

Reactivity of Pt(0) Bromosilylene Complexes Towards Ethylene

Pauline Hädinger^a and Alexander Hinz^{*,a}

^a Institute of Inorganic Chemistry (AOC), Karlsruhe Institute of Technology (KIT), Engesserstr.13,
76131 Karlsruhe

Electronic Supplementary Information

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1 Experimental

1.1 General Considerations

All manipulations were carried out using standard Schlenk and glove box techniques under an argon atmosphere. Toluene, *n*-pentane and *n*-hexane were dried over potassium and distilled prior to use. *n*-heptane was dried by using an MBraun solvent purification system (SPS-800). C₆D₆ was stored over 3 Å molecular sieves and distilled prior to use. The starting materials RSiBr^[1] and Pt(PCy₃)₂^[2] were prepared according to literature protocols. All other reagents were used as received.

NMR spectra were acquired on a Bruker Avance II 300 MHz or Bruker Avance 400 MHz spectrometer. Reported chemical shifts are referenced to the ¹H and ¹³C NMR resonances of the deuterated solvent.^[3] Coupling constants *J* are given in Hertz as positive values regardless of their real individual sign. ¹H, ¹³C, ²⁹Si, ³¹P and ¹⁹⁵Pt NMR spectra were obtained at 400.1, 100.6, 79.5, 162.0 and 85.6 MHz, respectively.

IR spectra were recorded on a Bruker Alpha spectrometer using the attenuated total reflection (ATR) technique on powdered samples.

UV-vis spectra were measured in solution using a Mettler-Toledo Spektralphotometer UV7 and quartz cuvettes (d = 1 cm). To subtract the solvent, the sample was measured relative to the pure solvent.

Elemental analyses were obtained with a Vario Micro Cube (Elementar Analysensysteme GmbH) in the institutional technical laboratories of the Karlsruhe Institute of Technology (KIT).

Single crystals were mounted in perfluoropolyalkyl ether oil on a cryo loop and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were collected using a Stoe IPDS II diffractometer and graphite-monochromated Mo-K_α (0.71073 Å) radiation or a Stoe STADIVARI diffractometer and Ga-K_α (1.34134 Å) radiation. The structures were solved by direct methods with SHELXS^[4] or intrinsic phasing with SHELXT^[5] followed by full-matrix least-squares refinement using SHELXL-2018/3^[6] and the ShelXle GUI.^[7] All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model. For molecule R(Br)Si(C₂H₄)₂Pt(PCy₃)₂ (**3**) the program SQUEEZE was used to remove electron contribution of disordered solvent molecules.^[8]

1.2 Syntheses

R(Br)Si(C₂H₄)Pt(PPh₃)₂ (1**)**

In a Schlenk tube, RSiBr (255 mg, 0.341 mmol) and (η^2 -C₂H₄)Pt(PPh₃)₂ (260 mg, 0.341 mmol) were combined as solids. 7 mL of toluene were added and the resulting dark orange solution was stirred at ambient temperature for 12 hours. Then, the solvent was removed under reduced pressure and the residue was washed with 1 mL of *n*-hexane. The product was isolated as a pale brown powder (427 mg, 83 %). Orange crystals were obtained after 1 week *via* concentrating a toluene solution of **1** to approximately 0.5 mL and subsequent vapour diffusion with approximately 4 mL of *n*-pentane in a H-shaped Schlenk tube.

¹H NMR (400.1 MHz, C₆D₆): δ (ppm) = 1.25 (m, 1H, Si-CH₂), 1.30 (s, 12 H, ^{*t*}BuH), 1.33 (m, 1H, Si-CH₂), 1.37 (s, 12 H, ^{*t*}BuH), 1.47 (s br, 12 H, ^{*t*}BuH), 1.62 (s, 18 H, ^{*t*}BuH), 1.68 (m, 1H, Pt-CH₂), 2.08 (m, 1H, Pt-CH₂), 5.91-7.19 (m br, 30H, Ph-H), 7.36 (d, $J_{\text{HH}} = 2.0$ Hz, 1 H, CH), 7.50 (d, $J_{\text{HH}} = 2.1$ Hz, 1 H, CH), 7.56 (t, $J_{\text{HH}} = 1.8$ Hz, 1 H, CH), 7.80 (t, $J_{\text{HH}} = 1.8$ Hz, 1 H, CH), 7.92 (s br, 1H, CH), 8.26 (d, $J_{\text{HH}} = 2.0$ Hz, 1 H, CH), 8.34 (d, $J_{\text{HH}} = 2.1$ Hz, 1 H, CH), 8.45 (s br, 1H, CH), 8.55 (s br, 1H, CH). **¹³C{¹H} NMR** (100.6 MHz, C₆D₆): δ (ppm) = 3.50 (dd, Si-CH₂), 32.0 (s, ^{*t*}Bu-CH), 32.1 (s, ^{*t*}Bu-CH), 32.5 (s, ^{*t*}Bu-CH), 33.3 (d, Pt-CH₂), 34.5 (s, ^{*t*}Bu-C), 34.6 (s, ^{*t*}Bu-C), 35.7 (s, ^{*t*}Bu-C), 114.7 (s, CH), 114.8 (s, CH), 120.3 (s, CH), 121.7 (s, CH), 122.6 (s br, CH), 124.7 (s br, CH), 128.6 (s, Ph-C), 128.9 (s, CH), 129.5 (s br), 130.3 (s), 131.3 (s), 132.7 (s), 134.1 (s), 134.9 (s br), 143.1 (s), 143.9 (s), 144.1 (s), 144.5 (s), 146.0 (s), 146.2 (s), 149.4 (s), 150.2 (s), 150.5 (s). **²⁹Si{¹H} NMR** (79.5 MHz, C₆D₆): δ (ppm) = -35.9 (d, $^2J_{\text{SiPt}} = 263.4$ Hz, $^1J_{\text{SiPt}} = 1510$ Hz). **³¹P{¹H} NMR** (162.0 MHz, C₆D₆): δ (ppm) = 26.4 (dd, $^2J_{\text{P1P2}} = 9.8$ Hz, $^2J_{\text{P1Si}} = 269.6$ Hz, $^1J_{\text{P1Pt}} = 1504.9$ Hz, $^1J_{\text{P2Pt}} = 2076.0$ Hz). **¹⁹⁵Pt NMR** (85.6 MHz, C₆D₆): δ (ppm) = -4617.7 (dd, $^1J_{\text{PtP1}} = 1504.9$ Hz, $^1J_{\text{PtP2}} = 2076.0$ Hz).

IR (ATR): $\tilde{\nu}(\text{cm}^{-1}) = 3054$ (vw), 2953 (w), 2904 (vw), 2864 (vw), 1587 (vw), 1478 (w), 1434 (m), 1390 (vw), 1376 (vw), 1362 (w), 1288 (vw), 1245 (vw), 1198 (w), 1181 (vw), 1153 (vw), 1092 (w), 1074 (vw), 1029 (vw), 999 (vw), 927 (vw), 891 (vw), 876 (w), 864 (w), 843 (w), 795 (vw), 743 (m), 717 (w), 694 (vs), 662 (vw), 638 (vw), 558 (vw), 530 (m), 519 (s), 508 (vs), 454 (m), 408 (w).

EA [C₈₆H₉₈BrNP₂PtSi] found (calc.): C 68.60 (68.37) H 6.66 (6.54) N 0.83 (0.93).

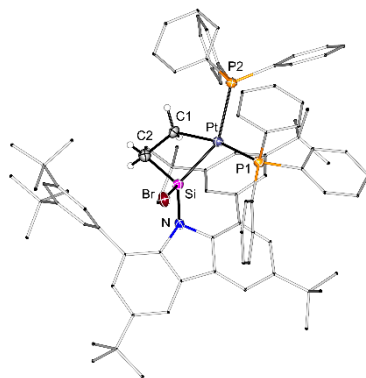


Figure S1: Molecular structure of **1**.

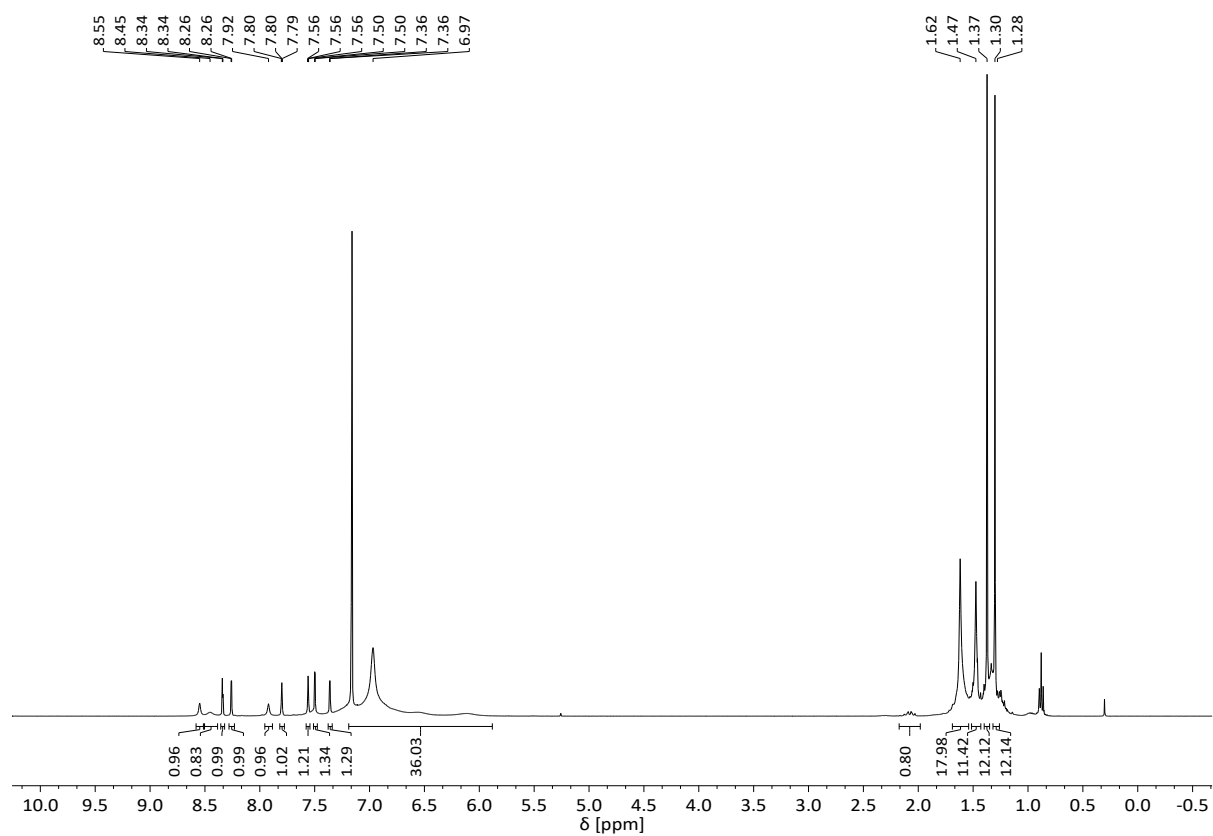


Figure S2: ¹H NMR spectrum of 1.

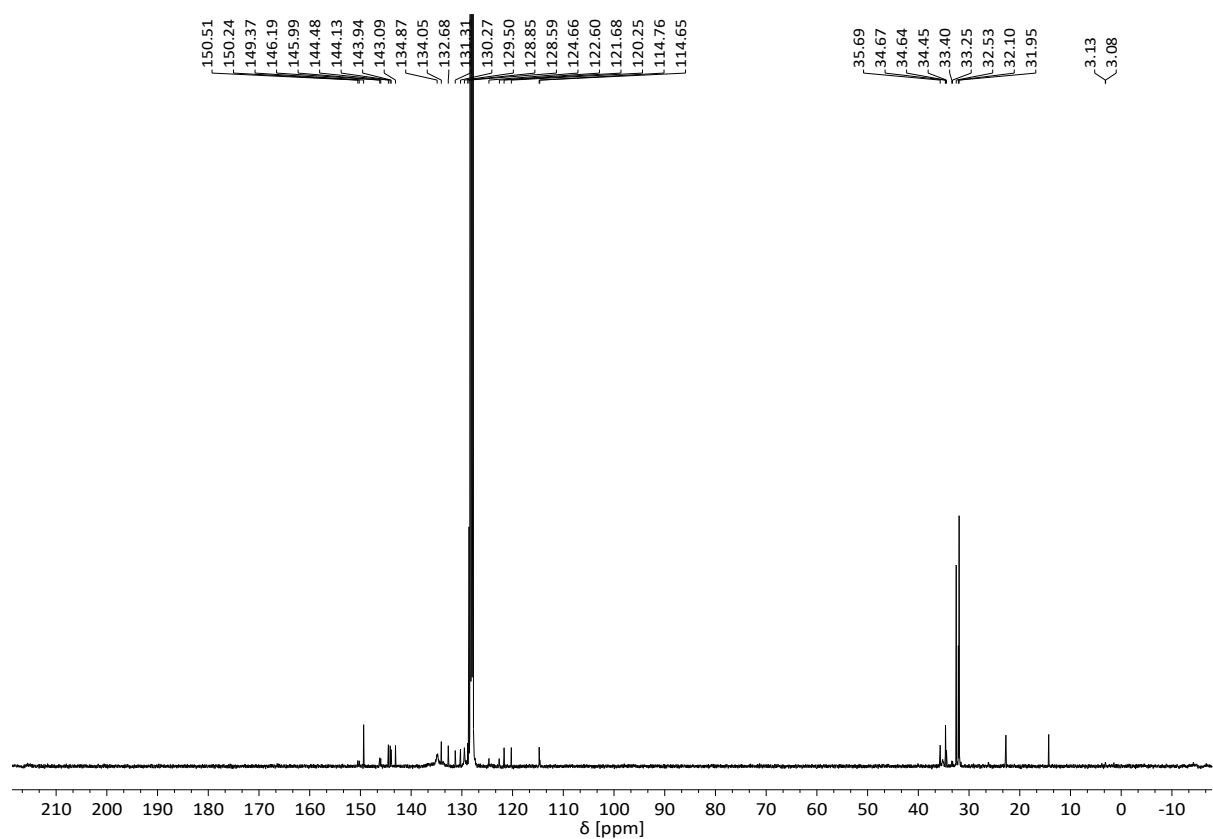


Figure S3: ¹³C{¹H} NMR spectrum of 1.

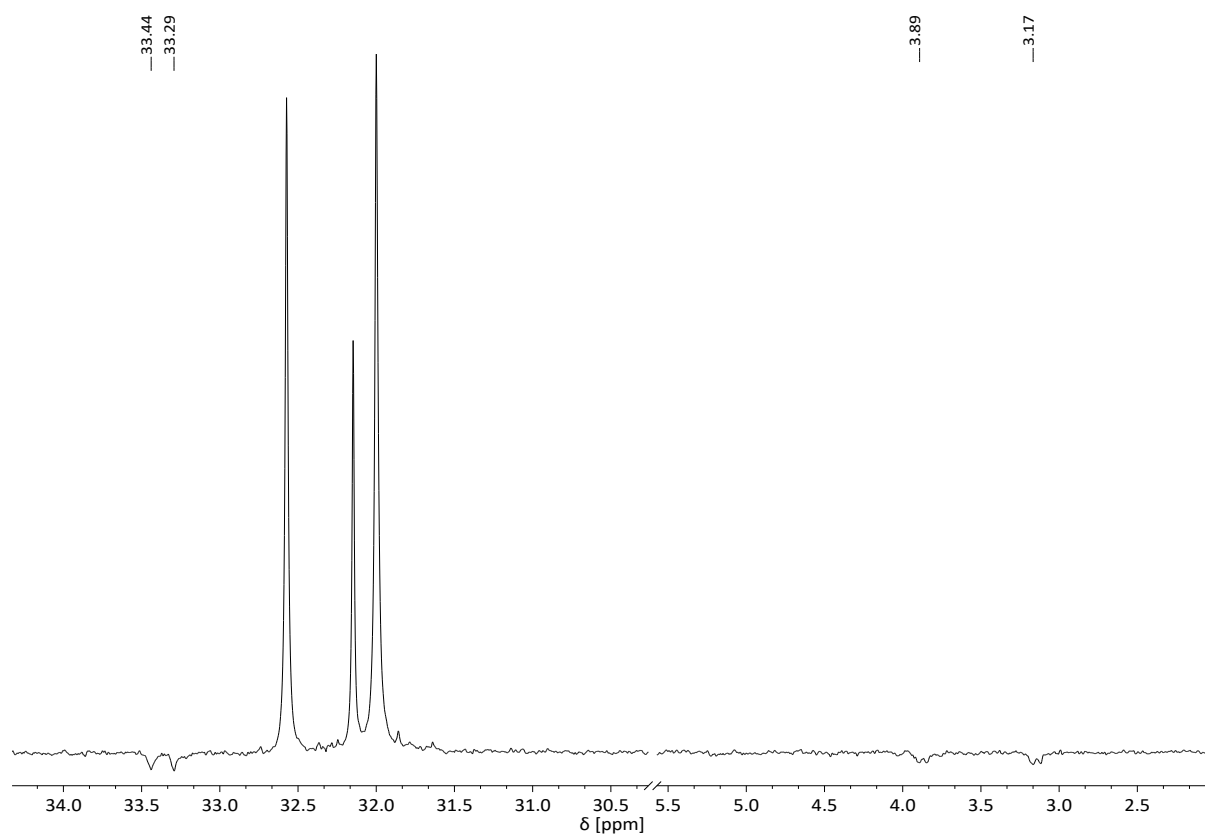


Figure S4: Extract of the DEPT-135 NMR spectrum of **1**.

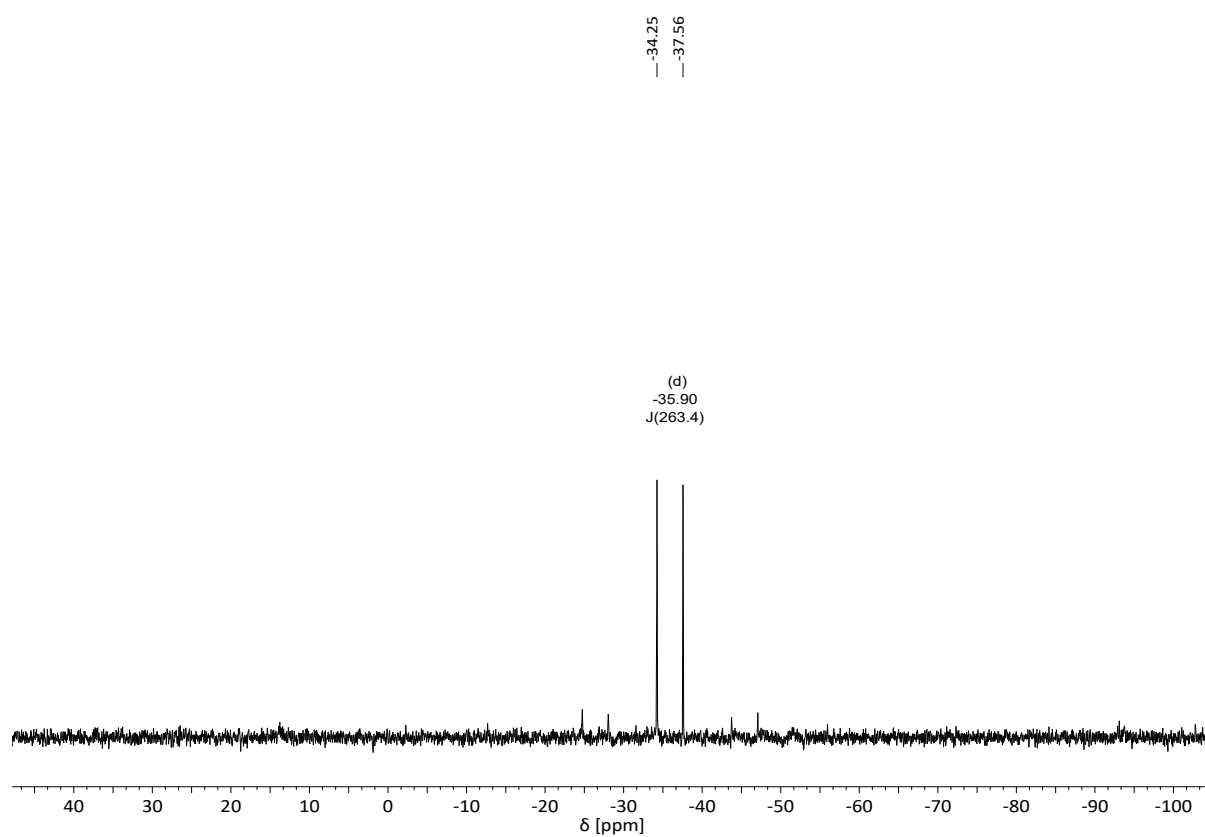


Figure S5: $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **1**.

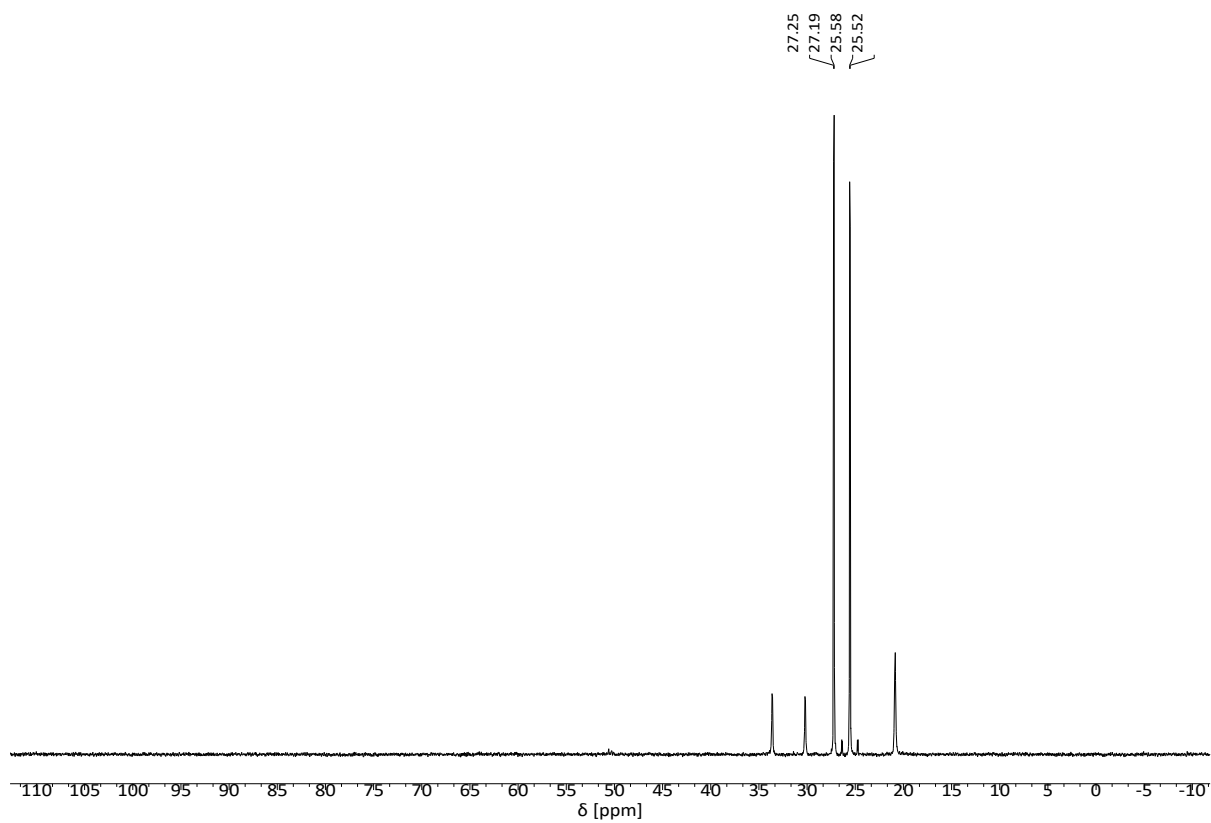


Figure S6: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1**.

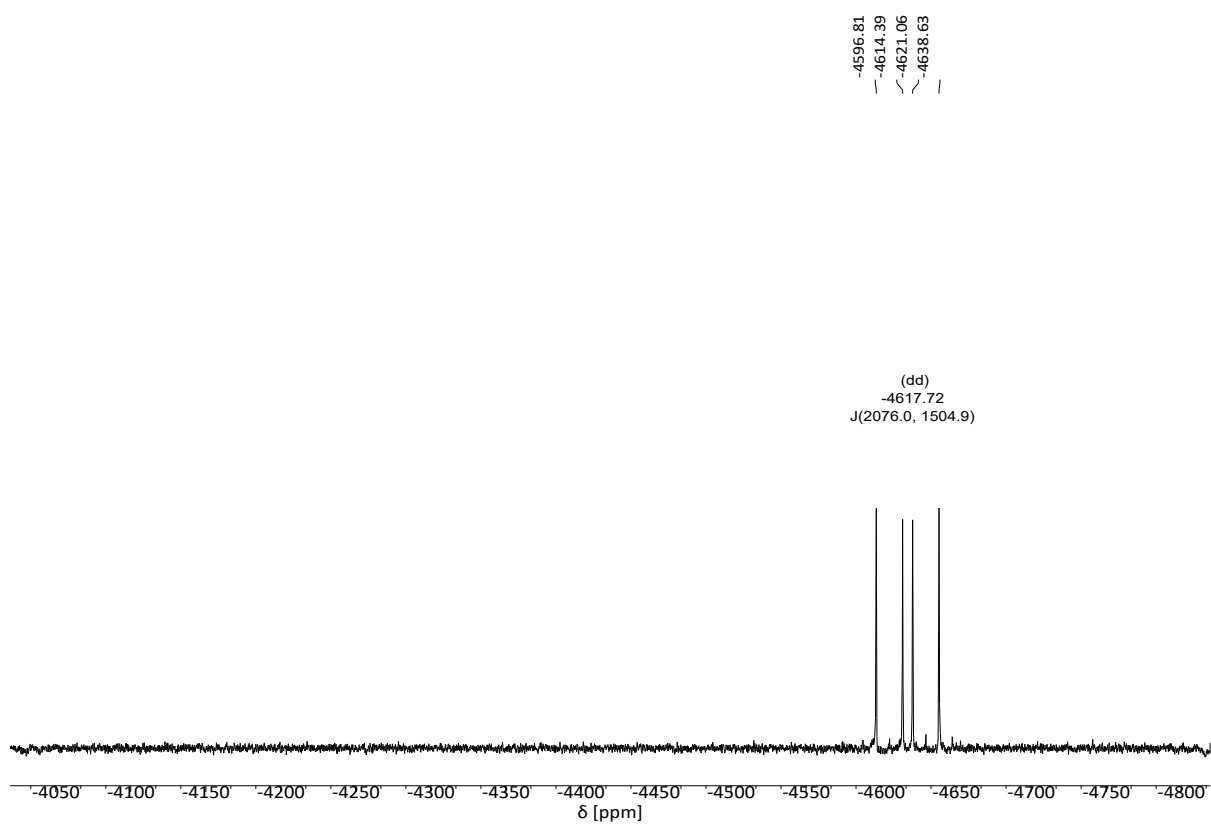


Figure S7: ^{195}Pt NMR spectrum of **1**.

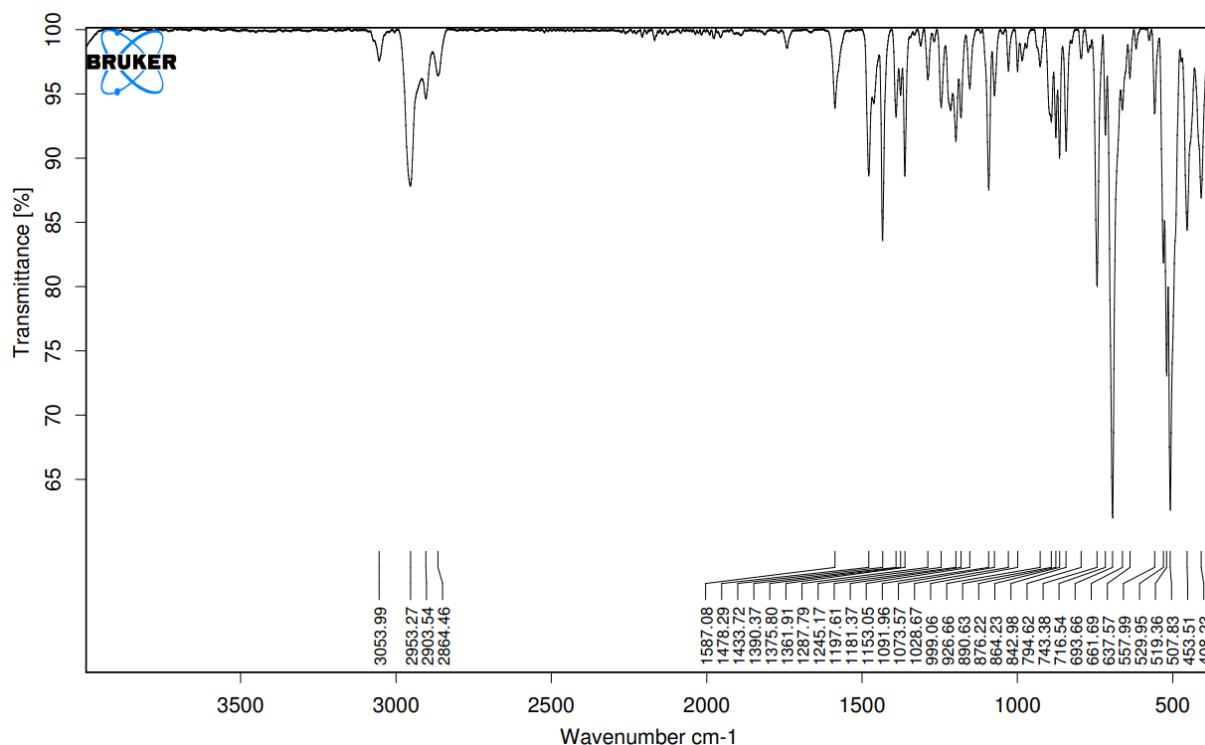


Figure S8: IR spectrum of **1**.

R(Br)SiPt(PCy₃)₂ (2**)**

In a Schlenk tube, RSiBr (115 mg, 0.151 mmol) and Pt(PCy₃)₂ (100 mg, 0.132 mmol) were combined as solids. 2.5 mL of toluene were added and the resulting orange solution was sonicated for 15 minutes. Then, the solvent was removed under reduced pressure and the residue was treated with 1 mL of *n*-hexane. Immediate concentration to approximately 0.5 mL and storage at −40 °C yielded orange crystals after 24 hours (63.5 mg, 0.042 mmol, 32 %).

¹H NMR (400.1 MHz, C₆D₆): δ(ppm) = 1.25-1.43 (m br, Cy-H), 1.45 (s, 18 H, Carb-^{*t*}BuH), 1.53 (s, 36 H, Ar-^{*t*}BuH), 1.60-1.94 (s (m br, Cy-H), 7.64 (t, *J*_{HH} = 1.8 Hz, 2 H, *p*-CH), 7.76 (d, *J*_{HH} = 2.0 Hz, 2 H, C^{2,7}H), 8.14 (d, *J*_{HH} = 2.0 Hz, 2 H, C^{4,5}H), 8.22 (d, *J*_{HH} = 1.8 Hz, 4 H, *o*-CH). **¹³C{¹H} NMR** (100.6 MHz, C₆D₆): δ(ppm) = 27.1 (m br, Cy-C), 28.3 (m br, Cy-C), 30.5 (m br, Cy-C), 32.0 (s, Carb-C(CH₃)), 32.2 (s, Ar-C(CH₃)), 34.8 (s, Carb-C(CH₃)), 35.4 (s, Ar-C(CH₃)), 39.3 (m br, Cy-C), 115.3 (s, C^{4,5}H), 121.9 (s, *p*-CH), 123.9 (s, *o*-CH), 133.4 (s), 133.5 (s), 142.5 (s br), 142.6 (s), 144.7 (s, C^{3,6}), 150.4 (s, *m*-C). **²⁹Si{¹H} NMR** (79.5 MHz, C₆D₆): δ(ppm) = 235.5 (t, ²*J*_{SIP} = 146.5 Hz, ¹*J*_{SIPt} = 3569.3 Hz). **³¹P{¹H} NMR** (162.0 MHz, C₆D₆): δ(ppm) = 59.8 (s, ²*J*_{SIP} = 146.5 Hz, ¹*J*_{Pt} = 3833.2 Hz). **¹⁹⁵Pt NMR** (85.6 MHz, C₆D₆): δ(ppm) = −4644.9 (t, ¹*J*_{Pt} = 3833.2 Hz).

IR (ATR): $\tilde{\nu}$ (cm^{−1}) = 2923 (vs), 2849 (s), 1592 (w), 1478 (w), 1446 (s), 1392 (w), 1362 (m), 1289 (w), 1266 (vw), 1246 (w), 1201 (w), 1174 (w), 1003 (w), 913 (vw), 886 (m), 867 (vs), 849 (s), 835 (m), 735 (w), 718 (m), 704 (w), 648 (vw), 558 (w), 536 (w), 511 (s), 472 (w), 443 (w), 425 (m), 409 (w), 396 (w), 385 (m).

UV-vis (*n*-hexane, 1·10^{−5} mol·L^{−1}): λ_{max} (nm) = 393.

EA [C₈₄H₁₃₀BrNP₂PtSi] found (calc.): C 66.50 (66.42) H 8.45 (8.63) N 0.65 (0.92).

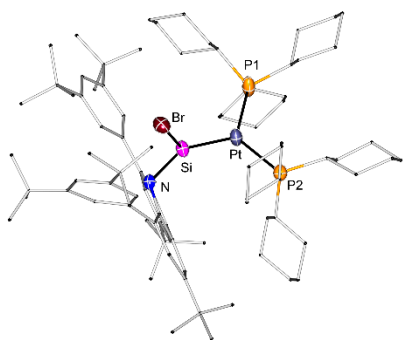


Figure S9: Molecular structure of **2**.

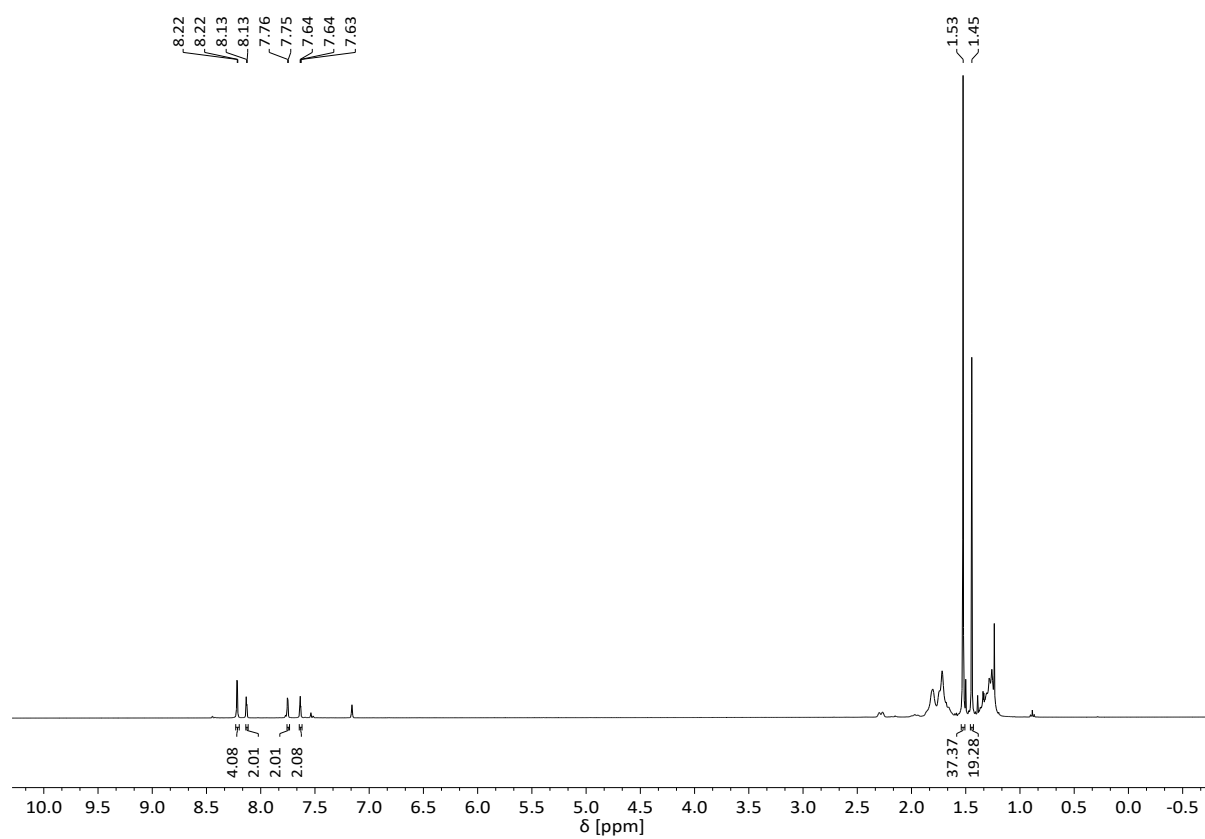


Figure S10: ^1H NMR spectrum of **2**.

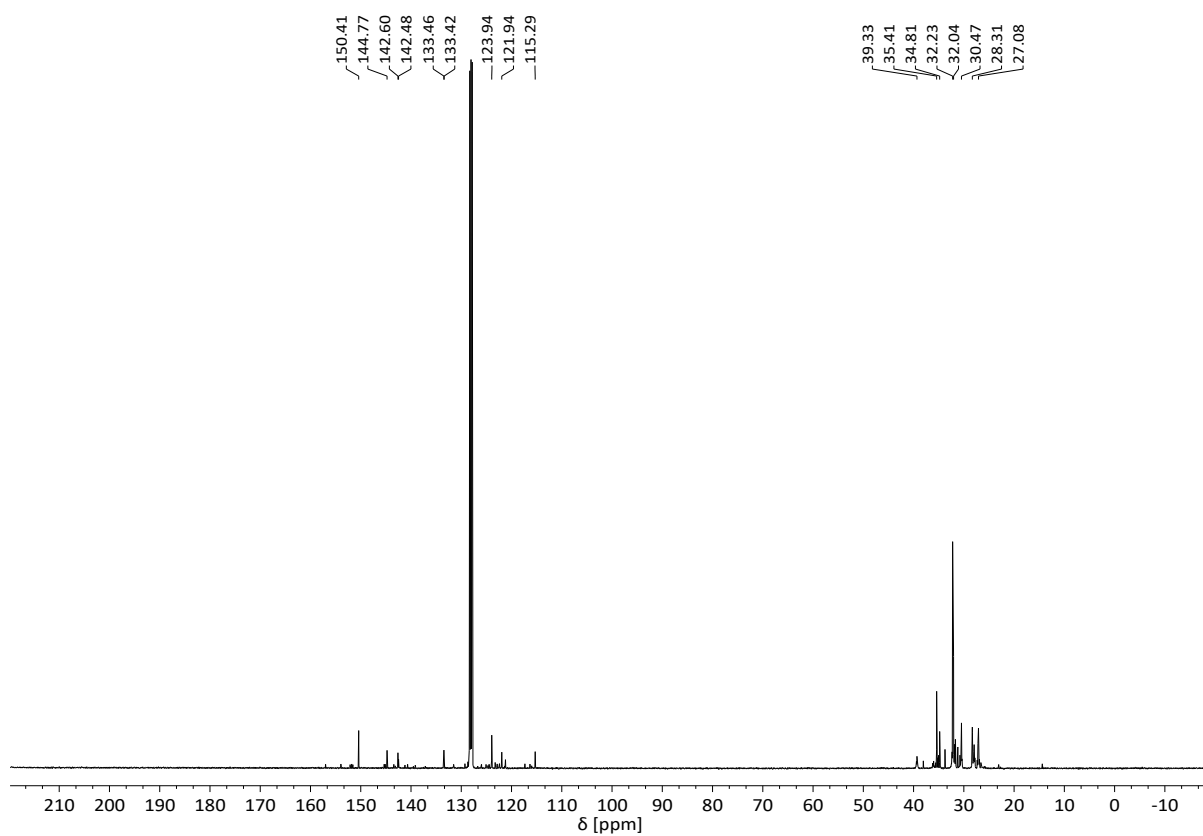


Figure S11: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2**.

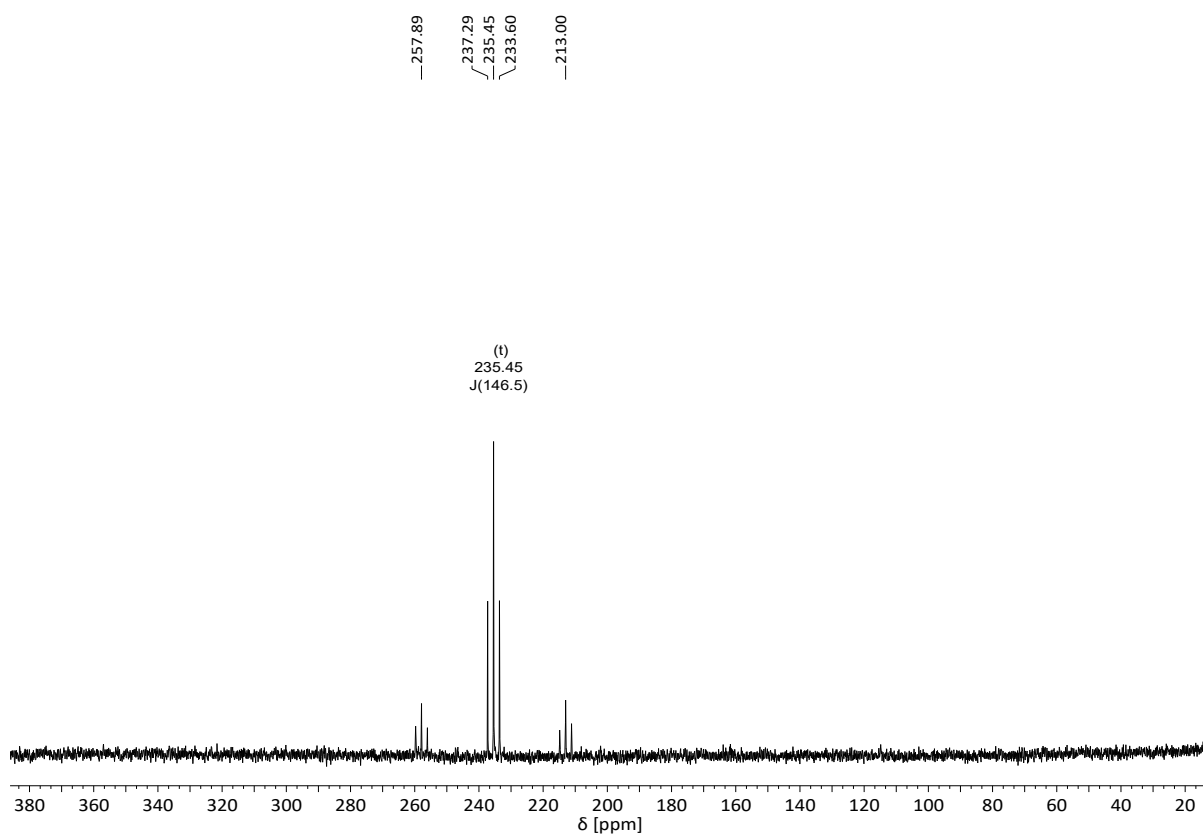


Figure S12: $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **2**.

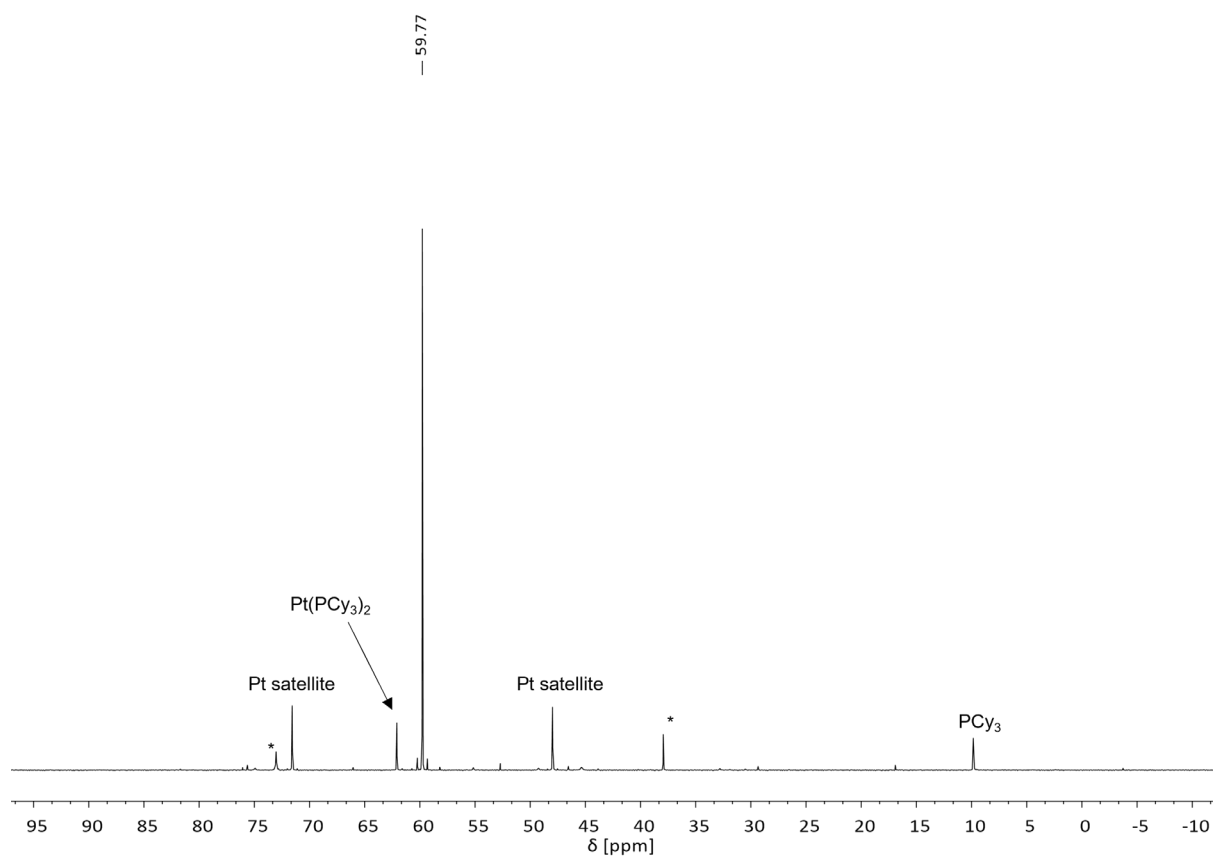


Figure S13: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2**. Resonances marked with * correspond to unknown impurities.

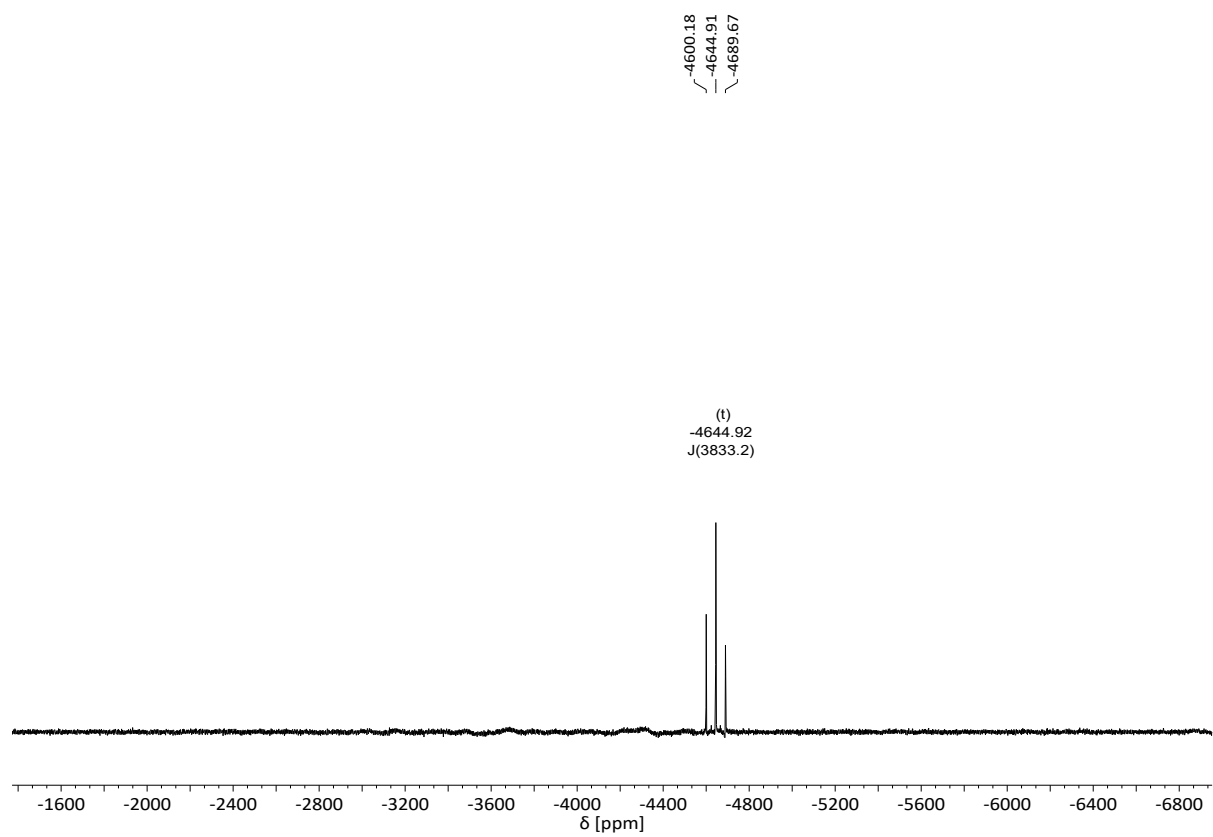


Figure S14: ^{195}Pt NMR spectrum of **2**.

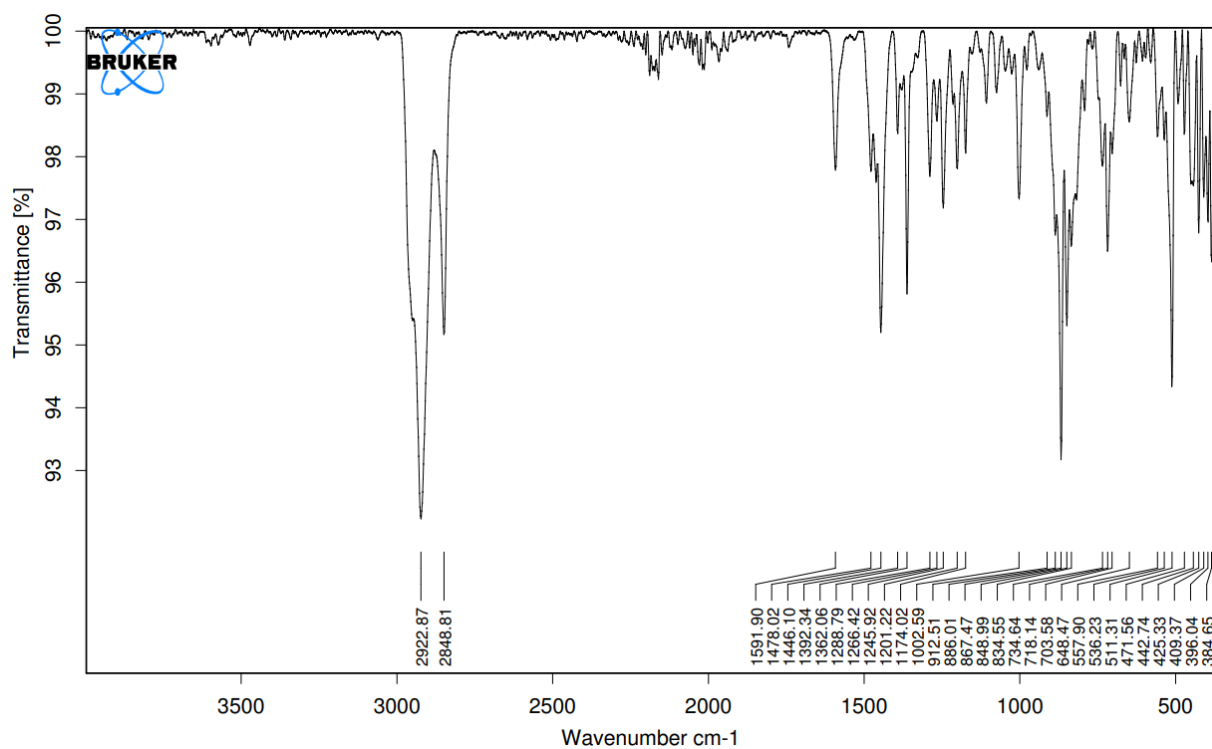


Figure S15: IR spectrum of **2**.

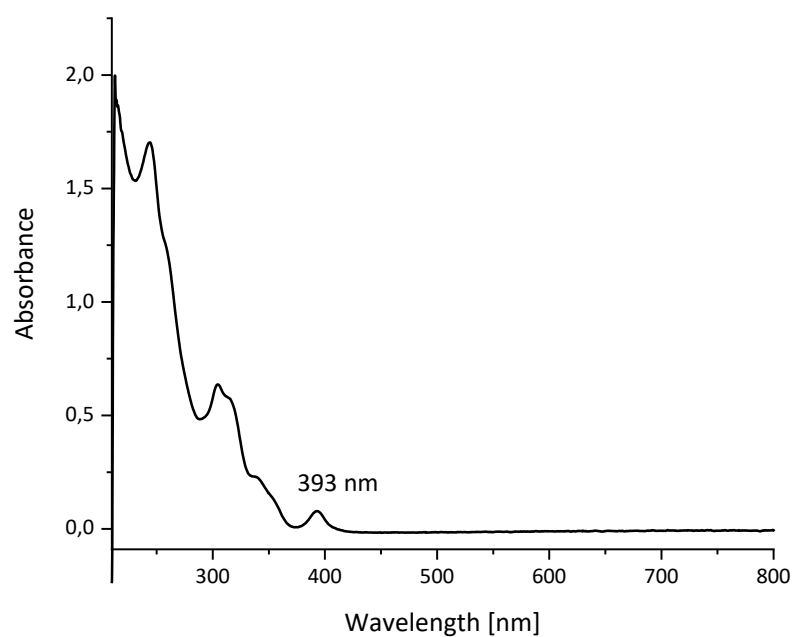
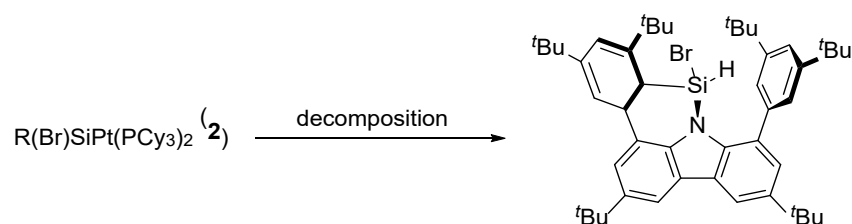


Figure S16: UV-vis spectrum of **2** in *n*-hexane ($1 \cdot 10^{-5}$ mol·L⁻¹).

R(Br)SiPt(PCy₃)₂ decomposition product (2-I)



R(Br)SiPt(PCy₃)₂ fully decomposes in solution at ambient temperature over a period of 72 hours, yielding free Pt(PCy₃)₂ and C-H insertion product **2-I**, which was confirmed by NMR spectroscopy. The decomposition product **2-I** could not be isolated from Pt(PCy₃)₂ completely. Independent structural proof could be obtained and allowed identification.

¹H NMR (400.1 MHz, C₆D₆): δ(ppm) = 1.20 (s, 9 H, ^tBuH), 1.33 (s, 9 H, ^tBuH), 1.41 (s, 9 H, ^tBuH), 1.43 (s, 9 H, ^tBuH), 1.45 (s, 9 H, ^tBuH), 1.46 (s, 9 H, ^tBuH), 5.40 (s, *J*_{SiH} = 300.6 Hz, 1 H, SiH), 7.47 (t, *J*_{HH} = 1.7 Hz, 1 H, CH), 7.65 (d, *J*_{HH} = 1.7 Hz, 1 H, CH), 7.71 (t, *J*_{HH} = 1.9 Hz, 1 H, CH), 7.72 (d, *J*_{HH} = 2.0 Hz, 1 H, CH), 7.85 (t, *J*_{HH} = 1.7 Hz, 1 H, CH), 8.28 (d, *J*_{HH} = 1.6 Hz, 1 H, CH), 8.36 (d, *J*_{HH} = 1.6 Hz, 1 H, CH), 8.39 (d, *J*_{HH} = 1.9 Hz, 2 H, CH). **¹³C{¹H} NMR** (100.6 MHz, C₆D₆): δ(ppm) = 31.2 (s, C(CH₃)), 31.7 (s, C(CH₃)), 31.9 (s, C(CH₃)), 32.1 (m br, Cy-C), 32.2 (s, C(CH₃)), 33.7 (s, C(CH₃)), 35.0 (s, C(CH₃)), 35.0 (s, C(CH₃)), 35.2 (s, C(CH₃)), 35.3 (s, C(CH₃)), 38.1 (s, C(CH₃)), 116.3 (s, CH), 117.3 (s, CH), 121.2 (s, CH), 122.4 (s, CH), 122.8 (s, CH), 123.9 (s, CH), 124.5 (s, CH), 125.1 (s, CH), 126.0 (s, CH), 128.7 (s), 129.3 (s), 131.5 (s), 139.2 (s), 140.7 (s), 141.2 (s), 143.4 (s), 145.1 (s), 145.3 (s), 151.6 (s), 152.1 (s), 154.0 (s), 157.0 (s). **²⁹Si{¹H} NMR** (79.5 MHz, C₆D₆): δ(ppm) = -30.8 (s).

IR (ATR): $\tilde{\nu}(\text{cm}^{-1})$ = 2951 (vs), 2925 (vs), 2851 (m), 1592 (w), 1478 (m), 1462 (w), 1446 (m), 1392 (w), 1362 (s), 1287 (w), 1245 (m), 1200 (w), 1001 (w), 887 (w), 867 (vs), 849 (m), 717 (m), 704 (w), 549 (w), 512 (vs), 488 (s), 458 (vs), 415 (vs), 407 (vs), 391 (s), 385 (s).

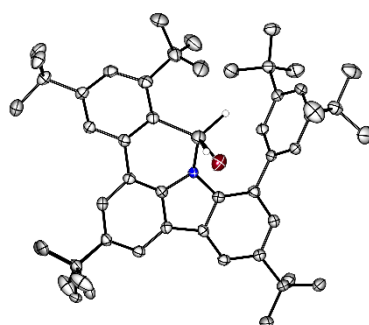


Figure S17: Molecular structure of **2-I**, including the H/Br disorder in the crystalline material.

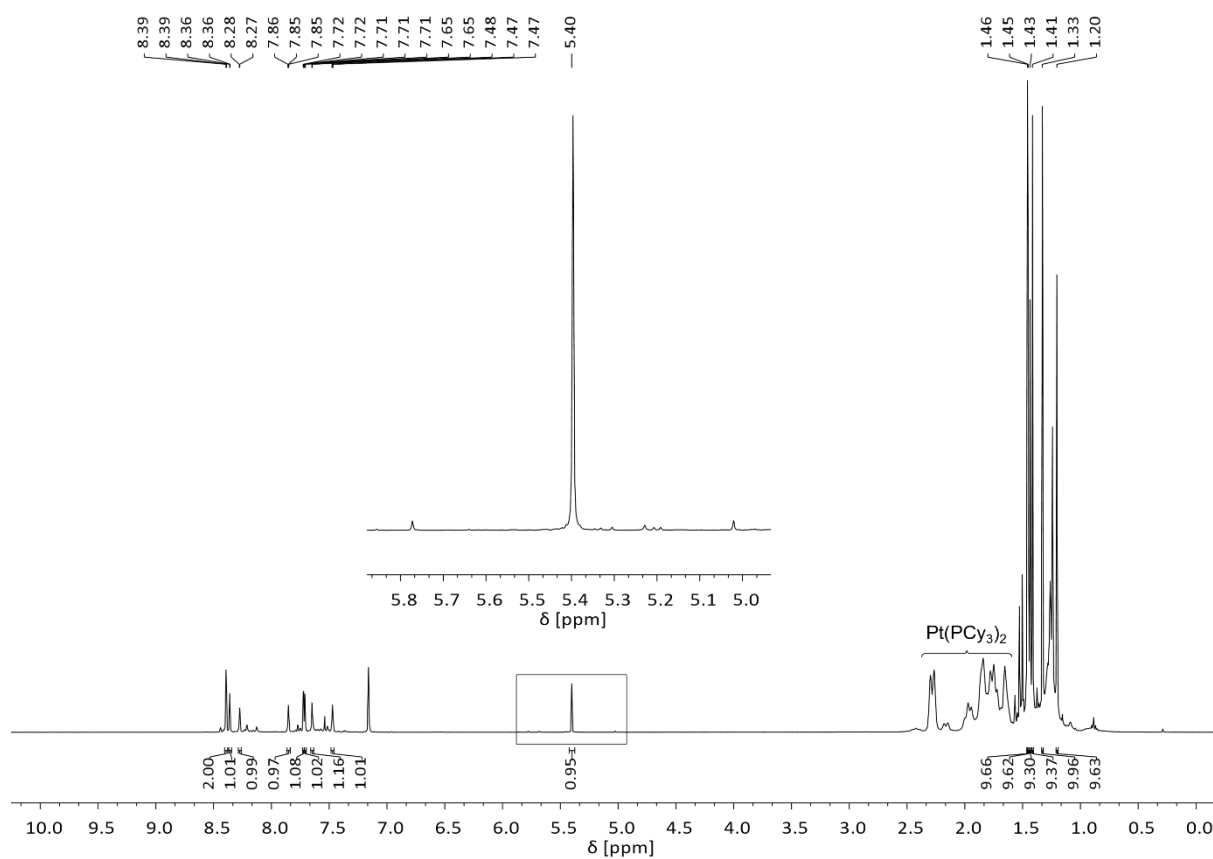


Figure S18: ¹H NMR spectrum of **2-I**.

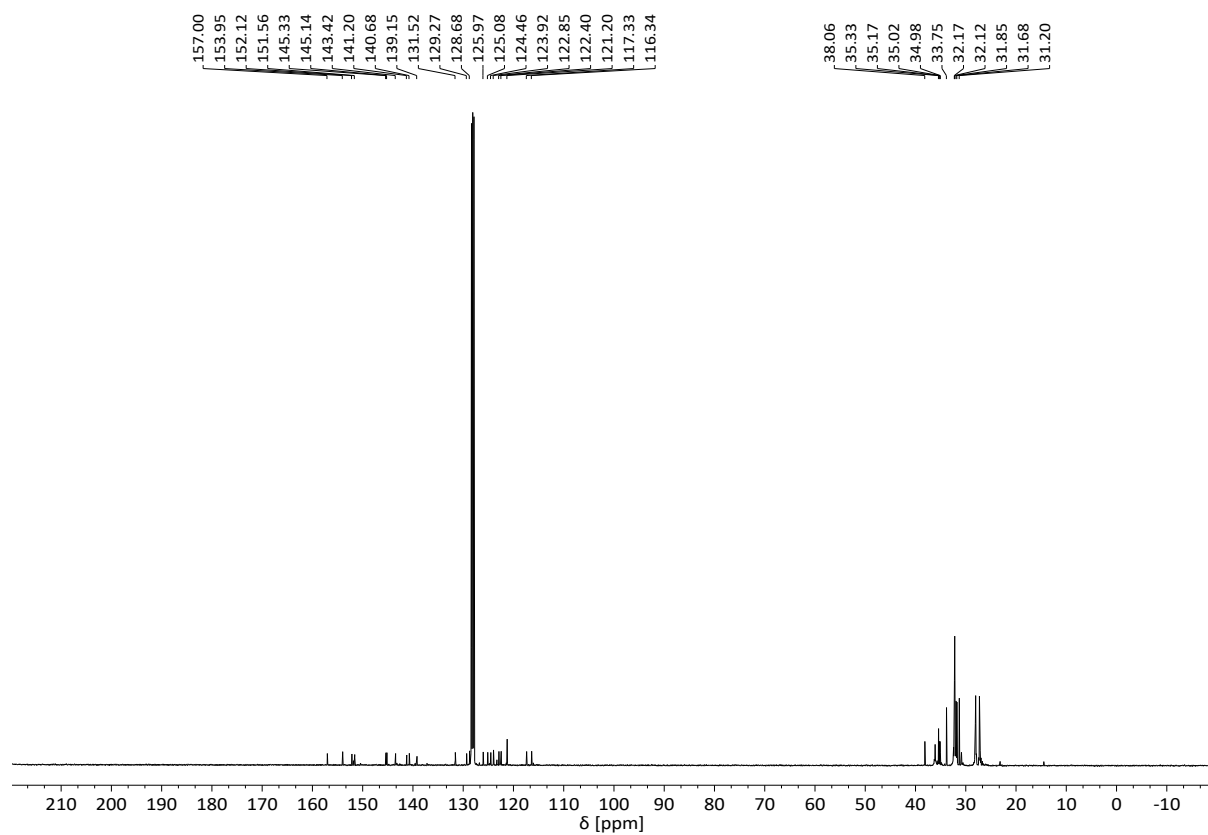


Figure S19: ¹³C{¹H} NMR spectrum of **2-I**.

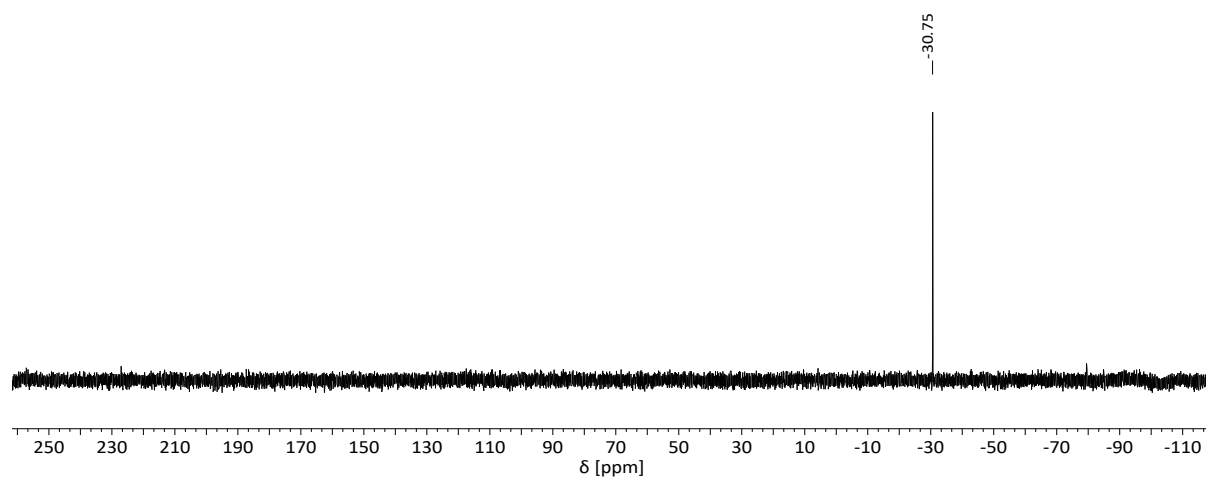


Figure S20: $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of 2-I.

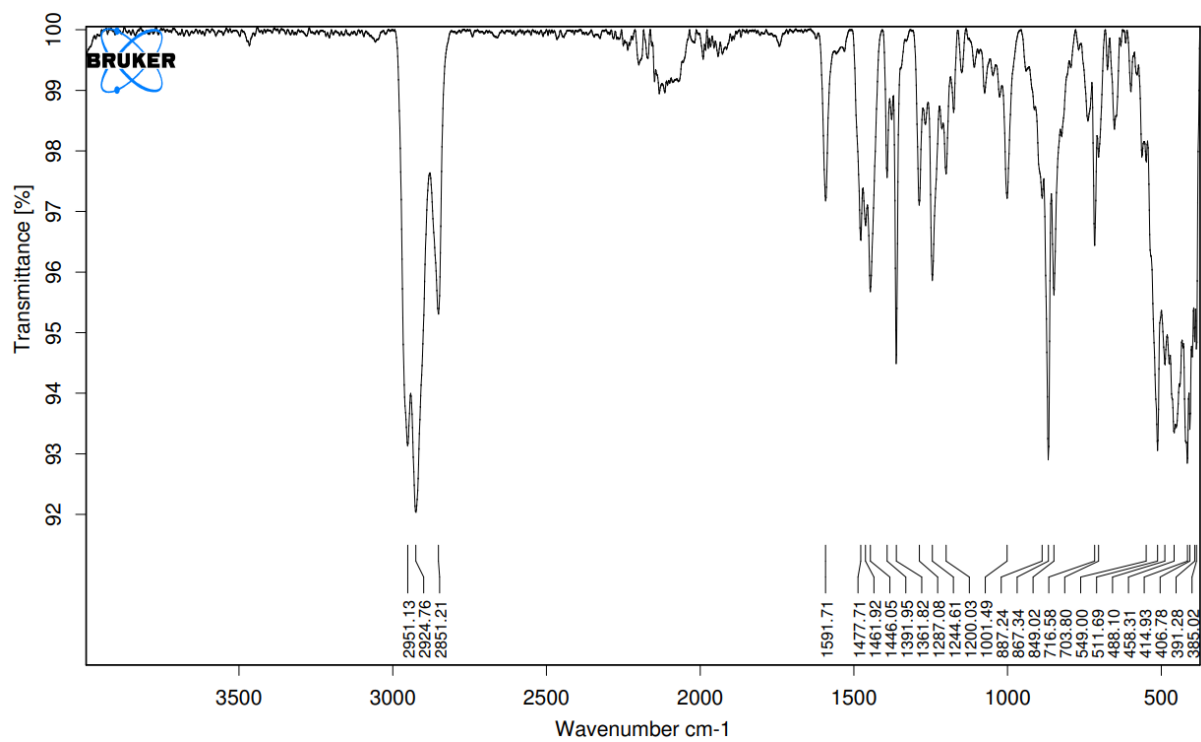


Figure S21: IR spectrum of 2-I.

R(Br)Si(C₂H₄)₂Pt(PCy₃)₂ (3)

In a Young tube, RSiBr (222 mg, 0.291 mmol) and Pt(PCy₃)₂ (220 mg, 0.291 mmol) were mixed and 6 mL of toluene were added. The solution was sonicated for 15 minutes and then exposed to one atmosphere of C₂H₄. Upon stirring at ambient temperature for 12 hours the solution turned yellow. The solvent was removed under reduced pressure and the residue was treated with 4 mL of *n*-heptane. Then, the solution was concentrated to approximately 1 mL and after storage at ambient temperature for 24 hours colourless crystals were obtained (75 mg, 0.047 mmol, 16 %).

¹H NMR (400.1 MHz, C₆D₆): δ(ppm) = 1.13 (m br, 4H, Si-CH₂), 1.28 (m br, 4H, Pt-CH₂), 1.16-1.33 (m br, Cy-H), 1.45 (s, 18 H, Carb-^{*t*}BuH), 1.53 (s, 36 H, Ar-^{*t*}BuH), 1.58-2.32 (m br, Cy-H), 7.59 (d, *J*_{HH} = 2.1 Hz, 2 H, C^{2,7}H), 7.65 (t, *J*_{HH} = 1.8 Hz, 2 H, *p*-CH), 7.89 (d, *J*_{HH} = 1.8 Hz, 4 H, *o*-CH), 8.23 (d, *J*_{HH} = 2.1 Hz, 2 H, C^{4,5}H). **¹³C{¹H} NMR** (100.6 MHz, C₆D₆): δ(ppm) = 7.0 (m, Si-CH₂), 22.0 (s br, Pt-CH₂), 27.1 (m br, Cy-C), 28.3 (m br, Cy-C), 30.9 (m br, Cy-C), 32.0 (s, Ar-C(CH₃)), 32.1 (s, Carb-C(CH₃)), 34.7 (s, Carb-C(CH₃)), 35.2 (s, Ar-C(CH₃)), 35.7 (m br, Cy-C), 114.8 (s, C^{4,5}H), 121.9 (s, *p*-CH), 125.5 (s, *o*-CH), 128.7 (s, C^{2,7}H), 130.5 (s), 132.8 (s), 142.7 (s), 144.4 (s), 145.2 (s), 150.3 (s). **²⁹Si{¹H} NMR** (79.5 MHz, C₆D₆): δ(ppm) = 15.5 (s). **³¹P{¹H} NMR** (162.0 MHz, C₆D₆): δ(ppm) = 21.0 (s, ¹*J*_{Pt} = 1641.8 Hz). **¹⁹⁵Pt NMR** (85.6 MHz, C₆D₆): δ(ppm) = -4655.5 (t, ¹*J*_{Pt} = 1667.1 Hz).

IR (ATR): $\tilde{\nu}(\text{cm}^{-1})$ = 2923 (vs), 2850 (s), 1593 (w), 1478 (w), 1446 (m), 1391 (w), 1377 (w), 1362 (m), 1290 (w), 1267 (vw), 1247 (w), 1214 (w), 1199 (m), 1174 (w), 1075 (vw), 1003 (w), 892 (w), 868 (s), 846 (s), 796 (w), 729 (w), 716 (m), 704 (w), 676 (vw), 645 (w), 525 (m), 511 (m), 490 (m), 464 (w), 453 (w), 413 (w), 390 (m).

EA [C₈₈H₁₃₈BrNP₂PtSi] found (calc.): C 67.01 (67.10) H 8.77 (8.83) N 0.80 (0.89).

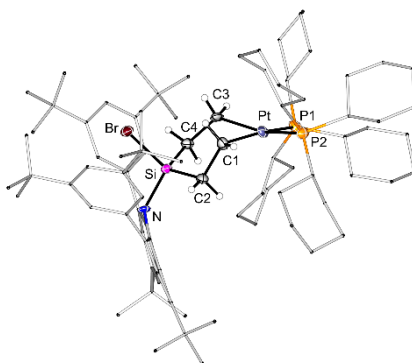


Figure S22: Molecular structure of **3**.

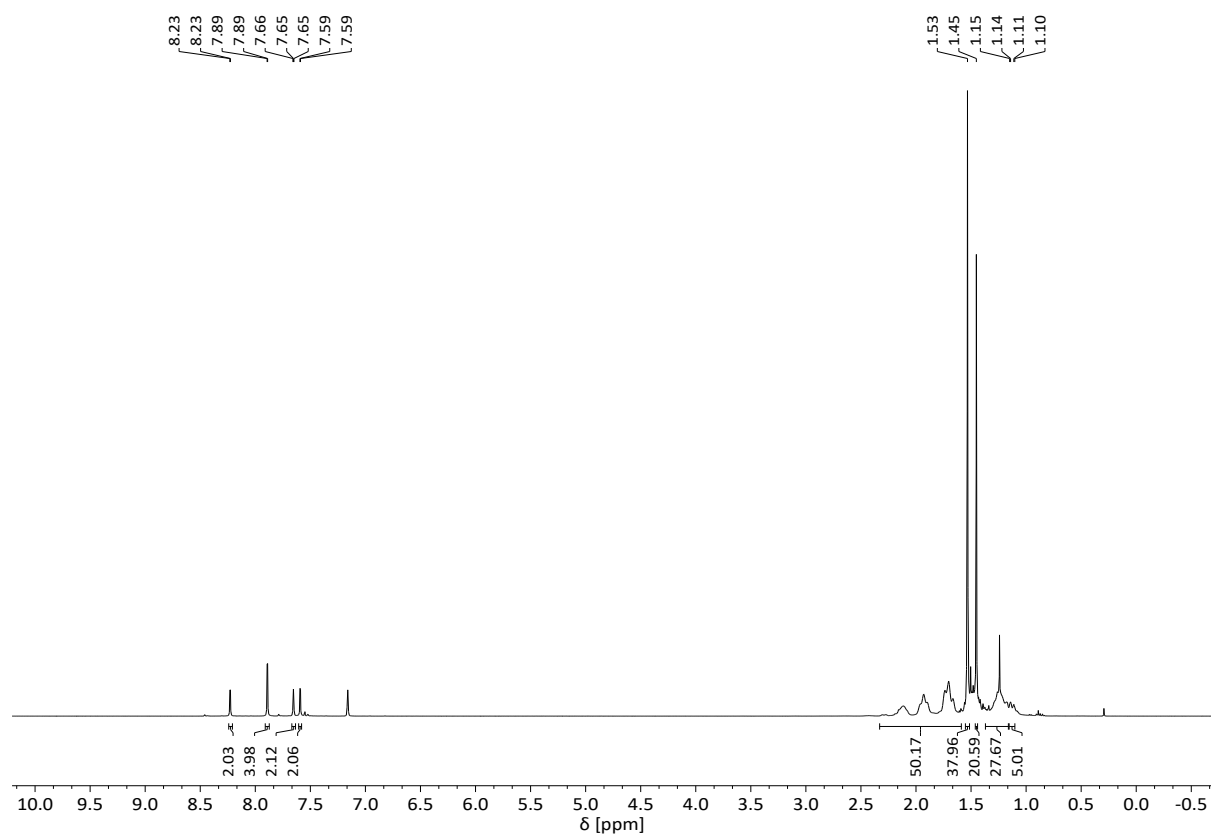


Figure S23: ¹H NMR spectrum of **3**.

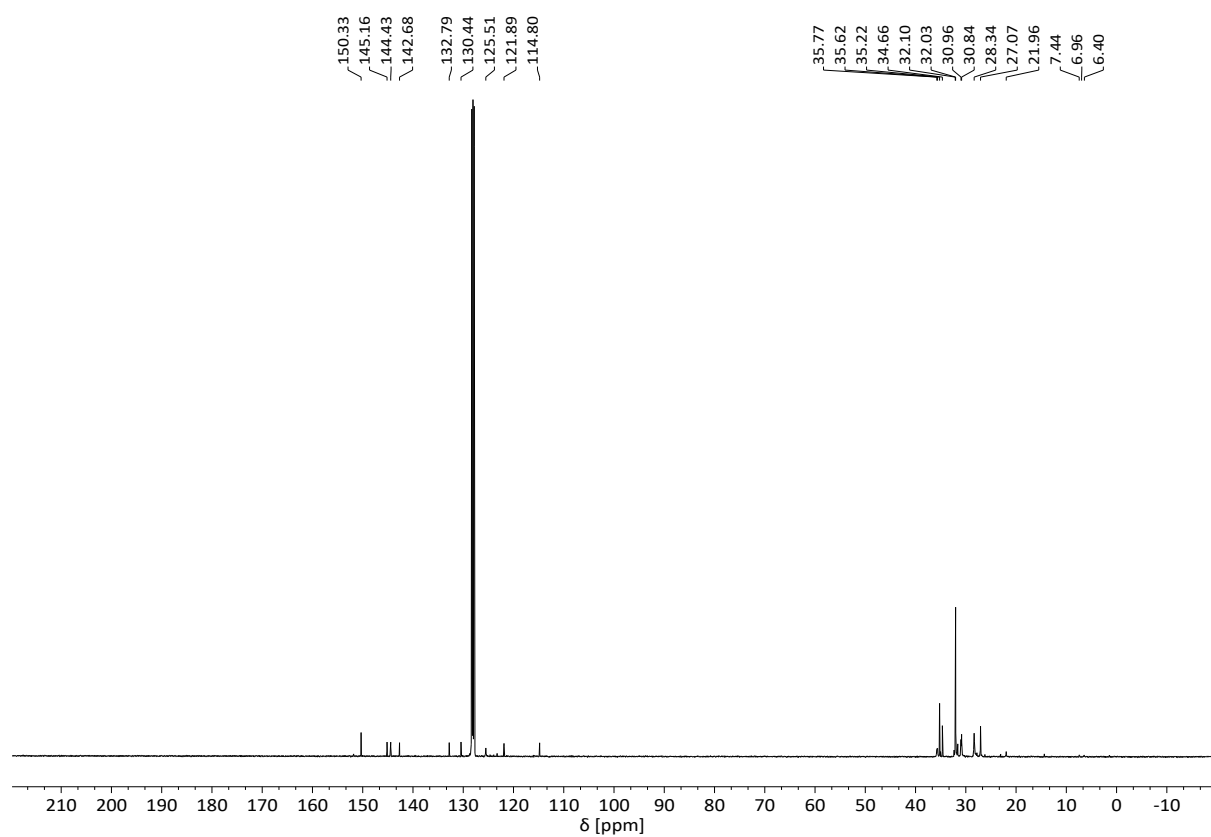


Figure S24: ¹³C{¹H} NMR spectrum of **3**.

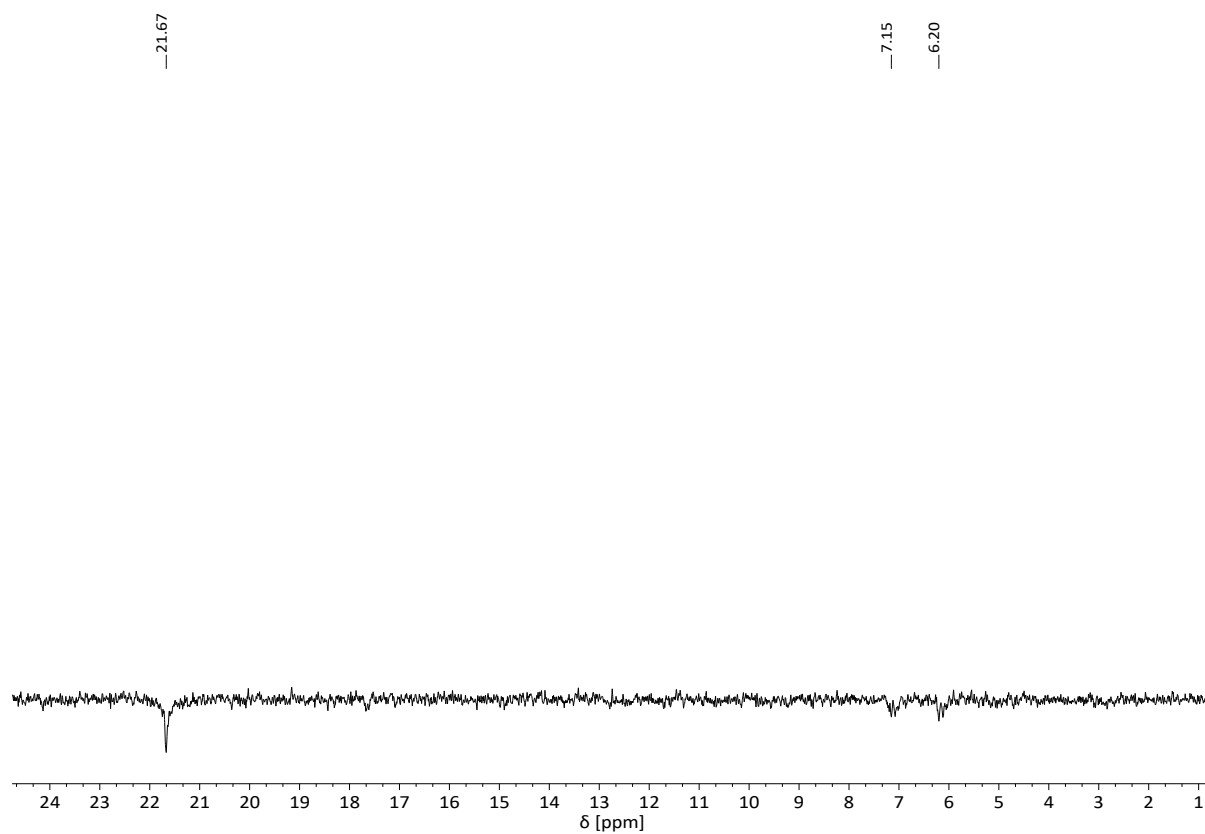


Figure S25: Extract of the DEPT-135 NMR spectrum of **3**.

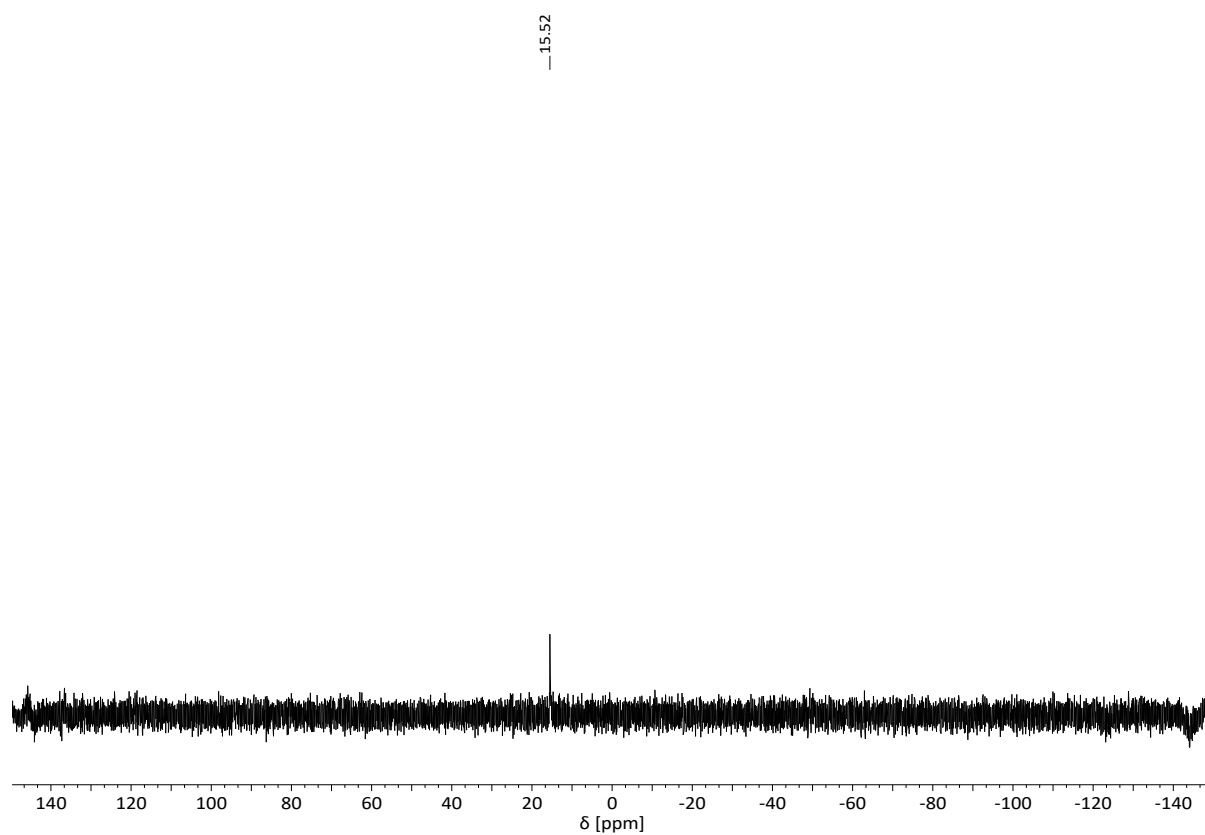


Figure S26: $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **3**.

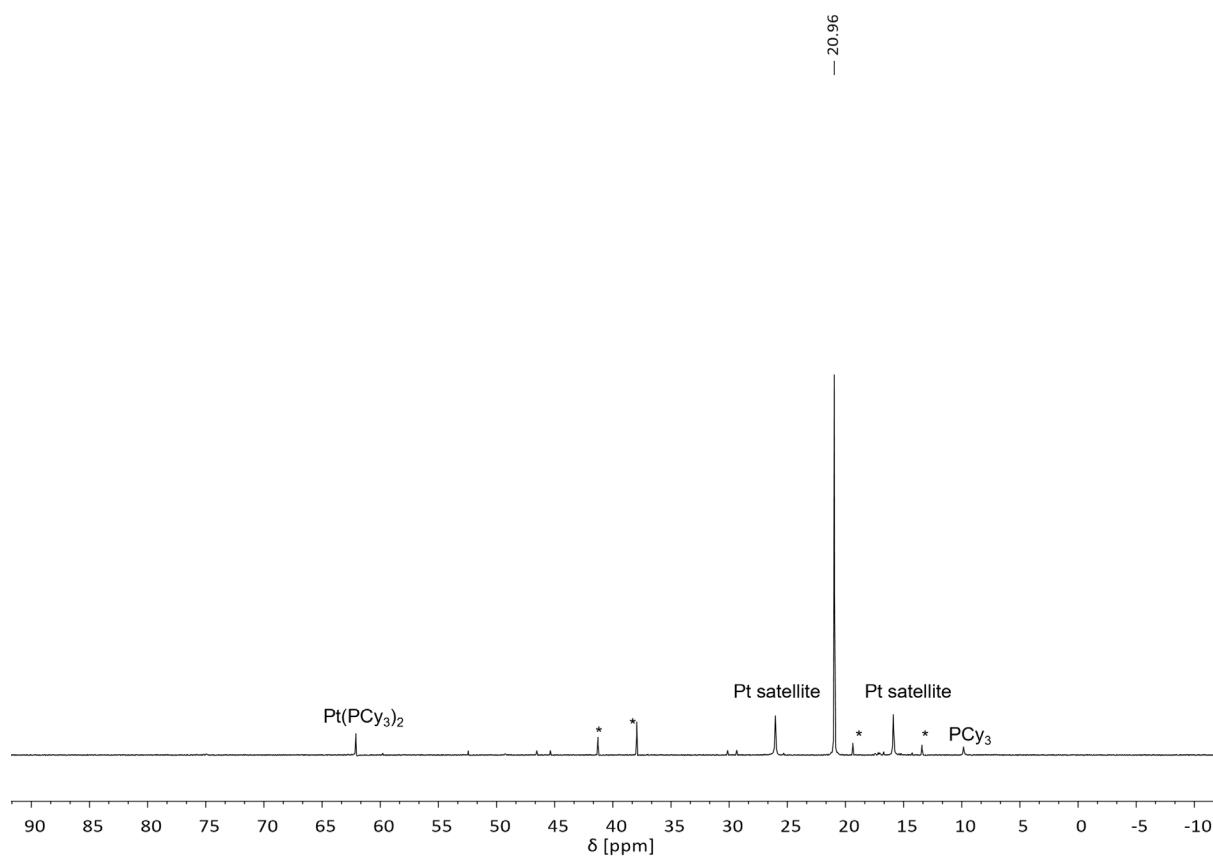


Figure S27: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **3**. Resonances marked with * correspond to unknown impurities

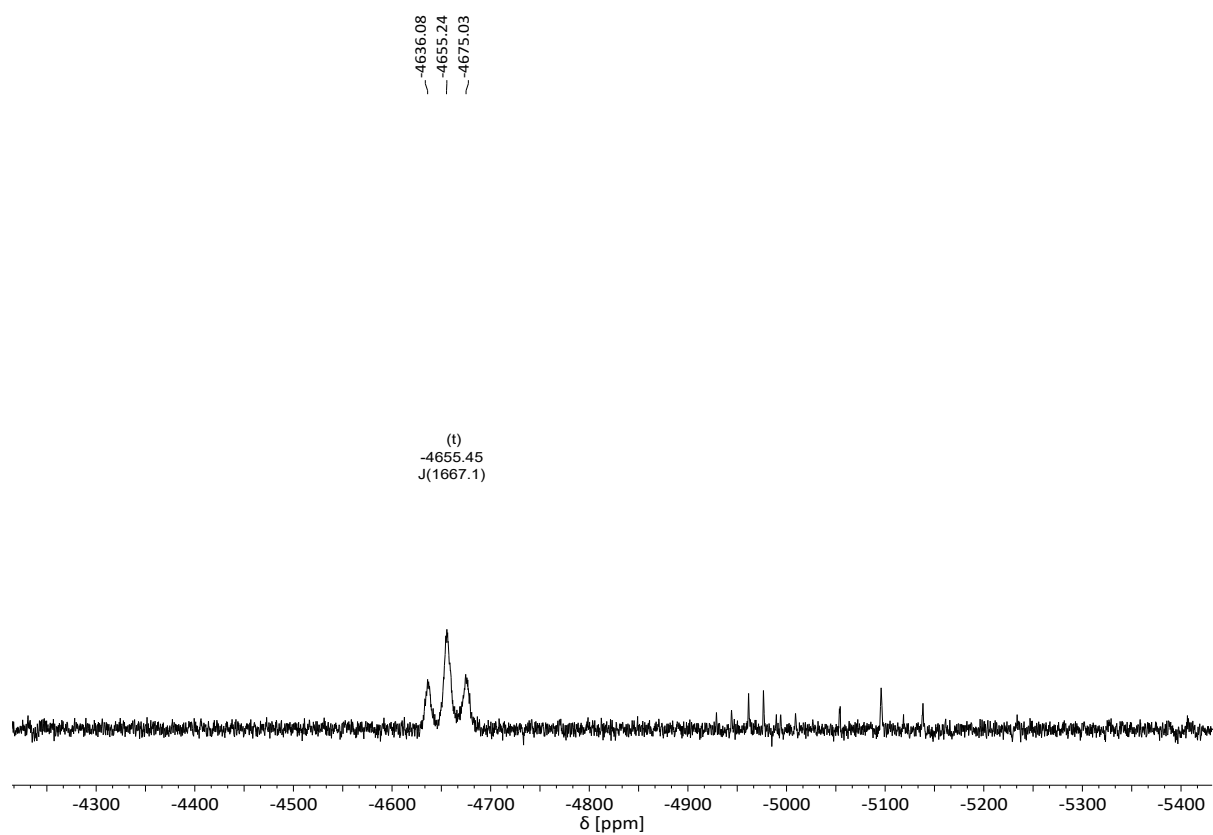


Figure S28: ^{195}Pt NMR spectrum of **3**.

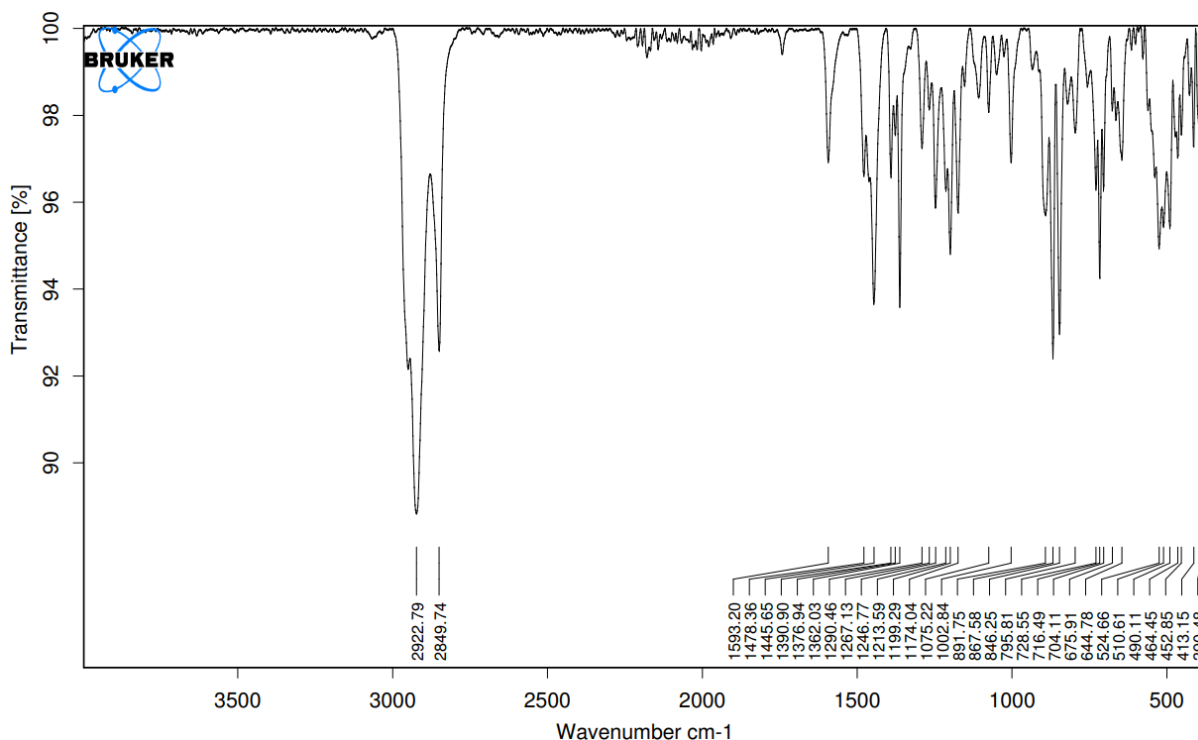


Figure S29: IR spectrum of **3**.

R(Br)Si(C₂H₄)₂Pt(PPh₃)₂ (4**)**

In a Young NMR tube, R(Br)Si(C₂H₄)Pt(PPh₃)₂ (**1**) (30.7 mg, 0.02 mmol) were dissolved in 0.5 mL of C₆D₆. The solution was exposed to one atmosphere of C₂H₄ and heated to 80 °C for 72 hours. As the NMR spectra indicate, six-membered platinasilacycle (**4**) has formed.

¹H NMR (400.1 MHz, C₆D₆): δ(ppm) = 1.41 (s, 36 H, Carb-^{*t*}BuH), 1.47 (s, 18 H, Carb-^{*t*}BuH), 1.53 (s, 36 H, Ar-^{*t*}BuH), 6.86-6.98 (m br, 15 H, Ph-H), 7.17-7.27 (m br, 15 H, Ph-H), 7.56 (d, *J*_{HH} = 2.1 Hz, 2 H, C^{2,7}H), 7.58 (t, *J*_{HH} = 1.8 Hz, 2 H, *p*-CH), 7.64 (s br, 4 H, *o*-CH), 8.27 (d, *J*_{HH} = 2.1 Hz, 2 H, C^{4,5}H). **¹³C{¹H} NMR** (100.6 MHz, C₆D₆): δ(ppm) = 15.6 (m, Si-CH₂), 22.2 (s br, Pt-CH₂), 34.7 (s, Carb-C(CH₃)), 35.2 (s, Ar-C(CH₃)), 115.1 (s, C^{4,5}H), 121.7 (s, *p*-CH), 125.6 (s br, *o*-CH), 126.7 (s, Ph-C), 128.5 (s, C^{2,7}H), 127.7 (s, Ph-C), 128.6 (s, Ph-C), 130.5 (s), 133.1 (s), 133.4 (s, Ph-C), 133.8 (s, Ph-C), 134.9 (m, Ph-C), 142.5 (s), 144.1 (s), 145.2 (s), 150.1 (s br). **²⁹Si{¹H} NMR** (79.5 MHz, C₆D₆): δ(ppm) = n. obs. **³¹P{¹H} NMR** (162.0 MHz, C₆D₆): δ(ppm) = 26.8 (s, ¹*J*_{Pt} = 1761.7 Hz).

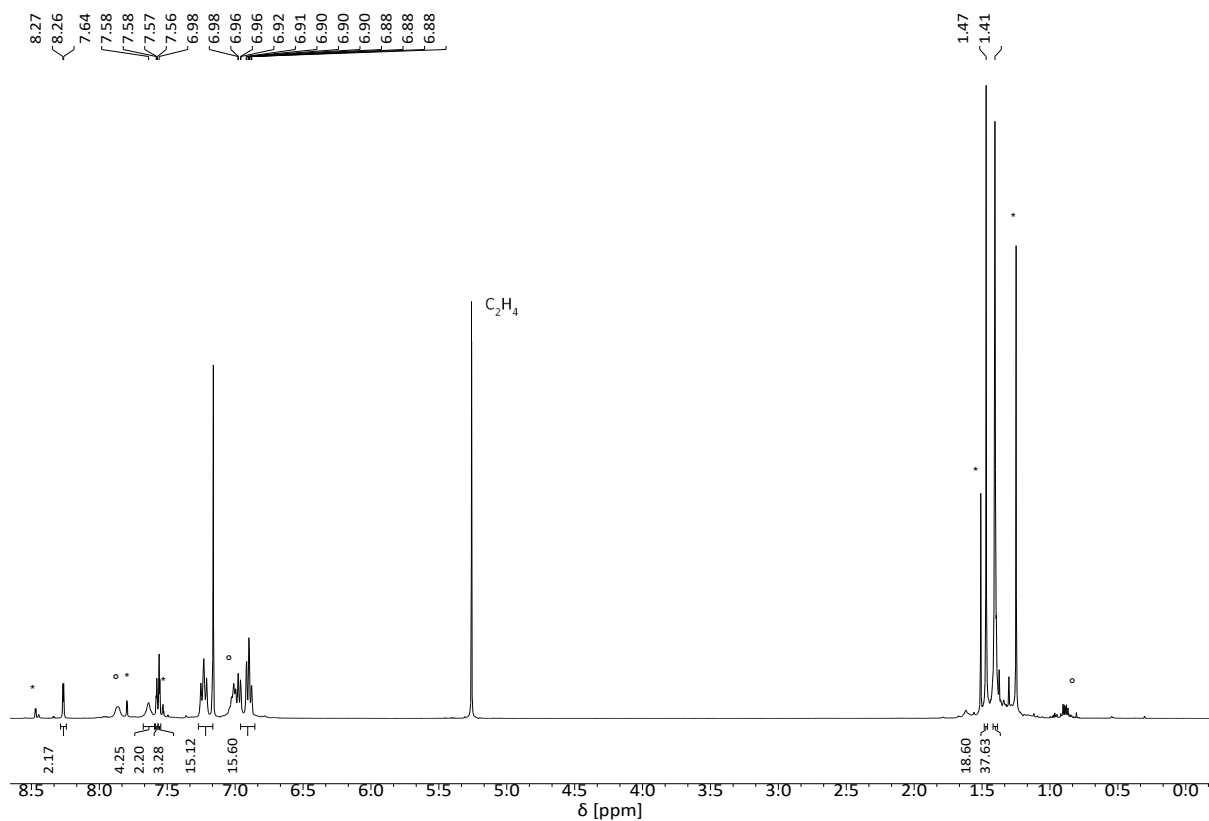


Figure S30: ¹H NMR spectrum of **4**. Resonances marked with * correspond to free ligand RH, ° belong to an unknown impurity.

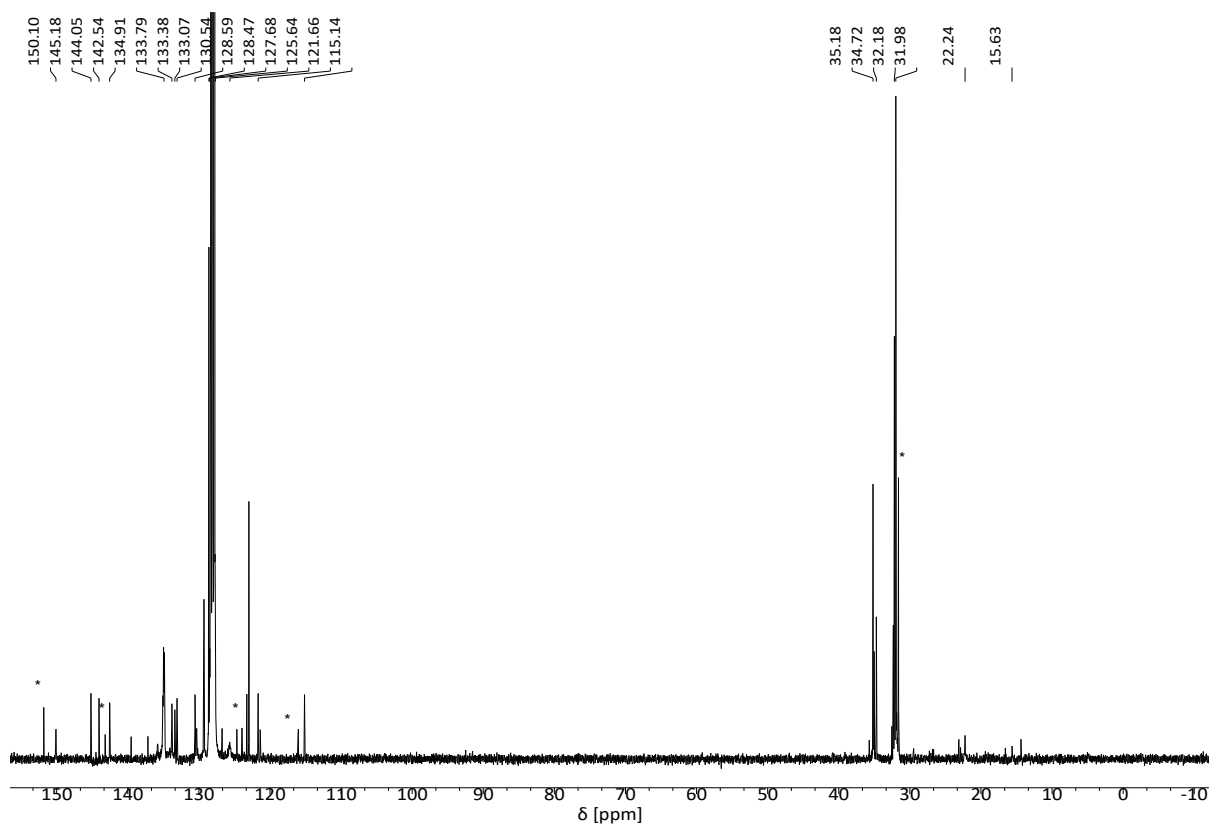


Figure S31: ¹³C{¹H} NMR spectrum of **4**. Resonances marked with * correspond to free ligand RH.

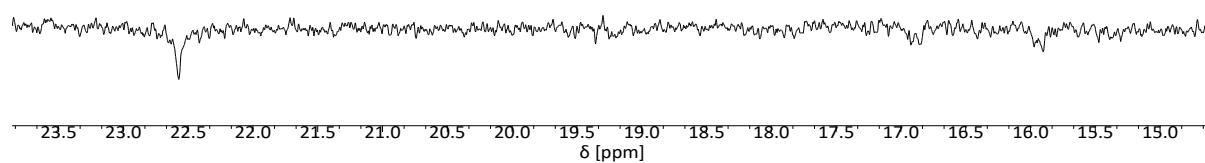


Figure S32: Extract of the DEPT-135 NMR spectrum of **4**.

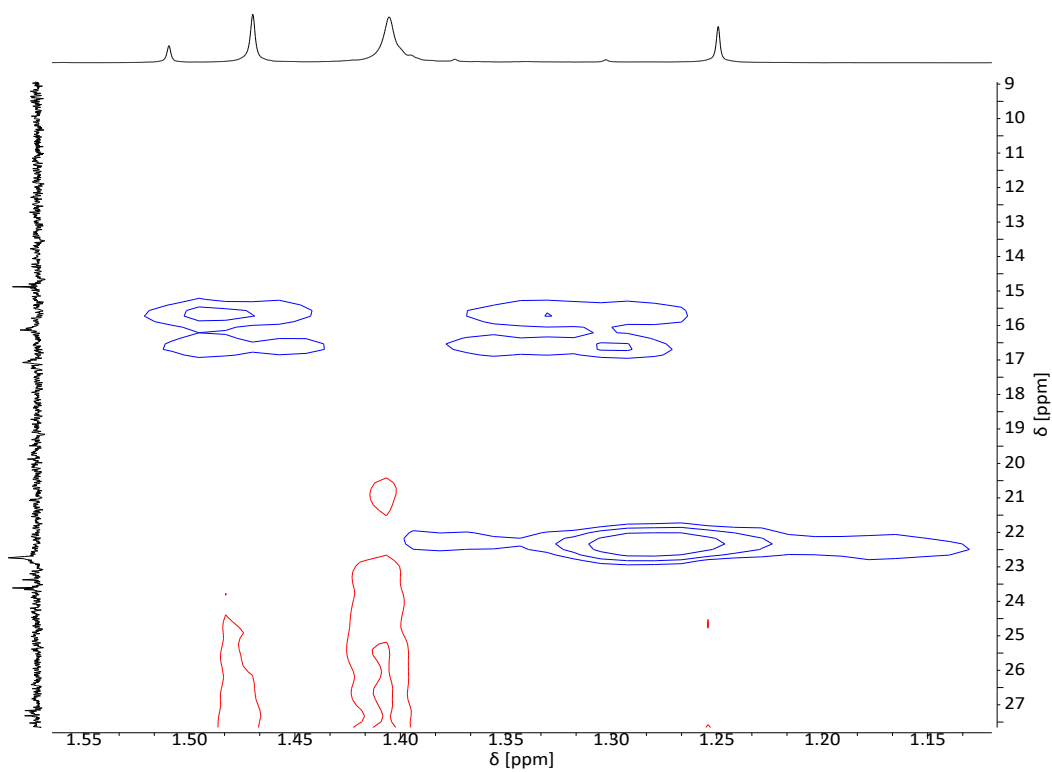


Figure S33: Extract of the ^1H - $^{13}\text{C}\{^1\text{H}\}$ HSQC NMR spectrum of **4**.

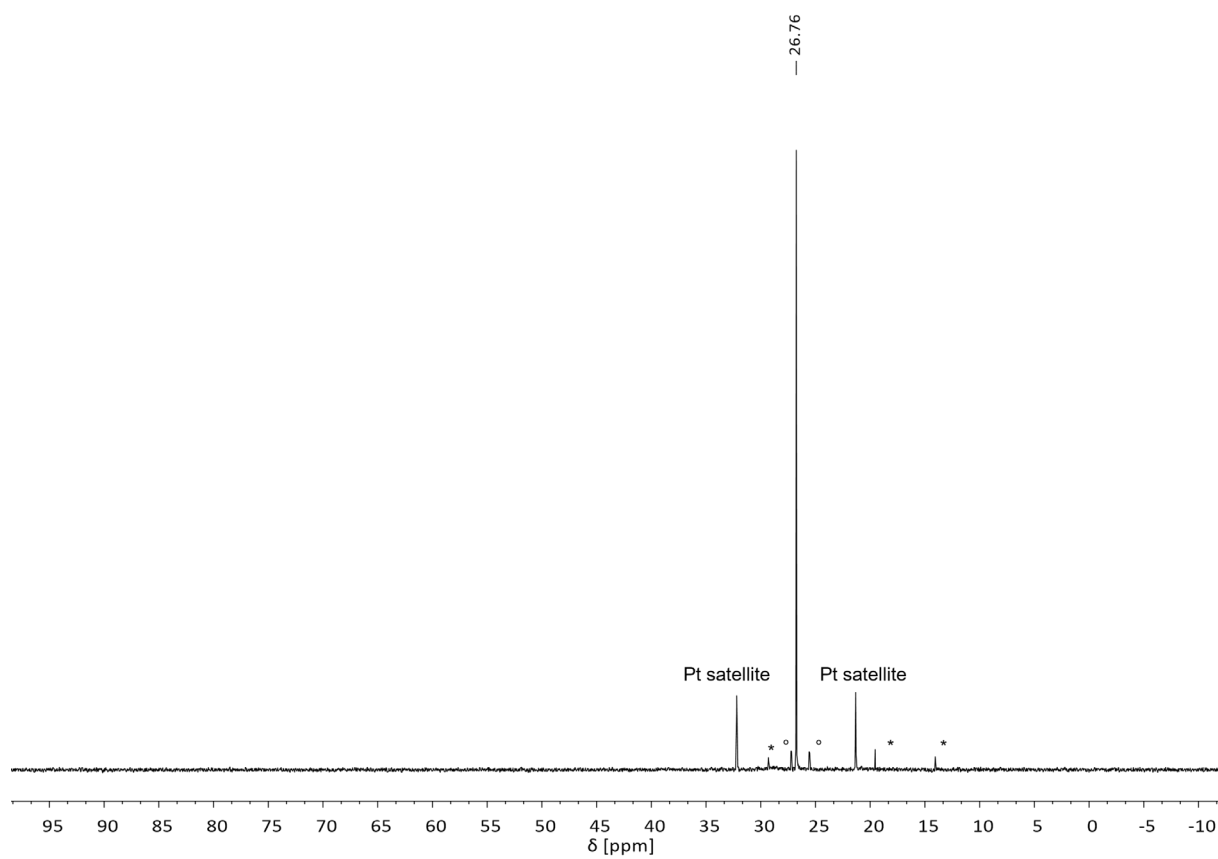


Figure S34: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **4**. Resonances marked with * correspond to unknown impurities, ° belong to starting material.

2 Crystallographic data

	R(Br)Si(C₂H₄)Pt(PPh₃)₂ (1)	R(Br)SiPt(PCy₃)₂ (2)
CDCC #		
Empirical formula	C ₉₈ H ₁₁₀ NSiBrP ₂ Pt	C ₉₆ H ₁₅₈ NSiBrP ₂ Pt
FW [g·mol ⁻¹]	1666.89	1691.25
Wavelength [Å]	1.34143	1.34143
Temperature [K]	150(2)	150(2)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a [Å]	12.5070(2)	12.8841(8)
b [Å]	18.5677(4)	14.2936(6)
c [Å]	19.0009(4)	25.1199(12)
α [°]	79.425(2)	86.724(4)
β [°]	76.139(2)	85.053(4)
γ [°]	88.150(2)	87.610(4)
V [Å ³]	4210.94(15)	4598.2(4)
Z	2	2
ρ _{calc} [g·cm ⁻³]	1.315	1.222
μ [mm ⁻³]	3.058	2.875
F(000)	1724.0	1796.0
Crystal size [mm ³]	0.180 × 0.070 × 0.060	0.080 × 0.070 × 0.030
2θ _{max} [°]	120	120
Reflections collected	45663	59317
Independent reflections	18499	20031
R _{int}	0.0236	0.0326
R _{sigma}	0.0193	0.0265
Parameters	1054	1224
Restraints	564	1362
Goof	1.052	1.054
R ₁	0.0335	0.0281
R ₁ (all)	0.0346	0.0350
wR ₂	0.0853	0.0749
wR ₂ (all)	0.0859	0.0767
Largest diff. peak/hole [e ⁻ ·Å ⁻³]	1.78/−2.54	0.91/−1.17

	2-I	R(Br)Si(C ₂ H ₄) ₂ Pt(PCy ₃) ₂ (3)
CDCC #		
Empirical formula	C ₄₈ H _{64.83} NSiBr _{0.17}	C ₉₅ H ₁₅₄ NSiP ₂ BrPt
FW [g·mol ⁻¹]	697.66	1675.21
Wavelength [Å]	0.71073	0.71073
Temperature [K]	100(2)	100(2)
Crystal system	monoclinic	triclinic
Space group	P21/c	P-1
a [Å]	13.9653(9)	15.2690(10)
b [Å]	15.3055(9)	15.7982(9)
c [Å]	20.3949(15)	22.2137(14)
α [°]	90	106.144(5)
β [°]	103.984(6)	109.170(5)
γ [°]	90	90.351(5)
V [Å ³]	4230.1(5)	4833.6(5)
Z	4	2
ρ _{calc} [g·cm ⁻³]	1.095	1.151
μ [mm ⁻³]	0.250	1.950
F(000)	1519.0	1776.0
Crystal size [mm ³]	0.190 × 0.140 × 0.110	0.180 × 0.080 × 0.060
2θ _{max} [°]	52	51
Reflections collected	33959	53174
Independent reflections	8274	17578
R _{int}	0.0535	0.0497
R _{sigma}	0.0576	0.0510
Parameters	519	915
Restraints	168	336
GooF	1.020	1.156
R ₁	0.0639	0.0780
R ₁ (all)	0.1045	0.0898
wR ₂	0.1517	0.1925
wR ₂ (all)	0.1747	0.1999
Largest diff. peak/hole [e ⁻ ·Å ⁻³]	0.34/−0.61	4.60/−2.05

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