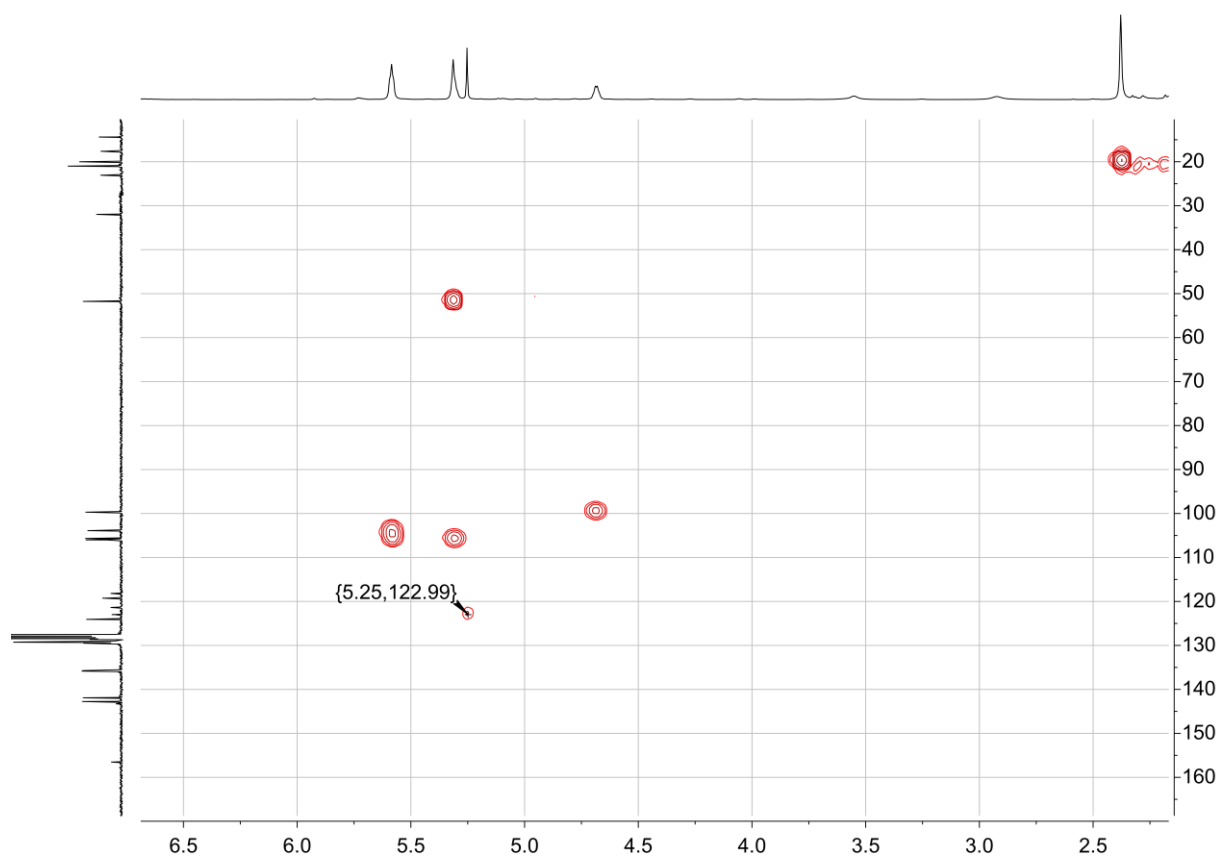


Figure S9: $^1\text{H},^{13}\text{C}$ -HMQC NMR spectra (75 MHz, 300 MHz, 75 MHz, C_6D_6 , 295 K) of the reaction mixture of **4**, showing that the $\delta^1\text{H} = 5.25$ ppm protons are attached to the $\delta^{13}\text{C} = 123.0$ ppm carbon atom.

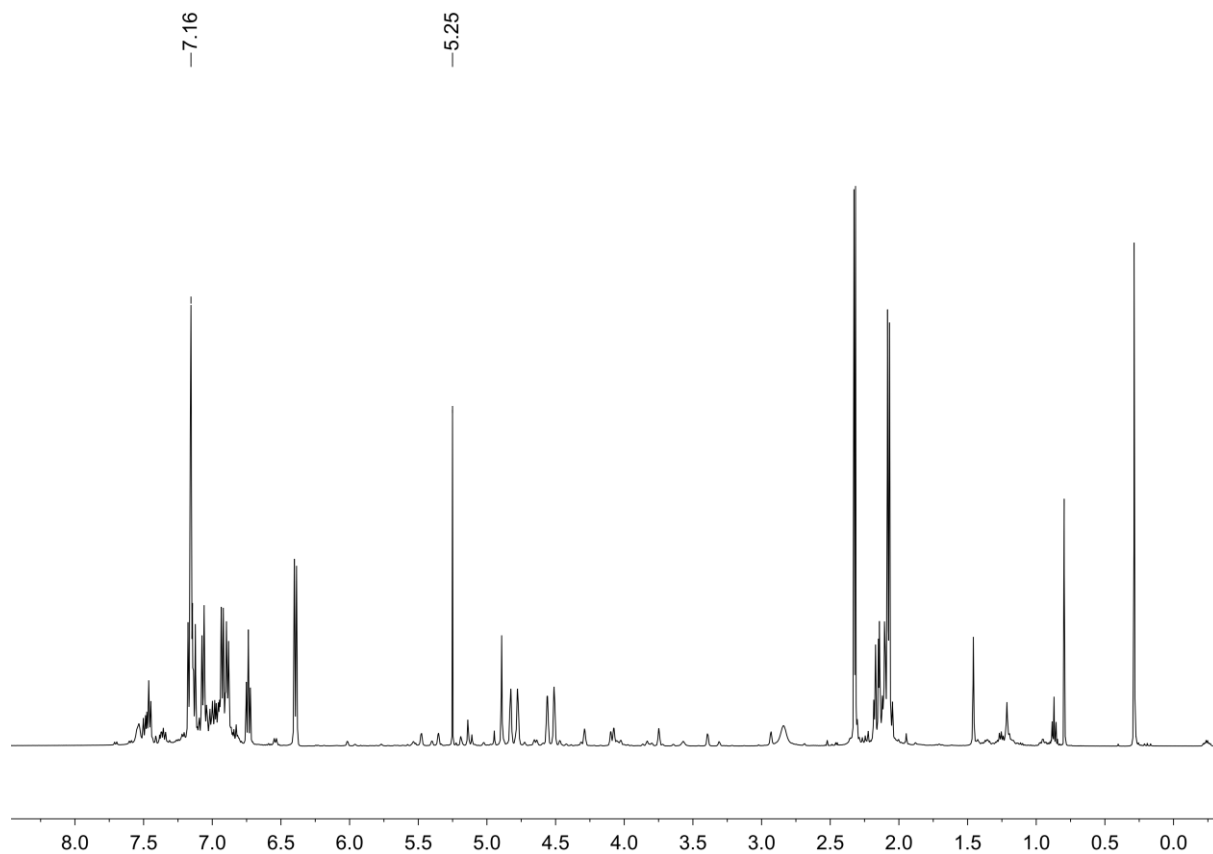


Figure S10: ^1H NMR spectra (500 MHz, C_6D_6 , 305 K) of the reaction mixture of **5**. Ethylene signal at $\delta = 5.25$ ppm.

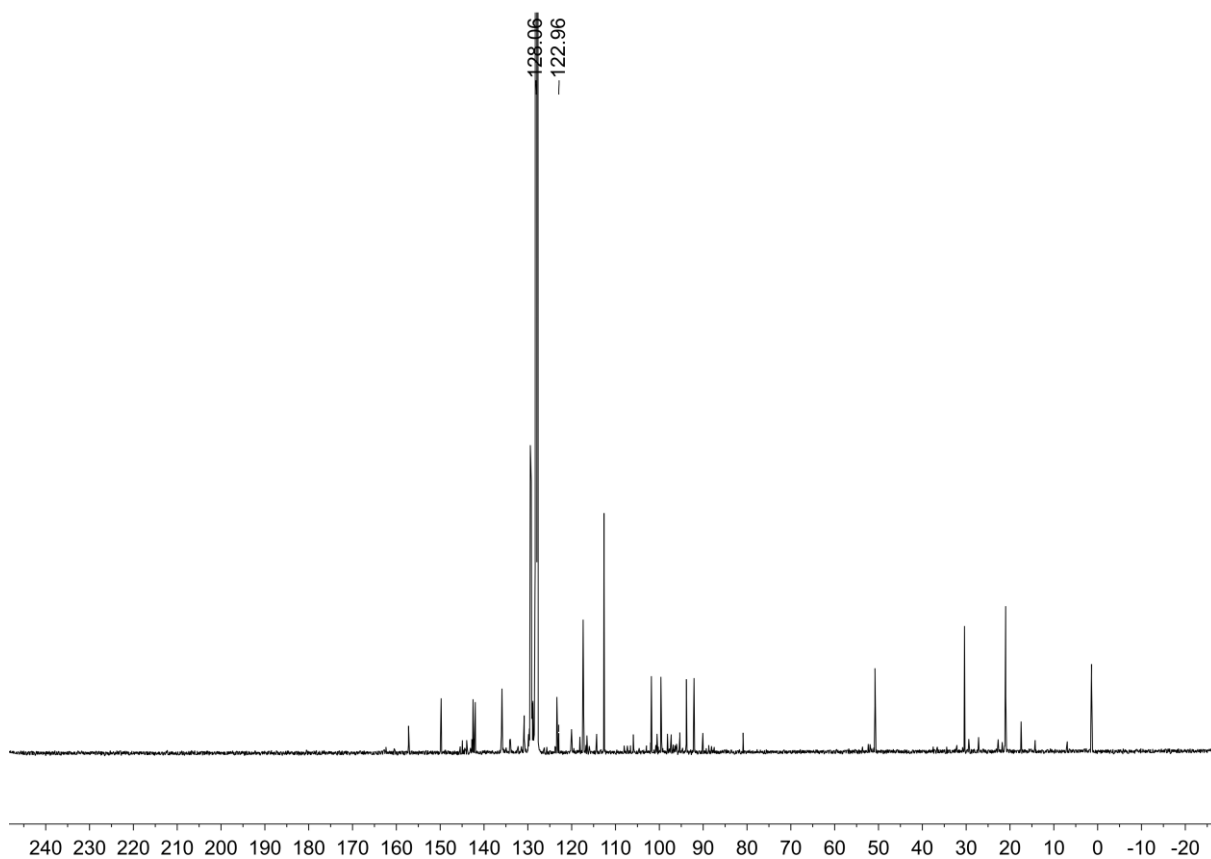


Figure S11: ^{13}C NMR spectra (126 MHz, C_6D_6 , 305 K) of the reaction mixture of **5**. Ethylene signal at $\delta = 123.0$ ppm.

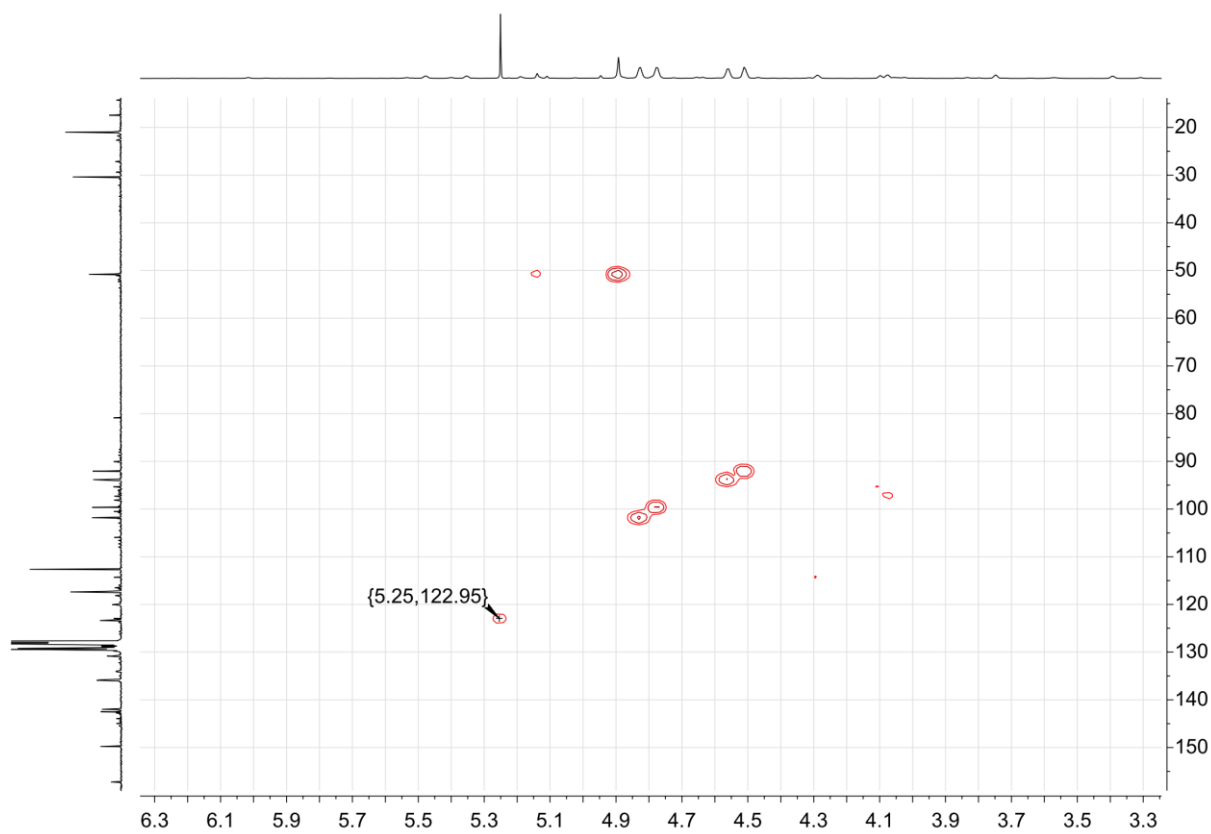


Figure S12: ^1H , ^{13}C -HMOC NMR spectra (126 MHz, 500 MHz, 126 MHz, C_6D_6 , 305 K) of the reaction mixture of **5**, showing that the $\delta^1\text{H} = 5.25$ ppm protons are attached to the $\delta^{13}\text{C} = 123.0$ ppm carbon atom.

β -Hydride elimination experiment: To investigate if niobocene imido-ethyl complex **7** is an intermediate in the formation of **4**, a portion of **7** was dissolved in C_6D_6 and stored first at $60^\circ C$ for one week and subsequently at $80^\circ C$ for another week, while being shaken occasionally. Shown by the 1H NMR spectra (**Figure S13**) no conversion of **7** or liberation of ethylene is detected.

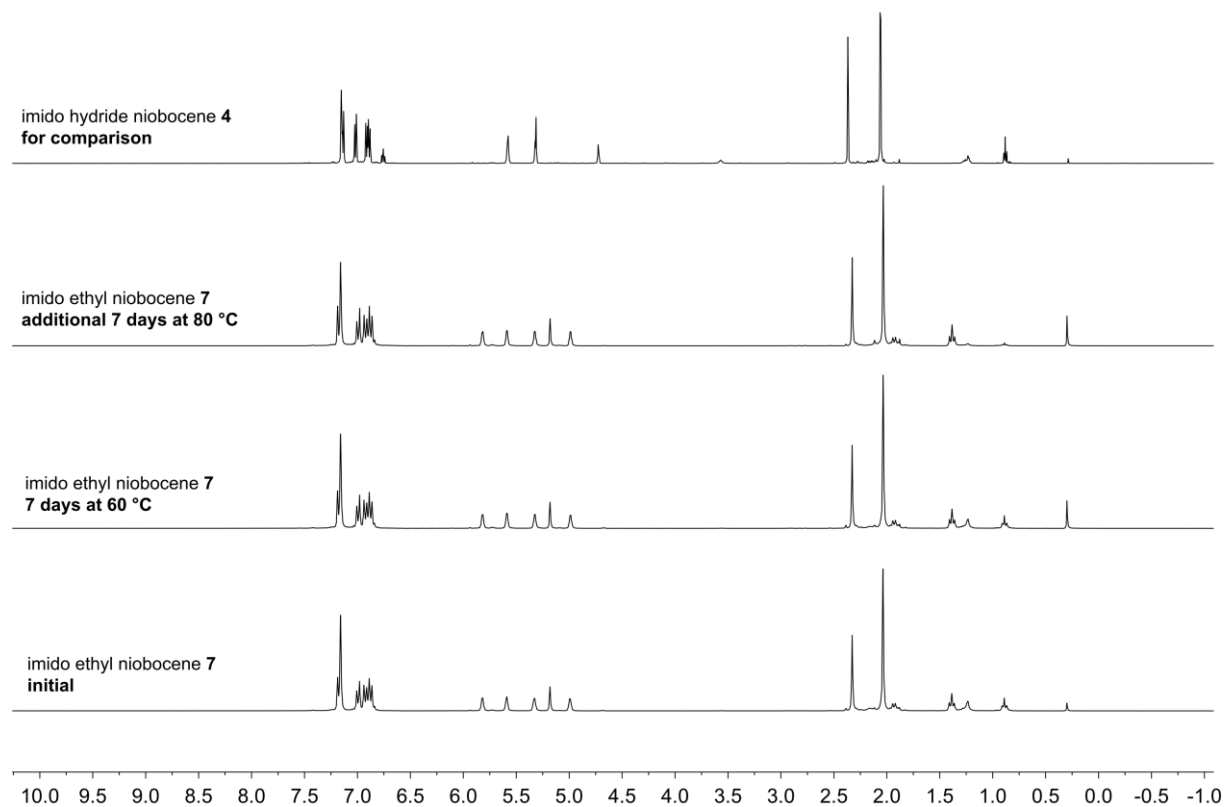


Figure S13: 1H NMR spectra from bottom to top: **7** initial (300 MHz, C_6D_6 , 295 K), **7** after 7 days at $60^\circ C$ (300 MHz, C_6D_6 , 293 K), **7** after additional 7 days at $80^\circ C$ (300 MHz, C_6D_6 , 293 K), **4** for comparison (500 MHz, C_6D_6 , 305 K).

Crystallographic Data

Single crystal X-ray data were measured at a temperature of 100 K on a Bruker AXS D8 Venture diffractometer (multilayer optics, Mo-K α or Cu-K α radiation with $\lambda = 0.71073$ Å and 1.54178 Å respectively, Kappa 4-circle goniometer, Photon III C14 CPAD detector). Absorption corrections using equivalent reflections were performed with the program SADABS.² The structures were solved with the program SHELXS³ and refined with SHELXL⁴ using the OLEX2⁵ GUI.

Unless stated otherwise, all non H atoms were refined using anisotropic atomic displacement parameters, H atoms bonded to C were located in the difference Fourier maps and placed on idealized geometric positions with idealized atomic displacement parameters using the riding model.

2 (*Pna2*₁) has been refined as an inversion twin (BASF 0.420(19)). The structure shows whole molecule disorder (~ 80 : 20), and the minor component has been refined with isotropic displacement parameters and with restraints on the geometry and constraints on atomic displacement parameters as generated by the SAME and EADP instructions, respectively, in SHELXL.

The solvent in **3** (hexane) is completely disordered. It has been treated with the solvent masking routine as implemented in SHELXL/OLEX2 where the solvent contribution is subtracted from the observed data. The such computed electron count amounts to 133.6 e⁻ per unit cell, which corresponds to 2/3 molecules of hexane per formula unit.

7 (*Cmc2*₁) has been refined as an inversion twin (BASF 0.40(3)). Aside from the toluene groups of the Cp-ligand, the structure is disordered (~ 66 : 34). The minor component has been refined with isotropic displacement parameters using geometry restraints generated by the SAME instruction in SHELXL.

The crystallographic data can be obtained free of charge from <https://www.ccdc.cam.ac.uk/structures/> quoting the CCDC numbers 2180949-2180953.

Table S1: Crystal Structure Data for Compounds **2**, **3**, and **4**.

	2	3	4
CCDC	2180950	2180951	2180949
empirical formula	C ₄₂ H ₄₁ Nb	C ₄₆ H _{52.33} NbO	C ₄₈ H ₄₈ NNb
fw	638.66	714.11	731.78
color	yellow	colorless	yellow
Habit	rod	plate	plate
cryst dimens, mm	0.14x0.06x0.02	0.12x0.07x0.04	0.06x0.04x0.015
cryst syst	orthorhombic	monoclinic	triclinic
space group	<i>Pna</i> 2 ₁	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1
<i>a</i> , Å	24.1670(15)	18.9136(15)	12.2019(3)
<i>b</i> , Å	14.2843(10)	6.3645(5)	12.2626(3)
<i>c</i> , Å	18.8613(12)	32.438(3)	14.3100(4)
α , deg	90	90	80.0722(18)
β , deg	90	100.554(3)	88.089(2)
γ , deg	90	90	63.2622(18)
<i>V</i> , Å ³	6511.1(7)	3838.7(5)	1881.20(9)
<i>Z</i>	8	4	2
ρ_{calc} , g cm ⁻³	1.303	1.236	1.292
μ , mm ⁻¹	3.207	2.790	2.851
<i>T</i> , K	100(2)	100(2)	100(2)
λ , Å	1.54178	1.54178	1.54178
θ range, deg	3.594 – 74.495	2.376 – 74.495	3.139 – 66.595
no. of rflns collected	100489	70482	24109
no. of indep rflns (<i>R</i> (int))	13195 (0.0651)	7828 (0.0481)	6607 (0.0553)
no. of rflns with $I > 2\sigma(I)$	12270	7319	5657
abs cor	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
max, min transmission	1.0000 and 0.7913	0.8290 and 0.6517	1.0000 and 0.8518
final <i>R</i> indices [$I > 2\sigma(I)$]	<i>R</i> 1 = 0.0589 <i>wR</i> 2 = 0.1583	<i>R</i> 1 = 0.0477 <i>wR</i> 2 = 0.1343	<i>R</i> 1 = 0.0386 <i>wR</i> 2 = 0.0887
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0627 <i>wR</i> 2 = 0.1625	<i>R</i> 1 = 0.0497 <i>wR</i> 2 = 0.1367	<i>R</i> 1 = 0.0492 <i>wR</i> 2 = 0.0931
GOF on <i>F</i> ²	1.111	1.063	1.081
largest diff peak / hole (e.Å ⁻³)	2.611/ -0.550	1.903/ -0.723	1.281 / -0.866

Table S2: Crystal Structure Data for Compounds **6** and **7**.

	6	7
CCDC	2180953	2180952
empirical formula	C ₅₁ H ₅₄ CINNb	C ₅₀ H ₅₂ NNb
fw	809.31	759.83
color	yellow	yellow
Habit	rod	block
cryst dimens, mm	0.12x0.06x0.02	0.20x0.14x0.12
cryst syst	orthorhombic	Orthorhombic
space group	<i>Pbca</i>	<i>Cmc2₁</i>
<i>a</i> , Å	14.5460(4)	17.0160(6)
<i>b</i> , Å	22.2303(7)	11.6364(4)
<i>c</i> , Å	25.7237(9)	20.0189(7)
α , deg	90	90
β , deg	90	90
γ , deg	90	90
<i>V</i> , Å ³	8318.1(5)	3963.8(2)
<i>Z</i>	8	4
ρ calc, g cm ⁻³	1.293	1.273
μ , mm ⁻¹	0.389	0.339
<i>T</i> , K	100(2)	100(2)
λ , Å	0.71073	0.71073
θ range, deg	1.583 – 28.699	2.035 – 40.246
no. of rflns collected	247663	168977
no. of indep rflns (<i>R</i> (int))	10738 (0.0986)	12752 (0.0332)
no. of rflns with $I > 2\sigma(I)$	9076	12042
abs cor	Semi-empirical from equivalents	Semi-empirical from equivalents
max, min transmission	1.0000 and 0.9366	1.0000 and 0.9032
final <i>R</i> indices[$I > 2\sigma(I)$]	<i>R</i> 1 = 0.0484 w <i>R</i> 2 = 0.0868	<i>R</i> 1 = 0.0316 w <i>R</i> 2 = 0.0799
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0615 w <i>R</i> 2 = 0.0911	<i>R</i> 1 = 0.0340 w <i>R</i> 2 = 0.0815
GOF on <i>F</i> ²	1.123	1.113
largest diff peak / hole (e.Å ⁻³)	0.462 / -0.963	1.491 / -0.762

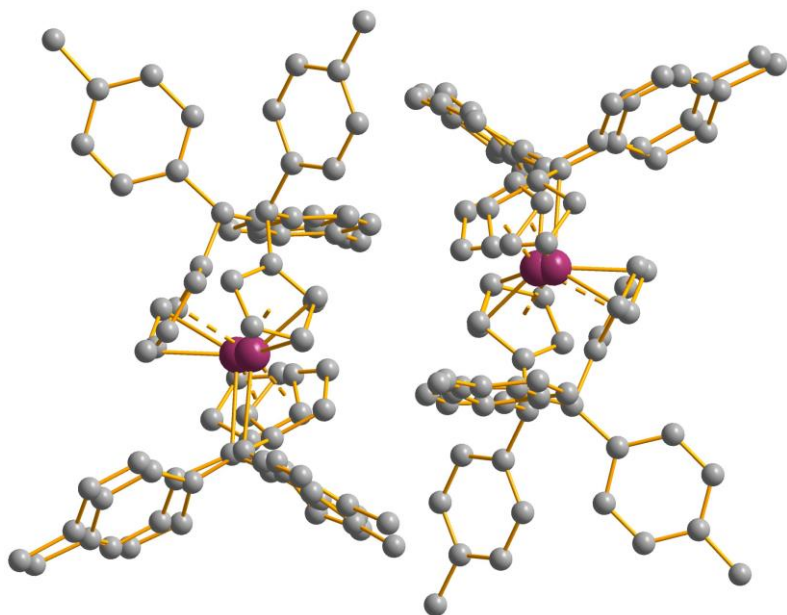


Figure S14: Molecular structure of **2**. Hydrogen atoms are omitted.

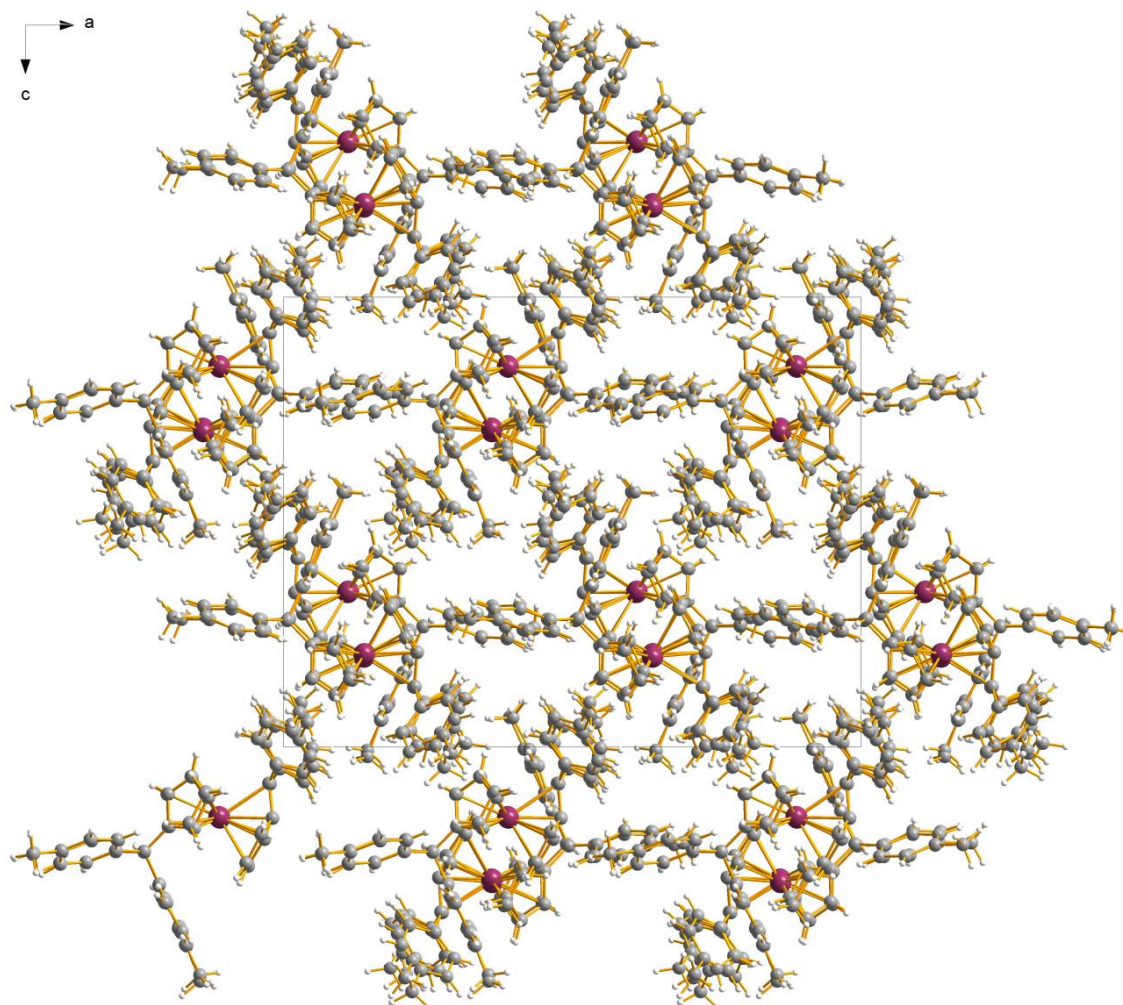


Figure S15: View along the b axis showing the packing of molecules in the crystal structure of complex **2**.

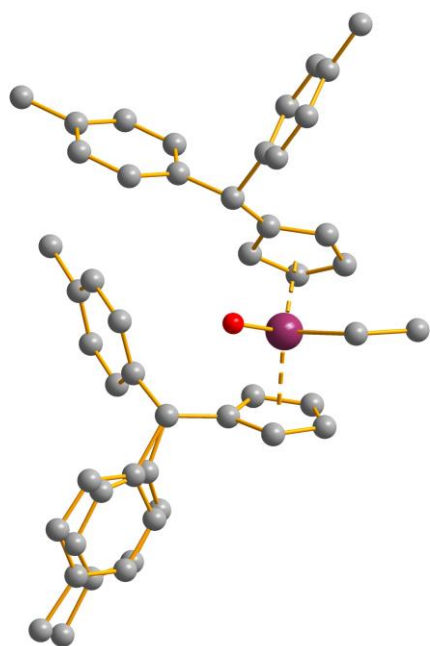


Figure S16: Molecular structure of **3**. Hydrogen atoms are omitted. One *p*-tolyl substituent is distorted.

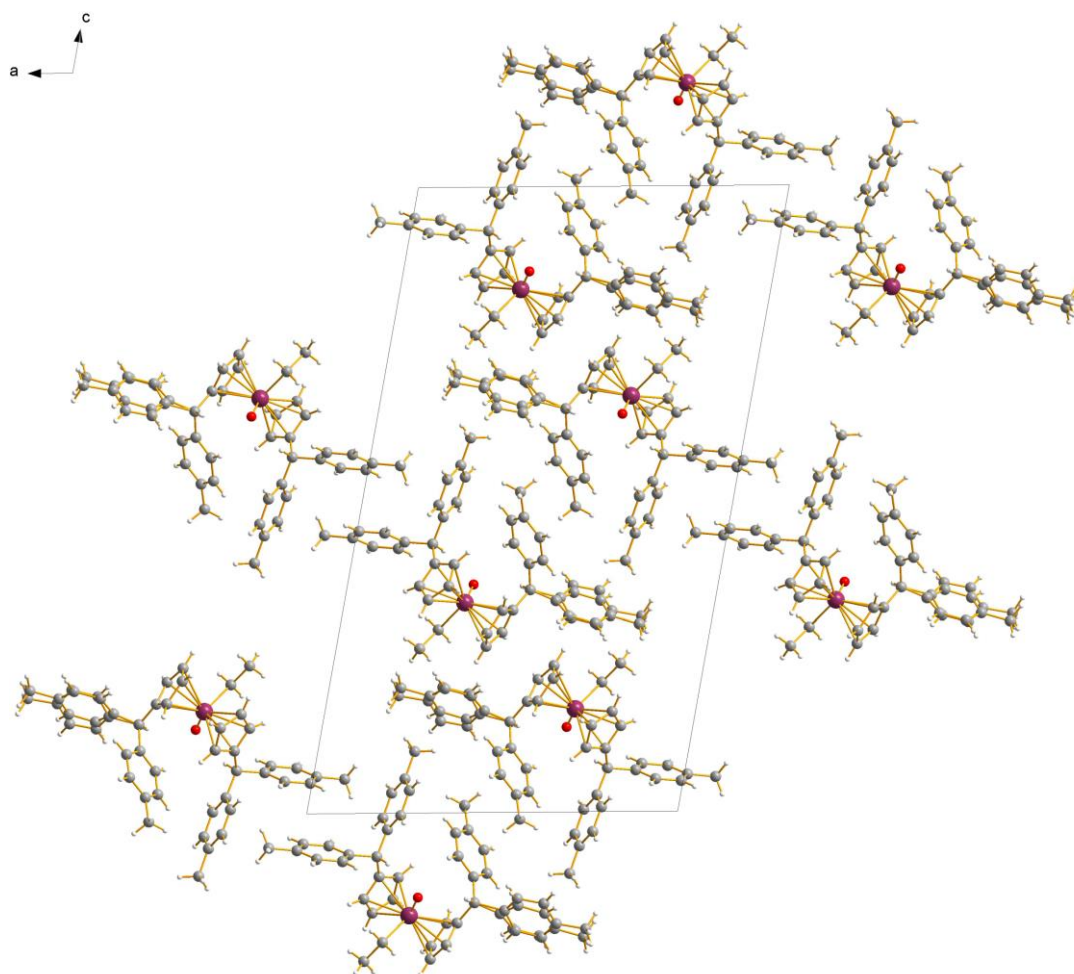


Figure S17: View along the *b* axis showing the packing of molecules in the crystal structure of complex **3**.

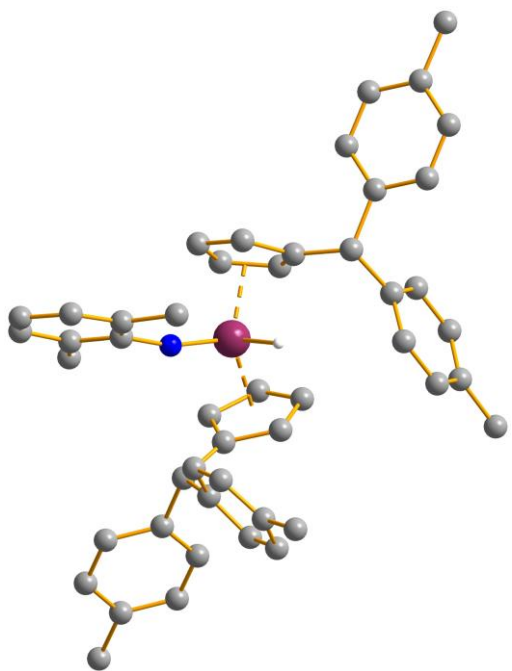


Figure S18: Molecular structure of **4**. Hydrogen atoms are omitted.

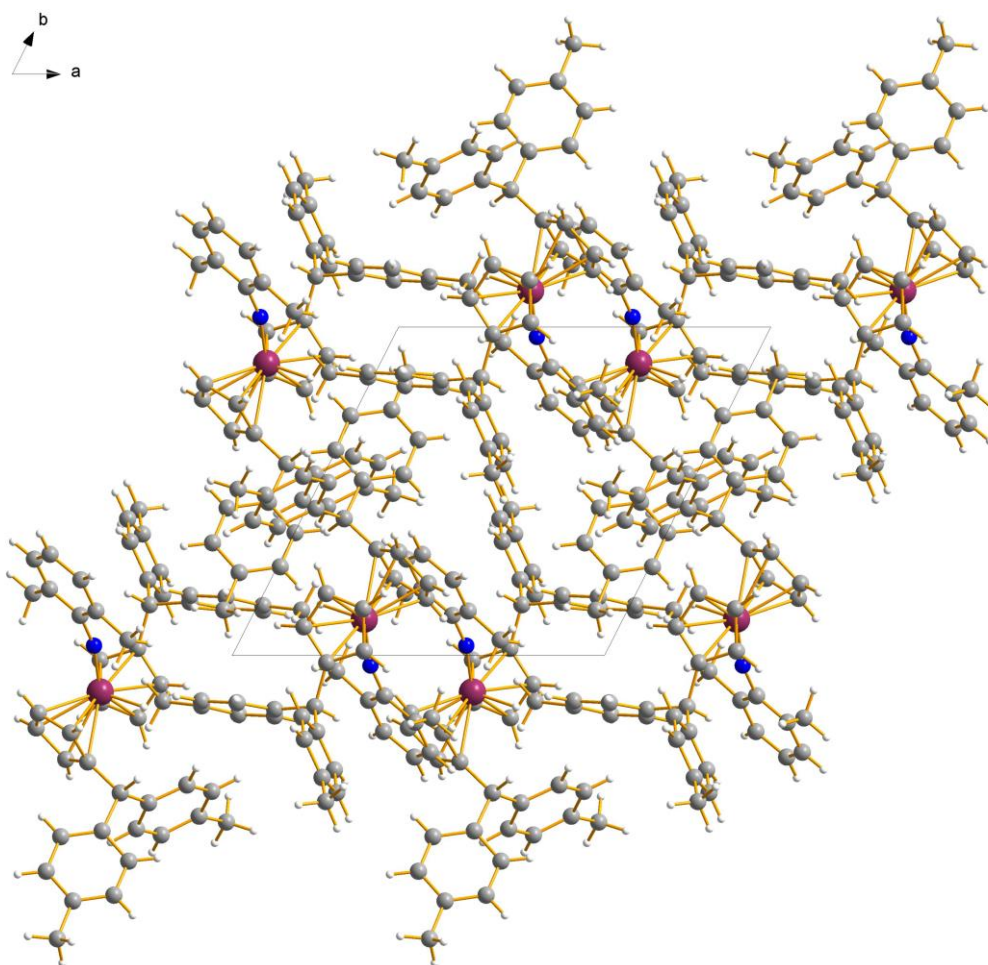


Figure S19: View along the c axis showing the packing of molecules in the crystal structure of complex **4**.

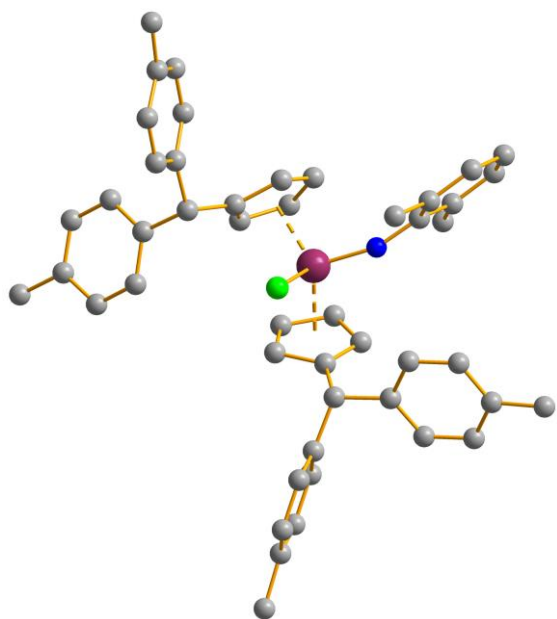


Figure S20: Molecular structure of **6**. Hydrogen atoms are omitted.

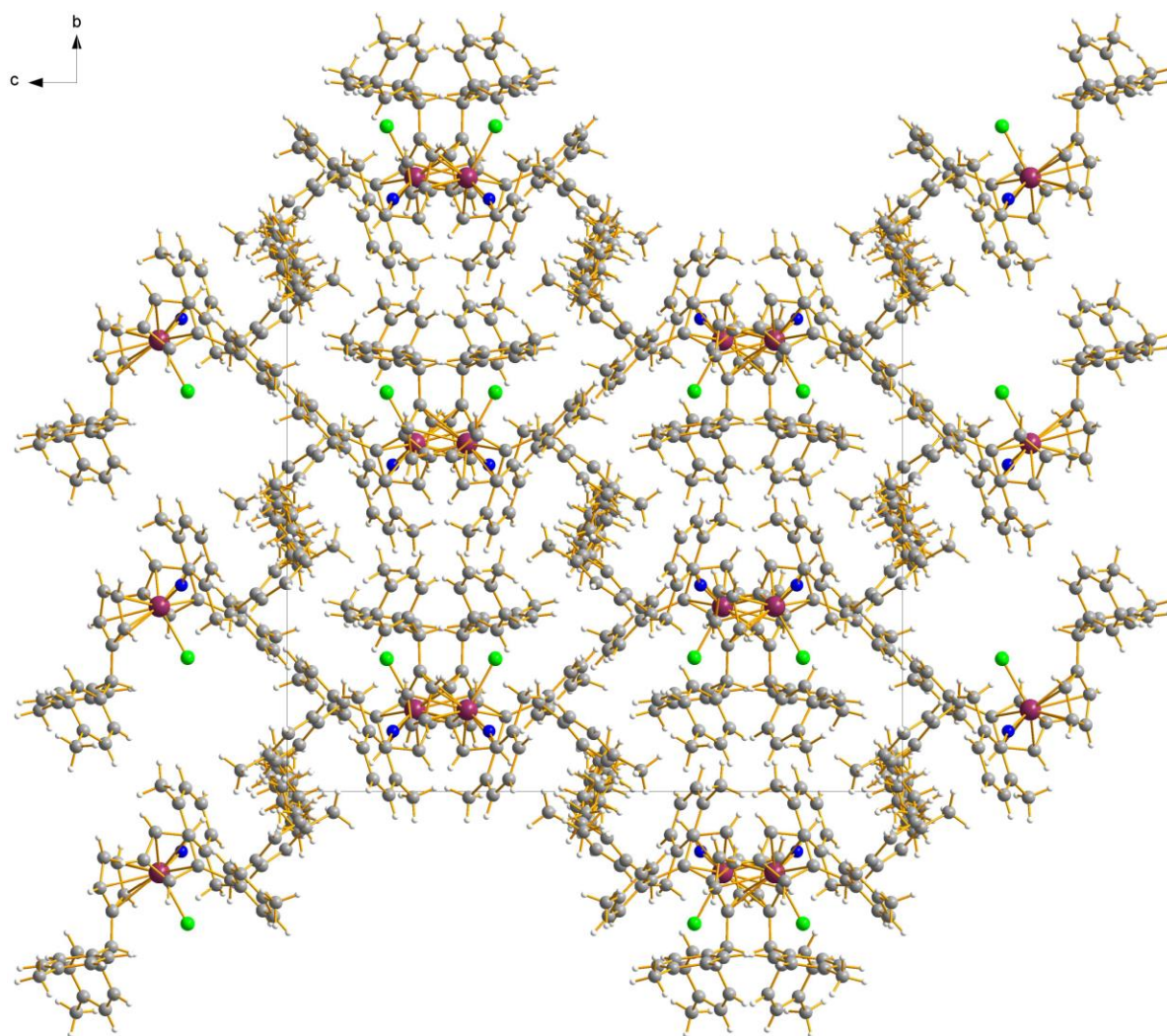


Figure S21: View along the b axis showing the packing of molecules in the crystal structure of complex **6**.

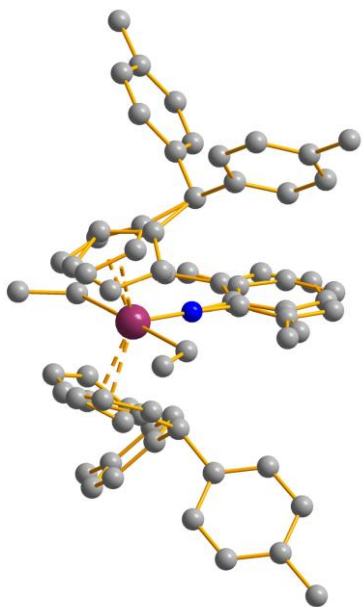


Figure S22: Molecular structure of **7**. Hydrogen atoms are omitted. Middle section is symmetrically distorted.

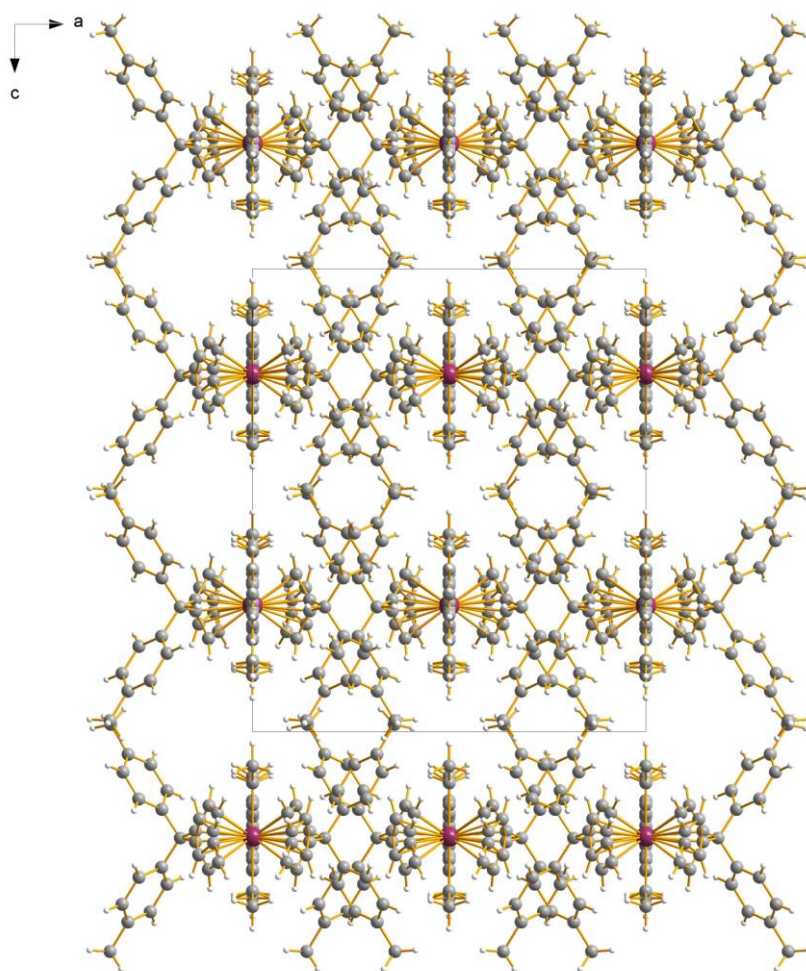


Figure S23: View along the b axis showing the packing of molecules in the crystal structure of complex **7**.

Supplementary NMR Spectra

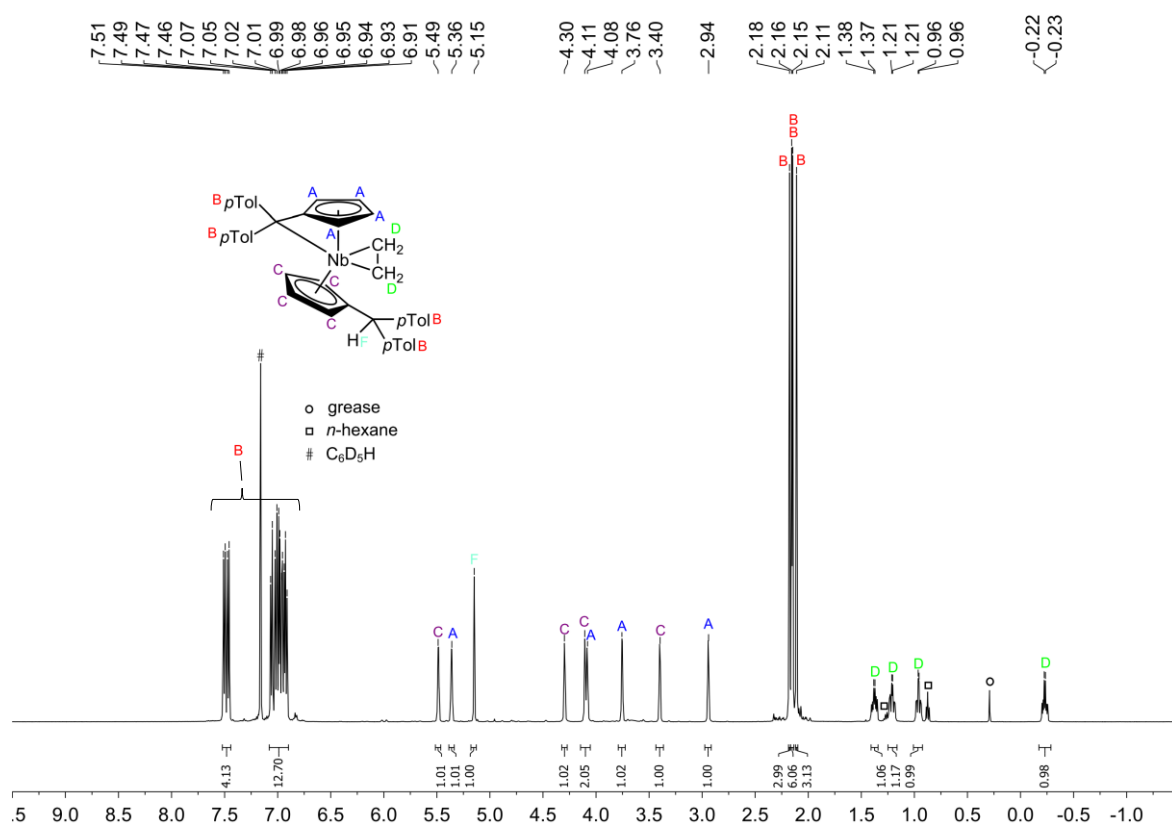


Figure S24: ¹H NMR spectrum of **2** (500 MHz, C₆D₆, 305 K).

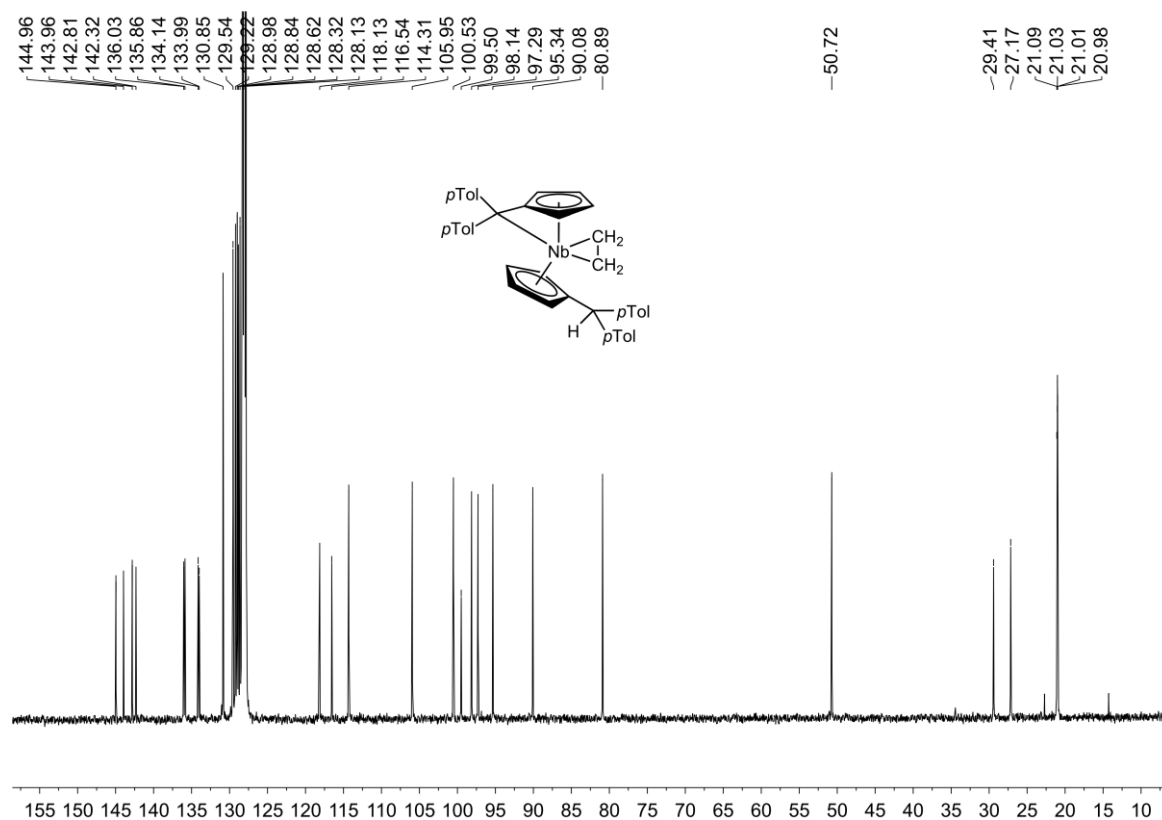


Figure S25: ¹³C{¹H} NMR spectrum of **2** (126 MHz, C₆D₆, 305 K).

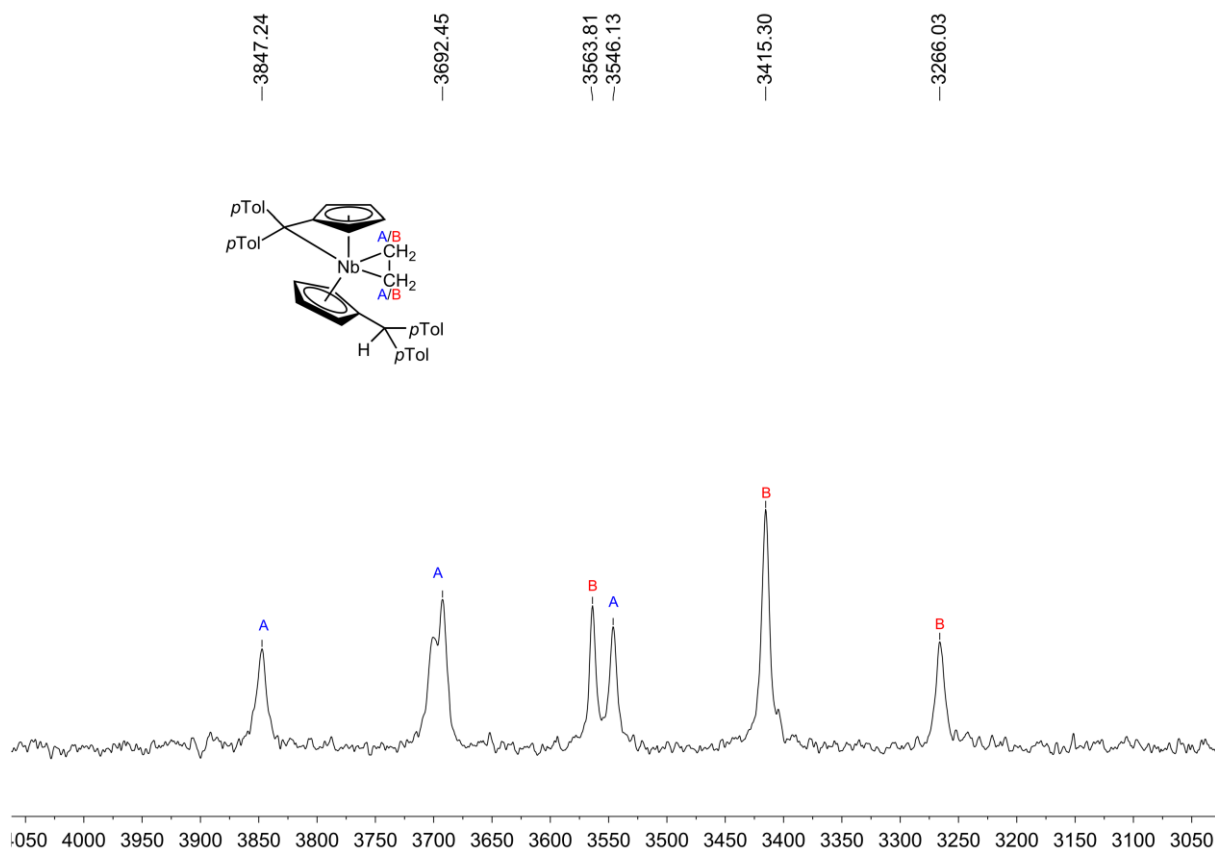


Figure S26: Excerpt of the ^{13}C NMR spectrum of **2** (126 MHz, C_6D_6 , 305 K). Scale depicted in Hz.

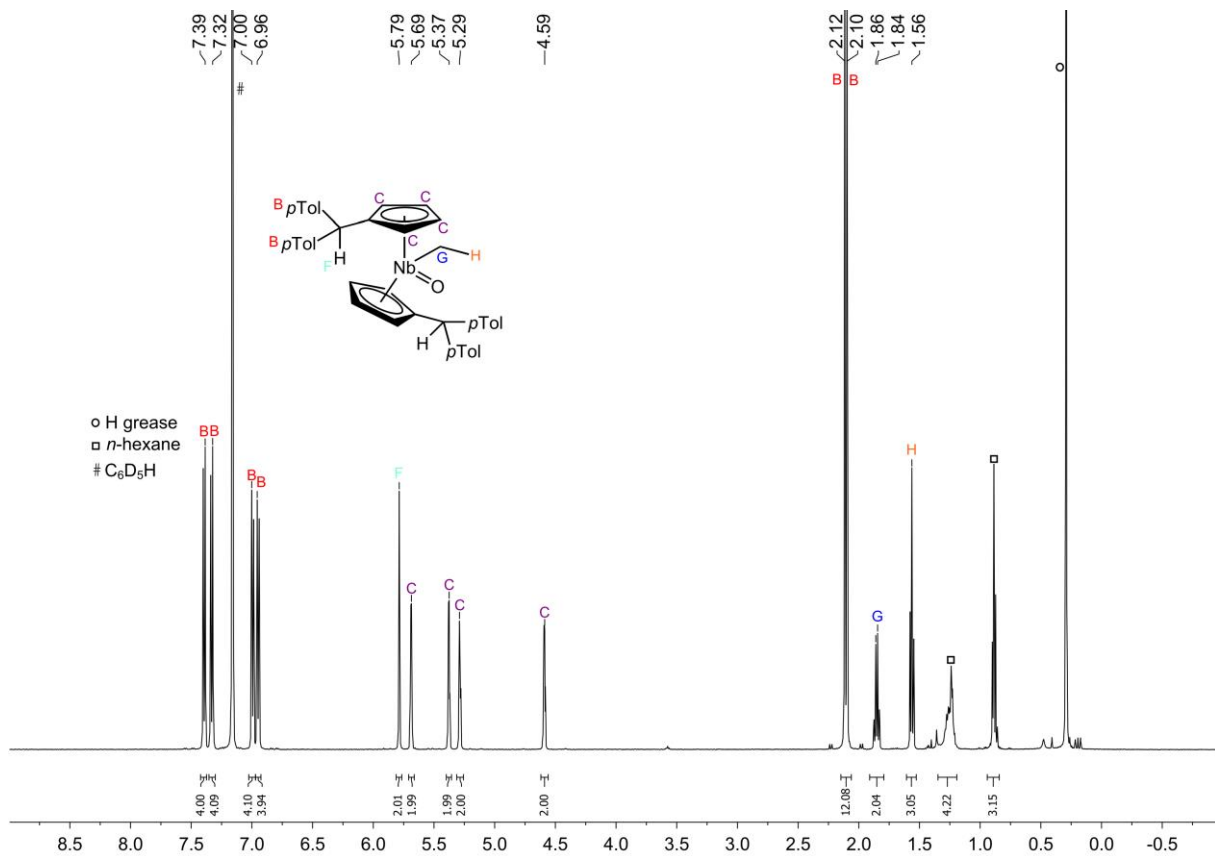


Figure S27: ^1H NMR spectrum of **3** (500 MHz, C_6D_6 , 305 K).

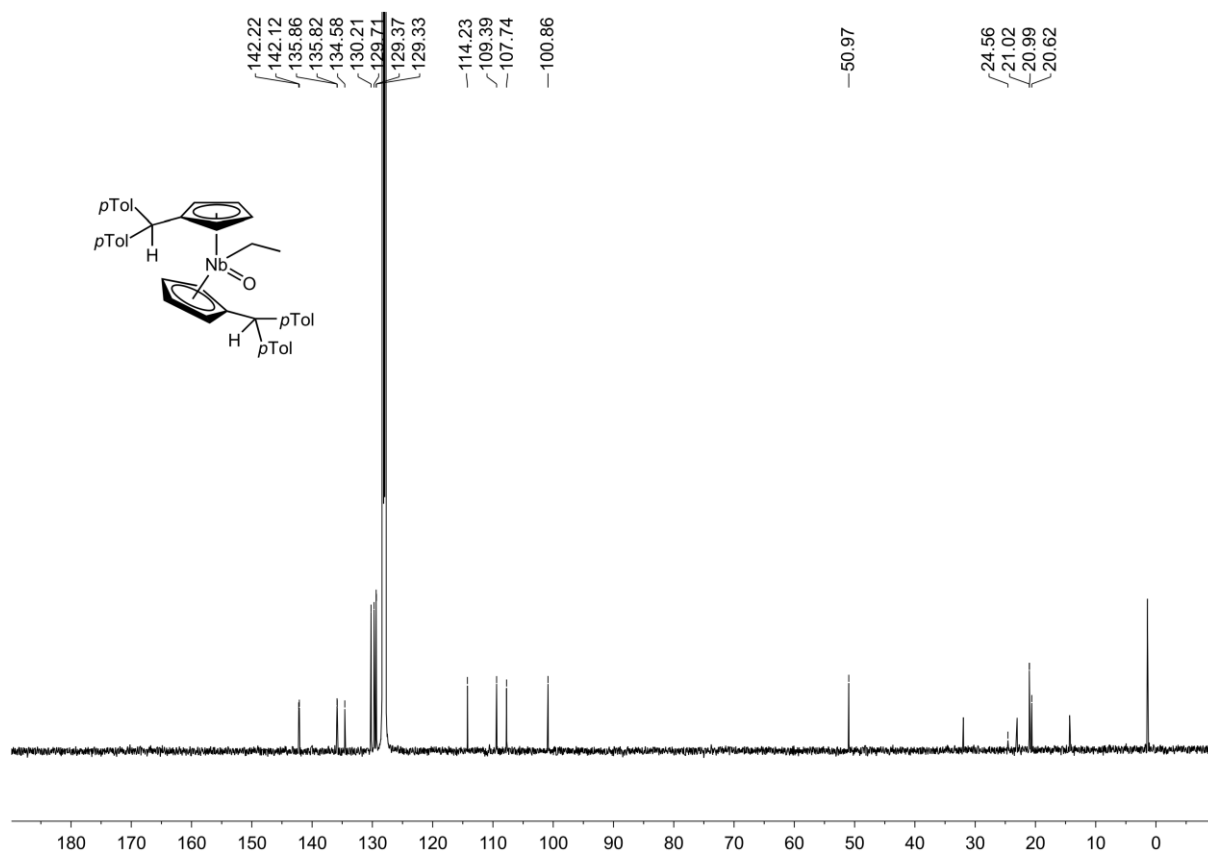


Figure S28: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (126 MHz, C_6D_6 , 305 K).

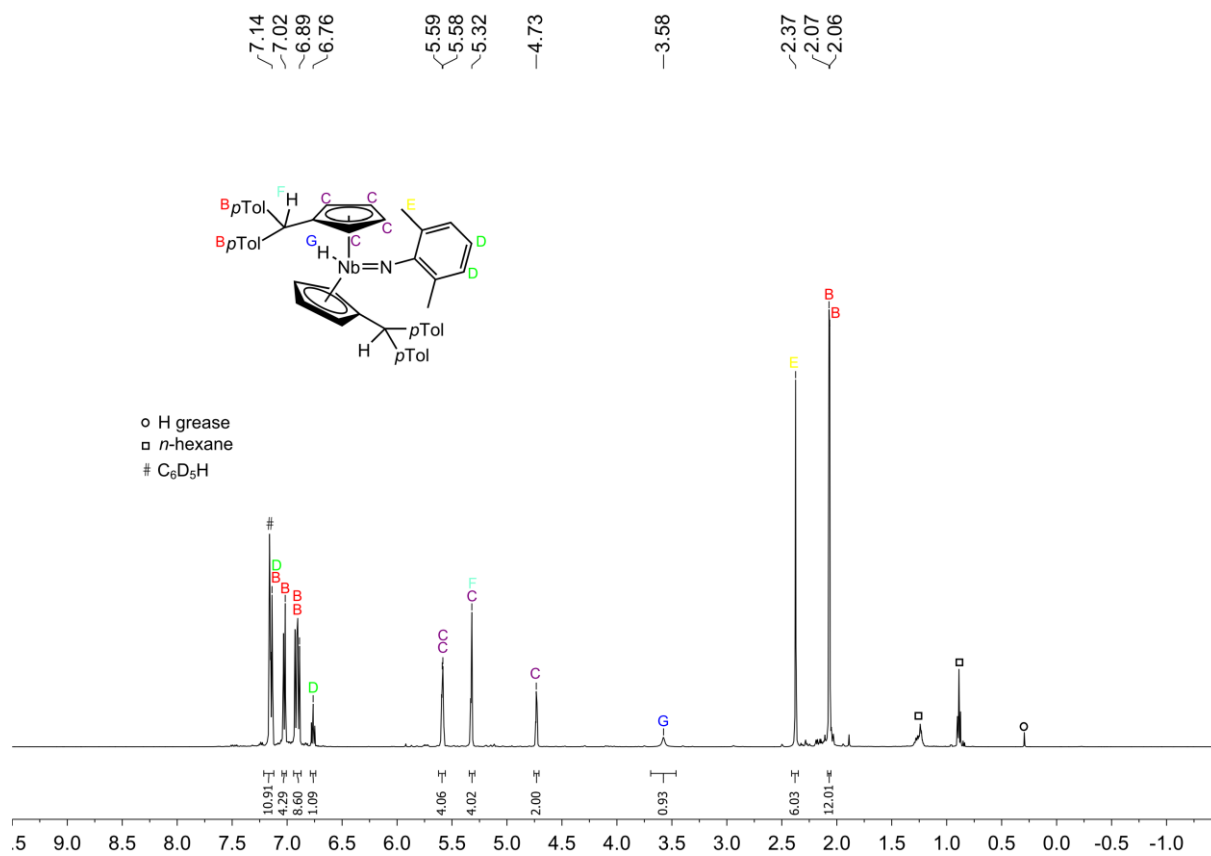


Figure S29: ^1H NMR spectrum of **4** (500 MHz, C_6D_6 , 305 K).

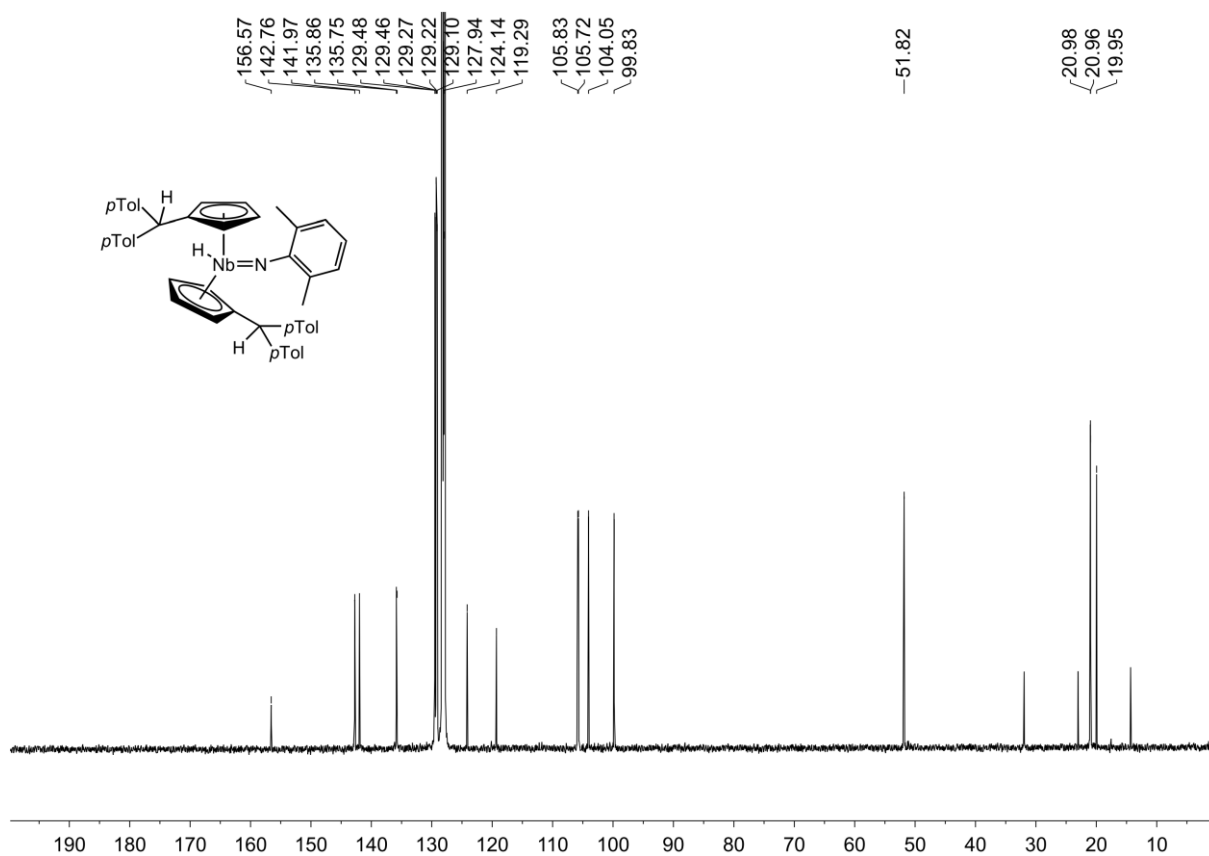


Figure S30: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** (126 MHz, C_6D_6 , 305 K).

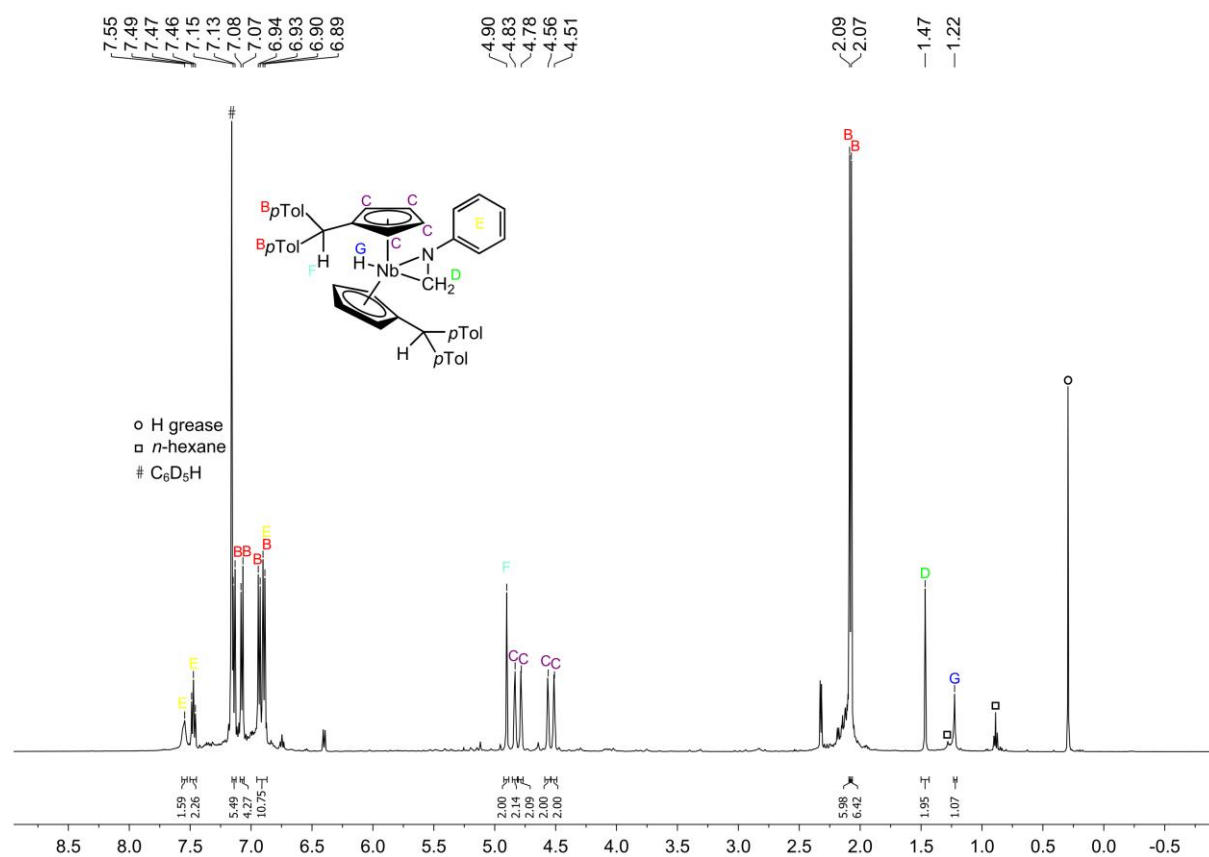


Figure S31: ^1H NMR spectrum of **5** (500 MHz, C_6D_6 , 305 K).

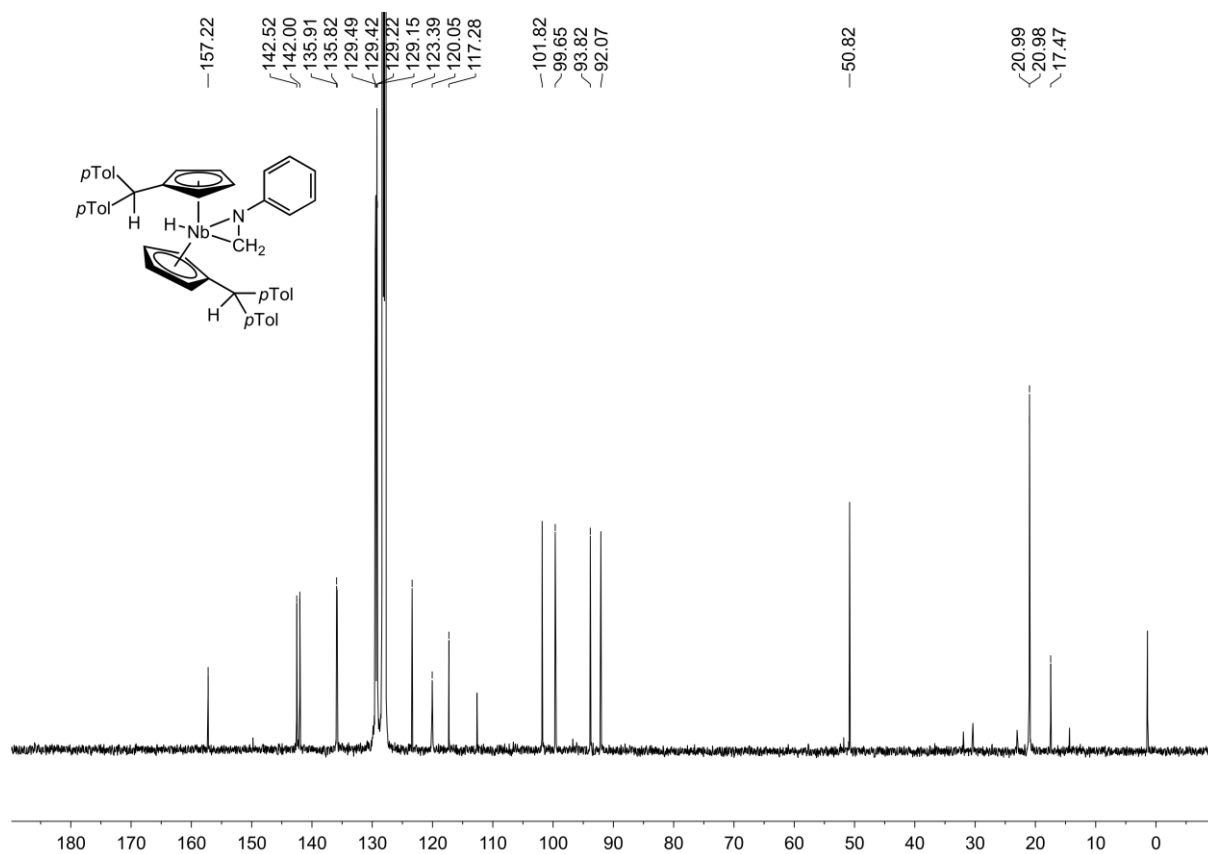


Figure S32: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** (126 MHz, C_6D_6 , 305 K).

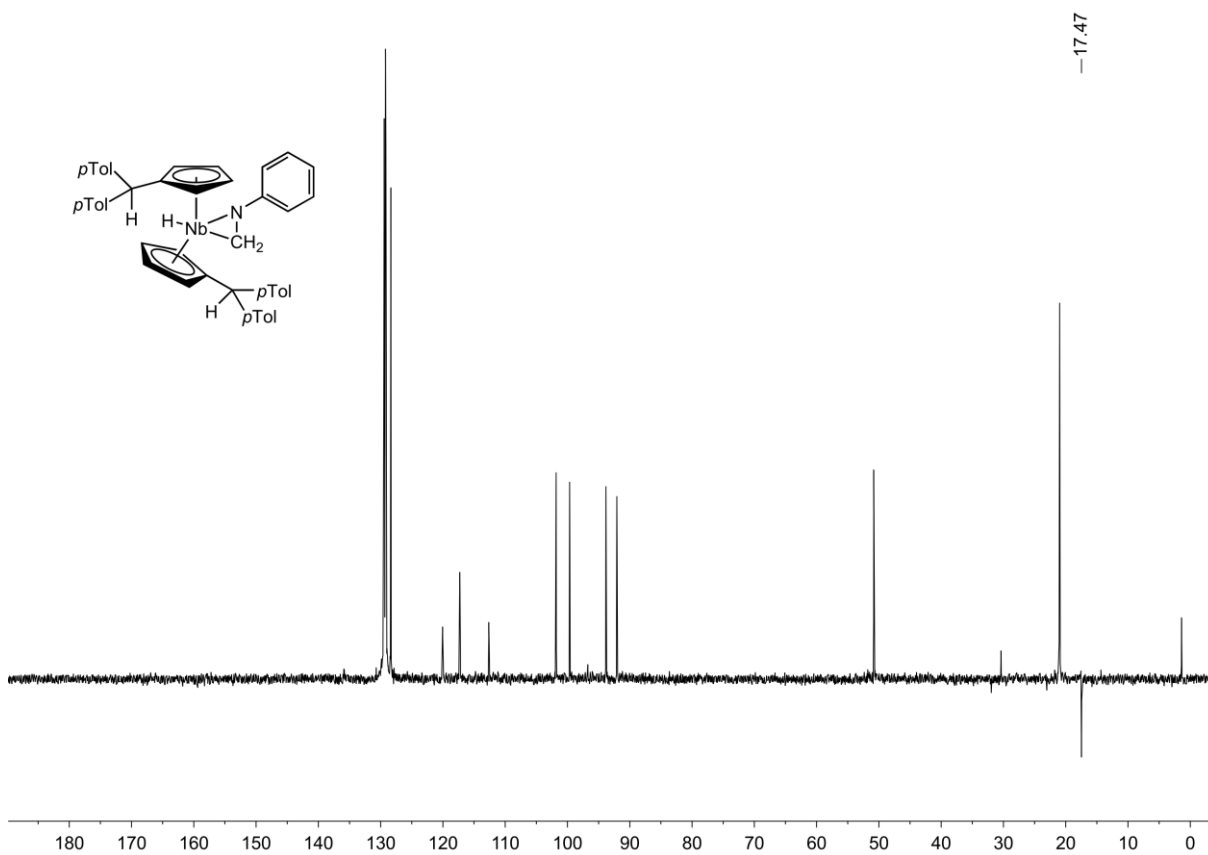


Figure S33: $^1\text{H}, ^{13}\text{C}$ dept135 NMR spectrum of **5** (126 MHz, C_6D_6 , 305 K) identifying the signal at 17.47 ppm as a methylene group.

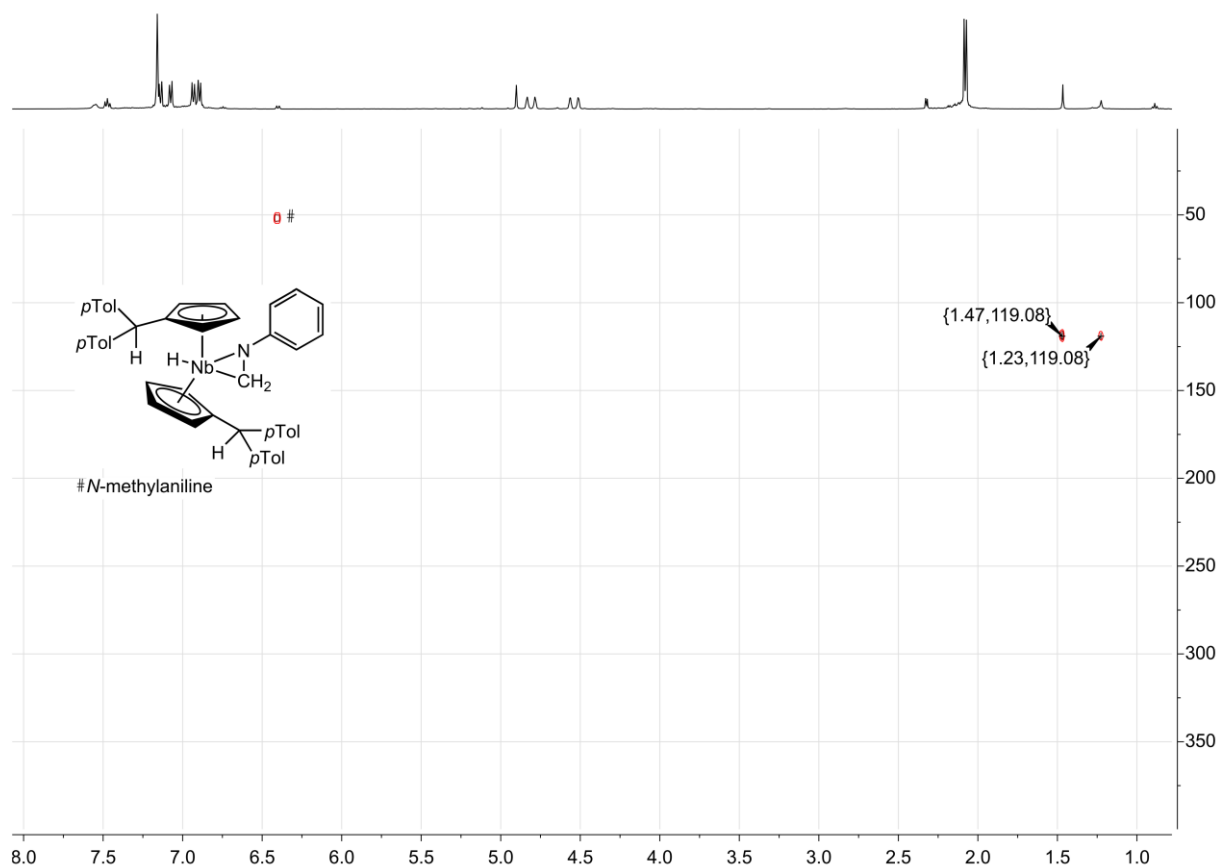


Figure S34: ^1H , ^{15}N HMBC NMR spectrum of **5** (51 MHz, 500 MHz, C_6D_6 , 305 K).

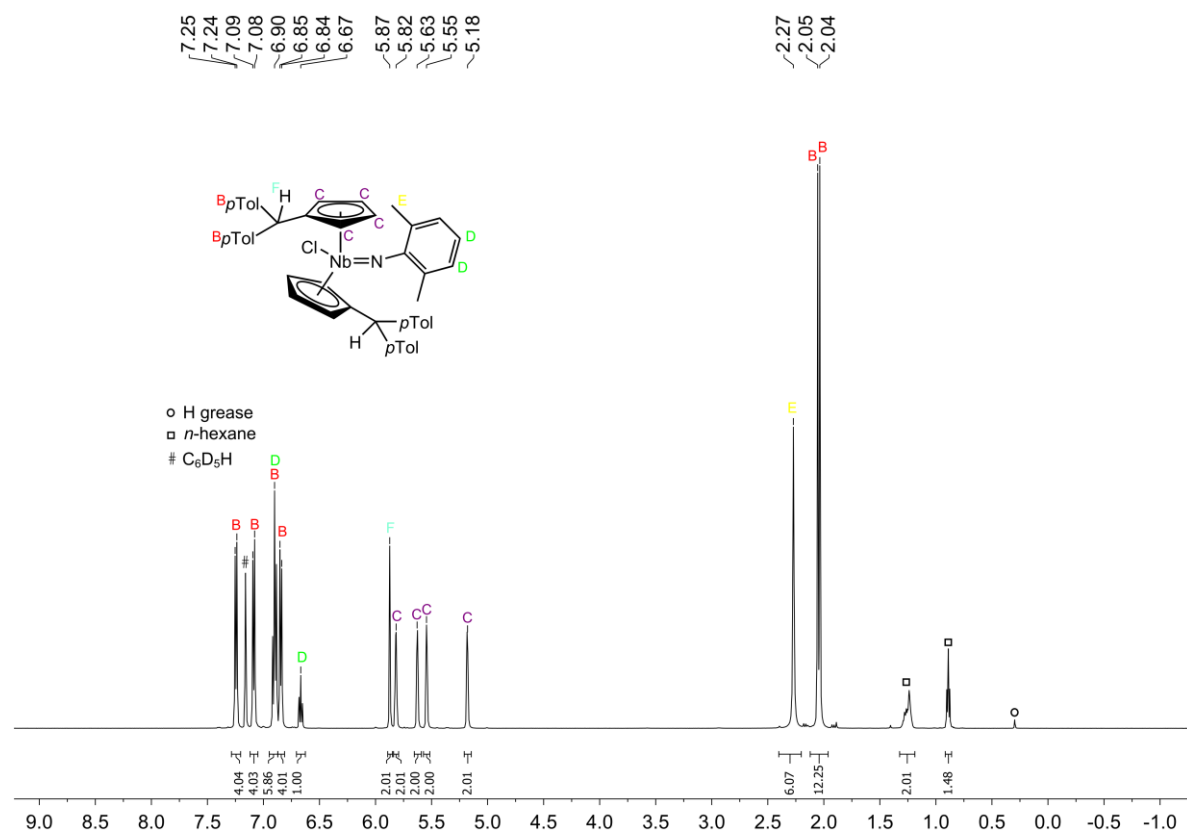


Figure S35: ^1H NMR spectrum of **6** (500 MHz, C_6D_6 , 305 K).

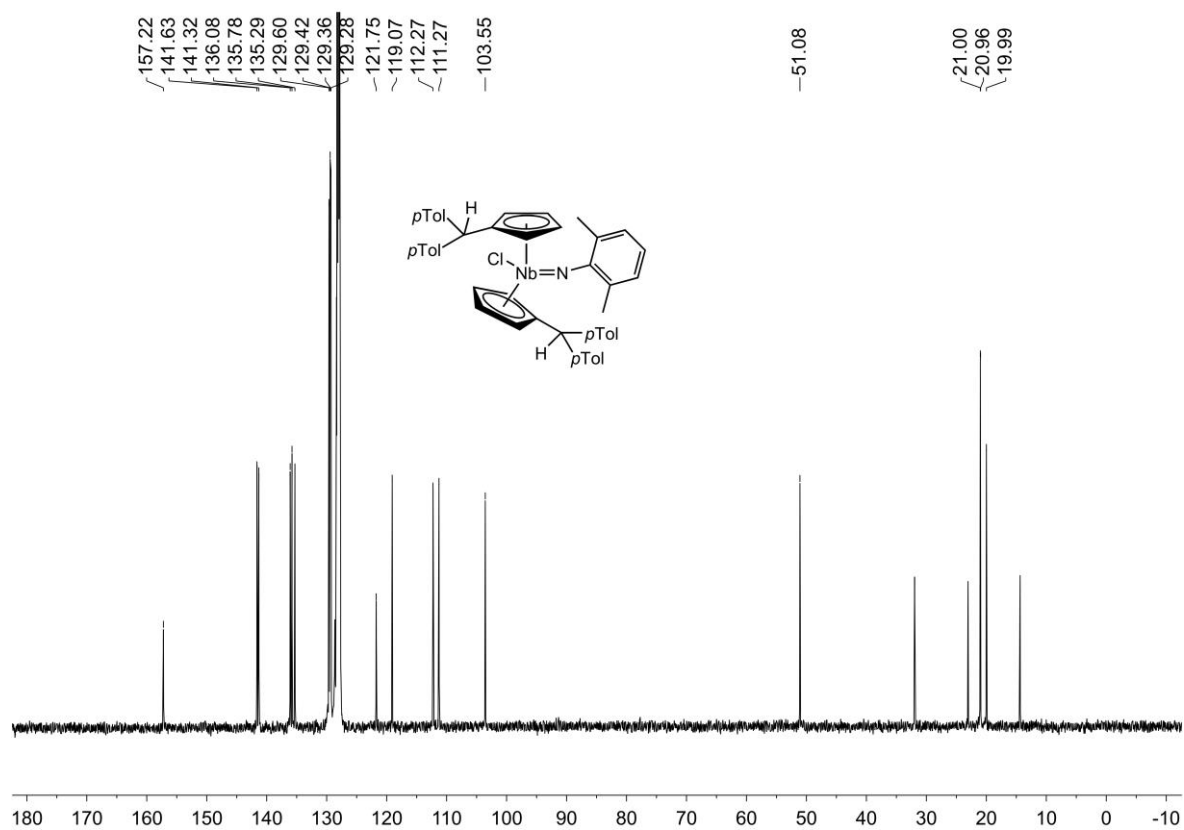


Figure S36: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** (126 MHz, C_6D_6 , 305 K).

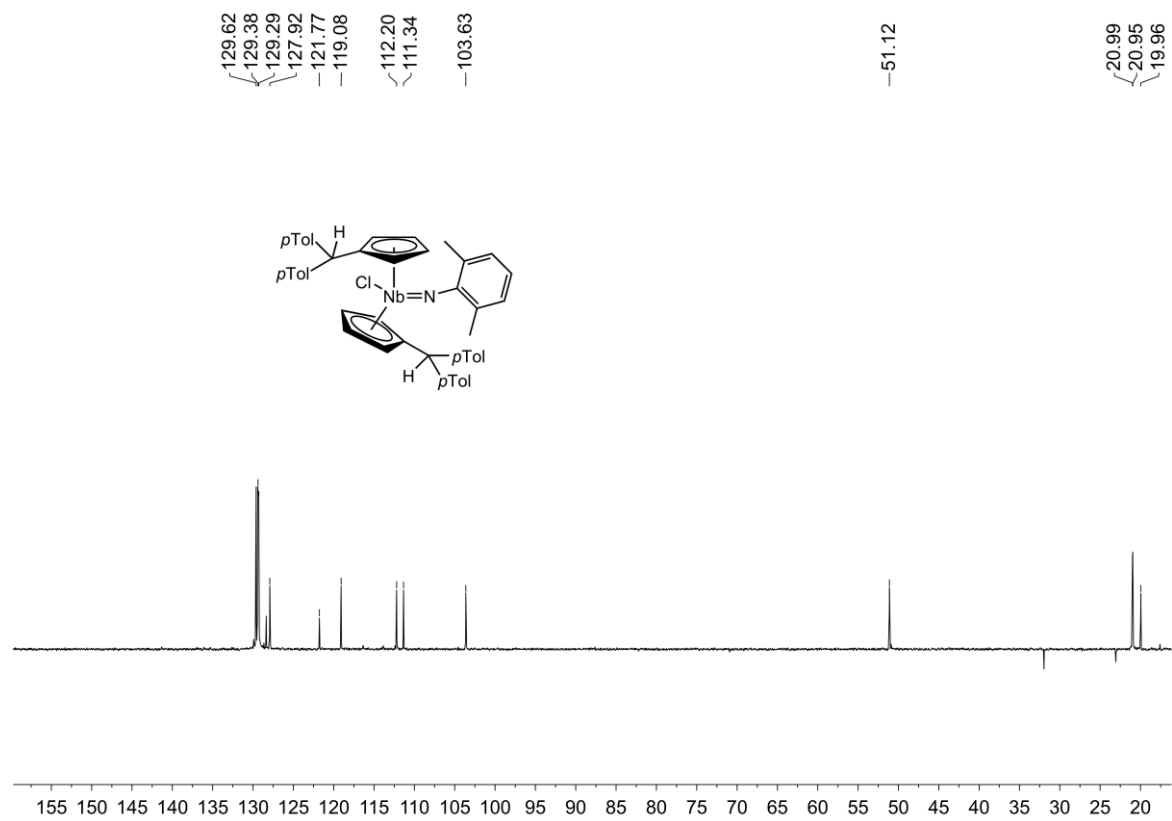


Figure S37: $^1\text{H}, ^{13}\text{C}$ dept135 NMR spectrum of **6** (126 MHz, C_6D_6 , 305 K) showing signal at 127.92 ppm.

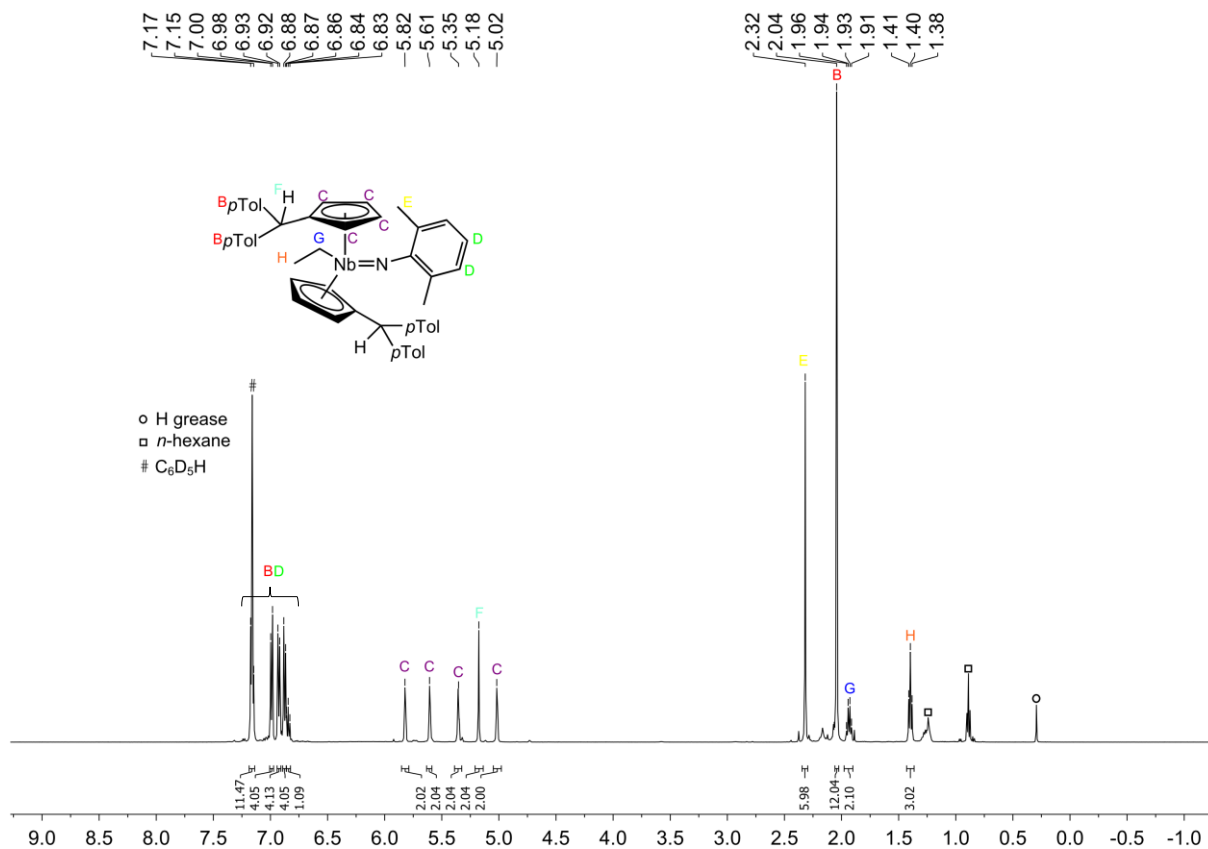


Figure 38: ¹H NMR spectrum of **7** (500 MHz, C₆D₆, 305 K).

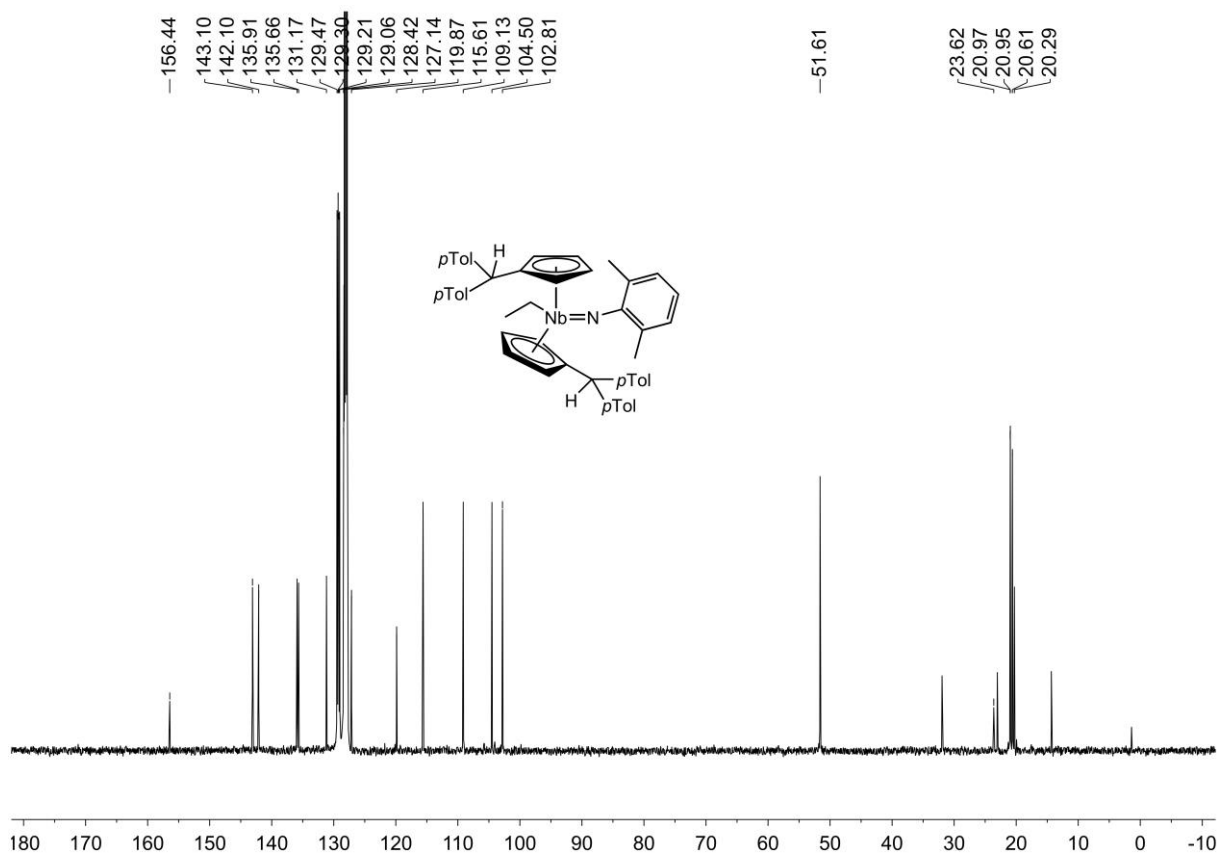


Figure 39: ¹³C{¹H} NMR spectrum of **7** (126 MHz, C₆D₆, 305 K).

Quantum Chemical Calculations

All DFT (density functional theory) calculations were performed with the B3LYP/Def2-TZVP level of theory. The optimized ground state geometry of complex **2** was calculated in gas phase and compared with experimental parameters (**Tables S3-4**).

Table S3: Cartesian coordinates for optimized molecular structure of **2**

Atom type	Coordinates (Å)		
	X	Y	Z
Nb	8.706675	11.096353	5.536689
C	10.739207	9.755628	4.906808
C	9.573815	8.95535	4.790747
C	9.005642	8.777713	6.082946
C	9.822987	9.47208	7.009853
C	10.867788	10.079906	6.285972
C	6.469843	11.465314	5.617255
C	6.654996	10.450697	4.610031
C	7.328807	11.014394	3.49492
C	7.542043	12.379208	3.753775
C	7.021973	12.668338	5.039212
C	6.559091	11.205634	7.026256
C	9.534614	12.848794	6.738539
C	10.10734	12.902043	5.424186
C	11.761142	10.087631	3.8373
H	9.195364	8.533775	3.873908
H	8.129694	8.198289	6.322692
H	9.665415	9.53619	8.073628
H	11.646794	10.695315	6.707479
H	6.388394	9.413372	4.714819
H	7.61353	10.493824	2.594442
H	8.013533	13.081435	3.086805
H	7.068601	13.621447	5.535962
C	6.380088	12.359197	7.972722
C	6.049022	9.901234	7.562784
H	8.807842	13.593185	7.034342
H	10.15301	12.526391	7.569382
H	11.155178	12.657204	5.28975
H	9.779286	13.683618	4.748945
H	12.037711	11.135739	3.977556
C	13.054438	9.285014	4.003093
C	11.205532	9.979416	2.418805
C	5.320008	13.25303	7.790841
C	7.19263	12.561765	9.094187
C	6.591749	9.304983	8.710378
C	4.951528	9.253288	6.983142
C	13.097701	8.025214	4.593615

C	14.252874	9.820642	3.52387
C	10.783496	11.12354	1.745029
C	11.100539	8.756765	1.75249
H	4.656765	13.12227	6.944178
C	5.086733	14.297878	8.679915
C	6.952777	13.596638	9.985639
H	8.046487	11.917552	9.254115
H	7.427294	9.775369	9.210213
C	6.085316	8.1225	9.22687
C	4.447563	8.063595	7.500014
H	4.462738	9.698392	6.125981
H	12.192788	7.585582	4.994178
C	14.295725	7.321516	4.692783
C	15.445048	9.120271	3.626397
H	14.250654	10.802054	3.062088
H	10.860153	12.087489	2.234713
C	10.266576	11.050696	0.455039
C	10.577726	8.684507	0.468157
H	11.447681	7.85096	2.234264
H	4.253232	14.968723	8.50164
C	5.894046	14.48881	9.798148
H	7.611144	13.722218	10.838864
H	6.540085	7.697598	10.115634
C	5.004777	7.468598	8.628708
H	3.591458	7.600964	7.020577
H	14.297156	6.343212	5.160657
C	15.489902	7.85166	4.211636
H	16.358576	9.567616	3.249508
H	9.95644	11.961368	-0.045532
C	10.148935	9.82997	-0.206938
H	10.513467	7.720057	-0.024265
C	5.64357	15.610853	10.77188
C	4.471286	6.175392	9.187183
C	16.786921	7.091708	4.312282
C	9.581455	9.741338	-1.599957
H	4.803211	16.229981	10.455471
H	6.519248	16.258549	10.866907
H	5.417756	15.227246	11.770744
H	5.18097	5.355663	9.040512
H	3.535106	5.891723	8.704604
H	4.286352	6.251481	10.2615
H	17.564463	7.692707	4.790276
H	17.159353	6.811963	3.32272
H	16.666297	6.176182	4.892454
H	8.605449	9.247426	-1.599592
H	10.233683	9.163594	-2.259054
H	9.451072	10.731028	-2.039143

Table S4: Comparison of the calculated bond length with the found bond length of the four molecules found in the crystal structure of **2**. Experimental bond length are marked by the central atom of the complex. Deviations are omitted but can be found in the provided CCDC entries. C–H bonds are omitted. Atom identifiers for the bonds (column 1) are given for the molecule containing Nb1A.

Bond in Nb1A	Nb1A	Nb2A	Nb1B	Nb2B	Calculated	Nb1A%	Nb2A%	Nb1B%	Nb2B%	Average	Average%
Nb(1A)-C(21A)	2.226	2.240	2.23	2.21	2.2685	1.9%	1.3%	1.7%	2.6%	2.227	1.9%
Nb(1A)-C(41A)	2.245	2.286	2.26	2.24	2.2806	1.6%	0.2%	0.9%	1.8%	2.258	1.0%
Nb(1A)-C(42A)	2.262	2.261	2.19	2.22	2.2880	1.1%	1.2%	4.5%	3.1%	2.233	2.5%
Nb(1A)-C(22A)	2.301	2.319	2.3	2.28	2.3420	1.8%	1.0%	1.8%	2.7%	2.300	1.8%
Nb(1A)-C(25A)	2.325	2.304	2.36	2.27	2.3573	1.4%	2.3%	0.1%	3.8%	2.315	1.8%
Nb(1A)-C(3A)	2.374	2.421	2.4	2.44	2.4008	1.1%	0.8%	0.0%	1.6%	2.409	0.3%
Nb(1A)-C(2A)	2.398	2.464	2.45	2.43	2.4274	1.2%	1.5%	0.9%	0.1%	2.436	0.3%
Nb(1A)-C(23A)	2.409	2.432	2.47	2.37	2.4646	2.3%	1.3%	0.2%	4.0%	2.420	1.8%
Nb(1A)-C(4A)	2.413	2.362	2.39	2.48	2.4606	2.0%	4.2%	3.0%	0.8%	2.411	2.0%
Nb(1A)-C(5A)	2.445	2.388	2.46	2.49	2.5030	2.4%	4.8%	1.7%	0.5%	2.446	2.3%
Nb(1A)-C(1A)	2.452	2.449	2.49	2.47	2.5151	2.6%	2.7%	1.0%	1.8%	2.465	2.0%
Nb(1A)-C(24A)	2.459	2.440	2.51	2.4	2.4861	1.1%	1.9%	1.0%	3.6%	2.452	1.4%
Nb(1A)-C(26A)	2.525	2.512	2.44	2.55	2.6159	3.6%	4.1%	7.2%	2.6%	2.507	4.4%
C(1A)-C(2A)	1.392	1.429	1.45	1.39	1.4185	1.9%	0.7%	2.2%	2.1%	1.415	0.2%
C(1A)-C(5A)	1.440	1.428	1.43	1.45	1.4226	1.2%	0.4%	0.5%	1.9%	1.437	1.0%
C(1A)-C(6A)	1.533	1.513	1.51	1.54	1.5161	1.1%	0.2%	0.4%	1.6%	1.524	0.5%
C(2A)-C(3A)	1.423	1.391	1.38	1.43	1.4227	0.0%	2.3%	3.1%	0.5%	1.406	1.2%
C(3A)-C(4A)	1.397	1.408	1.42	1.4	1.4175	1.5%	0.7%	0.2%	1.3%	1.406	0.8%
C(4A)-C(5A)	1.381	1.411	1.4	1.37	1.4089	2.0%	0.1%	0.6%	2.8%	1.391	1.3%
C(6A)-C(14A)	1.511	1.526	1.54	1.52	1.5273	1.1%	0.1%	0.8%	0.5%	1.524	0.2%
C(6A)-C(7A)	1.534	1.525	1.53	1.52	1.5311	0.2%	0.4%	0.1%	0.7%	1.527	0.3%
C(7A)-C(8A)	1.394	1.407	1.41	1.4	1.3920	0.1%	1.1%	1.3%	0.6%	1.403	0.8%
C(7A)-C(12A)	1.405	1.362	1.38	1.4	1.3974	0.5%	2.6%	1.3%	0.2%	1.387	0.8%
C(8A)-C(9A)	1.391	1.381	1.38	1.38	1.3929	0.1%	0.9%	0.9%	0.9%	1.383	0.7%
C(9A)-C(10A)	1.398	1.396	1.39	1.38	1.3923	0.4%	0.3%	0.2%	0.9%	1.391	0.1%
C(10A)-C(11A)	1.372	1.372	1.38	1.38	1.3978	1.9%	1.9%	1.3%	1.3%	1.376	1.6%
C(10A)-C(13A)	1.510	1.620	1.62	1.51	1.5066	0.2%	7.0%	7.0%	0.2%	1.565	3.7%
C(11A)-C(12A)	1.398	1.414	1.41	1.38	1.3865	0.8%	1.9%	1.7%	0.5%	1.401	1.0%
C(14A)-C(15A)	1.381	1.400	1.39	1.38	1.3932	0.9%	0.5%	0.2%	1.0%	1.388	0.4%
C(14A)-C(19A)	1.396	1.404	1.41	1.41	1.3964	0.0%	0.5%	1.0%	1.0%	1.405	0.6%
C(15A)-C(16A)	1.402	1.391	1.4	1.41	1.3916	0.7%	0.0%	0.6%	1.3%	1.401	0.7%
C(16A)-C(17A)	1.397	1.386	1.39	1.41	1.3936	0.2%	0.5%	0.3%	1.2%	1.396	0.2%
C(17A)-C(18A)	1.397	1.405	1.41	1.39	1.3970	0.0%	0.6%	0.9%	0.5%	1.401	0.2%
C(17A)-C(20A)	1.460	1.507	1.51	1.47	1.5068	3.2%	0.0%	0.2%	2.5%	1.487	1.3%
C(18A)-C(19A)	1.393	1.400	1.41	1.41	1.3885	0.3%	0.8%	1.5%	1.5%	1.403	1.1%
C(21A)-C(25A)	1.417	1.414	1.4	1.4	1.4444	1.9%	2.1%	3.2%	3.2%	1.408	2.6%
C(21A)-C(22A)	1.425	1.449	1.45	1.41	1.4416	1.2%	0.5%	0.6%	2.2%	1.434	0.6%
C(21A)-C(26A)	1.455	1.457	1.46	1.46	1.4355	1.3%	1.5%	1.7%	1.7%	1.458	1.5%
C(22A)-C(23A)	1.401	1.413	1.43	1.41	1.4196	1.3%	0.5%	0.7%	0.7%	1.414	0.4%
C(23A)-C(24A)	1.427	1.402	1.41	1.42	1.4054	1.5%	0.2%	0.3%	1.0%	1.415	0.7%
C(24A)-C(25A)	1.433	1.422	1.42	1.44	1.4165	1.2%	0.4%	0.2%	1.6%	1.429	0.9%
C(26A)-C(34A)	1.479	1.503	1.49	1.48	1.4998	1.4%	0.2%	0.7%	1.3%	1.488	0.8%
C(26A)-C(27A)	1.500	1.493	1.48	1.5	1.5028	0.2%	0.7%	1.5%	0.2%	1.493	0.6%
C(27A)-C(32A)	1.386	1.403	1.39	1.38	1.3996	1.0%	0.2%	0.7%	1.4%	1.390	0.7%
C(27A)-C(28A)	1.402	1.391	1.39	1.4	1.3985	0.2%	0.5%	0.6%	0.1%	1.396	0.2%
C(28A)-C(29A)	1.373	1.393	1.39	1.36	1.3916	1.4%	0.1%	0.1%	2.3%	1.379	0.9%
C(29A)-C(30A)	1.403	1.370	1.36	1.39	1.3924	0.8%	1.6%	2.4%	0.2%	1.381	0.8%
C(30A)-C(31A)	1.376	1.390	1.39	1.38	1.3972	1.5%	0.5%	0.5%	1.2%	1.384	1.0%
C(30A)-C(33A)	1.515	1.523	1.51	1.51	1.5066	0.6%	1.1%	0.2%	0.2%	1.515	0.5%
C(31A)-C(32A)	1.376	1.390	1.39	1.37	1.3868	0.8%	0.2%	0.2%	1.2%	1.382	0.4%
C(34A)-C(35A)	1.380	1.411	1.4	1.36	1.4025	1.6%	0.6%	0.2%	3.1%	1.388	1.1%
C(34A)-C(39A)	1.415	1.401	1.41	1.43	1.4001	1.1%	0.1%	0.7%	2.1%	1.414	1.0%
C(35A)-C(36A)	1.431	1.384	1.38	1.43	1.3862	3.1%	0.2%	0.4%	3.1%	1.406	1.4%
C(36A)-C(37A)	1.383	1.412	1.41	1.4	1.3975	1.0%	1.0%	0.9%	0.2%	1.401	0.3%
C(37A)-C(38A)	1.360	1.379	1.38	1.35	1.3923	2.4%	1.0%	0.9%	3.1%	1.367	1.8%
C(37A)-C(40A)	1.540	1.504	1.5	1.54	1.5063	2.2%	0.2%	0.4%	2.2%	1.521	1.0%
C(38A)-C(39A)	1.400	1.377	1.38	1.4	1.3916	0.6%	1.1%	0.8%	0.6%	1.389	0.2%
C(41A)-C(42A)	1.429	1.438	1.42	1.43	1.4347	0.4%	0.2%	1.0%	0.3%	1.429	0.4%

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