Supporting Information

A Transient Lanthanum Phosphinidene Complex

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1. Experimental Section

General Remarks. If not otherwise mentioned, all transformations were carried out under inert conditions using an argon filled glovebox. All glassware (including glass-fibre filters) was stored in an oven at 150 °C for at least 12 h prior to use. Solvents were dried by a MBraun SPS system, degassed and stored over activated molecular sieves (3 Å) for at least 24 h prior to use. Cyclohexene and THF-d_8 were degassed by three freeze-pump-thaw cycles and then dried by storage over activated molecular sieves (3 Å) for at least 24 h. D_2O was degassed by sonication and sparging with argon prior to use. IR spectra were recorded at room temperature under inert conditions using a Bruker Vertex 70 with ATR equipment. If not otherwise stated, the NMR spectra were collected at 303 K on a Bruker AV-500 or an Ascent 700 spectrometer using a J-Young NMR tube. All chemical shifts (δ) are reported in ppm and coupling constants are given in Hz. ^{1}H and ^{13}C chemical shifts were calibrated to residual solvent peaks. ^{15}N chemical shifts (obtained by ^{1}H–^{15}N HMBC NMR spectroscopy) were calibrated externally to liquid ammonia (NH_3). ^{31}P chemical shifts were calibrated externally to phosphoric acid (H_3PO_4, 85% in water). Elemental analyses were performed using an Elementar vario microcube instrument at the Paderborn University. Starting materials KPHMes,[1a,b] $(PN)_2LaCl$,[1c] **1**,[1c] **4**[1c] and KBn[2] were synthesised following literature known procedures. 18-crown-6 (18C6) was recrystallised twice from hot acetonitrile, washed with diethyl ether and dried *in vacuo* prior to use. KHMDS and 2.2.2-cryptand were used as received.

Synthetic Procedures

Preparation of KPDMes.

A suspension of KPHMes (632 mg, 3.32 mmol, 1 eq.) in toluene (10 mL) was cooled to 0 °C and D_2O (0.1 mL, 5.54 mmol, 1.67 eq.) was added dropwise. After stirring for 15 min toluene and residual D_2O were carefully removed *in vacuo* at room temperature. The oily residue was extracted with *n*-hexane (2 x 3 mL), filtered and the solvent removed *in vacuo*. The mixture of H_2PMes (≈12%), HDPMes (≈47%) and D_2PMes (≈41%) was then reacted again with KHMDS (1 eq.) in toluene. The whole cycle was repeated two more times and KPDMes of >95% isotopic purity was finally isolated by filtration, washing with *n*-hexane (2 x 2 mL) and drying *in vacuo*. Yield: 200 mg (1.05 mmol, 32%).

Preparation of $(PN)_2$La(PDMes) (1-d).

Toluene (6 mL) was added to $(PN)_2$LaCl (171 mg, 200 µmol, 1 eq.) and KPDMes (46 mg, 240 µmol, 1.2 eq.) and the resulting yellow reaction mixture stirred for 3 d at room temperature. After centrifugation the solution was filtered and another portion of KPDMes (10 mg, 52 µmol, 0.26 eq.) was added. After stirring for another 24 h at room temperature the reaction mixture was again centrifuged, the solution filtered and all volatiles were removed *in vacuo*. The remaining solid was washed with –40 °C cold *n*-pentane (1 mL) and dried *in vacuo* to give the mono-deuterated complex **1-*d*** in ≈97% purity and ≈86–88% isotopic purity. Yield: 164 mg (169 µmol, 85%). ^{1}H NMR (C_6D_6, 303 K, 500 MHz, in ppm): δ = 0.85–0.98 (br. s, CH_{3iPr}, 12 H), 1.01–1.09 (br. s, CH_{3iPr}, 12 H), 1.72–1.91 (br. s, CH_{iPr}, 4 H), 2.14 (s, CH_{3Ar}, 6 H), 2.15 (s, CH_{3Ar}, 6 H), 2.25 (s, CH_{3Ar}, 3 H), 2.29–2.42 (br. s, CH_{3Ar}, 12 H), 2.44 (s, CH_{3Ar}, 6 H), 5.66–5.70 (m, CH_{Ar}, 2 H), 6.81 (dd, J = 8.4 Hz, J = 1.9 Hz, CH_{Ar}, 2 H), 6.83 (s, CH_{Ar}, 2 H), 6.84–6.87 (m, CH_{Ar}, 2 H), 6.89 (s, CH_{Ar}, 4 H); ^{31}P{^{1}H} NMR (C_6D_6, 303 K, 202 MHz, in ppm): δ = –38.2 (t, $^1J_{PD}$ = 28.6 Hz, *P*DMes, 1 P), 11.2 (s, P(^{i}Pr)$_2$, 2 P).

Preparation of [K(18C6)][(PN)(PN_{cyclo})La(PHMes)] (3a).

Route A: A solution of either KHMDS (20 mg, 100 µmol, 1 eq.) or KBn (13 mg, 100 µmol, 1 eq.) in DME (1 mL) was added dropwise to a mixture of **1** (97 mg, 100 µmol, 1 eq.) and 18-crown-6 (26 mg, 100 µmol, 1 eq.) in DME (3 mL) at room temperature, giving an orange-coloured solution. After 10 min the reaction mixture was filtered through a glass-fibre filter and most of the volatiles were removed *in vacuo* until an oily residue was obtained. Diethyl ether (3 mL) was added, which caused the dissolution

of the oil followed by the formation of orange-coloured crystalline blocks at –40 °C within 1 h. The crystals were isolated from the mother liquor, washed with diethyl ether (3 x 2 mL) and left to dry in the glovebox atmosphere, since prolonged drying *in vacuo* caused significant decomposition. Over a period of several hours to days, slow decomposition was also observed when storing a NMR sample of **3a** in, e.g., THF-d_8 at room temperature. NMR spectroscopic analysis of the obtained material in THF-d_8 revealed the presence of significant amounts (ca. 15%) of a second, as yet unidentified C–H-activated product, which could not be removed by repeated recrystallisation or washing. Attempts to optimise the reaction with THF, diethyl ether or toluene as alternative solvents, different rate of addition of base, stoichiometry of base or larger scaled batches as well as low temperature experiments at –40 °C did not yield better results and reaction monitoring of the DME reaction solution (with C_6D_6 capillary) by means of $^{31}P\{^1H\}$ NMR spectroscopy indicated that the formation of the unknown side product occurs already before work-up (see Fig. S3). Even though the NMR spectroscopic features of **3a** could still be assigned, due to the impurity no useful IR data or elemental analysis could be obtained. Single crystals of **3a** suitable for X-ray structure determination were obtained during work-up as described above. Yield: 67 mg (53 µmol, 53%, crude); ^{1}H NMR (THF-d_8, 303 K, 700 MHz, in ppm): δ = 0.26 (dd, J = 15.7 Hz, J = 6.9 Hz, CH_{3iPr}, 3 H), 0.64 (dd, J = 14.3 Hz, J = 6.9 Hz, CH_{3iPr}, 3 H), 0.76–0.81 (m, CH_{3iPr}, 6 H), 0.88–0.90 (m, CH_{3iPr}, 3 H), 1.02 (dd, J = 13.3 Hz, J = 7.0 Hz, CH_{3iPr}, 3 H), 1.07 (dd, $^2J_{HH}$ = 4.8 Hz, J = 3.1 Hz, C$H_{2Mes(PNcyclo)}$, 3 H), 1.15 (dd, J = 15.8 Hz, J = 6.9 Hz, CH_{3iPr}, 3 H), 1.25 (dd, J = 15.3 Hz, J = 6.8 Hz, CH_{3iPr}, 3 H), 1.41–1.44 (br. m, CH_{iPr}, 1 H), 1.73 (s, CH_{3Ar}, 3 H), 1.79–1.83 (m, CH_{iPr}, 1 H), 1.86 (s, CH_{3Ar}, 3 H), 1.99 (s, CH_{3Ar}, 3 H), 2.01 (s, CH_{3Ar}, 3 H), 2.08 (s, CH_{3Ar}, 3 H), 2.09 (s, CH_{3Ar}, 3 H), 2.10–2.17 (br. m, CH_{iPr}, 2 H), 2.19 (s, CH_{3Ar}, 6 H), 2.22 (s, CH_{3Ar}, 3 H), 2.48 (s, CH_{3Ar}, 3 H), 2.58 (d, $^1J_{PH}$ = 181.6 Hz, PHMes, 1 H), 2.78 (dd, $^2J_{HH}$ = 4.8 Hz, J = 0.8 Hz, C$H_{2Mes(PNcyclo)}$, 1 H), 3.54 (s, C$H_{2(18C6)}$, 24 H), 5.09 (dd, J = 8.6 Hz, J = 4.9 Hz, CH_{Ar}, 1 H), 5.52 (dd, J = 8.5 Hz, J = 5.0 Hz, CH_{Ar}, 1 H), 6.07–6.09 (m, CH_{Ar}, 1 H), 6.36 (dd, J = 8.6 Hz, J = 1.9 Hz, CH_{Ar}, 1 H), 6.37–6.38 (m, CH_{Ar}, 1 H), 6.41–6.44 (m, CH_{Ar}, 3 H), 6.53 (dd, J = 5.0 Hz, J = 1.8 Hz, CH_{Ar}, 1 H), 6.63 (dd, J = 4.9 Hz, J = 1.9 Hz, CH_{Ar}, 1 H), 6.79–6.80 (m, CH_{Ar}, 1 H), 6.90–6.92 (m, CH_{Ar}, 1 H); $^{13}C\{^1H\}$ NMR (THF-d_8, 303 K, 176 MHz, in ppm): δ = 16.5 (d, J_{CP} = 5.4 Hz, CH$_{3iPr}$), 16.6 (d, J_{CP} = 3.8 Hz, CH$_{3iPr}$), 19.2 (m, CH$_{3iPr}$), 19.3 (m, CH$_{3iPr}$), 19.4 (m, CH$_{3iPr}$), 19.5 (s, CH$_{3Ar}$), 19.9 (m, CH$_{3iPr}$), 20.4 (m, CH$_{3iPr}$), 20.5 (s, CH$_{3Ar}$), 20.7 (s, CH$_{3Ar}$), 20.9 (s, CH$_{3Ar}$), 21.11 (s, CH$_{3Ar}$), 21.15 (s, CH$_{3Ar}$), 21.27 (s, CH$_{3Ar}$), 21.28 (m, CH$_{3iPr}$), 21.8 (s, CH$_{iPr}$), 22.1 (s, CH$_{3Ar}$), 22.6 (d, J_{CP} = 2.9 Hz, CH$_{iPr}$), 24.4 (d, J_{CP} = 2.5 Hz, CH$_{iPr}$), 25.9 (s, CH$_{iPr}$), 65.4 (s, CH$_{2Mes(PNcyclo)}$), 71.3 (s, CH$_{2(18C6)}$), 111.9 (d, J_{CP} = 7.1 Hz, CH$_{Ar}$), 112.7 (d, J_{CP} = 6.3 Hz, CH$_{Ar}$), 114.7 (d, J_{CP} = 8.7 Hz, C_{qAr}), 115.6 (d, J_{CP} = 10.7 Hz, C_{qAr}), 118.5 (s, C_{qAr}), 120.1 (s, CH$_{Ar}$), 125.0 (s, CH$_{Ar}$), 126.5 (s, C_{qAr}), 127.2 (s, CH$_{Ar}$), 130.5 (s, CH$_{Ar}$), 131.3 (s, CH$_{Ar}$), 131.7 (s, CH$_{Ar}$), 132.2 (s, CH$_{Ar}$), 132.3 (s, C_{qAr}), 133.2 (s, CH$_{Ar}$), 133.3 (s, C_{qAr}), 134.0 (s, CH$_{Ar}$), 136.7 (d, J_{CP} = 9.0 Hz, C_{qAr}), 137.3 (s, C_{qAr}), 138.8 (s, C_{qAr}), 139.1 (s, C_{qAr}), 143.8 (s, C_{qAr}), 146.4 (s, C_{qAr}), 150.8 (d, J_{CP} = 42.9 Hz, C_{qAr}), 162.0 (d, J_{CP} = 21.8 Hz, C_{qAr}), 163.4 (d, J_{CP} = 24.1 Hz, C_{qAr}); ^{31}P NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –87.4 (dd, $^1J_{PH}$ = 181.6 Hz, $^2J_{PP}$ = 22.6 Hz, PHMes, 1 P), 2.6–3.8 (br. m, P(^{i}Pr)$_2$, 2 P); $^{31}P\{^1H\}$ NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –87.4 (d, $^2J_{PP}$ = 22.6 Hz, PHMes, 1 P), 3.0 (dd, $^2J_{PP}$ = 36.8 Hz, $^2J_{PP}$ = 22.6 Hz, P(^{i}Pr)$_2$, 1 P), 3.4 (d, $^2J_{PP}$ = 36.8 Hz, P(^{i}Pr)$_2$, 1 P).

Route B: A solution of KHMDS (10 mg, 50 µmol, 1. eq.) in cyclohexene (1 mL) was added dropwise to a mixture of **1-*d*** (49 mg, 50 µmol, 1 eq.) and 18-crown-6 (13 mg, 50 µmol, 1 eq.) in cyclohexene (2 mL) at room temperature, giving an orange-coloured solution. The reaction solution was allowed to rest at room temperature for 3 d, during which orange-coloured crystals formed. The crystalline material was separated from the mother liquor, washed with *n*-pentane (4 x 2 mL) and left to dry in the glovebox atmosphere for 2 h, yielding **3a** of ≈94% purity (see Fig. S18–S24). The obtained material gave satisfying elemental analysis results and therefore was also used to collect an IR spectrum. Yield: 32 mg (25 µmol, 50%); elemental analysis (in %): $C_{65}H_{97}KLaN_2O_6P_3$: calcd.: C 61.31, H 7.68, N 2.20; found: C 61.56, H 7.41, N 2.11.

Preparation of [K(2.2.2-cryptand)][(PN)(PN$_{cyclo}$)La(PHMes)] (3b).

A solution of either KHMDS (20 mg, 100 µmol, 1 eq.) or KBn (13 mg, 100 µmol, 1 eq.) in DME (1 mL) was added dropwise to a mixture of **1** (97 mg, 100 µmol, 1 eq.) and 2.2.2-cryptand (38 mg, 100 µmol, 1 eq.) in DME (3 mL) at room temperature, giving an orange-coloured solution. After 10 min the reaction mixture was filtered through a glass-fibre filter and most of the volatiles were removed *in vacuo* until an oily residue was obtained. Since crystallisation from DME/diethyl ether was not feasible due to the formation of a layer of oil, the residue was extracted with toluene (2 mL). The extract was concentrated *in vacuo* and triturated with *n*-hexane (3 x 2 mL) to give a light orange-coloured solid which was washed with *n*-pentane (2 x 2 mL) and left to dry in the glovebox atmosphere. Recrystallisation of this raw product in useful quantities was not possible due to the poor crystallisation behaviour of **3b**, i.e., the formation of mainly oily precipitates from different solvent combinations of DME, THF or toluene with diethyl ether, *n*-hexane or *n*-pentane. Since **3b** was found to be very difficult to isolate as pure material and prone to decomposition, a full characterisation was not feasible. The ^{1}H NMR resonances are assigned as well as possible by comparison with the spectrum of **3a**. Single crystals of **3b** suitable for X-ray structure determination were obtained by gas phase diffusion of *n*-hexane into a THF solution of **3b** (ca. 15 mg in 300 µL) at room temperature overnight. Yield: 128 mg (92 µmol, 92%, crude); ^{1}H NMR (THF-d_8, 303 K, 500 MHz, in ppm): δ = 0.28 (dd, J = 15.2 Hz, J = 7.0 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 0.65 (dd, J = 13.8 Hz, J = 6.9 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 0.75–0.85 (m, C$H_{3i\mathrm{Pr}}$, 6 H), 0.95–1.06 (m, C$H_{3i\mathrm{Pr}}$, 6 H), 1.11–1.16 (dd, J = 15.2 Hz, J = 6.8 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 1.23–1.28 (dd, J = 13.8 Hz, J = 6.9 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 1.41–1.46 (br. m, C$H_{i\mathrm{Pr}}$, 1 H), 1.74 (s, C$H_{3\mathrm{Ar}}$, 3 H), 1.79–1.84 (br. m, C$H_{i\mathrm{Pr}}$, 1 H), 1.86 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.00 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.01 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.08 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.09 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.10–2.15 (br. m, C$H_{i\mathrm{Pr}}$, 2 H), 2.20 (s, C$H_{3\mathrm{Ar}}$, 6 H), 2.22 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.48–2.49 (m, C$H_{2(2.2.2\text{-cryptand})}$, 12 H; s, C$H_{3\mathrm{Ar}}$), 2.59 (d, $^{1}J_{\mathrm{PH}}$ = 180.8 Hz, P*H*Mes, 1 H), 2.78 (dd, $^{2}J_{\mathrm{HH}}$ = 4.9 Hz, J = 0.7 Hz, C$H_{2\mathrm{Mes(PNcyclo)}}$, 1 H), 3.46–3.48 (m, C$H_{2(2.2.2\text{-cryptand})}$, 12 H), 3.52 (s, C$H_{2(2.2.2\text{-cryptand})}$, 12 H), 5.09 (dd, J = 8.5 Hz, J = 4.9 Hz, CH_{Ar}, 1 H), 5.53 (dd, J = 8.5 Hz, J = 4.8 Hz, CH_{Ar}, 1 H), 6.07–6.09 (m, CH_{Ar}, 1 H), 6.35–6.39 (m, CH_{Ar}, 2 H), 6.42–6.45 (m, CH_{Ar}, 3 H), 6.54 (dd, J = 5.1 Hz, J = 2.0 Hz, CH_{Ar}, 1 H), 6.64 (dd, J = 4.9 Hz, J = 2.1 Hz, CH_{Ar}, 1 H), 6.79–6.81 (m, CH_{Ar}, 1 H), 6.90–6.92 (m, CH_{Ar}, 1 H) (One of the C$H_{2\mathrm{Mes(PNcyclo)}}$ resonances is obscured by the C$H_{3i\mathrm{Pr}}$ multiplet resonances and therefore cannot be assigned.); ^{31}P NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –86.9 (dd, $^{1}J_{\mathrm{PH}}$ = 180.8 Hz, $^{2}J_{\mathrm{PP}}$ = 21.6 Hz, *P*HMes, 1 P), 2.7–4.0 (br. m, $P(^{i}\mathrm{Pr})_2$, 2 P); ^{31}P{^{1}H} NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –86.9 (d, $^{2}J_{\mathrm{PP}}$ = 21.6 Hz, *P*HMes, 1 P), 3.2 (dd, $^{2}J_{\mathrm{PP}}$ = 36.7 Hz, $^{2}J_{\mathrm{PP}}$ = 22.7 Hz, $P(^{i}\mathrm{Pr})_2$, 1 P), 3.6 (d, $^{2}J_{\mathrm{PP}}$ = 36.7 Hz, $P(^{i}\mathrm{Pr})_2$, 1 P).

Preparation of [K(18C6)][(PN)(PN$_{cyclo}$)La(OMes)] (5a).

A solution of either KHMDS (25 mg, 126 µmol, 1.05 eq.) or KBn (17 mg, 126 µmol, 1.05 eq.) in DME (1 mL) was added dropwise to a mixture of **4** (115 mg, 120 µmol, 1 eq.) and 18-crown-6 (32 mg, 120 µmol, 1 eq.) in DME (3 mL) at room temperature, causing the dissolution of **4** and formation of a deep-yellow solution. After 10 min the reaction mixture was filtered through a glass-fibre filter and most of the volatiles were removed *in vacuo* until an oily residue was obtained. Diethyl ether (3 mL) was added, which caused the dissolution of the oil followed by the formation of yellow crystals in the form of radially growing aggregates of needles within 1 h. The crystalline material was isolated from the mother liquor, washed with diethyl ether (3 x 1 mL) and dried *in vacuo* to give analytically pure **5a** as a yellow microcrystalline powder. Single crystals of **5a** suitable for X-ray structure determination were obtained by gas phase diffusion of *n*-hexane into a concentrated benzene solution of **5a** (ca. 15 mg in 300 µL) at room temperature over a period of two days. Yield: 111 mg (88 µmol, 74%); ^{1}H NMR (THF-d_8, 303 K, 700 MHz, in ppm): δ = 0.43 (dd, J = 14.8 Hz, J = 6.9 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 0.68 (dd, J = 15.3 Hz, J = 6.9 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 0.72–0.79 (m, C$H_{3i\mathrm{Pr}}$, 6 H), 0.82 (*pseudo*-t, J = 7.3 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 0.93–0.99 (m, C$H_{3i\mathrm{Pr}}$, 6 H), 1.15 (dd, J = 15.1 Hz, J = 6.9 Hz, C$H_{3i\mathrm{Pr}}$, 3 H), 1.34 (dd, $^{2}J_{\mathrm{HH}}$ = 5.0 Hz, J = 3.1 Hz, C$H_{2\mathrm{Mes(PNcyclo)}}$, 1 H), 1.63 (s, C$H_{3\mathrm{Ar}}$, 3 H), 1.65–1.70 (m, C$H_{i\mathrm{Pr}}$, 1 H), 1.74 (s, C$H_{3\mathrm{Ar}}$, 3 H), 1.97 (s, C$H_{3\mathrm{Ar}}$, 3 H), 1.99 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.01–2.06 (br. m, C$H_{i\mathrm{Pr}}$, 2 H), 2.03 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.05 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.06 (s, C$H_{3\mathrm{Ar}}$, 6 H), 2.09–2.12 (br. m, C$H_{i\mathrm{Pr}}$, 1 H), 2.13 (dd, $^{2}J_{\mathrm{HH}}$ = 5.0 Hz, J = 1.6 Hz, C$H_{2\mathrm{Mes(PNcyclo)}}$, 1 H), 2.20 (s, C$H_{3\mathrm{Ar}}$, 3 H), 2.36 (s, C$H_{3\mathrm{Ar}}$, 3 H), 3.57 (s, C$H_{2(18\mathrm{C6})}$, 24 H), 5.11 (dd, J = 8.6 Hz, J = 5.2 Hz, CH_{Ar}, 1 H), 5.53 (dd,

J = 8.3 Hz, J = 5.2 Hz, CH_{Ar}, 1 H), 5.94–5.96 (m, CH_{Ar}, 1 H), 6.33 (dd, J = 8.6 Hz, J = 1.9 Hz, CH_{Ar}, 1 H), 6.35–6.38 (m, CH_{Ar}, 2 H), 6.46 (s, CH_{Ar}, 2 H), 6.52 (dd, J = 5.2 Hz, J = 1.9 Hz, CH_{Ar}, 1 H), 6.66 (dd, J = 5.2 Hz, J = 2.1 Hz, CH_{Ar}, 1 H), 6.75–6.77 (m, CH_{Ar}, 1 H), 6.82–6.85 (m, CH_{Ar}, 1 H); ^{13}C{^{1}H} NMR (THF-d_8, 303 K, 176 MHz, in ppm): δ = 16.5 (d, J_{CP} = 4.5 Hz, CH$_{3iPr}$), 17.2 (d, J_{CP} = 2.1 Hz, CH$_{3iPr}$), 18.7 (d, J_{CP} = 11.7 Hz, CH$_{3iPr}$), 19.0 (d, J_{CP} = 10.9 Hz, CH$_{3iPr}$), 19.2 (d, J_{CP} = 16.7 Hz, CH$_{3iPr}$), 19.7 (d, J_{CP} = 16.2 Hz, CH$_{3iPr}$), 19.72 (s, CH$_{3Ar}$), 20.3 (s, CH$_{3Ar}$), 20.34 (s, CH$_{3Ar}$; d, J_{CP} = 9.3 Hz, CH$_{3iPr}$), 20.8 (s, CH$_{3Ar}$), 21.0 (s, CH$_{3Ar}$), 21.02 (d, J_{CP} = 11.1 Hz, CH$_{3iPr}$), 21.1 (d, J_{CP} = 3.8 Hz, CH$_{3Ar}$), 21.2 (s, CH$_{3Ar}$), 21.5 (s, CH_{3Ar}), 22.3 (s, CH$_{3Ar}$), 23.1 (s, CH$_{iPr}$), 25.9 (s, CH$_{iPr}$), 26.2 (d, J_{CP} = 4.3 Hz, CH$_{iPr}$), 61.2 (s, CH$_{2Mes(PNcyclo)}$), 71.3 (s, CH$_{2(18C6)}$), 111.7 (d, J_{CP} = 7.3 Hz, CH$_{Ar}$), 112.0 (d, J_{CP} = 6.3 Hz, CH$_{Ar}$), 114.9 (d, J_{CP} = 10.8 Hz, C_{qAr}), 115.2 (d, J_{CP} = 7.9 Hz, C_{qAr}), 116.2 (d, J_{CP} = 2.7 Hz, C_{qAr}), 117.6 (d, J_{CP} = 2.5 Hz, C_{qAr}), 118.7 (s, CH$_{Ar}$), 121.0 (s, C_{qAr}), 123.8 (s, CH$_{Ar}$), 126.3 (s, C_{qAr}), 128.7 (s, CH$_{Ar}$), 130.2 (s, CH$_{Ar}$), 130.9 (s, CH$_{Ar}$),131.8 (s, C_{qAr}), 131.82 (s, CH$_{Ar}$), 131.9 (s, C_{qAr}), 132.2 (s, CH$_{Ar}$), 133.3 (d, J_{CP} = 3.3 Hz, CH$_{Ar}$), 133.6 (d, J_{CP} = 2.8 Hz, CH$_{Ar}$), 136.1 (d, J_{CP} = 3.1 Hz, C_{qAr}), 136.5 (s, C_{qAr}), 137.3 (s, C_{qAr}), 139.1 (s, C_{qAr}), 146.7 (d, J_{CP} = 2.9 Hz, C_{qAr}), 147.0 (s, C_{qAr}), 162.6 (d, J_{CP} = 21.4 Hz, C_{qAr}), 163.9 (d, J_{CP} = 24.8 Hz, C_{qAr}),164.2 (s, C_{qAr}); ^{31}P{^{1}H} NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –1.4 (d, $^2J_{PP}$ = 33.7 Hz, $P(^i$Pr$)_2$, 1 P), 1.1 (d, $^2J_{PP}$ = 33.7 Hz, $P(^i$Pr$)_2$, 1 P); elemental analysis (in %): $C_{65}H_{96}KLaN_2O_7P_2$: calcd.: C 62.09, H 7.70, N 2.23; found: C 61.67, H 7.66, N 2.38.

Preparation of [K(2.2.2-cryptand)][(PN)(PN$_{cyclo}$)La(OMes)] (5b).

A solution of either KHMDS (28 mg, 142 µmol, 1.15 eq.) or KBn (19 mg, 142 µmol, 1.15 eq.) in DME (1 mL) was added dropwise to a mixture of **4** (118 mg, 124 µmol, 1 eq.) and 2.2.2-cryptand (47 mg, 124 µmol, 1 eq.) in DME (3 mL) at room temperature, causing the dissolution of **4** and formation of a deep-yellow solution. After 20 min the reaction mixture was filtered through a glass-fibre filter and most of the volatiles were removed *in vacuo* until an oily residue was obtained. Diethyl ether (2 mL) was added, which caused the dissolution of the oil followed by the formation of yellow crystals in the form of radially growing aggregates of very thin needles after 2 d. The crystalline material was isolated from the mother liquor, washed with diethyl ether (2 x 2 mL) and dried *in vacuo* to give analytically pure **5b** as a yellow microcrystalline powder. Yield: 152 mg (111 µmol, 89%); ^{1}H NMR (THF-d_8, 303 K, 700 MHz, in ppm): δ = 0.44 (dd, J = 14.8 Hz, J = 7.0 Hz, CH_{3iPr}, 3 H), 0.68 (dd, J = 15.4 Hz, J = 7.0 Hz, CH_{3iPr}, 3 H), 0.72–0.80 (m, CH_{3iPr}, 6 H), 0.82 (*pseudo*-t, J = 7.3 Hz, CH_{3iPr}, 3 H), 0.95–0.99 (m, CH_{3iPr}, 6 H), 1.16 (dd, J = 15.1 Hz, J = 6.9 Hz, CH_{3iPr}, 3 H), 1.35 (dd, $^2J_{HH}$ = 5.0 Hz, J = 3.1 Hz, C$H_{2Mes(PNcyclo)}$, 1 H), 1.63 (s, CH_{3Ar}, 3 H), 1.65–1.71 (m, CH_{iPr}, 1 H), 1.75 (s, CH_{3Ar}, 3 H), 1.98 (s, CH_{3Ar}, 3 H), 1.99 (s, CH_{3Ar}, 3 H), 2.01–2.07 (br. m, CH_{iPr}, 2 H), 2.04 (s, CH_{3Ar}, 3 H), 2.06 (s, CH_{3Ar}, 3 H), 2.08 (s, CH_{3Ar}, 6 H), 2.11–2.13 (br. m, CH_{iPr}, 1 H), 2.14 (dd, $^2J_{HH}$ = 5.0 Hz, J = 1.6 Hz, C$H_{2Mes(PNcyclo)}$, 1 H), 2.20 (s, CH_{3Ar}, 3 H), 2.36 (s, CH_{3Ar}, 3 H), 2.51–2.54 (m, C$H_{2(2.2.2-cryptand)}$, 12 H), 3.49–3.52 (m, C$H_{2(2.2.2-cryptand)}$, 12 H), 3.55 (s, C$H_{2(2.2.2-cryptand)}$, 12 H), 5.11 (dd, J = 8.6 Hz, J = 5.2 Hz, CH_{Ar}, 1 H), 5.55 (dd, J = 8.5 Hz, J = 5.2 Hz, CH_{Ar}, 1 H), 5.94–5.96 (m, CH_{Ar}, 1 H), 6.34 (dd, J = 8.6 Hz, J = 1.8 Hz, CH_{Ar}, 1 H), 6.36–6.40 (m, CH_{Ar}, 2 H), 6.46 (s, CH_{Ar}, 2 H), 6.52 (dd, J = 5.2 Hz, J = 1.8 Hz, CH_{Ar}, 1 H), 6.66 (dd, J = 5.2 Hz, J = 2.1 Hz, CH_{Ar}, 1 H), 6.75–6.78 (m, CH_{Ar}, 1 H), 6.83–6.85 (m, CH_{Ar}, 1 H); ^{13}C{^{1}H} NMR (THF-d_8, 303 K, 176 MHz, in ppm): δ = 16.5 (d, J_{CP} = 4.4 Hz, CH$_{3iPr}$), 17.2 (d, J_{CP} = 1.9 Hz, CH$_{3iPr}$), 18.7 (d, J_{CP} = 11.6 Hz, CH$_{3iPr}$), 19.0 (d, J_{CP} = 11.0 Hz, CH$_{3iPr}$), 19.2 (d, J_{CP} = 16.7 Hz, CH$_{3iPr}$), 19.7 (d, J_{CP} = 16.2 Hz, CH$_{3iPr}$), 19.8 (s, CH_{3Ar}), 20.3 (s, CH_{3Ar}), 20.4 (s, CH_{3Ar}; d, J_{CP} = 9.1 Hz, CH$_{3iPr}$), 20.8 (s, CH_{3Ar}), 21.0 (s, CH_{3Ar}), 21.03 (s, CH_{3Ar}), 21.04 (d, J_{CP} = 11.1 Hz, CH$_{3iPr}$), 21.1 (d, J_{CP} = 3.7 Hz, CH$_{3Ar}$), 21.2 (s, CH_{3Ar}), 21.5 (s, CH_{3Ar}), 22.2 (s, CH_{3Ar}), 23.1 (s, CH$_{iPr}$), 25.9 (s, CH$_{iPr}$), 26.2 (d, J_{CP} = 4.2 Hz, CH$_{iPr}$), 54.9 (s, CH$_{2(2.2.2-cryptand)}$), 61.3 (s, CH$_{2Mes(PNcyclo)}$), 68.7 (s, CH$_{2(2.2.2-cryptand)}$), 71.5 (s, CH$_{2(2.2.2-cryptand)}$), 111.7 (d, J_{CP} = 7.1 Hz, CH$_{Ar}$), 112.0 (d, J_{CP} = 6.3 Hz, CH$_{Ar}$), 114.9 (d, J_{CP} = 11.0 Hz, C_{qAr}), 115.2 (d, J_{CP} = 7.9 Hz, C_{qAr}), 116.2 (d, J_{CP} = 2.6 Hz, C_{qAr}), 117.6 (d, J_{CP} = 2.3 Hz, C_{qAr}), 118.7 (s, CH$_{Ar}$), 121.0 (s, C_{qAr}), 123.8 (s, CH$_{Ar}$), 126.3 (s, C_{qAr}), 128.7 (s, CH$_{Ar}$), 130.2 (s, CH$_{Ar}$), 130.9 (s, CH$_{Ar}$), 131.8 (s, C_{qAr}), 131.9 (s, CH$_{Ar}$), 132.2 (s, CH$_{Ar}$), 133.3 (d, J_{CP} = 3.4 Hz, CH$_{Ar}$), 133.6 (d, J_{CP} = 2.7 Hz, CH$_{Ar}$), 136.2 (d, J_{CP} = 3.4 Hz, C_{qAr}), 136.5 (s, C_{qAr}), 137.3 (s, C_{qAr}), 139.1 (s, C_{qAr}), 146.7 (d, J_{CP} = 2.6 Hz, C_{qAr}), 147.0 (s, C_{qAr}), 162.6 (d, J_{CP} = 21.4 Hz, C_{qAr}), 163.9 (d, J_{CP} = 24.7 Hz, C_{qAr}), 164.2 (s, C_{qAr}); ^{31}P{^{1}H} NMR (THF-d_8, 303 K, 283 MHz, in ppm): δ = –1.4 (d, $^2J_{PP}$ = 33.3 Hz, $P(^i$Pr$)_2$, 1 P), 1.0 (d, $^2J_{PP}$ = 33.3 Hz, $P(^i$Pr$)_2$, 1 P); elemental analysis (in %): $C_{71}H_{108}KLaN_4O_7P_2$: calcd.: C 62.26, H 7.95, N 4.09; found: C 61.83, H 7.53, N 4.10.

Isotope labelling experiment: Reaction of 1-d with KHMDS in the presence of 18-crown-6.

A solution of KHMDS (5 mg, 25 µmol, 1. eq.) in DME (0.5 mL) was added dropwise to a mixture of **1-*d*** (24 mg, 25 µmol, 1 eq.) and 18-crown-6 (6.6 mg, 25 µmol, 1 eq.) in DME (0.5 mL) at room temperature, giving an orange-coloured solution. After 10 min an aliquot of ≈0.6 mL was transferred to a J-Young NMR tube equipped with a sealed C_6D_6 capillary and $^{31}P\{^1H\}$, ^{31}P and ^2H NMR spectra were measured to determine the deuteration level of the product and to check for $DN(SiMe_3)_2$ (Fig. S60–S65). Prior to the experiment the respective NMR data of the starting material **1-*d*** in DME with a sealed C_6D_6 capillary were collected as a reference.

Trapping experiment: Reaction of 1-d with KHMDS in the presence of 18-crown-6 in cyclohexene.

A solution of KHMDS (10 mg, 50 µmol, 1. eq.) in cyclohexene (1 mL) was added dropwise to a mixture of **1-*d*** (49 mg, 50 µmol, 1 eq.) and 18-crown-6 (13 mg, 50 µmol, 1 eq.) in cyclohexene (2 mL) at room temperature, giving an orange-coloured solution. After 10 min an aliquot of ≈0.6 mL was transferred to a J-Young NMR tube equipped with a sealed C_6D_6 capillary. $^{31}P\{^1H\}$ as well as ^{31}P NMR spectra were measured (Fig. S66 and S67) which indicated quite clean formation of **3a** (see also: Preparation of **3a**, Route B), but no trapping of transient phosphinidene complex **2** with cyclohexene in significant amounts. (Notably, >99% conversion of the *PD* group in **1-*d*** to the *PH* group in **3a** had occurred. After 3 d, no D/H scrambling between **3a** and DHMDS was observed and only **3a** containing >99% *PH* was crystallised from the reaction mixture (see Fig. S24).)

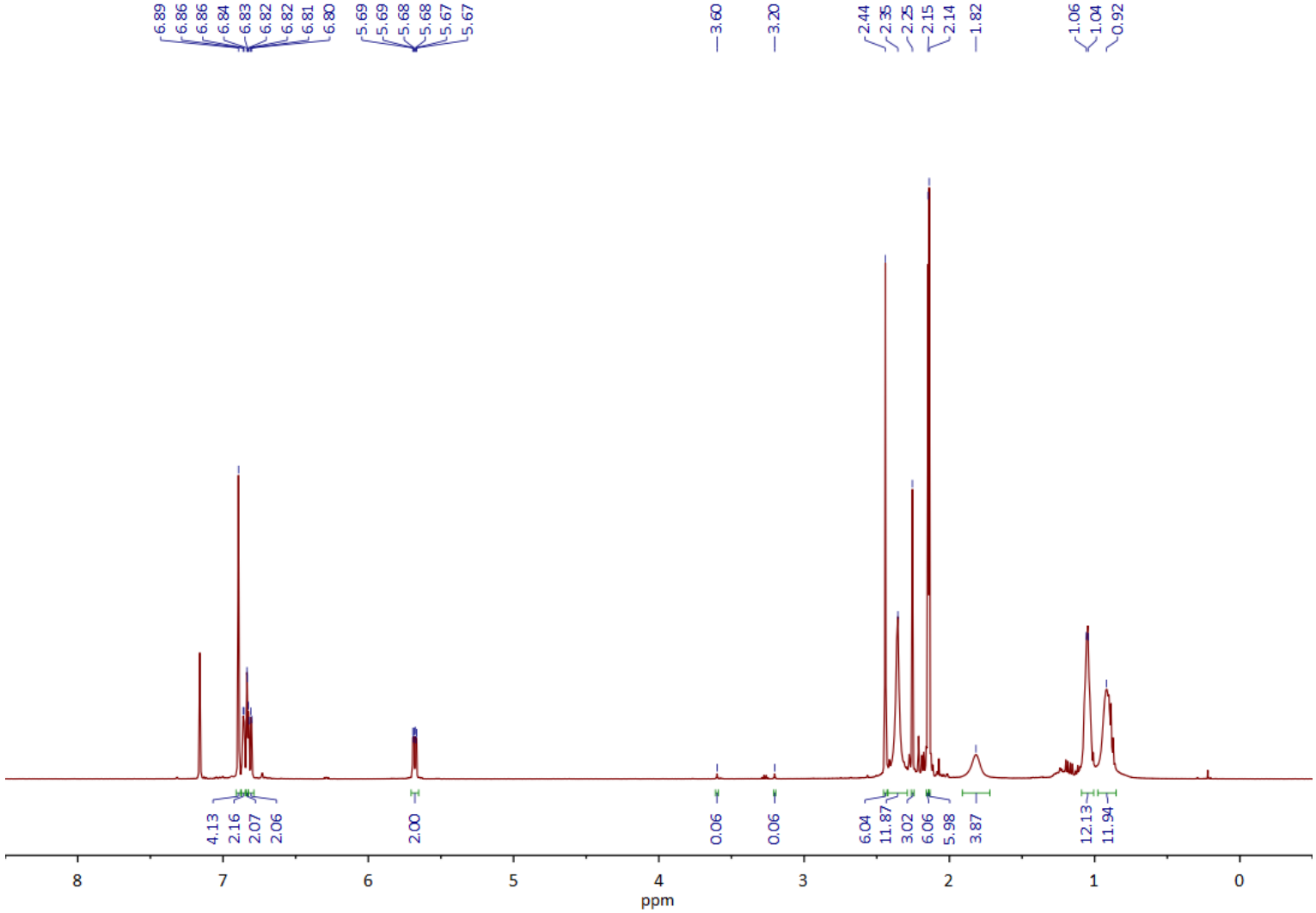
NMR scale conversion of 3b into [K(2.2.2-cryptand)][(PN)$_2$La(P$_2$Mes$_2$)] (6).

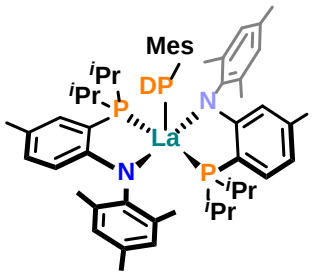
A solution of **3b** (25 mg, 18 µmol) in THF-d_8 (0.6 mL) was transferred to a J-Young NMR tube and heated at 50 °C for 3 d. The progress of the reaction was regularly controlled by means of $^{31}P\{^1H\}$ NMR spectroscopy (Fig. S68). After full consumption of starting material **3b**, gas diffusion of *n*-hexane into the reaction solution at room temperature overnight yielded only a layer of orange-coloured oil. Therefore, all volatiles were removed *in vacuo*, the residue extracted with diethyl ether (1 mL) and filtered through a glass-fibre filter. Concentrating the filtrate to ca. 0.2 mL and storing it at room temperature for 2 d yielded orange-coloured crystals of **6** suitable for X-ray structure determination. Despite the low X-ray quality of the crystals, the connectivity of **6** could be unambiguously determined. No yield could be determined. $^{31}P\{^1H\}$ NMR (THF-d_8, 303 K, 202 MHz, in ppm): δ = 9.3 (s, *P*N$^-$, 2 P), 30.5 (br. s, $P_2Mes_2^{2-}$, 2 P).

X-ray Crystallography

Single crystals for X-ray diffraction experiments were measured at the analytical facility of the Paderborn University using a Bruker Smart AXS or a Bruker D8 Venture instrument. All crystals were kept at 130(2) K or 120(2) K throughout data collection. Data collection was performed using either the APEXIII or the Smart software package. Data refinement and reduction were performed with Bruker Saint (V8.34A). All structures were solved with SHELXT[3,4] and refined using the OLEX 2 software package.[5] All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were included at the geometrically calculated positions and refined using a riding model. All structures have been submitted to the CCDC and can be obtained under the numbers presented in Table S1. For further crystallographic details regarding crystal measurements, please check Tables S1 and S2.

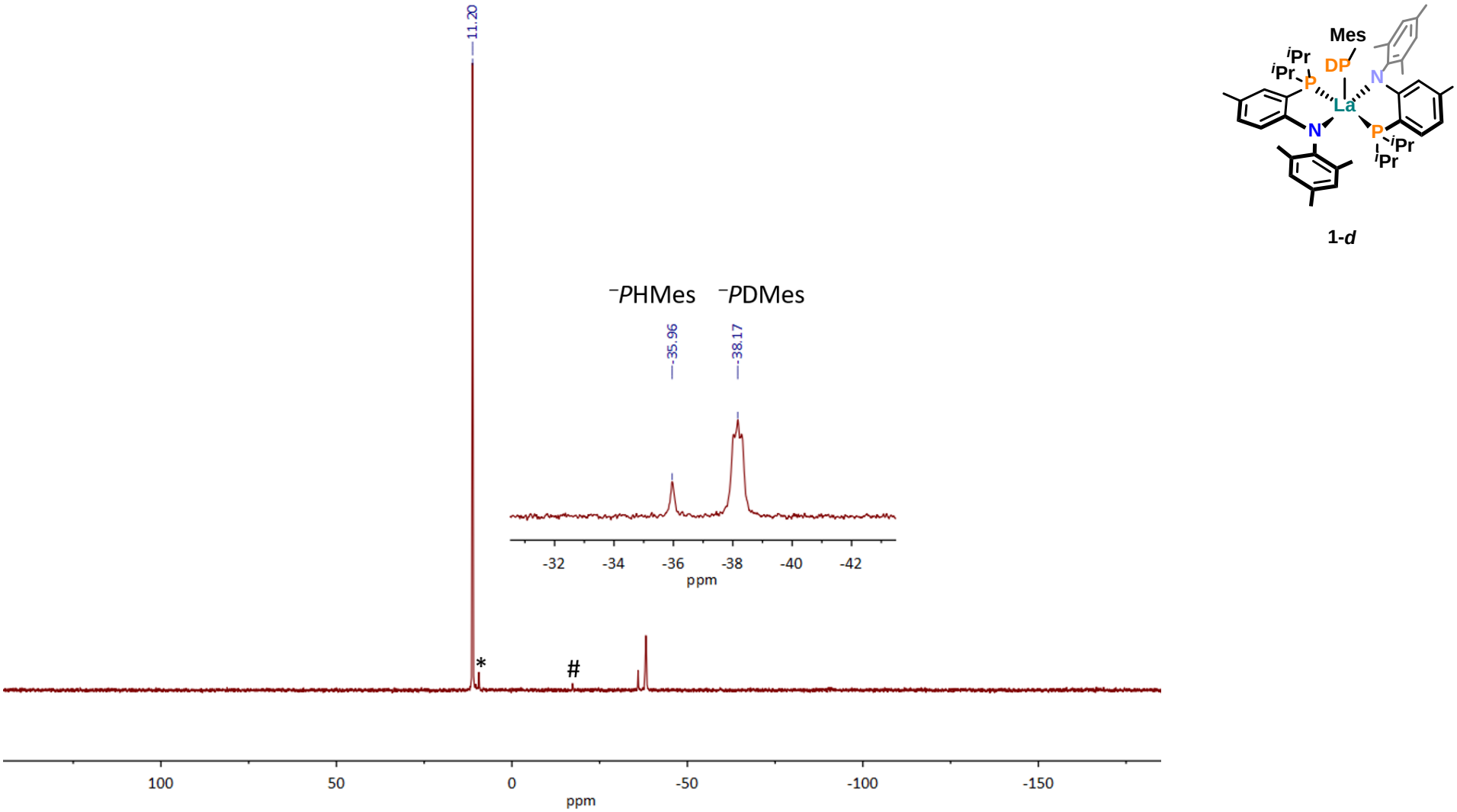
2. NMR Spectra





1-*d*

Fig. S1: *^{1}H NMR spectrum of **1-d** (≈86–88% isotopic purity) in C_6D_6 (303 K). The integral values of the doublet at δ = 3.40 ppm ($^{1}J_{PH}$ = 198.5 Hz) of 0.06 each correspond to in total ≈12% remaining PH groups.*



1-*d*

Fig. S2: *$^{31}P\{^{1}H\}$ NMR spectrum of **1-d** (≈86–88% isotopic purity) in C_6D_6 (303 K). The enlargement shows the resonances of the ⁻PDMes ligand as well as residual ⁻PHMes ligand (see caption of Fig. S1). Traces of starting complex $(PN)_2LaCl$ are marked by an asterisk (*). Traces of protonated ligand HPN are marked by #.*

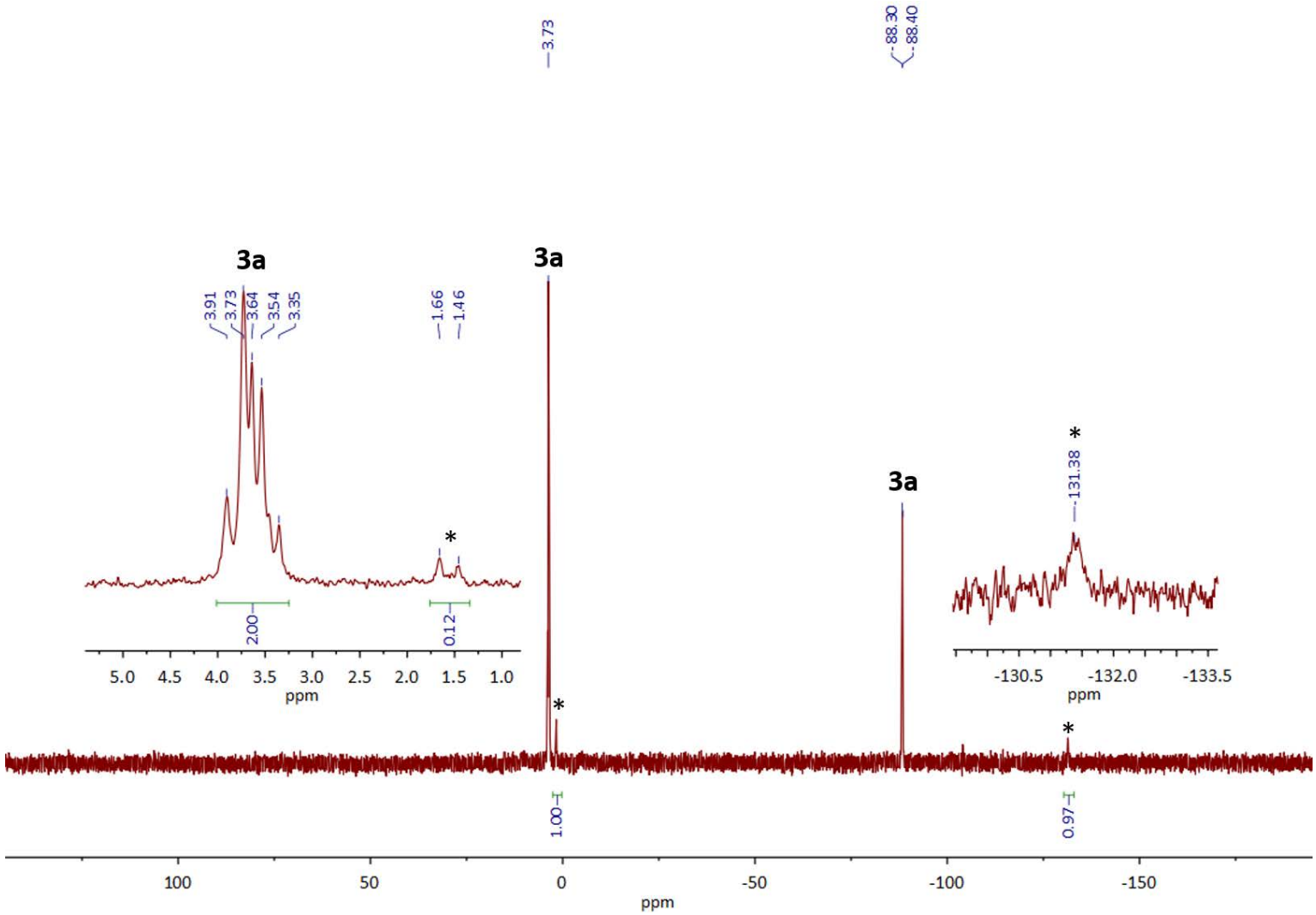
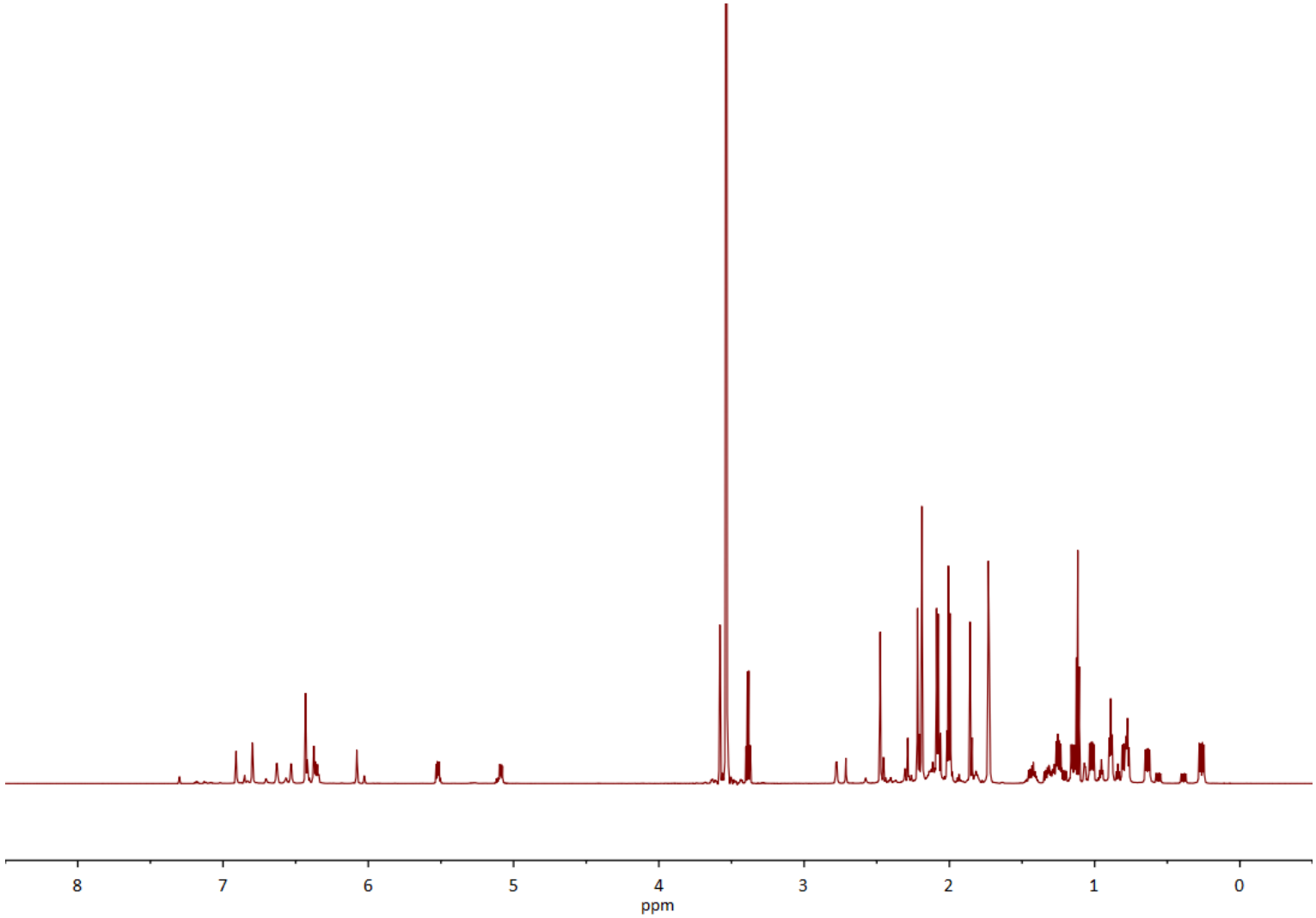
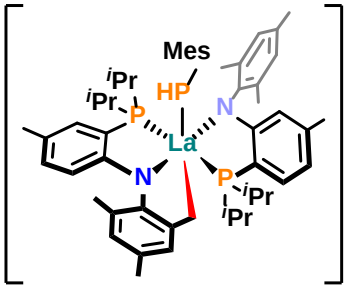


Fig. S3: $^{31}P\{^{1}H\}$ *NMR spectrum of the reaction mixture (after 10 min reaction time) of* ***1****, 18-crown-6* and *benzyl potassium in DME (Route A) with a sealed* C_6D_6 *capillary (303 K). Besides the main product* ***3a****, significant amounts of an unknown C–H activated side product (δ = 1.6 ppm; ≈12%) form along with the appearance of a new resonance at δ = 131.4 ppm (see the two enlargements). The impurities seem to form in a defined ratio of ≈1:1 as indicated by the integral values given at the bottom.*



[K(18C6)]



3a

Fig. S4: *^{1}H NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K).*

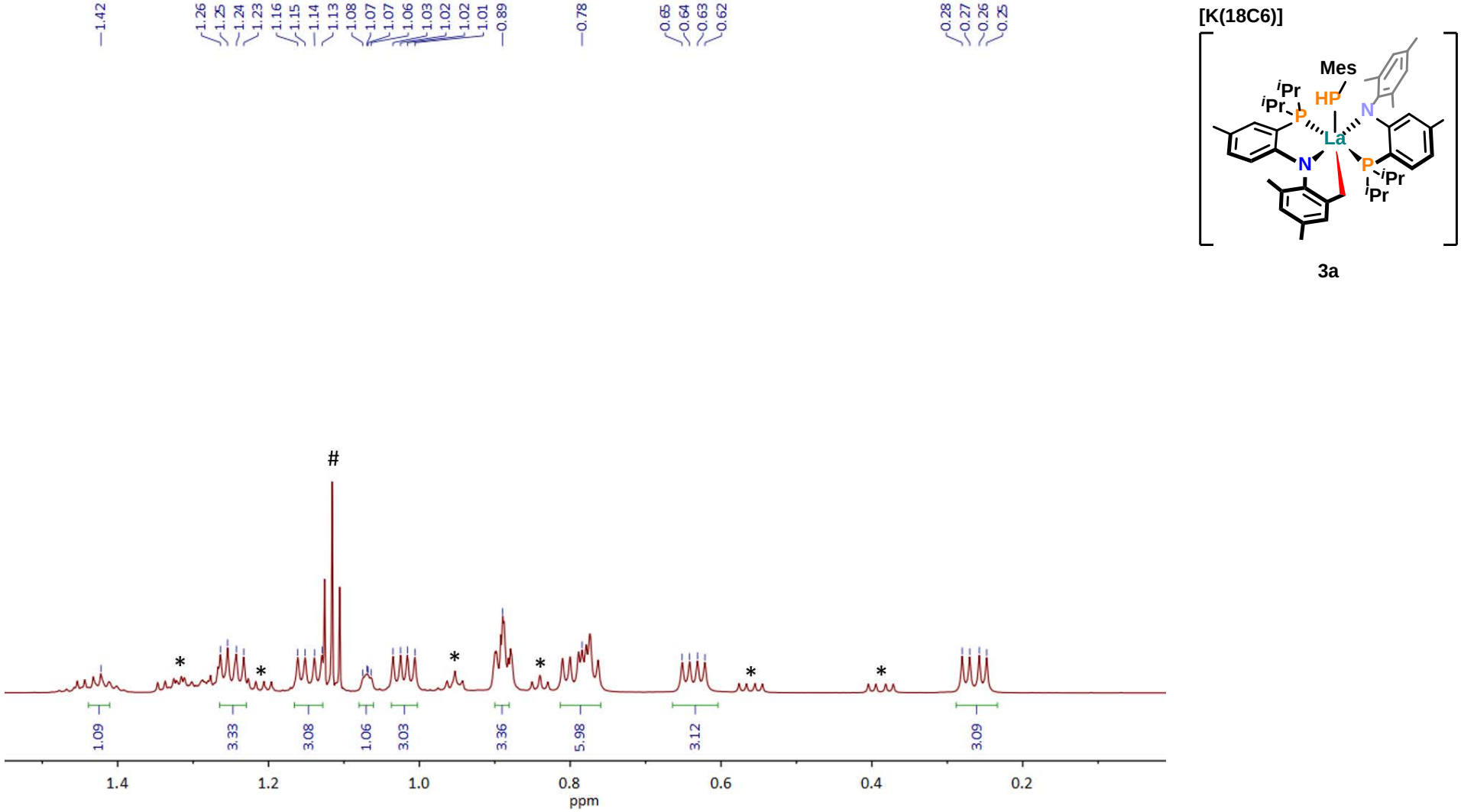
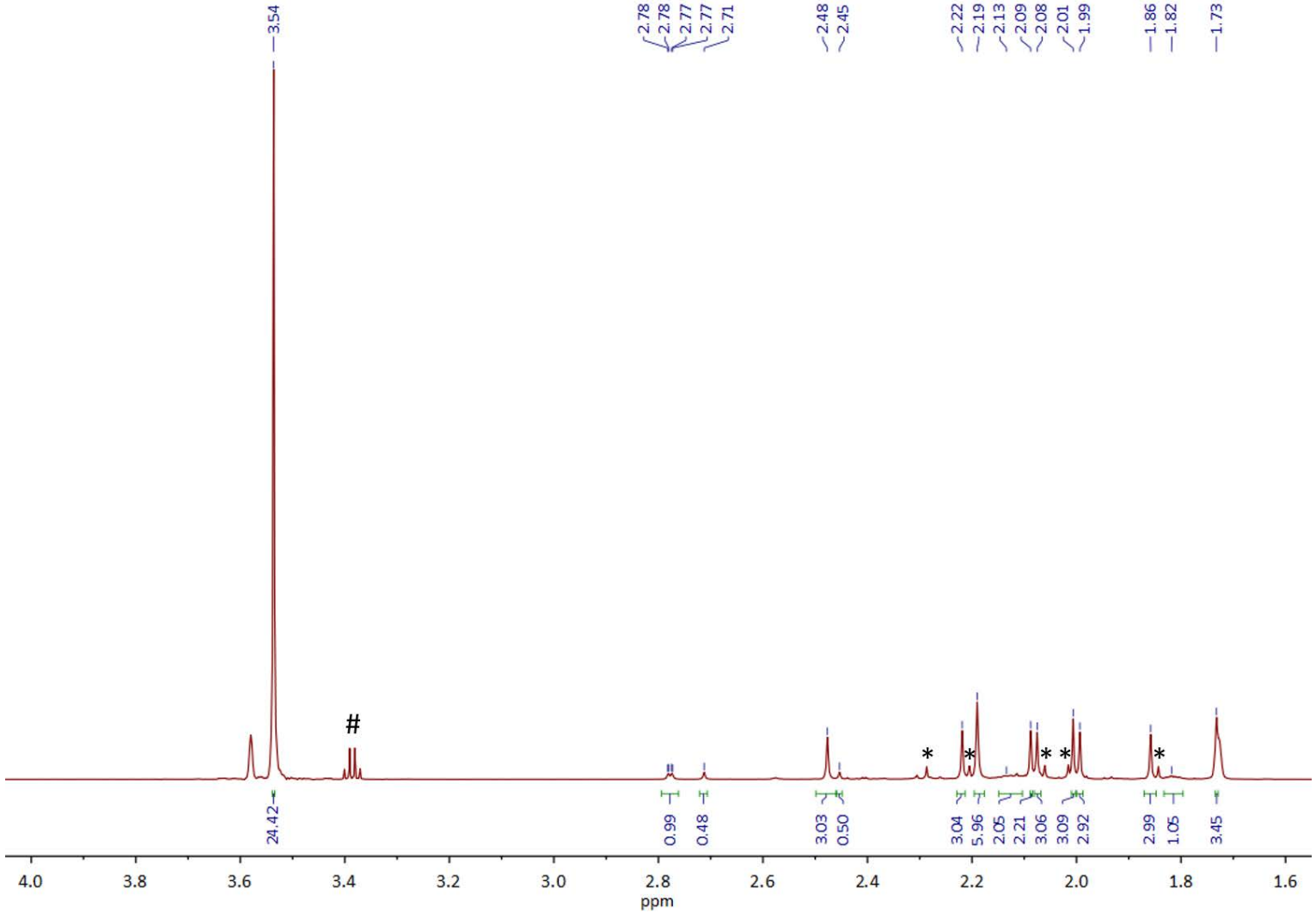
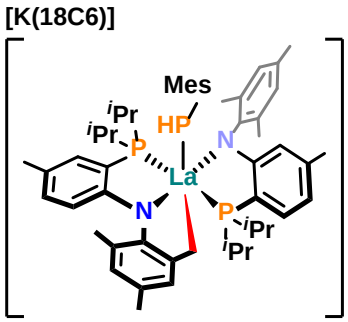


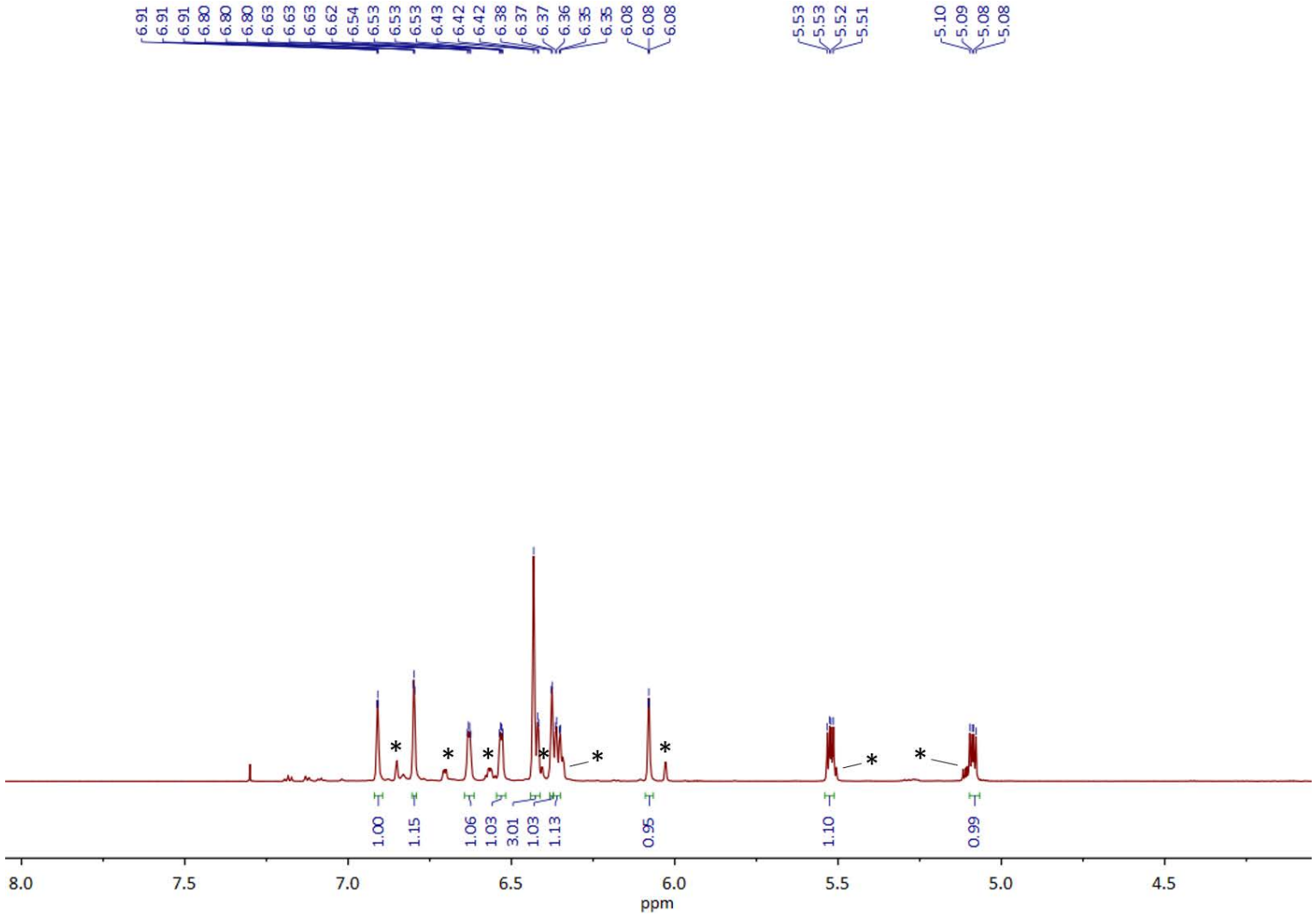
Fig. S5: *Section of the ^{1}H NMR spectrum (δ = 0.1 – 1.55 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonances of an as yet unidentified C–H activated side product are marked by asterisks (*). Residual diethyl ether from work-up is marked by #.*

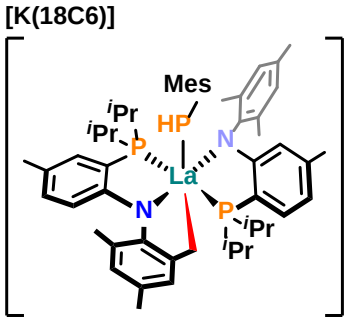




3a

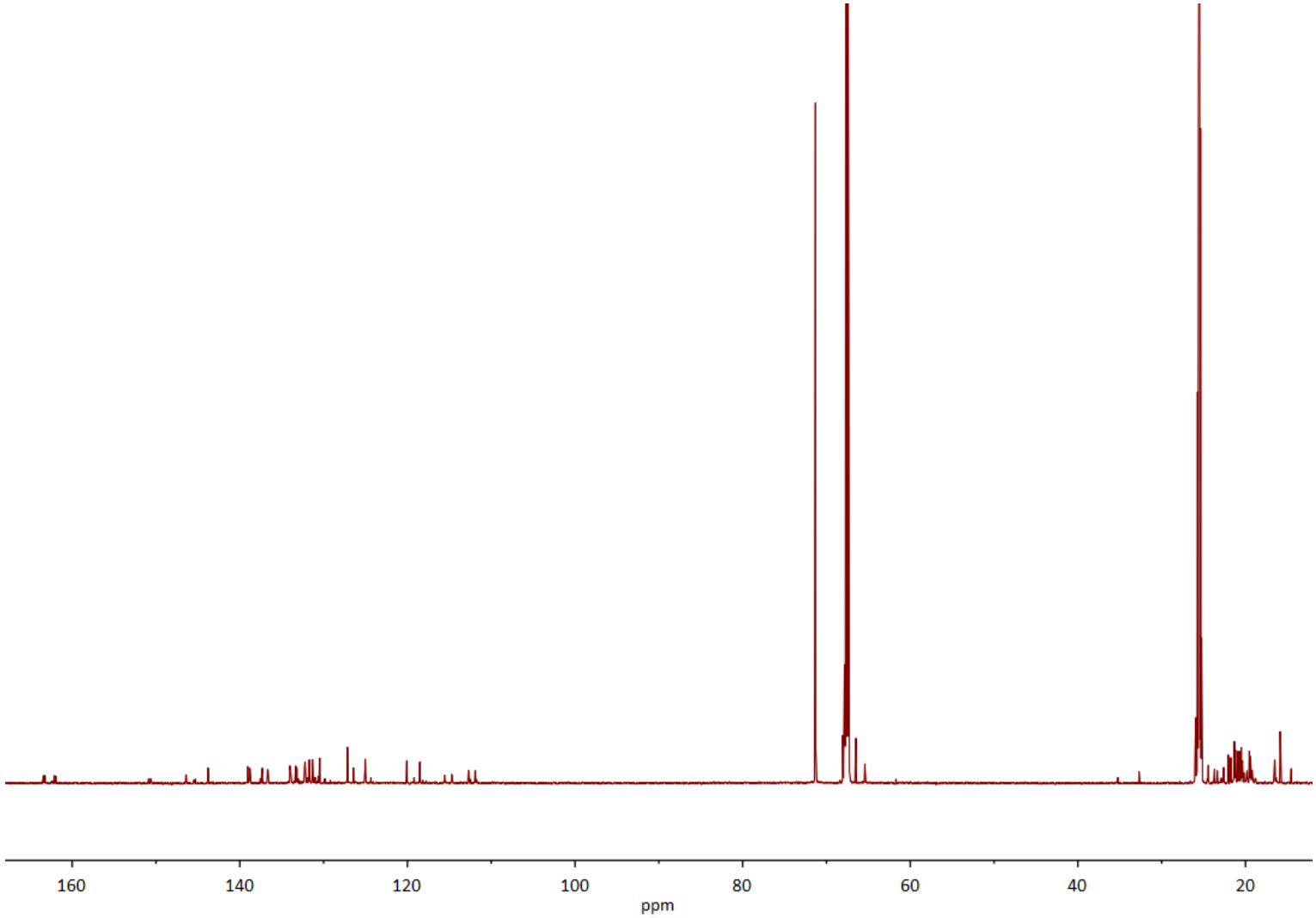
Fig. S6: *Section of the ^{1}H NMR spectrum (δ = 1.55 – 4.05 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonances of an as yet unidentified C–H activated side product are marked by asterisks (*). Residual diethyl ether from work-up is marked by #.*

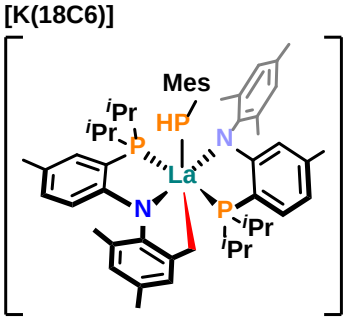




3a

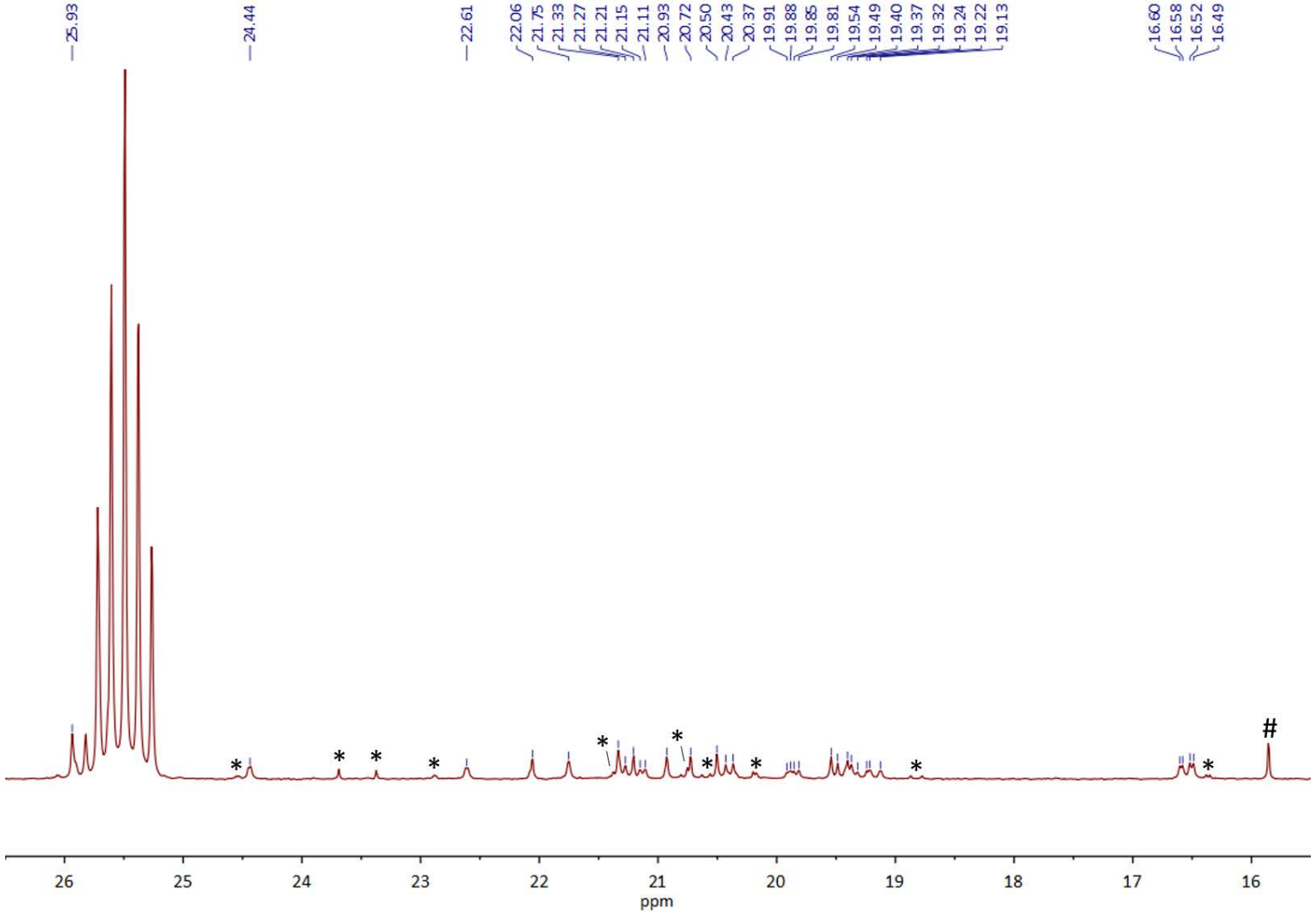
Fig. S7: *Section of the ^{1}H NMR spectrum (δ = 4.05 – 8.05 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonances of an as yet unidentified C–H activated side product are marked by asterisks (*).*

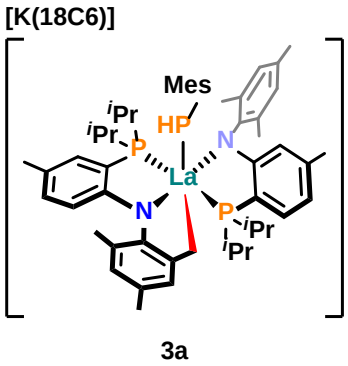




3a

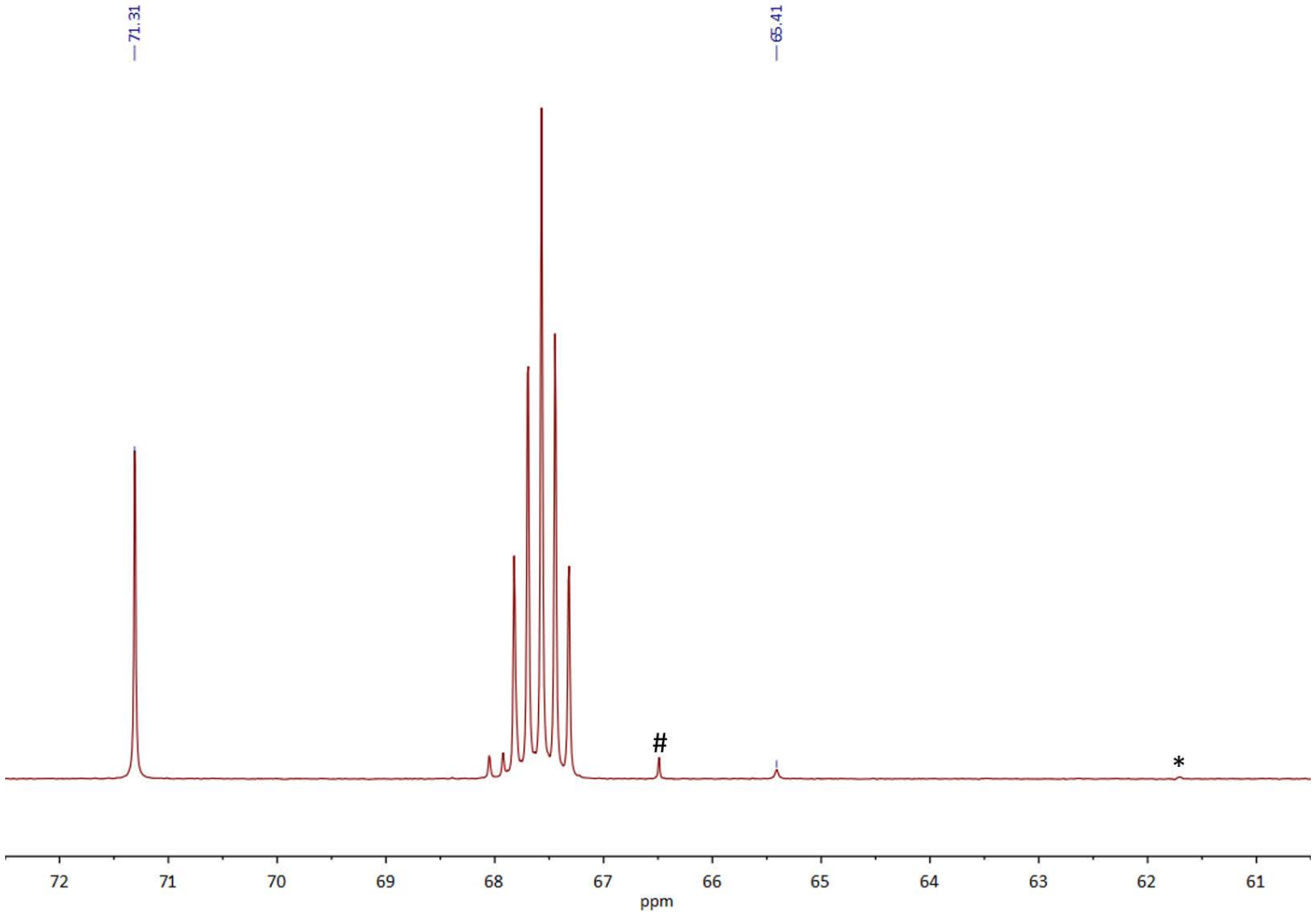
Fig. S8: *$^{13}C\{^{1}H\}$ NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K).*

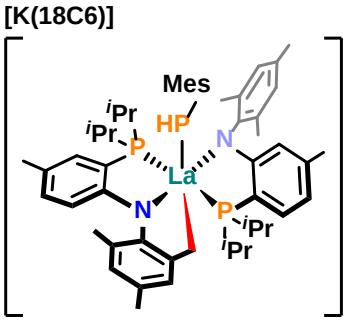




3a

Fig. S9: *Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 15.5 – 26.5 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonances of an as yet unidentified C–H activated side product are marked by asterisks (*). Residual diethyl ether from work-up is marked by #.*





3a

Fig. S10: *Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 60.5 – 72.5 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonance of an as yet unidentified C–H activated side product is marked by an asterisk (*). Residual diethyl ether from work-up is marked by #.*

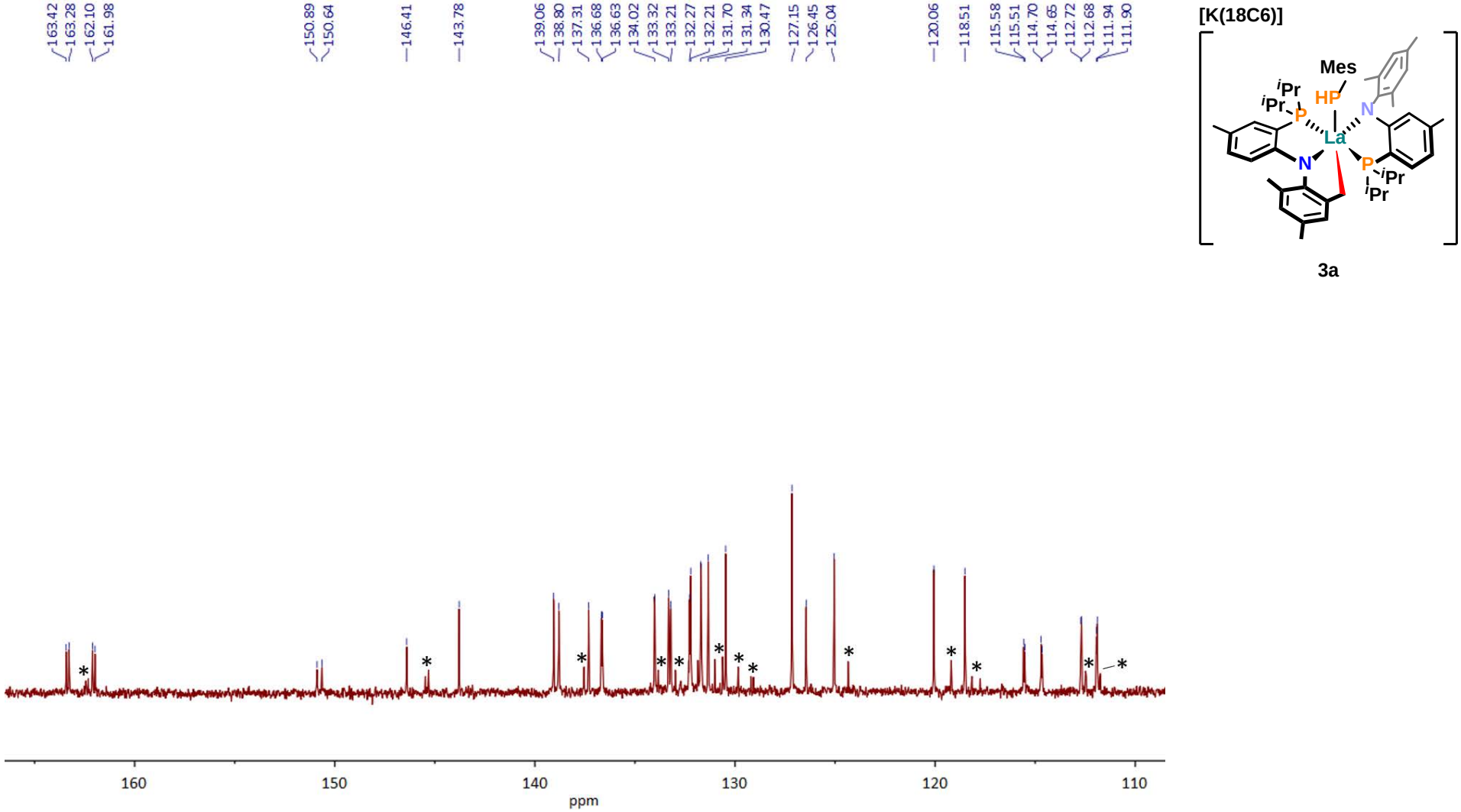
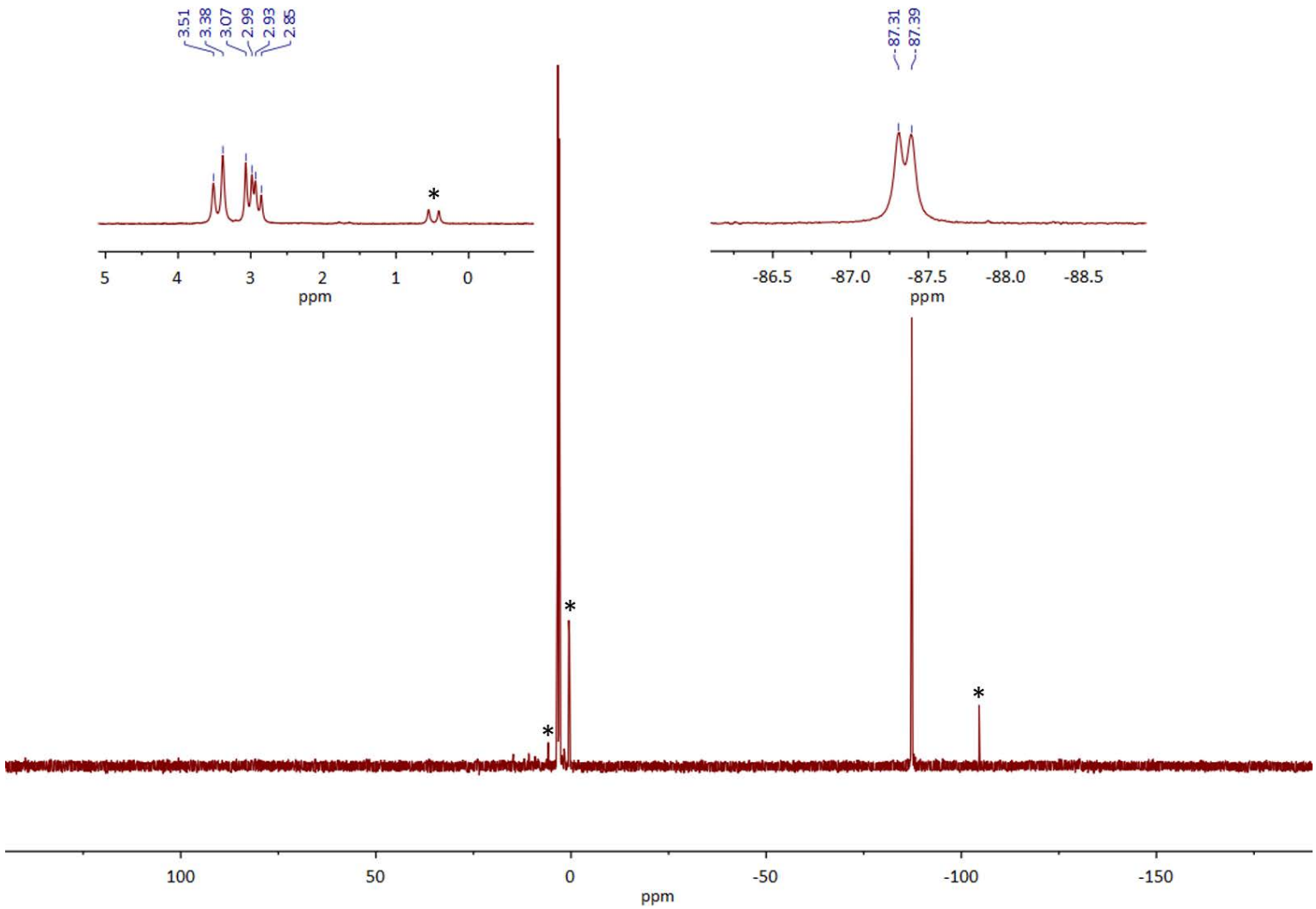
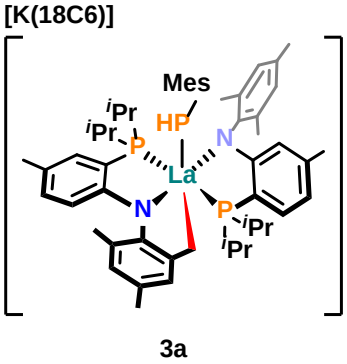


Fig. S11: *Section of the $^{13}C\{^1H\}$ NMR spectrum (δ = 108.5 – 166.5 ppm) of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The resonances of an as yet unidentified C–H activated side product are marked by asterisks (*). Residual diethyl ether from work-up is marked by #.*





3a

Fig. S12: *$^{31}P\{^{1}H\}$ NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The two enlargements show the main product's multiplet at δ = 2.7 –3.7 ppm (left) and doublet at δ = –87.4 ppm (right). In the left enlargement one resonance of the as yet unidentified C–H activated side product is marked by an asterisk (*), the other one is obscured by the resonances of **3a** at δ = 2.7 –3.7 ppm. Other unknown impurities are also marked by asterisks (*).*

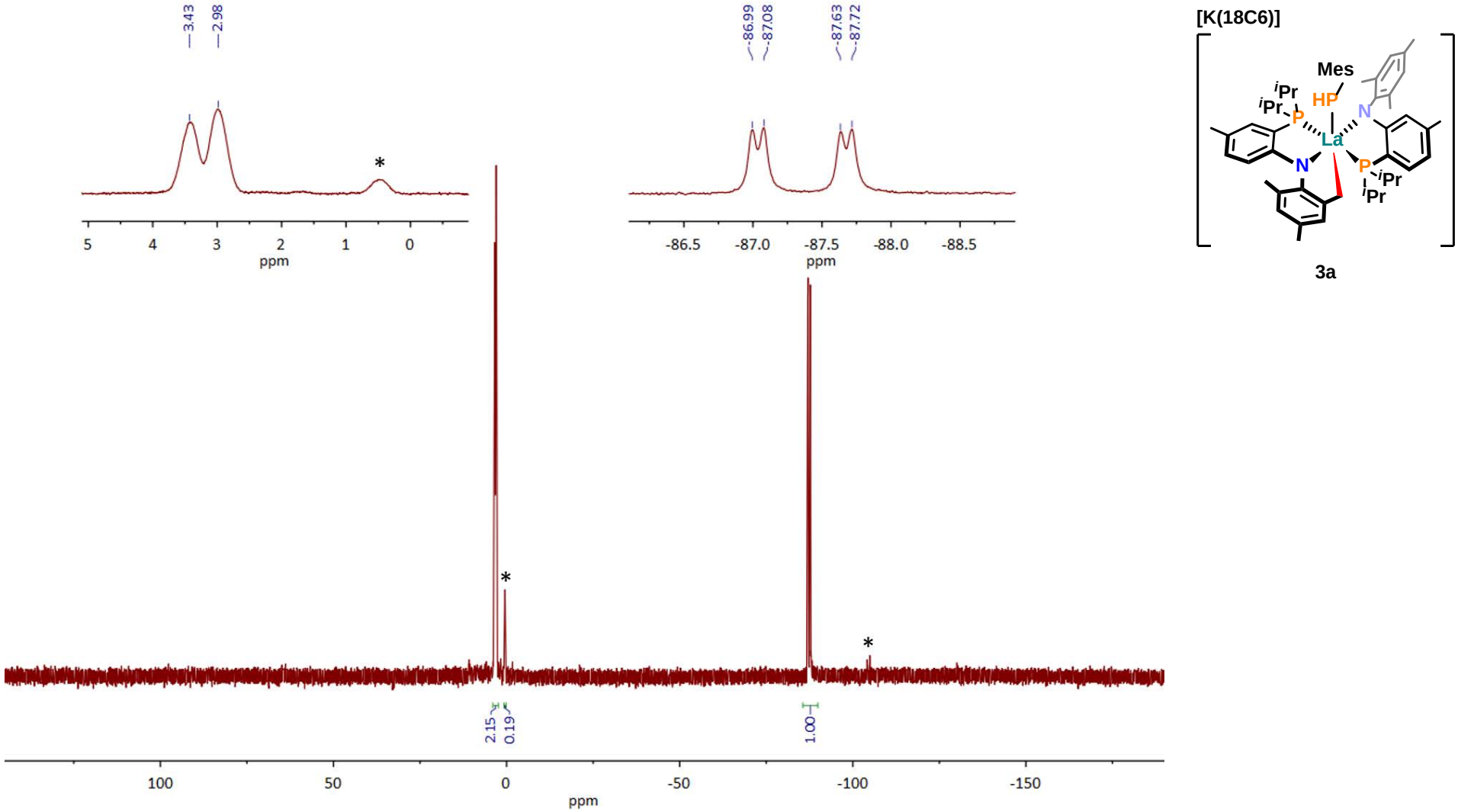
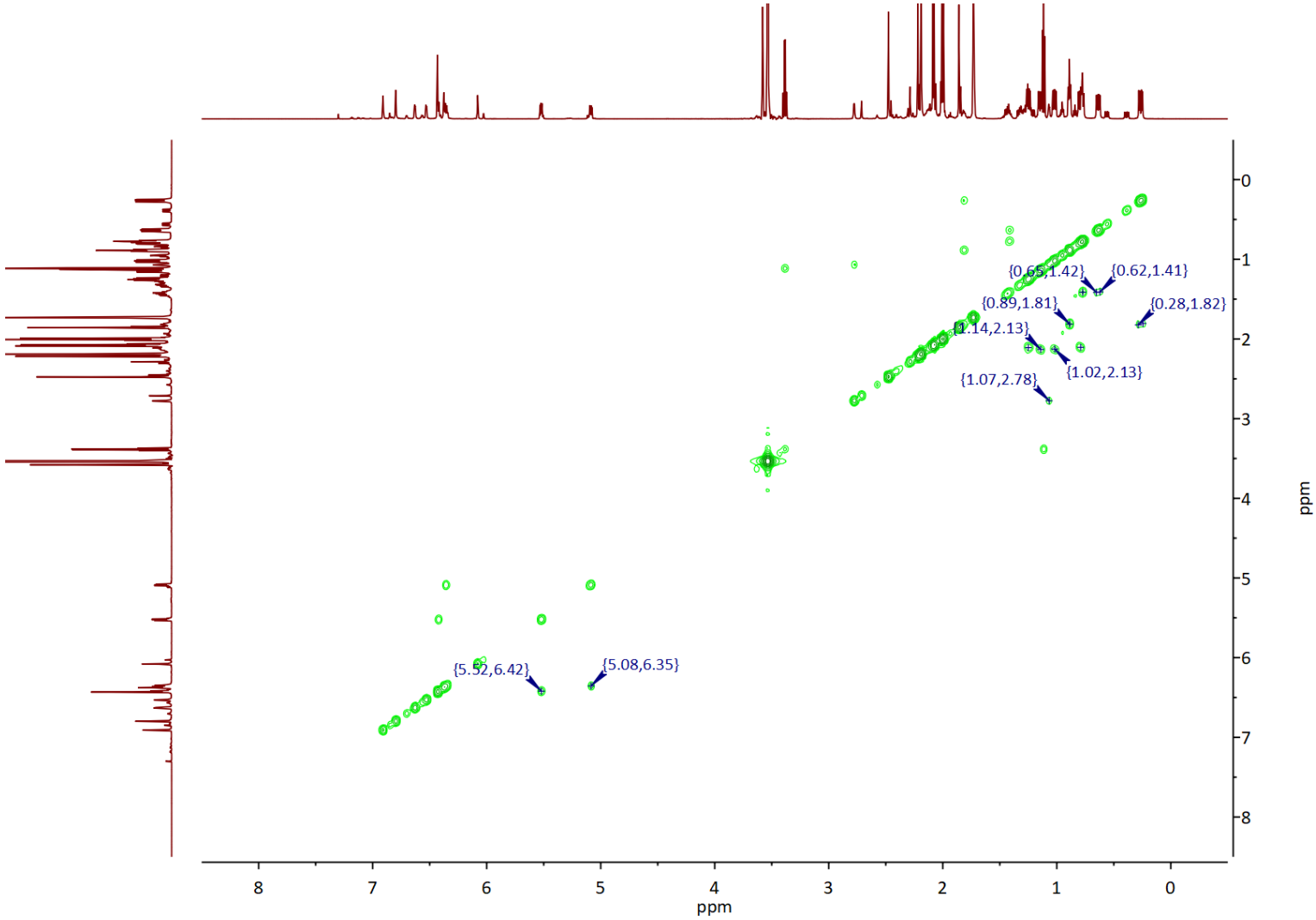
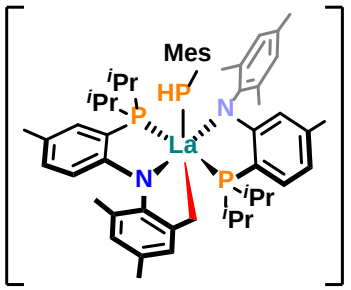


Fig. S13: *^{31}P NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The two enlargements show the main product's broad multiplet at δ = 2.7 –3.7 ppm (left) and the doublet of doublets at δ = –87.4 ppm (right). In the left enlargement one resonance of the as yet unidentified C–H activated side product is marked by an asterisk (*), the other one is obscured by the resonances of **3a** at δ = 2.7 –3.7 ppm. Other unknown impurities are also marked by asterisks (*).*



[K(18C6)]



3a

Fig. S14: *^{1}H–^{1}H COSY NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K).*

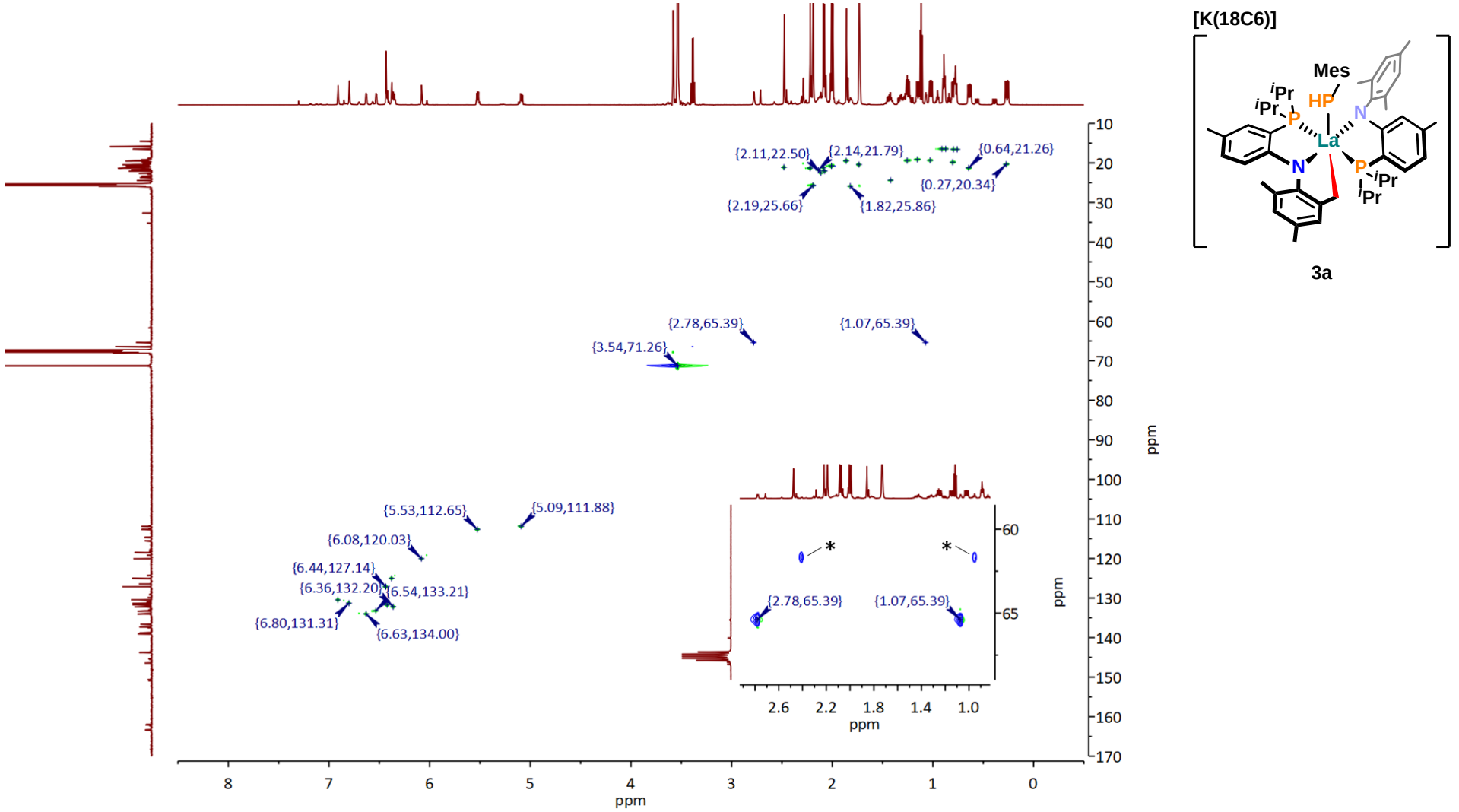
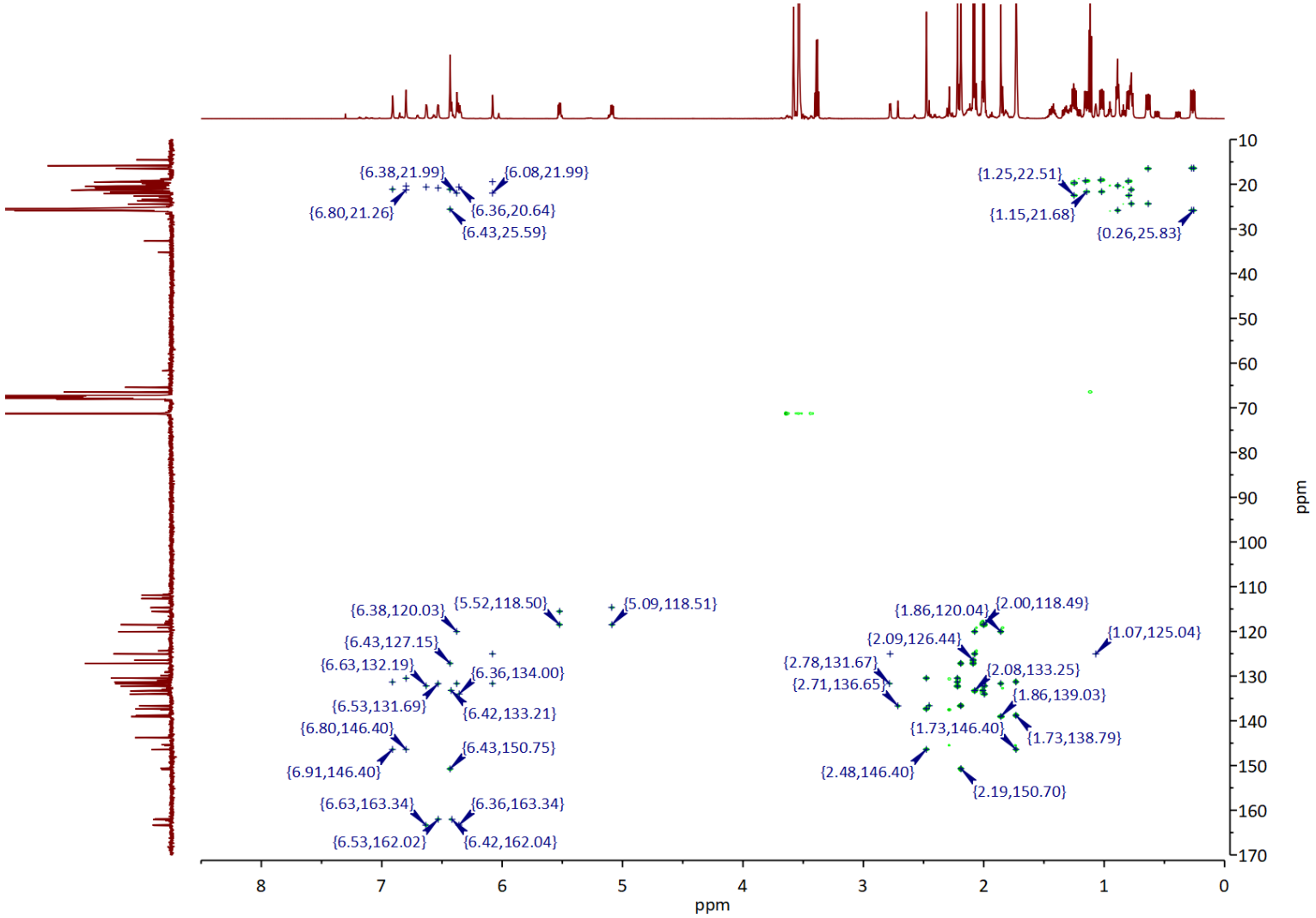
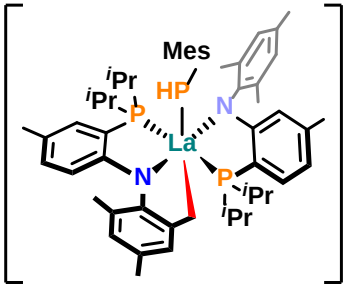


Fig. S15: *^{1}H–^{13}C HSQC NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K). The enlargement shows the two cross peaks for the $CH_{2Mes(PNcyclo)}$ methylene protons of **3a**, the analogous cross peaks of the as yet unidentified C–H activated side product are marked by asterisks (*).*

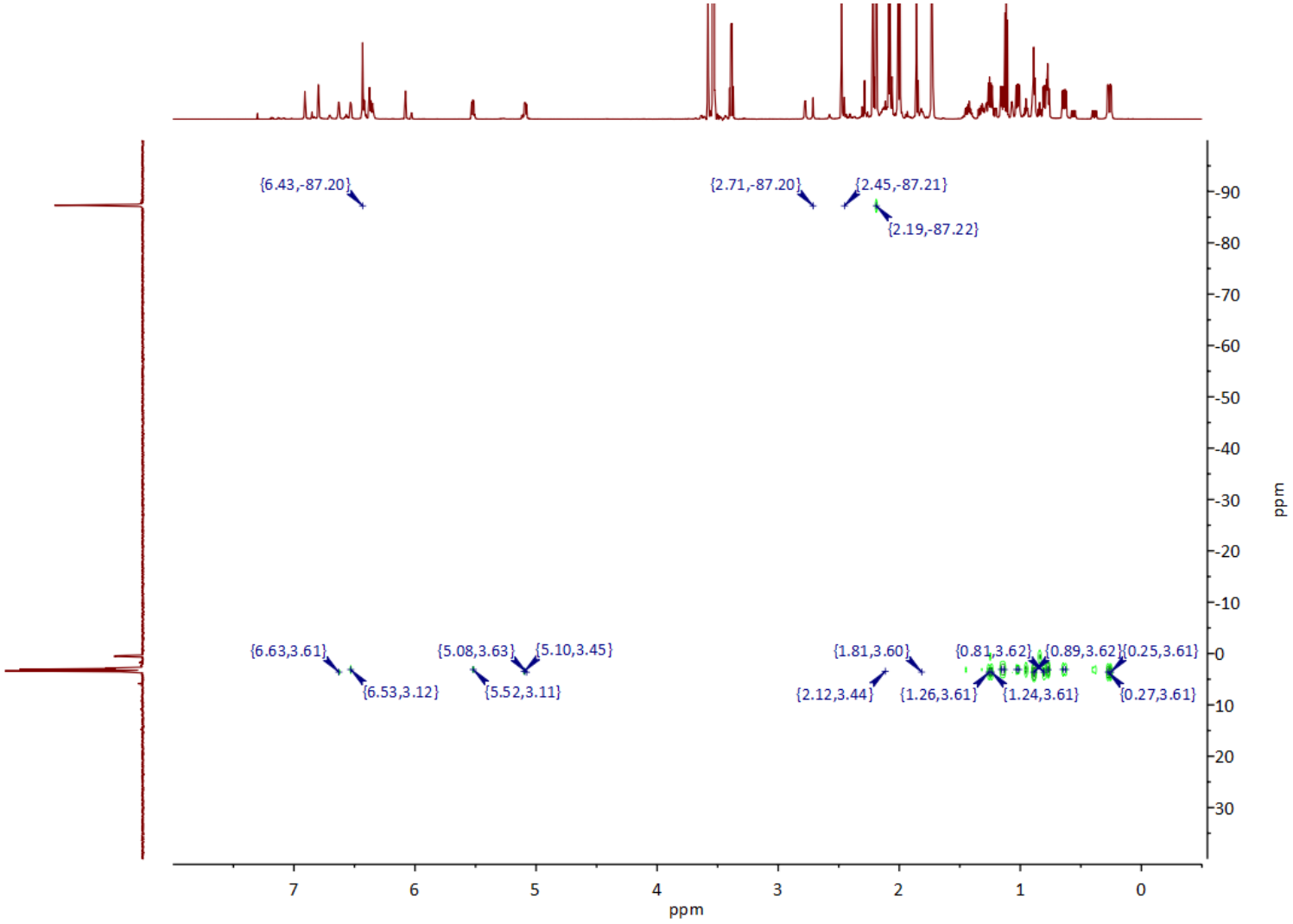


[K(18C6)]



3a

Fig. S16: *^{1}H–^{13}C HMBC NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K).*



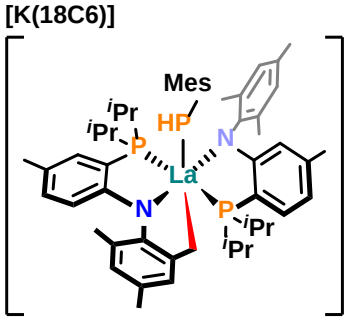
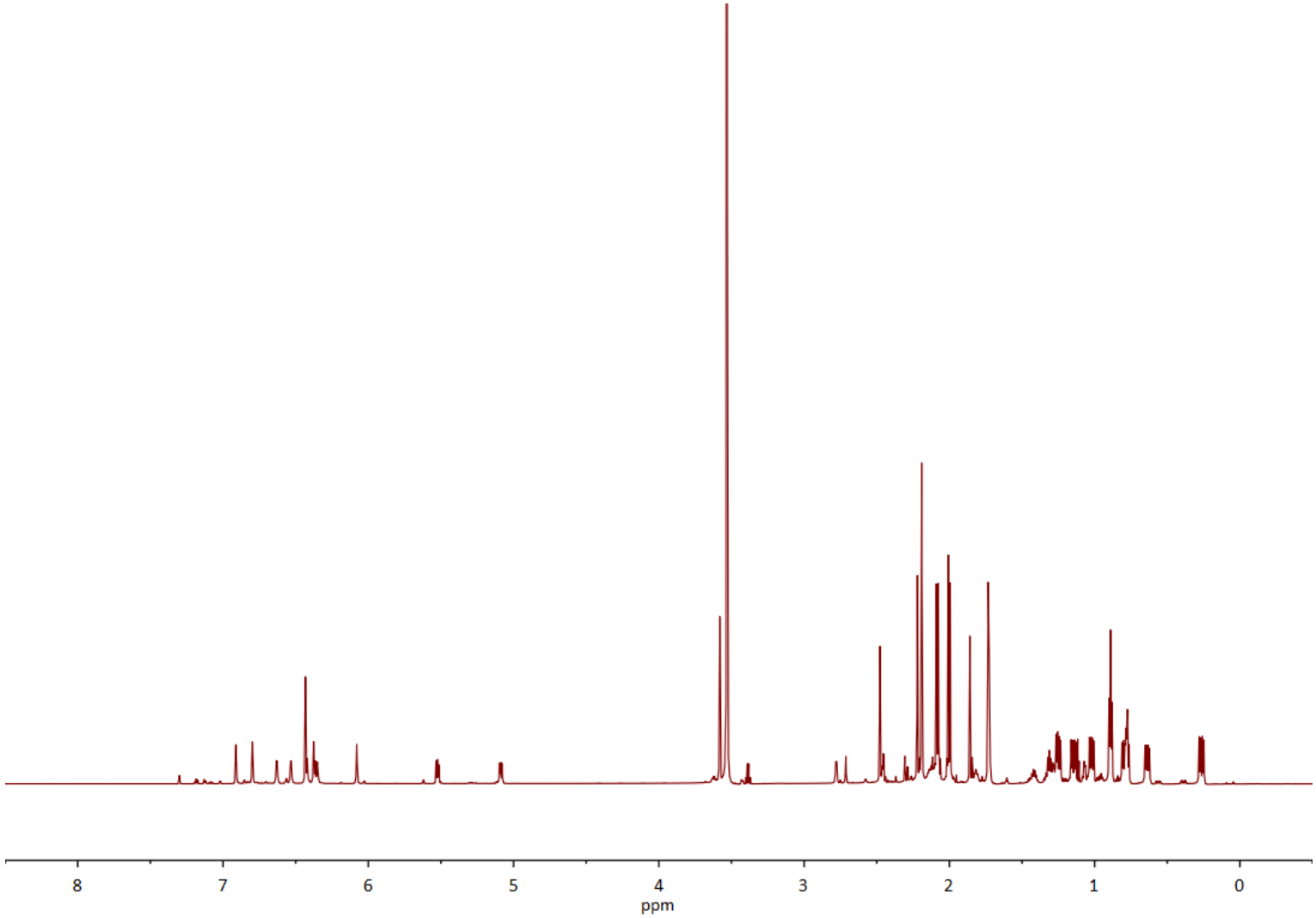
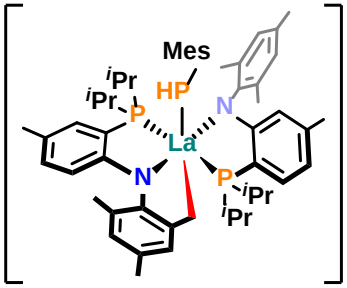


Fig. S17: *^{1}H–^{31}P HMBC NMR spectrum of **3a** (≈85% purity, obtained by Route A) in THF-d_8 (303 K).*



[K(18C6)]



3a

Fig. S18: *^{1}H NMR spectrum of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K).*

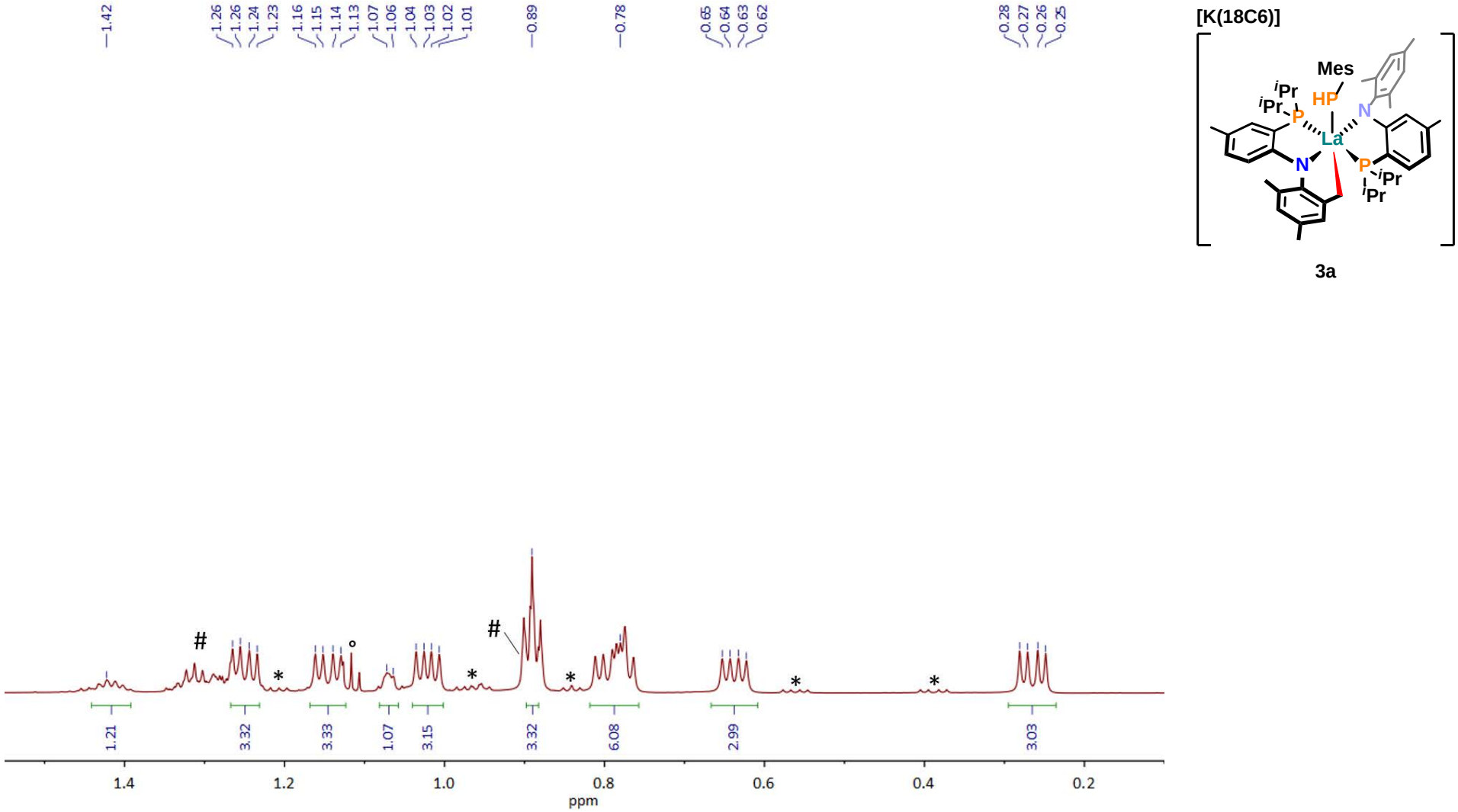
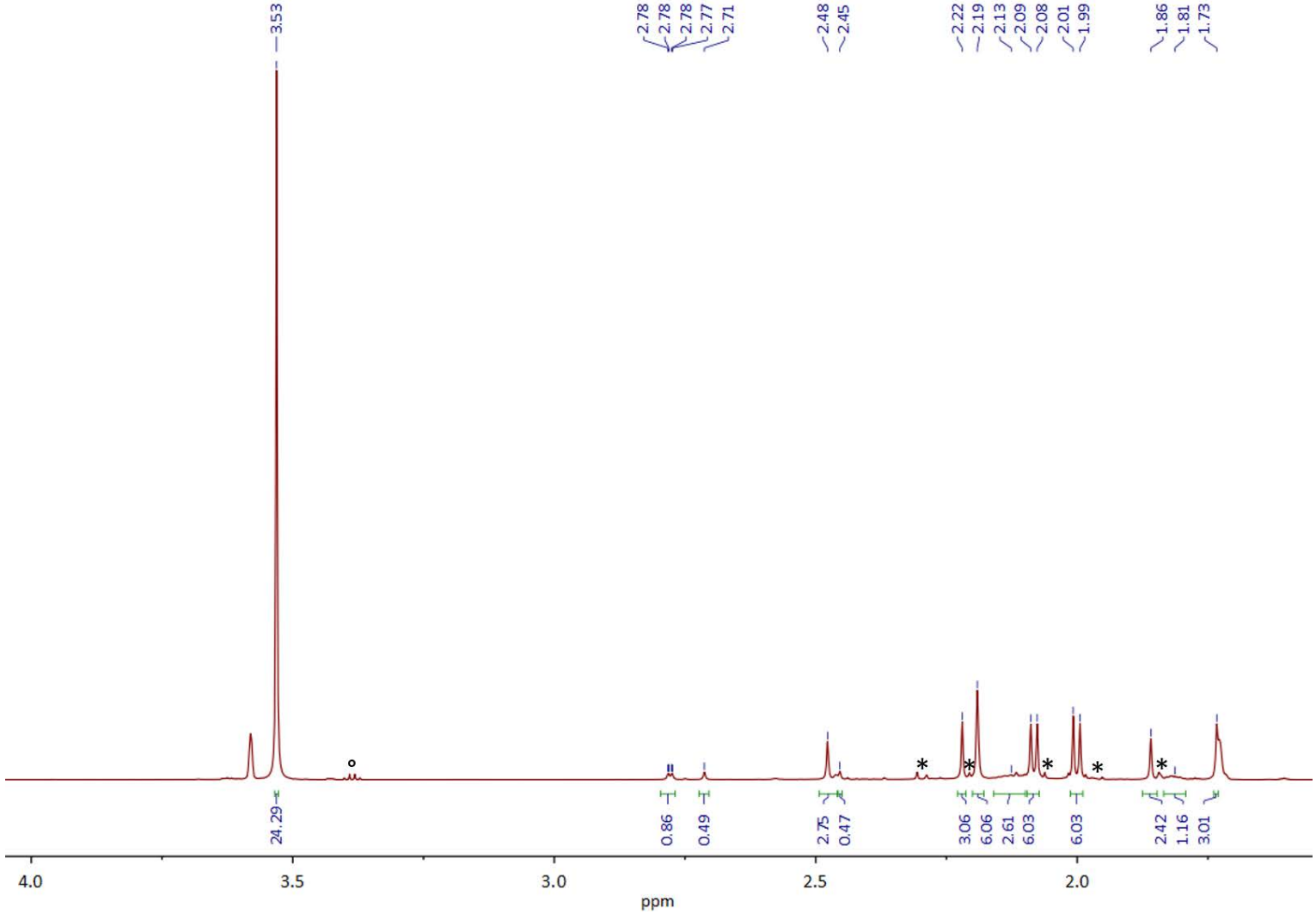
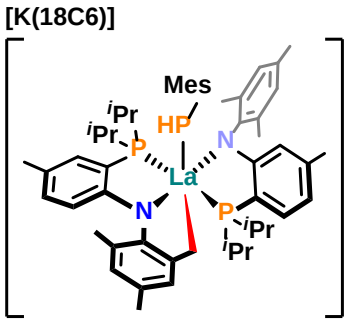


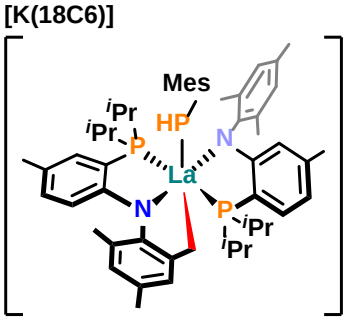
Fig. S19: *Section of the ^{1}H NMR spectrum (δ = 0.1 – 1.55 ppm) of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). The peak at δ = 0.89 ppm overlaps with a peak of n-pentane. Residual n-pentane from work-up is marked by #. Traces of diethyl ether are marked by °. Traces of unknown impurities are marked by asterisks (*).*





3a

Fig. S20: *Section of the ^{1}H NMR spectrum (δ = 1.55 – 4.05 ppm) of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). Traces of diethyl ether are marked by °. Traces of unknown impurities are marked by asterisks (*).*



3a

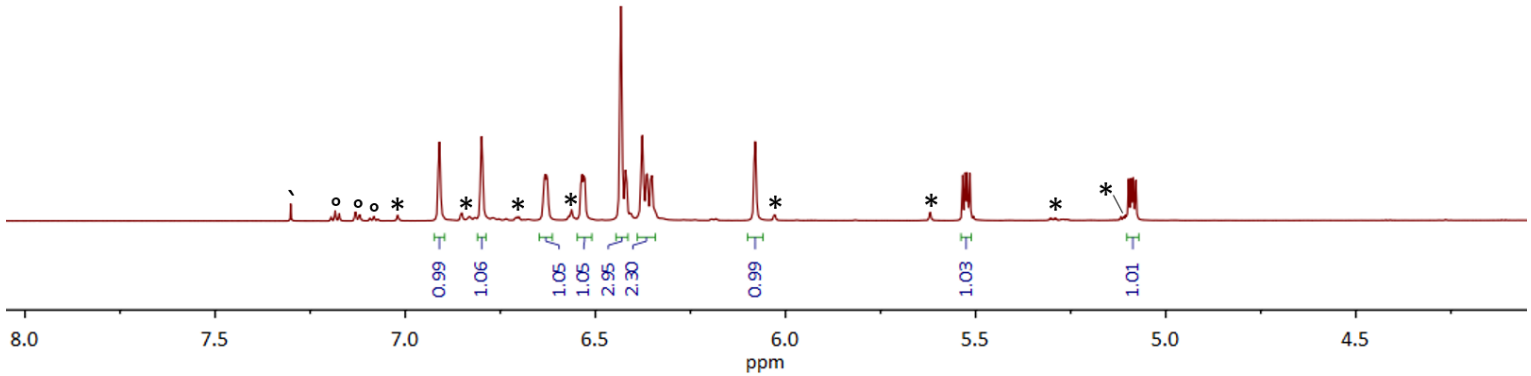
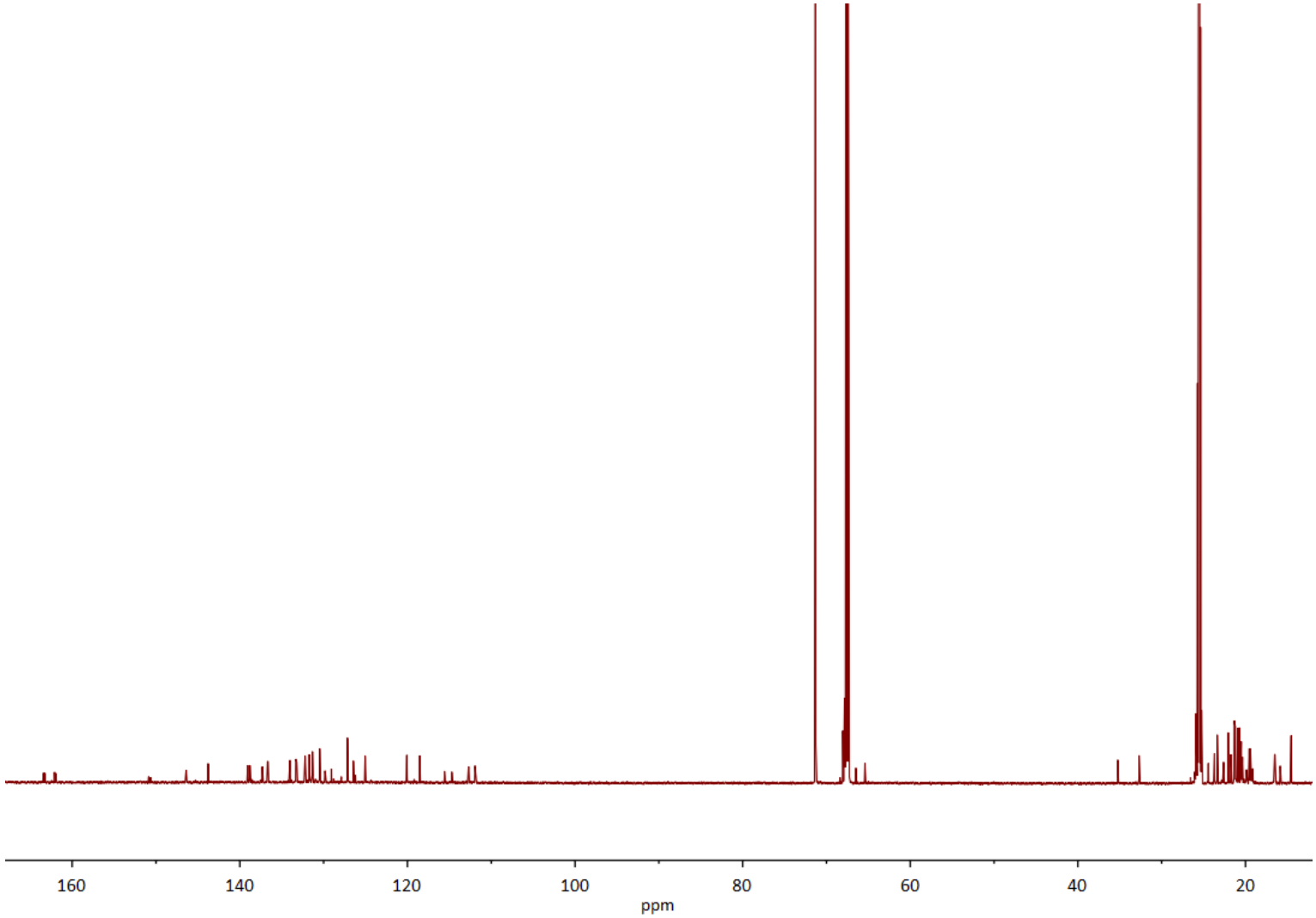
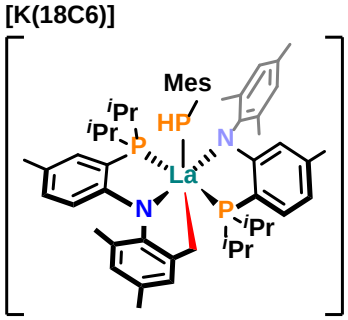


Fig. S21: *Section of the ^{1}H NMR spectrum (δ = 4.05 – 8.05 ppm) of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). Traces of toluene are marked by °. Traces of benzene are marked by `. Traces of unknown impurities are marked by asterisks (*).*





3a

Fig. S22: *$^{13}C\{^{1}H\}$ NMR spectrum of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). For assignments please see the corresponding $^{13}C\{^{1}H\}$ NMR data of material obtained by Route A (Fig. S9–S11).*

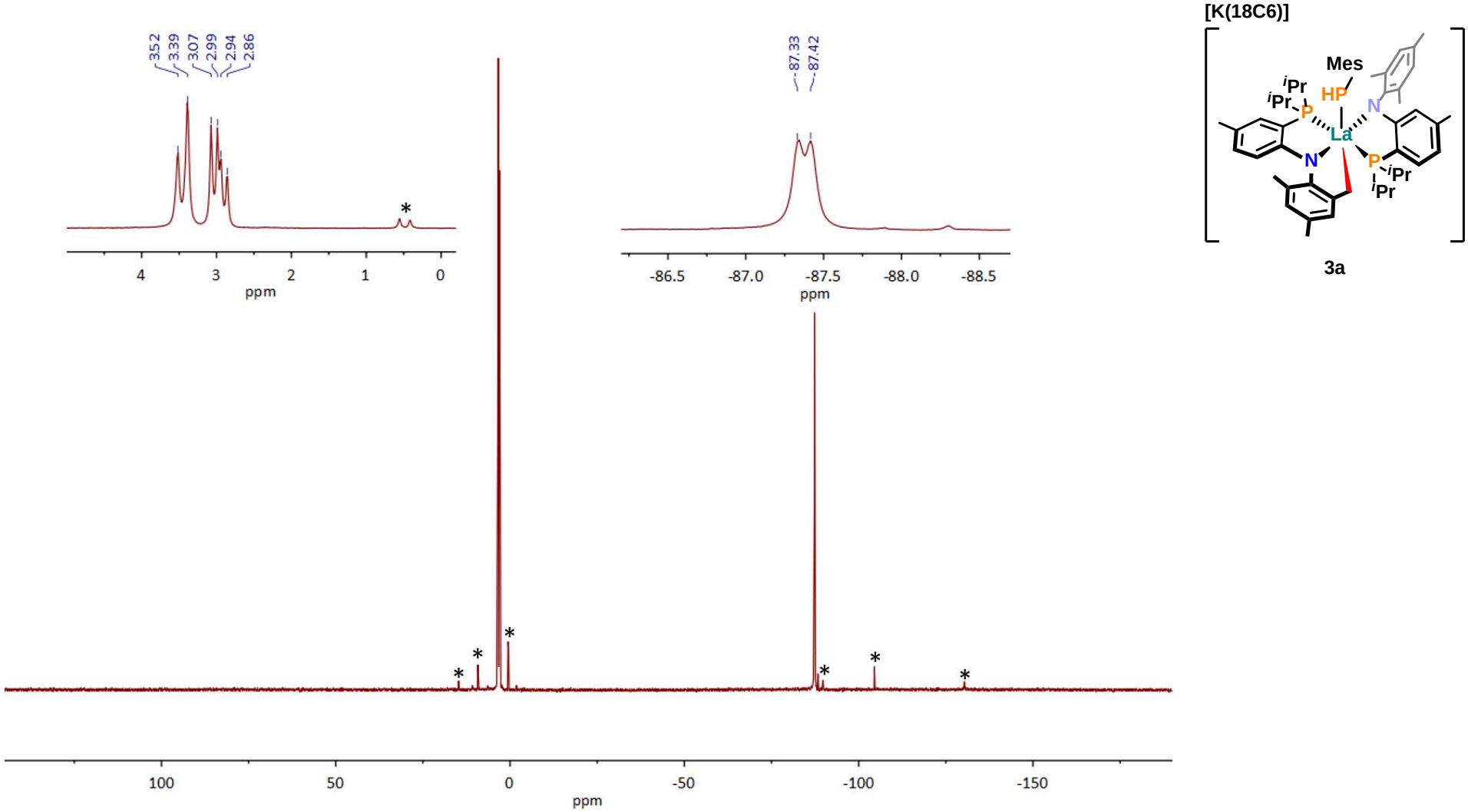
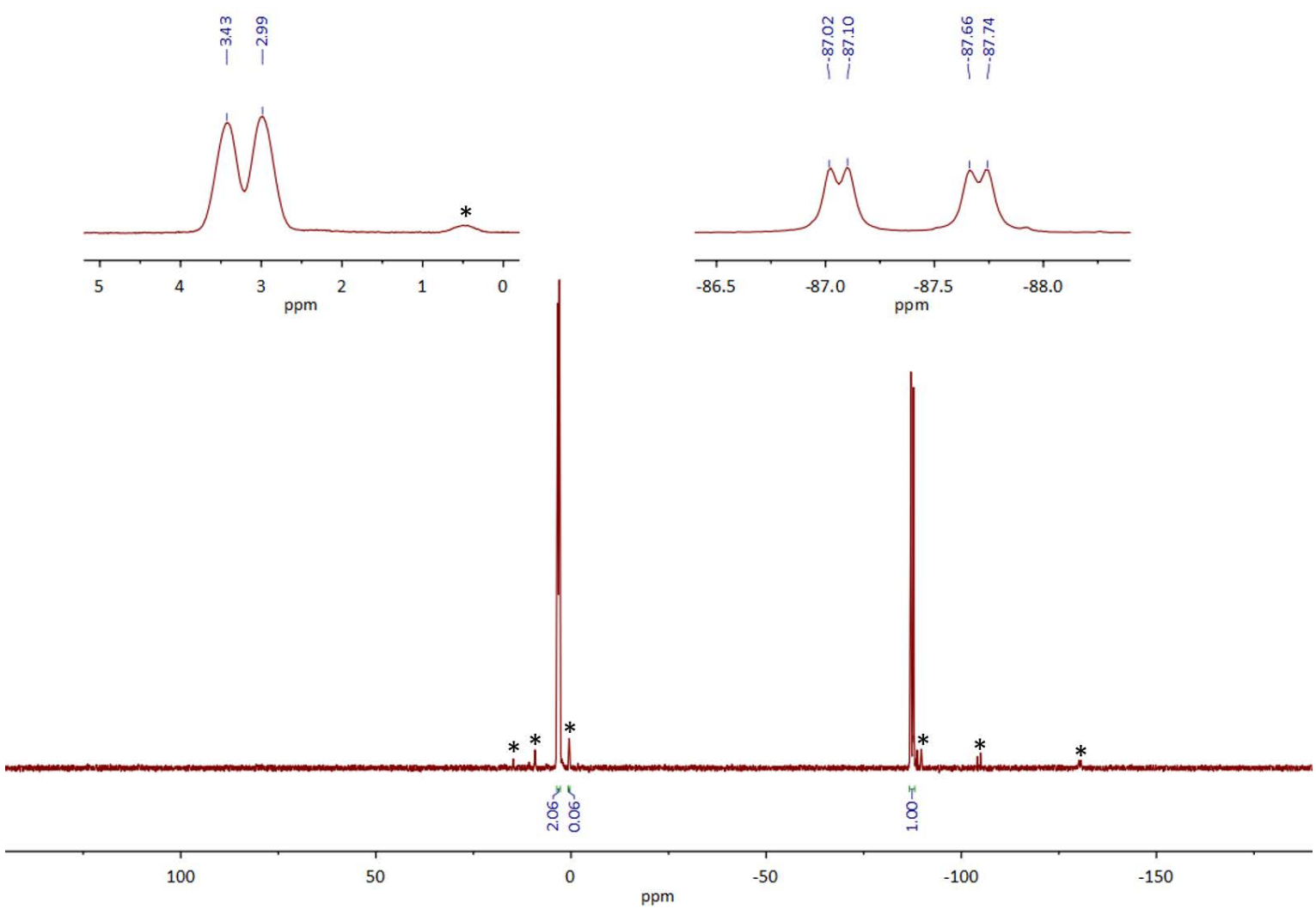


Fig. S23: *$^{31}P\{^{1}H\}$ NMR spectrum of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). The two enlargements show the main product's multiplet at δ = 2.7 –3.7 ppm (left) and doublet at δ = –87.4 ppm (right). In the left enlargement one resonance of the as yet unidentified C–H activated side product is marked by an asterisk (*), the other one is obscured by the resonances of **3a** at δ = 2.7 –3.7 ppm. Other traces of unknown impurities are also marked by asterisks (*).*



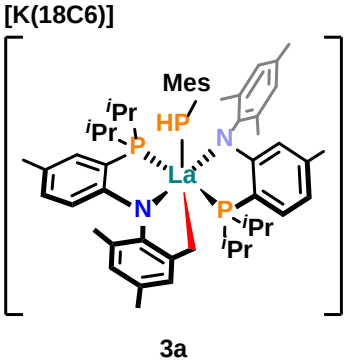
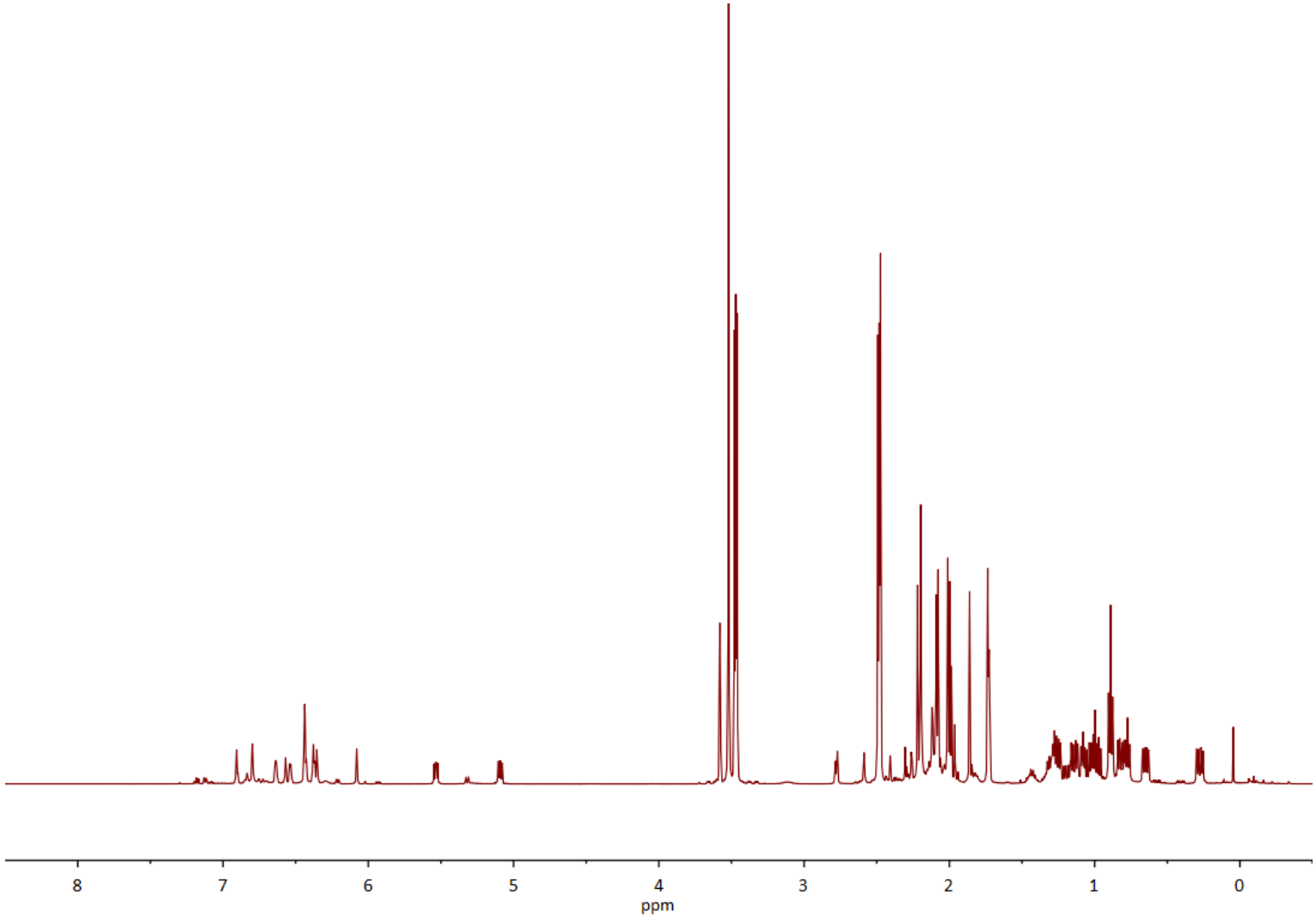
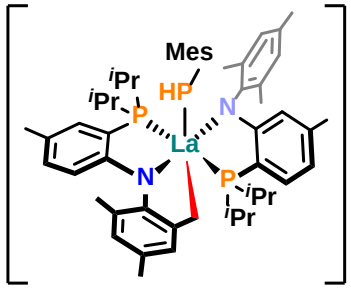


Fig. S24: *^{31}P NMR spectrum of **3a** (≈94% purity, obtained by Route B) in THF-d_8 (303 K). The two enlargements show the main product's broad multiplet at δ = 2.7 –3.7 ppm (left) and the doublet of doublets at δ = –87.4 ppm (right). In the left enlargement one resonance of the as yet unidentified C–H activated side product is marked by an asterisk (*), the other one is obscured by the resonances of **3a** at δ = 2.7 –3.7 ppm. Other traces of unknown impurities are also marked by asterisks (*).*



[K(2.2.2-cryptand)]



3b

Fig. S25: *^{1}H NMR spectrum of **3b** (crude) in THF-d_8 (303 K).*

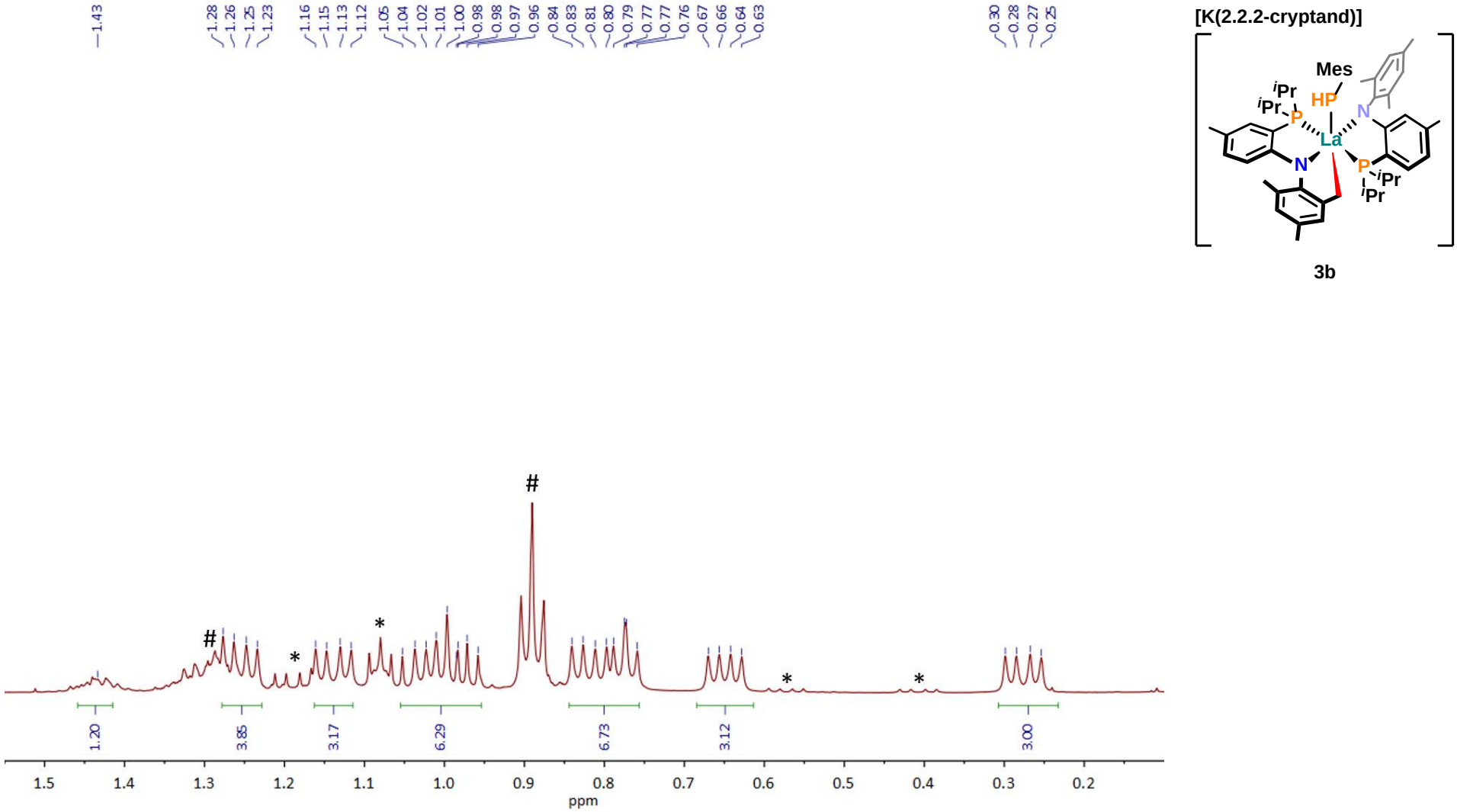
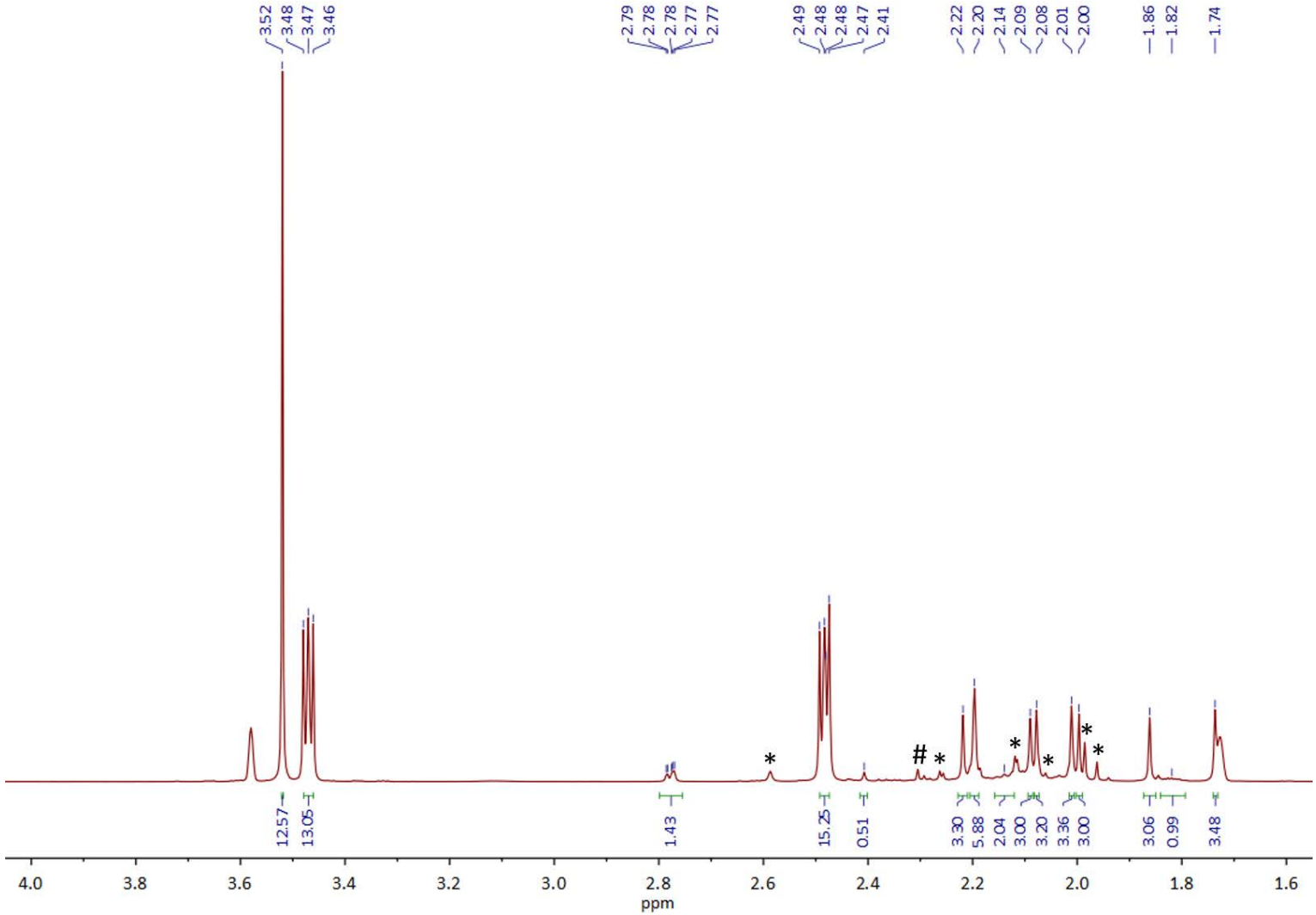
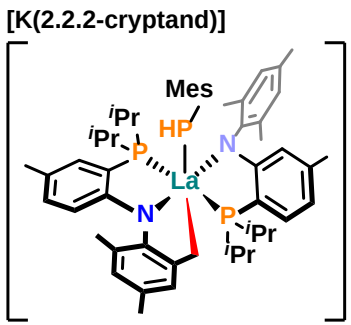


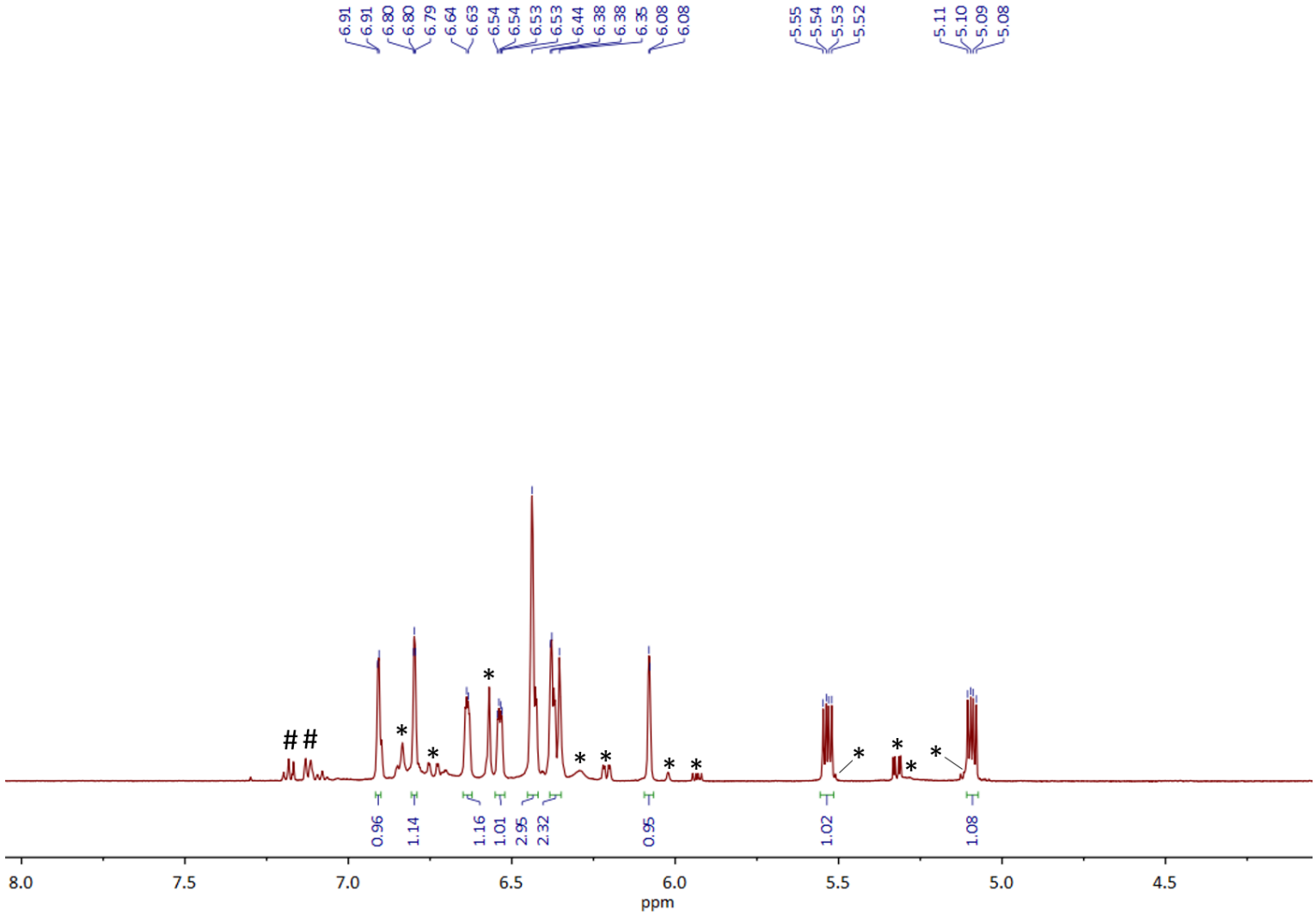
Fig. S26: *Section of the ^{1}H NMR spectrum (δ = 0.1 – 1.55 ppm) of **3b** (crude) in THF-d_8 (303 K). The integration values are only estimates, due to the presence of obscured resonances of unknown impurities underneath the main product's peaks. Well separated resonances of unknown impurities are marked by asterisks (*). Residual n-pentane from work-up is marked by #.*



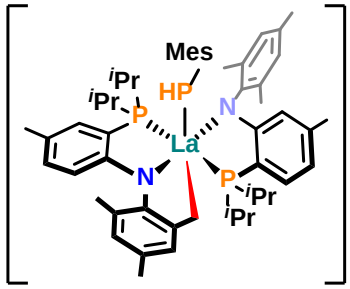


3b

Fig. S27: *Section of the ^{1}H NMR spectrum (δ = 1.55 – 4.05 ppm) of **3b** (crude) in THF-d_8 (303 K). The resonances of unknown impurities are marked by asterisks (*). Residual toluene from work-up is marked by #.*

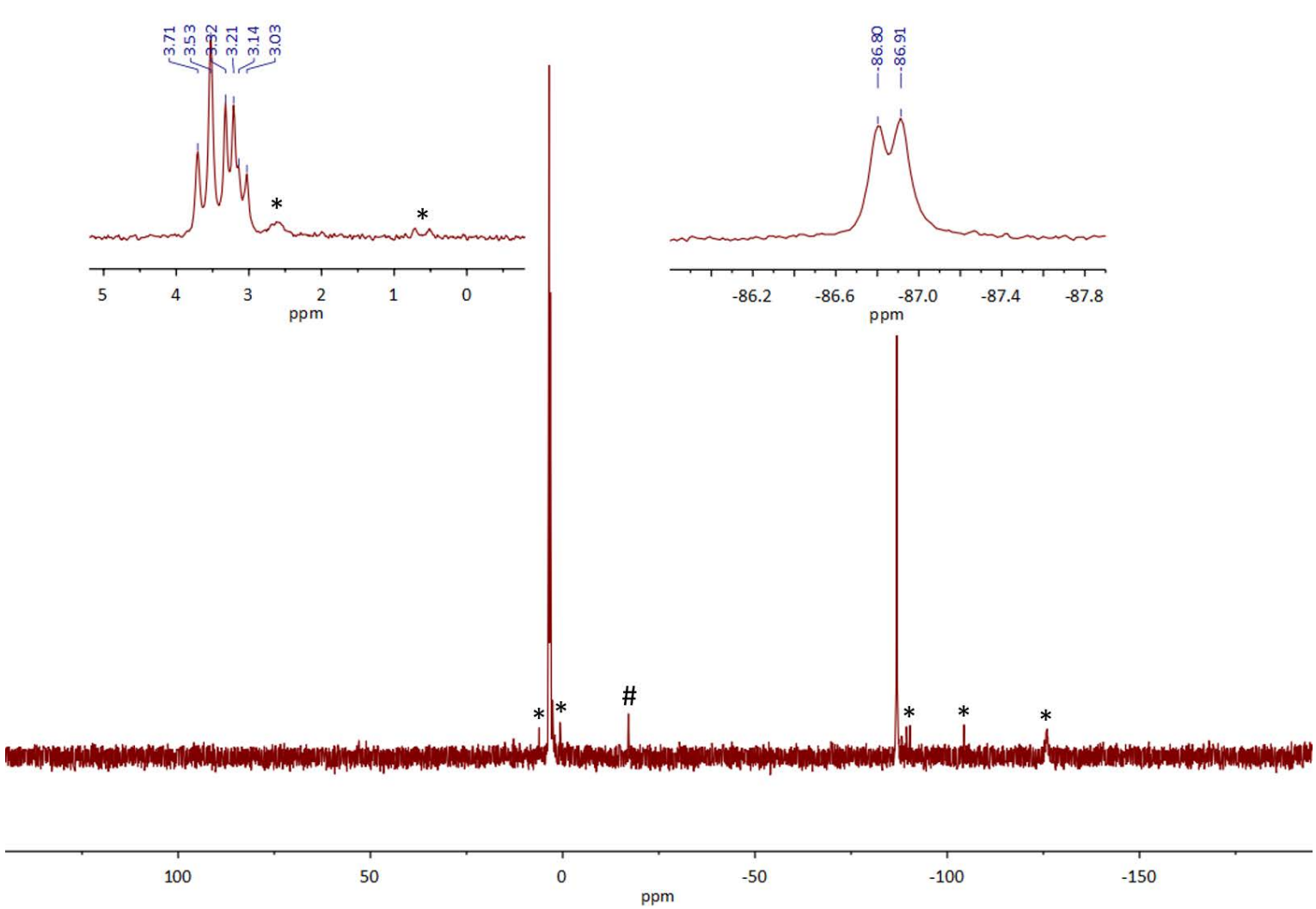


[K(2.2.2-cryptand)]

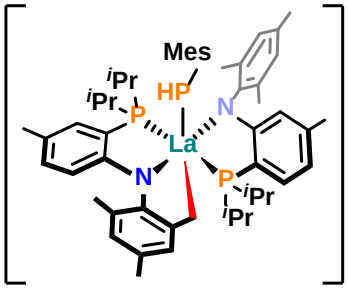


3b

Fig. S28: *Section of the ^{1}H NMR spectrum (δ = 4.05 – 8.05 ppm) of **3b** (crude) in THF-d_8 (303 K). The resonances of unknown impurities are marked by asterisks (*). Residual toluene from work-up is marked by #.*



[K(2.2.2-cryptand)]



3b

Fig. S29: *$^{31}P\{^{1}H\}$ NMR spectrum of **3b** (crude) in THF-d_8 (303 K). The two enlargements show the main product's multiplet at δ = 2.9 –3.9 ppm (left) and the doublet at δ = –86.9 ppm (right). The resonances of unknown impurities are marked by asterisks (*). Traces of protonated ligand HPN are marked by #.*

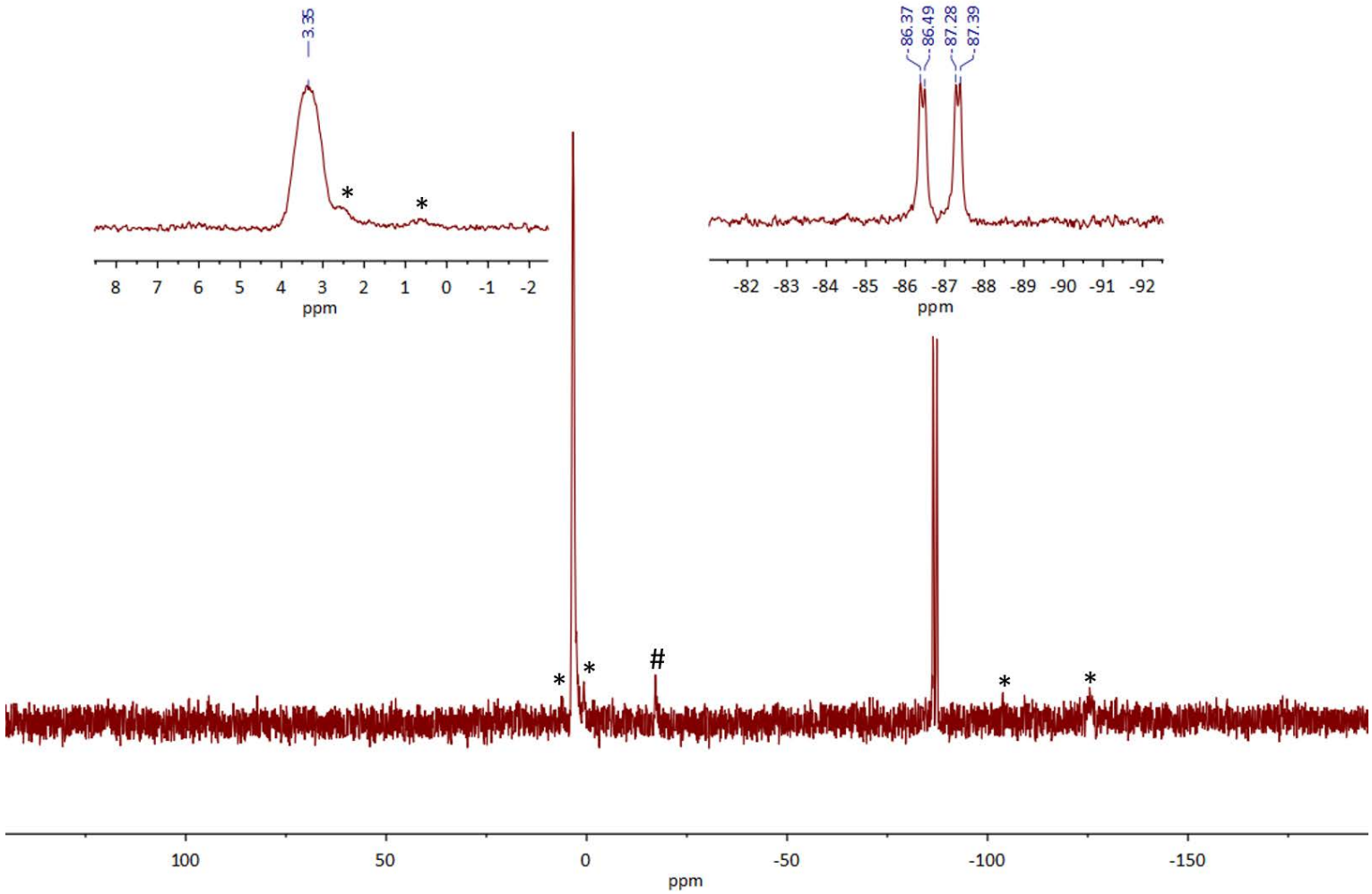
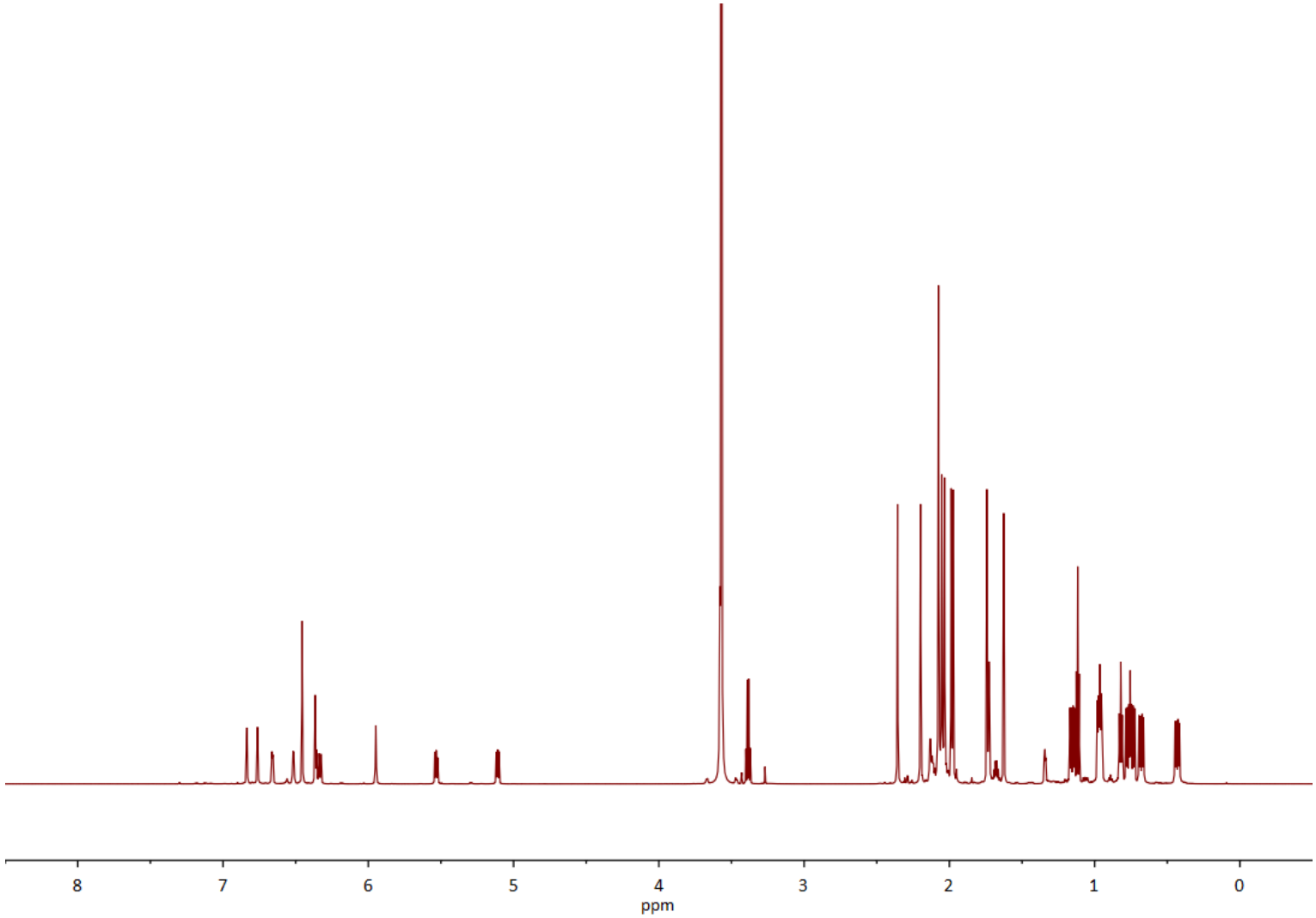
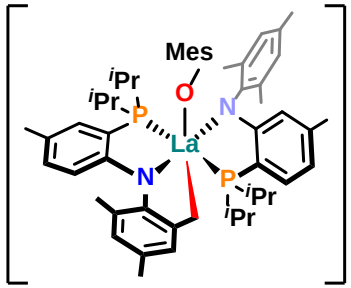


Fig. S30: *^{31}P NMR spectrum of **3b** (crude) in THF-d_8 (303 K). The two enlargements show the main product's broad multiplet at δ = 2.9 –3.9 ppm (left) and the doublet of doublets at δ = –86.9 ppm (right). The resonances of unknown impurities are marked by asterisks (*). Traces of protonated ligand HPN are marked by #.*

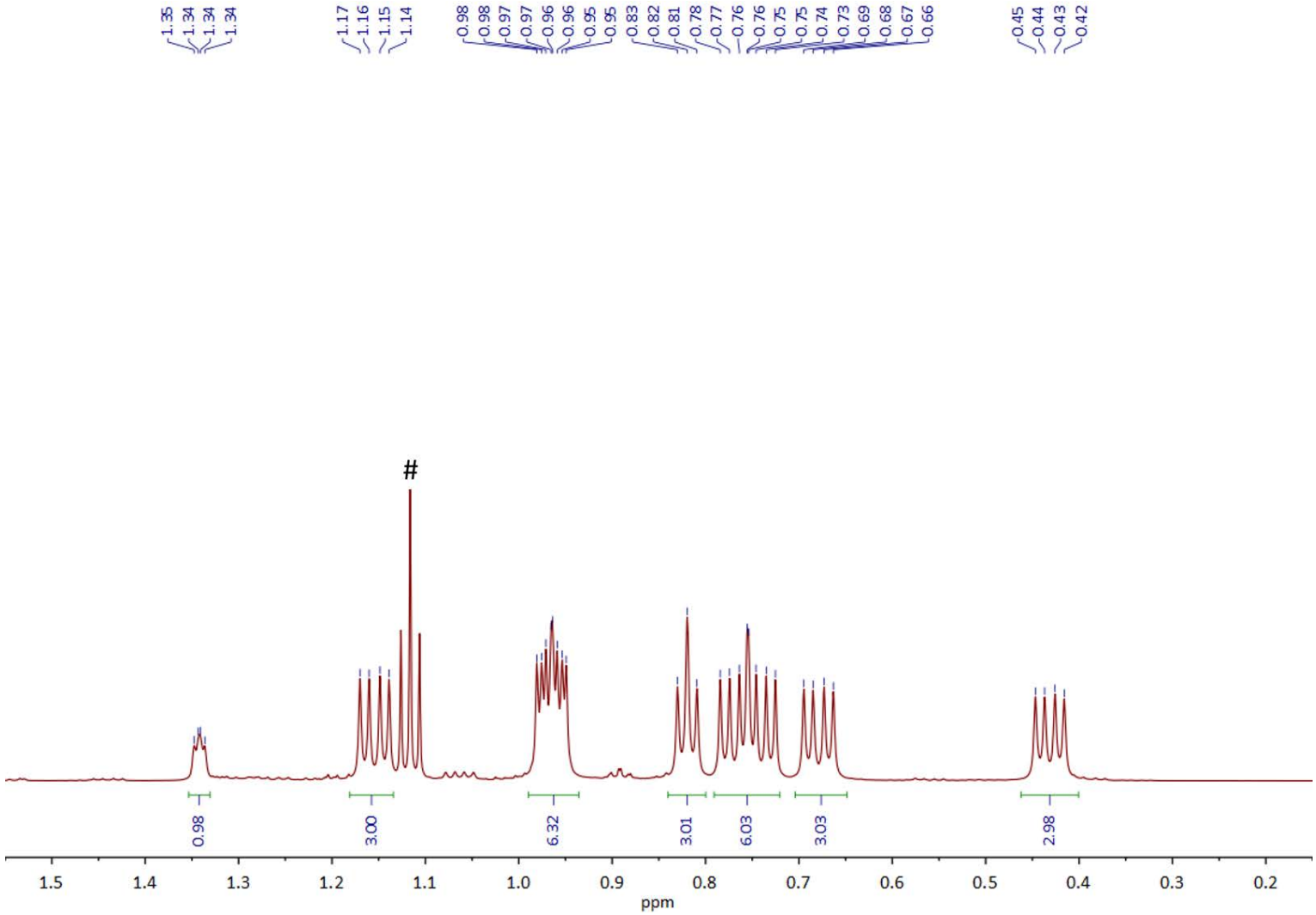


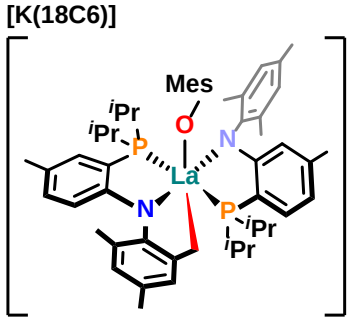
[K(18C6)]



5a

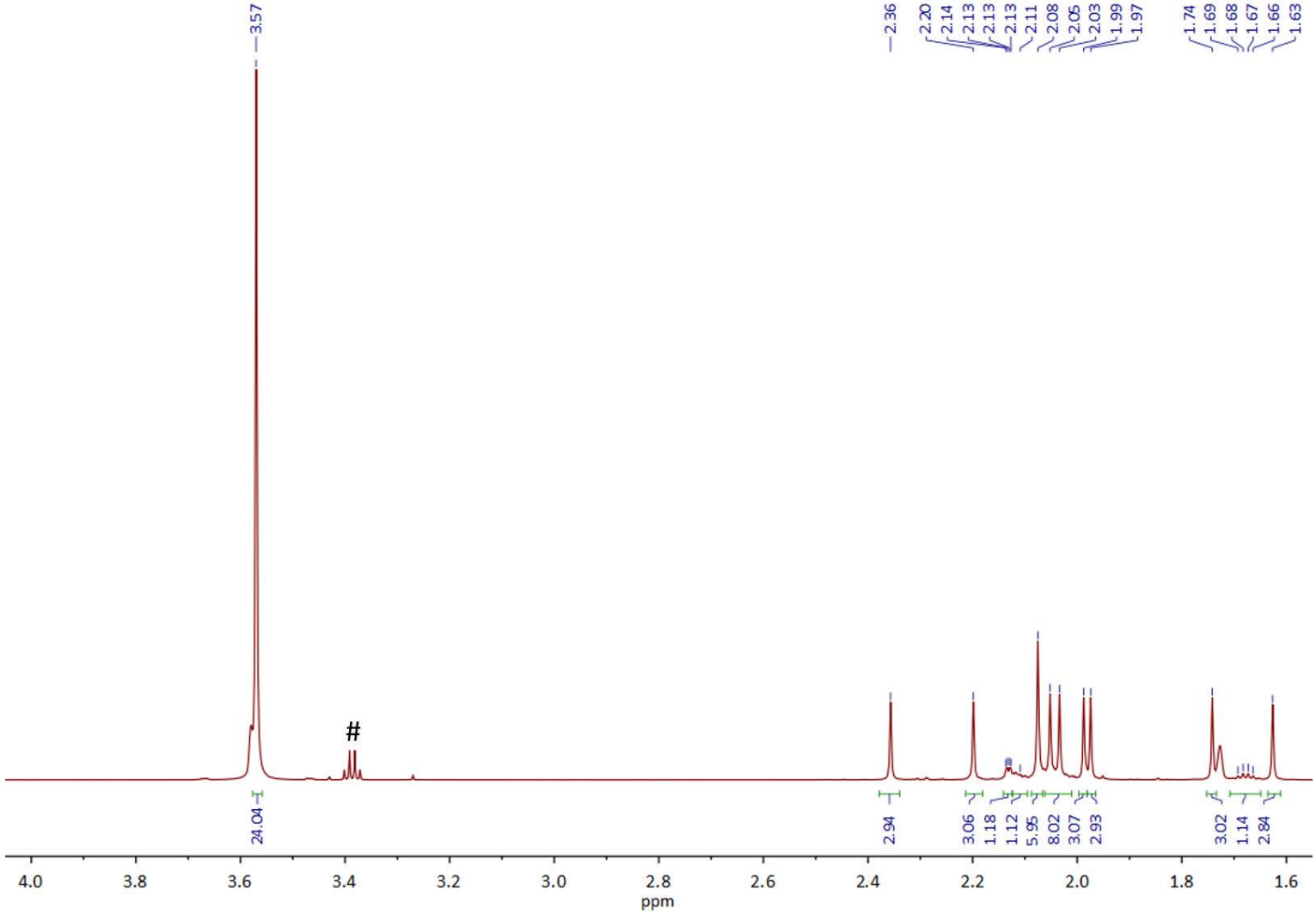
Fig. S31: *^{1}H NMR spectrum of **5a** in THF-d_8 (303 K).*

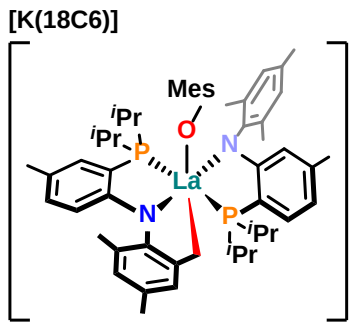




5a

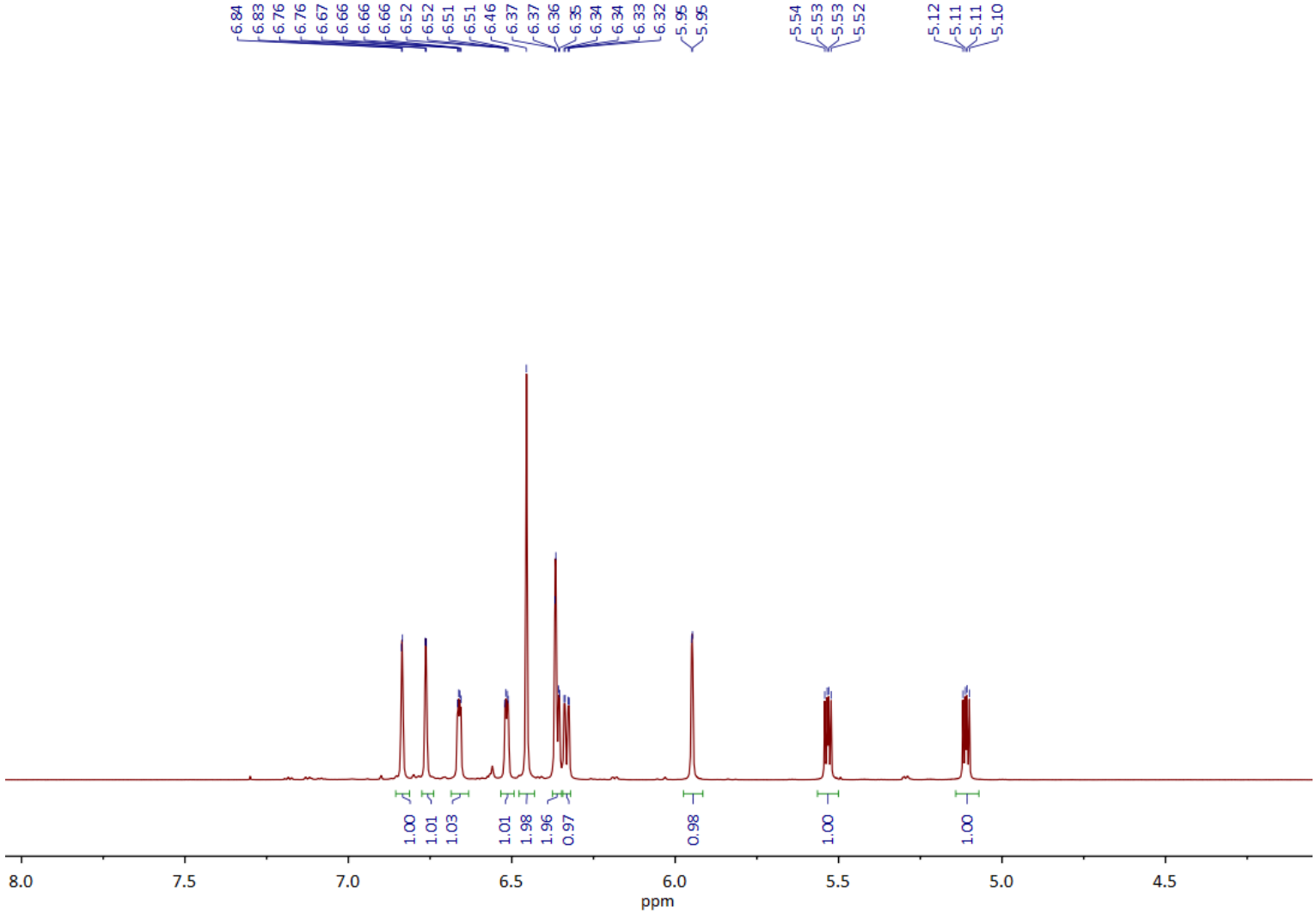
*Fig. S32: Section of the ^{1}H NMR spectrum (δ = 0.15 – 1.55 ppm) of **5a** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

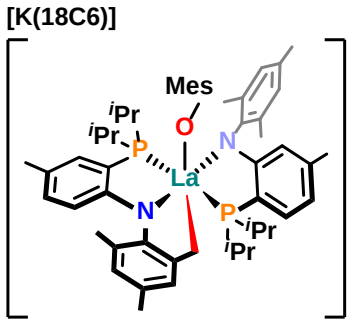




5a

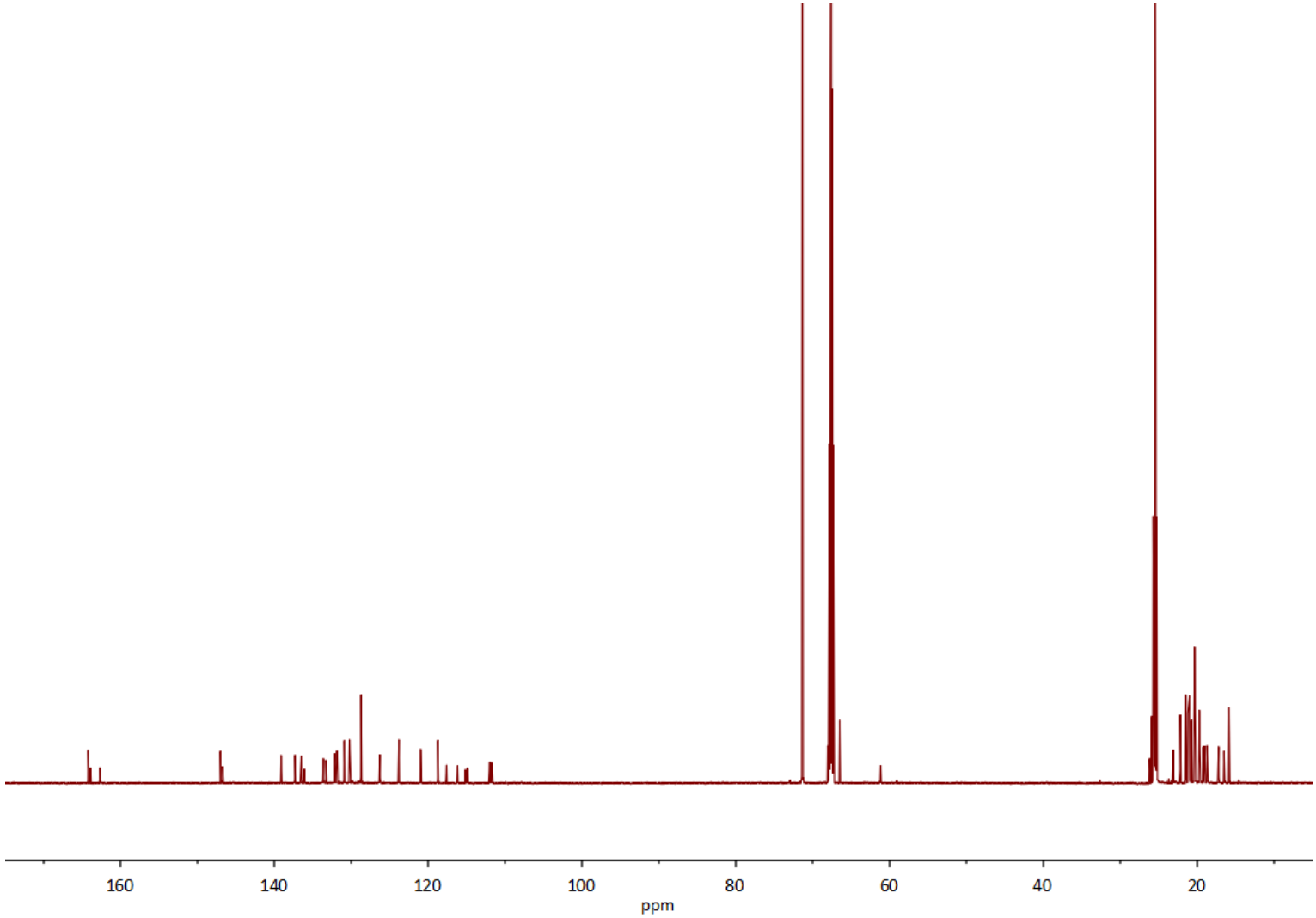
*Fig. S33: Section of the ^{1}H NMR spectrum (δ = 1.55 – 4.05 ppm) of **5a** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

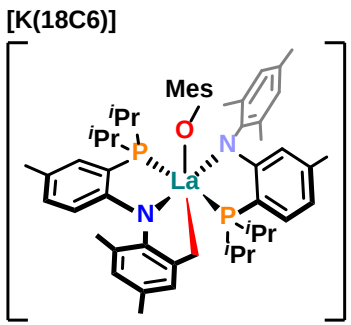




5a

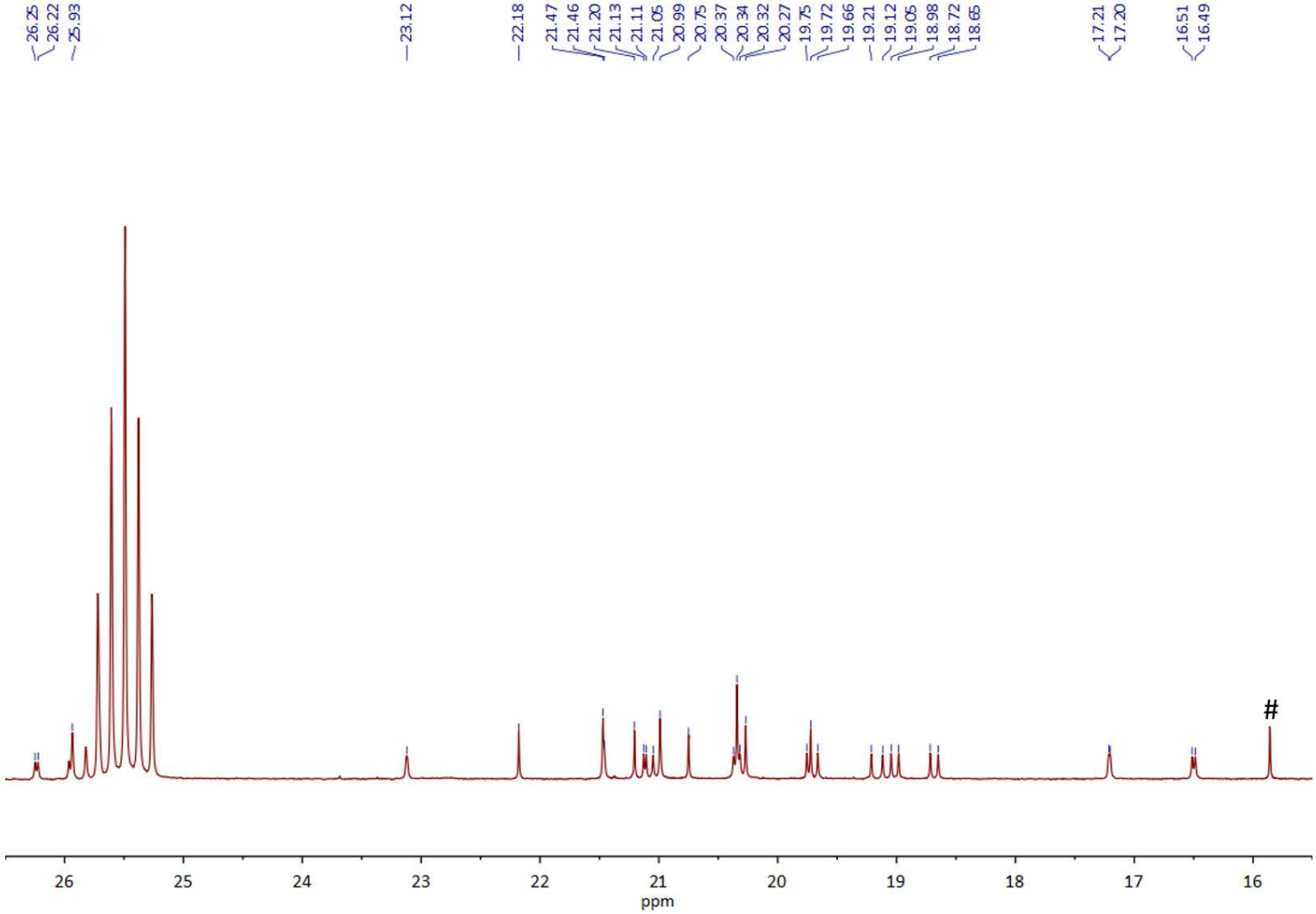
Fig. S34: *Section of the ^{1}H NMR spectrum (δ = 4.05 – 8.05 ppm) of **5a** in THF-d_8 (303 K).*

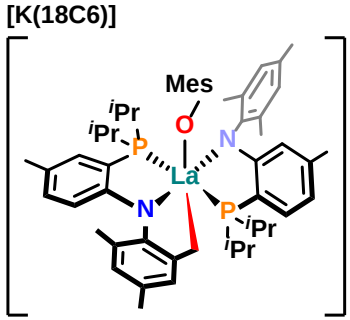




5a

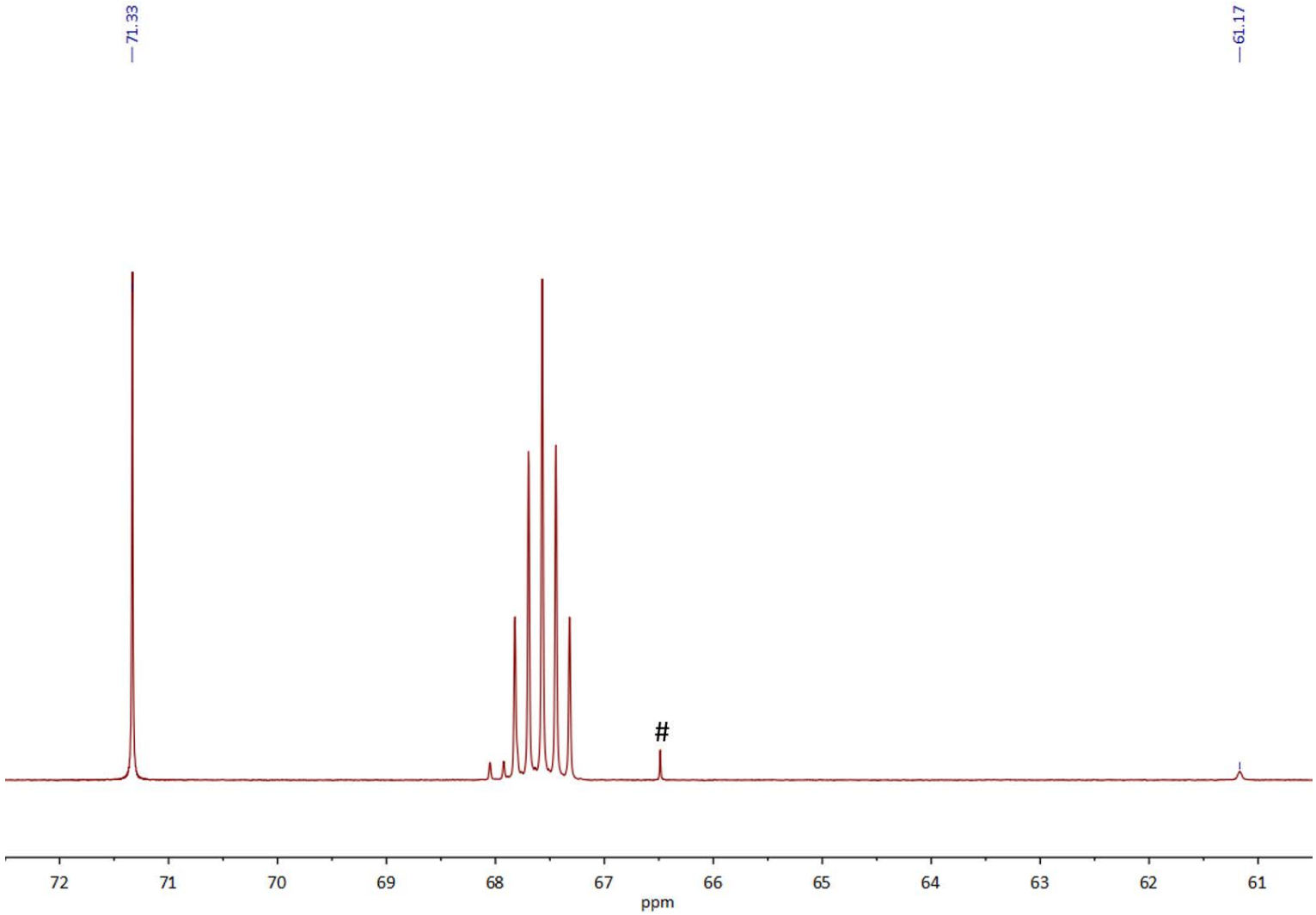
Fig. S35: *$^{13}C\{^{1}H\}$ NMR spectrum of **5a** in THF-d_8 (303 K).*

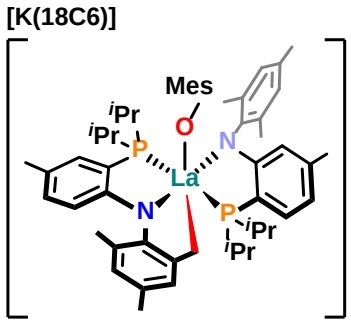




5a

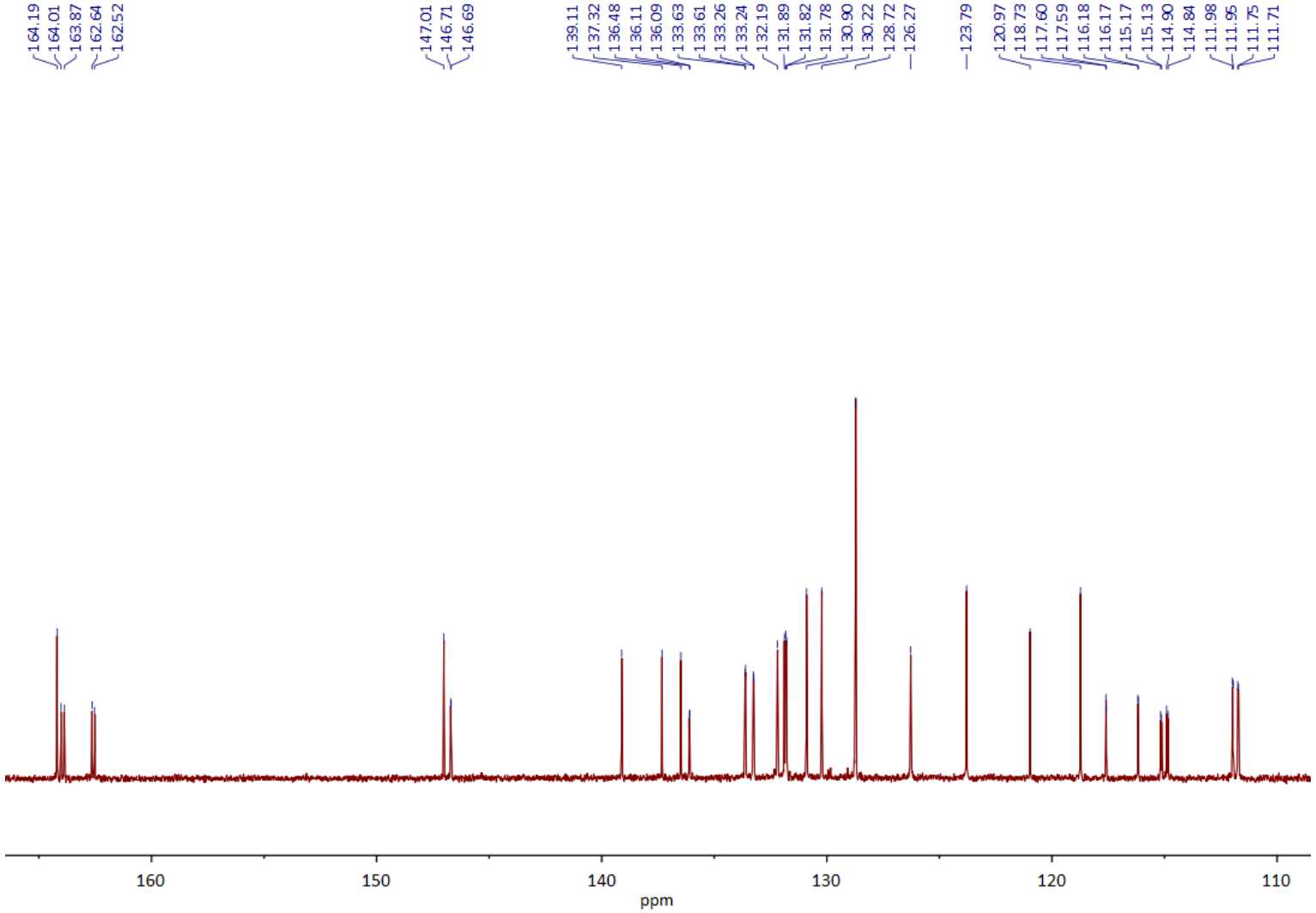
*Fig. S36: Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 15.5 – 26.5 ppm) of **5a** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

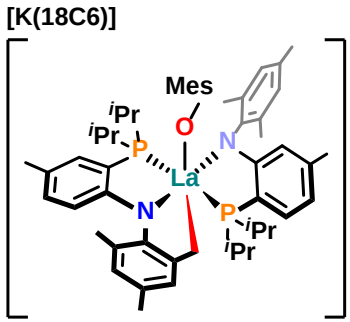




5a

*Fig. S37: Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 60.5 – 72.5 ppm) of **5a** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*





5a

Fig. S38: *Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 108.5 – 166.5 ppm) of **5a** in THF-d_8 (303 K).*

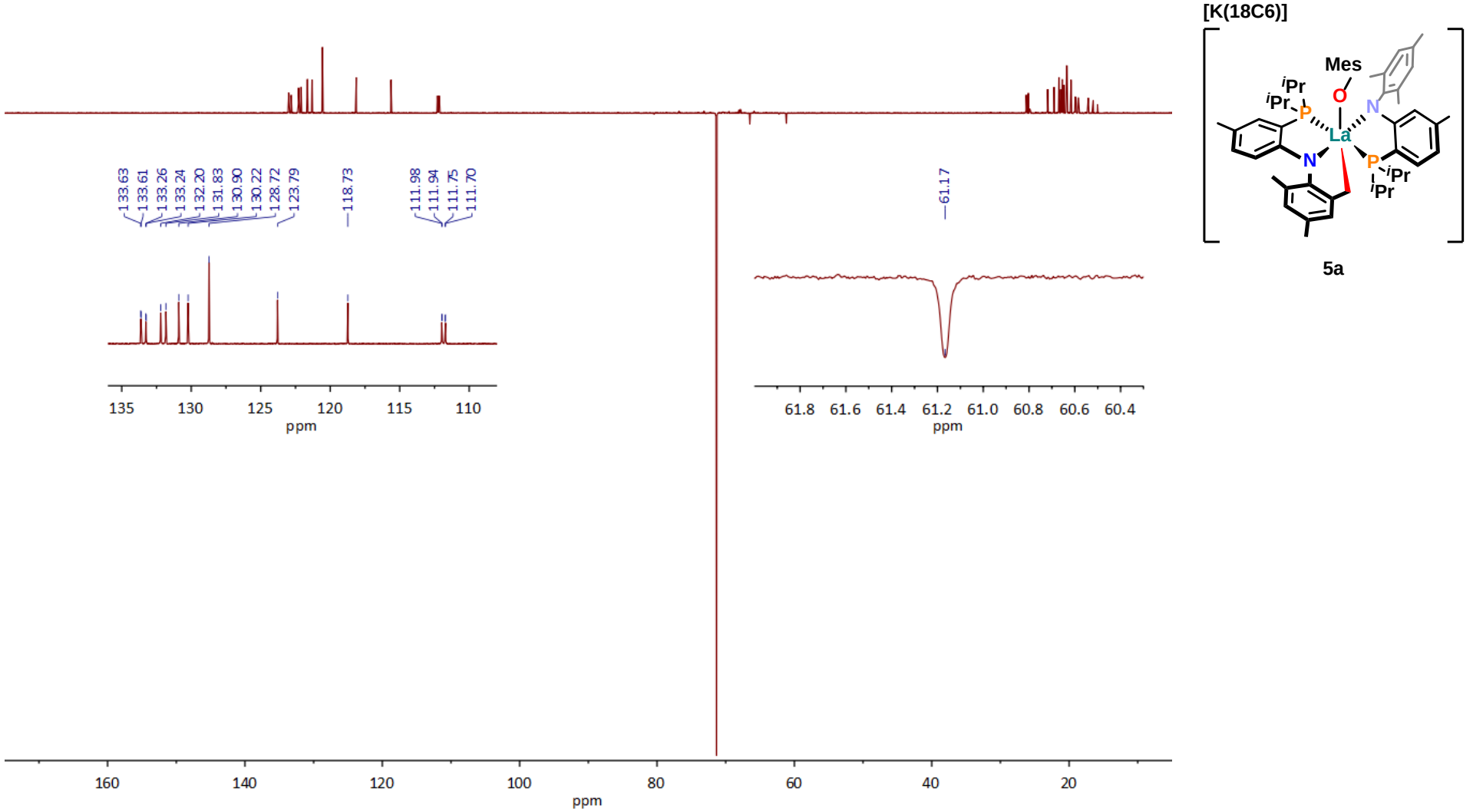
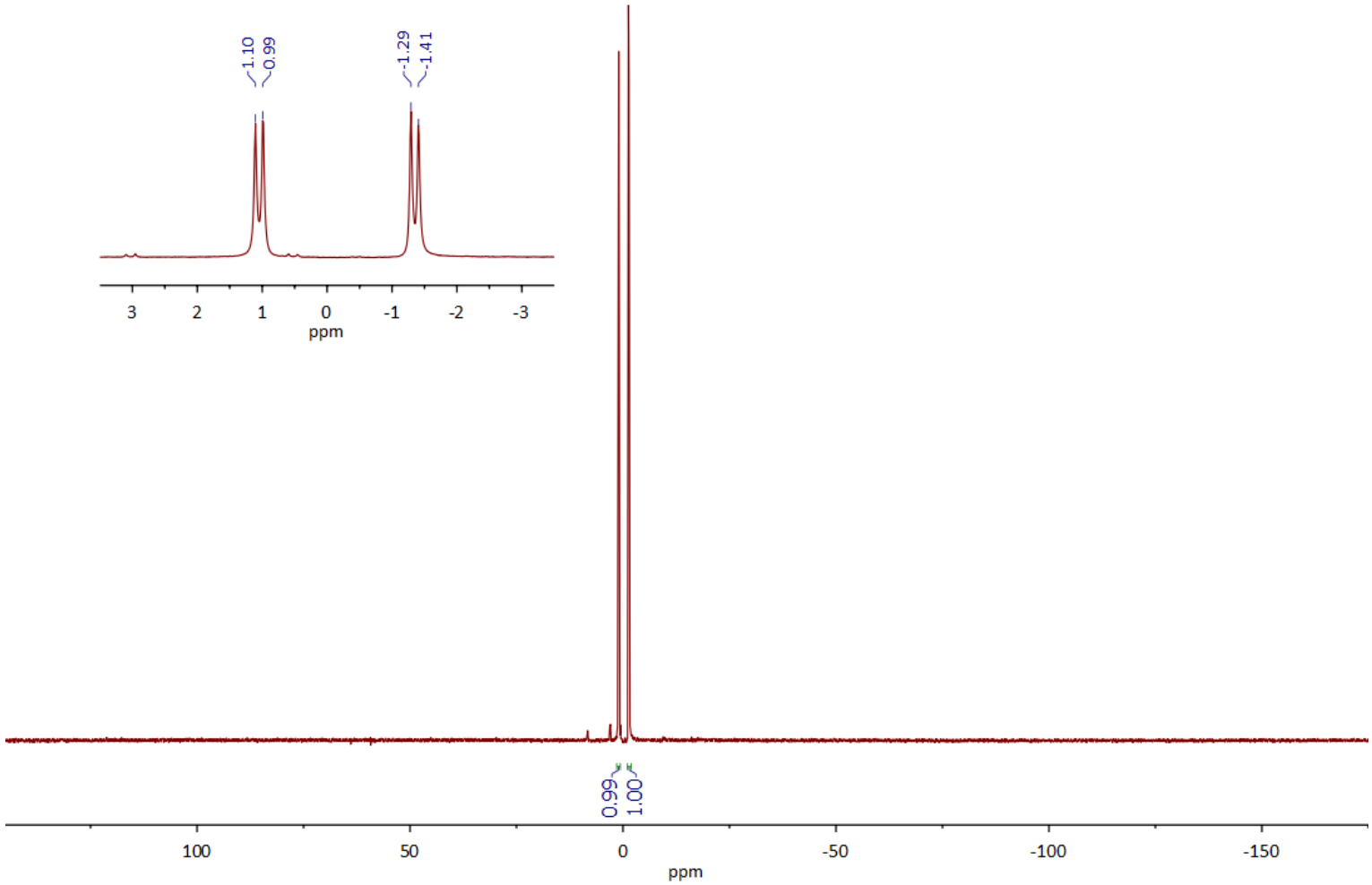
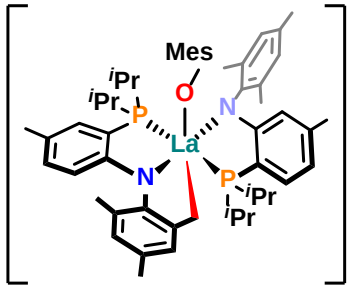


Fig. S39: *$^{13}C\{^{1}H\}$ DEPT135 NMR spectrum of **5a** in THF-d_8 (303 K). The two enlargements show the ^{13}C chemical shifts of the CH groups in the aromatic region (left) and a close-up of the peak for the $CH_{2Mes(PNcyclo)}$ methylene group at δ = 61.2 ppm (right) of **5a**.*

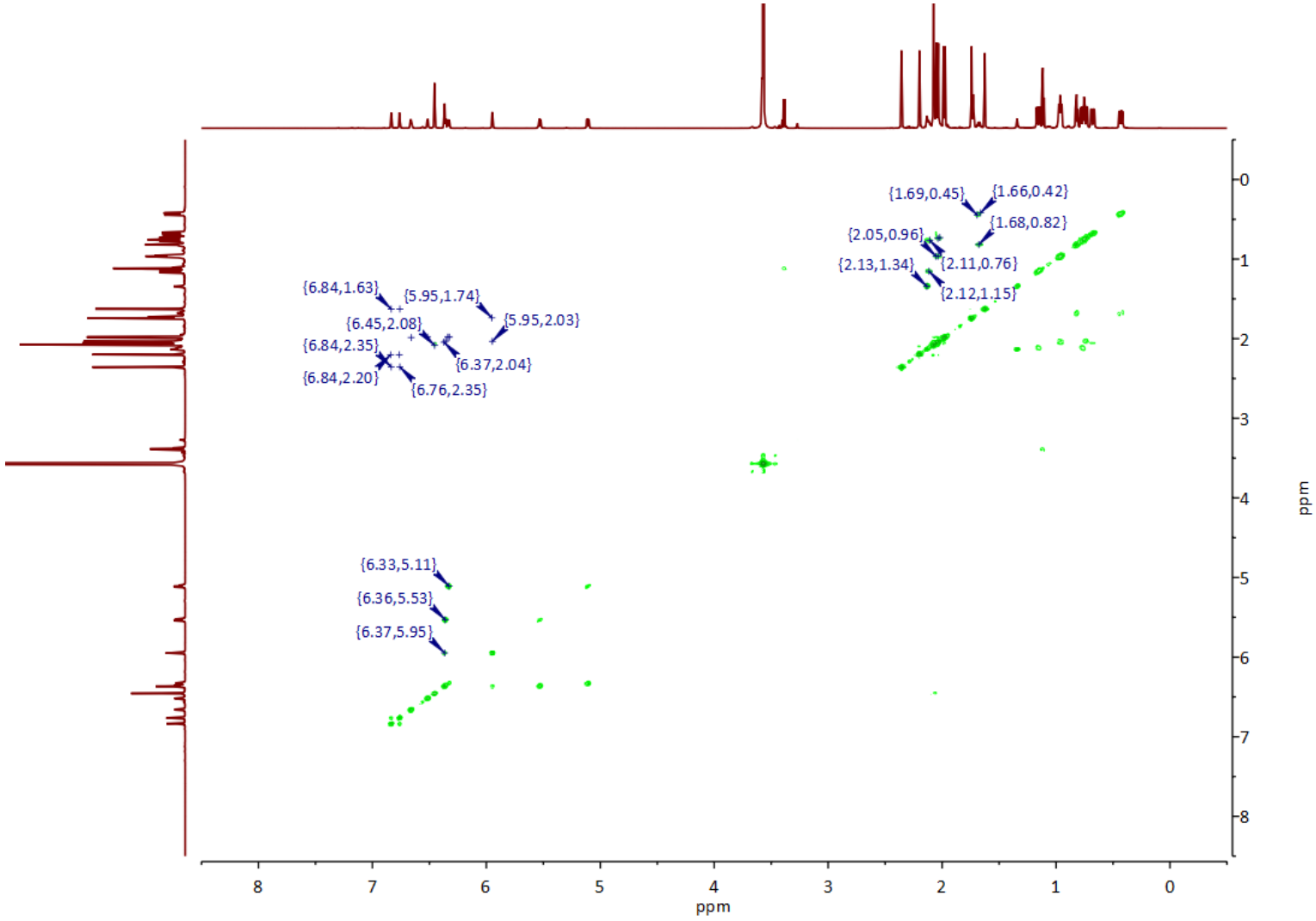


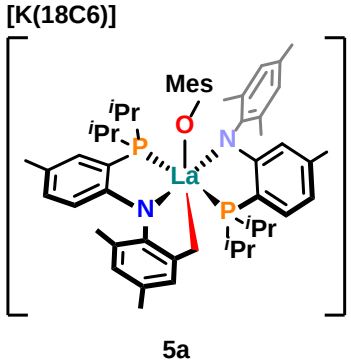
[K(18C6)]



5a

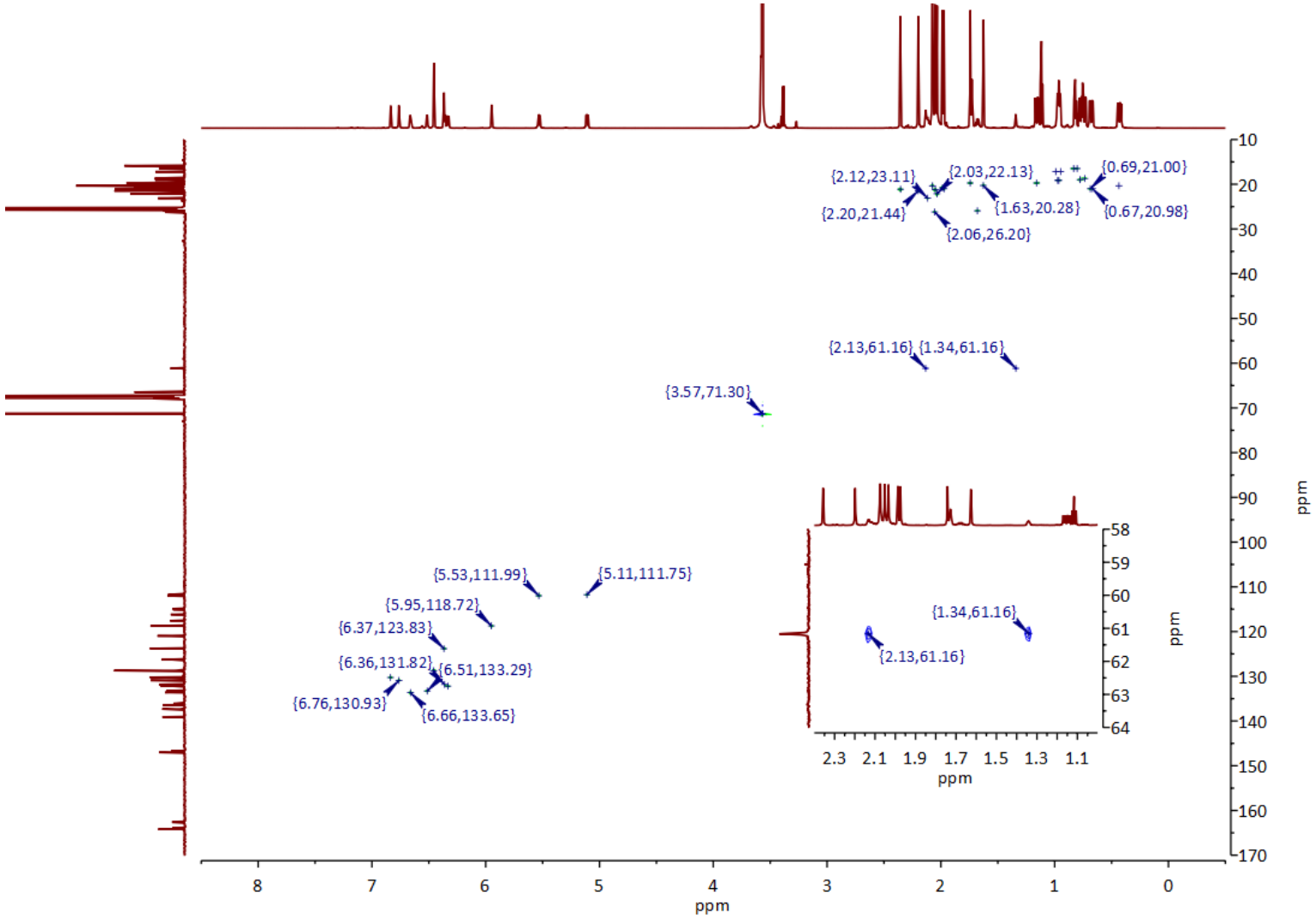
Fig. S40: *$^{31}P\{^{1}H\}$ NMR spectrum of **5a** in THF-d_8 (303 K). The enlargement shows the doublet splitting of the resonances at δ = –1.4 and 1.1 ppm.*

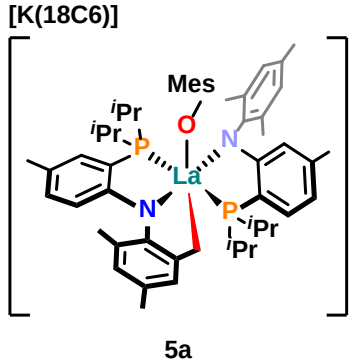




5a

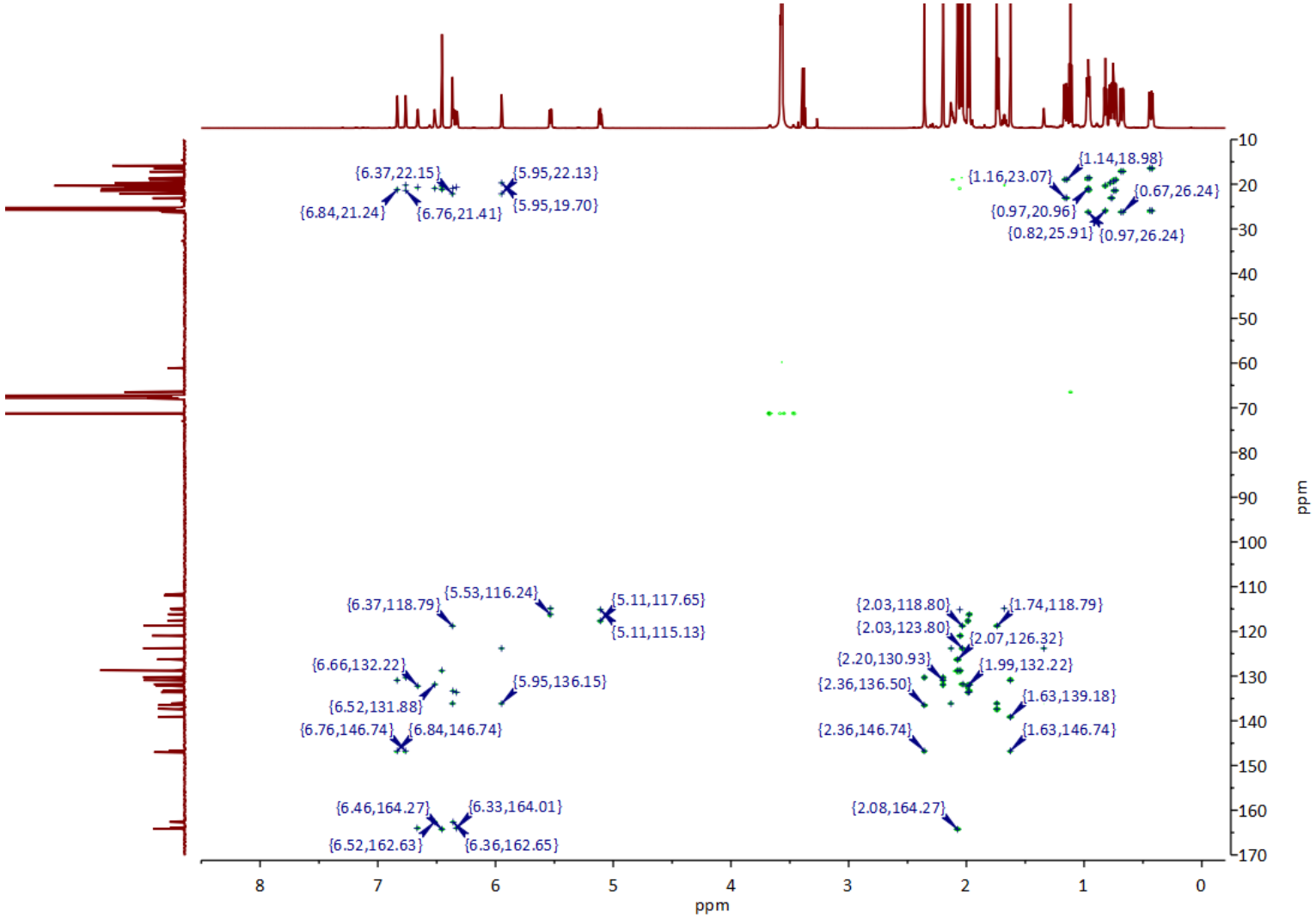
Fig. S41: *^{1}H–^{1}H COSY NMR spectrum of **5a** in THF-d_8 (303 K).*

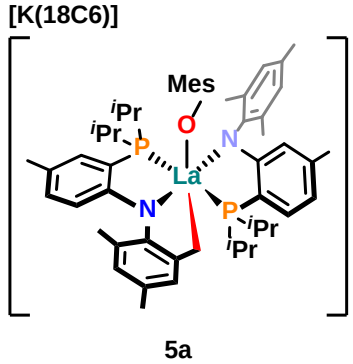




5a

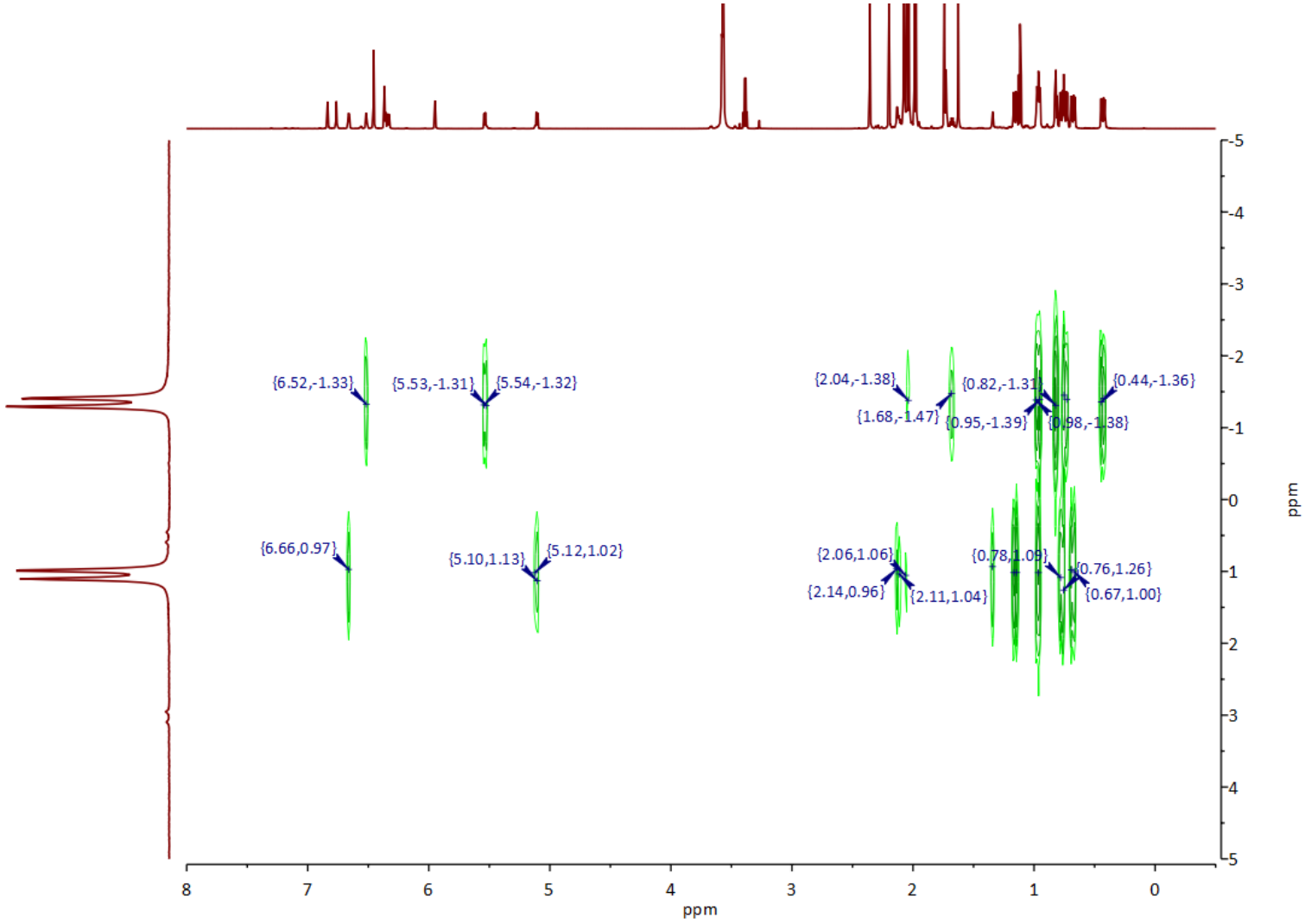
Fig. S42: *^{1}H–^{13}C HSQC NMR spectrum of **5a** in THF-d_8 (303 K). The enlargement shows the two cross peaks for the $CH_{2Mes(PNcyclo)}$ methylene protons of **5a**.*



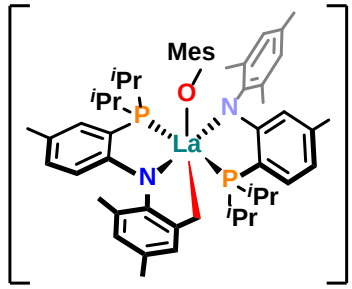


5a

Fig. S43: *^{1}H–^{13}C HMBC NMR spectrum of **5a** in THF-d_8 (303 K).*

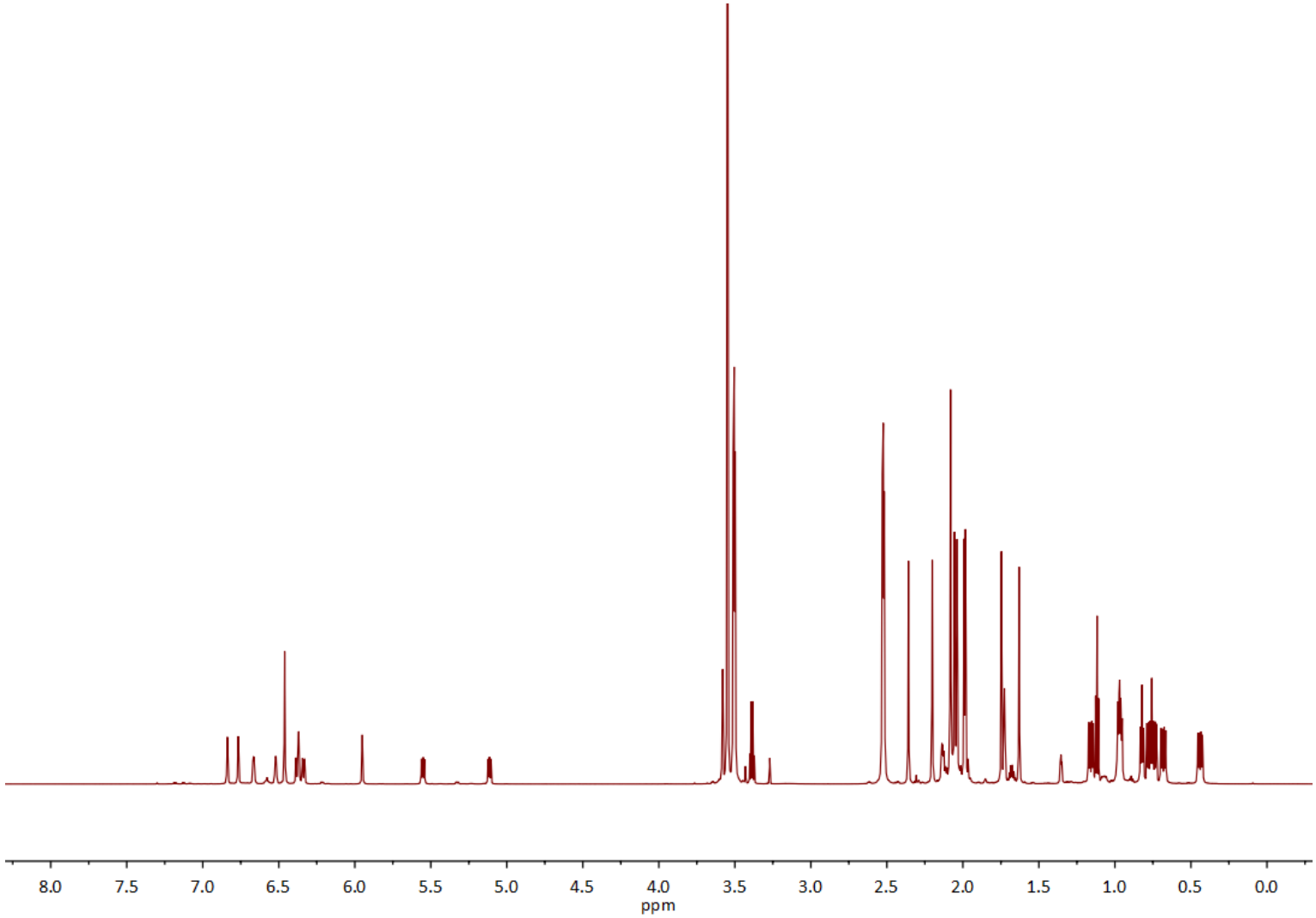


[K(18C6)]

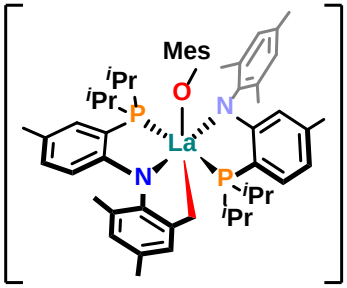


5a

Fig. S44: *^{1}H–^{31}P HMBC NMR spectrum of **5a** in THF-d_8 (303 K).*

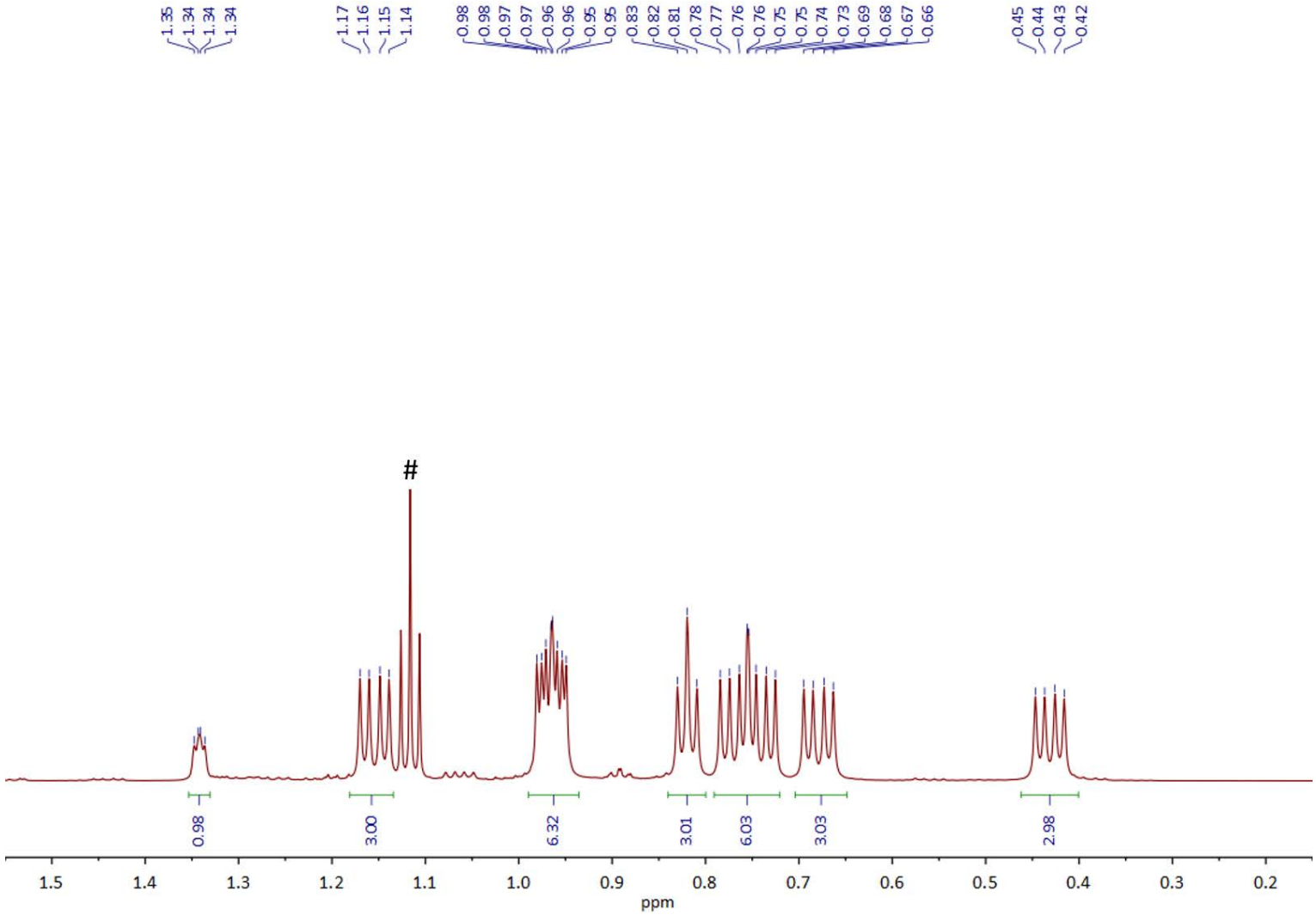


[K(2.2.2-cryptand)]

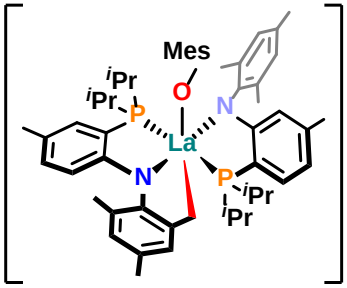


5b

Fig. S45: *^{1}H NMR spectrum of **5b** in THF-d_8 (303 K).*

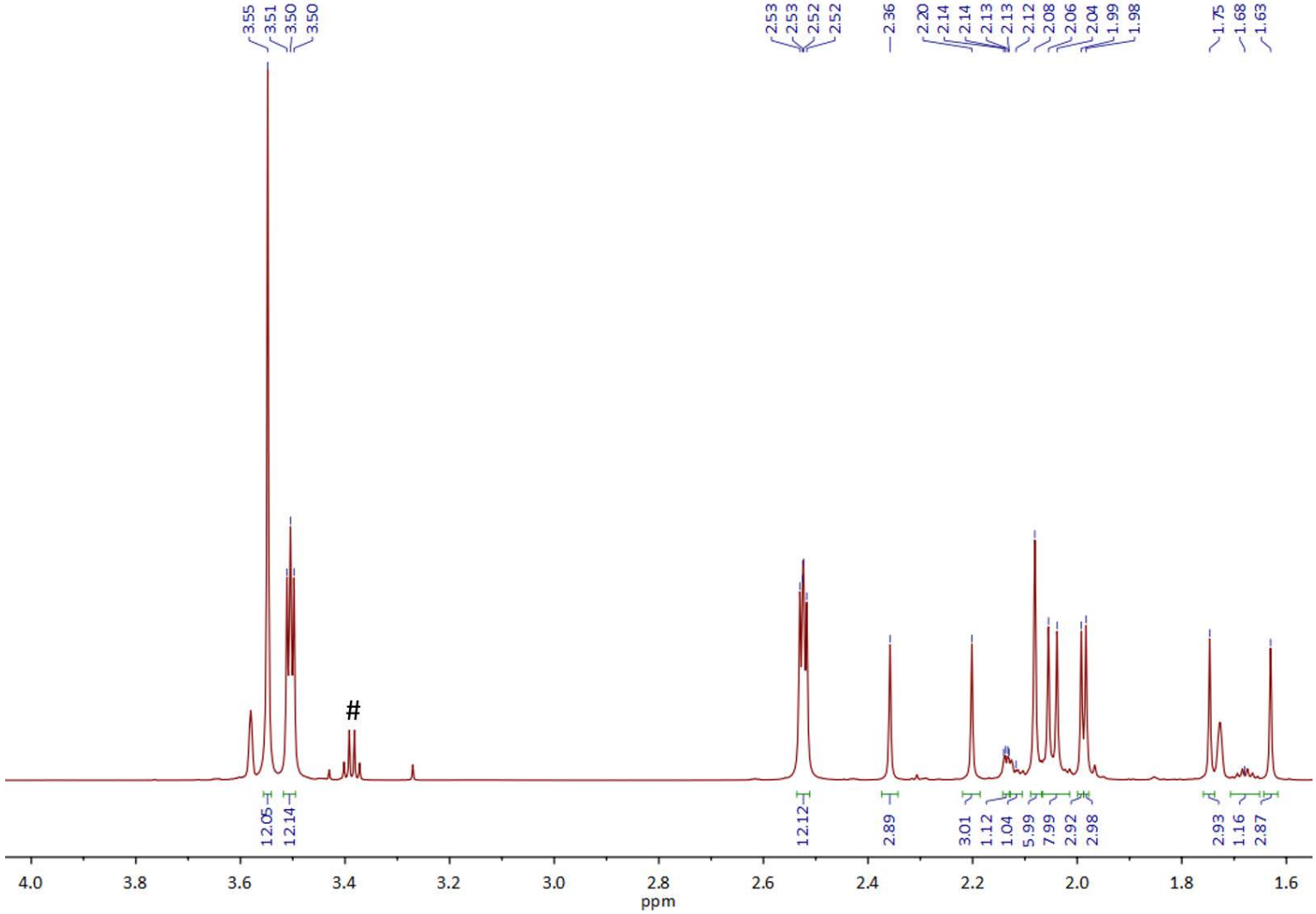


[K(2.2.2-cryptand)]

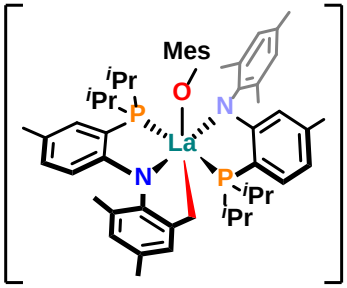


5b

*Fig. S46: Section of the ^{1}H NMR spectrum (δ = 0.15 – 1.55 ppm) of **5b** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

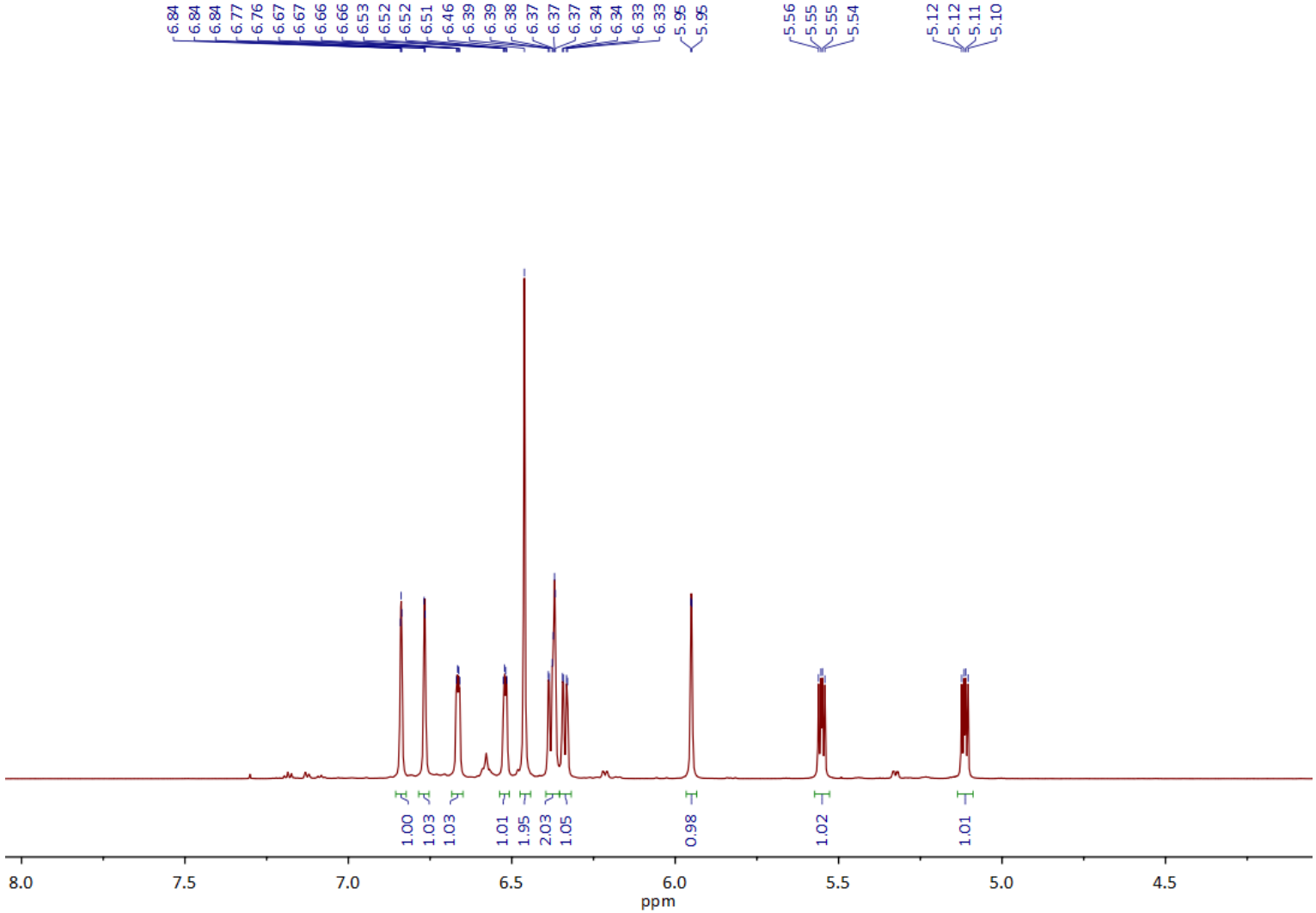


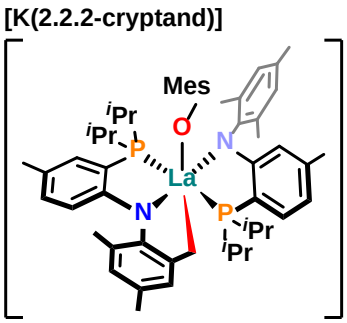
[K(2.2.2-cryptand)]



5b

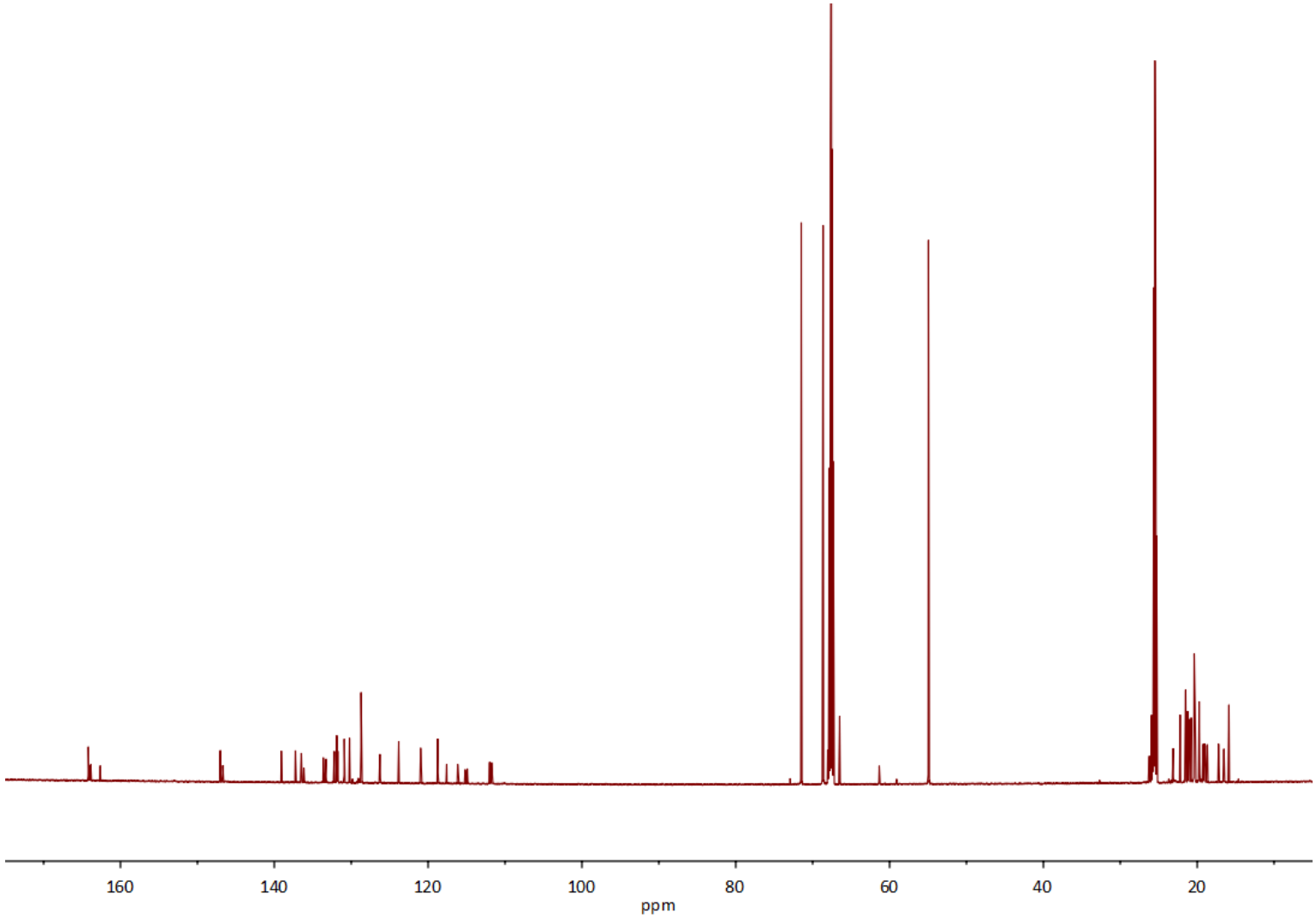
*Fig. S47: Section of the ^{1}H NMR spectrum (δ = 1.55 – 4.05 ppm) of **5b** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*



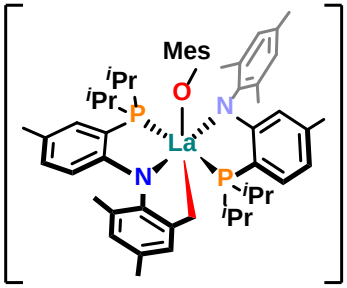


5b

Fig. S48: *Section of the ^{1}H NMR spectrum (δ = 4.05 – 8.05 ppm) of **5b** in THF-d_8 (303 K).*

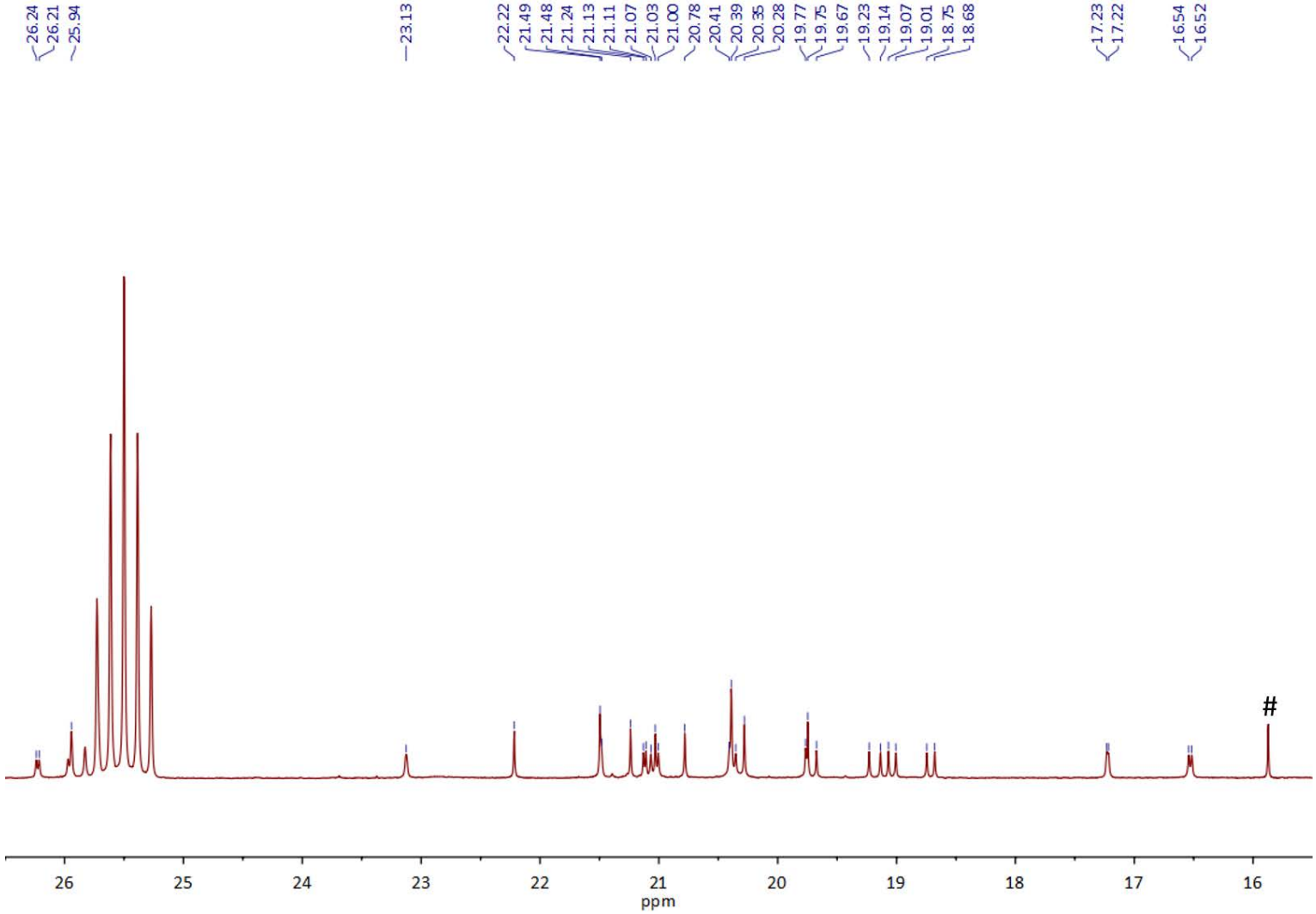


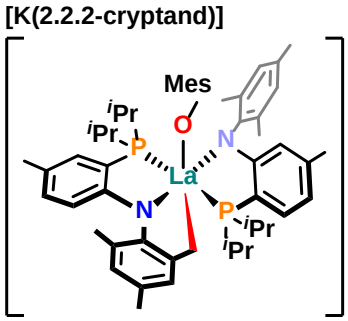
[K(2.2.2-cryptand)]



5b

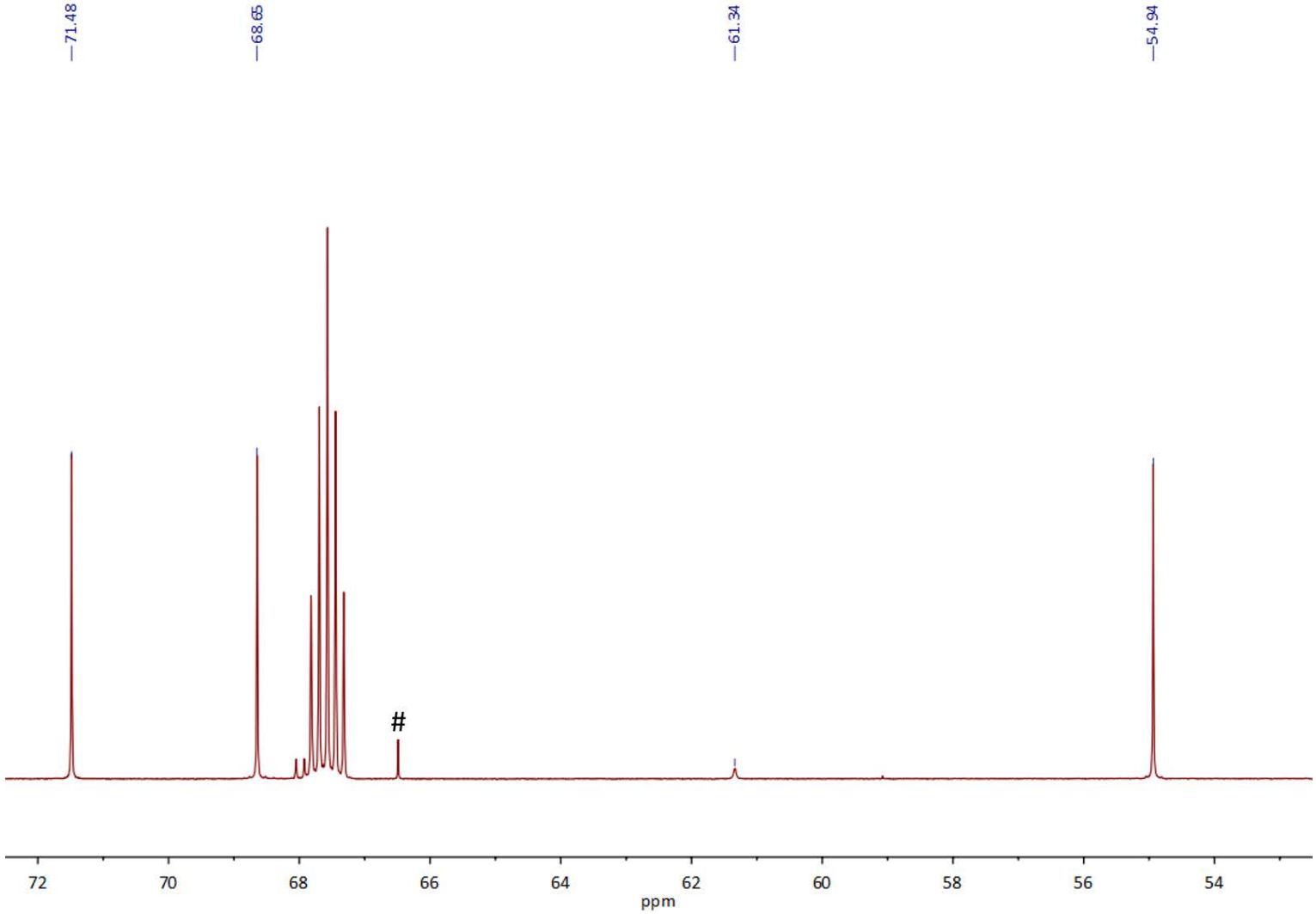
Fig. S49: *$^{13}C\{^{1}H\}$ NMR spectrum of **5b** in THF-d_8 (303 K).*



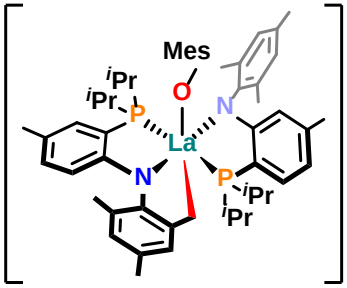


5b

*Fig. S50: Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 15.5 – 26.5 ppm) of **5b** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

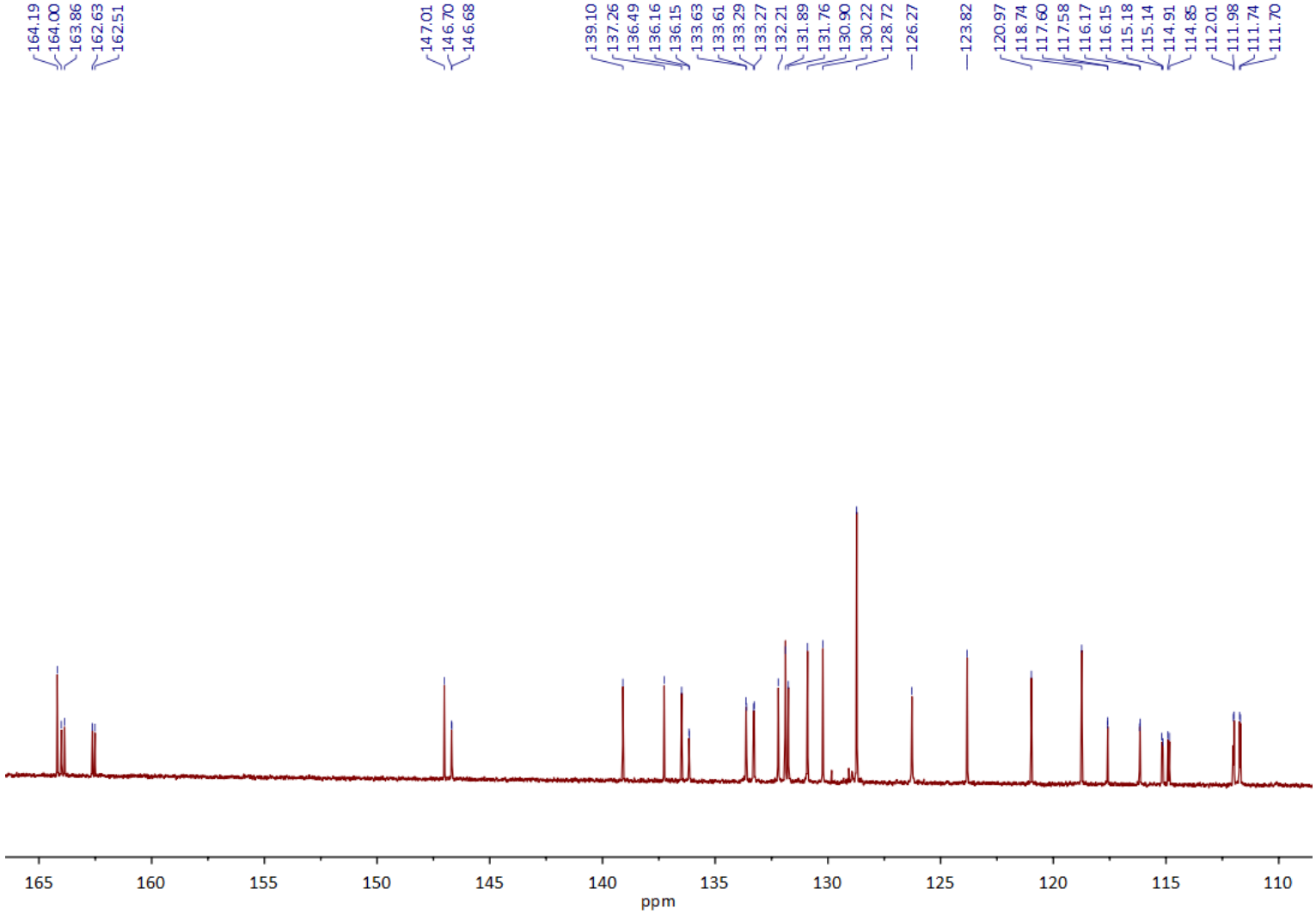


[K(2.2.2-cryptand)]

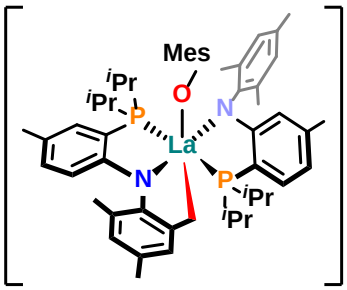


5b

*Fig. S51: Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 52.5 – 72.5 ppm) of **5b** in THF-d_8 (303 K). Residual diethyl ether from work-up is marked by #.*

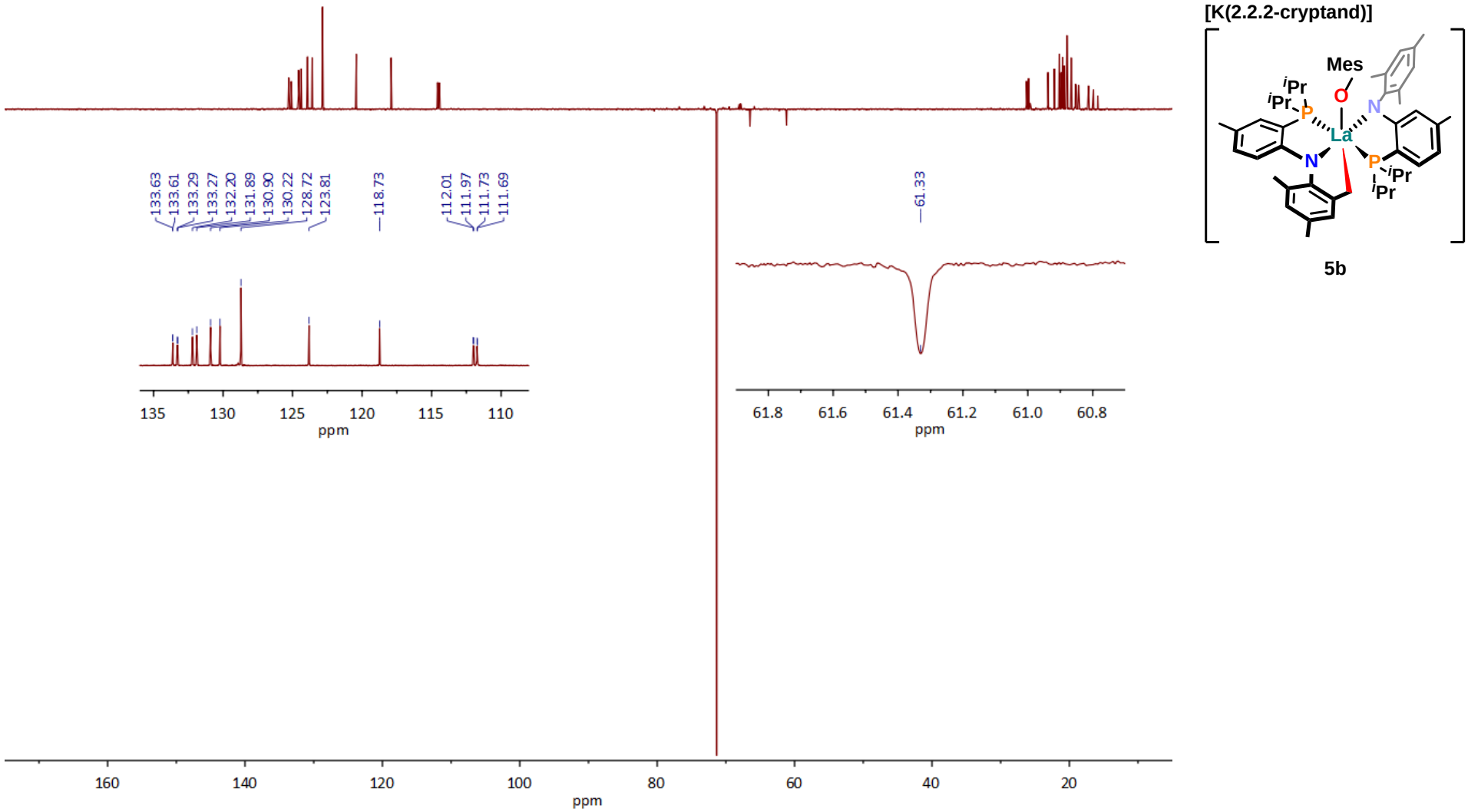


[K(2.2.2-cryptand)]



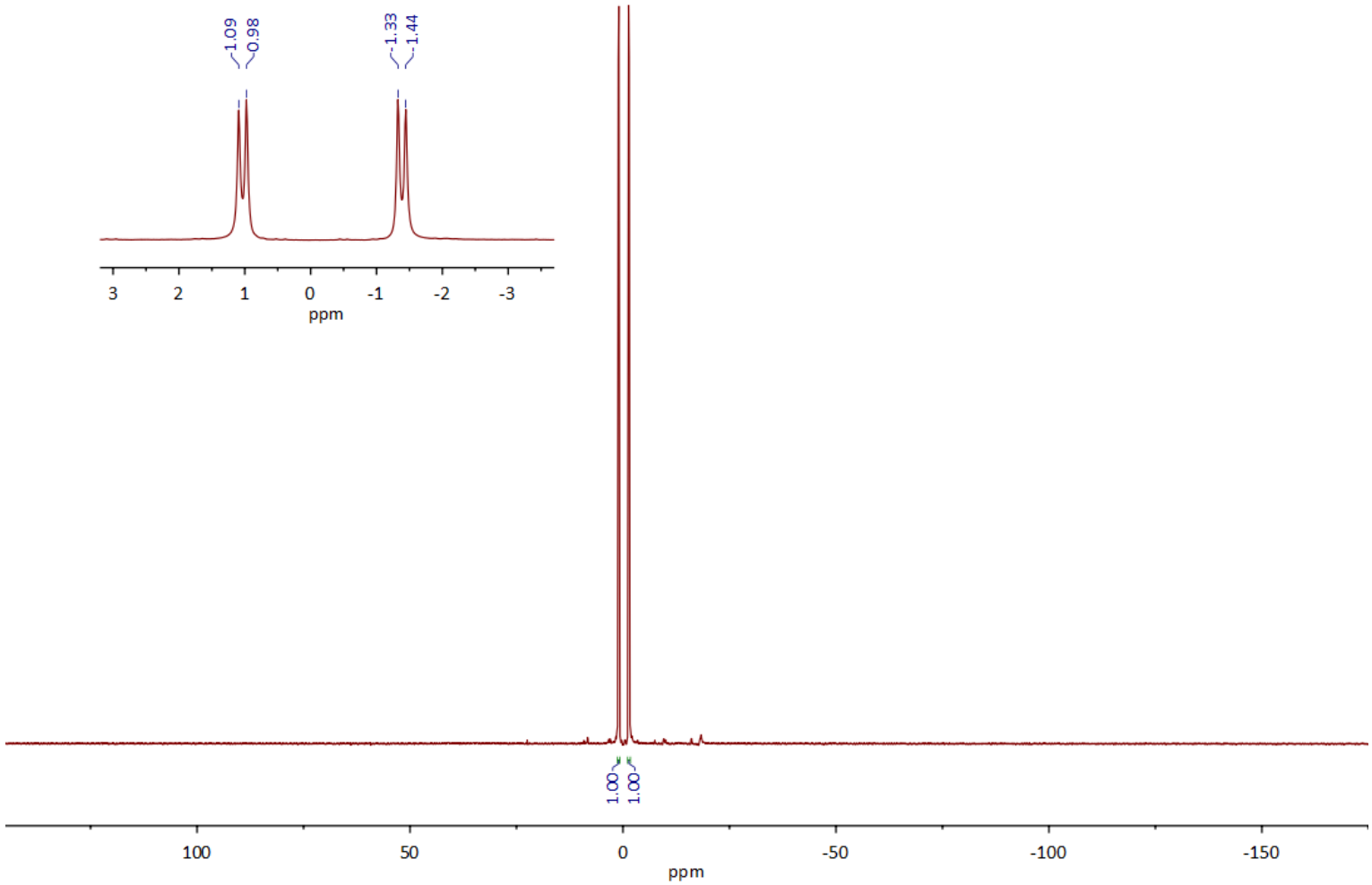
5b

Fig. S52: *Section of the $^{13}C\{^{1}H\}$ NMR spectrum (δ = 108.5 – 166.5 ppm) of **5b** in THF-d_8 (303 K).*

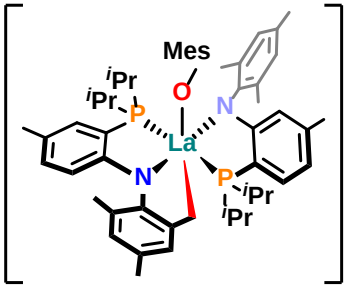


5b

Fig. S53: *$^{13}C\{^1H\}$ DEPT135 NMR spectrum of **5b** in THF-d_8 (303 K). The two enlargements show the ^{13}C chemical shifts of the CH groups in the aromatic region (left) and a close-up of the peak for the $CH_{2Mes(PNcyclo)}$ methylene group at δ = 61.3 ppm (right) of **5b**.*

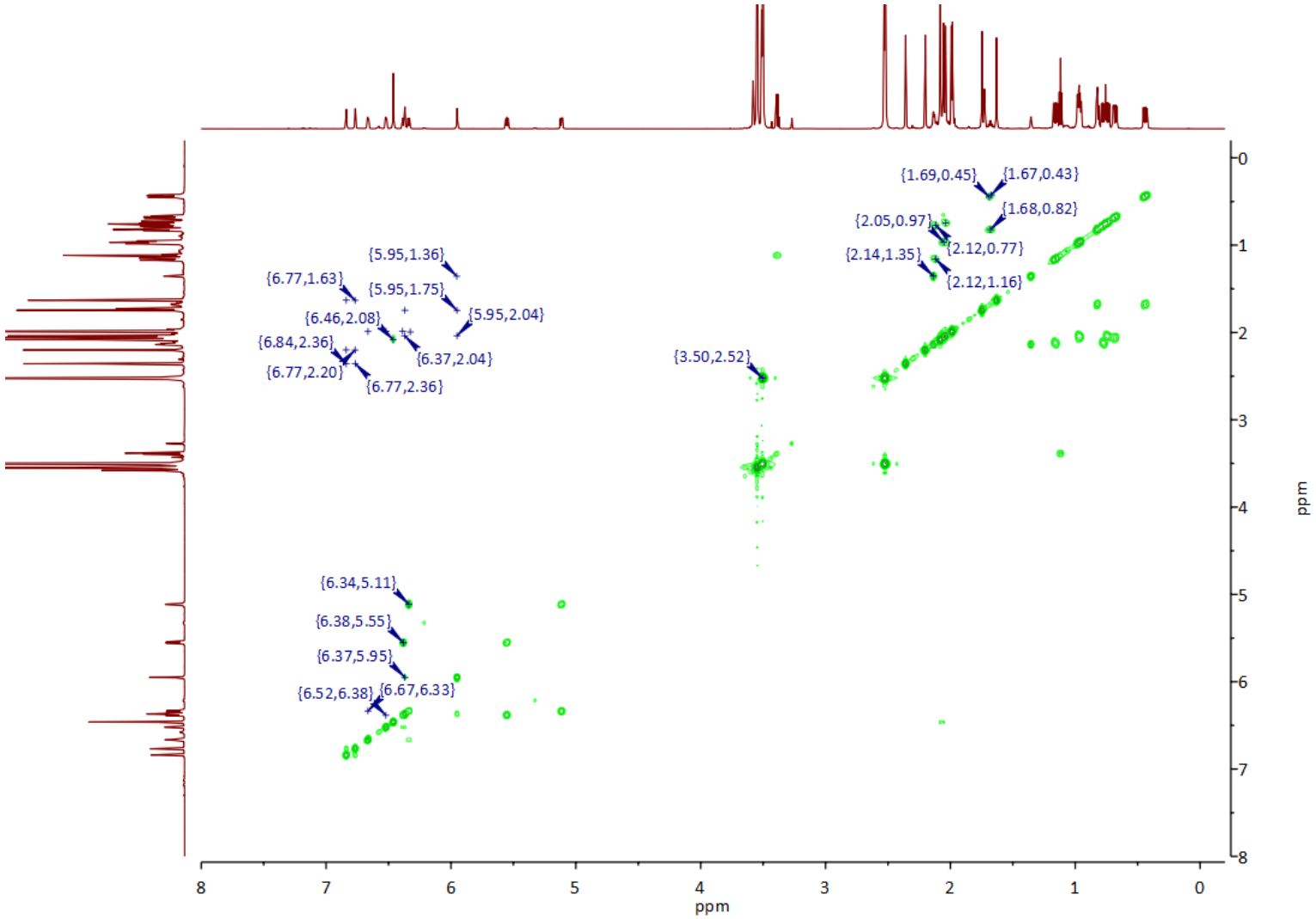


[K(2.2.2-cryptand)]

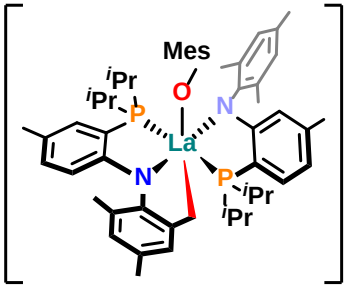


5b

Fig. S54: *$^{31}P\{^{1}H\}$ NMR spectrum of **5b** in THF-d_8 (303 K). The enlargement shows the doublet splitting of the resonances at δ = –1.4 and 1.0 ppm.*

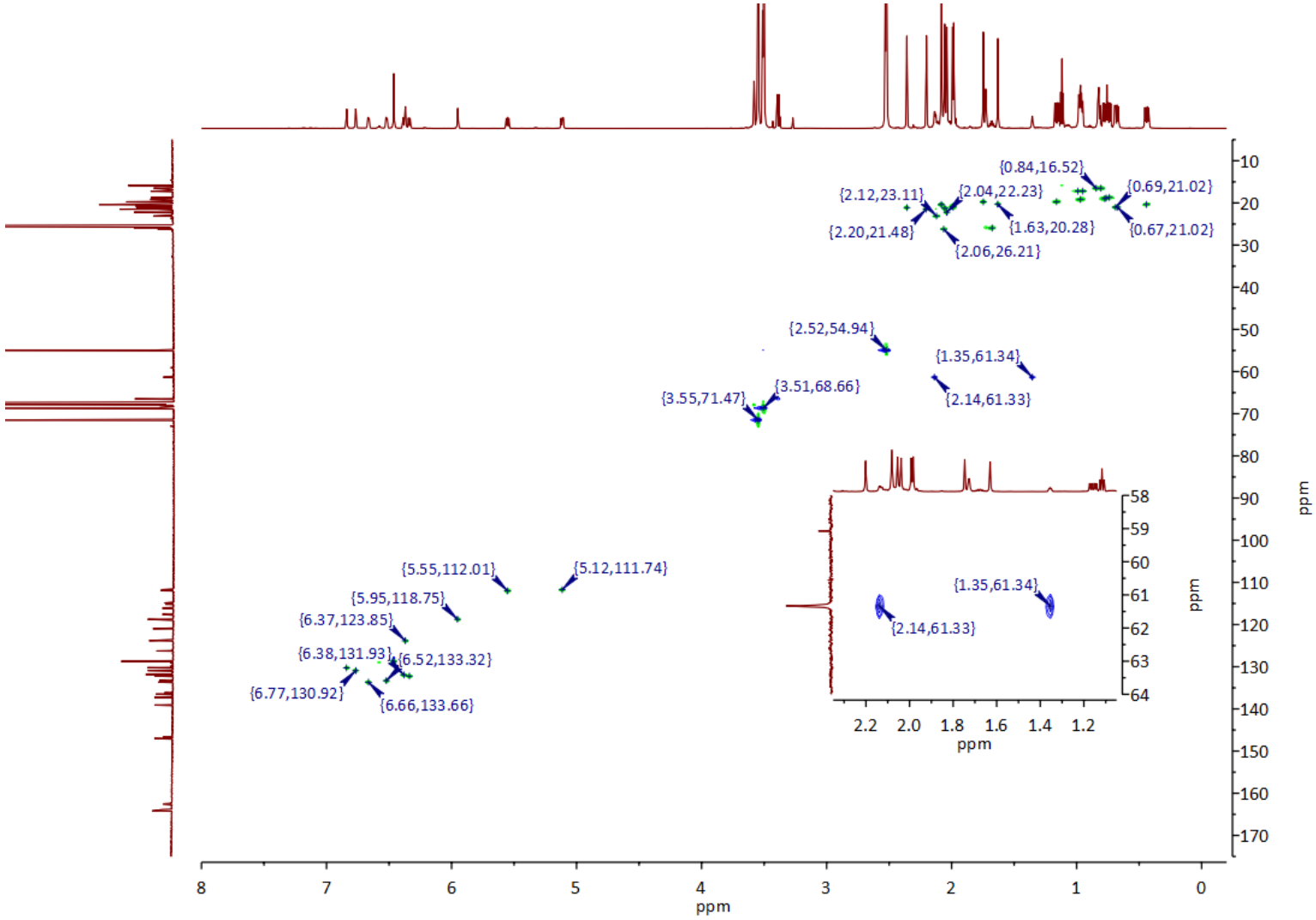


[K(2.2.2-cryptand)]

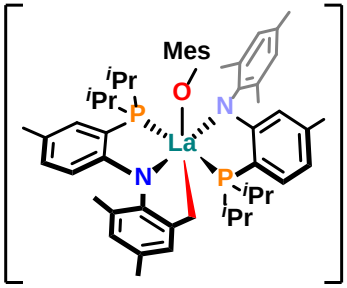


5b

Fig. S55: *^{1}H–^{1}H COSY NMR spectrum of **5b** in THF-d_8 (303 K).*

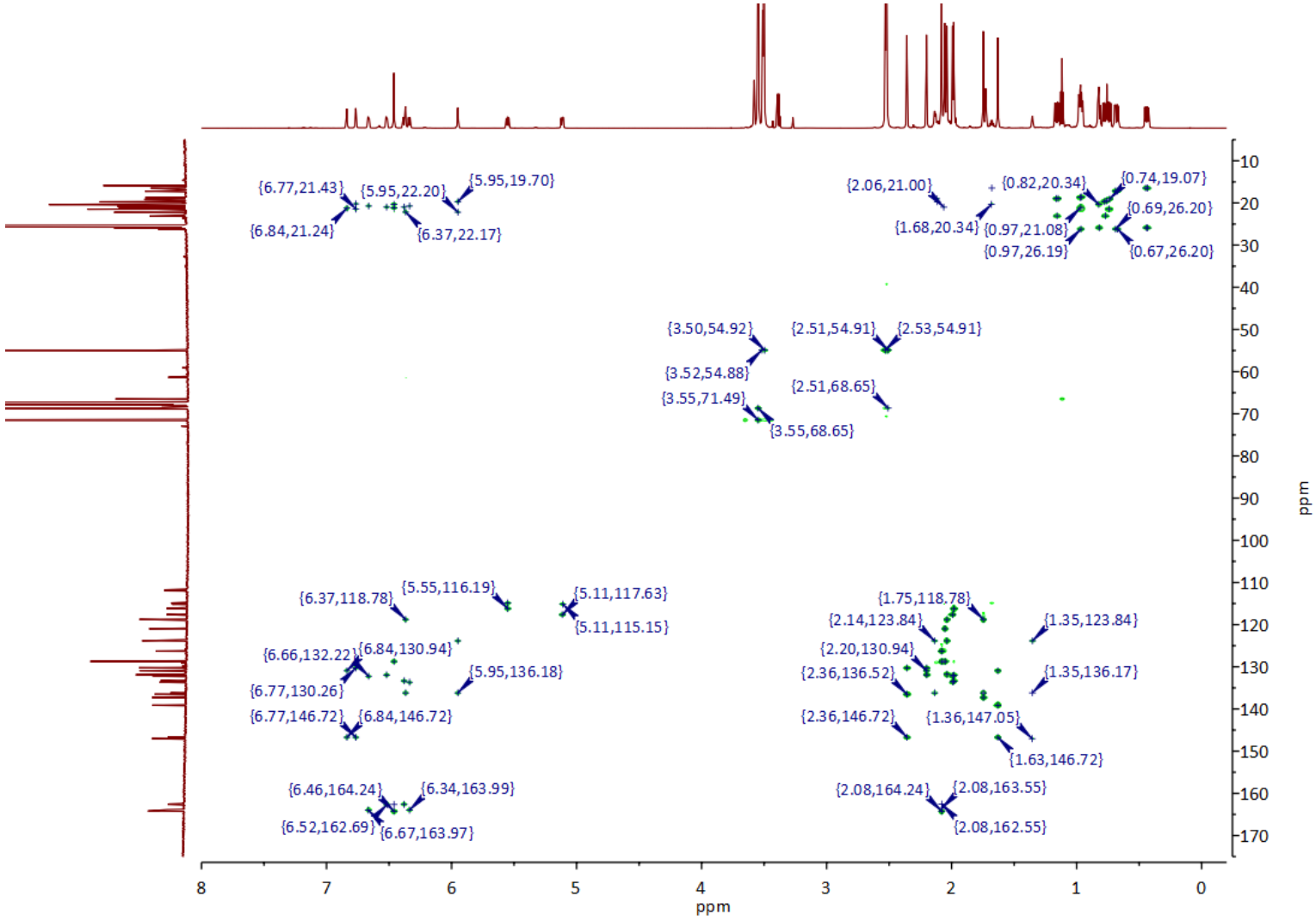


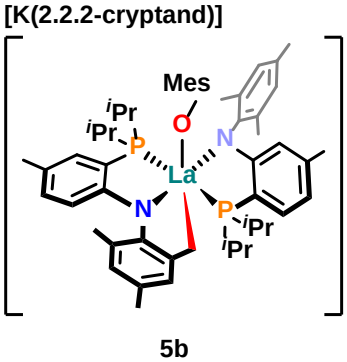
[K(2.2.2-cryptand)]



5b

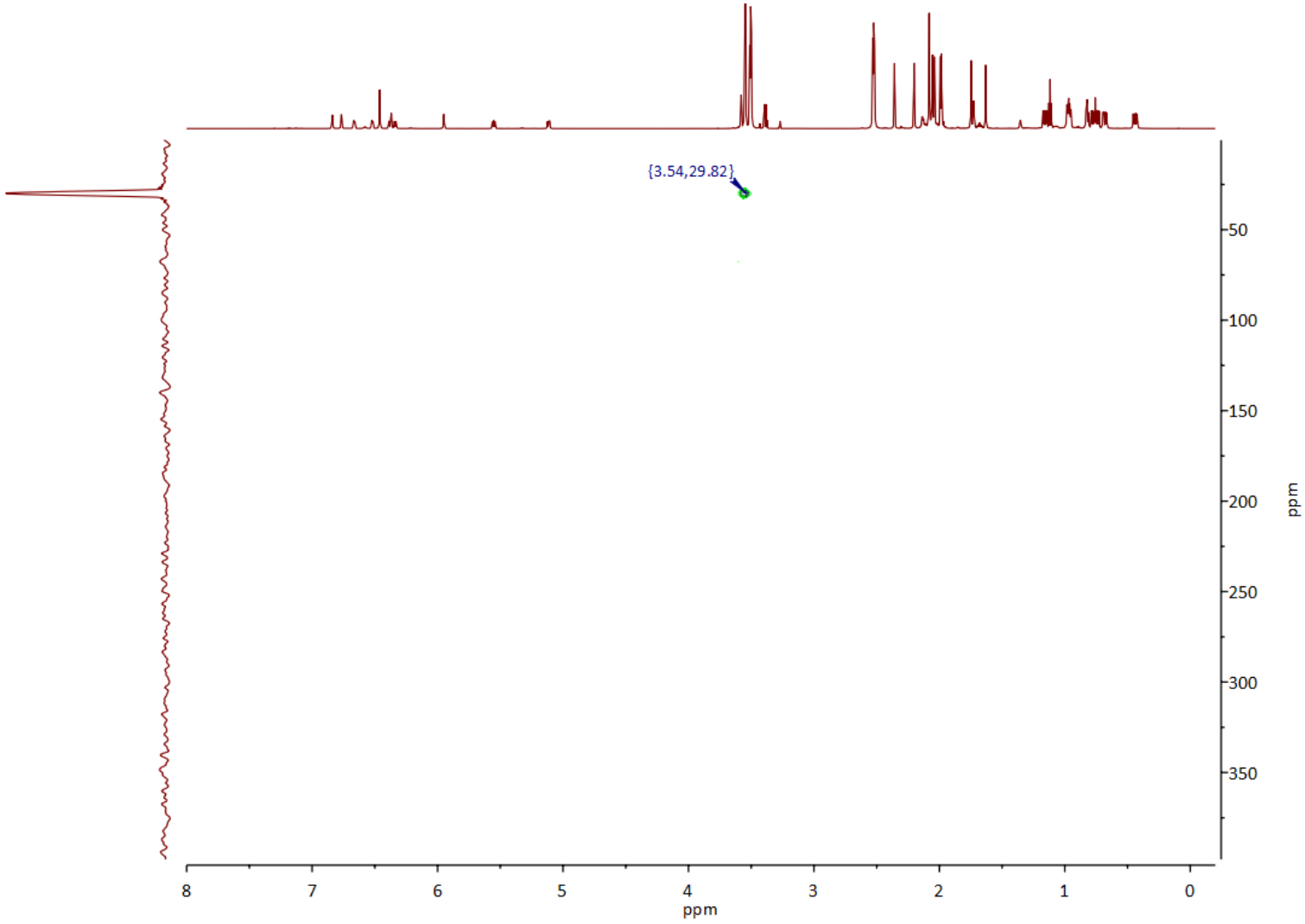
Fig. S56: *^{1}H–^{13}C HSQC NMR spectrum of **5b** in THF-d_8 (303 K). The enlargement shows the two cross peaks for the $CH_{2Mes(PNcyclo)}$ methylene protons of **5b**.*



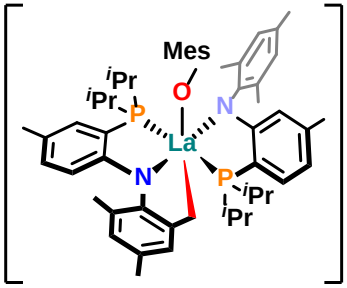


5b

Fig. S57: *^{1}H–^{13}C HMBC NMR spectrum of **5b** in THF-d_8 (303 K).*

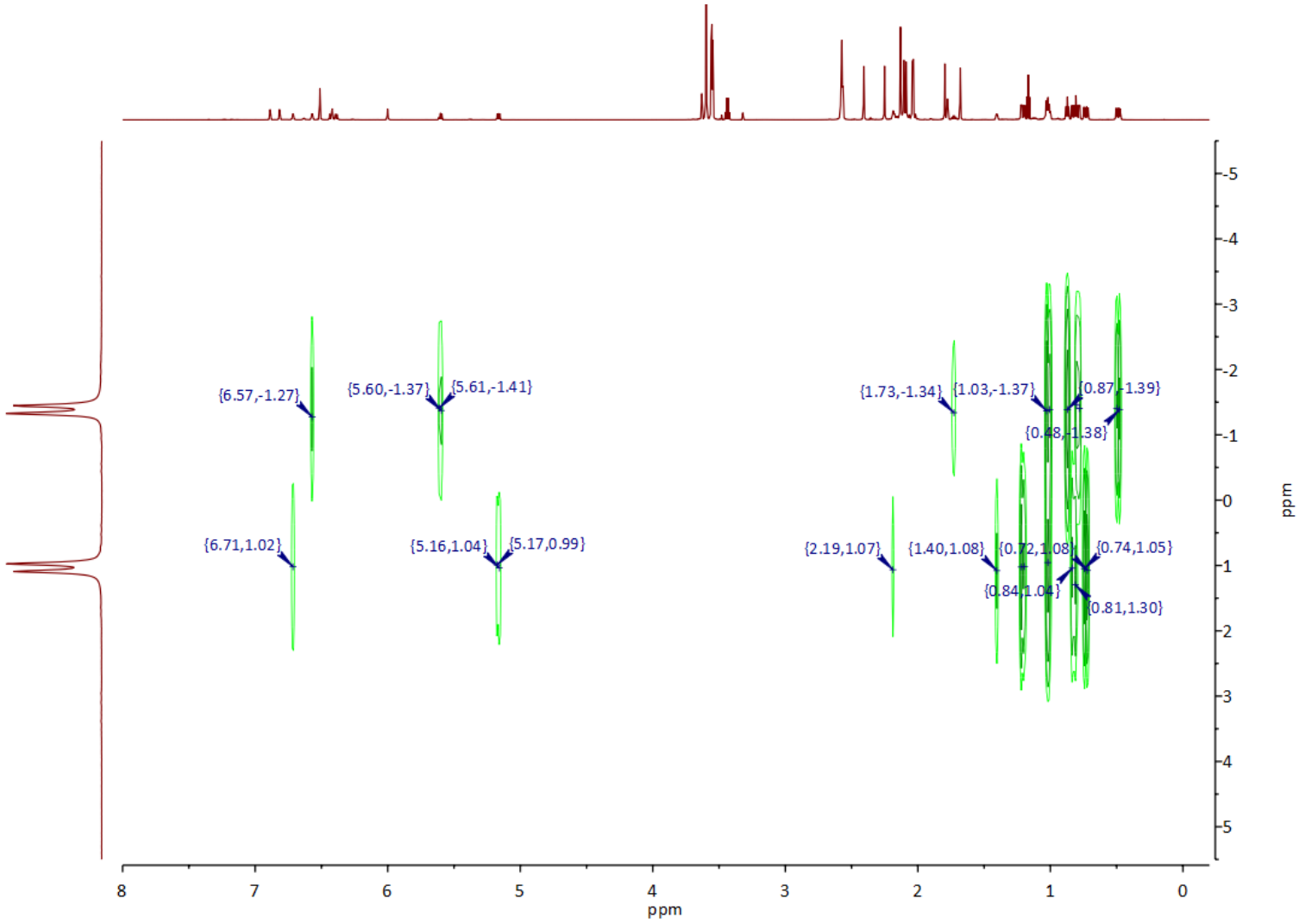


[K(2.2.2-cryptand)]

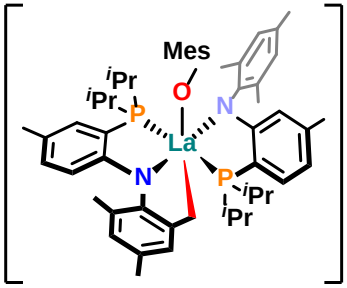


5b

Fig. S58: *^{1}H–^{15}N HMBC NMR spectrum of **5b** in THF-d_8 (303 K).*



[K(2.2.2-cryptand)]



5b

Fig. S59: *^{1}H–^{31}P HMBC NMR spectrum of **5b** in THF-d_8 (303 K).*

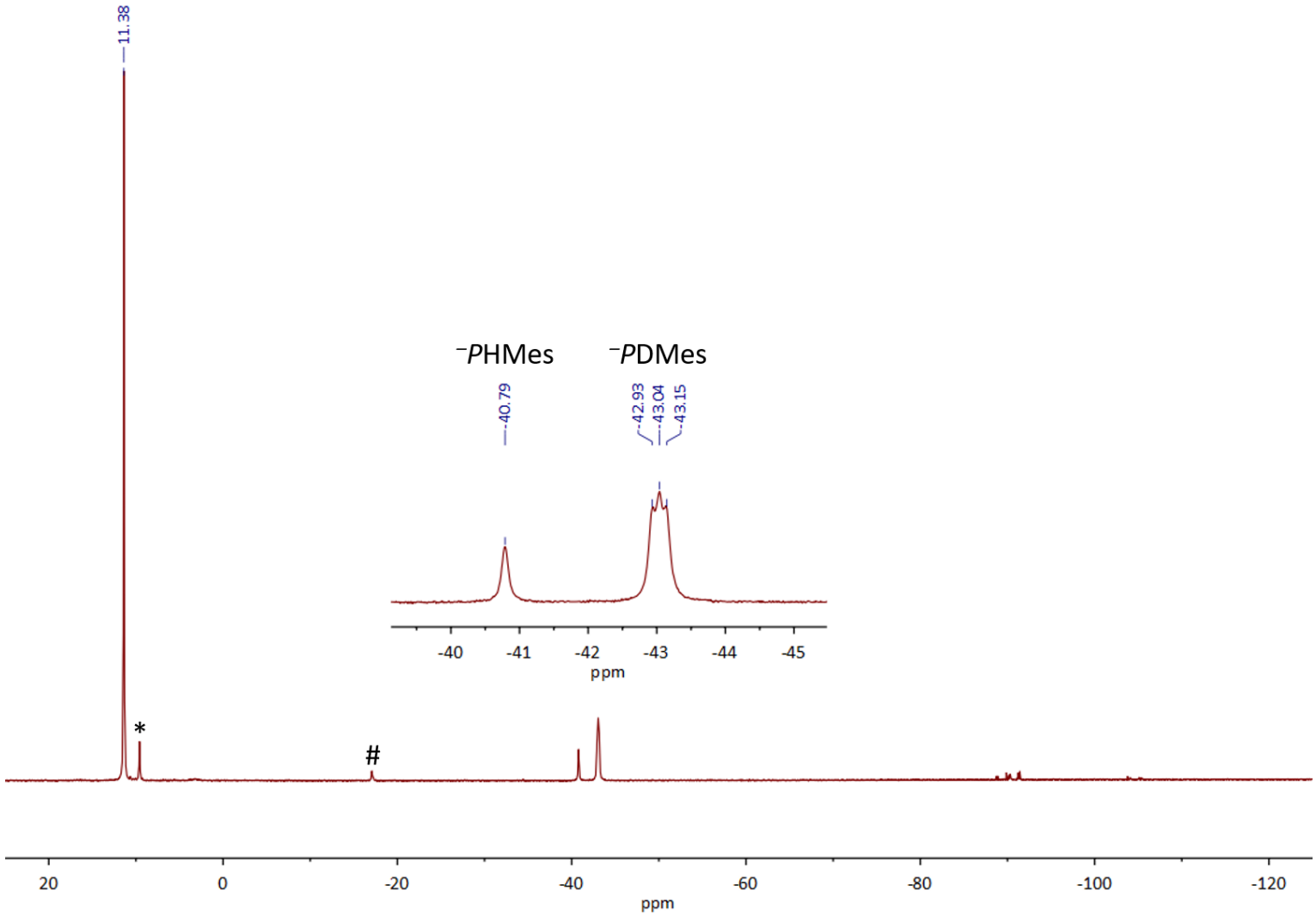


Fig. S60: *Reference for the isotope labelling experiment: $^{31}P\{^{1}H\}$ NMR spectrum of **1-d** (≈86% isotopic purity) in DME with a sealed C_6D_6 capillary (303 K). The enlargement shows the singlet resonance at δ = –40.8 ppm for the ⁻PHMes ligand and the triplet resonance at δ = –43.0 ppm for the ⁻PDMes ligand. Traces of precursor complex $(PN)_2LaCl$ are marked by an asterisk (*). Traces of protonated ligand HPN are denoted as #.*

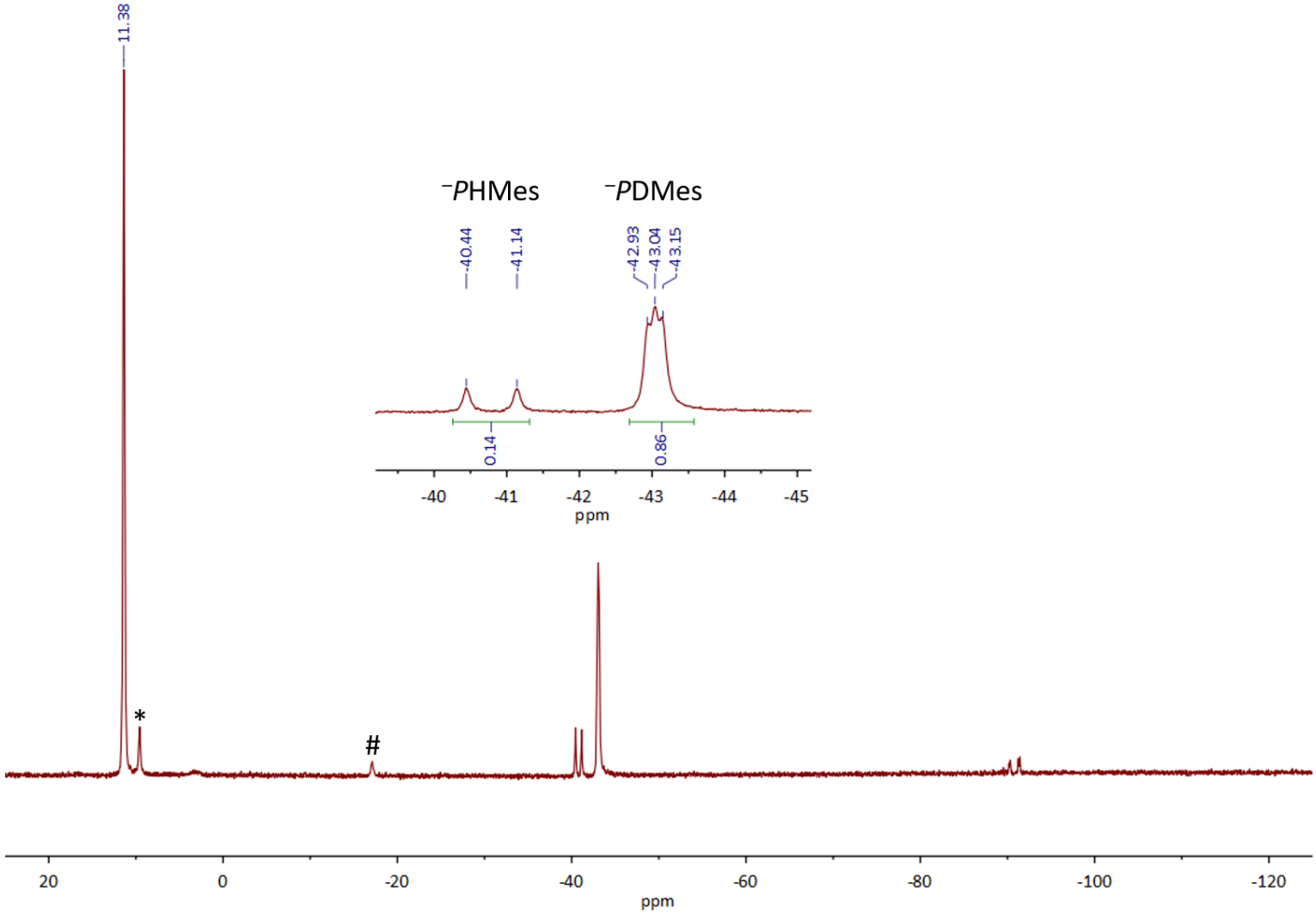


Fig. S61: *Reference for the isotope labelling experiment: ^{31}P NMR spectrum of **1-d** (≈86% isotopic purity) in DME with a sealed C_6D_6 capillary (303 K). The enlargement shows the doublet resonance at δ = –40.8 ppm for the ⁻PHMes ligand and the triplet resonance at δ = –43.0 ppm for the ⁻PDMes ligand. Traces of precursor complex $(PN)_2LaCl$ are marked by an asterisk (*). Traces of protonated ligand HPN are denoted as #.*

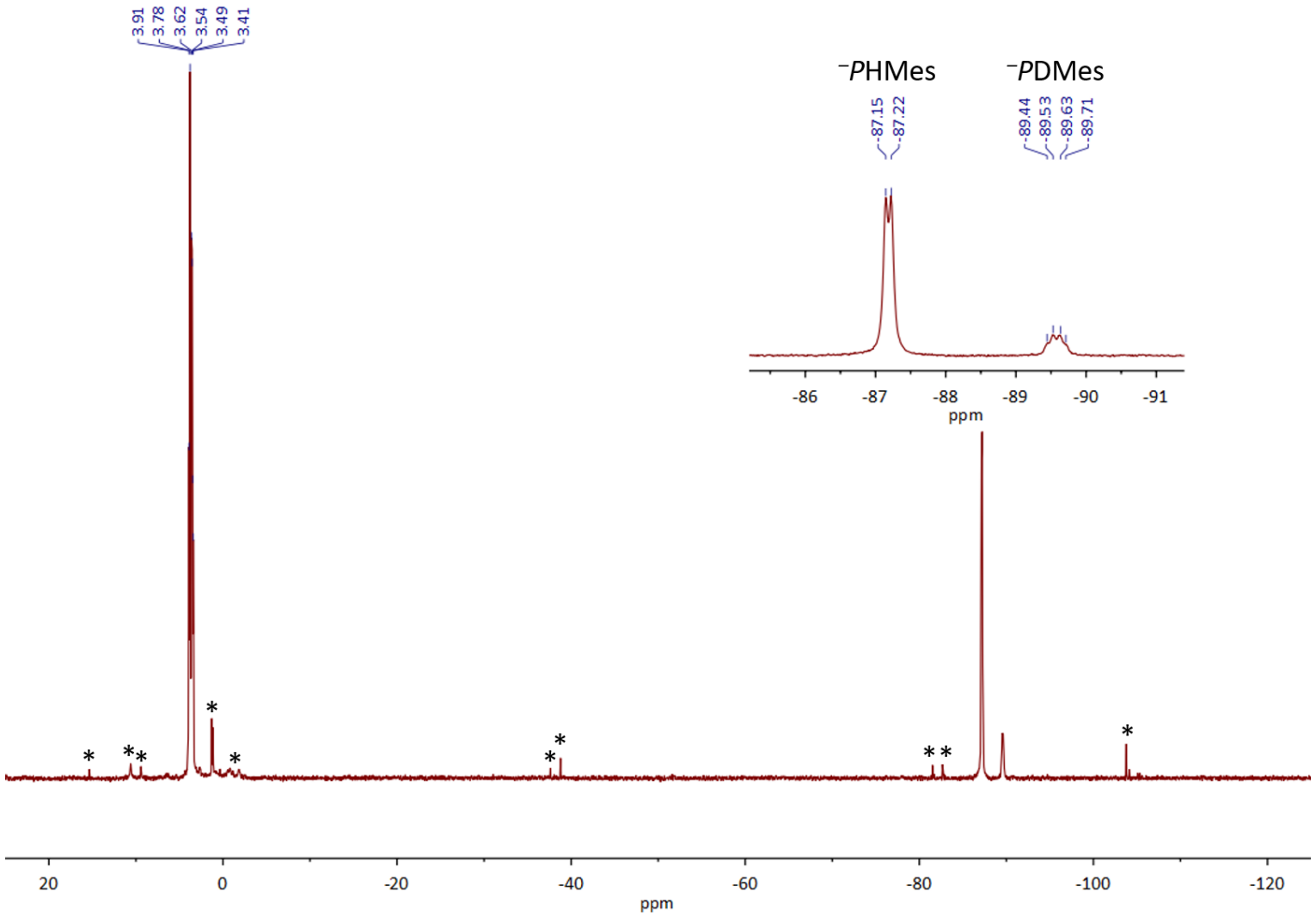


Fig. S62: *Isotope labelling experiment: $^{31}P\{^{1}H\}$ NMR spectrum of the reaction between **1-d** (≈86% isotopic purity) and KHMDS in the presence of 18-crown-6 in DME with a sealed C_6D_6 capillary (303 K). The enlargement shows the doublet resonance at δ = –87.2 ppm ($^{2}J_{PP}$ = 22.6 Hz) for the ⁻PHMes ligand and the multiplet resonance at δ = –89.6 ppm for the ⁻PDMes ligand. Traces of unknown impurities are marked by asterisks (*).*

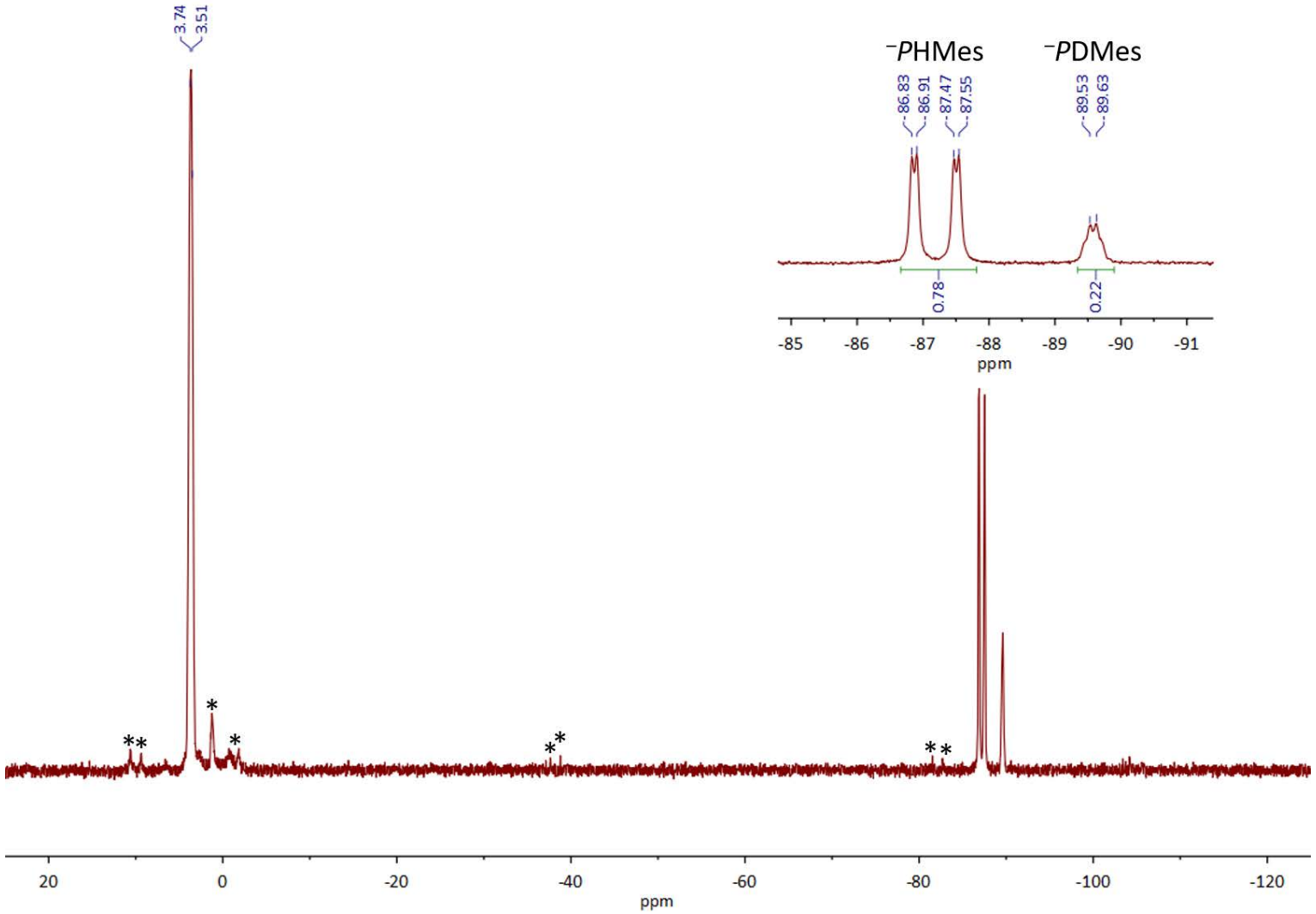


Fig. S63: *Isotope labelling experiment: ^{31}P NMR spectrum of the reaction between **1-d** (≈86% isotopic purity) and KHMDS in the presence of 18-crown-6 in DME with a sealed C_6D_6 capillary (303 K). The enlargement shows the doublet of doublets at δ = –87.2 ppm for the ⁻PHMes ligand and the multiplet resonance at δ = –89.6 ppm for the ⁻PDMes ligand. Note the drastic changes in the integral values for the PH and PD groups compared to the ones found for starting material **1-d** (see reference spectrum in Fig. 61). Traces of unknown impurities are marked by asterisks (*).*

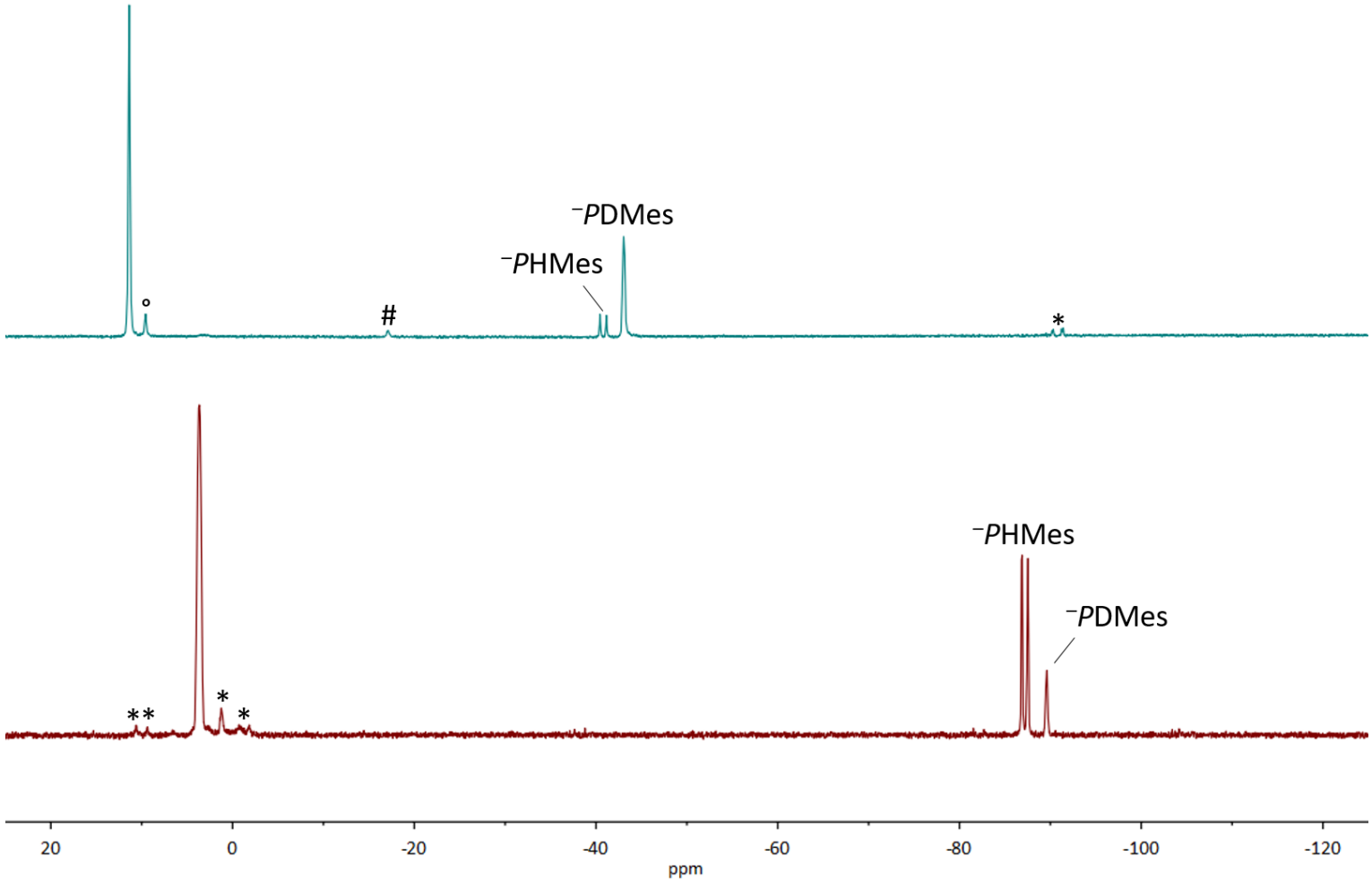


Fig. S64: *Isotope labelling experiment: Stacked ^{31}P NMR spectra of **1-d** (≈86% isotopic purity, top) and the reaction between **1-d** (≈86% isotopic purity) and KHMDS in the presence of 18-crown-6 (bottom) in DME with a sealed C_6D_6 capillary (303 K). The direct comparison clearly shows the inversion of the D/H isotopic ratio at phosphorous (for integral values see Fig. S61 and S63). Traces of precursor complex $(PN)_2LaCl$ are marked by ° and traces of protonated ligand HPN are labelled by # (top). Traces of unknown impurities are marked by asterisks (*).*

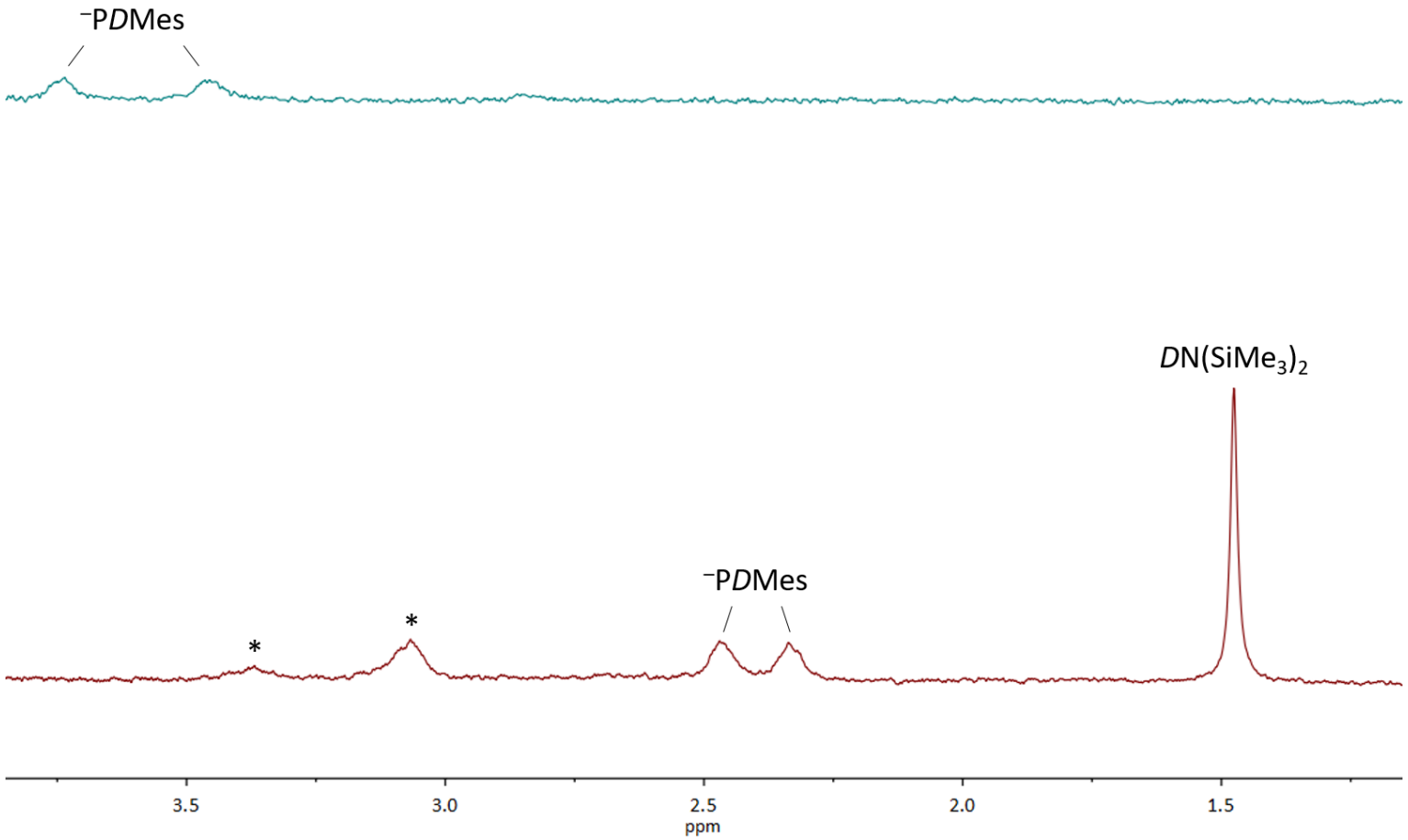


Fig. S65: *Isotope labelling experiment: Stacked details of the ^2H NMR spectra of* **1-d** *(≈86% isotopic purity, top) and the reaction between* ***1-d*** *(≈86% isotopic purity) and KHMDS in the presence of 18-crown-6 (bottom) in DME with a sealed C_6D_6 capillary (303 K). The new intense singlet resonance at δ = 1.48 ppm can be assigned to $DN(SiMe_3)_2$. Unknown deuterated compounds are marked by asterisks (*).*

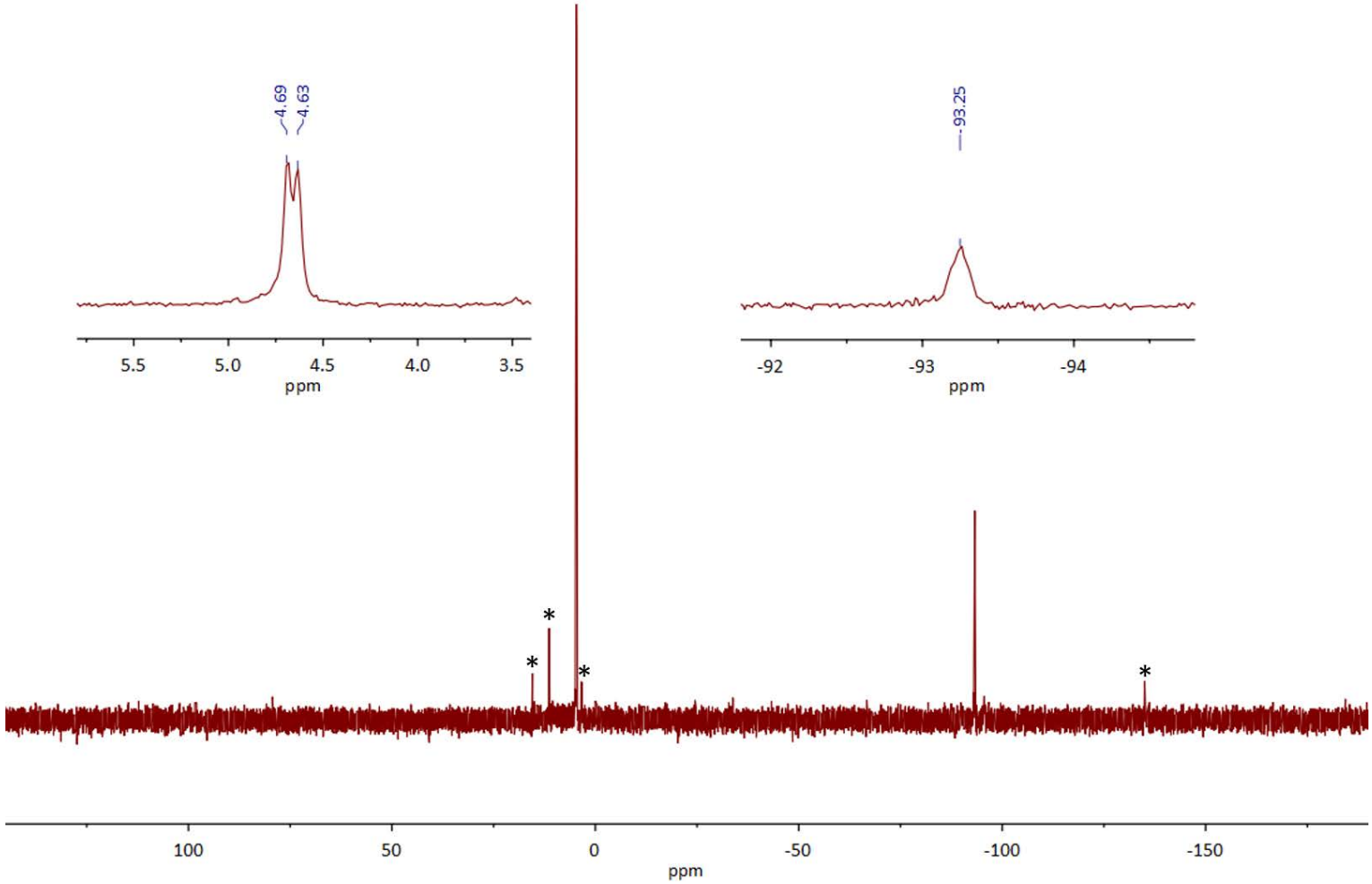


Fig. S66: *Trapping experiment: $^{31}P\{^{1}H\}$ NMR spectrum of the reaction between **1-d** and KHMDS in the presence of 18-crown-6 in cyclohexene with a sealed C_6D_6 capillary (303 K). The enlargements show the resonances of the main product **3a**. Traces of unknown impurities are marked by asterisks (*).*

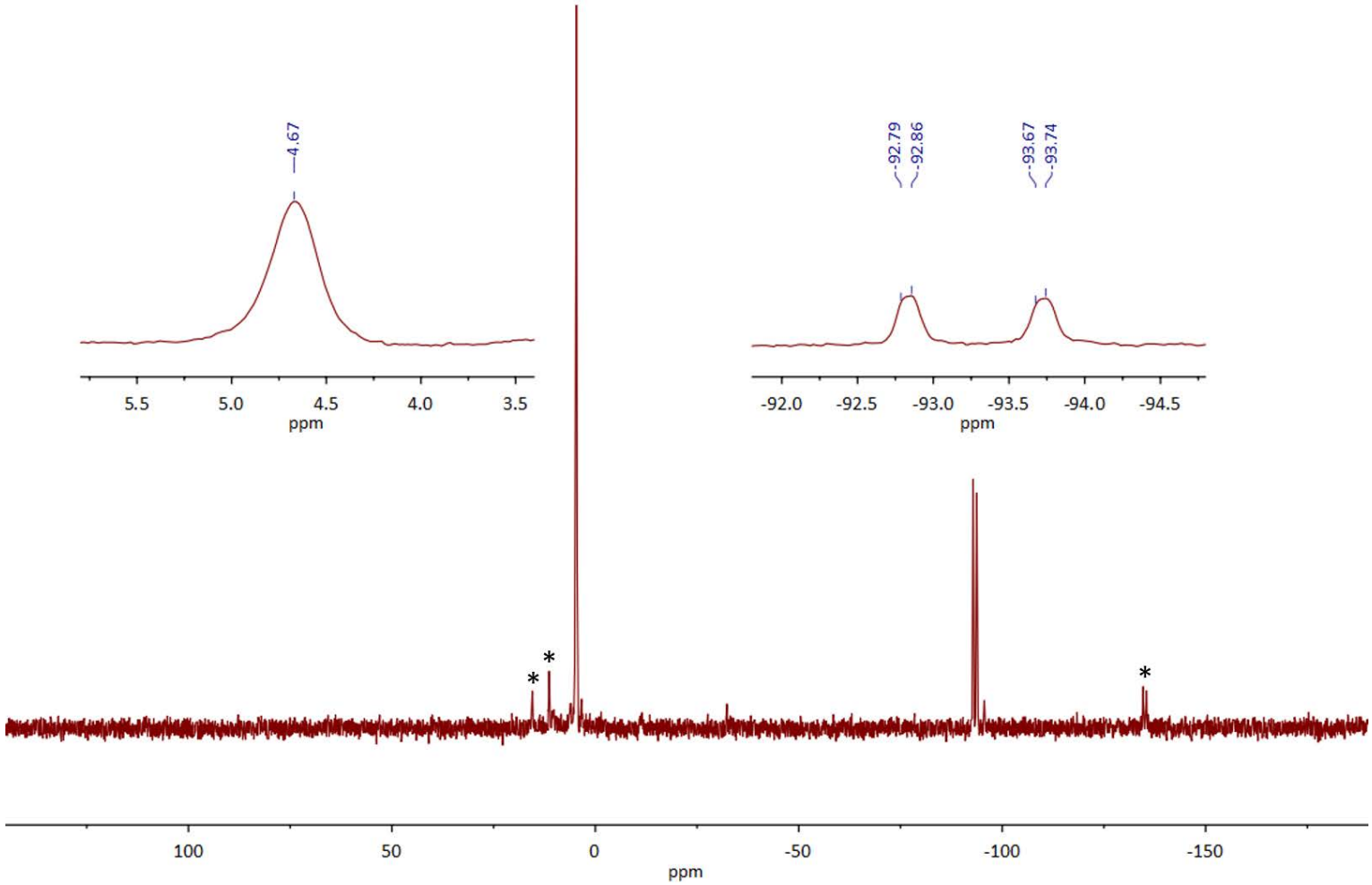


Fig. S67: *Trapping experiment: ^{31}P NMR spectrum of the reaction between **1-d** and KHMDS in the presence of 18-crown-6 in cyclohexene with a sealed C_6D_6 capillary (303 K). The enlargements show the resonances of the main product **3a**. Note also the >99% conversion of the PD groups into PH groups as is obvious by the doublet splitting in the right enlargement. Traces of unknown impurities are marked by asterisks (*).*

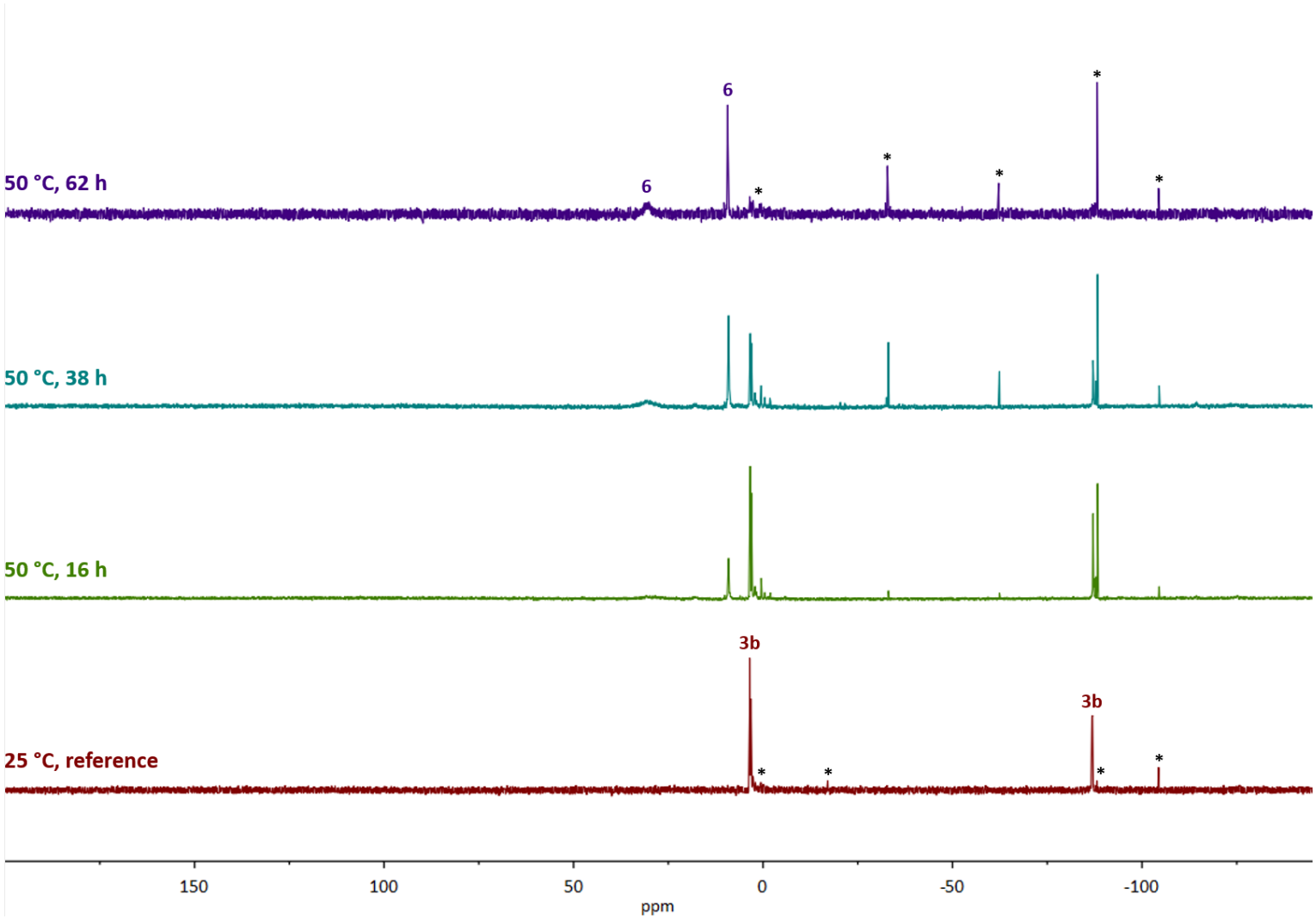
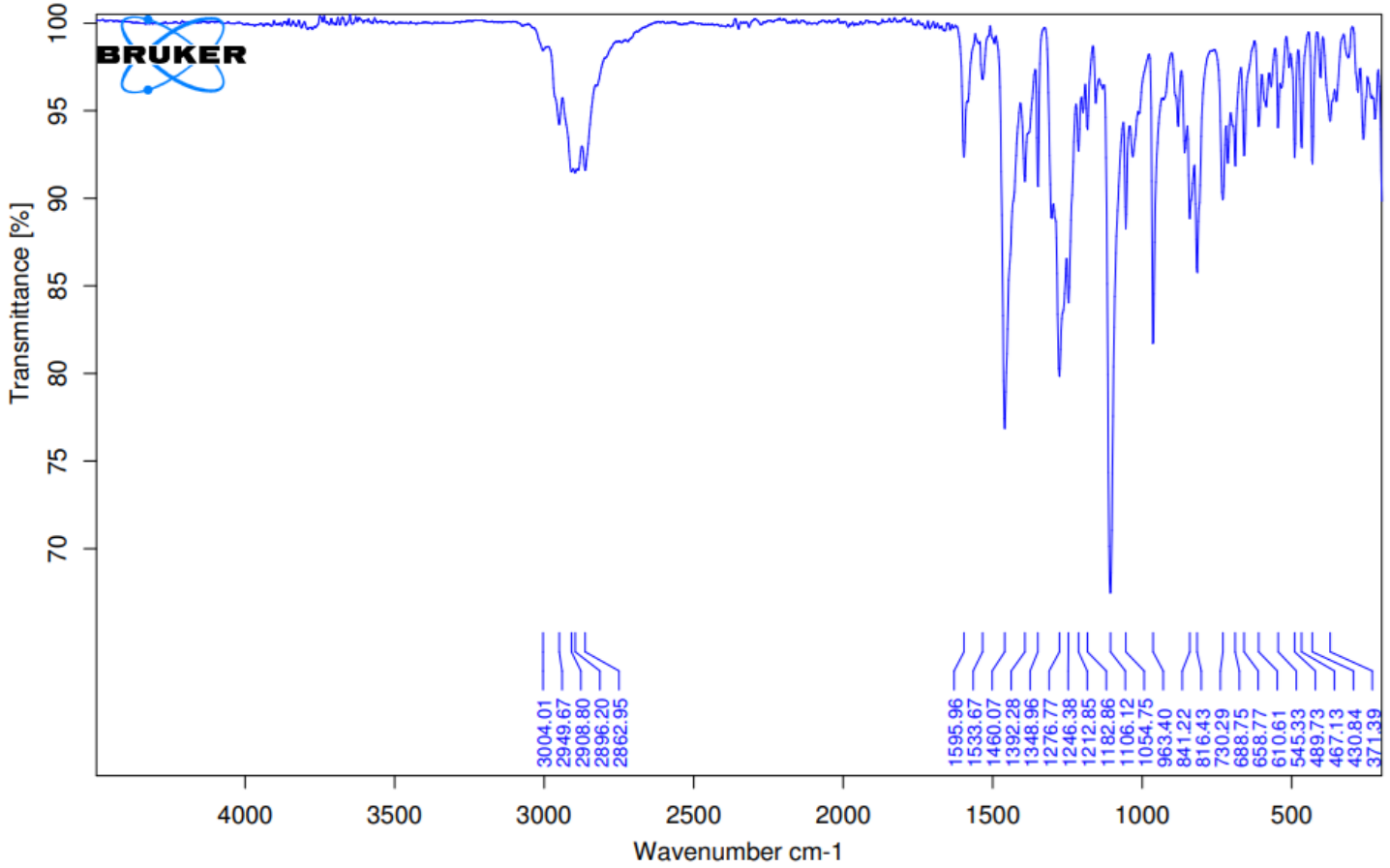
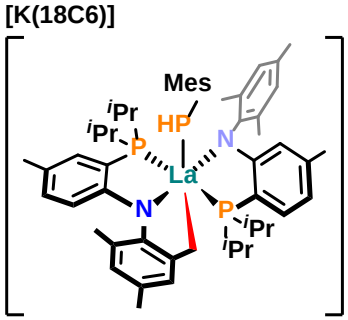


Fig. S68: *Stacked reaction control $^{31}P\{^{1}H\}$ NMR spectra of the conversion of **3b** to **6** (THF-d_8, 303 K). The resonances of freshly prepared starting material **3b** (reference) and main product **6** are labelled in the bottom and top spectrum, respectively. Unknown impurities in the starting material and after full conversion of **3b** are marked with asterisks (*). The temperature and reaction times are specified on the left.*

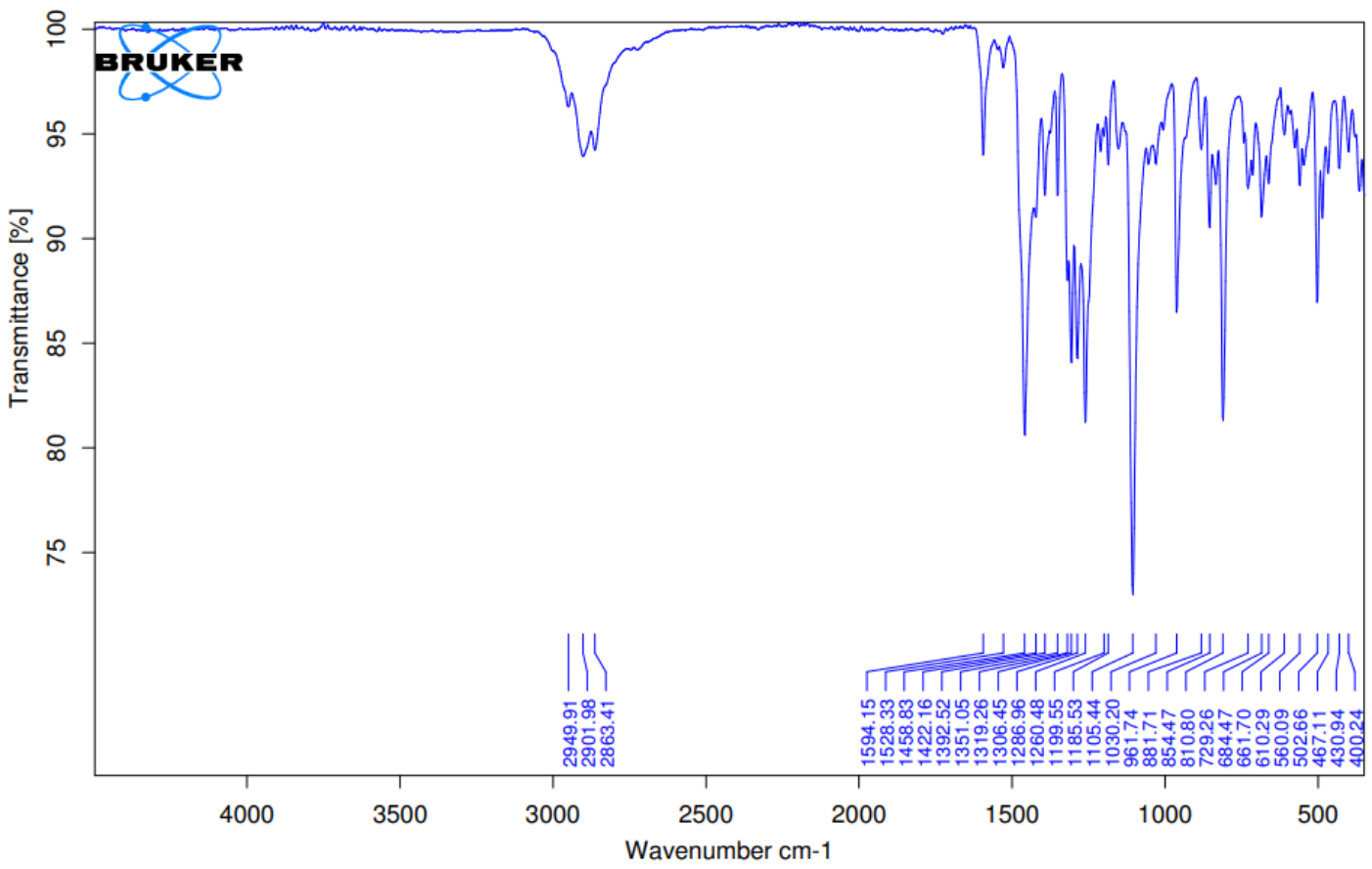
3. IR Spectra

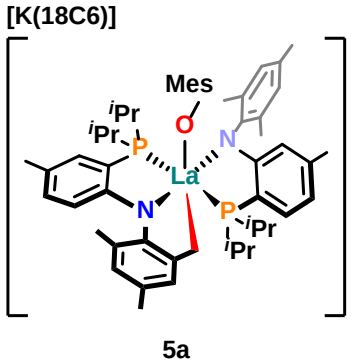




3a

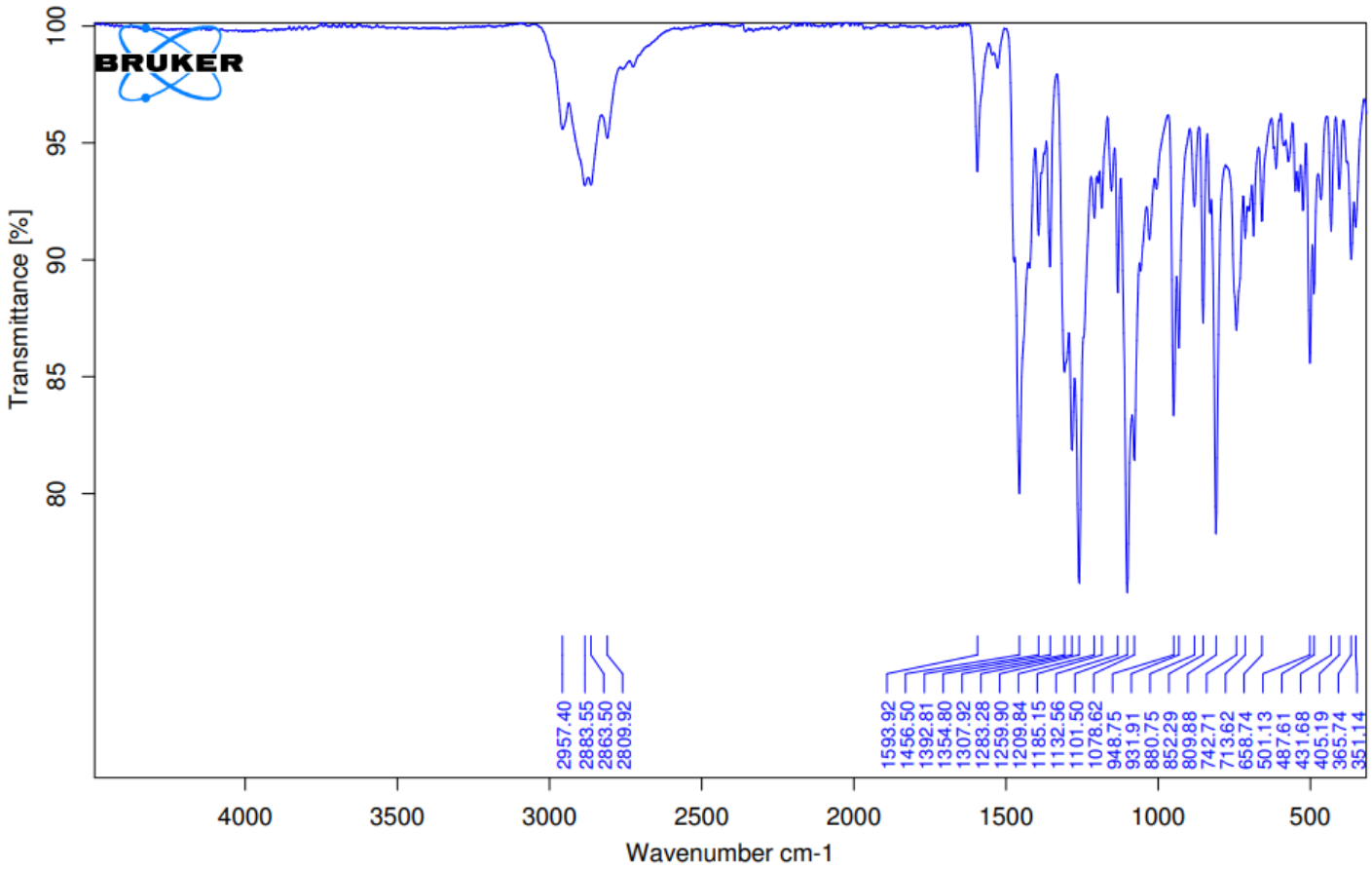
*Fig. S69: IR spectrum (ATR) of **3a**.*

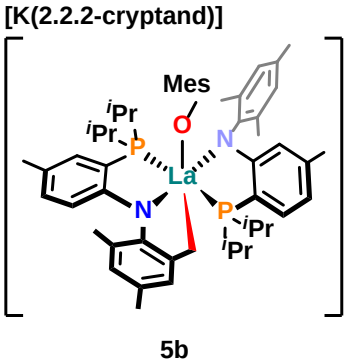




5a

*Fig. S70: IR spectrum (ATR) of **5a**.*





5b

*Fig. S71: IR spectrum (ATR) of **5b**.*

4. Crystallographic Details

*Table S1: Crystallographic details on complexes **3a**, **3b**, **5a** and **6**.*

	3a	**3b**	**5a**	**6*[#]**
Chemical formula	2 ($C_{65}H_{97}N_2O_6P_3KLa$) · ($C_4H_{10}O$)	$C_{71}H_{109}N_4O_6P_3KLa$	2 ($C_{65}H_{96}N_2O_7P_2KLa$)	$C_{80}H_{120}N_4O_6P_4KLa$
M_r	2620.84	1385.54	2514.76	1535.68
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*–1	*P*–1	*P*–1	*P*–1
a (Å)	14.0506(8)	12.7500(8)	13.3178(9)	14.168(15)
b (Å)	14.3744(8)	15.9812(8)	25.286(2)	18.79(2)
c (Å)	18.1614(10)	21.2031(14)	25.521(2)	19.86(2)
α (°)	99.417(2)	105.285(2)	116.117(2)	105.16(3)
β (°)	90.617(2)	94.133(3)	98.326(2)	97.23(3)
γ (°)	91.294(2)	109.532(3)	99.911(2)	104.28(3)
V (Å^3)	3617.3(4)	3866.2(4)	7361.7(9)	4841(9)
Z	1	2	2	2
Densitiy (g cm^{-3})	1.203	1.190	1.134	1.053
F(000)	1382	1464	2648	1624
Radiation Type	MoKα	MoKα	MoKα	MoKα
μ (mm^{-1})	0.71073	0.71073	0.71073	0.593
Crystal size	0.22x0.18x0.17	0.35x0.32x0.28	0.26x0.22x0.04	0.02x0.01x0.005
Meas. Refl.	337081	266834	672658	53580
Indep. Refl.	14757	17757	32352	16395
Obsvd. [$I > 2\sigma(I)$]	13249	15847	24047	6842
R_{int}	0.0530	0.0709	0.0938	0.3354
R [$F^2 > 2\sigma(F^2)$]	0.0326	0.0303	0.0518	0.0981
wR(F^2)	0.0979	0.0861	0.1437	0.2883
S	1.124	1.097	1.088	0.959
$\Delta\rho_{max}$	1.842	0.545	4.627	1.839
$\Delta\rho_{min}$	–0.553	–0.704	–1.625	–2.263
CCDC	2020114	2020113	2021044	2020112

[#]Due to strong disorder of three diethyl ether molecules, the SQUEEZE technique had to be applied for this crystal.

*Despite numerous attempts, only low quality crystals could be obtained, which did not diffract very well. This results in the high R_{int} as well as the moderately good R1 and wR2 values. Nevertheless, the model as such can be considered as reliable in combination with the other analytical data obtained.

*Table S2: Selected bond lengths in Å and angles in ° of complexes **3a**, **3b**, **5a** and **6**.*

	3a	**3b**	**5a**	**6**
La1 – P1	3.285(1)	3.169(1)	3.240(1)	3.237(4)
La1 – P2	3.191(1)	3.175(1)	3.160(1)	3.241(4)
La1 – P70 / O70	3.049(1)	3.025(1)	2.283(3)	2.921(4)
La1 – P80	-	-	-	2.914(4)
La1 – N1	2.395(2)	2.433(2)	2.440(3)	2.454(9)
La1 – N2	2.473(2)	2.514(2)	2.498(3)	2.511(10)
La1 – C25	2.634(3)	2.617(2)	2.653(4)	-
P70 – P80	-	-	-	2.168(5)
N1 – La1 – N2	113.80(7)	122.31(6)	109.9(1)	124.3(3)
P1 – La1 – P2	172.25(2)	172.39(1)	171.46(3)	172.5(1)
N1 – La1 – P1	59.81(5)	61.87(4)	59.29(8)	62.6(2)
C70 – P70 / O70 – La1	129.20(1)	128.10(8)	166.3(3)	126.6(4)
C80 – P80 – La1	-	-	-	128.8(4)

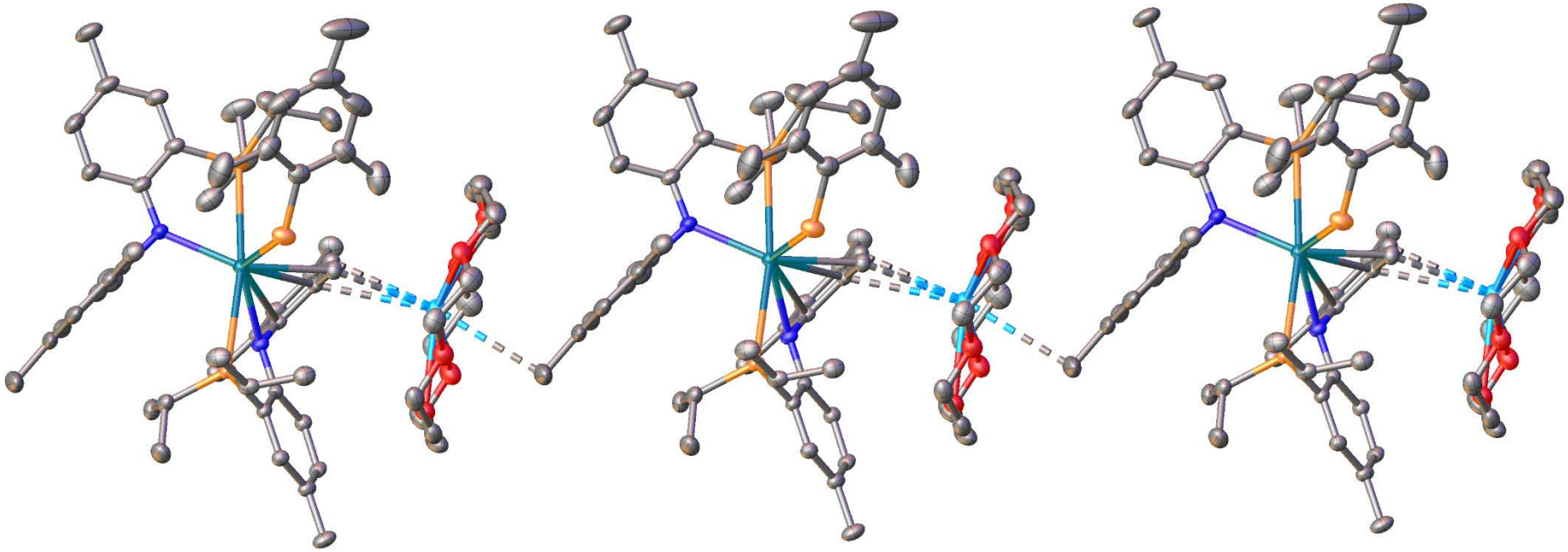


Fig. S72: *Molecular view of the polymeric chain structure of complex **3a**. Hydrogen atoms and solvent molecules have been omitted for clarity. Thermal ellipsoids are shown at a probability level of 50%.*

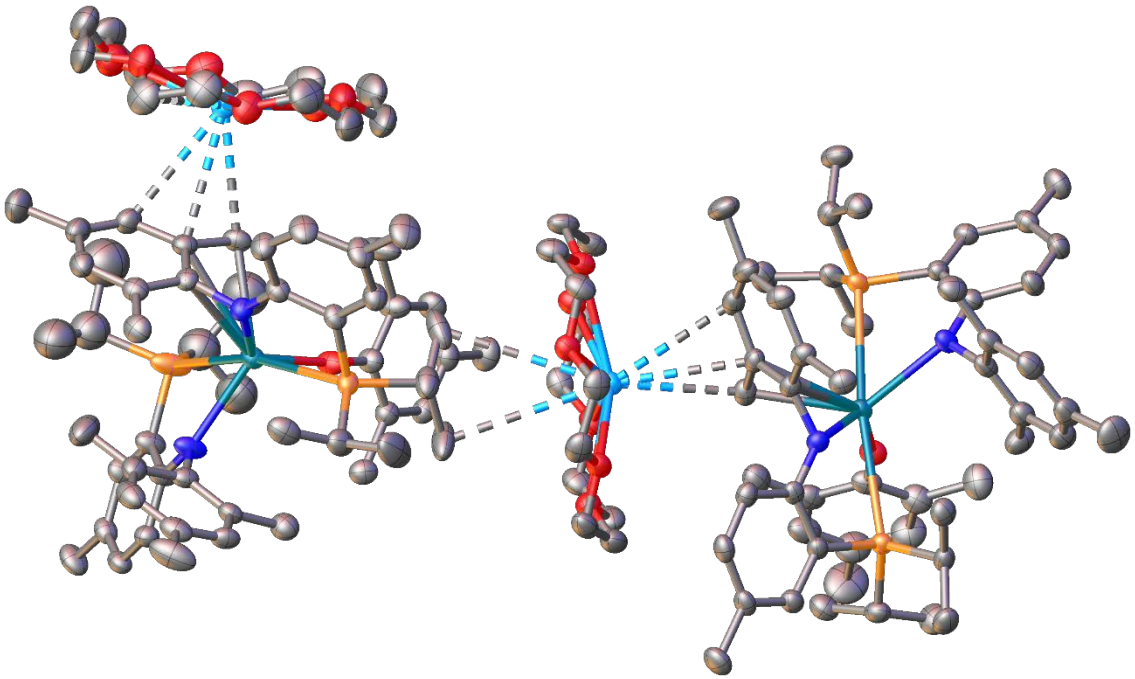


*Fig. S73: Molecular view of the polymeric chain structure of complex **5a**. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at a probability level of 50%.*

5. Computational Details

All DFT calculations were performed with Gaussian 09.[6] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[7] Si and La atoms were treated with a Stuttgart effective core potential[8] augmented with a polarization function (ζ_d = 0.284 for Si and ζ_f = 1.000 for La).[9] For P, N, C and H atoms, Pople's double-ζ basis set 6-31G(d,p) was used.[10] Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. Analytical frequency calculations at 298.15 K and 1 atm were systematically done in order to characterize the nature of stationary points. IRC calculations were carried out in order to confirm the connectivity between reactant(s), transition state and product(s).

! H abstraction by HMDS on the adjacent methyl group - Adduct !

P	3.796169	-0.854550	-0.338321
La	0.607123	-0.517065	-0.757602
N	1.688266	1.108460	0.588847
C	0.675214	2.086104	0.814228
C	-0.412710	1.820170	1.680357
C	-0.512394	0.535984	2.468355
H	-1.208223	0.684438	3.302971
N	-3.124719	2.175856	4.530615
Si	-4.705274	1.525845	4.466468
C	-4.826495	-0.381864	4.798034
H	-4.192380	-0.938359	4.098919
C	-5.466898	1.758238	2.704360
C	-6.044627	2.274620	5.658009
Si	-2.319859	2.751371	5.929650
C	-2.957581	4.448895	6.622004
N	0.351518	-2.464602	0.552811
C	0.105721	-3.822311	0.643919
C	0.145621	-4.615400	-0.530981
C	-0.092259	-5.986590	-0.463700
C	-0.374688	-6.634229	0.740507
C	-0.401455	-5.847416	1.895601
C	-0.170670	-4.473083	1.878147

C	-1.388649	2.801990	1.905180
C	-1.316625	4.043448	1.272594
C	-0.240167	4.297183	0.413088
C	0.758608	3.352998	0.180181
C	0.479934	-3.951217	-1.830110
C	-0.667267	-8.111304	0.789683
C	-0.218402	-3.680713	3.156260
N	0.060942	-0.072415	-3.145508
C	1.158974	0.446563	-3.886391
C	2.190348	-0.395570	-4.362853
C	3.265424	0.151127	-5.073686
C	3.361152	1.514757	-5.341488
C	2.325680	2.335839	-4.887030
C	1.232204	1.833360	-4.181233
P	-2.484548	-0.458713	-1.405213
C	-3.526416	1.100462	-1.081302
C	-4.966827	1.061242	-1.585045
C	5.064059	-0.135337	-1.569757
C	4.664013	1.298937	-1.911531
C	3.911317	0.259888	1.128899
C	2.816883	1.138712	1.378490
C	2.949897	2.019193	2.483473
C	4.072022	2.006809	3.294381
C	5.140926	1.127131	3.069915
C	5.026495	0.268791	1.977149
C	4.621554	-2.458709	0.234287
C	3.860441	-3.068476	1.411213
C	2.124339	-1.886108	-4.167438
C	4.537382	2.088952	-6.086637
C	0.116752	2.755915	-3.781532
C	-2.369507	5.089389	1.531149

C	1.951406	3.702568	-0.667052
C	6.347476	1.108899	3.971271
C	6.528206	-0.199646	-1.138901
C	-2.331135	1.588556	7.486641
C	-0.446589	3.054872	5.574939
C	-1.091078	-0.330830	-3.872329
C	-1.085628	-0.369879	-5.293255
C	-2.214987	-0.680606	-6.032345
C	-3.438549	-0.978573	-5.420094
C	-3.466001	-0.918490	-4.027170
C	-2.349607	-0.589667	-3.246395
C	-4.657672	-1.345098	-6.224798
C	-3.665950	-1.851903	-0.911666
C	-3.148713	-3.219675	-1.351215
C	-3.902970	-1.810732	0.599470
C	-2.794503	2.326627	-1.618741
C	4.727359	-3.442767	-0.932245
H	0.410377	-2.080450	1.496864
H	-2.158733	2.605409	2.668618
H	-0.156139	-0.159936	-5.813109
H	-4.405332	-1.138314	-3.524794
H	-2.948623	-3.256504	-2.425970
H	-3.896473	-3.988436	-1.121000
H	-2.234991	-3.491622	-0.814963
H	5.635237	-2.203211	0.566674
H	-2.139783	-0.701579	-7.119075
H	-5.004672	0.986515	-2.676868
H	-5.475466	1.989231	-1.297942
H	-5.545598	0.237295	-1.158367
H	-3.532531	1.165588	0.013833
H	-0.050683	-6.566950	-1.385392

H	3.653418	1.354549	-2.324092
H	5.347957	1.712214	-2.662155
H	4.710528	1.937078	-1.023578
H	-0.159312	5.271224	-0.069248
H	4.929009	-0.751597	-2.468934
H	2.361819	3.403676	-5.098345
H	-0.612929	-6.321932	2.853634
H	1.098194	-2.252583	-4.248568
H	2.504337	-2.185612	-3.182838
H	2.739019	-2.402004	-4.911724
H	4.041012	-0.519078	-5.442495
H	-1.798342	2.431718	-1.180858
H	-3.354862	3.234149	-1.367061
H	-2.698690	2.280853	-2.708221
H	3.839701	-2.389505	2.268152
H	4.343327	-4.001176	1.727534
H	2.826950	-3.298671	1.135749
H	-4.616214	-1.657831	-1.424000
H	0.462761	0.224229	2.857078
H	-0.923053	-0.296274	1.875904
H	-0.277997	-3.212156	-2.129503
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H	1.439782	-3.422119	-1.752884
H	5.839694	-0.428109	1.785115
H	2.866553	3.722396	-0.063607
H	1.827355	4.687854	-1.126257
H	2.119891	2.971671	-1.463152
H	-2.963381	-1.956865	1.142190
H	-4.582752	-2.618384	0.895108
H	-4.346084	-0.870505	0.938647
H	-4.888561	-0.586063	-6.982349

H	-5.539064	-1.448854	-5.584329
H	-4.526122	-2.296584	-6.756246
H	4.111731	2.693478	4.138605
H	-0.816181	2.477177	-4.283515
H	0.351194	3.790972	-4.045735
H	-0.081251	2.713448	-2.707522
H	0.739204	-3.188566	3.376133
H	-0.453473	-4.324593	4.008042
H	-0.980306	-2.891250	3.123229
H	-0.333467	-8.556020	1.733602
H	-0.167022	-8.646200	-0.025018
H	-1.742076	-8.320258	0.699258
H	2.133753	2.698635	2.709194
H	4.221334	2.840027	-6.818790
H	5.091238	1.310603	-6.620491
H	5.241081	2.582743	-5.404496
H	6.700020	0.398753	-0.238720
H	7.164967	0.212958	-1.932124
H	6.872389	-1.220073	-0.944531
H	3.734699	-3.725695	-1.298172
H	5.227183	-4.363150	-0.606615
H	5.297125	-3.038111	-1.775274
H	-1.927177	6.085308	1.648164
H	-2.934539	4.847564	2.434975
H	-3.082595	5.149892	0.698538
H	7.076035	0.359882	3.644506
H	6.076928	0.873509	5.008162
H	6.859122	2.079550	3.988652
H	-2.376498	4.772439	7.495015
H	-2.882043	5.226299	5.853538
H	-4.009537	4.377356	6.918817

H	-1.765320	2.028032	8.317859
H	-3.354436	1.404817	7.833568
H	-1.884455	0.617830	7.244410
H	0.051763	3.495388	6.447029
H	0.062553	2.116163	5.331290
H	-0.317865	3.733863	4.725626
H	-5.855524	-0.749185	4.694796
H	-4.481300	-0.615016	5.811408
H	-6.436621	1.254727	2.610882
H	-5.607748	2.821389	2.481368
H	-4.792451	1.348641	1.944597
H	-7.021931	1.802017	5.498002
H	-5.766425	2.127666	6.707744
H	-6.153491	3.351775	5.490867

! H abstraction by HMDS on the adjacent methyl group - Transition State !

P	14.680505	5.437210	18.843804
La	11.461936	5.915087	18.250703
N	12.709899	7.615249	19.407263
C	11.708365	8.612813	19.430243
C	10.414176	8.275123	19.926732
C	10.126912	7.010570	20.644661
H	9.592755	7.266993	21.887698
N	9.071860	7.470363	23.117480
Si	7.356957	7.505122	23.360351
C	6.648260	6.066309	24.439259
H	6.919753	5.097062	24.007801
C	6.420678	7.342017	21.685315
C	6.667940	9.122577	24.165945
Si	10.244881	7.779746	24.364620

C	10.753735	9.635795	24.506034
N	11.098811	3.911137	19.509620
C	11.067202	2.535733	19.528749
C	11.401379	1.817247	18.351149
C	11.385369	0.424279	18.341913
C	11.042062	-0.322528	19.470985
C	10.717596	0.390617	20.629731
C	10.722027	1.782514	20.687954
C	9.391707	9.243648	19.813568
C	9.608161	10.506313	19.281700
C	10.895586	10.821755	18.819747
C	11.936607	9.900421	18.870412
C	11.775875	2.602421	17.134414
C	10.991942	-1.827922	19.435500
C	10.370275	2.491703	21.967071
N	11.129985	6.237667	15.748043
C	12.264724	6.814118	15.107090
C	13.323360	6.019672	14.605367
C	14.405285	6.628120	13.959951
C	14.490942	8.009156	13.793116
C	13.435927	8.783239	14.279390
C	12.328336	8.217031	14.914263
P	8.459384	5.602120	17.179022
C	7.210730	7.044081	17.298976
C	5.813808	6.783403	16.738432
C	16.045614	5.905308	17.593511
C	15.809773	7.344182	17.134408
C	14.842486	6.731761	20.151140
C	13.795466	7.694131	20.240404
C	13.936932	8.695185	21.237146
C	15.034861	8.734229	22.080502

C	16.063253	7.784540	22.003341
C	15.931425	6.795340	21.028207
C	15.372842	3.887349	19.683262
C	14.532047	3.526862	20.908475
C	13.288024	4.518954	14.707159
C	15.681044	8.645828	13.124550
C	11.182613	9.094842	15.330998
C	8.500011	11.524627	19.206240
C	13.288028	10.259979	18.317770
C	17.238870	7.819460	22.944230
C	17.486682	5.718347	18.064842
C	9.700917	7.274092	26.149398
C	11.856622	6.789926	24.037597
C	10.104719	5.867964	14.896538
C	10.255083	5.869169	13.479597
C	9.256627	5.438841	12.622183
C	8.022339	4.975806	13.094653
C	7.840132	5.011734	14.476421
C	8.818925	5.458339	15.374165
C	6.955544	4.465719	12.162199
C	7.369150	4.101266	17.563996
C	8.068981	2.784725	17.235603
C	6.938588	4.146411	19.031028
C	7.820818	8.290342	16.661639
C	15.441970	2.721995	18.693908
H	10.848504	4.261644	20.432943
H	8.416224	8.996827	20.223471
H	11.194106	6.210584	13.056899
H	6.885969	4.671581	14.873820
H	8.403681	2.749993	16.194849
H	7.377436	1.947884	17.394896

H 8.931882 2.617892 17.885913

H 16.391705 4.126940 20.012547

H 9.447548 5.456791 11.549399

H 5.849664 6.579704 15.663258

H 5.190840 7.675554 16.881242

H 5.302819 5.951790 17.232084

H 7.132941 7.212606 18.381010

H 11.648689 -0.092361 17.418698

H 14.804891 7.483436 16.728022

H 16.524806 7.612233 16.347595

H 15.942351 8.041584 17.967643

H 11.086587 11.808032 18.398257

H 15.861890 5.237467 16.741036

H 13.461232 9.863484 14.142396

H 10.450813 -0.160847 21.531666

H 12.273076 4.132676 14.590956

H 13.660280 4.173213 15.678189

H 13.923245 4.065114 13.939777

H 15.199997 5.994887 13.566756

H 8.789503 8.538295 17.100956

H 7.160239 9.152689 16.812167

H 7.952952 8.149038 15.583939

H 14.558686 4.319950 21.660419

H 14.911984 2.606120 21.368176

H 13.487789 3.358351 20.627881

H 6.477603 4.188071 16.931040

H 11.016300 6.413810 20.872603

H 9.311547 6.409634 20.220456

H 10.944337 3.224377 16.770668

H 12.084999 1.960849 16.304018

H 12.615504 3.277335 17.356442

H 16.706542 6.034209 20.964501

H 14.055718 10.274108 19.099955

H 13.264015 11.246222 17.844256

H 13.614687 9.526974 17.572968

H 7.811156 4.098164 19.690882

H 6.298343 3.287118 19.264930

H 6.377830 5.052673 19.278846

H 6.756262 5.171505 11.346355

H 6.011769 4.300473 12.691922

H 7.237797 3.512142 11.696212

H 15.085664 9.517162 22.835895

H 10.249417 8.761519 14.867129

H 11.362348 10.133001 15.036396

H 11.024907 9.081958 16.413682

H 11.196650 3.114668 22.335300

H 10.122786 1.777116 22.757202

H 9.507259 3.160159 21.847588

H 11.309768 -2.265041 20.389043

H 11.644275 -2.231134 18.653153

H 9.978894 -2.203781 19.234103

H 13.143975 9.428784 21.347992

H 15.390085 9.523614 12.537813

H 16.186395 7.943837 12.453501

H 16.421351 8.982240 13.861728

H 17.705341 6.361845 18.922828

H 18.178946 6.000149 17.260647

H 17.714703 4.684839 18.343521

H 14.439278 2.396367 18.400469

H 15.935828 1.860933 19.160967

H 16.001922 2.969924 17.785527

H 8.799689 12.475344 19.662674

H	7.602891	11.174616	19.724620
H	8.222423	11.741243	18.166778
H	17.963679	7.035581	22.701531
H	16.931553	7.669461	23.987172
H	17.767763	8.780179	22.903015
H	11.549293	9.778769	25.247148
H	11.110526	10.006770	23.539925
H	9.895305	10.249202	24.800302
H	10.504101	7.499366	26.861240
H	8.803581	7.809620	26.476422
H	9.491349	6.200798	26.201208
H	12.588365	6.968431	24.833701
H	11.639871	5.716858	24.006776
H	12.321017	7.072197	23.088759
H	5.554035	6.124277	24.492521
H	7.039983	6.097563	25.460629
H	5.352026	7.182177	21.866446
H	6.524693	8.241657	21.070292
H	6.799277	6.489780	21.113174
H	5.574576	9.089143	24.240120
H	7.069118	9.271092	25.174501
H	6.947118	9.994866	23.565838

! H abstraction by HMDS on the adjacent methyl group - Product !

P	3.483382	-0.856315	0.002756
La	0.252794	-0.340448	-0.649901
N	1.570457	1.389089	0.528621
C	0.583291	2.402950	0.587765
C	-0.724954	2.019862	1.026990
C	-0.967022	0.638415	1.435953

H	-2.156951	1.148348	4.048702
N	-2.474184	1.401245	4.982074
Si	-4.231250	1.368317	5.192167
C	-4.752860	0.153600	6.576320
H	-4.389639	-0.853523	6.350132
C	-5.003646	0.782945	3.547882
C	-4.934875	3.096999	5.628344
Si	-1.208660	2.143056	5.984679
C	-0.915434	3.979414	5.535175
N	-0.103356	-2.478176	0.424163
C	-0.085967	-3.846819	0.505893
C	0.295049	-4.613769	-0.631712
C	0.327051	-6.003885	-0.567936
C	-0.009563	-6.710018	0.591007
C	-0.380249	-5.953863	1.706165
C	-0.426488	-4.561123	1.692885
C	-1.743044	2.998279	0.965992
C	-1.509029	4.302460	0.537759
C	-0.214153	4.654050	0.139053
C	0.828008	3.722463	0.145875
C	0.669446	-3.885665	-1.885106
C	-0.002986	-8.216317	0.625724
C	-0.825491	-3.804838	2.930391
N	-0.153678	0.104759	-3.172903
C	0.986419	0.680549	-3.795828
C	2.025191	-0.116431	-4.333674
C	3.125987	0.493075	-4.945068
C	3.248872	1.878108	-5.043360
C	2.214876	2.655923	-4.518869
C	1.091517	2.089463	-3.912964
P	-2.746958	-0.581624	-1.711014

C	-3.994698	0.851608	-1.497206
C	-5.411648	0.604511	-2.012974
C	4.846530	-0.340936	-1.230774
C	4.565393	1.088788	-1.693839
C	3.634599	0.405343	1.345050
C	2.606480	1.396391	1.417531
C	2.729466	2.348549	2.469492
C	3.787032	2.323934	3.363225
C	4.798054	1.355078	3.291251
C	4.683923	0.409945	2.269834
C	4.197480	-2.419599	0.801656
C	3.337508	-2.842355	1.993540
C	1.947392	-1.618276	-4.292917
C	4.458090	2.515064	-5.677126
C	-0.023820	2.975507	-3.434215
C	-2.628180	5.311479	0.483034
C	2.195362	4.117261	-0.340234
C	5.939855	1.328877	4.273291
C	6.285203	-0.474415	-0.735797
C	-1.738727	2.044541	7.822125
C	0.410767	1.169410	5.746637
C	-1.189431	-0.219921	-4.019258
C	-1.075657	-0.146488	-5.439450
C	-2.095348	-0.539769	-6.289668
C	-3.316947	-1.029899	-5.809788
C	-3.465797	-1.058933	-4.422849
C	-2.464757	-0.655488	-3.531325
C	-4.402900	-1.505070	-6.738665
C	-3.820628	-2.094903	-1.332847
C	-3.104627	-3.389678	-1.710854
C	-4.196320	-2.085717	0.150793

C	-3.414751	2.121665	-2.116107
C	4.307474	-3.548184	-0.225839
H	-0.429661	-2.094300	1.311864
H	-2.740666	2.723998	1.307039
H	-0.149042	0.222447	-5.867221
H	-4.410725	-1.417212	-4.017605
H	-2.826369	-3.401868	-2.768697
H	-3.759382	-4.250190	-1.523272
H	-2.201009	-3.527712	-1.110835
H	5.205511	-2.177607	1.161459
H	-1.933117	-0.468813	-7.365325
H	-5.413397	0.437277	-3.094994
H	-6.034522	1.487684	-1.818804
H	-5.900303	-0.248362	-1.532561
H	-4.029161	0.985925	-0.407972
H	0.625867	-6.555711	-1.459938
H	3.559333	1.196421	-2.107102
H	5.278106	1.381223	-2.474419
H	4.667613	1.790133	-0.859469
H	-0.013188	5.668431	-0.203241
H	4.698143	-1.014816	-2.085560
H	2.272025	3.740924	-4.598068
H	-0.642578	-6.469748	2.630695
H	0.928273	-1.972729	-4.464068
H	2.268694	-2.009958	-3.321269
H	2.602414	-2.060952	-5.050249
H	3.906565	-0.140950	-5.364854
H	-2.437957	2.367673	-1.694489
H	-4.080891	2.972865	-1.927085
H	-3.308940	2.009507	-3.200230
H	3.321769	-2.071637	2.769050

H	3.732481	-3.765221	2.436833
H	2.306731	-3.034719	1.680046
H	-4.735231	-2.011824	-1.933249
H	-0.238585	0.262846	2.165879
H	-1.994543	0.432469	1.746590
H	-0.159876	-3.275471	-2.267873
H	0.974600	-4.570938	-2.682148
H	1.504299	-3.197034	-1.697466
H	5.445180	-0.365498	2.207039
H	2.928359	4.133508	0.475632
H	2.175504	5.110299	-0.800298
H	2.566666	3.397766	-1.077121
H	-3.294344	-2.121264	0.770575
H	-4.808057	-2.963054	0.395545
H	-4.765003	-1.194081	0.434618
H	-4.587441	-0.789873	-7.549957
H	-5.348213	-1.646253	-6.203976
H	-4.153125	-2.464679	-7.212102
H	3.823848	3.076611	4.150711
H	-0.975860	2.682753	-3.886889
H	0.174035	4.020877	-3.689844
H	-0.153937	2.920853	-2.348661
H	-0.035338	-3.119723	3.267666
H	-1.043033	-4.488805	3.756315
H	-1.722132	-3.190201	2.768218
H	0.135721	-8.592196	1.645679
H	0.803288	-8.630902	0.009281
H	-0.943020	-8.646448	0.251036
H	1.954748	3.103393	2.570591
H	4.188951	3.413382	-6.243418
H	4.962028	1.824340	-6.360997

H	5.193544	2.820046	-4.921381
H	6.458956	0.166658	0.134552
H	6.982011	-0.155330	-1.522296
H	6.549202	-1.501245	-0.463703
H	3.317297	-3.872851	-0.559687
H	4.798521	-4.420549	0.223343
H	4.889161	-3.260564	-1.108264
H	-2.278621	6.314347	0.752942
H	-3.441170	5.044121	1.165993
H	-3.058789	5.380780	-0.524700
H	6.618086	0.494291	4.066956
H	5.590615	1.216833	5.308238
H	6.536433	2.250281	4.238177
H	-0.085707	4.398901	6.115001
H	-0.674502	4.074365	4.472050
H	-1.809918	4.578782	5.732287
H	-0.975706	2.513761	8.452479
H	-2.685641	2.560733	8.008306
H	-1.846817	1.002484	8.137149
H	1.206939	1.579382	6.377238
H	0.267510	0.117647	6.012381
H	0.753353	1.216633	4.708614
H	-5.844377	0.115140	6.664708
H	-4.343507	0.449878	7.546534
H	-6.092562	0.709028	3.637601
H	-4.774467	1.481208	2.737464
H	-4.618652	-0.201603	3.265581
H	-6.022861	3.052087	5.749854
H	-4.509210	3.482498	6.560195
H	-4.705567	3.812443	4.832782

! Direct N - H abstraction by the HMDS anion - Adduct !

C	-1.259297	3.107817	1.564421
C	-0.052381	3.039862	0.827914
C	0.174243	4.001688	-0.189780
C	-0.789116	4.977983	-0.448434
C	-1.988657	5.046491	0.265382
C	-2.199522	4.100196	1.268306
N	0.884297	2.015938	1.077445
C	1.944255	2.310754	1.888763
C	3.020744	1.385871	2.086390
C	4.049359	1.685284	2.987499
C	4.122153	2.881487	3.702413
C	3.094764	3.807165	3.471645
C	2.049893	3.540720	2.604142
P	3.014242	-0.183737	1.109760
C	4.466066	0.022217	-0.108922
C	5.861072	0.153974	0.497586
C	5.235973	3.159399	4.677490
C	1.463490	3.986280	-0.962717
C	-3.022290	6.096608	-0.049635
C	-1.496530	2.159344	2.708587
La	-0.049926	-0.226830	0.151494
N	-0.512897	-1.769754	1.490548
C	-0.782035	-2.801234	2.334145
C	-0.695365	-4.170642	1.910648
C	-0.973201	-5.212547	2.792291
C	-1.343734	-4.997151	4.123021
C	-1.423474	-3.667206	4.546892
C	-1.160785	-2.590689	3.702717
C	-0.283476	-4.473435	0.500804

C	-1.673770	-6.141100	5.046166
C	-1.271547	-1.188298	4.222574
N	-0.435529	-0.555055	-2.405192
C	-1.529730	-0.968579	-3.116448
C	-1.432643	-1.496397	-4.437990
C	-2.530890	-1.980357	-5.126981
C	-3.815930	-1.982763	-4.566480
C	-3.932887	-1.444355	-3.284536
C	-2.850519	-0.926013	-2.562841
C	-5.001337	-2.549230	-5.302951
P	-3.075451	-0.169445	-0.891558
C	-4.362481	-1.272470	-0.051556
C	-4.712094	-0.689876	1.319433
C	0.787505	-0.442282	-3.095768
C	1.055974	0.663889	-3.945204
C	2.295176	0.768860	-4.577945
C	3.301568	-0.186626	-4.411880
C	3.027199	-1.272989	-3.582014
C	1.799888	-1.418021	-2.926785
C	-0.000019	1.706244	-4.181487
C	1.534898	-2.642754	-2.093130
C	4.638570	-0.035201	-5.089830
C	-4.044646	1.439325	-1.229685
C	-3.176020	2.364453	-2.080259
C	-5.436369	1.287225	-1.838602
C	3.643980	-1.487813	2.327751
C	3.788046	-2.832315	1.612125
C	2.687320	-1.598552	3.515138
C	4.156752	1.199824	-1.032508
C	-3.828924	-2.698572	0.078900
H	-3.115216	4.144912	1.857275

H	-0.451967	-1.539573	-4.903340
H	-4.918553	-1.434455	-2.823017
H	-3.617660	-3.137776	-0.900242
H	-4.569157	-3.332041	0.583738
H	-2.908131	-2.716825	0.670824
H	4.630651	-1.170327	2.689822
H	-2.383733	-2.383377	-6.129207
H	-5.381821	0.844569	-2.838435
H	-5.909549	2.273020	-1.941041
H	-6.101364	0.669649	-1.226723
H	-4.138238	1.885684	-0.230632
H	-0.895556	-6.237647	2.424804
H	3.205301	1.064384	-1.554553
H	4.938662	1.305767	-1.794588
H	4.108534	2.135062	-0.465161
H	-0.593414	5.710206	-1.231479
H	4.423689	-0.897841	-0.707335
H	2.477888	1.626483	-5.225190
H	-1.700874	-3.458654	5.582092
H	1.574458	-2.442905	-1.013086
H	2.284371	-3.416642	-2.287099
H	0.543572	-3.055156	-2.297766
H	3.782986	-2.047089	-3.451572
H	-2.213749	2.569700	-1.602638
H	-3.678947	3.327005	-2.235866
H	-2.987015	1.920939	-3.063316
H	2.619875	-0.654991	4.064040
H	3.037828	-2.372738	4.209283
H	1.681440	-1.874657	3.182017
H	-5.265543	-1.282695	-0.675987
H	-2.392369	2.442050	3.270264

H	-0.643986	2.151753	3.394608
H	-1.636808	1.119971	2.386744
H	-0.873722	-3.894264	-0.219004
H	-0.392875	-5.539718	0.272331
H	0.763642	-4.196443	0.320495
H	4.832817	0.946931	3.148015
H	2.319913	4.157155	-0.300587
H	1.467145	4.760523	-1.736099
H	1.631475	3.016755	-1.441638
H	-3.818797	-0.643650	1.951740
H	-5.443682	-1.329414	1.828516
H	-5.140107	0.316469	1.254210
H	-5.933242	-2.352479	-4.762519
H	-4.926095	-3.637465	-5.433045
H	-5.106698	-2.116748	-6.306319
H	3.107696	4.762407	3.996907
H	-0.852221	1.287457	-4.729838
H	0.398370	2.547074	-4.757582
H	-0.397625	2.086286	-3.236315
H	-0.384147	-0.598979	3.964729
H	-1.403879	-1.174616	5.310441
H	-2.124029	-0.659578	3.775284
H	-1.097531	-7.040087	4.796332
H	-2.736427	-6.423845	5.003253
H	-1.455413	-5.890066	6.091055
H	1.266355	4.281562	2.472381
H	5.152139	-0.997951	-5.179478
H	5.302246	0.636042	-4.529130
H	4.534211	0.384432	-6.096530
H	5.941742	1.061842	1.103510
H	6.611215	0.223806	-0.301488

H 6.132653 -0.701257 1.124587

H 2.816967 -3.169531 1.234217

H 4.151732 -3.596529 2.310116

H 4.489021 -2.790262 0.771385

H -2.556759 7.054109 -0.308134

H -3.690093 6.267129 0.800993

H -3.649687 5.804039 -0.901686

H 4.876997 3.204397 5.714792

H 5.732377 4.116795 4.472449

H 6.002338 2.378299 4.634680

! Direct N - H abstraction by the HMDS anion - Transition State !

C 10.281666 8.719068 19.234771

C 11.478254 9.155243 18.593272

C 11.476578 10.339683 17.821239

C 10.299741 11.081307 17.699146

C 9.107196 10.664650 18.303278

C 9.116821 9.491018 19.054724

N 12.604114 8.312614 18.661559

C 13.611713 8.562327 19.541509

C 14.710725 7.654412 19.653846

C 15.729501 7.896148 20.580561

C 15.746099 9.010720 21.422395

C 14.671132 9.903894 21.302667

C 13.640667 9.695944 20.401801

P 14.677779 6.177248 18.540604

C 16.036226 6.561652 17.258932

C 17.452276 6.703216 17.813262

C 16.855428 9.238579 22.415714

C 12.746496 10.795274 17.156933

C	7.841158	11.465831	18.133293
C	10.310016	7.517541	20.124365
La	11.461050	6.270735	17.834937
N	10.975736	4.861598	19.425747
C	10.652286	3.822672	20.252025
C	10.435098	2.513823	19.700664
C	10.064600	1.443385	20.510381
C	9.913992	1.563619	21.894560
C	10.188097	2.816136	22.446689
C	10.552633	3.922750	21.679597
C	10.667716	2.285937	18.236624
C	9.470741	0.402697	22.745785
C	10.878856	5.212323	22.379826
N	11.202718	5.751954	15.284580
C	10.132714	5.233863	14.599112
C	10.276594	4.566300	13.346718
C	9.208259	3.986339	12.684545
C	7.906777	4.022878	13.202075
C	7.740520	4.706045	14.407479
C	8.791107	5.318290	15.101007
C	6.754710	3.351148	12.502230
P	8.496391	6.288145	16.647214
C	7.048127	5.418362	17.504339
C	6.598970	6.240744	18.714815
C	12.447362	5.748459	14.611757
C	12.810976	6.812464	13.747999
C	14.058929	6.805834	13.122141
C	14.980392	5.773052	13.308223
C	14.607687	4.720964	14.144863
C	13.367889	4.688615	14.791139
C	11.844238	7.929910	13.476659

C	12.994405	3.502107	15.635793
C	16.332147	5.804136	12.643550
C	7.674452	7.893949	16.031303
C	8.684444	8.693690	15.212648
C	6.362756	7.722846	15.268095
C	15.450069	4.803068	19.587862
C	15.685155	3.556490	18.732426
C	14.541789	4.495844	20.778675
C	15.632503	7.808013	16.469752
C	7.436170	4.002703	17.926058
H	8.206283	9.178018	19.563518
H	11.268936	4.498480	12.910988
H	6.738015	4.762510	14.827008
H	7.747771	3.397452	17.070258
H	6.580305	3.503696	18.398204
H	8.254895	4.017033	18.652763
H	16.419744	5.158453	19.959579
H	9.393414	3.479345	11.737370
H	6.514210	7.146458	14.349829
H	5.966099	8.705643	14.980415
H	5.590127	7.221874	15.860324
H	7.486877	8.444637	16.961714
H	9.898327	0.472137	20.041586
H	14.666629	7.678783	15.974380
H	16.376194	8.022618	15.692100
H	15.568581	8.681483	17.127119
H	10.311664	11.999789	17.113297
H	15.998685	5.703214	16.575566
H	14.315880	7.634598	12.463014
H	10.125079	2.940087	23.529280
H	12.994858	3.742599	16.706437

H 13.706095 2.682465 15.495952

H 11.991619 3.139975 15.392843

H 15.292995 3.886095 14.288943

H 9.587298 8.909092 15.790956

H 8.252715 9.654820 14.905659

H 8.970334 8.149945 14.307072

H 14.436224 5.366916 21.431054

H 14.959012 3.673298 21.373363

H 13.538940 4.204504 20.448458

H 6.216851 5.362455 16.789951

H 9.350142 7.425553 20.643749

H 11.091023 7.662962 20.879972

H 10.550428 6.297210 19.867709

H 10.155680 3.029314 17.616418

H 10.334717 1.288231 17.929876

H 11.735322 2.371640 17.995285

H 16.542556 7.177499 20.667853

H 13.497508 11.096837 17.897273

H 12.562924 11.643558 16.490094

H 13.197168 9.981406 16.579605

H 7.422475 6.362053 19.425949

H 5.782007 5.726534 19.236445

H 6.239081 7.236857 18.438399

H 5.796675 3.646414 12.943073

H 6.814622 2.255753 12.563729

H 6.718613 3.607321 11.435831

H 14.635533 10.784502 21.944361

H 10.934610 7.552261 12.996361

H 12.289367 8.684186 12.820320

H 11.526658 8.419230 14.401480

H 11.763883 5.683958 21.938419

H 11.070628 5.039137 23.444624

H 10.068424 5.947904 22.312158

H 9.826209 -0.552861 22.341931

H 8.375353 0.329615 22.815836

H 9.849139 0.489320 23.771062

H 12.811793 10.397481 20.356431

H 16.735669 4.795061 12.509475

H 17.061578 6.368220 13.239331

H 16.284273 6.280748 11.658451

H 17.516862 7.543893 18.511530

H 18.158471 6.898443 16.995111

H 17.795672 5.802363 18.332379

H 14.742322 3.178715 18.322908

H 16.121456 2.755288 19.342011

H 16.365029 3.742973 17.894367

H 8.047171 12.541806 18.112222

H 7.134846 11.274828 18.947843

H 7.328834 11.218436 17.193965

H 16.480090 9.300626 23.445719

H 17.401018 10.171857 22.220830

H 17.586143 8.423396 22.385083

! Direct N - H abstraction by the HMDS anion - Product !

C -1.052995 3.031725 0.924821

C 0.282441 3.139204 0.418411

C 0.625780 4.182181 -0.469825

C -0.347277 5.106826 -0.859789

C -1.667337 5.012131 -0.401884

C -1.998327 3.980039 0.471279

N 1.199276 2.121802 0.783192

C	2.188450	2.396414	1.683173
C	3.127981	1.387047	2.061750
C	4.133041	1.673196	2.991790
C	4.280908	2.923845	3.594915
C	3.350716	3.908492	3.231171
C	2.341460	3.662601	2.316456
P	2.909385	-0.280263	1.294031
C	4.349162	-0.376555	0.043375
C	5.753071	-0.411191	0.643617
C	5.378904	3.202059	4.587792
C	2.027564	4.287025	-1.005067
C	-2.708826	6.001190	-0.861288
C	-1.393591	1.926009	1.812950
La	-0.237899	0.169091	0.302546
N	-0.825526	-1.361887	2.085398
C	-0.931076	-2.588042	2.687830
C	-0.597860	-3.761868	1.953729
C	-0.692841	-5.017480	2.546479
C	-1.113874	-5.193454	3.868236
C	-1.434563	-4.039133	4.587901
C	-1.355390	-2.760638	4.039397
C	-0.130948	-3.604655	0.540316
C	-1.246692	-6.565084	4.477475
C	-1.708805	-1.556325	4.868581
N	-0.544416	-0.368741	-2.234135
C	-1.594266	-0.899205	-2.946215
C	-1.454613	-1.397034	-4.276063
C	-2.498001	-1.999483	-4.959094
C	-3.770713	-2.149617	-4.393141
C	-3.942543	-1.613922	-3.116008
C	-2.917429	-0.986109	-2.399796

C	-4.885648	-2.856184	-5.118098
P	-3.216073	-0.165752	-0.775480
C	-4.455960	-1.286838	0.111271
C	-4.839528	-0.649676	1.449316
C	0.670103	-0.204220	-2.951662
C	0.963339	1.040205	-3.564787
C	2.164712	1.211077	-4.255988
C	3.100181	0.182997	-4.387466
C	2.791990	-1.045032	-3.804452
C	1.604497	-1.258092	-3.095903
C	-0.038244	2.159533	-3.522852
C	1.319974	-2.626998	-2.539836
C	4.396594	0.400005	-5.123451
C	-4.283710	1.353537	-1.224180
C	-3.545147	2.196630	-2.261227
C	-5.713114	1.068761	-1.681901
C	3.461147	-1.462448	2.668867
C	3.509212	-2.902013	2.152659
C	2.526605	-1.340408	3.873156
C	4.214750	0.779978	-0.947167
C	-3.872160	-2.682674	0.319766
H	-3.013549	3.919580	0.862593
H	-0.488917	-1.310539	-4.764112
H	-4.925916	-1.692283	-2.655076
H	-3.597381	-3.151448	-0.629532
H	-4.606207	-3.328903	0.817686
H	-2.984118	-2.639207	0.956456
H	4.473224	-1.169733	2.976222
H	-2.314424	-2.371133	-5.967418
H	-5.722378	0.485401	-2.608648
H	-6.231133	2.014918	-1.887887

H	-6.303377	0.532022	-0.932883
H	-4.313086	1.918822	-0.283727
H	-0.427239	-5.891795	1.951024
H	3.234040	0.796717	-1.428682
H	4.972044	0.692049	-1.735471
H	4.360295	1.739249	-0.440085
H	-0.071177	5.906840	-1.545659
H	4.167391	-1.314901	-0.498278
H	2.365184	2.175964	-4.720447
H	-1.759181	-4.136229	5.624788
H	1.512389	-2.676826	-1.463438
H	1.959471	-3.376855	-3.016610
H	0.276728	-2.913479	-2.694830
H	3.490121	-1.874894	-3.911347
H	-2.550550	2.483621	-1.913532
H	-4.103874	3.118369	-2.466597
H	-3.441010	1.646767	-3.202376
H	2.535247	-0.327112	4.284420
H	2.836677	-2.033993	4.665115
H	1.498100	-1.588672	3.593383
H	-5.351716	-1.368179	-0.517296
H	-2.423205	1.953297	2.177324
H	-0.685378	1.818151	2.645207
H	-1.139573	-0.638609	2.733201
H	-0.893906	-3.136652	-0.096490
H	0.137719	-4.564363	0.087645
H	0.754050	-2.954430	0.497409
H	4.826670	0.884346	3.277565
H	2.742349	4.555755	-0.217486
H	2.090464	5.042708	-1.794573
H	2.360910	3.326889	-1.412005

H	-3.950289	-0.522025	2.075503
H	-5.543781	-1.293925	1.990664
H	-5.311062	0.331624	1.329772
H	-5.855029	-2.652822	-4.650451
H	-4.752826	-3.947143	-5.122425
H	-4.953585	-2.541029	-6.166722
H	3.413054	4.895862	3.689123
H	-1.007349	1.828045	-3.907382
H	0.301809	3.007589	-4.124964
H	-0.206062	2.524665	-2.504569
H	-0.870555	-0.850172	4.946857
H	-1.991637	-1.847668	5.884851
H	-2.550667	-0.993831	4.440757
H	-0.494923	-7.257140	4.080355
H	-2.229988	-7.016197	4.280211
H	-1.123157	-6.533758	5.566044
H	1.623649	4.443020	2.080305
H	4.836479	-0.548711	-5.447632
H	5.138529	0.904486	-4.490928
H	4.254291	1.026059	-6.011301
H	5.951092	0.496726	1.222574
H	6.501800	-0.458923	-0.158363
H	5.916940	-1.275640	1.294740
H	2.507692	-3.258978	1.894142
H	3.899103	-3.569779	2.931175
H	4.150764	-3.012187	1.271736
H	-2.296529	7.013963	-0.936841
H	-3.558710	6.035110	-0.171685
H	-3.103416	5.740205	-1.852183
H	4.988770	3.624458	5.522791
H	6.117473	3.917954	4.201145

H 5.920762 2.285728 4.845031

! Direct P-H abstraction - Adduct !

C 13.385569000 9.685506301 20.684915000
C 13.369793699 8.519131000 19.889961301
C 14.443746699 7.602215000 20.083750301
C 15.416513000 7.876110000 21.033325301
C 15.428717000 9.035964000 21.826818000
C 14.372364301 9.947945000 21.607852000
N 12.345907699 8.247916000 18.981887601
C 11.357106000 9.239894301 18.778198301
C 10.111700000 9.148188902 19.448876301
C 9.128470301 10.130683902 19.208523000
C 9.357072301 11.195943601 18.355187399
C 10.599908301 11.267109301 17.696485699
C 11.589979301 10.328794000 17.898510000
C 9.857648699 8.057678504 20.452529902
C 8.284171601 12.236677601 18.102715098
C 12.928610301 10.480582699 17.229527000
P 14.507207699 6.090696000 19.020406301
C 15.251014301 4.761938000 20.136798000
C 14.358862601 4.495811399 21.350905000
C 16.461173301 9.272248000 22.879244000
La 11.418525098 6.248563098 18.127460504
P 10.562168594 4.415977007 20.123549511
C 10.295758098 2.621137406 20.253395105
C 10.862894000 1.831527308 19.231600804
C 10.765839902 0.452913007 19.285628601
C 10.117794601 -0.197200196 20.326438699
C 9.514908699 0.587310902 21.321958699

C	9.563542098	1.981459902	21.321689601
C	11.550311301	2.512493909	18.086163406
C	10.070586203	-1.703391196	20.401752496
C	8.802946196	2.763348399	22.356601902
N	11.311937000	5.971579399	15.678677601
C	12.537666000	6.261047699	15.022602601
C	13.597083000	5.326578699	14.978873301
C	14.775508000	5.653076699	14.297887301
C	14.969058699	6.880534699	13.661591301
C	13.910590699	7.790388699	13.713910301
C	12.716169699	7.504763699	14.376693301
C	13.449839000	3.936902000	15.559224601
C	16.254149699	7.202158000	12.971442000
C	11.586807699	8.493825699	14.312925601
C	10.307145000	5.506936699	14.849838301
C	10.578893000	5.075489000	13.515398301
C	9.595477000	4.586202000	12.672313301
C	8.262810000	4.464266000	13.102736000
C	7.977104000	4.883354000	14.401020000
C	8.941504000	5.420012699	15.257624301
P	8.494466699	6.006847699	16.946480301
C	7.448302699	7.576545699	16.672026000
C	6.099403000	7.382812699	15.966052699
C	7.199631000	3.907402000	12.193084000
C	7.194460699	4.754478699	17.533358000
C	7.713376601	3.321402000	17.517154203
C	6.665225098	5.156198000	18.925530399
C	15.920754699	6.487363000	17.798379301
C	15.590386699	7.779158000	17.074278000
C	17.323237699	6.559790000	18.418168000
C	15.508767601	3.501555000	19.330681699

C	8.279068000	8.611944000	15.946993301
N	9.531133804	5.847295496	23.774291286
Si	8.038508504	6.526783496	24.131151091
C	6.808568601	6.405014699	22.620505294
Si	10.969752203	5.796234797	24.654562391
C	12.281049601	7.143753699	24.204439594
C	10.849440496	5.926658098	26.606109790
C	11.943297902	4.132673797	24.374251895
C	7.970519007	8.423818895	24.579863895
C	7.039645706	5.688849594	25.583396091
H	10.099697895	4.769587112	21.178643623
H	8.201833000	10.048163504	19.747484000
H	11.599262000	5.134044000	13.151086301
H	6.951023000	4.797387000	14.750760000
H	8.080846504	3.029074699	16.538503504
H	6.900203902	2.630943699	17.779792203
H	8.502736301	3.168227203	18.270806504
H	16.229738000	5.162099000	20.483792000
H	9.857999301	4.278244000	11.665507301
H	6.233887301	7.005040000	14.943311699
H	5.574541000	8.344564699	15.898714699
H	5.432284000	6.704061399	16.499516399
H	7.246981699	7.926055699	17.693315000
H	11.229499504	-0.151459790	18.476225601
H	14.618143699	7.740491699	16.579757000
H	16.343935699	7.976152000	16.302930000
H	15.597080399	8.629487000	17.763247000
H	10.791711601	12.104896000	17.028472399
H	15.881158699	5.660511000	17.077473301
H	14.009782699	8.751344699	13.210674301
H	8.972340399	0.103764000	22.140628797

H	13.690497098	3.923192301	16.639818601
H	14.113658902	3.240229000	15.061126504
H	12.405427601	3.581519399	15.457653699
H	15.570210000	4.891500000	14.247382301
H	9.203967699	8.871197699	16.489921601
H	7.709459000	9.542085000	15.832236301
H	8.569000000	8.271106000	14.948124301
H	14.257263000	5.377046399	21.981580000
H	14.788039203	3.694686699	21.961594000
H	13.361437601	4.206272496	21.057217000
H	6.356605301	4.813877098	16.820507399
H	9.059716000	8.327029406	21.145008902
H	10.721727000	7.816295504	21.068308601
H	9.496845399	7.110116504	20.015380203
H	10.842867301	3.136491007	17.496812804
H	12.005763504	1.806079210	17.401544706
H	12.340154399	3.186770511	18.466391007
H	16.229100699	7.149487000	21.206469000
H	13.720702301	10.656016399	17.988442699
H	12.935677301	11.344586399	16.553817699
H	13.212183000	9.594005399	16.676124000
H	7.475037797	5.150213301	19.664232699
H	5.903647098	4.456463699	19.252927399
H	6.213104797	6.162799699	18.921241098
H	6.217209000	3.924040000	12.675345000
H	7.407271000	2.867355000	11.910563000
H	7.100138301	4.480514000	11.260781000
H	14.337089301	10.850334301	22.206769699
H	10.717045000	8.084470699	13.776303301
H	11.898464699	9.421540699	13.824130601
H	11.220657699	8.756701399	15.313295601

H	7.922806797	3.215945601	21.889892902
H	9.350007196	3.632361895	22.813491406
H	8.466231993	2.094608496	23.160762399
H	10.345887504	-2.161945294	19.445275196
H	9.059042504	-2.063335797	20.678730895
H	10.747599504	-2.094715496	21.165290196
H	12.566174301	10.408623301	20.566921000
H	16.070661699	7.798239000	12.053085301
H	16.797481699	6.299803000	12.673584000
H	16.923956699	7.805998699	13.614259000
H	17.388912699	7.338015301	19.166447000
H	18.049806699	6.774586301	17.628859000
H	17.622135000	5.604210301	18.884514000
H	14.578680601	3.062778000	18.955159699
H	15.993049601	2.743723000	19.958123699
H	16.182058301	3.671489301	18.473362699
H	7.543026601	12.252924902	18.906799098
H	7.763484301	12.045505301	17.169724098
H	8.722404601	13.235618601	18.021816797
H	16.758276601	10.321630000	22.925806699
H	17.352553301	8.662188000	22.717587699
H	16.090099301	9.000816301	23.880667000
H	11.849473895	5.872002699	27.093997391
H	10.391891594	6.874690797	26.895080489
H	10.228201797	5.127195496	27.012863189
H	12.936182601	4.153435098	24.857312196
H	11.384812601	3.275846399	24.797075196
H	12.067694504	3.946181895	23.301269196
H	13.218986000	7.026185000	24.785549196
H	12.529686504	7.114390000	23.134312895
H	11.873206000	8.142875399	24.406739594

H	6.050020706	6.151924294	25.729892391
H	6.884612007	4.626465594	25.372392790
H	7.585004007	5.776521294	26.519284091
H	5.828894203	6.847930000	22.864484496
H	7.205358000	6.902027301	21.736124294
H	6.633611000	5.355051000	22.359185692
H	6.927861609	8.763985895	24.764169399
H	8.550197210	8.619074993	25.503006993
H	8.399376105	9.038427496	23.782158895

! Direct P-H abstraction - Transition State !

C	13.385569000	9.703576000	20.684915000
C	13.351724000	8.519131000	19.908031000
C	14.425677000	7.602215000	20.101820000
C	15.416513000	7.876110000	21.051395000
C	15.428717000	9.035964000	21.826818000
C	14.390434000	9.947945000	21.607852000
N	12.327838000	8.247916000	19.018027000
C	11.357106000	9.257964000	18.796268000
C	10.111700000	9.202398000	19.466946000
C	9.146540000	10.184893000	19.208523000
C	9.375142000	11.232083000	18.319048000
C	10.617978000	11.285179000	17.678416000
C	11.608049000	10.328794000	17.898510000
C	9.839579000	8.148027000	20.506739000
C	8.320311000	12.272817000	18.048506000
C	12.946680000	10.462513000	17.229527000
P	14.489138000	6.090696000	19.038476000
C	15.269084000	4.761938000	20.136798000
C	14.395002000	4.459672000	21.350905000

C	16.479243000	9.272248000	22.879244000
La	11.364316000	6.194354000	18.217809000
P	10.417611000	4.596674000	20.394595000
C	10.241549000	2.765695000	20.379883000
C	10.862894000	2.030294000	19.340019000
C	10.820049000	0.633610000	19.321768000
C	10.153934000	-0.088782000	20.308369000
C	9.496839000	0.641520000	21.303889000
C	9.509333000	2.035669000	21.357829000
C	11.568381000	2.747400000	18.230721000
C	10.142865000	-1.594973000	20.311404000
C	8.694528000	2.727209000	22.410811000
N	11.311937000	5.935440000	15.714817000
C	12.537666000	6.242978000	15.058742000
C	13.597083000	5.308509000	14.996943000
C	14.775508000	5.635007000	14.315957000
C	14.950989000	6.862465000	13.679661000
C	13.892521000	7.772319000	13.731980000
C	12.698100000	7.486694000	14.394763000
C	13.449839000	3.936902000	15.595364000
C	16.236080000	7.202158000	12.971442000
C	11.568738000	8.475756000	14.349065000
C	10.307145000	5.488867000	14.867908000
C	10.578893000	5.075489000	13.533468000
C	9.595477000	4.586202000	12.690383000
C	8.262810000	4.464266000	13.102736000
C	7.977104000	4.883354000	14.401020000
C	8.941504000	5.401943000	15.275694000
P	8.476397000	5.988778000	16.964550000
C	7.430233000	7.558476000	16.672026000
C	6.099403000	7.364743000	15.947983000

C	7.199631000	3.907402000	12.193084000
C	7.176391000	4.736409000	17.533358000
C	7.749516000	3.321402000	17.589433000
C	6.611016000	5.156198000	18.889391000
C	15.902685000	6.487363000	17.816449000
C	15.572317000	7.779158000	17.074278000
C	17.305168000	6.559790000	18.418168000
C	15.544907000	3.501555000	19.312612000
C	8.279068000	8.611944000	15.965063000
N	9.639552000	5.756947000	23.430967000
Si	8.128857000	6.436435000	23.896245000
C	6.844708000	6.386945000	22.457878000
Si	11.042031000	5.723956000	24.437726000
C	12.317189000	7.125684000	24.059882000
C	10.759092000	5.872449000	26.353134000
C	11.997507000	4.060395000	24.247764000
C	8.151216000	8.297331000	24.453376000
C	7.202273000	5.544292000	25.348490000
H	9.973210000	5.076772000	21.756874000
H	8.201833000	10.138512000	19.747484000
H	11.599262000	5.134044000	13.169156000
H	6.951023000	4.797387000	14.750760000
H	8.171195000	3.011005000	16.628852000
H	6.954413000	2.612874000	17.852071000
H	8.520806000	3.240506000	18.361155000
H	16.229738000	5.162099000	20.483792000
H	9.876069000	4.278244000	11.683577000
H	6.251957000	7.005040000	14.925242000
H	5.574541000	8.326495000	15.880645000
H	5.432284000	6.667922000	16.463377000
H	7.228912000	7.907986000	17.693315000

H	11.319848000	0.101516000	18.512365000
H	14.600074000	7.722422000	16.579757000
H	16.325866000	7.976152000	16.302930000
H	15.560941000	8.629487000	17.763247000
H	10.827851000	12.104896000	16.992333000
H	15.863089000	5.660511000	17.095543000
H	13.991713000	8.733275000	13.228744000
H	8.936201000	0.103764000	22.068350000
H	13.636288000	3.941262000	16.675958000
H	14.167868000	3.240229000	15.151475000
H	12.441567000	3.545380000	15.439584000
H	15.570210000	4.891500000	14.265452000
H	9.185898000	8.853128000	16.526061000
H	7.709459000	9.542085000	15.850306000
H	8.569000000	8.271106000	14.966194000
H	14.257263000	5.340907000	21.981580000
H	14.860318000	3.676617000	21.961594000
H	13.397577000	4.115924000	21.057217000
H	6.374675000	4.759668000	16.784368000
H	9.059716000	8.471587000	21.199218000
H	10.721727000	7.906644000	21.104448000
H	9.460706000	7.200465000	20.087659000
H	10.860937000	3.317188000	17.605231000
H	12.096112000	2.059055000	17.564172000
H	12.304015000	3.457816000	18.647088000
H	16.211031000	7.149487000	21.206469000
H	13.738772000	10.619877000	17.970373000
H	12.953747000	11.308447000	16.535748000
H	13.212183000	9.557866000	16.676124000
H	7.402759000	5.168283000	19.646163000
H	5.849438000	4.438394000	19.216788000

H	6.140826000	6.144730000	18.867032000
H	6.217209000	3.924040000	12.675345000
H	7.407271000	2.867355000	11.910563000
H	7.118208000	4.480514000	11.260781000
H	14.355159000	10.868404000	22.188700000
H	10.717045000	8.066401000	13.794373000
H	11.880395000	9.403471000	13.860270000
H	11.202588000	8.720562000	15.349435000
H	7.850528000	3.252085000	21.944102000
H	9.241589000	3.505874000	22.958049000
H	8.285535000	2.004260000	23.124623000
H	10.436236000	-1.999318000	19.336857000
H	9.149391000	-1.991057000	20.552243000
H	10.837948000	-2.004367000	21.056872000
H	12.584244000	10.426693000	20.566921000
H	16.052592000	7.798239000	12.071155000
H	16.779412000	6.299803000	12.673584000
H	16.905887000	7.787929000	13.614259000
H	17.370843000	7.356085000	19.166447000
H	18.031737000	6.792656000	17.628859000
H	17.622135000	5.622280000	18.884514000
H	14.614820000	3.062778000	18.937090000
H	16.029189000	2.743723000	19.940054000
H	16.200128000	3.689559000	18.455293000
H	7.579166000	12.307134000	18.852590000
H	7.781554000	12.063575000	17.115515000
H	8.758544000	13.271758000	17.949538000
H	16.794416000	10.321630000	22.907737000
H	17.370623000	8.662188000	22.699518000
H	16.108169000	9.018886000	23.880667000
H	11.722986000	5.853933000	26.877161000

H	10.247334000	6.802412000	26.624035000
H	10.155923000	5.036847000	26.723748000
H	12.972322000	4.099226000	24.748894000
H	11.420952000	3.239707000	24.688657000
H	12.158043000	3.819694000	23.192851000
H	13.218986000	7.026185000	24.677131000
H	12.620035000	7.114390000	23.007825000
H	11.873206000	8.106736000	24.262182000
H	6.212648000	5.989297000	25.513056000
H	7.065309000	4.481908000	25.119417000
H	7.765701000	5.613894000	26.284378000
H	5.901173000	6.847930000	22.774136000
H	7.205358000	6.920097000	21.573497000
H	6.633611000	5.355051000	22.160419000
H	7.144698000	8.637498000	24.728030000
H	8.803173000	8.438378000	25.322310000
H	8.525864000	8.948079000	23.655671000

! Direct P-H abstraction - Product !

C	13.385569000	9.719644828	20.684915000
C	13.335655172	8.519131000	19.924099828
C	14.409608172	7.602215000	20.117888828
C	15.416513000	7.876110000	21.067463828
C	15.428717000	9.035964000	21.826818000
C	14.406502828	9.947945000	21.607852000
N	12.311769172	8.247916000	19.050164656
C	11.357106000	9.274032828	18.812336828
C	10.111700000	9.250604484	19.483014828
C	9.162608828	10.233099484	19.208523000
C	9.391210828	11.264220656	18.286910344

C	10.634046828	11.301247828	17.662347172
C	11.624117828	10.328794000	17.898510000
C	9.823510172	8.228371140	20.554945484
C	8.352448656	12.304954656	18.000299516
C	12.962748828	10.446444172	17.229527000
P	14.473069172	6.090696000	19.054544828
C	15.285152828	4.761938000	20.136798000
C	14.427139656	4.427534344	21.350905000
C	16.495311828	9.272248000	22.879244000
La	11.316109516	6.146147516	18.298153140
P	10.289060376	4.757362280	20.635627420
C	10.193342516	2.894245624	20.492364796
C	10.862894000	2.207051108	19.436431968
C	10.868255484	0.794298280	19.353905656
C	10.186071656	0.007630968	20.292300172
C	9.480770172	0.689726484	21.287820172
C	9.461126516	2.083875484	21.389966656
C	11.584449828	2.956294764	18.359271624
C	10.207140312	-1.498560032	20.231059860
C	8.598115032	2.695071344	22.459017484
N	11.311937000	5.903302344	15.746954656
C	12.537666000	6.226909172	15.090879656
C	13.597083000	5.292440172	15.013011828
C	14.775508000	5.618938172	14.332025828
C	14.934920172	6.846396172	13.695729828
C	13.876452172	7.756250172	13.748048828
C	12.682031172	7.470625172	14.410831828
C	13.449839000	3.936902000	15.627501656
C	16.220011172	7.202158000	12.971442000
C	11.552669172	8.459687172	14.381202656
C	10.307145000	5.472798172	14.883976828

C	10.578893000	5.075489000	13.549536828
C	9.595477000	4.586202000	12.706451828
C	8.262810000	4.464266000	13.102736000
C	7.977104000	4.883354000	14.401020000
C	8.941504000	5.385874172	15.291762828
P	8.460328172	5.972709172	16.980618828
C	7.414164172	7.542407172	16.672026000
C	6.099403000	7.348674172	15.931914172
C	7.199631000	3.907402000	12.193084000
C	7.160322172	4.720340172	17.533358000
C	7.781653656	3.321402000	17.653708312
C	6.562809516	5.156198000	18.857253344
C	15.886616172	6.487363000	17.832517828
C	15.556248172	7.779158000	17.074278000
C	17.289099172	6.559790000	18.418168000
C	15.577044656	3.501555000	19.296543172
C	8.279068000	8.611944000	15.981131828
N	9.735964968	5.676602860	23.125659268
Si	8.209201140	6.356090860	23.687350236
C	6.876845656	6.370876172	22.313258548
Si	11.106306312	5.659680688	24.244900064
C	12.349326656	7.109615172	23.931331376
C	10.678747860	5.824242516	26.128170408
C	12.045713484	3.996119688	24.135282204
C	8.311904280	8.184849204	24.340894204
C	7.346892452	5.415741376	25.139595236
H	9.860728204	5.349942076	22.271076496
H	8.201833000	10.218856140	19.747484000
H	11.599262000	5.134044000	13.185224828
H	6.951023000	4.797387000	14.750760000
H	8.251539140	2.994936172	16.709196140

H	7.002619484	2.596805172	17.916346312
H	8.536874828	3.304781312	18.441499140
H	16.229738000	5.162099000	20.483792000
H	9.892137828	4.278244000	11.699645828
H	6.268025828	7.005040000	14.909173172
H	5.574541000	8.310426172	15.864576172
H	5.432284000	6.635784344	16.431239344
H	7.212843172	7.891917172	17.693315000
H	11.400192140	0.326479592	18.544502656
H	14.584005172	7.706353172	16.579757000
H	16.309797172	7.976152000	16.302930000
H	15.528803344	8.629487000	17.763247000
H	10.859988656	12.104896000	16.960195344
H	15.847020172	5.660511000	17.111611828
H	13.975644172	8.717206172	13.244812828
H	8.904063344	0.103764000	22.004074688
H	13.588081516	3.957330828	16.708095656
H	14.216074484	3.240229000	15.231819140
H	12.473704656	3.513242344	15.423515172
H	15.570210000	4.891500000	14.281520828
H	9.169829172	8.837059172	16.558198656
H	7.709459000	9.542085000	15.866374828
H	8.569000000	8.271106000	14.982262828
H	14.257263000	5.308769344	21.981580000
H	14.924593312	3.660548172	21.961594000
H	13.429714656	4.035579860	21.057217000
H	6.390743828	4.711461516	16.752230344
H	9.059716000	8.600137624	21.247424484
H	10.721727000	7.986988140	21.136585656
H	9.428568344	7.280809140	20.151934312
H	10.877005828	3.477876280	17.701643968

H	12.176456140	2.284018592	17.708791452
H	12.271877344	3.698848420	18.807776280
H	16.194962172	7.149487000	21.206469000
H	13.754840828	10.587739344	17.954304172
H	12.969815828	11.276309344	16.519679172
H	13.212183000	9.525728344	16.676124000
H	7.338483688	5.184351828	19.630094172
H	5.801231516	4.422325172	19.184650344
H	6.076550688	6.128661172	18.818825516
H	6.217209000	3.924040000	12.675345000
H	7.407271000	2.867355000	11.910563000
H	7.134276828	4.480514000	11.260781000
H	14.371227828	10.884472828	22.172631172
H	10.717045000	8.050332172	13.810441828
H	11.864326172	9.387402172	13.892407656
H	11.186519172	8.688424344	15.381572656
H	7.786252688	3.284222656	21.992308484
H	9.145176032	3.393392204	23.086599624
H	8.124846720	1.923915860	23.092485344
H	10.516580140	-1.854698548	19.240444032
H	9.229735140	-1.926781688	20.439761204
H	10.918292140	-1.924022860	20.960459032
H	12.600312828	10.442761828	20.566921000
H	16.036523172	7.798239000	12.087223828
H	16.763343172	6.299803000	12.673584000
H	16.889818172	7.771860172	13.614259000
H	17.354774172	7.372153828	19.166447000
H	18.015668172	6.808724828	17.628859000
H	17.622135000	5.638348828	18.884514000
H	14.646957656	3.062778000	18.921021172
H	16.061326656	2.743723000	19.923985172

H	16.216196828	3.705627828	18.439224172
H	7.611303656	12.355340484	18.804383516
H	7.797622828	12.079643828	17.067308516
H	8.790681656	13.303895656	17.885262688
H	16.826553656	10.321630000	22.891668172
H	17.386691828	8.662188000	22.683449172
H	16.124237828	9.034954828	23.880667000
H	11.610504204	5.837864172	26.684335064
H	10.118783376	6.738136688	26.383002580
H	10.091647688	4.956502860	26.466646752
H	13.004459656	4.051019516	24.652481032
H	11.453089656	3.207569344	24.592244032
H	12.238387140	3.707212204	23.096438032
H	13.218986000	7.026185000	24.580718032
H	12.700379140	7.114390000	22.895343204
H	11.873206000	8.074598344	24.133631376
H	6.357267452	5.844677548	25.320230064
H	7.225997280	4.353357376	24.894453408
H	7.926389280	5.469274548	26.075483236
H	5.965448312	6.847930000	22.693791860
H	7.205358000	6.936165828	21.428877548
H	6.633611000	5.355051000	21.983661892
H	7.337523936	8.525016204	24.695892344
H	9.028136592	8.277689720	25.161621720
H	8.638345796	8.867734860	23.543189204

! Internal C-H activation from the Phosphido - Adduct !

C	13.380569000	9.683176000	20.580206000
C	13.501339000	8.648258000	19.603469000
C	14.770542000	8.017253000	19.503492000

C	15.830962000	8.381855000	20.318071000
C	15.714901000	9.392551000	21.282649000
C	14.471844000	10.023897000	21.382988000
N	12.431531000	8.327141000	18.811746000
C	12.570185000	7.384455000	17.776790000
C	12.715295000	7.880150000	16.447513000
C	12.734186000	6.955650000	15.387967000
C	12.645949000	5.578911000	15.604082000
C	12.519317000	5.112650000	16.920504000
C	12.464538000	5.991894000	18.002584000
C	12.914149000	9.357327000	16.219991000
C	12.683732000	4.607370000	14.451390000
C	12.328785000	5.471774000	19.407081000
C	16.877197000	9.786469000	22.156307000
P	11.729685000	10.506823000	20.674305000
C	12.121283000	12.293977000	21.158089000
C	12.960371000	12.973561000	20.076510000
La	10.607450000	9.574410000	17.734427000
P	10.916707000	11.966274000	16.584346000
C	11.725863000	13.455342000	15.860696000
C	10.888086000	14.530650000	15.451226000
C	11.446953000	15.695386000	14.924498000
C	12.825792000	15.862593000	14.779620000
C	13.642757000	14.813595000	15.200052000
C	13.128570000	13.628234000	15.732743000
C	9.391905000	14.447727000	15.589953000
C	13.404055000	17.115309000	14.174854000
C	14.092103000	12.561657000	16.167211000
N	8.111470000	9.069270000	18.148465000
C	7.794290000	9.347786000	19.499242000
C	7.526237000	10.671231000	19.927717000

C	7.222801000	10.908925000	21.271887000
C	7.160287000	9.881002000	22.215204000
C	7.411459000	8.579272000	21.775469000
C	7.725090000	8.296819000	20.444168000
C	7.490757000	11.801367000	18.934904000
C	6.848405000	10.167750000	23.661578000
C	7.928060000	6.874920000	19.996576000
C	7.042643000	8.862555000	17.313408000
C	7.217737000	8.565018000	15.925273000
C	6.107549000	8.420282000	15.085473000
C	4.789235000	8.519584000	15.531921000
C	4.615568000	8.764213000	16.900672000
C	5.689062000	8.927126000	17.759554000
P	8.941970000	8.363645000	15.307203000
C	9.074955000	6.497992000	14.938726000
C	8.145922000	5.945374000	13.860388000
C	3.618726000	8.387448000	14.593449000
C	8.914002000	9.136215000	13.578325000
C	8.502741000	10.605810000	13.650498000
C	10.290237000	8.980782000	12.927349000
C	10.994347000	9.779005000	22.280550000
C	10.990716000	8.253717000	22.174144000
C	11.662597000	10.222966000	23.580418000
C	10.812965000	13.053825000	21.389042000
C	8.907134000	5.728494000	16.248933000
H	12.870188000	7.322017000	14.373952000
H	5.498209000	9.124042000	18.810023000
H	6.275958000	8.231805000	14.026783000
H	7.489602000	10.721672000	14.045150000
H	8.534409000	11.053148000	12.648435000
H	9.185810000	11.165094000	14.306386000

H	12.692816000	12.272905000	22.094952000
H	3.606594000	8.836522000	17.307082000
H	7.095592000	6.053544000	14.149381000
H	8.338186000	4.873643000	13.717000000
H	8.286086000	6.431949000	12.889812000
H	10.116245000	6.386653000	14.612390000
H	10.779057000	16.501551000	14.620009000
H	10.500231000	7.915648000	21.258473000
H	10.454345000	7.814487000	23.024430000
H	12.013101000	7.862065000	22.172889000
H	12.454847000	4.041177000	17.105775000
H	9.953188000	10.124156000	22.269831000
H	7.350720000	7.755738000	22.486298000
H	14.724847000	14.918601000	15.117650000
H	8.446206000	11.942449000	18.413363000
H	7.235941000	12.743494000	19.430352000
H	6.743790000	11.609261000	18.156737000
H	7.008211000	11.930353000	21.584304000
H	9.638798000	6.044773000	16.997445000
H	9.053397000	4.653859000	16.082867000
H	7.903011000	5.873974000	16.661538000
H	13.912789000	12.458937000	19.920557000
H	13.177076000	14.010412000	20.364531000
H	12.421754000	12.991708000	19.122118000
H	8.174611000	8.587139000	12.981249000
H	13.250929000	9.510066000	15.186023000
H	13.715595000	9.707845000	16.885718000
H	12.235296000	10.131841000	16.267172000
H	14.360615000	10.830730000	22.105576000
H	13.241797000	5.649731000	19.988274000
H	12.123712000	4.396768000	19.412139000

H	11.523734000	5.987078000	19.940379000
H	11.053309000	9.506376000	13.515674000
H	10.285324000	9.420873000	11.922214000
H	10.592227000	7.932560000	12.829677000
H	2.870434000	7.678034000	14.969286000
H	3.939630000	8.033483000	13.607987000
H	3.100251000	9.343965000	14.440454000
H	16.785671000	7.870442000	20.194555000
H	7.172588000	6.588001000	19.256703000
H	7.864310000	6.182737000	20.841840000
H	8.899113000	6.735412000	19.510404000
H	14.083835000	11.708163000	15.475099000
H	13.823568000	12.167568000	17.153355000
H	15.116561000	12.946950000	16.207144000
H	12.814242000	18.000232000	14.439785000
H	13.430207000	17.065349000	13.077308000
H	14.432019000	17.285196000	14.513154000
H	14.906132000	7.244307000	18.751650000
H	6.311624000	9.334915000	24.128357000
H	6.232067000	11.066616000	23.767280000
H	7.762082000	10.331470000	24.247886000
H	12.718647000	9.932753000	23.600232000
H	11.174468000	9.737871000	24.436445000
H	11.601499000	11.303752000	23.741279000
H	10.220928000	13.082697000	20.468247000
H	11.022906000	14.090319000	21.682089000
H	10.194783000	12.603688000	22.172732000
H	13.044530000	5.087752000	13.536511000
H	11.688513000	4.196951000	14.236276000
H	13.340655000	3.756255000	14.665133000
H	16.604704000	10.605391000	22.830302000

H 17.739922000 10.123464000 21.566739000

H 17.225803000 8.952936000 22.780715000

H 8.912543000 15.357739000 15.212168000

H 8.987396000 13.585390000 15.048381000

H 9.101286000 14.303754000 16.636984000

! Internal C-H activation from the Phosphido - Transition State !

C 13.409670 9.669542 20.547414

C 13.512249 8.630155 19.572510

C 14.776124 7.992309 19.458237

C 15.848083 8.351617 20.261027

C 15.748639 9.362324 21.226352

C 14.511231 10.004488 21.337368

N 12.431364 8.316437 18.797955

C 12.544764 7.367394 17.761562

C 12.687248 7.859639 16.426765

C 12.678309 6.919206 15.373144

C 12.588044 5.548658 15.598794

C 12.479141 5.090973 16.919238

C 12.442826 5.976811 17.997134

C 12.880509 9.305198 16.193052

C 12.601135 4.571325 14.450445

C 12.325573 5.464985 19.406234

C 16.912181 9.729651 22.109828

P 11.767260 10.508931 20.653229

C 12.179860 12.294885 21.124472

C 13.015974 12.961349 20.032475

La 10.601645 9.574953 17.736724

P 10.918953 11.962986 16.582333

C 11.731041 13.443723 15.845527

C 10.897232 14.527938 15.449265

C 11.458842 15.686505 14.913615

C 12.837550 15.839952 14.746847

C 13.649991 14.782750 15.153111

C 13.132474 13.602068 15.694572

C 9.402694 14.459225 15.611653

C 13.416971 17.091209 14.140068

C 14.092148 12.525529 16.112668

N 8.107280 9.085267 18.172216

C 7.806326 9.368699 19.525622

C 7.550979 10.695216 19.953768

C 7.265176 10.938228 21.300462

C 7.207846 9.912788 22.247367

C 7.445946 8.608784 21.808224

C 7.742071 8.320815 20.473734

C 7.510764 11.822626 18.958108

C 6.914851 10.207034 23.696212

C 7.932079 6.896608 20.027637

C 7.028562 8.886818 17.348034

C 7.187978 8.589199 15.958019

C 6.068758 8.452626 15.129181

C 4.755504 8.560623 15.588728

C 4.597010 8.804589 16.959292

C 5.680107 8.959463 17.807762

P 8.904799 8.375546 15.323012

C 9.020076 6.508383 14.957159

C 8.065110 5.957035 13.901085

C 3.575119 8.441063 14.660995

C 8.863387 9.144485 13.592624

C 8.462541 10.616948 13.666527

C 10.231223 8.979204 12.926539

C	11.041843	9.795312	22.270541
C	11.021299	8.269687	22.171413
C	11.727996	10.237952	23.561511
C	10.881038	13.068438	21.363617
C	8.876882	5.744562	16.273589
H	12.807615	7.283924	14.355136
H	5.500836	9.155450	18.860461
H	6.225582	8.262973	14.068902
H	7.454260	10.740170	14.071241
H	8.487115	11.062648	12.663541
H	9.155666	11.172799	14.309625
H	12.759222	12.272901	22.056504
H	3.592595	8.882578	17.375824
H	7.022010	6.069645	14.213493
H	8.250325	4.884355	13.755479
H	8.184901	6.441313	12.926603
H	10.053458	6.390631	14.608672
H	10.793908	16.499000	14.619489
H	10.513127	7.932117	21.265283
H	10.493326	7.840067	23.031798
H	12.039494	7.867528	22.156668
H	12.413797	4.020833	17.111631
H	10.004179	10.151016	22.269312
H	7.389031	7.787639	22.522075
H	14.731487	14.876398	15.051909
H	8.460813	11.955805	18.424727
H	7.267979	12.767814	19.453741
H	6.753305	11.633008	18.189563
H	7.060321	11.961755	21.612646
H	9.628076	6.058060	17.003805
H	9.011408	4.668274	16.108329

H 7.883556 5.898756 16.708651

H 13.963284 12.438487 19.872895

H 13.242632 13.998269 20.312471

H 12.470428 12.977616 19.081945

H 8.114059 8.598953 13.004647

H 13.156512 9.499983 15.153152

H 13.651804 9.703637 16.858203

H 11.995181 10.554449 16.269926

H 14.414134 10.815513 22.057326

H 13.251948 5.631268 19.969562

H 12.104149 4.393304 19.420253

H 11.538848 5.995536 19.951697

H 11.004048 9.496872 13.504540

H 10.217322 9.416731 11.920358

H 10.526021 7.929040 12.827958

H 3.089624 9.410157 14.480328

H 2.804909 7.770963 15.063255

H 3.877078 8.045498 13.685411

H 16.799220 7.836599 20.125864

H 7.172645 6.615097 19.289854

H 7.864370 6.206211 20.874071

H 8.901045 6.747825 19.539856

H 14.064381 11.672404 15.425536

H 13.835436 12.133760 17.102909

H 15.120944 12.900497 16.136311

H 12.953089 17.994799 14.553531

H 13.266123 17.125582 13.052332

H 14.495080 17.158578 14.319892

H 14.900310 7.221408 18.702362

H 6.238302 11.061758 23.802664

H 7.829814 10.449217 24.252493

H 6.452519 9.347970 24.193540

H 12.781231 9.937073 23.572008

H 11.243704 9.761391 24.424461

H 11.679460 11.319954 23.718338

H 10.282805 13.102985 20.447026

H 11.103888 14.102911 21.654242

H 10.263906 12.625391 22.152167

H 13.041659 5.016277 13.552512

H 11.586957 4.242365 14.187980

H 13.175768 3.671294 14.696592

H 17.857844 9.731016 21.554808

H 17.036224 9.029448 22.948270

H 16.783859 10.727886 22.542108

H 8.926147 15.374036 15.241994

H 8.981472 13.600922 15.076447

H 9.122448 14.322533 16.663178

! Internal C-H activation from the Phosphido - Product !

C 13.380569000 9.683176000 20.580206000

C 13.501339000 8.648258000 19.603469000

C 14.770542000 8.017253000 19.503492000

C 15.830962000 8.381855000 20.318071000

C 15.714901000 9.392551000 21.282649000

C 14.471844000 10.023897000 21.382988000

N 12.431531000 8.327141000 18.821720755

C 12.560210245 7.384455000 17.776790000

C 12.735244510 7.890124755 16.447513000

C 12.734186000 6.945675245 15.387967000

C 12.645949000 5.578911000 15.604082000

C 12.519317000 5.112650000 16.920504000

C	12.464538000	5.991894000	18.002584000
C	12.914149000	9.307453225	16.229965755
C	12.683732000	4.607370000	14.451390000
C	12.328785000	5.471774000	19.407081000
C	16.877197000	9.786469000	22.156307000
P	11.729685000	10.506823000	20.674305000
C	12.121283000	12.293977000	21.158089000
C	12.960371000	12.973561000	20.076510000
La	10.607450000	9.574410000	17.734427000
P	10.916707000	11.966274000	16.584346000
C	11.725863000	13.455342000	15.860696000
C	10.888086000	14.530650000	15.451226000
C	11.446953000	15.695386000	14.924498000
C	12.825792000	15.862593000	14.779620000
C	13.642757000	14.813595000	15.200052000
C	13.128570000	13.628234000	15.732743000
C	9.391905000	14.447727000	15.589953000
C	13.404055000	17.115309000	14.174854000
C	14.092103000	12.561657000	16.167211000
N	8.111470000	9.069270000	18.148465000
C	7.794290000	9.347786000	19.499242000
C	7.526237000	10.671231000	19.927717000
C	7.222801000	10.908925000	21.271887000
C	7.160287000	9.881002000	22.215204000
C	7.411459000	8.579272000	21.775469000
C	7.725090000	8.296819000	20.444168000
C	7.490757000	11.801367000	18.934904000
C	6.848405000	10.167750000	23.661578000
C	7.928060000	6.874920000	19.996576000
C	7.042643000	8.862555000	17.313408000
C	7.217737000	8.565018000	15.925273000

C	6.107549000	8.420282000	15.085473000
C	4.789235000	8.519584000	15.531921000
C	4.615568000	8.764213000	16.900672000
C	5.689062000	8.927126000	17.759554000
P	8.941970000	8.363645000	15.307203000
C	9.074955000	6.497992000	14.938726000
C	8.145922000	5.945374000	13.860388000
C	3.618726000	8.387448000	14.593449000
C	8.914002000	9.136215000	13.578325000
C	8.502741000	10.605810000	13.650498000
C	10.290237000	8.980782000	12.927349000
C	10.994347000	9.779005000	22.280550000
C	10.990716000	8.253717000	22.174144000
C	11.662597000	10.222966000	23.580418000
C	10.812965000	13.053825000	21.389042000
C	8.907134000	5.728494000	16.248933000
H	12.880162755	7.322017000	14.373952000
H	5.498209000	9.124042000	18.810023000
H	6.275958000	8.231805000	14.026783000
H	7.489602000	10.721672000	14.045150000
H	8.534409000	11.053148000	12.648435000
H	9.185810000	11.165094000	14.296411245
H	12.692816000	12.272905000	22.094952000
H	3.606594000	8.836522000	17.307082000
H	7.095592000	6.053544000	14.149381000
H	8.338186000	4.873643000	13.717000000
H	8.286086000	6.431949000	12.889812000
H	10.116245000	6.386653000	14.612390000
H	10.779057000	16.501551000	14.620009000
H	10.500231000	7.915648000	21.258473000
H	10.454345000	7.814487000	23.024430000

H	12.013101000	7.862065000	22.172889000
H	12.454847000	4.041177000	17.105775000
H	9.953188000	10.124156000	22.269831000
H	7.350720000	7.755738000	22.486298000
H	14.724847000	14.918601000	15.117650000
H	8.446206000	11.942449000	18.413363000
H	7.235941000	12.743494000	19.430352000
H	6.743790000	11.609261000	18.156737000
H	7.008211000	11.930353000	21.584304000
H	9.638798000	6.044773000	16.997445000
H	9.053397000	4.653859000	16.082867000
H	7.903011000	5.873974000	16.661538000
H	13.912789000	12.458937000	19.920557000
H	13.177076000	14.010412000	20.364531000
H	12.421754000	12.991708000	19.122118000
H	8.174611000	8.587139000	12.981249000
H	13.161156204	9.559939775	15.195997755
H	13.625822204	9.757718775	16.925617020
H	11.796406776	11.009619447	16.317045775
H	14.360615000	10.830730000	22.105576000
H	13.241797000	5.649731000	19.988274000
H	12.123712000	4.396768000	19.412139000
H	11.523734000	5.987078000	19.940379000
H	11.053309000	9.496401245	13.515674000
H	10.285324000	9.420873000	11.922214000
H	10.592227000	7.932560000	12.829677000
H	2.870434000	7.678034000	14.969286000
H	3.939630000	8.033483000	13.607987000
H	3.100251000	9.343965000	14.440454000
H	16.785671000	7.870442000	20.194555000
H	7.172588000	6.588001000	19.256703000

H 7.864310000 6.182737000 20.841840000

H 8.899113000 6.735412000 19.510404000

H 14.083835000 11.708163000 15.485073755

H 13.823568000 12.167568000 17.153355000

H 15.116561000 12.946950000 16.207144000

H 12.814242000 18.000232000 14.439785000

H 13.430207000 17.065349000 13.077308000

H 14.432019000 17.285196000 14.513154000

H 14.906132000 7.244307000 18.751650000

H 6.311624000 9.334915000 24.128357000

H 6.232067000 11.066616000 23.767280000

H 7.762082000 10.331470000 24.247886000

H 12.718647000 9.932753000 23.600232000

H 11.174468000 9.737871000 24.436445000

H 11.601499000 11.303752000 23.741279000

H 10.220928000 13.082697000 20.468247000

H 11.022906000 14.090319000 21.682089000

H 10.194783000 12.603688000 22.172732000

H 13.044530000 5.087752000 13.536511000

H 11.688513000 4.196951000 14.236276000

H 13.340655000 3.756255000 14.665133000

H 16.604704000 10.605391000 22.830302000

H 17.739922000 10.123464000 21.566739000

H 17.225803000 8.952936000 22.780715000

H 8.912543000 15.357739000 15.212168000

H 8.987396000 13.585390000 15.048381000

H 9.091311245 14.313728755 16.636984000

! H abstraction by HMDS on the adjacent methyl group - Adduct !

C -0.380186000 -5.237164000 1.613583000

C	0.094947000	-4.687347000	0.395554000
C	-0.121847000	-5.412572000	-0.802104000
C	-0.786474000	-6.639052000	-0.767218000
C	-1.252321000	-7.194942000	0.424206000
C	-1.036768000	-6.470032000	1.597563000
P	1.025562000	-3.104032000	0.281697000
La	0.801161000	-0.316272000	-0.681916000
P	-2.321103000	-0.338115000	-1.189568000
C	-3.458141000	-1.726633000	-0.601726000
C	-3.625858000	-1.641101000	0.916825000
C	0.353795000	-4.867961000	-2.119260000
C	-1.938439000	-8.535652000	0.449590000
C	-0.211685000	-4.533904000	2.932731000
C	0.675216000	2.151232000	0.935695000
C	0.568056000	3.460012000	0.397896000
C	-0.541754000	4.235742000	0.727424000
C	-1.555410000	3.765552000	1.572919000
C	-1.449281000	2.473574000	2.093266000
C	-0.349450000	1.661592000	1.783098000
C	1.675122000	4.029894000	-0.446491000
N	1.810433000	1.340461000	0.649241000
C	2.958119000	1.542821000	1.390507000
C	4.141577000	0.806753000	1.107735000
C	5.287709000	0.991889000	1.890711000
C	5.340160000	1.895325000	2.952414000
C	4.172734000	2.623984000	3.218932000
C	3.018143000	2.458216000	2.471155000
C	-0.215442000	0.319205000	2.462796000
C	-2.734510000	4.621901000	1.950896000
P	4.064420000	-0.388215000	-0.294568000
C	5.127294000	-1.843355000	0.292082000

C	5.200181000	-2.904041000	-0.808623000
C	6.586491000	2.077141000	3.778343000
N	0.138910000	0.030234000	-2.987302000
C	-1.015442000	-0.294366000	-3.690089000
C	-2.251335000	-0.540724000	-3.026594000
C	-3.377906000	-0.924812000	-3.763511000
C	-3.372696000	-1.061110000	-5.152240000
C	-2.163528000	-0.789145000	-5.802385000
C	-1.024454000	-0.421211000	-5.102940000
C	-4.602856000	-1.479602000	-5.913779000
C	5.167362000	0.412567000	-1.631653000
C	6.655887000	0.514202000	-1.305262000
C	4.594166000	1.784835000	-1.981368000
C	1.255459000	0.428968000	-3.770325000
C	2.264027000	-0.504069000	-4.104860000
C	3.350983000	-0.095615000	-4.886404000
C	3.473967000	1.210529000	-5.358284000
C	2.464769000	2.119585000	-5.028379000
C	1.364365000	1.758665000	-4.250850000
C	2.136918000	-1.949609000	-3.698370000
C	4.658847000	1.634788000	-6.185670000
C	0.280551000	2.759574000	-3.967186000
C	-3.358222000	1.233043000	-0.924094000
C	-2.668980000	2.410851000	-1.609775000
C	-4.823981000	1.141346000	-1.341483000
C	-2.920947000	-3.090405000	-1.027243000
C	4.604272000	-2.441287000	1.597367000
N	-3.520766000	2.306215000	4.527634000
Si	-2.756718000	2.837375000	5.968064000
C	-3.410867000	4.520721000	6.679309000
Si	-5.090192000	1.632697000	4.417878000

C	-5.202033000	-0.271944000	4.770503000
C	-5.797793000	1.840558000	2.630218000
C	-6.474792000	2.379794000	5.556892000
C	-2.822128000	1.637874000	7.494546000
C	-0.870898000	3.139649000	5.684043000
H	-0.940938000	0.247027000	3.277249000
H	-4.524473000	-0.829909000	4.114878000
H	1.180823000	-2.803280000	1.669186000
H	-2.199761000	2.155165000	2.834953000
H	-0.105318000	-0.235523000	-5.649839000
H	-4.302482000	-1.133475000	-3.230218000
H	-2.844049000	-3.179282000	-2.114493000
H	-3.587481000	-3.883383000	-0.668502000
H	-1.933377000	-3.275364000	-0.593802000
H	6.132793000	-1.442983000	0.471008000
H	-2.106016000	-0.876500000	-6.886710000
H	-4.923832000	0.977994000	-2.419864000
H	-5.326728000	2.085539000	-1.101320000
H	-5.367870000	0.352347000	-0.815069000
H	-3.302897000	1.390003000	0.159858000
H	-0.944016000	-7.173385000	-1.703620000
H	3.560262000	1.715070000	-2.329015000
H	5.178729000	2.246391000	-2.785867000
H	4.622969000	2.454117000	-1.115558000
H	-0.607983000	5.248081000	0.329208000
H	5.035283000	-0.242511000	-2.502472000
H	2.531367000	3.143090000	-5.394630000
H	-1.400507000	-6.873253000	2.542050000
H	1.134855000	-2.331204000	-3.912750000
H	2.327695000	-2.119029000	-2.629091000
H	2.862427000	-2.566990000	-4.236300000

H	4.108848000	-0.830953000	-5.153311000
H	-1.650690000	2.558312000	-1.240394000
H	-3.222385000	3.335125000	-1.408476000
H	-2.633460000	2.266854000	-2.694792000
H	4.544441000	-1.695052000	2.394162000
H	5.276254000	-3.241809000	1.931698000
H	3.612323000	-2.880192000	1.451765000
H	-4.434695000	-1.564554000	-1.074585000
H	0.789992000	0.172845000	2.869834000
H	-0.430227000	-0.546420000	1.809375000
H	-0.130452000	-3.910960000	-2.354479000
H	0.138714000	-5.560621000	-2.938508000
H	1.434713000	-4.677047000	-2.099843000
H	6.173613000	0.397285000	1.676683000
H	2.575052000	4.206792000	0.154961000
H	1.374147000	4.982323000	-0.892504000
H	1.970522000	3.347286000	-1.249059000
H	-2.665817000	-1.784849000	1.423786000
H	-4.301058000	-2.431718000	1.263552000
H	-4.042988000	-0.686586000	1.249258000
H	-5.453355000	-1.628916000	-5.241660000
H	-4.445233000	-2.419707000	-6.457262000
H	-4.898090000	-0.727245000	-6.655736000
H	4.160891000	3.332388000	4.045813000
H	-0.663720000	2.454227000	-4.431331000
H	0.548596000	3.747116000	-4.353143000
H	0.084494000	2.849177000	-2.895247000
H	0.845909000	-4.415710000	3.199109000
H	-0.697386000	-5.094373000	3.736887000
H	-0.646058000	-3.527643000	2.912490000
H	-2.707486000	-8.577930000	1.228253000

H	-1.229890000	-9.349958000	0.652620000
H	-2.419411000	-8.757385000	-0.508758000
H	2.127456000	3.023156000	2.728604000
H	5.420887000	2.128382000	-5.569219000
H	4.368172000	2.344962000	-6.966825000
H	5.136809000	0.777356000	-6.669393000
H	6.825187000	1.139484000	-0.422998000
H	7.185570000	0.983227000	-2.144455000
H	7.122740000	-0.460091000	-1.132339000
H	4.205280000	-3.320707000	-1.000717000
H	5.850390000	-3.729949000	-0.495073000
H	5.599294000	-2.508445000	-1.748953000
H	-2.431390000	5.658035000	2.141120000
H	-3.218548000	4.207348000	2.844155000
H	-3.477230000	4.646969000	1.142332000
H	7.370362000	1.376561000	3.473400000
H	6.393951000	1.912237000	4.845390000
H	6.996388000	3.090688000	3.681475000
H	-2.860287000	4.820557000	7.580075000
H	-3.306703000	5.316885000	5.933720000
H	-4.472944000	4.445302000	6.936496000
H	-2.277069000	2.054511000	8.350954000
H	-3.855602000	1.453692000	7.809435000
H	-2.374622000	0.670016000	7.242948000
H	-0.398524000	3.541766000	6.588516000
H	-0.360866000	2.206709000	5.420903000
H	-0.707137000	3.849528000	4.866660000
H	-6.219314000	-0.655149000	4.619435000
H	-4.907829000	-0.485755000	5.804065000
H	-6.753955000	1.316979000	2.511268000
H	-5.955715000	2.899843000	2.400143000

H -5.095726000 1.443715000 1.888922000

H -7.442595000 1.897553000 5.370260000

H -6.228941000 2.244496000 6.616217000

H -6.587034000 3.454650000 5.377199000

! H abstraction by HMDS on the adjacent methyl group - Transition State !

C 8.850269 5.463865 15.359350

C 10.140585 5.851415 14.874698

C 10.290753 5.828443 13.458309

C 9.286981 5.396194 12.607824

C 8.047734 4.954993 13.087710

C 7.866118 5.014839 14.468860

N 11.170277 6.223378 15.720273

C 12.309721 6.783601 15.073023

C 13.364275 5.976200 14.583593

C 14.452288 6.569475 13.934020

C 14.547628 7.947534 13.749969

C 13.496586 8.734611 14.224082

C 12.383997 8.183851 14.863582

C 13.319708 4.477046 14.703058

C 15.743237 8.567948 13.075995

C 11.245247 9.075644 15.269402

C 6.975941 4.438935 12.164334

P 8.491963 5.639903 17.161716

C 7.382774 4.160179 17.573037

C 6.960442 4.233353 19.041591

La 11.494796 5.917026 18.221725

P 11.045237 3.520475 19.754319

C 10.985342 1.682766 19.793859

C 11.302692 0.952585 18.619503

C	11.268013	-0.440375	18.619741
C	10.923823	-1.174733	19.756204
C	10.607688	-0.449349	20.910056
C	10.631009	0.942451	20.958790
C	11.671248	1.724757	17.392802
C	10.918185	-2.681468	19.751426
C	10.279908	1.665414	22.230376
P	14.701868	5.452113	18.831442
C	15.390477	3.902037	19.673117
C	15.462696	2.738714	18.681559
C	16.072928	5.920426	17.588253
C	17.510978	5.746107	18.073428
C	14.852634	6.747420	20.138872
C	13.804185	7.708955	20.218570
C	13.933143	8.707828	21.218970
C	15.021857	8.746009	22.074297
C	16.052177	7.797697	22.006069
C	15.932087	6.810221	21.027713
N	12.727361	7.631194	19.372688
C	11.724327	8.626893	19.392644
C	10.433319	8.293289	19.893687
C	9.408654	9.258156	19.784167
C	9.622717	10.518499	19.245125
C	10.908256	10.831667	18.776185
C	11.950577	9.912664	18.827800
C	10.150608	7.022490	20.608702
C	8.515341	11.537875	19.173234
C	13.302187	10.271316	18.275155
C	17.217344	7.832005	22.959879
C	7.261800	7.099260	17.260412
C	7.886460	8.327682	16.603311

C	5.860929	6.846982	16.705848
C	15.831501	7.354209	17.116369
C	14.544876	3.539287	20.894328
C	8.060437	2.828168	17.260841
N	8.978902	7.497497	23.217977
Si	10.136189	7.764372	24.479544
C	11.785675	6.858398	24.096350
Si	7.262936	7.472558	23.405077
C	6.518823	8.954427	24.401068
C	6.562121	5.887941	24.261685
C	6.377483	7.538437	21.694955
C	10.585404	9.623302	24.744464
C	9.605062	7.119825	26.224138
H	9.588236	7.279487	21.864764
H	6.846430	4.993353	23.697359
H	10.710336	4.019112	21.041021
H	8.436531	9.011076	20.201222
H	11.233618	6.152477	13.030381
H	6.907955	4.692770	14.871706
H	8.388281	2.772298	16.218865
H	7.356927	2.004837	17.437017
H	8.924572	2.657421	17.908540
H	16.408153	4.140654	20.006706
H	9.477442	5.395212	11.534839
H	5.892828	6.624190	15.634335
H	5.250163	7.749698	16.833773
H	5.339611	6.031021	17.214607
H	7.187363	7.286526	18.339632
H	11.515408	-0.966601	17.697607
H	14.831458	7.482131	16.694638
H	16.555497	7.622995	16.338038

H 15.946587 8.058502 17.946432

H 11.097100 11.816660 18.350661

H 15.900438 5.245149 16.739327

H 13.529566 9.812914 14.074012

H 10.329793 -0.990826 21.814690

H 12.301198 4.096487 14.601058

H 13.699889 4.140094 15.674237

H 13.944427 4.010157 13.934873

H 15.243775 5.925973 13.551193

H 8.860452 8.567249 17.035296

H 7.238924 9.201255 16.744999

H 8.011797 8.169902 15.527086

H 14.566942 4.331604 21.647253

H 14.924524 2.618869 21.354893

H 13.502157 3.369134 20.609117

H 6.489507 4.251494 16.943145

H 11.044994 6.438695 20.849297

H 9.352097 6.410269 20.169308

H 10.843371 2.355498 17.035558

H 11.961433 1.073745 16.562909

H 12.522600 2.389890 17.598945

H 16.708283 6.049653 20.971181

H 14.068778 10.285388 19.058435

H 13.279256 11.257383 17.801270

H 13.629405 9.537540 17.531343

H 7.834594 4.171853 19.698112

H 6.301242 3.392355 19.288682

H 6.422243 5.155230 19.282009

H 6.015713 4.347274 12.682292

H 7.222281 3.447644 11.760457

H 6.825301 5.103960 11.305318

H 15.063633 9.526956 22.832267

H 10.309086 8.743436 14.810932

H 11.432635 10.108411 14.960934

H 11.088369 9.078125 16.352358

H 11.111785 2.280615 22.599231

H 10.019129 0.959916 23.024305

H 9.426009 2.343542 22.100951

H 10.842604 -3.076212 18.732550

H 10.075586 -3.084681 20.325256

H 11.833399 -3.100288 20.192791

H 13.138019 9.440146 21.323511

H 16.481346 8.914628 13.810581

H 15.458317 9.436311 12.472501

H 16.249054 7.852464 12.419746

H 17.717855 6.396873 18.928858

H 18.208488 6.026635 17.273364

H 17.742992 4.716001 18.361326

H 14.460907 2.418818 18.378412

H 15.948337 1.874090 19.150595

H 16.031632 2.986323 17.778719

H 8.808429 12.479870 19.651690

H 7.611473 11.178228 19.672768

H 8.252451 11.774070 18.134322

H 17.943785 7.046975 22.726028

H 16.898003 7.683411 23.999349

H 17.747866 8.792018 22.923640

H 11.366143 9.745555 25.505079

H 10.943870 10.062499 23.807799

H 9.704593 10.191874 25.061942

H 10.388899 7.330348 26.961814

H 8.680386 7.591043 26.573671

H	9.442671	6.037159	26.200301
H	12.514704	7.020765	24.898846
H	11.612143	5.780761	24.006574
H	12.233730	7.209143	23.162154
H	5.467509	5.921196	24.325775
H	6.960355	5.781397	25.275791
H	5.309053	7.321339	21.807504
H	6.471616	8.529086	21.238200
H	6.804735	6.801884	21.007657
H	5.424684	8.889489	24.443295
H	6.894323	8.978560	25.429667
H	6.789521	9.903496	23.926356

! H abstraction by HMDS on the adjacent methyl group - Product !

C	-0.177572000	3.886846000	-0.052002000
C	-0.064638000	2.558827000	0.429399000
C	-1.222378000	1.864241000	0.913434000
C	-2.460977000	2.553478000	0.856321000
C	-2.571921000	3.862461000	0.408626000
C	-1.418108000	4.522124000	-0.044503000
La	0.294553000	-0.083424000	-0.752673000
C	-1.112578000	0.487185000	1.354690000
N	1.165733000	1.853789000	0.416058000
C	2.119611000	2.142793000	1.357553000
C	3.346487000	1.413481000	1.386360000
C	4.321761000	1.711956000	2.341565000
C	4.161275000	2.710476000	3.305992000
C	2.947636000	3.410124000	3.288677000
C	1.956327000	3.139808000	2.356960000
P	3.528952000	0.079378000	0.121320000

C	4.733930000	0.870988000	-1.136590000
C	4.174512000	2.221924000	-1.581245000
C	5.240695000	3.023663000	4.308910000
C	-3.903884000	4.569088000	0.397201000
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C	2.403085000	-0.809225000	-3.970723000
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C	2.086212000	-2.225634000	-3.574292000
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C	-0.813779000	-0.455521000	-4.209317000
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C	-3.829166000	-1.933748000	-7.045969000
C	-3.888569000	-1.579530000	-1.614463000
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C	-4.456637000	-1.291246000	-0.223240000
P	0.888960000	-2.955649000	0.203030000
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C	-0.642438000	-5.175643000	-0.558222000

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C	-2.130712000	-5.388556000	1.774412000
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C	4.943903000	-2.332071000	-0.029554000
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H	-3.700878000	3.244886000	6.575237000

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