Supporting Information for:

Metal-Free σ-Bond Metathesis in Ammonia Activation by a Diazadiphosphapentalene

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I. Synthesis, physical and spectroscopic data for all new compounds

General Materials and Methods. All reactions were performed under an atmosphere of argon using standard Schlenk or dry box techniques; solvents were dried over Na metal or CaH_2. Reagents were purchased from commercial suppliers and used without further purification. ^{1}H, ^{13}C, ^{11}B, and ^{31}P NMR spectra were recorded with Bruker AVIII 400MHz BBFO, Bruker Avance 400 or JEOL ECA400 spectrometers at 298 K unless otherwise stated. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal, sept = septet. Coupling constants *J* are given in Hz. Electrospray ionization (ESI) mass spectra were obtained at the Mass Spectrometry Laboratory at the Division of Chemistry and Biological Chemistry, Nanyang Technological University. Melting points were measured with OptiMelt Stanford Research System. Compound **1** was prepared according to the literature procedures.[1]

Compound 2: A mixture of nBuLi (1.6 M in hexane, 40 ml, 64 mmol) and TMEDA (9.6 ml, 64 mmol) was added dropwise to a hexane solution (200 ml) of compound **1** (16.6 g, 64 mmol) at −78 °C. The mixture was warmed to room temperature and stirred overnight to give a white suspension. To the reaction mixture, PCl_3 (2.8 ml, 32 mmol) in hexane (100 ml) was added slowly at −78 °C, and then stirred overnight at room temperature. After removing salts by filtration, the filtrate was dried under vacuum to give light yellow oil which slowly solidified to afford **2** as a light yellow solid (64%).

2: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.05−7.04 (m, 4H, *m*-C*H*), 7.00−6.96 (m, 2H, *p*-C*H*), 2.86 (br d, $^{2}J_{P\text{-}H}$ = 12.8 Hz, 2H, CH_2), 2.61−2.52 (br m, 4H, C*H*Me$_2$), 2.29−2.06 (br m, 2H, CH_2), 1.22−1.17 (br m, 18H, C*Me*$_3$), 1.09−1.03 (br m, 12H, CH*Me*$_2$).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 172.4 (br, *C*=N), 145.8 (*ipso-C*), 135.3 (*o-C*), 123.2 (*p-C*), 122.7, (*m-C*), 41.0 (br, *C*Me$_3$), 39.2 (br d, $^{1}J_{P\text{-}C}$ = 47.3 Hz, *C*H$_2$), 28.8 (d, $^{4}J_{P\text{-}C}$ = 3.6 Hz, C*Me*$_3$), 28.6 (d, $^{4}J_{P\text{-}C}$ = 3.4 Hz, C*Me*$_3$), 28.4 (C*H*Me$_2$), 23.3 (CH*Me*$_2$), 21.3 (CH*Me*$_2$).

^{31}P NMR (162 MHz, $CDCl_3$): δ = 101.4.

HRMS (ESI): calcd for $[C_{36}H_{56}ClN_2P+H]^+$: 583.3948; found: 583.3954. M.p.: 58 °C.

Compound 3: A hexane solution (50 ml) of compound **2** (14.58 g, 25 mmol) was added to a suspension of $LiAlH_4$ (0.76 g, 20 mmol) in hexane (50 ml) at −78 °C. The reaction mixture was stirred at room temperature overnight. After filtration, the filtrate was dried under vacuum to give light yellow oil. The ^{31}P NMR of this oil showed a double at −80.0 ppm (d, $^1J_{P\text{-}H}$ = 196.0 Hz) in $CDCl_3$ indicating reduction of the P−Cl of **2** to P−H. The oil was used for next reaction without further purification. To a hexane solution (50 ml) of the oil (10.97 g, 20 mmol), BH_3 in THF (1.0 M, 20ml, 20 mmol) was added at room temperature. The reaction mixture was stirred at room temperature overnight. After removal of all volatiles under vacuum, the residue was washed with hexane (10 ml) to afford **3** as colorless solid (72%).

3: ^1H NMR (400 MHz, $CDCl_3$): δ = 7.07−7.01 (m, 6H, *Ar*), 4.48 (d, 1H, $^1J_{P\text{-}H}$ = 377.1 Hz, P*H*), 2.60−2.24 (br m, 8H, C*H*Me$_2$ and PC*H*$_2$), 1.22−1.20 (m, 12H, CH*Me*$_2$), 1.14 (br s, 18H, C*Me*$_3$,), 1.06 (d, *J* = 6.1 Hz, 6H, CH*Me*$_2$), 1.00 (d, *J* = 6.1 Hz, 6H, CH*Me*$_2$). Signal for B*H*$_3$ could not be detected, presumably due to the overlap with other peaks.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 170.0 (*C*=N), 145.2 (*o-C*), 135.9 (*ipso-C*), 134.0 (*o-C*), 123.9 (*p-C*), 123.2 (*m-C*), 122.7 (*m-C*), 41.4 (br, *C*Me$_3$), 28.8 (C*Me*$_3$), 28.3 (CH*Me*$_2$), 23.6 (CH*Me*$_2$), 23.3 (CH*Me*$_2$), 21.4 (CH*Me*$_2$), 20.9 (CH*Me*$_2$).

^{31}P {^1H} NMR (162 MHz, $CDCl_3$): δ = −15.1 (d, $^1J_{P\text{-}H}$ = 377.1 Hz).

^{11}B NMR (120 MHz, $CDCl_3$): δ = −38.6 (br).

HRMS (ESI): calcd for $[C_{36}H_{60}BN_2P+H]^+$: 563.4665; found: 563.4661. M.p.: 115 °C.

Compound 4: To a toluene solution (100 ml) of compound **3** (3.82 g, 6.8 mmol), KHMDS (1.36g, 6.8 mmol) was added at –78 °C. The reaction mixture was allowed to warm up slowly to room temperature and stirred for 4h. The reaction mixture was cooled to –78 °C, and then Et_3N (0.95 ml, 6.8 mmol) and PCl_3 (0.6 ml, 6.8 mmol) were added. The reaction mixture was warmed to room temperature and stirred overnight. After removal of the salts by filtration, all volatiles were removed under vacuum to give light yellow oil. Single crystals of **4** (49%) was obtained by recrystallization from pentane.

4 (major-*trans*): ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32−7.28 (m, 1H, *Ar*), 7.27−7.22 (m, 1H, *Ar*), 7.18−7.14 (m, 2H, *Ar*), 7.08−7.04 (m, 2H, *Ar*), 5.21 (dd, J_{P-H} = 42.0 and 3.5 Hz, 1H, *H*C=C), 3.63 (sept, *J* = 6.7 Hz, 1H, C*H*Me$_2$), 3.06 (t, *J* = 12.3 Hz, 1H, C*H*$_2$), 2.95 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 2.76 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 2.46 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 2.21 (d, *J* = 13.3 Hz, 1H, C*H*$_2$), 1.41 (s, 9H, C*Me*$_3$), 1.36 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.32 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.30 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.27 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.20 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.16 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 1.14 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 0.93 (d, *J* = 6.8 Hz, 3H, CH*Me*$_2$), 0.87 (s, 9H, C*Me*$_3$).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 174.8 (dd, J_{P-C} = 9.7 and 6.2 Hz, *C*=N), 166.8 (dd, J_{P-C} = 11.1 and 4.6 Hz, C=*C*–N), 148.6 (d, J_{P-C} = 3.8 Hz, *o-C*), 148.5 (d, J_{P-C} = 5.5 Hz, *o-C*), 146.8 (*ipso–C*), 139.1 (dd, J_{P-C} = 16.0 and 1.9 Hz, *ipso–C*), 135.7 (*o-C*), 134.8 (*o-C*), 128.8 (d, J_{P-C} = 2.5 Hz, *m-C*), 125.0 (d, J_{P-C} = 2.3 Hz, *m-C*), 123.9 (d, J_{P-C} = 1.0 Hz, *p-C*), 123.3 (*p-C*), 123.1 (*m-C*), 122.8 (*m-C*), 104.2 (dd, J_{P-C} = 32.7 and 3.3 Hz, *C*=C–N), 41.2 (*C*Me$_3$), 37.1 (*C*Me$_3$), 31.2 (C*Me*$_3$), 30.4 (C*Me*$_3$), 29.1 (d, J_{P-C} = 5.4 Hz, *C*HMe$_2$), 29.0 (*C*HMe$_2$), 28.6 (C*Me*$_3$ and *C*HMe$_2$), 28.4 (C*Me*$_3$), 27.6 (d, J_{P-C} = 2.3 Hz, CH*Me*$_2$), 27.4 (*C*HMe$_2$), 27.0 (d, J_{P-C} = 4.9 Hz, CH*Me*$_2$), 25.3 (dd, J_{P-C} = 38.6 and 19.7 Hz, *C*H$_2$), 23.5 (CH*Me*$_2$), 23.2 (CH*Me*$_2$), 22.8 (CH*Me*$_2$), 22.2(CH*Me*$_2$), 21.7 (CH*Me*$_2$), 21.2 (CH*Me*$_2$).

^{31}P NMR (162 MHz, $CDCl_3$): δ = 160.4 (dd, $^{1}J_{P-P}$ = 273.2 and $^{2}J_{P-H}$ = 9.3 Hz, P*P*N), –19.1 (dd, $^{1}J_{P-P}$ = 273.3 and $^{2}J_{P-H}$ = 42.0 Hz, *P*C).

HRMS (ESI): calcd for $[C_{36}H_{55}ClN_2P_2+H]^+$: 613.3607; found: 613.3604. M.p.: 157 °C.

4 (minor-*cis*): (only detected in ^{31}P NMR); ^{31}P NMR (162 MHz, $CDCl_3$): δ = 203.7 (dd, $^{1}J_{P-P}$ = 219.8 and $^{2}J_{P-H}$ = 8.9 Hz, P*P*N), 0.2 (dd, $^{1}J_{P-P}$ = 219.8 and $^{2}J_{P-H}$ = 25.2 Hz, *P*C).

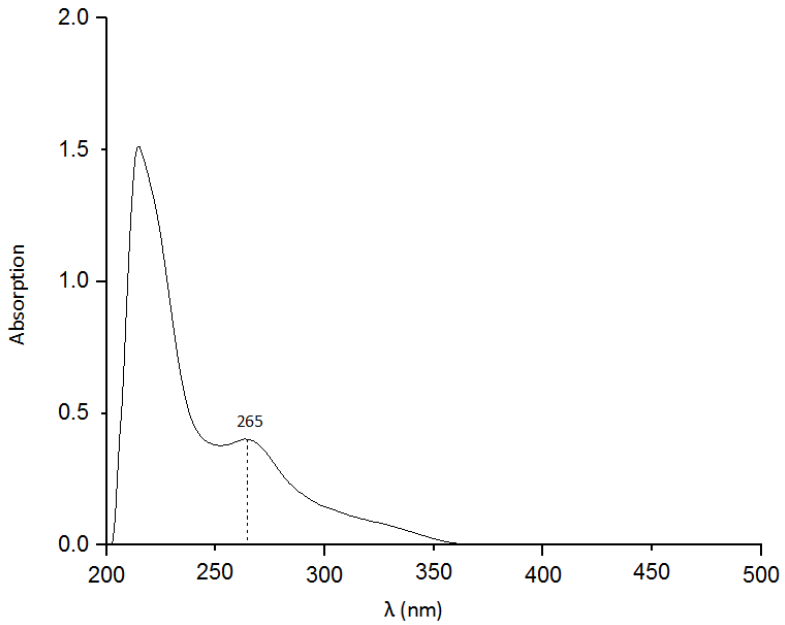
Compound 5: To a toluene solution (100 ml) of compound **4** (3.80 g, 6.19 mmol), KHMDS (1.24 g, 6.19 mmol) was added at –78 °C. The reaction mixture was allowed to warm up slowly to room temperature, and stirred overnight. After salts were filtered off, all volatiles were removed under vacuum. The residue was washed with pentane and dried under vacuum to afford **5** as a slightly yellowish white solid (67%).

5: ^{1}H NMR (400 MHz, C_6D_6): δ = 7.08 (t, *J* = 7.6 Hz, 2H, *p-Ar*), 7.01 (d, *J* = 7.6 Hz, 2H, *m-Ar*), 6.95 (d, *J* = 7.6 Hz, 2H, *m-Ar*), 5.58 (dd, J_{P-H}= 40.6 and 6.2 Hz, 1H, C=C*H*), 3.49, (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 3.26 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 1.28 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.25 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.23 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 0.98 (s, 18H, C*Me*$_3$), 0.85 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$). ^{13}C NMR (100 MHz, C_6D_6): δ = 165.7 (dd, J_{P-C} = 6.1, 2.2 Hz, ^{t}Bu*C*), 149.7 (d, J_{P-C} = 3.6 Hz, *o-C*), 148.6 (d, J_{P-C} = 2.9 Hz, *o-C*), 141.3 (dd, J_{P-C} = 14.2 and 1.5 Hz, *ipso-C*), 128.0 (*p-C*), 125.0 (d, J_{P-C} = 1.2 Hz, *m-C*), 124.7 (d, J_{P-C} = 1.9 Hz, *m-C*), 100.6 (br d, J_{P-C} = 30.6 Hz, *C*H=C^{t}Bu), 37.6 (dd, J_{P-C} = 3.5 and 0.9 Hz, *C*Me$_3$), 32.8 (C*Me*$_3$), 28.7 (*C*HMe$_2$), 28.2 (br t, J_{P-C} = 4.0 Hz, CH*Me*$_2$), 27.8 (dd, J_{P-C} = 9.1 and 1.4 Hz, *C*HMe$_2$), 24.5 (CH*Me*$_2$), 24.4 (CH*Me*$_2$), 23.4(CH*Me*$_2$).

^{31}P NMR (162 MHz, C_6D_6): δ = 173.2 (d, $^{1}J_{P-P}$ = 195.4 Hz, N*P*N), –30.8 (dd, $^{1}J_{P-P}$ = 195.4 and $^{2}J_{P-H}$ = 40.6 Hz, C*P*C).

HRMS (ESI): calcd for $[C_{36}H_{54}N_2P_2+H]^+$: 577.3840; found: 577.3848. M.p.: 124 °C.

UV-Vis spectrum of 5



UV-Vis absorption of compound **5** (10^{-5} mol/L in THF at 25 °C)

A broad absorption band with maximum of 265 nm corresponds to the HOMO-LUMO transition, which reasonably agrees with theoretical result; $\Delta E_{(HOMO-LUMO)}$ = 4.168 eV ≈ 268 nm.

Reaction of compound 5 with NH_3: To a degassed solution of compound **5** (144 mg, 0.25 mmol) in THF (20 ml), NH_3 gas was introduced at room temperature at 1atm. The reaction mixture was stirred at room temperature for 16 h. After all volatiles were removed under vacuum, the residual colorless oil was washed with pentane to afford **6** as a light brown powder (74%).

6: ^{1}H NMR (400 MHz, C_6D_6): δ = 7.32−7.09 (m, 6H, *Ar*), 5.30 (d, $^2J_{P\text{-}H}$ = 23.0 Hz, 1H, *H*C=CN), 4.95 (s, 1H, *H*N(Ar)C=CH), 4.63 (b, 1H, HN(Ar)C=C*H*), 3.99 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 3.56 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 3.40 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 3.25 (sept, *J* = 6.8 Hz, 1H, C*H*Me$_2$), 2.73 (br, 2H, N*H*$_2$), 1.61−1.33 (m, 18H, CH*Me*$_2$), 1.32 (s, 9H, C*Me*$_3$), 1.26−1.18 (m, 6H, CH*Me*$_2$), 1.04 (s, 9H, C*Me*$_3$).

^{13}C NMR (100 MHz, C_6D_6): δ = 162.0 (dd, $J_{P\text{-}C}$ = 12.6 and 4.3 Hz, ^{t}Bu*C*=C), 158.6 (dd, $J_{P\text{-}C}$ = 14.1 and 7.0 Hz, ^{t}Bu*C*$_{ring}$=C), 149.6 (d, $J_{P\text{-}C}$ = 4.1 Hz, *o-C*), 148.5 (d, $J_{P\text{-}C}$ = 7.4 Hz, *ipso–C*), 146.5 (d, $J_{P\text{-}C}$ = 3.0 Hz, *o-C*), 146.2 (*o-C*), 142.6 (dd, $J_{P\text{-}C}$ = 19.4 and 5.5 Hz, *ipso–C*), 136.7 (d, $J_{P\text{-}C}$ = 3.3 Hz, *o-C*), 127.8 (*p-C*), 126.9 (d, $J_{P\text{-}C}$ = 1.8 Hz, *p-C*), 124.4 (d, $J_{P\text{-}C}$ = 1.6 Hz, *m-C*), 123.5 (br, *m-C* x2), 123.4 (*m-C*), 104.9 (d, $J_{P\text{-}C}$ = 20.4 Hz, ^{t}BuC$_{ring}$=*C*H), 76.2 (d, $J_{P\text{-}C}$ = 33.6 Hz, ^{t}BuC=*C*H), 37.9 (d, $J_{P\text{-}C}$ = 3.9 Hz, *C*Me$_3$), 36.4 (*C*Me$_3$), 30.9 (C*Me*$_3$), 29.8 (C*Me*$_3$), 29.0 (br, *C*HMe$_2$), 28.8 (dd, $J_{P\text{-}C}$ = 4.2 and 2.4 Hz, CH*Me*$_2$), 28.7(*C*HMe$_2$), 28.6 (*C*HMe$_2$), 27.9 (d, *J* = 4.2 Hz, *C*HMe$_2$), 26.3 (d, $J_{P\text{-}C}$ = 5.6 Hz, CH*Me*$_2$), 25.4 (CH*Me*$_2$), 25.3 (CH*Me*$_2$), 23.3 (CH*Me*$_2$), 22.2 (d, $J_{P\text{-}C}$ = 3.4 Hz, CH*Me*$_2$), 22.1 (d, $J_{P\text{-}C}$ = 8.4 Hz, CH*Me*$_2$), 21.9 (CH*Me*$_2$).

^{31}P NMR (162 MHz, C_6D_6): δ = 108.9 (d, $^1J_{P\text{-}P}$ = 253.4 Hz, P*P*N), –40.1 (dd, $^1J_{P\text{-}P}$ = 253.4 and $^2J_{P\text{-}H}$ = 22.2 Hz, *P*C).

HRMS (ESI): calcd for $[C_{36}H_{57}N_3P_2+H]^+$: 594.4106; found: 594.4061. M.p.: 116 °C.

Isomerization of compound 6 to 7: Compound **6** was dissolved (0.25 mmol) in THF (10ml) and the solution was stirred at room temperature. Reaction was monitored by ^{31}P NMR. After the solvent was removed under vacuum, the oil residue was washed with acetonitrile, and then dried under vacuum to afford crude **7** as a white powder (crude yield: 81%), containing a slight amount of **8** due to the further isomerization.

7: ^{1}H NMR (400 MHz, C_6D_6): δ = 7.12−6.93 (m, 6H, *Ar*), 4.56 (d, $^{2}J_{P\text{-}H}$ = 21.9 Hz, 1H, *H*C=C), 3.61 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 3.33 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 3.07 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 2.98 (br t, *J* = 11.1 Hz, 1H, C*H*$_2$), 2.91 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 2.41 (dd, *J* = 13.0 and 3.9 Hz, 1H, C*H*$_2$), 1.94 (dd, 2H, $J_{P\text{-}H}$ = 10.1 and 3.7 Hz, N*H*$_2$), 1.36 (s, 9H, C*Me*$_3$), 1.30−1.10 (br m, 24H, CH*Me*$_2$), 0.78 (s, 9H, C*Me*$_3$).

^{13}C NMR (100 MHz, C_6D_6): δ = 177.1 (d, $J_{P\text{-}C}$ = 12.7 Hz, *C*=N), 160.7 (dd, $J_{P\text{-}C}$ = 12.0 and 7.9 Hz, ^{t}Bu*C*=C), 149.3 (d, $J_{P\text{-}C}$ = 4.4 Hz, o–*C*), 148.0 (*o*-*C*), 146.4 (d, $J_{P\text{-}C}$ = 3.2 Hz, *ipso*–*C*), 141.4 (dd, $J_{P\text{-}C}$ = 19.8 and 5.9 Hz, *ipso*–*C*), 136.0 (*o*-*C*), 135.2 (*o*-*C*), 127.5 (*p*–*C*), 124.6 (*p*-*C*), 123.8 (*m*-*C*), 123.6 (*m*-*C*), 123.3 (*m*-*C*), 123.1 (*m*-*C*), 101.9 (dd, $J_{P\text{-}C}$ = 28.8 and 4.4 Hz, H*C*=C), 41.4 (*C*Me$_3$), 36.6 (*C*Me$_3$), 30.7 (C*Me*$_3$), 29.0 (m, *C*HMe$_2$), 28.8 (C*Me*$_3$), 28.7 (br m, CH*Me*$_2$), 28.6 (br, *C*HMe$_2$), 28.3 (br m, *C*HMe$_2$), 28.1 (br m, C*H*Me$_2$), 26.3 (d, $J_{P\text{-}C}$ = 5.3 Hz, CH*Me*$_2$), 23.8 (CH*Me*$_2$), 23.5 (CH*Me*$_2$), 23.2 (CH*Me*$_2$), 22.0 (CH*Me*$_2$), 21.8 (d, $J_{P\text{-}C}$ = 3.6 Hz, CH*Me*$_2$), 21.4 (CH*Me*$_2$), 19.3 (d, $J_{P\text{-}C}$ = 40.5 Hz, *C*H$_2$).

^{31}P NMR (162 MHz, C_6D_6): δ = 106.1 (d, $^{1}J_{P\text{-}P}$ = 241.0 Hz, P*P*N), –28.2 (dd, $^{1}J_{P\text{-}P}$ = 241.0 and $^{2}J_{P\text{-}H}$ = 21.9 Hz, *P*C).

HRMS (ESI): calcd for $[C_{36}H_{57}N_3P_2+H]^+$: 594.4106; found: 594.4108.

Isomerization of compound 7 to 8: Compound **7** was dissolved (0.25 mmol) in THF (10ml) and the solution was stirred at room temperature. Reaction was monitored by ^{31}P NMR. After the solvent was removed under vacuum, the residue was recrystallized from hexane solution to afford **8** as a light yellow solid (46%).

8: ^{1}H NMR (400 MHz, C_6D_6): δ = 7.27 (dd, *J* = 6.9 and 1.2 Hz, 1H, *m*-*Ar*), 7.19 (dd, 7.6 and 1.2 Hz, 1H, *m*-*Ar*), 7.13−7.09 (m, 2H, *p*-*Ar*), 7.06 (dd, 7.6 and 1.6 Hz, 1H, *m*-*Ar*), 6.94 (dd, 7.6 and 1.6 Hz, 1H, *m*-*Ar*), 4.91 (dd, $J_{P\text{-}H}$ = 39.4 and 4.8 Hz, 1H, *H*C=CN), 3.72 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 3.38 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 3.26 (td, *J* = 12.8 and 2.8 Hz, 1H, C*H*$_2$), 2.95 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 2.73 (sept, *J* = 6.9 Hz, 1H, C*H*Me$_2$), 2.41 (dt, *J* = 12.8 and 2.8 Hz, 1H, C*H*$_2$), 2.22 (dd, $J_{P\text{-}H}$ = 18.0 and 6.4 Hz, 2H, N*H*$_2$), 1.50 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.44 (s, 9H, C*Me*$_3$), 1.40 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.36 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.24 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.23 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.17 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.08 (d, *J* = 6.9 Hz, 3H, CH*Me*$_2$), 1.05 (d, *J* = 6.9 Hz,

3H, CH*Me*$_2$), 0.86 (s, 9H, C*Me*$_3$).

^{13}C NMR (100 MHz, C_6D_6): δ = 176.6 (m, *C*=N), 166.5 (m, C=*C*–N), 149.0 (d, $J_{P\text{-}C}$ = 3.9 Hz, *o*-*C*), 148.0 (d, $J_{P\text{-}C}$ = 3.1 Hz, *o*-*C*), 147.7 (*ipso*–*C*), 141.7 (d, $J_{P\text{-}C}$ = 14.3 Hz, *ipso*–*C*), 136.3 (*o*-*C*), 134.9 (*o*-*C*), 127.6 (d, $J_{P\text{-}C}$ = 1.9 Hz, *p*-*C*), 124.4 (d, $J_{P\text{-}C}$ = 1.9 Hz, *m*-*C*), 124.1 (d, $J_{P\text{-}C}$ = 1.4 Hz, *m*-*C*), 123.6 (*p*-*C*), 123.4 (*m*-*C*), 123.0 (*m*-*C*), 97.5 (d, $J_{P\text{-}C}$ = 26.3 Hz, *C*=C–N), 41.1 (*C*Me$_3$), 37.1 (d, $J_{P\text{-}C}$ = 2.4 Hz, *C*Me$_3$), 31.6 (C*Me*$_3$), 29.5 (d, *J* = 6.0 Hz, *C*HMe$_2$), 28.8 (CH*Me*$_2$), 28.7 (d, *J* = 1.7 Hz, *C*HMe$_2$ x2), 28.7 (C*Me*$_3$), 27.4 (*C*HMe$_2$), 27.2 (d, *J* = 2.7 Hz, CH*Me*$_2$), 27.0 (d, *J* = 5.6 Hz, CH*Me*$_2$), 26.7 (dd, $J_{P\text{-}C}$ = 35.7 and 20.7 Hz, *C*H$_2$), 23.7 (d, *J* = 3.2 Hz, CH*Me*$_2$), 22.8 (CH*Me*$_2$), 22.4 (CH*Me*$_2$), 22.1 (CH*Me*$_2$), 21.5 (d, *J* = 1.8 Hz, CH*Me*$_2$).

^{31}P NMR (162 MHz, C_6D_6): δ = 90.6 (d, $^1J_{P\text{-}P}$ = 218.0 Hz, P*P*N), –32.7 (dm, $^1J_{P\text{-}P}$ = 218.0 Hz, *P*C).

HRMS (ESI): calcd for $[C_{36}H_{57}N_3P_2+H]^+$: 594.4106; found: 594.4110. M.p.: 123 °C.

II. Crystallographic Procedure and Data

Intensity data for all compounds was collected using a Bruker APEX II diffractometer. The structure was solved by direct phase determination (SHELXS-97) and refined for all data by full-matrix least squares methods on F^2.[2] All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were generated geometrically and allowed to ride in their respective parent atoms; they were assigned appropriate isotropic thermal parameters and included in the structure-factor calculations. CCDC- 1021264-1021270 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Single crystals of compound **7** were obtained as co-crystals with **8** as a disorder because of the isomerization from **7** to **8** during recrystallization.

Table S1. X-ray data for compounds **2**, **3**, and **4**.

Compounds	**2**	**3**	**4**
Formula	C36H56ClN2P	C36H60BN2P	C36H55ClN2P2
Fw	583.24	562.64	613.21
T/K	103(2)	103(2)	103(2)
Size (mm^3)	0.100 x 0.400 x 0.420	0.240 x 0.260 x 0.410	0.200 x 0.380 x 0.420
Cryst syst	monoclinic	monoclinic	monoclinic
Space group	P 1 21/n 1	P 1 21/c 1	P 1 21/c 1
a, Å	15.829(8)	16.3011(11)	19.1008(13)
b, Å	12.119(6)	12.2497(7)	9.3723(6)
c, Å	19.547(10)	19.4830(9)	20.0296(15)
α, deg	90	90	90
β, deg	113.612(6)	113.7205(18)	101.868(3)
γ, deg	90	90	90
V, A^3	3436.(3)	3561.8(4)	3509.0(4)
Z	4	4	4
d_{calcd} g·cm-3	1.128	1.049	1.161
μ, mm^{-1}	0.184	0.102	0.226
Refl collected	25922	51768	40141
Indepen. refl	6609	10878	11730
[R int]	0.0879	0.0711	0.1144
T_{max}/ T_{min}	0.9820/0.9270	0.9760/0.9590	0.9560/0.9110
R1 (I>2σ(I))	0.0873	0.0641	0.0638
wR2 (I>2σ(I))	0.232	0.1578	0.1457
GOF	1.119	1.038	1.034
Largest diff. peak/ hole[e. $Å^{-3}$]	0.981/-0.717	0.744/-0.466	1.188/-0.676

Table S2. X-ray data for compounds **5**, **6**, **7** and **8**.

Compounds	**5**	**6**	**7(&8)**	**8**
Formula	C36H54N2P2	C36H57N3P2	C36H57N3P2	C36H57N3P2
Fw	576.75	593.78	593.78	593.78
T/K	296(2)	296(2)	103(2)	173(2)
Size (mm^3)	0.120 x 0.380 x 0.400	0.140 x 0.200 x 0.400	0.060 x 0.120 x 0.400	0.220 x 0.280 x 0.360
Cryst syst	monoclinic	monoclinic	triclinic	triclinic
Space group	P 1 21/c 1	P 1 21/c 1	P -1	P -1
a, Å	17.287(4)	12.9755(6)	9.5581(18)	9.7159(7)
b, Å	11.975(3)	16.0657(7)	13.979(3)	12.9229(10)
c, Å	18.283(4)	17.3774(7)	14.962(3)	16.3051(16)
α, deg	90	90	114.231(8)	67.064(6)
β, deg	114.7164(18)	90.158(3)	90.678(8)	81.934(6)
γ, deg	90	90	95.787(8)	70.631(5)
V, A^3	3438.1(14)	3622.5(3)	1810.6(6)	1778.5(3)
Z	4	4	2	2
d_{calcd} $g \cdot cm^{-3}$	1.114	1.089	1.089	1.109
μ, mm^{-1}	0.152	0.147	0.147	0.149
Refl collected	27336	52945	41401	23044
Indep. Refl.	10402	7257	7231	8054
[R int]	0.0745	0.1778	0.1671	0.1002
T_{max}/T_{min}	0.9820/0.9420	0.9800/0.7200	0.9910/0.9440	0.9480/0.9680
R1 (I>2σ(I))	0.0582	0.0807	0.0722	0.0979
wR2 (I>2σ(I))	0.1184	0.1498	0.1991	0.2259
GOF	0.968	1.020	0.970	1.061
Largest diff. peak/hole[e. $Å^{-3}$]	0.244/-0.227	0.270/-0.391	0.263/-0.284	0.418/-0.513

III. Kinetics studies.

Eying Kinetics

In a J-Young NMR tube, compound **5** was mixed with a saturated THF solution of NH_3 (excess). The reaction was monitored by $^{31}P\{^1H\}$ NMR spectroscopy at fixed intervals over the a temperature range from 0 to 50 °C. Based on the integration of compound **5** (Ph_3P was employed as an internal standard), the concentration of **5** was plotted against time which followed first-order kinetics, and provided the reaction rate k_{obs} at each temperature (Table S3). Eyring plot (Figure S1) was obtained based on the rate at each temperature and plotted against inverse of time.

Table S3. Eyring data.

Temp (K)	1/T	k_{obs} （S^{-1}）	ln(k/T)
273.15	0.003660992	0.00001385	-16.797246420
283.15	0.003531697	0.00003896	-15.798951872
293.15	0.003411223	0.00006237	-15.363110591
303.15	0.003298697	0.00015975	-14.456128197
313.15	0.003193358	0.00032071	-13.791655579
323.15	0.003094538	0.00101672*	-12.669290131

***** For the reaction at 50 °C, a NH_3 solution diluted to 1/4 concentration from the original saturated solution was used. The reaction analysis gave a k_{obs}' value of 0.00025418 S^{-1}. The k_{obs} (0.00101672 S^{-1}) was then obtained from the calculation of k_{obs}' x 4.

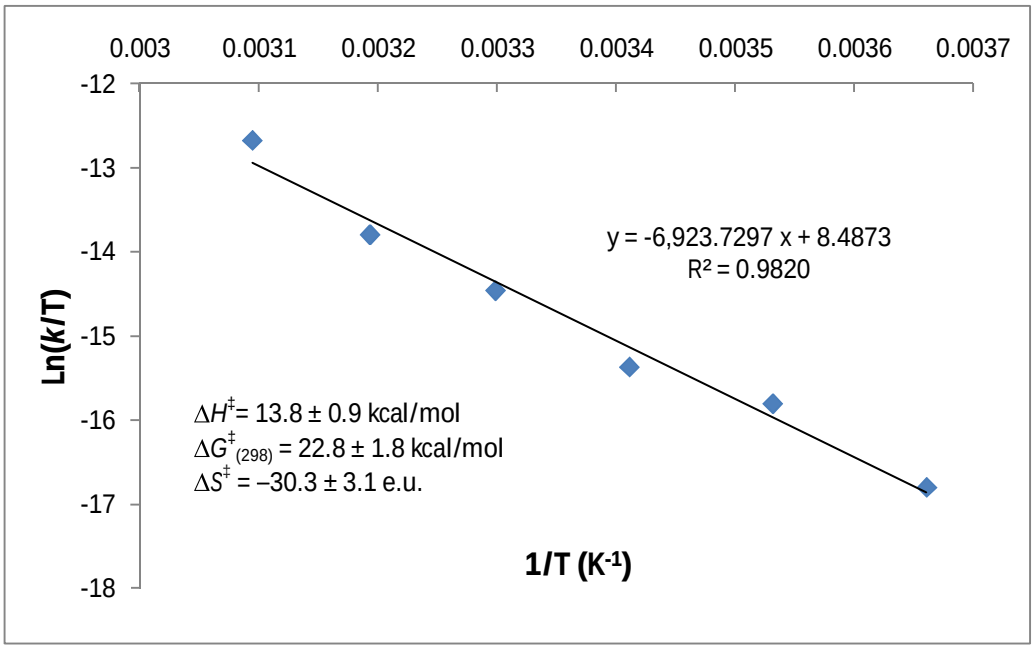


Figure S1. Plot of Ln(k/T) vs 1/T for the reaction of **5** and NH_3.

Reaction order of NH_3

In a J-Young NMR tube, compound **5** was mixed with THF solutions of varying concentrations of NH_3 (0.08 – 0.40 M, 9.4 – 48.2 equiv.). $^{31}P\{^1H\}$ spectra were measured at 450 second intervals over the course of 50% conversion at 40 °C (313.15K). Ph_3P was employed as an internal standard.

Table S4. Effect of NH_3 concentration on observed rate.

5 (mg)	[**5**] (M)	$[NH_3]$ (M)	$[NH_3]^2$ (M^2)	$[NH_3]^3$ (M^3)	k_{obs} (S^{-1})
12.0	0.0083	0.4000	0.1600	0.064000	0.00036827
14.8	0.0103	0.3200	0.1024	0.032768	0.00032269
14.4	0.0100	0.2400	0.0576	0.013824	0.00029018
11.5	0.0080	0.1600	0.0256	0.004096	0.00025010
12.3	0.0085	0.0800	0.0064	0.000512	0.00021908

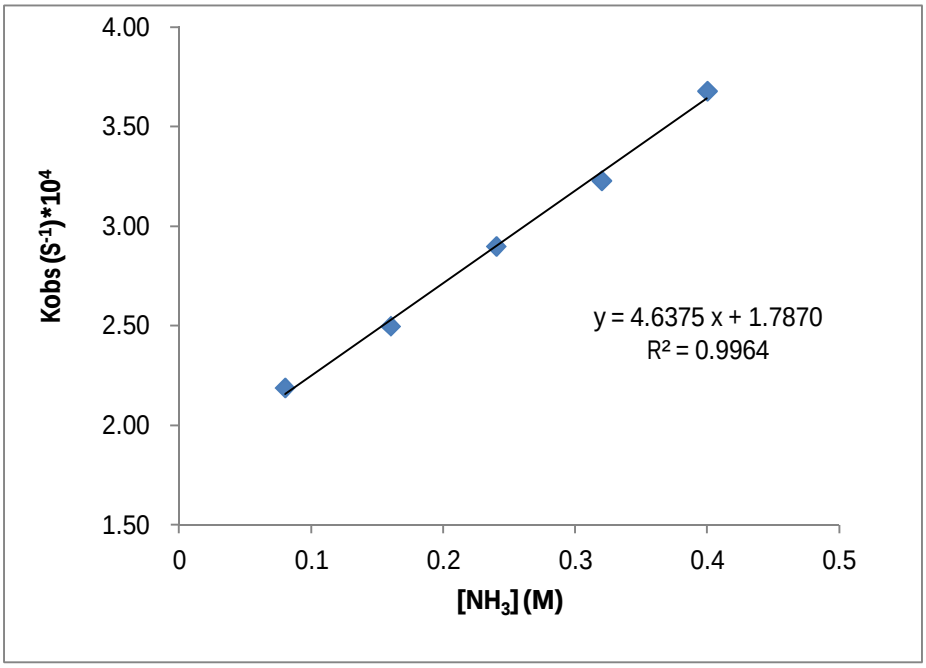


Figure S2. Plot of k_{obs} vs $[NH_3]$ with attempted linear fit.

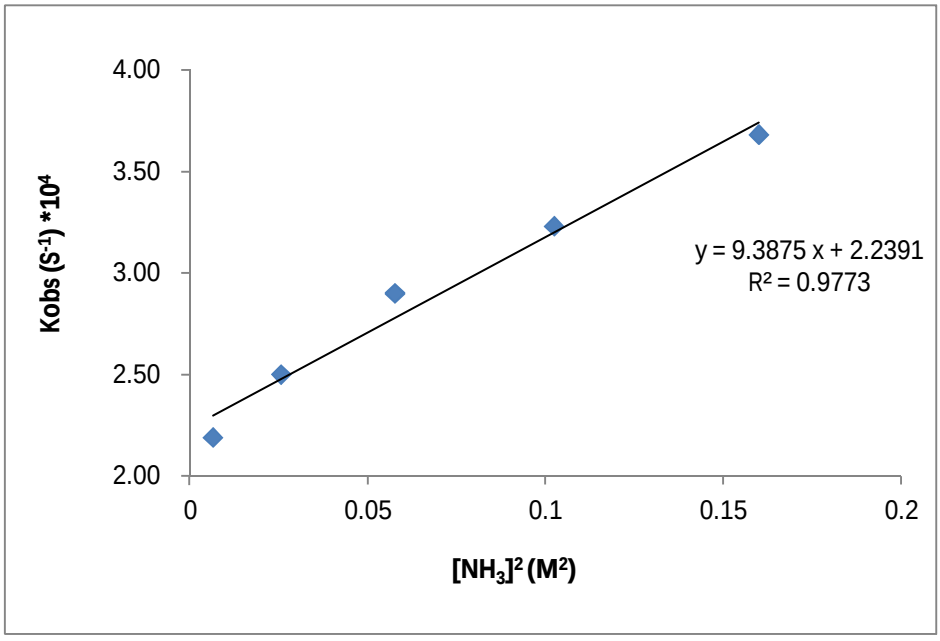


Figure S3. Plot of k_{obs} vs $[NH_3]^2$ with attempted linear fit.

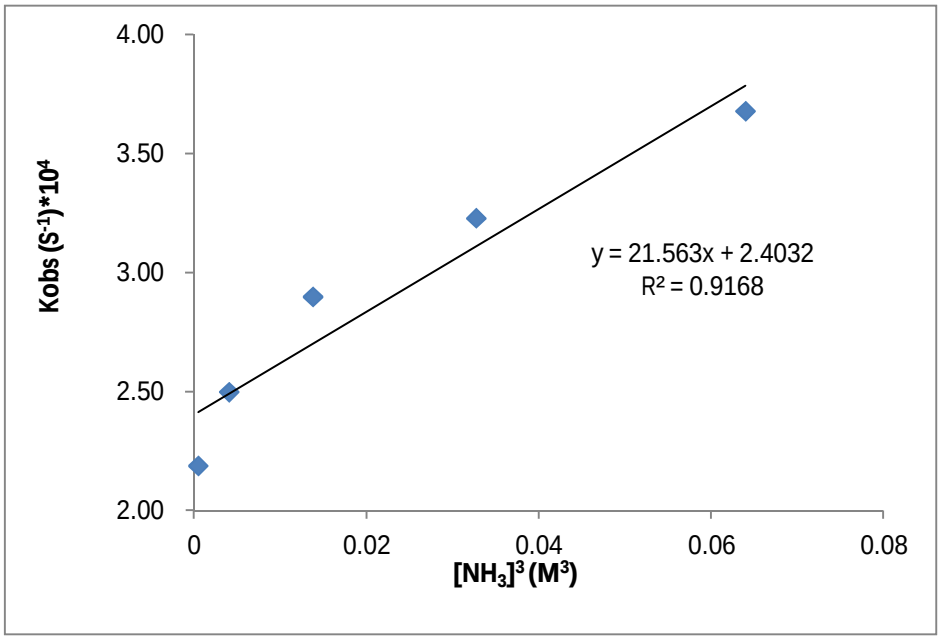


Figure S4. Plot of k_{obs} vs $[NH_3]^3$ with attempted linear fit.

IV. DFT Calculation

Method[3,4]

Gaussian 09 was used for density functional theory (DFT) calculations with the B3LYP functional.[3,4] Two basis sets, B1 and B2 were used for geometry optimization and refined energy evaluation, respectively. B1 utilizes the 6-311+G(d,p) basis set for the heavy atoms in the bicycle moiety and NH_3 and the 6-31G(d) basis set for the remaining atoms. B2 designates the 6-311+G(d,p) basis set used for all atoms.[5] The B3LYP/B1 calculations yielded free energy correction values (G_{corr}) for all species. The optimized geometries were subsequently subjected to single-point energy calculations at the B3LYP/6-311+G(d,p) (i.e., B3LYP/B2) level with the solvent effect of tetrahydrofuran included using a self-consistent reaction field (SCRF) method called IEFECM.[6] These single-point energy calculations yielded energy values (E(B2)) of all species. Furthermore, dispersion correction (E_{disp}) was estimated using the DFT-D3 method with Becke-Johnson (BJ) damping.[7] The following quantity G was used to evaluate the relative stability of different species.

$$G = E(B2) + G_{corr} + E_{disp}$$

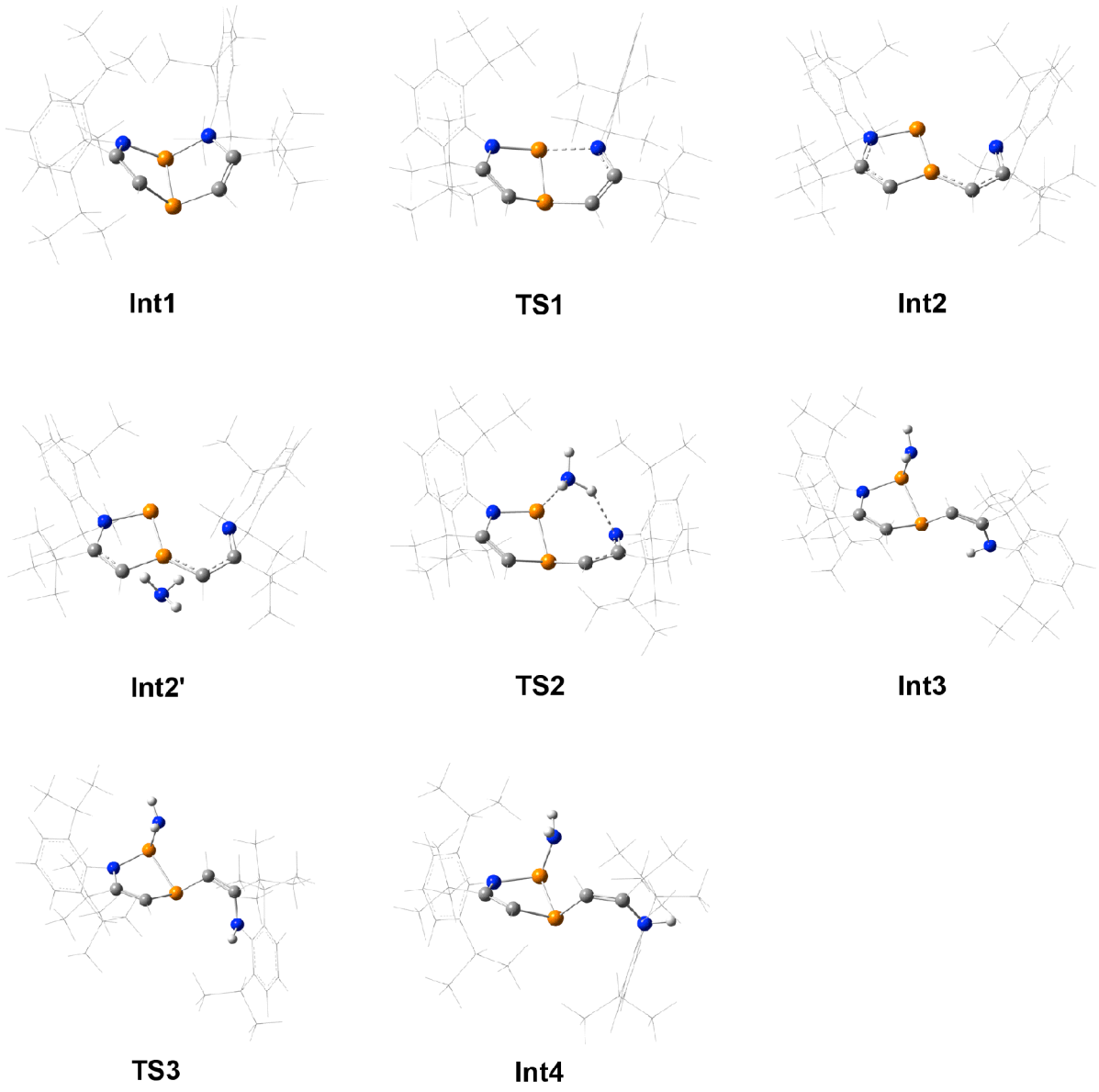


Figure S5. Optimized geometries (from **Int1** to **Int4**).

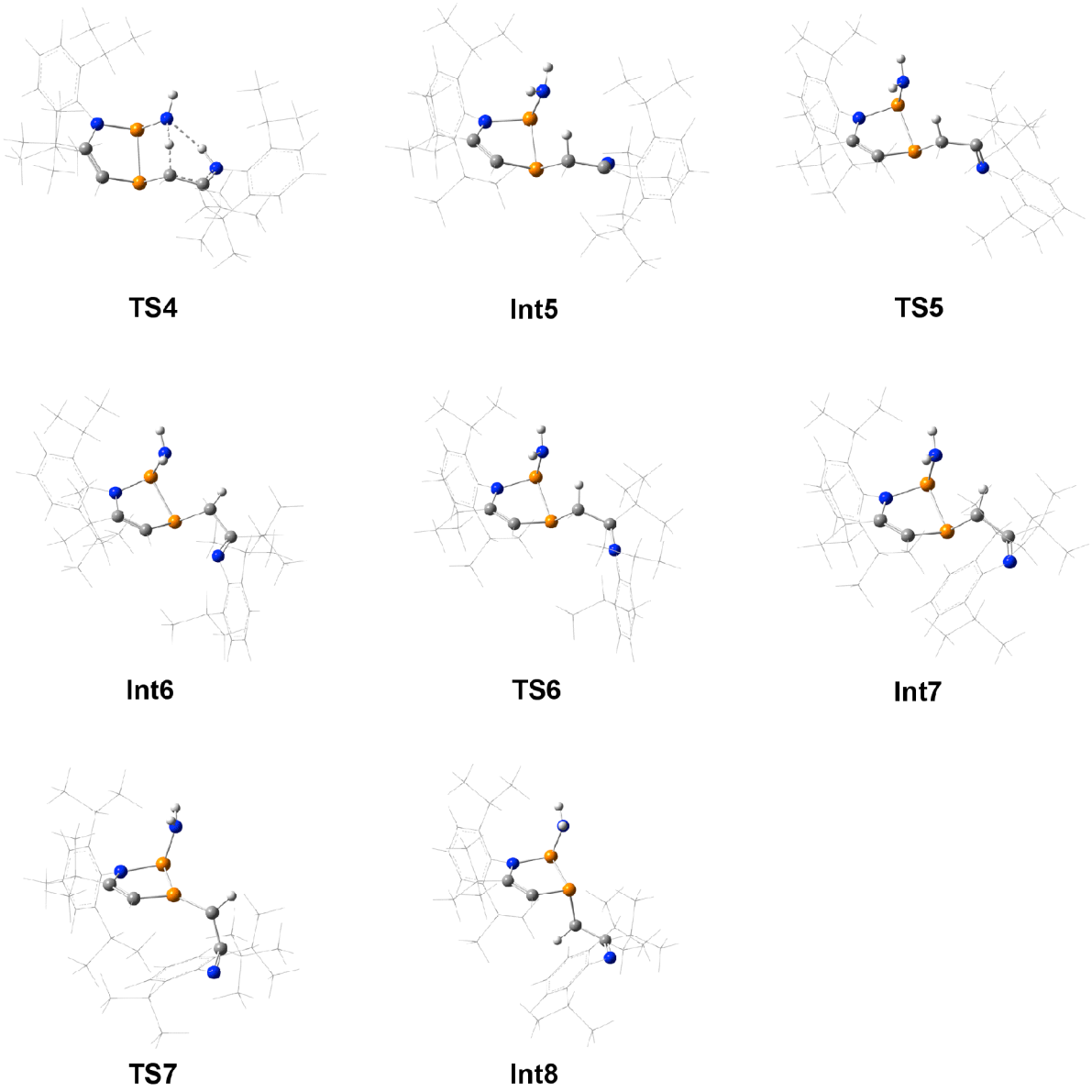


Figure S6. Optimized geometries (from **TS4** to **Int8**).

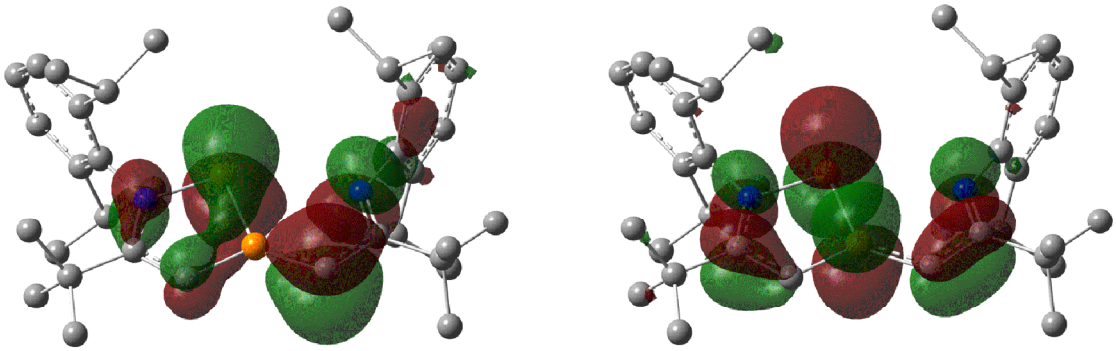


Figure S7. HOMO and LUMO of **Int2** obtained at the B3LYP/B1 level.

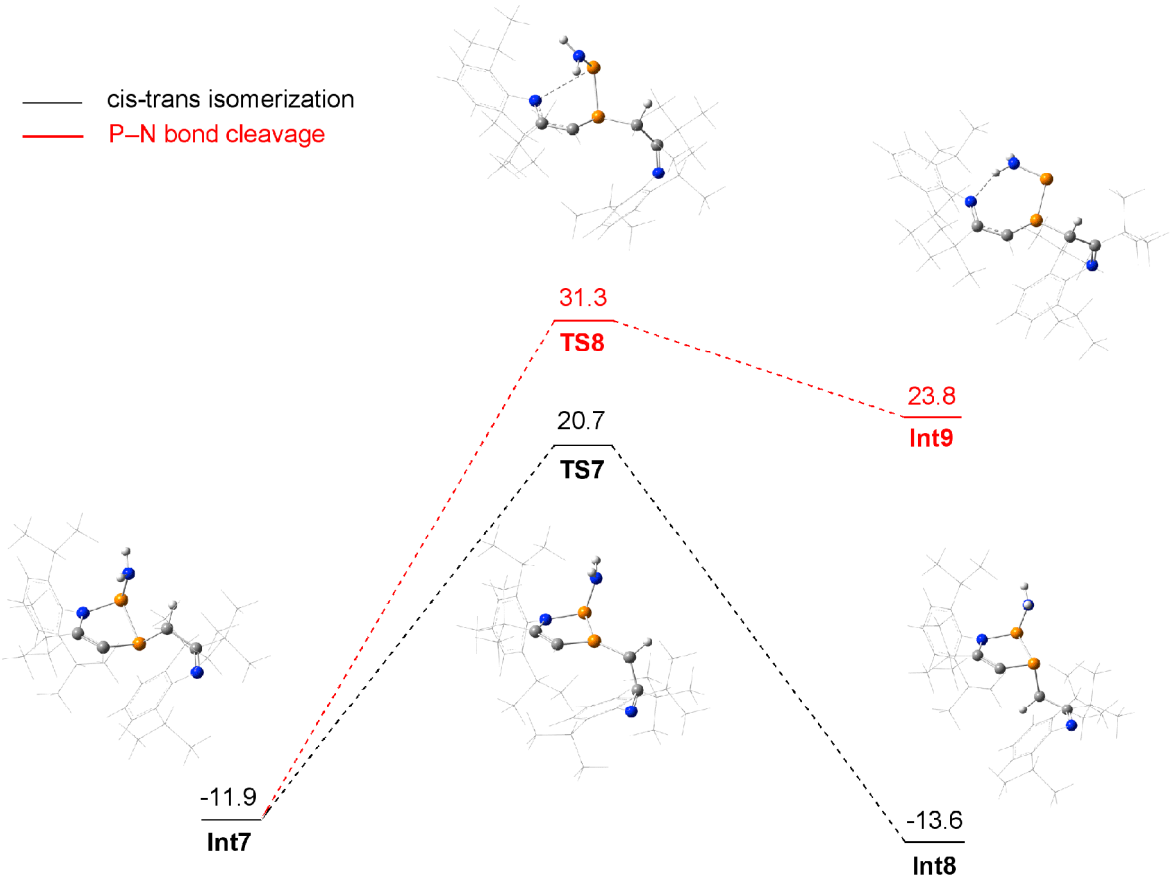


Figure S8. P–N cleavage pathway from **Int7** and its comparison with the cis-trans isomerization pathway. Energy values are given in kcal mol^{-1}.

Table S5. Raw energy data

	E(B1) [au]	E(B2) [au]	ZPE [au]	Gcorr [au]	Edisp [au]	ΔG [kcal/mol]
Int1 + NH_3	-2253.214285	-2253.570019	0.863843	0.771226	-0.261350	0.0
TS1 + NH_3	-2253.196647	-2253.548349	0.861690	0.768272	-0.251518	17.9
Int2 + NH_3	-2253.212942	-2253.568296	0.862074	0.765374	-0.240759	10.3
Int2’	-2253.215891	-2253.573098	0.862954	0.776170	-0.244779	11.6
TS2	-2253.186293	-2253.544300	0.863953	0.784714	-0.255557	28.2
Int3	-2253.243805	-2253.597930	0.866813	0.785001	-0.249134	-1.2
TS3	-2253.230162	-2253.585935	0.866184	0.787025	-0.249068	7.6
Int4	-2253.247219	-2253.601704	0.865830	0.784110	-0.251463	-5.6
TS4	-2253.195150	-2253.549600	0.862048	0.782238	-0.251269	26.0
Int5	-2253.249406	-2253.604800	0.865880	0.785105	-0.250633	-6.4
TS5	-2253.245183	-2253.601069	0.865559	0.786803	-0.248814	-1.8
Int6	-2253.248515	-2253.603677	0.866032	0.785040	-0.249200	-4.8
TS6	-2253.230634	-2253.586949	0.864218	0.782732	-0.245512	6.5
Int7	-2253.258265	-2253.611211	0.865900	0.783645	-0.251521	-11.9
TS7	-2253.209150	-2253.563480	0.865032	0.785873	-0.249597	20.7
Int8	-2253.260772	-2253.613845	0.866139	0.784886	-0.252861	-13.6
TS8	-2253.188117	-2253.542781	0.863560	0.781917	-0.249428	31.3
Int9	-2253.202968	-2253.558409	0.865222	0.783227	-0.247106	23.8

XYZ Coordinates of Optimized Geometries

=== **NH3** ===

N	0.481505	-3.126616	3.924589
H	-0.447485	-3.492759	4.104832
H	1.134227	-3.902913	3.953699
H	0.490188	-2.746430	2.984114

=== **Int1** ===

C	3.523003	-1.975785	2.431942
C	3.394297	-0.799002	1.431756
C	4.048037	0.424179	2.108515
C	4.248785	-1.109780	0.172906
C	1.900835	-0.694474	0.961676
C	1.359373	-1.808700	0.416230
C	-1.524691	-1.940813	0.749191
C	-2.311545	-0.905830	1.093245
C	-3.563054	-1.120541	1.986966
C	-4.015061	0.135261	2.754535
C	-4.749520	-1.601847	1.118664
C	-3.265767	-2.215284	3.042862
C	-2.908640	1.283358	-0.029054
C	-3.586429	0.894614	-1.220398
C	-3.212688	-0.336027	-2.051021
C	-2.337246	0.088984	-3.252476
C	-4.419181	-1.148529	-2.561534
C	-4.579347	1.738878	-1.736040
C	-4.879824	2.959647	-1.143638
C	-4.156940	3.367400	-0.029966
C	-3.166171	2.558026	0.542115
C	-2.377524	3.133930	1.713466
C	-3.263279	3.650251	2.864826
C	-1.460483	4.272079	1.220570
C	1.499292	1.760460	1.487330
C	1.987277	2.784816	0.635525
C	2.277786	2.577935	-0.852866
C	3.764236	2.828526	-1.185483
C	1.384101	3.456575	-1.750658
C	2.267408	4.038407	1.196354
C	2.091175	4.282186	2.553488
C	1.649772	3.256163	3.385919
C	1.356068	1.983458	2.882754
C	0.962666	0.864055	3.852353
C	-0.549313	0.835471	4.127990
C	1.728274	0.918733	5.189382
N	1.116934	0.484291	0.931612
N	-1.920708	0.389181	0.587265
P	-0.197106	-1.721291	-0.491393
P	-0.319540	0.503290	-0.191181
H	3.200726	-2.928352	2.003820
H	2.925911	-1.796501	3.332794
H	4.570715	-2.084182	2.737699
H	3.574571	0.689734	3.053026
H	4.059906	1.311014	1.474448
H	5.089915	0.162082	2.328468
H	5.306554	-1.192391	0.452190
H	4.158725	-0.310205	-0.570736
H	3.947326	-2.044727	-0.306171
H	1.925090	-2.729803	0.348034
H	-1.724687	-2.949147	1.095254
H	-3.219222	0.541120	3.383011
H	-4.851013	-0.134236	3.411067
H	-4.363884	0.920666	2.084514
H	-5.063774	-0.827563	0.413644
H	-5.607386	-1.839324	1.760450
H	-4.486647	-2.500929	0.551262
H	-3.098804	-3.198439	2.592269
H	-4.125498	-2.311468	3.716350
H	-2.386674	-1.961669	3.644419
H	-2.622772	-1.013325	-1.432556
H	-2.904179	0.733180	-3.935644
H	-2.004633	-0.793652	-3.811994
H	-1.449014	0.641752	-2.930513
H	-5.092522	-1.442443	-1.751524
H	-4.062780	-2.062462	-3.051048
H	-5.005343	-0.594729	-3.303896
H	-5.108254	1.442401	-2.636596
H	-5.652668	3.598710	-1.562885
H	-4.361320	4.338901	0.410474
H	-1.741739	2.341568	2.109069
H	-3.869857	4.510228	2.557257
H	-2.631068	3.983178	3.696754
H	-3.942129	2.881394	3.244111
H	-0.792105	3.930171	0.426237
H	-0.840289	4.647142	2.041559
H	-2.050852	5.109447	0.828352
H	2.064947	1.533253	-1.098939
H	4.049161	3.872315	-1.009156
H	3.953375	2.609390	-2.243128
H	4.429395	2.197105	-0.587315
H	0.324089	3.247018	-1.581407
H	1.602930	3.262415	-2.807834
H	1.558984	4.523427	-1.565585
H	2.639797	4.833634	0.556467
H	2.313190	5.262820	2.966527
H	1.548056	3.445892	4.450024
H	1.210024	-0.087749	3.373075
H	-0.891082	1.782428	4.564075
H	-0.793142	0.031520	4.833759
H	-1.103827	0.657502	3.206120
H	2.811224	1.002825	5.049796
H	1.531892	0.005124	5.762437
H	1.406166	1.762029	5.811329

=== **TS1** ===

C	4.267646	-1.750135	1.396709
C	3.868972	-0.753822	0.282443
C	4.725235	0.513321	0.474923
C	4.258733	-1.349663	-1.096674
C	2.314284	-0.553426	0.253154
C	1.557507	-1.712864	0.206735
C	-1.469760	-1.998305	0.771182
C	-2.432028	-1.051717	0.967937
C	-3.683242	-1.359807	1.826292
C	-3.800497	-0.332730	2.971332
C	-4.987582	-1.351959	0.997284
C	-3.571790	-2.759535	2.472737
C	-3.123058	1.213470	0.053849
C	-3.830741	1.018214	-1.165661
C	-3.552138	-0.156809	-2.105483
C	-2.661992	0.303525	-3.281472
C	-4.827866	-0.824972	-2.655362
C	-4.771706	1.977138	-1.554995
C	-4.994590	3.124239	-0.798638
C	-4.248142	3.337402	0.353217
C	-3.297627	2.406705	0.799287
C	-2.442577	2.775114	2.009182
C	-3.255208	3.307550	3.206696
C	-1.378060	3.818527	1.606468
C	2.133368	1.933611	0.470765
C	2.268602	2.907035	-0.551956
C	2.111814	2.563788	-2.032102

C	3.421142	2.797056	-2.813704
C	0.951450	3.339668	-2.685782
C	2.588252	4.222199	-0.189749
C	2.763551	4.585560	1.141003
C	2.630161	3.621814	2.138902
C	2.317905	2.292424	1.835188
C	2.174942	1.273338	2.969001
C	0.755323	1.278969	3.568373
C	3.218426	1.453744	4.088006
N	1.662082	0.637521	0.114947
N	-2.138010	0.218283	0.433704
P	-0.121013	-1.515208	-0.288955
P	-0.433189	0.579566	-0.195627
H	3.788826	-2.726388	1.281520
H	4.005286	-1.364155	2.387639
H	5.352652	-1.909778	1.375544
H	4.570992	0.988679	1.444810
H	4.546734	1.262630	-0.298441
H	5.780334	0.219454	0.415701
H	5.345181	-1.494412	-1.145530
H	3.970290	-0.674299	-1.910206
H	3.777312	-2.314850	-1.278169
H	2.013852	-2.693393	0.161044
H	-1.561454	-3.021898	1.105265
H	-2.880864	-0.289208	3.565990
H	-4.622341	-0.620632	3.637857
H	-4.016260	0.665288	2.592090
H	-5.200385	-0.372990	0.565222
H	-5.829820	-1.623468	1.645482
H	-4.938828	-2.086960	0.186614
H	-3.557543	-3.560318	1.725087
H	-4.447592	-2.926493	3.109577
H	-2.679705	-2.851784	3.101960
H	-2.998089	-0.919308	-1.551514
H	-3.181471	1.054021	-3.889870
H	-2.414139	-0.546195	-3.929584
H	-1.725922	0.745695	-2.926900
H	-5.517035	-1.117503	-1.857666
H	-4.560453	-1.725914	-3.220013
H	-5.371211	-0.165474	-3.341995
H	-5.327159	1.832017	-2.476683
H	-5.729318	3.858097	-1.119480
H	-4.394808	4.252791	0.918563
H	-1.921802	1.872328	2.337698
H	-3.704025	4.284318	2.992798
H	-2.594457	3.439866	4.071391
H	-4.061562	2.627928	3.500299
H	-0.741072	3.456443	0.794089
H	-0.732024	4.060781	2.457862
H	-1.856398	4.746654	1.269919
H	1.873484	1.498189	-2.098101
H	3.714264	3.853750	-2.804340
H	3.298423	2.496449	-3.861377
H	4.251587	2.219004	-2.392979
H	0.006248	3.146195	-2.168431
H	0.834666	3.038734	-3.734386
H	1.131264	4.421669	-2.670303
H	2.702730	4.973617	-0.966745
H	3.006776	5.612270	1.401951
H	2.774090	3.912577	3.175380
H	2.327493	0.276776	2.547003
H	0.507257	2.261943	3.986999
H	0.675468	0.537141	4.373026
H	0.008184	1.033561	2.807988
H	4.239823	1.495558	3.693815
H	3.160453	0.613317	4.789831
H	3.047183	2.368163	4.667687

=== **Int2** ===

C	4.408521	-1.278645	2.849910
C	4.230955	-1.450678	1.320631
C	5.376091	-0.688939	0.628003
C	4.372019	-2.947386	0.952541
C	2.800923	-0.966075	0.940217
C	1.723653	-1.685591	1.566913
C	-1.320628	-1.875012	1.745024
C	-2.460788	-1.232876	1.281430
C	-3.862142	-1.797401	1.636797
C	-4.711086	-0.793030	2.445691
C	-4.630274	-2.197838	0.358658
C	-3.733111	-3.071503	2.504621
C	-3.230750	0.789833	-0.052004
C	-3.687978	0.630595	-1.384424
C	-3.160028	-0.450072	-2.328979
C	-2.178795	0.170743	-3.347900
C	-4.269658	-1.205589	-3.087999
C	-4.614207	1.560122	-1.877272
C	-5.051033	2.629435	-1.103064
C	-4.541559	2.807153	0.179724
C	-3.616002	1.910851	0.728432
C	-3.016084	2.215675	2.102197
C	-4.062267	2.638690	3.153160
C	-1.939745	3.317276	1.987008
C	3.192933	0.862667	-0.668432
C	3.501048	0.479345	-2.002178
C	3.102308	-0.889899	-2.549914
C	4.239859	-1.598907	-3.308630
C	1.848021	-0.773915	-3.439756
C	4.139661	1.402023	-2.837335
C	4.470973	2.680810	-2.394609
C	4.141107	3.055574	-1.094989
C	3.496243	2.174369	-0.219582
C	3.107247	2.652692	1.177151
C	2.047596	3.769905	1.102689
C	4.320981	3.113777	2.007373
N	2.437986	0.002033	0.148990
N	-2.238596	-0.131705	0.478846
P	0.156438	-1.168542	1.196587
P	-0.555654	0.382878	0.041227
H	3.679246	-1.859947	3.422444
H	4.301053	-0.228113	3.143311
H	5.411363	-1.610438	3.146250
H	5.362786	0.379513	0.852851
H	5.352064	-0.799160	-0.458154
H	6.330349	-1.095779	0.985446
H	5.376399	-3.299664	1.218532
H	4.234940	-3.103428	-0.123389
H	3.647148	-3.577852	1.476248
H	1.850064	-2.521927	2.243164
H	-1.347484	-2.753858	2.371207
H	-4.187692	-0.469537	3.351783
H	-5.645302	-1.278040	2.752986
H	-4.973331	0.088076	1.859858
H	-4.896231	-1.327812	-0.241461
H	-5.560838	-2.705718	0.638795
H	-4.043598	-2.885289	-0.260708
H	-3.193147	-3.872060	1.987762
H	-4.738313	-3.445040	2.727672
H	-3.238717	-2.872382	3.461612
H	-2.602388	-1.178961	-1.732835
H	-2.692741	0.898069	-3.988055
H	-1.756793	-0.608856	-3.993000
H	-1.351127	0.682979	-2.849327
H	-5.019004	-1.635553	-2.417103

H	-3.827483	-2.023968	-3.667885
H	-4.790707	-0.553380	-3.797984
H	-4.986420	1.451145	-2.891497
H	-5.770190	3.337313	-1.506749
H	-4.858934	3.666143	0.762937
H	-2.522082	1.309196	2.465707
H	-4.493731	3.619614	2.922901
H	-3.583489	2.722684	4.135672
H	-4.885306	1.923489	3.238586
H	-1.140274	3.028651	1.299901
H	-1.489568	3.510330	2.968320
H	-2.380243	4.255089	1.627115
H	2.831688	-1.524831	-1.700579
H	4.519152	-1.063429	-4.223553
H	3.925456	-2.606847	-3.605984
H	5.141265	-1.693984	-2.692379
H	1.014278	-0.338512	-2.879668
H	1.537325	-1.761271	-3.805760
H	2.041994	-0.136157	-4.311149
H	4.380294	1.115419	-3.857925
H	4.970485	3.380545	-3.059462
H	4.384348	4.058450	-0.751775
H	2.648688	1.807532	1.700090
H	2.441989	4.662136	0.601125
H	1.724605	4.066768	2.108516
H	1.166368	3.434341	0.545682
H	5.067776	2.317950	2.106969
H	4.006027	3.409502	3.015912
H	4.818286	3.977999	1.550834

=== **Int2'** ===

C	4.482341	-1.587602	2.641051
C	4.237247	-1.561217	1.113098
C	5.379266	-0.753763	0.468674
C	4.313245	-3.004971	0.556822
C	2.808242	-1.005660	0.839180
C	1.735728	-1.741584	1.455311
C	-1.296694	-1.859187	1.778505
C	-2.445668	-1.209884	1.350471
C	-3.830169	-1.671030	1.876596
C	-4.531373	-0.540246	2.659990
C	-4.754285	-2.145736	0.734183
C	-3.672082	-2.864782	2.847060
C	-3.260372	0.665677	-0.163738
C	-3.761407	0.272592	-1.431655
C	-3.264362	-0.966938	-2.177430
C	-2.264021	-0.561718	-3.282285
C	-4.396132	-1.809314	-2.799079
C	-4.706310	1.100635	-2.050965
C	-5.124369	2.290468	-1.463189
C	-4.575423	2.691597	-0.249773
C	-3.625833	1.906352	0.417681
C	-2.974258	2.459140	1.685960
C	-3.983898	3.012576	2.711594
C	-1.960210	3.566047	1.321113
C	3.199879	0.986555	-0.560624
C	3.419183	0.847274	-1.956498
C	2.930212	-0.378791	-2.724366
C	4.063785	-1.104865	-3.474525
C	1.795900	-0.000248	-3.697228
C	4.071324	1.877190	-2.643469
C	4.490149	3.035806	-1.994367
C	4.240825	3.178153	-0.631329
C	3.596390	2.178027	0.104841
C	3.293572	2.407881	1.584371
C	2.162780	3.442327	1.756277
C	4.533311	2.825953	2.398193
N	2.442865	0.019883	0.125609
N	-2.246074	-0.152993	0.482419
P	0.162052	-1.203581	1.131222
P	-0.577138	0.341087	-0.017537
H	3.769381	-2.231077	3.165868
H	4.408133	-0.581724	3.070112
H	5.490288	-1.968270	2.847885
H	5.426524	0.272208	0.838999
H	5.294621	-0.709168	-0.618921
H	6.331044	-1.242634	0.711828
H	5.314514	-3.416845	0.733766
H	4.128905	-3.020479	-0.523419
H	3.587153	-3.673770	1.028773
H	1.857972	-2.648201	2.035062
H	-1.292260	-2.678008	2.482309
H	-3.892499	-0.157052	3.463530
H	-5.449145	-0.930046	3.116325
H	-4.810940	0.289576	2.010801
H	-5.043923	-1.328212	0.073713
H	-5.671245	-2.566159	1.164258
H	-4.275437	-2.928350	0.135982
H	-3.225819	-3.737648	2.358788
H	-4.665555	-3.159260	3.201893
H	-3.070185	-2.611344	3.725856
H	-2.728393	-1.600117	-1.463613
H	-2.750044	0.071228	-4.034757
H	-1.878002	-1.454031	-3.789885
H	-1.412905	-0.011628	-2.872385
H	-5.165414	-2.078445	-2.069840
H	-3.981087	-2.736173	-3.211696
H	-4.887534	-1.282998	-3.625544
H	-5.110543	0.814248	-3.017033
H	-5.860042	2.915871	-1.962093
H	-4.877526	3.640328	0.183320
H	-2.419644	1.645322	2.163458
H	-4.491990	3.908433	2.336725
H	-3.456444	3.302170	3.627915
H	-4.750793	2.280675	2.980683
H	-1.205722	3.204009	0.617122
H	-1.443481	3.920621	2.220910
H	-2.468908	4.423402	0.863789
H	2.510920	-1.080001	-1.995861
H	4.514321	-0.465778	-4.243161
H	3.678153	-2.001081	-3.976252
H	4.864041	-1.417116	-2.794096
H	0.967546	0.476417	-3.162820
H	1.407371	-0.890666	-4.207547
H	2.147938	0.699741	-4.464768
H	4.249765	1.771656	-3.711079
H	4.994878	3.824263	-2.546413
H	4.549735	4.090858	-0.127417
H	2.929955	1.463618	2.001351
H	2.456262	4.418670	1.351156
H	1.918231	3.578554	2.817850
H	1.255968	3.119642	1.234846
H	5.345605	2.096416	2.304035
H	4.278610	2.912828	3.461798
H	4.923911	3.798405	2.076294
N	0.534960	-2.275391	4.893912
H	1.068435	-1.720471	4.229816
H	1.181247	-2.619094	5.597271
H	-0.115374	-1.650299	5.359507

=== **TS2** ===

C	3.825526	-2.186140	2.655881
C	3.989667	-1.863305	1.149313
C	5.209042	-0.934308	1.007676

C	4.288520	-3.172991	0.385962	H	-2.396838	0.801407	3.023714
C	2.650068	-1.240012	0.645083	H	-4.464558	2.732762	4.216570
C	1.513558	-2.040098	0.689473	H	-3.386304	1.645562	5.089680
C	-1.377212	-2.243660	0.450890	H	-4.691371	0.982579	4.093247
C	-2.457300	-1.494544	0.764542	H	-1.233309	2.915435	2.265453
C	-3.794986	-2.110829	1.225703	H	-1.417108	2.857249	4.037121
C	-4.253682	-1.501736	2.567643	H	-2.486415	3.871144	3.059199
C	-4.921712	-1.938288	0.180199	H	2.781738	-1.227382	-1.802766
C	-3.625064	-3.631410	1.450802	H	4.819720	-0.625296	-4.014814
C	-3.269254	0.943535	0.513757	H	4.011666	-2.164654	-3.700337
C	-3.815470	1.134758	-0.782028	H	5.174672	-1.514061	-2.528176
C	-3.307707	0.380180	-2.011756	H	1.256683	0.310929	-3.008223
C	-2.308879	1.261282	-2.796023	H	1.750812	-1.040497	-4.045624
C	-4.428625	-0.095090	-2.956105	H	2.480220	0.562725	-4.267743
C	-4.802418	2.114089	-0.944707	H	4.693374	1.521326	-3.445172
C	-5.221029	2.907252	0.119883	H	5.392512	3.615920	-2.330769
C	-4.631884	2.748630	1.368860	H	4.763911	4.007271	0.029948
C	-3.644096	1.779399	1.594002	H	3.065461	1.483591	2.169885
C	-2.959912	1.737864	2.960443	H	2.403601	4.371276	1.369393
C	-3.938461	1.773908	4.151159	H	1.837794	3.556140	2.836467
C	-1.960294	2.909808	3.083925	H	1.296669	3.002472	1.228817
C	3.315937	0.927018	-0.367346	H	5.403250	2.322318	2.493022
C	3.679644	0.712967	-1.731705	H	4.240300	3.075003	3.602983
C	3.218436	-0.518711	-2.510046	H	4.846849	3.978284	2.213334
C	4.374512	-1.243873	-3.226619	N	0.398717	0.381117	2.550328
C	2.110666	-0.147548	-3.517726	H	1.331274	0.368953	2.119187
C	4.425489	1.687438	-2.404255	H	0.251062	-0.489950	3.049487
C	4.818749	2.870795	-1.785915	H	0.300806	1.174974	3.174066
C	4.459601	3.084656	-0.458317				
C	3.724445	2.139450	0.264078	=== **Int3** ===			
C	3.357952	2.436370	1.714464	C	4.122317	0.505369	3.928197
C	2.149921	3.392702	1.794927	C	3.652683	-0.618970	2.972872
C	4.531467	2.983591	2.548809	C	4.884379	-1.240293	2.276442
N	2.447357	0.043949	0.294269	C	3.017045	-1.718137	3.852739
N	-2.226291	-0.064030	0.690404	C	2.655184	-0.088953	1.914017
P	0.095256	-1.416570	-0.182569	C	1.340035	-0.446646	1.944466
P	-0.616858	0.505167	0.490668	C	-0.922128	-1.341973	0.415246
H	3.024799	-2.911220	2.834736	C	-2.263343	-1.209787	0.488664
H	3.594966	-1.279382	3.229286	C	-3.228813	-2.367674	0.157379
H	4.757272	-2.605268	3.057452	C	-4.216341	-2.584819	1.322010
H	5.073407	0.005010	1.550358	C	-4.026768	-2.112349	-1.143632
H	5.425708	-0.686753	-0.033934	C	-2.449317	-3.686172	-0.046636
H	6.089771	-1.438809	1.425672	C	-3.925637	0.735360	0.554925
H	5.225381	-3.614830	0.749708	C	-3.968771	1.283838	-0.756102
H	4.397706	-2.988382	-0.687949	C	-2.763313	1.257255	-1.695747
H	3.492816	-3.912849	0.515027	C	-2.002158	2.599211	-1.610370
H	1.458345	-3.031738	1.126730	C	-3.123640	0.951441	-3.162025
H	-1.406641	-3.325722	0.478447	C	-5.129488	1.947576	-1.170051
H	-3.468588	-1.573804	3.329509	C	-6.215890	2.112979	-0.316195
H	-5.130478	-2.047400	2.935871	C	-6.142789	1.626928	0.983785
H	-4.539977	-0.456101	2.458012	C	-5.011494	0.941007	1.447533
H	-5.185368	-0.891410	0.022068	C	-4.974046	0.512136	2.913746
H	-5.822048	-2.459419	0.528073	C	-6.259235	-0.197888	3.383516
H	-4.632142	-2.374224	-0.781927	C	-4.694529	1.727732	3.825260
H	-3.379332	-4.161390	0.524480	C	4.162442	1.670350	0.782316
H	-4.571214	-4.042343	1.819502	C	5.254284	1.450670	-0.092532
H	-2.852031	-3.852021	2.195184	C	5.321182	0.214545	-0.985064
H	-2.767327	-0.508528	-1.673310	C	6.732483	-0.385255	-1.110060
H	-2.806374	2.158612	-3.183595	C	4.745222	0.535072	-2.381459
H	-1.897014	0.705103	-3.646104	C	6.245594	2.436982	-0.183362
H	-1.472393	1.586322	-2.169063	C	6.158499	3.613575	0.553637
H	-5.190575	-0.679660	-2.431999	C	5.051302	3.842622	1.366901
H	-4.001162	-0.724449	-3.745070	C	4.025552	2.896017	1.481750
H	-4.929680	0.743986	-3.452066	C	2.750976	3.236991	2.252262
H	-5.239051	2.270317	-1.926201	C	1.737605	3.921300	1.307714
H	-5.988480	3.661856	-0.030139	C	2.984573	4.104950	3.500656
H	-4.936117	3.396309	2.185513	N	3.133154	0.666708	0.839599

N	-2.740540	0.040984	1.011471
P	0.117426	0.122886	0.732762
P	-1.570604	1.019914	1.937466
H	3.270058	0.971445	4.434311
H	4.686169	1.282744	3.409094
H	4.776135	0.076033	4.697482
H	5.464435	-0.494626	1.730088
H	4.586997	-2.029617	1.576333
H	5.542981	-1.687845	3.030332
H	3.772766	-2.090484	4.553533
H	2.665750	-2.567838	3.257283
H	2.179619	-1.338873	4.447814
H	1.004317	-1.142596	2.701018
H	-0.443123	-2.260535	0.098979
H	-3.687785	-2.741564	2.269862
H	-4.829569	-3.472600	1.125722
H	-4.888466	-1.735083	1.438461
H	-4.675272	-1.237679	-1.070367
H	-4.659160	-2.982839	-1.358416
H	-3.350238	-1.970721	-1.993397
H	-1.772670	-3.635381	-0.906462
H	-3.161413	-4.496537	-0.239909
H	-1.864979	-3.957021	0.839708
H	-2.081619	0.471695	-1.362718
H	-2.633994	3.425878	-1.958383
H	-1.102051	2.570701	-2.236610
H	-1.692524	2.822241	-0.584079
H	-3.715977	0.035495	-3.254915
H	-2.206992	0.823293	-3.749787
H	-3.691055	1.766765	-3.625994
H	-5.175679	2.361069	-2.172986
H	-7.106018	2.635492	-0.656912
H	-6.979686	1.786346	1.657525
H	-4.144853	-0.191330	3.029721
H	-7.119656	0.480857	3.399293
H	-6.126159	-0.573507	4.405164
H	-6.518147	-1.047681	2.743679
H	-3.777654	2.250645	3.531717
H	-4.597679	1.411512	4.872386
H	-5.516060	2.452191	3.771708
H	4.673515	-0.543380	-0.535841
H	7.417604	0.277414	-1.651855
H	6.689618	-1.328684	-1.666853
H	7.172745	-0.592427	-0.128363
H	3.713582	0.900193	-2.315699
H	4.746516	-0.360638	-3.014790
H	5.339775	1.307177	-2.884997
H	7.094708	2.283572	-0.842742
H	6.941734	4.363584	0.477800
H	4.975054	4.782342	1.905118
H	2.292966	2.303743	2.590147
H	2.136491	4.870816	0.930142
H	0.799507	4.129772	1.836641
H	1.500659	3.288488	0.445356
H	3.739096	3.668878	4.164410
H	2.050284	4.198693	4.066173
H	3.307120	5.120581	3.243250
N	-1.369220	0.238423	3.447702
H	2.409977	0.804730	0.140026
H	-1.252585	-0.766110	3.498277
H	-1.925200	0.596475	4.211822

=== **TS3** ===

C	4.666662	0.697151	3.840236
C	3.477066	-0.255375	3.592258
C	4.036137	-1.623643	3.122004
C	2.732083	-0.468759	4.923043
C	2.552757	0.279004	2.478345
C	1.214028	0.289992	2.569810
C	-0.571171	-0.904707	0.672372
C	-1.910509	-1.006742	0.536724
C	-2.596151	-2.285226	0.010038
C	-3.702101	-2.736282	0.985858
C	-3.210582	-2.081420	-1.395525
C	-1.577539	-3.440931	-0.106957
C	-3.884149	0.620908	0.413022
C	-3.832347	1.242136	-0.864318
C	-2.515872	1.498835	-1.597020
C	-2.044459	2.946921	-1.334910
C	-2.584133	1.235174	-3.113152
C	-5.022133	1.717055	-1.428788
C	-6.234453	1.625857	-0.751611
C	-6.265509	1.074631	0.523953
C	-5.107360	0.572366	1.133347
C	-5.204834	0.067308	2.572182
C	-6.396910	-0.878580	2.818141
C	-5.279560	1.256481	3.556165
C	3.762779	1.683836	0.622608
C	4.489627	1.443026	-0.591003
C	4.621370	0.032447	-1.173119
C	5.859368	-0.172159	-2.063744
C	3.345846	-0.377228	-1.946135
C	5.048407	2.519904	-1.278069
C	4.921133	3.828212	-0.818377
C	4.230674	4.049007	0.363603
C	3.650898	3.013832	1.113300
C	2.916536	3.426683	2.392577
C	1.593090	4.153116	2.073813
C	3.789314	4.297015	3.321021
N	3.175435	0.546930	1.210503
N	-2.671324	0.111888	1.019328
P	0.128118	0.720103	1.151934
P	-1.835125	1.199052	2.154053
H	4.340524	1.630537	4.308649
H	5.187543	0.945436	2.910819
H	5.386497	0.219903	4.516237
H	4.657952	-1.520390	2.225349
H	3.225767	-2.329940	2.904791
H	4.666172	-2.060026	3.906125
H	3.441110	-0.797662	5.691779
H	1.955218	-1.237624	4.842982
H	2.262419	0.456469	5.276104
H	0.737057	0.043894	3.513342
H	0.102972	-1.707980	0.401402
H	-3.310470	-2.863397	2.002306
H	-4.112179	-3.699527	0.659287
H	-4.522276	-2.019687	1.018963
H	-4.002411	-1.330398	-1.398475
H	-3.642866	-3.027695	-1.744044
H	-2.443106	-1.776893	-2.115315
H	-0.793673	-3.226337	-0.841267
H	-2.098865	-4.344824	-0.441858
H	-1.101844	-3.664751	0.854370
H	-1.755983	0.828509	-1.189379
H	-2.757330	3.668016	-1.753823
H	-1.066531	3.122276	-1.799041
H	-1.950186	3.152721	-0.263575
H	-2.968831	0.235052	-3.337537
H	-1.581456	1.318359	-3.548481
H	-3.220006	1.963336	-3.630149
H	-4.995578	2.185508	-2.407976
H	-7.146134	2.003168	-1.207554
H	-7.207406	1.038021	1.063404
H	-4.289092	-0.490136	2.788000

H	-7.357334	-0.357781	2.731410
H	-6.344016	-1.289433	3.833482
H	-6.409337	-1.718305	2.115791
H	-4.436055	1.943640	3.426773
H	-5.283982	0.899252	4.594533
H	-6.198777	1.833419	3.399027
H	4.757518	-0.678273	-0.341829
H	5.778836	0.373497	-3.010592
H	5.963905	-1.234363	-2.313151
H	6.776267	0.152519	-1.560278
H	2.440772	-0.258849	-1.340632
H	3.406757	-1.421111	-2.279595
H	3.230653	0.256121	-2.833528
H	5.596678	2.335194	-2.195931
H	5.357772	4.655400	-1.370590
H	4.130227	5.066713	0.730284
H	2.656944	2.531973	2.956874
H	1.778722	5.086952	1.529263
H	1.056416	4.404609	2.997746
H	0.938924	3.532101	1.453622
H	4.754057	3.823040	3.530925
H	3.273984	4.463702	4.275232
H	3.993170	5.282863	2.888243
N	-1.721535	0.323607	3.631483
H	3.440380	-0.305023	0.747767
H	-1.533119	-0.672405	3.603169
H	-2.431493	0.545630	4.316746

=== **Int4** ===

C	3.802623	0.404921	4.672062
C	3.583648	-0.623908	3.534161
C	4.953077	-1.143784	3.029652
C	2.830317	-1.823924	4.138869
C	2.816736	0.046600	2.362520
C	1.595840	-0.401825	1.967960
C	-0.510188	-1.360308	0.393758
C	-1.854352	-1.251648	0.395971
C	-2.784010	-2.462231	0.164006
C	-3.807502	-2.568752	1.313680
C	-3.542170	-2.376703	-1.182331
C	-1.974105	-3.777832	0.139229
C	-3.552019	0.643810	0.169474
C	-3.547847	1.035393	-1.197416
C	-2.298551	0.935836	-2.072248
C	-1.578835	2.302249	-2.112793
C	-2.578467	0.446331	-3.505760
C	-4.702981	1.614833	-1.735611
C	-5.831177	1.847132	-0.954370
C	-5.805650	1.519841	0.396213
C	-4.680533	0.925935	0.985038
C	-4.694358	0.680429	2.492983
C	-5.980020	-0.003824	2.998225
C	-4.482985	2.007254	3.255717
C	3.150708	2.006051	0.765182
C	3.455782	1.679163	-0.574293
C	4.114801	0.352853	-0.938092
C	5.635259	0.534264	-1.124683
C	3.487289	-0.312959	-2.176257
C	3.165042	2.622876	-1.565961
C	2.585956	3.847852	-1.244116
C	2.289013	4.154618	0.081600
C	2.564072	3.245673	1.111080
C	2.291543	3.608749	2.568309
C	1.009031	4.434049	2.771000
C	3.504655	4.344731	3.176990
N	3.527846	1.096437	1.810759
N	-2.376024	0.037073	0.754270
P	0.518181	0.137878	0.602492
P	-1.258442	1.155690	1.588735
H	2.843909	0.790883	5.035643
H	4.411381	1.262405	4.363219
H	4.320606	-0.071552	5.512723
H	5.595917	-0.344861	2.644604
H	4.818507	-1.876325	2.225841
H	5.493007	-1.632622	3.849237
H	3.431387	-2.252624	4.948783
H	2.658539	-2.613607	3.399902
H	1.865300	-1.529525	4.564828
H	1.203199	-1.245037	2.522689
H	-0.007653	-2.301120	0.202325
H	-3.308747	-2.590597	2.290011
H	-4.387601	-3.493708	1.208502
H	-4.508238	-1.734204	1.303184
H	-4.208468	-1.513808	-1.231119
H	-4.151174	-3.279867	-1.315263
H	-2.840661	-2.318960	-2.021614
H	-1.262443	-3.808184	-0.692925
H	-2.663286	-4.620226	0.010150
H	-1.422880	-3.935114	1.072937
H	-1.612476	0.218474	-1.616538
H	-2.216197	3.061674	-2.583024
H	-0.648978	2.230254	-2.689436
H	-1.323971	2.651694	-1.107221
H	-3.141663	-0.492395	-3.515004
H	-1.630698	0.278118	-4.030897
H	-3.142827	1.181946	-4.090813
H	-4.712878	1.909198	-2.780934
H	-6.716789	2.300829	-1.391944
H	-6.675194	1.734834	1.010683
H	-3.852417	0.022353	2.725419
H	-6.856739	0.646317	2.897327
H	-5.880358	-0.247535	4.062866
H	-6.191889	-0.932779	2.459109
H	-3.566563	2.514774	2.935003
H	-4.424669	1.827089	4.337488
H	-5.317762	2.695938	3.077750
H	3.964508	-0.327584	-0.094757
H	5.850576	1.220598	-1.952822
H	6.115420	-0.426242	-1.349122
H	6.102792	0.945040	-0.222253
H	2.403621	-0.419480	-2.057551
H	3.918171	-1.310911	-2.322378
H	3.675471	0.258105	-3.093247
H	3.394941	2.398918	-2.603544
H	2.368735	4.568404	-2.028578
H	1.841360	5.115137	0.317288
H	2.159982	2.671506	3.119284
H	1.092480	5.441012	2.344990
H	0.810927	4.552755	3.842911
H	0.142039	3.941384	2.318307
H	4.423612	3.751074	3.098483
H	3.334362	4.563313	4.238296
H	3.683215	5.295236	2.659653
N	-1.110454	0.619759	3.208662
H	4.360790	1.359149	2.309265
H	-0.896700	-0.346279	3.422063
H	-1.745556	1.030447	3.878950

=== **TS4** ===

C	3.565505	-2.159775	2.643388
C	3.687876	-1.852571	1.125600
C	5.125156	-1.357214	0.871099
C	3.479172	-3.158795	0.319640
C	2.558862	-0.874416	0.766146

C	1.191152	-1.237411	0.974528	H	-3.431504	2.098831	4.773443
C	-1.376023	-2.067346	0.159483	H	-4.658924	1.053899	4.040658
C	-2.469302	-1.425033	0.650913	H	-1.910764	3.350825	1.556757
C	-3.582733	-2.215783	1.389067	H	-1.838891	3.470018	3.331426
C	-3.837942	-1.561336	2.763676	H	-3.209209	4.157638	2.442050
C	-4.911122	-2.280720	0.601361	H	2.918061	-0.642624	-1.902630
C	-3.154599	-3.677710	1.652618	H	5.124616	-0.193341	-3.987760
C	-3.694489	0.770106	0.359164	H	3.959179	-1.517733	-3.924977
C	-4.405266	0.701024	-0.872211	H	5.203563	-1.372527	-2.669940
C	-3.926000	-0.141909	-2.056407	H	1.847778	1.402034	-2.818112
C	-3.163952	0.742271	-3.069490	H	2.040620	0.154917	-4.060342
C	-5.059057	-0.892967	-2.783792	H	3.139435	1.550162	-4.024461
C	-5.546407	1.495162	-1.036094	H	5.611982	1.725669	-2.999285
C	-5.973074	2.371022	-0.041898	H	6.704988	3.362572	-1.510974
C	-5.233973	2.484903	1.129547	H	5.950910	3.612500	0.827316
C	-4.086315	1.710324	1.349479	H	3.344128	1.425650	2.410498
C	-3.261950	1.973570	2.608810	H	3.629994	4.443325	1.965166
C	-4.093326	1.981302	3.906802	H	2.701147	3.666812	3.262203
C	-2.507492	3.315156	2.474441	H	2.204298	3.466241	1.570807
C	3.850235	1.131170	-0.159009	H	5.773111	1.479439	3.085133
C	4.244314	0.993146	-1.508554	H	4.720603	2.405931	4.171069
C	3.539597	0.048292	-2.479383	H	5.741557	3.247733	3.003543
C	4.518059	-0.803859	-3.308964	N	0.076798	1.073771	1.273222
C	2.585705	0.838813	-3.399501	H	1.840100	0.921547	0.421176
C	5.286532	1.809649	-1.966694	H	0.662849	-0.210515	1.519393
C	5.901138	2.737688	-1.130983	H	-0.075635	1.893737	1.851666
C	5.475658	2.875081	0.187394				
C	4.442439	2.082183	0.701163	=== **Int5** ===			
C	3.963544	2.286057	2.136482	C	4.038011	-2.254409	2.466516
C	3.070270	3.540392	2.237336	C	4.088756	-1.802921	0.985804
C	5.120132	2.357319	3.151513	C	5.389026	-1.002604	0.782496
N	2.721635	0.378314	0.325083	C	4.144894	-3.054856	0.074213
N	-2.500654	-0.018769	0.563501	C	2.793904	-1.019814	0.651142
P	0.030155	-1.170669	-0.549784	C	1.491324	-1.674118	1.090628
P	-0.974096	0.837133	-0.004481	C	-1.323403	-2.106463	0.712522
H	2.598730	-2.597797	2.905052	C	-2.467984	-1.461781	1.028562
H	3.700146	-1.252068	3.242520	C	-3.735111	-2.202833	1.506184
H	4.347656	-2.872597	2.929449	C	-4.225602	-1.608307	2.842614
H	5.360879	-0.449605	1.431974	C	-4.882716	-2.134533	0.470017
H	5.321977	-1.162563	-0.185518	C	-3.435102	-3.699631	1.744825
H	5.819466	-2.139843	1.198759	C	-3.472518	0.850631	0.581152
H	4.253088	-3.884171	0.596291	C	-3.875011	0.873364	-0.781933
H	3.556083	-2.976719	-0.758009	C	-3.148386	0.074258	-1.863014
H	2.502794	-3.610843	0.513798	C	-2.122021	0.979190	-2.580547
H	1.032748	-2.176626	1.498899	C	-4.086985	-0.577843	-2.895422
H	-1.290642	-3.145137	0.226837	C	-4.917466	1.727468	-1.160950
H	-2.907814	-1.462000	3.335058	C	-5.534534	2.571817	-0.242794
H	-4.531392	-2.182179	3.344071	C	-5.092373	2.589248	1.074762
H	-4.283537	-0.572792	2.658245	C	-4.059895	1.747781	1.512233
H	-5.349930	-1.295375	0.439918	C	-3.563689	1.893509	2.949808
H	-5.635430	-2.882857	1.164344	C	-4.695505	1.948673	3.994904
H	-4.764241	-2.759632	-0.372569	C	-2.673871	3.149066	3.085951
H	-3.018728	-4.244886	0.725193	C	3.567490	1.012933	-0.472033
H	-3.942318	-4.178924	2.226915	C	3.935542	0.914314	-1.838062
H	-2.228596	-3.734363	2.235013	C	3.405727	-0.203263	-2.733766
H	-3.224297	-0.892828	-1.684240	C	4.498014	-0.859041	-3.598529
H	-3.827883	1.506692	-3.492339	C	2.245443	0.312437	-3.609712
H	-2.782206	0.130679	-3.896968	C	4.757915	1.910274	-2.376790
H	-2.317691	1.252070	-2.599530	C	5.197767	2.987012	-1.611417
H	-5.673001	-1.481957	-2.095778	C	4.794859	3.088173	-0.282258
H	-4.632226	-1.576256	-3.527560	C	3.972614	2.123870	0.310071
H	-5.723772	-0.207636	-3.323010	C	3.487208	2.312466	1.745734
H	-6.101315	1.439853	-1.967889	C	2.374571	3.380373	1.800925
H	-6.862425	2.978072	-0.191087	C	4.620293	2.657697	2.730254
H	-5.544992	3.198524	1.887477	N	2.638059	0.096100	0.061292
H	-2.516686	1.177108	2.687623	N	-2.401474	-0.026843	1.005850
H	-4.807397	2.812949	3.929669	P	0.058361	-1.133935	0.007020

P	-0.768958	0.687059	1.039697
H	3.199634	-2.926741	2.673361
H	3.958005	-1.394186	3.141756
H	4.961126	-2.790330	2.716444
H	5.418393	-0.103023	1.403210
H	5.533792	-0.695951	-0.255193
H	6.238481	-1.635006	1.069149
H	5.041942	-3.639255	0.311410
H	4.197613	-2.775118	-0.983273
H	3.278925	-3.711514	0.208350
H	1.540351	-2.767627	1.048242
H	-1.252452	-3.187535	0.747867
H	-3.430259	-1.614152	3.597748
H	-5.061073	-2.205009	3.228166
H	-4.577114	-0.584311	2.719642
H	-5.228827	-1.113882	0.298556
H	-5.735256	-2.722275	0.832879
H	-4.567018	-2.558034	-0.489523
H	-3.149128	-4.214588	0.821317
H	-4.338938	-4.189399	2.124505
H	-2.639700	-3.844647	2.484363
H	-2.592001	-0.733292	-1.381904
H	-2.627378	1.800128	-3.104149
H	-1.551443	0.402390	-3.318220
H	-1.411027	1.420085	-1.874109
H	-4.864184	-1.182749	-2.417259
H	-3.509114	-1.231678	-3.559194
H	-4.582870	0.165579	-3.530295
H	-5.239311	1.747299	-2.197799
H	-6.341079	3.228470	-0.558629
H	-5.553402	3.275270	1.779405
H	-2.945906	1.019801	3.174557
H	-5.292469	2.863205	3.903324
H	-4.270862	1.941330	5.005953
H	-5.377619	1.096393	3.910245
H	-1.845252	3.136237	2.369607
H	-2.259128	3.221024	4.100156
H	-3.254998	4.059981	2.898526
H	2.989458	-0.985672	-2.092272
H	4.913779	-0.162223	-4.335501
H	4.081084	-1.707572	-4.154294
H	5.329445	-1.229389	-2.987150
H	1.433956	0.704920	-2.988379
H	1.838976	-0.497389	-4.228746
H	2.582666	1.114288	-4.278059
H	5.052925	1.844930	-3.420618
H	5.837284	3.747858	-2.050638
H	5.121010	3.940410	0.308099
H	3.040800	1.371074	2.080705
H	2.751019	4.356513	1.471361
H	1.997227	3.493880	2.825717
H	1.534186	3.105709	1.154528
H	5.421366	1.910065	2.703440
H	4.231318	2.700887	3.754802
H	5.070552	3.633094	2.512508
N	-0.221946	0.445336	2.656792
H	1.303406	-1.401918	2.132736
H	-0.509103	-0.395215	3.146282
H	-0.290649	1.258699	3.253833

=== **TS5** ===

C	3.319288	0.968873	2.560774
C	3.905235	-0.265579	1.830061
C	5.319031	0.097529	1.338623
C	4.042425	-1.441109	2.830990
C	2.919066	-0.677449	0.706336
C	1.566465	-1.211442	1.192029
C	-1.177109	-1.916396	0.673709
C	-2.398935	-1.428042	0.975848
C	-3.592121	-2.336428	1.336433
C	-4.231095	-1.879083	2.663982
C	-4.674395	-2.345619	0.230227
C	-3.127901	-3.798780	1.522234
C	-3.638869	0.792444	0.644428
C	-3.999533	0.865881	-0.728394
C	-3.161552	0.219313	-1.831017
C	-2.207974	1.268038	-2.446029
C	-3.996568	-0.445292	-2.941789
C	-5.113660	1.632501	-1.090037
C	-5.842220	2.346996	-0.143808
C	-5.446266	2.318514	1.188106
C	-4.347594	1.556522	1.609481
C	-3.921569	1.646389	3.073933
C	-5.087044	1.487931	4.070056
C	-3.190398	2.981065	3.341124
C	4.175042	-0.354174	-1.367218
C	5.040881	-1.398179	-1.785656
C	4.821915	-2.825661	-1.288394
C	6.086341	-3.699310	-1.305656
C	3.685662	-3.504176	-2.084755
C	6.057368	-1.090496	-2.695086
C	6.213444	0.197445	-3.203618
C	5.331408	1.200789	-2.811382
C	4.296213	0.952279	-1.903095
C	3.285664	2.038908	-1.545116
C	2.073443	1.974007	-2.498754
C	3.877689	3.458091	-1.515177
N	3.074985	-0.675801	-0.553458
N	-2.492176	0.005120	1.049420
P	0.106878	-0.751163	0.091816
P	-0.955634	0.882046	1.236443
H	2.316900	0.790845	2.960531
H	3.261567	1.831451	1.886659
H	3.975502	1.243136	3.395956
H	5.315861	0.948731	0.654465
H	5.809528	-0.736413	0.829688
H	5.931971	0.367293	2.207582
H	4.751225	-1.166108	3.620750
H	4.428675	-2.340348	2.335856
H	3.095007	-1.699685	3.313681
H	1.618103	-2.308442	1.149107
H	-0.976876	-2.981129	0.641354
H	-3.488383	-1.830284	3.469383
H	-5.007683	-2.592571	2.964870
H	-4.699728	-0.900103	2.565762
H	-5.124421	-1.362722	0.080426
H	-5.474209	-3.042538	0.510071
H	-4.253713	-2.682299	-0.723333
H	-2.729156	-4.225916	0.595806
H	-3.986978	-4.411014	1.819128
H	-2.365387	-3.889790	2.303873
H	-2.543357	-0.562121	-1.383589
H	-2.776551	2.069099	-2.934391
H	-1.558025	0.802243	-3.196036
H	-1.568196	1.726683	-1.685006
H	-4.728359	-1.151537	-2.536776
H	-3.334912	-0.994141	-3.622102
H	-4.538849	0.290750	-3.546604
H	-5.403853	1.688394	-2.134784
H	-6.701613	2.939181	-0.447378
H	-5.997725	2.903831	1.918177
H	-3.213771	0.833784	3.260114
H	-5.786914	2.329940	4.019684
H	-4.699643	1.452135	5.095352

H	-5.657405	0.570532	3.893473
H	-2.341441	3.119195	2.662519
H	-2.822776	3.020788	4.375126
H	-3.866940	3.831743	3.196016
H	4.491582	-2.768543	-0.243115
H	6.421133	-3.915036	-2.327053
H	5.880831	-4.662800	-0.824851
H	6.917349	-3.223693	-0.772041
H	2.765579	-2.912972	-2.036398
H	3.476495	-4.505819	-1.687380
H	3.967877	-3.610293	-3.139330
H	6.740589	-1.871031	-3.014934
H	7.012411	0.414764	-3.907327
H	5.449089	2.199366	-3.221331
H	2.910592	1.830080	-0.536460
H	2.385647	2.175032	-3.531091
H	1.318942	2.720463	-2.219710
H	1.603435	0.986040	-2.467257
H	4.762597	3.516273	-0.870611
H	3.132107	4.165616	-1.133722
H	4.167181	3.804481	-2.514250
N	-0.453501	0.576620	2.858305
H	1.361887	-0.943732	2.225218
H	-0.633785	-0.339433	3.255709
H	-0.683098	1.309449	3.517251

=== **Int6** ===

C	3.984846	0.533146	-1.347142
C	4.315058	-0.671674	-0.430019
C	5.298373	-1.586843	-1.182851
C	5.026041	-0.165903	0.850905
C	2.984651	-1.351772	-0.023831
C	1.989363	-0.473046	0.735681
C	-0.672552	-1.640236	0.329320
C	-1.912746	-1.352217	0.775837
C	-2.917043	-2.447373	1.191904
C	-3.442692	-2.170143	2.615164
C	-4.114943	-2.546676	0.217183
C	-2.234415	-3.833256	1.207269
C	-3.486324	0.668549	0.688781
C	-3.966066	0.757693	-0.646188
C	-3.134690	0.305782	-1.846536
C	-2.406938	1.519263	-2.467678
C	-3.949779	-0.427375	-2.928598
C	-5.208568	1.360361	-0.875018
C	-5.956159	1.901514	0.166542
C	-5.451473	1.865320	1.460911
C	-4.219201	1.262537	1.750376
C	-3.690588	1.343342	3.181882
C	-4.735705	0.965885	4.250249
C	-3.140400	2.757228	3.474820
C	3.189767	-3.656560	-0.826268
C	3.905121	-4.574501	-0.011485
C	4.090087	-4.301748	1.480028
C	5.327411	-4.975845	2.094039
C	2.817859	-4.694842	2.262076
C	4.387846	-5.746882	-0.600447
C	4.160015	-6.034329	-1.945515
C	3.426084	-5.141494	-2.719736
C	2.922213	-3.949192	-2.185781
C	2.064920	-3.028438	-3.051155
C	0.656714	-3.625917	-3.251334
C	2.712495	-2.698323	-4.409009
N	2.579798	-2.541968	-0.218421
N	-2.206898	0.045367	0.957959
P	0.384007	-0.263872	-0.232491
P	-0.810143	1.138521	1.065853
H	3.350003	1.278150	-0.857467
H	3.475494	0.207530	-2.260979
H	4.915838	1.033166	-1.639248
H	4.880783	-1.964470	-2.118797
H	5.606679	-2.447869	-0.584557
H	6.198049	-1.008275	-1.426152
H	5.964796	0.328731	0.574838
H	5.272654	-0.997289	1.521740
H	4.426509	0.556077	1.414087
H	1.786664	-0.936133	1.705308
H	-0.304182	-2.650657	0.212667
H	-2.618144	-2.066214	3.330780
H	-4.073248	-3.004378	2.945441
H	-4.045640	-1.263187	2.649497
H	-4.719097	-1.637799	0.201549
H	-4.764176	-3.376153	0.524105
H	-3.770899	-2.750109	-0.802535
H	-1.890485	-4.134377	0.212221
H	-2.958195	-4.584184	1.543892
H	-1.379416	-3.860911	1.891520
H	-2.370067	-0.390475	-1.495255
H	-3.129673	2.240355	-2.869271
H	-1.753997	1.196179	-3.287563
H	-1.788108	2.040445	-1.729671
H	-4.524691	-1.260706	-2.512291
H	-3.273921	-0.830342	-3.691975
H	-4.650559	0.241888	-3.441052
H	-5.589301	1.425585	-1.889743
H	-6.917341	2.367749	-0.033875
H	-6.022282	2.319721	2.265492
H	-2.860255	0.636638	3.266647
H	-5.551308	1.696212	4.301642
H	-4.264744	0.938545	5.240192
H	-5.180546	-0.016536	4.062023
H	-2.379476	3.054931	2.744868
H	-2.698006	2.799150	4.478955
H	-3.942547	3.503834	3.433622
H	4.223094	-3.220206	1.607937
H	5.224125	-6.066577	2.131949
H	5.467250	-4.630741	3.125071
H	6.238689	-4.743058	1.531179
H	1.939568	-4.172103	1.869693
H	2.922152	-4.445567	3.325881
H	2.636925	-5.773673	2.182625
H	4.951335	-6.452966	0.001487
H	4.544912	-6.952115	-2.381690
H	3.234860	-5.375346	-3.763835
H	1.934735	-2.082379	-2.516916
H	0.705848	-4.581927	-3.786967
H	0.025206	-2.942862	-3.832899
H	0.165249	-3.805362	-2.288915
H	3.711592	-2.264723	-4.285437
H	2.095414	-1.975974	-4.956940
H	2.813112	-3.587750	-5.042004
N	-0.099197	0.869200	2.607664
H	2.371091	0.527046	0.928588
H	-0.028709	-0.075533	2.967905
H	-0.375455	1.520615	3.330356

=== **TS6** ===

C	2.942111	0.280257	-0.161838
C	3.607988	-1.056659	0.231346
C	4.702216	-1.401161	-0.791079
C	4.245482	-0.920868	1.634310
C	2.547637	-2.188929	0.276878
C	1.287241	-1.944534	1.113806
C	-1.602383	-2.234545	0.935275

C	-2.681796	-1.484465	1.242228	H	-1.704703	3.198452	1.995749
C	-3.954634	-2.083470	1.875355	H	-2.013806	3.508510	3.722555
C	-4.344392	-1.288396	3.137941	H	-3.027387	4.262758	2.480727
C	-5.147459	-2.090728	0.889117	H	4.355059	-4.229176	1.248519
C	-3.714244	-3.549298	2.301721	H	5.180379	-7.165838	1.534444
C	-3.577427	0.822646	0.578950	H	5.754482	-5.785441	2.469151
C	-4.066303	0.707542	-0.750493	H	6.157824	-5.915923	0.744929
C	-3.463107	-0.264149	-1.764469	H	2.088122	-5.006999	1.986161
C	-2.427077	0.472875	-2.642882	H	3.331285	-5.356325	3.205285
C	-4.506189	-0.962258	-2.657489	H	2.715649	-6.652224	2.158371
C	-5.078140	1.578856	-1.171230	H	4.288496	-7.526702	-0.428996
C	-5.579135	2.568901	-0.331382	H	3.413545	-7.895857	-2.712783
C	-5.051045	2.714604	0.945954	H	2.216833	-6.062042	-3.871923
C	-4.046368	1.862416	1.425116	H	1.602685	-2.678402	-2.362687
C	-3.455473	2.140540	2.806527	H	0.158389	-4.822474	-4.003904
C	-4.517247	2.385432	3.896645	H	-0.321894	-3.124153	-3.838037
C	-2.489321	3.345011	2.746412	H	-0.354438	-4.198187	-2.426942
C	2.887354	-4.459172	-0.941930	H	3.430427	-2.816778	-4.060961
C	3.590797	-5.507059	-0.269648	H	1.893433	-2.301088	-4.787220
C	4.097886	-5.292645	1.151489	H	2.470926	-3.960689	-5.009146
C	5.370611	-6.087254	1.487351	N	-0.207627	0.468981	2.495850
C	2.992696	-5.591418	2.187830	H	1.441739	-1.204540	1.898290
C	3.757263	-6.723841	-0.932166	H	-0.439903	-0.316760	3.093700
C	3.267642	-6.939137	-2.219826	H	-0.224741	1.340630	3.008981
C	2.594870	-5.904061	-2.864131				
C	2.387801	-4.660936	-2.262013	=== **Int7** ===			
C	1.653385	-3.556733	-3.014148	C	2.850692	-0.552520	-0.929224
C	0.199551	-3.950870	-3.339505	C	3.342853	-1.801047	-0.162086
C	2.406896	-3.134420	-4.291032	C	4.187555	-2.668944	-1.110125
N	2.704504	-3.272691	-0.317138	C	4.229442	-1.352302	1.026528
N	-2.533531	-0.068469	1.045768	C	2.152723	-2.597872	0.399754
P	-0.209138	-1.445186	0.056841	C	1.093213	-1.838182	1.178851
P	-0.870451	0.542024	0.909101	C	-1.819222	-2.056331	1.055273
H	2.200308	0.607379	0.574303	C	-2.847169	-1.241784	1.371931
H	2.449900	0.211309	-1.139306	C	-4.120585	-1.751838	2.077935
H	3.703499	1.066922	-0.227574	C	-4.413617	-0.896862	3.328207
H	4.287789	-1.501864	-1.799983	C	-5.355811	-1.728841	1.145643
H	5.201911	-2.343205	-0.543976	C	-3.935648	-3.213095	2.544152
H	5.457724	-0.607028	-0.810220	C	-3.661140	1.074760	0.642597
H	5.013634	-0.138124	1.618843	C	-4.196073	0.926496	-0.665730
H	4.726359	-1.856417	1.943845	C	-3.663664	-0.108528	-1.656290
H	3.510082	-0.646333	2.398473	C	-2.634432	0.553089	-2.600185
H	1.012589	-2.893904	1.582612	C	-4.761464	-0.805262	-2.482329
H	-1.581519	-3.306842	1.089843	C	-5.185632	1.820351	-1.091849
H	-3.512098	-1.237027	3.850165	C	-5.620537	2.863043	-0.279292
H	-5.186630	-1.780847	3.638502	C	-5.046101	3.039170	0.974049
H	-4.651702	-0.272430	2.891643	C	-4.060912	2.166913	1.457587
H	-5.449367	-1.084549	0.593194	C	-3.411736	2.477816	2.805463
H	-6.009309	-2.573656	1.366001	C	-4.423956	2.816294	3.917550
H	-4.901611	-2.658484	-0.014726	C	-2.398162	3.635058	2.661324
H	-3.508089	-4.200440	1.445533	C	1.103967	-4.698492	0.721733
H	-4.617946	-3.931239	2.789870	C	1.148372	-5.171737	2.057063
H	-2.886294	-3.637820	3.013861	C	2.280346	-4.792376	3.010800
H	-2.933209	-1.049256	-1.220349	C	3.294939	-5.948828	3.127682
H	-2.912240	1.257182	-3.236874	C	1.782645	-4.357919	4.401946
H	-1.941313	-0.227780	-3.332606	C	0.157804	-6.069440	2.477111
H	-1.647429	0.946306	-2.036713	C	-0.847493	-6.499101	1.615725
H	-5.296323	-1.437924	-2.067815	C	-0.859085	-6.048629	0.295660
H	-4.017510	-1.737808	-3.258485	C	0.110475	-5.160237	-0.181522
H	-4.981902	-0.265853	-3.357740	C	0.156262	-4.758943	-1.655068
H	-5.467166	1.494494	-2.181418	C	-1.222373	-4.697412	-2.331727
H	-6.362851	3.236793	-0.679255	C	1.103246	-5.702450	-2.427367
H	-5.422528	3.510089	1.585299	N	2.129285	-3.860719	0.221811
H	-2.876352	1.260244	3.099372	N	-2.641934	0.159757	1.116771
H	-5.070367	3.316246	3.727469	P	-0.415311	-1.361641	0.115903
H	-4.033014	2.471499	4.876662	P	-0.961759	0.688073	0.894711
H	-5.245883	1.570327	3.951212	H	2.299750	0.145496	-0.289045

H	2.201619	-0.827563	-1.768182
H	3.712650	-0.008981	-1.334068
H	3.596352	-3.013889	-1.964635
H	4.575465	-3.555238	-0.601149
H	5.033332	-2.082285	-1.488746
H	5.088968	-0.782908	0.653114
H	4.613084	-2.218241	1.578527
H	3.688996	-0.709547	1.730573
H	0.722253	-2.460672	1.996424
H	-1.835555	-3.121873	1.249863
H	-3.548883	-0.864444	4.001929
H	-5.255387	-1.330840	3.880972
H	-4.682031	0.125204	3.061939
H	-5.619778	-0.719338	0.825690
H	-6.218374	-2.149110	1.677570
H	-5.180907	-2.340331	0.253904
H	-3.792827	-3.900112	1.703825
H	-4.837103	-3.533231	3.079007
H	-3.084581	-3.321231	3.225170
H	-3.143304	-0.888915	-1.096714
H	-3.114585	1.324678	-3.214633
H	-2.193106	-0.193752	-3.271242
H	-1.821329	1.028252	-2.041237
H	-5.542388	-1.233742	-1.845909
H	-4.320895	-1.617972	-3.071454
H	-5.242640	-0.120174	-3.189974
H	-5.609366	1.711284	-2.085639
H	-6.388175	3.547531	-0.630812
H	-5.364511	3.875043	1.590122
H	-2.860777	1.586136	3.117858
H	-4.939435	3.764448	3.726681
H	-3.903732	2.919980	4.877265
H	-5.187192	2.039678	4.030825
H	-1.647300	3.422386	1.892304
H	-1.882390	3.817726	3.613304
H	-2.905491	4.563849	2.374222
H	2.816688	-3.941365	2.581427
H	2.824390	-6.842431	3.555481
H	4.134561	-5.666363	3.775131
H	3.696054	-6.218956	2.144869
H	1.062101	-3.534053	4.332141
H	2.624804	-4.019319	5.017268
H	1.295835	-5.179633	4.939770
H	0.180227	-6.444205	3.496965
H	-1.607163	-7.194148	1.963294
H	-1.631288	-6.406166	-0.378591
H	0.581828	-3.751925	-1.715212
H	-1.687522	-5.686522	-2.419215
H	-1.117779	-4.300809	-3.348472
H	-1.909409	-4.042891	-1.783214
H	2.105314	-5.696800	-1.986961
H	1.186544	-5.392994	-3.476805
H	0.725937	-6.732441	-2.406636
N	-0.229814	0.656706	2.450909
H	1.493922	-0.924331	1.613746
H	-0.443141	-0.103883	3.086677
H	-0.198258	1.545489	2.932894

=== **TS7** ===

C	0.619078	0.159548	-3.185060
C	1.473187	-1.124480	-3.230883
C	0.973599	-2.013955	-4.383389
C	2.948449	-0.731340	-3.504339
C	1.458279	-1.899186	-1.899018
C	1.508283	-1.106154	-0.597278
C	-1.132669	-1.508206	1.220032
C	-2.276757	-0.877374	1.589768
C	-3.107109	-1.355649	2.802070
C	-2.729540	-0.483897	4.024894
C	-4.639036	-1.299191	2.599520
C	-2.761250	-2.821528	3.147846
C	-3.814699	0.839886	0.540997
C	-4.460303	0.168021	-0.527595
C	-3.789368	-0.936241	-1.342156
C	-3.470055	-0.424622	-2.763180
C	-4.629812	-2.225028	-1.414075
C	-5.741830	0.587221	-0.906814
C	-6.368669	1.662438	-0.285757
C	-5.702665	2.351492	0.721930
C	-4.426239	1.965023	1.151794
C	-3.750739	2.791777	2.243327
C	-4.619520	2.928423	3.509523
C	-3.358308	4.187727	1.714875
C	1.637293	-4.014529	-0.810523
C	2.879450	-4.178091	-0.146344
C	4.149237	-3.457973	-0.599411
C	5.058611	-4.419657	-1.392726
C	4.925493	-2.803647	0.559277
C	2.951167	-5.098148	0.909538
C	1.844208	-5.840501	1.304375
C	0.639592	-5.696885	0.615485
C	0.513457	-4.808616	-0.456962
C	-0.768933	-4.734615	-1.283753
C	-2.024073	-5.218242	-0.542355
C	-0.597494	-5.524135	-2.600710
N	1.519797	-3.171239	-1.940851
N	-2.497103	0.413744	0.978287
P	-0.092924	-0.549995	0.160323
P	-1.191159	1.315986	0.169605
H	0.969361	0.876686	-2.434449
H	-0.432150	-0.059090	-2.976498
H	0.674789	0.662402	-4.157877
H	-0.063869	-2.324831	-4.218941
H	1.579850	-2.917475	-4.481273
H	1.018169	-1.455185	-5.325885
H	3.013334	-0.160735	-4.438467
H	3.579166	-1.621422	-3.603784
H	3.364165	-0.103204	-2.706625
H	1.997873	-1.698256	0.179670
H	-0.789906	-2.440346	1.648444
H	-1.657356	-0.561701	4.239742
H	-3.280824	-0.815767	4.914043
H	-2.965528	0.569480	3.857448
H	-5.010881	-0.283185	2.464876
H	-5.131400	-1.718420	3.485808
H	-4.951534	-1.889782	1.732586
H	-2.942479	-3.489702	2.298754
H	-3.393940	-3.155660	3.977873
H	-1.720631	-2.941740	3.467312
H	-2.839572	-1.189898	-0.867084
H	-4.385650	-0.189758	-3.319653
H	-2.921008	-1.187080	-3.329697
H	-2.857909	0.483021	-2.727159
H	-4.833742	-2.628636	-0.416915
H	-4.092624	-2.992589	-1.983344
H	-5.592017	-2.060209	-1.913278
H	-6.248302	0.074545	-1.719988
H	-7.361936	1.973723	-0.598704
H	-6.182985	3.208087	1.186818
H	-2.829633	2.275493	2.525774
H	-5.534548	3.499862	3.315367
H	-4.064826	3.455760	4.295086
H	-4.915924	1.950618	3.903483
H	-2.730456	4.115345	0.819200

H	-2.808892	4.750484	2.480585
H	-4.245213	4.773053	1.444736
H	3.864226	-2.656472	-1.286374
H	5.394616	-5.252627	-0.763544
H	5.948905	-3.895718	-1.762283
H	4.527838	-4.842531	-2.252588
H	4.295096	-2.108988	1.127258
H	5.782914	-2.241562	0.170118
H	5.316282	-3.546928	1.263161
H	3.896615	-5.237786	1.426636
H	1.920472	-6.540981	2.131598
H	-0.212280	-6.299716	0.912958
H	-0.934823	-3.683463	-1.550174
H	-1.990187	-6.295018	-0.337447
H	-2.911277	-5.036581	-1.158835
H	-2.163343	-4.693412	0.408872
H	0.260117	-5.157509	-3.171360
H	-1.494225	-5.428668	-3.225818
H	-0.444008	-6.589901	-2.390854
N	-0.238451	2.184492	1.308958
H	2.093459	-0.193019	-0.714337
H	0.133609	1.729359	2.134453
H	-0.479920	3.156801	1.461212

=== **Int8** ===

C	0.449433	-1.335559	-4.581155
C	1.400953	-1.529103	-3.374653
C	2.682140	-2.225617	-3.864076
C	1.773512	-0.147306	-2.788800
C	0.685409	-2.377669	-2.310370
C	-0.505316	-1.765654	-1.592427
C	-1.352101	-1.776783	1.208263
C	-2.407150	-1.030538	1.617873
C	-3.377997	-1.544352	2.710500
C	-3.484490	-0.505055	3.845932
C	-4.791703	-1.845472	2.160669
C	-2.857324	-2.858644	3.336108
C	-3.764878	0.968857	0.806433
C	-4.605655	0.523368	-0.248754
C	-4.204205	-0.597942	-1.206852
C	-3.678947	0.012540	-2.525895
C	-5.338679	-1.594443	-1.514157
C	-5.811392	1.196926	-0.479531
C	-6.179587	2.305615	0.275860
C	-5.319019	2.777826	1.259891
C	-4.102736	2.138736	1.537760
C	-3.161071	2.784821	2.553111
C	-3.848179	3.201834	3.868466
C	-2.472181	4.016098	1.922292
C	0.514180	-4.424178	-1.135837
C	1.161419	-4.593224	0.114811
C	2.479500	-3.878084	0.408690
C	3.657473	-4.686989	-0.175934
C	2.713252	-3.576112	1.897161
C	0.604494	-5.492423	1.032113
C	-0.539449	-6.227146	0.725967
C	-1.134286	-6.085727	-0.526140
C	-0.624130	-5.197579	-1.480923
C	-1.218187	-5.123811	-2.887195
C	-2.708022	-5.494522	-2.963489
C	-0.393219	-5.997108	-3.857320
N	1.105638	-3.562341	-2.090697
N	-2.512834	0.287751	1.080396
P	-0.066222	-1.073092	0.140290
P	-1.090055	0.922749	0.210592
H	-0.471195	-0.807510	-4.308564
H	0.172077	-2.300071	-5.022202
H	0.949980	-0.742480	-5.355792
H	2.462358	-3.199403	-4.310352
H	3.383111	-2.393591	-3.040466
H	3.175370	-1.598745	-4.616850
H	2.293162	0.446624	-3.550043
H	2.441705	-0.247409	-1.925760
H	0.896119	0.427027	-2.471588
H	-0.951837	-0.966299	-2.185989
H	-1.163217	-2.762473	1.614721
H	-2.495188	-0.234529	4.233345
H	-4.069056	-0.923120	4.674255
H	-3.985598	0.402877	3.511641
H	-5.291520	-0.955659	1.775206
H	-5.412105	-2.255866	2.966962
H	-4.745931	-2.593337	1.361894
H	-2.810094	-3.674936	2.607940
H	-3.546216	-3.168570	4.130263
H	-1.865275	-2.734502	3.783205
H	-3.389451	-1.164867	-0.749322
H	-4.471955	0.574659	-3.033707
H	-3.338681	-0.776966	-3.208134
H	-2.846070	0.701420	-2.348174
H	-5.783097	-2.003815	-0.602379
H	-4.947348	-2.430773	-2.105570
H	-6.141477	-1.133843	-2.101488
H	-6.466161	0.857571	-1.276692
H	-7.120778	2.813141	0.081285
H	-5.591469	3.668047	1.819281
H	-2.387044	2.052276	2.797776
H	-4.561959	4.019388	3.716547
H	-3.097508	3.558274	4.583796
H	-4.387235	2.371101	4.334241
H	-1.978739	3.766615	0.975937
H	-1.725763	4.437834	2.608310
H	-3.204685	4.802731	1.705409
H	2.458989	-2.913662	-0.108903
H	3.731549	-5.669305	0.306869
H	4.606117	-4.158863	-0.016999
H	3.528544	-4.844378	-1.251469
H	1.876427	-3.014935	2.328495
H	3.619973	-2.970858	2.013412
H	2.856853	-4.487364	2.490074
H	1.079962	-5.630576	1.998352
H	-0.953249	-6.922321	1.451687
H	-2.008612	-6.683050	-0.765344
H	-1.132033	-4.089172	-3.238774
H	-2.879428	-6.557239	-2.756060
H	-3.087920	-5.299618	-3.973054
H	-3.309618	-4.911956	-2.255663
H	0.658873	-5.694819	-3.859270
H	-0.778931	-5.911342	-4.881077
H	-0.443797	-7.052389	-3.562771
N	-0.001623	1.563328	1.371163
H	-1.265889	-2.526278	-1.423958
H	0.359065	0.995101	2.127988
H	-0.151344	2.522514	1.649836

=== **TS8** ===

C	2.886890	-0.603965	-0.829697
C	3.327502	-1.997861	-0.330883
C	3.802538	-2.830081	-1.534354
C	4.510028	-1.833623	0.656900
C	2.177531	-2.707716	0.406502
C	1.432165	-1.932180	1.482831
C	-1.421893	-1.545529	1.837355
C	-2.676031	-0.902127	1.696787
C	-3.965243	-1.683763	2.116506

C	-4.859867	-0.804612	3.015073	H	-3.442798	4.693699	2.266920
C	-4.769178	-2.117195	0.870428	H	3.069984	-4.313555	2.296654
C	-3.625473	-2.959587	2.919009	H	2.903667	-7.263644	3.091406
C	-3.686723	1.079075	0.633884	H	4.362033	-6.254302	3.128775
C	-4.019076	0.851477	-0.735652	H	3.578157	-6.632796	1.580225
C	-3.237351	-0.145932	-1.589048	H	1.723665	-3.848827	4.364800
C	-2.080621	0.582621	-2.307591	H	3.307636	-4.563658	4.719878
C	-4.098082	-0.911442	-2.609758	H	1.848805	-5.553482	4.822357
C	-4.996796	1.651042	-1.337046	H	0.385041	-6.624695	3.526674
C	-5.634030	2.675676	-0.642960	H	-1.719873	-7.073966	2.313091
C	-5.257613	2.939628	0.670561	H	-2.093663	-6.077579	0.084332
C	-4.280046	2.179381	1.320541	H	-0.005248	-3.446882	-1.400866
C	-3.832178	2.588039	2.721380	H	-2.329126	-5.363816	-1.963549
C	-4.990854	2.872950	3.694705	H	-1.927139	-3.870503	-2.809057
C	-2.898675	3.815834	2.635115	H	-2.483087	-3.805478	-1.127338
C	0.955376	-4.718495	0.763282	H	1.466742	-5.334290	-2.106053
C	1.197787	-5.314302	2.025438	H	0.329609	-4.887688	-3.396217
C	2.519489	-5.131478	2.770632	H	0.035258	-6.338077	-2.416684
C	3.393278	-6.395758	2.633552	N	-0.414195	1.349441	2.923270
C	2.334008	-4.753009	4.252287	H	2.102748	-1.241641	1.989284
C	0.213979	-6.158326	2.560126	H	-0.749718	0.535315	3.429076
C	-0.969424	-6.419545	1.877961	H	-0.920437	2.193943	3.155106
C	-1.177381	-5.851941	0.620335				
C	-0.227022	-5.011549	0.033453	=== **Int9** ===			
C	-0.409457	-4.466573	-1.381951	C	4.067702	-0.636396	0.399425
C	-1.873214	-4.374556	-1.837255	C	4.012833	-2.118260	0.834155
C	0.409757	-5.307450	-2.385601	C	4.884799	-2.948842	-0.122663
N	1.945293	-3.929666	0.130193	C	4.579780	-2.255107	2.270095
N	-2.654907	0.345529	1.244928	C	2.563746	-2.633718	0.834657
P	-0.083496	-0.950764	0.881129	C	1.547849	-1.882866	1.702902
P	0.229685	1.176758	1.394365	C	-1.288785	-1.505319	1.931044
H	2.603280	0.065078	-0.008355	C	-2.611365	-0.949919	1.896527
H	2.042170	-0.674327	-1.523864	C	-3.635671	-1.532857	2.933399
H	3.717516	-0.123618	-1.359907	C	-4.113679	-0.419897	3.890635
H	2.994010	-2.979893	-2.257107	C	-4.854609	-2.130180	2.196618
H	4.153028	-3.817947	-1.224251	C	-3.042080	-2.660833	3.807782
H	4.624548	-2.308705	-2.039468	C	-4.036027	0.738132	0.795357
H	5.351552	-1.348518	0.148459	C	-4.924702	0.321730	-0.236064
H	4.853866	-2.807118	1.024567	C	-4.659199	-0.938827	-1.059732
H	4.250272	-1.213413	1.522737	C	-3.988437	-0.570189	-2.400219
H	1.042734	-2.627853	2.228896	C	-5.917007	-1.788451	-1.318885
H	-1.316500	-2.505759	2.325484	C	-6.020768	1.133138	-0.550404
H	-4.320442	-0.473364	3.910604	C	-6.240146	2.345648	0.097037
H	-5.730223	-1.384701	3.345525	C	-5.330553	2.776655	1.058149
H	-5.227761	0.076106	2.487434	C	-4.216588	2.007391	1.415075
H	-5.141613	-1.259191	0.306922	C	-3.187322	2.583651	2.388515
H	-5.634552	-2.714094	1.184966	C	-3.814330	3.229589	3.638718
H	-4.161827	-2.736122	0.201243	C	-2.277209	3.604425	1.670663
H	-3.077275	-3.695986	2.323130	C	1.014340	-4.308068	0.180023
H	-4.559674	-3.431653	3.244787	C	0.596317	-5.129767	1.256566
H	-3.039898	-2.736657	3.818761	C	1.497349	-5.417136	2.457560
H	-2.783417	-0.886748	-0.924652	C	2.140951	-6.813151	2.318932
H	-2.468226	1.336631	-3.003833	C	0.776912	-5.284292	3.812466
H	-1.471777	-0.129370	-2.879413	C	-0.645566	-5.771260	1.153864
H	-1.427308	1.085806	-1.587984	C	-1.450300	-5.622825	0.028386
H	-4.950253	-1.409219	-2.134775	C	-1.001317	-4.850028	-1.042049
H	-3.492647	-1.679161	-3.105543	C	0.235048	-4.199302	-1.003125
H	-4.488788	-0.254071	-3.395324	C	0.780508	-3.455257	-2.219871
H	-5.256744	1.476215	-2.376900	C	-0.304168	-2.882625	-3.145046
H	-6.396911	3.278102	-1.128700	C	1.738042	-4.372468	-3.012216
H	-5.726897	3.763873	1.201041	N	2.292193	-3.698753	0.194318
H	-3.255457	1.755089	3.134850	N	-2.856450	0.000607	1.037488
H	-5.576577	3.748434	3.391599	P	0.024331	-1.196507	0.875869
H	-4.599023	3.078808	4.698448	P	0.593675	0.375958	-0.401412
H	-5.675391	2.021788	3.766997	H	3.495718	0.024072	1.060200
H	-2.068516	3.640857	1.939938	H	3.683211	-0.504965	-0.617760
H	-2.489747	4.073951	3.622216	H	5.107846	-0.290492	0.413665

H	4.515665	-2.886312	-1.150875	H	-4.383690	4.132731	3.390119
H	4.894499	-4.005389	0.158931	H	-3.026240	3.529438	4.339914
H	5.913838	-2.570784	-0.100014	H	-4.489065	2.543418	4.160943
H	5.617731	-1.903490	2.290807	H	-1.758141	3.153857	0.818914
H	4.572930	-3.300879	2.599232	H	-1.519690	3.996064	2.361728
H	4.019623	-1.663388	3.003321	H	-2.864142	4.453553	1.299041
H	1.146544	-2.575935	2.448764	H	2.317412	-4.692586	2.454596
H	-1.059443	-2.309450	2.617423	H	1.376085	-7.598921	2.318574
H	-3.270013	0.046780	4.411936	H	2.826942	-7.009323	3.152287
H	-4.777901	-0.852844	4.649109	H	2.705460	-6.894147	1.383849
H	-4.669140	0.357587	3.364741	H	0.313174	-4.297696	3.933740
H	-5.412931	-1.369328	1.649987	H	1.487822	-5.425259	4.635264
H	-5.534569	-2.583454	2.928584	H	-0.012108	-6.034997	3.932783
H	-4.549872	-2.913753	1.493624	H	-0.981484	-6.409578	1.966711
H	-2.706441	-3.516304	3.211713	H	-2.411964	-6.125834	-0.026550
H	-3.820334	-3.022498	4.489647	H	-1.620080	-4.763621	-1.929213
H	-2.207187	-2.312182	4.426382	H	1.368667	-2.605786	-1.856319
H	-3.949210	-1.559739	-0.506117	H	-0.870131	-3.671233	-3.655554
H	-4.645662	0.065446	-3.005963	H	0.162140	-2.267331	-3.923364
H	-3.757410	-1.471583	-2.981514	H	-1.013456	-2.253665	-2.595647
H	-3.052784	-0.025449	-2.235842	H	2.551693	-4.735327	-2.376722
H	-6.435144	-2.043508	-0.388727	H	2.177883	-3.829804	-3.858183
H	-5.641189	-2.723724	-1.820898	H	1.200085	-5.241540	-3.410370
H	-6.632793	-1.273075	-1.969803	N	-0.843656	1.182890	-0.809923
H	-6.710906	0.814678	-1.326945	H	2.019577	-1.070837	2.251413
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H	-5.481916	3.741121	1.535325	H	-1.047345	1.233170	-1.800283
H	-2.547951	1.762722	2.726485				

V. References

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[3] Complete List of Authors of Gaussian 09 **(**Gaussian 09, Revision B.01);
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

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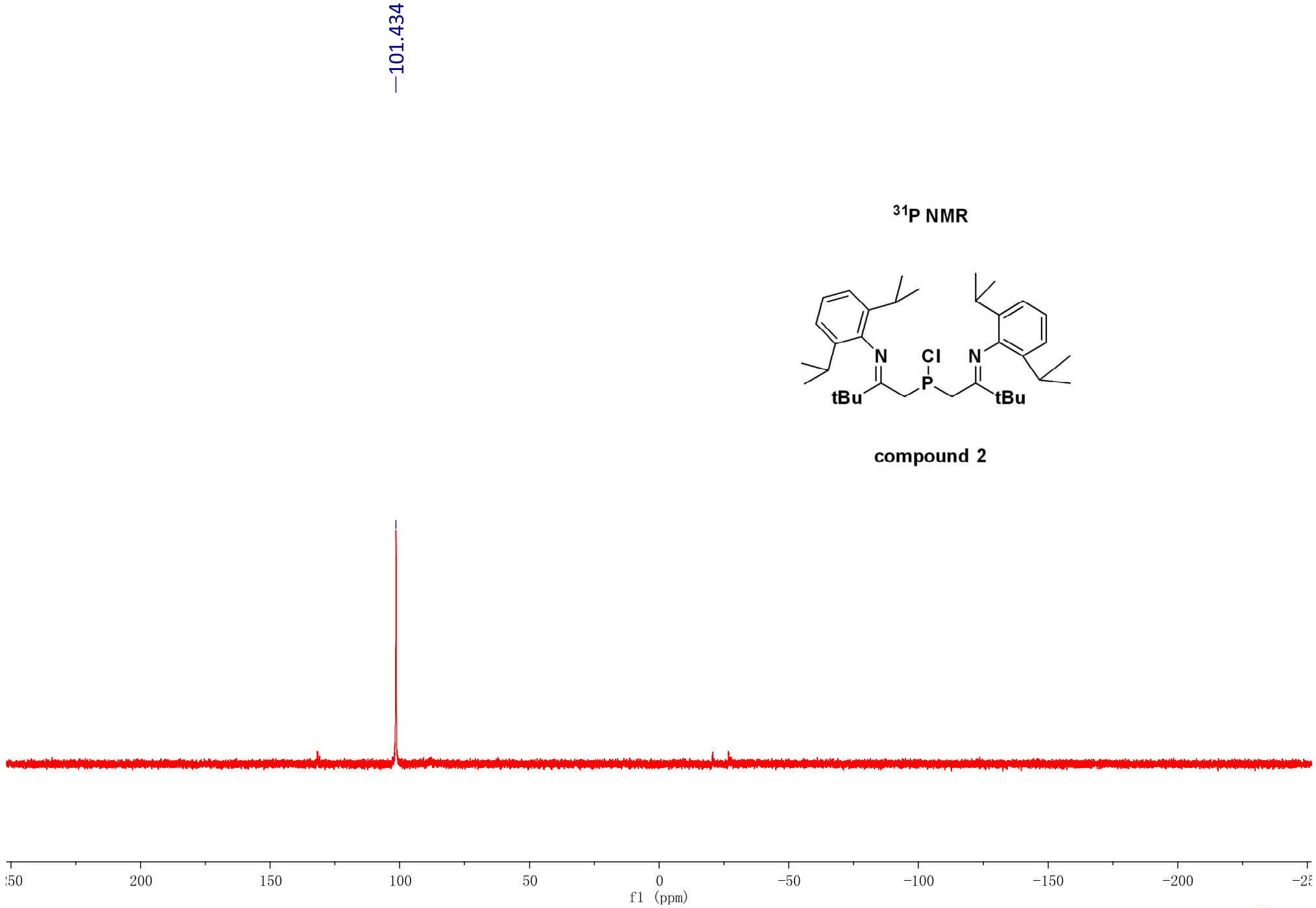
[7] (a) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104. (c) Johnson, E. R.; Becke, A. D. *J. Chem. Phys.* **2006**, *124*, 174104. (d) Becke, A. D.; Johnson, E. R. *J. Chem. Phys.* **2005**, *123*, 154101. (e) Johnson, E. R.; Becke, A. D. *J. Chem. Phys.* **2005**, *123*, 024101.

VI. NMR spectra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N
Cl
N
P
tBu
tBu
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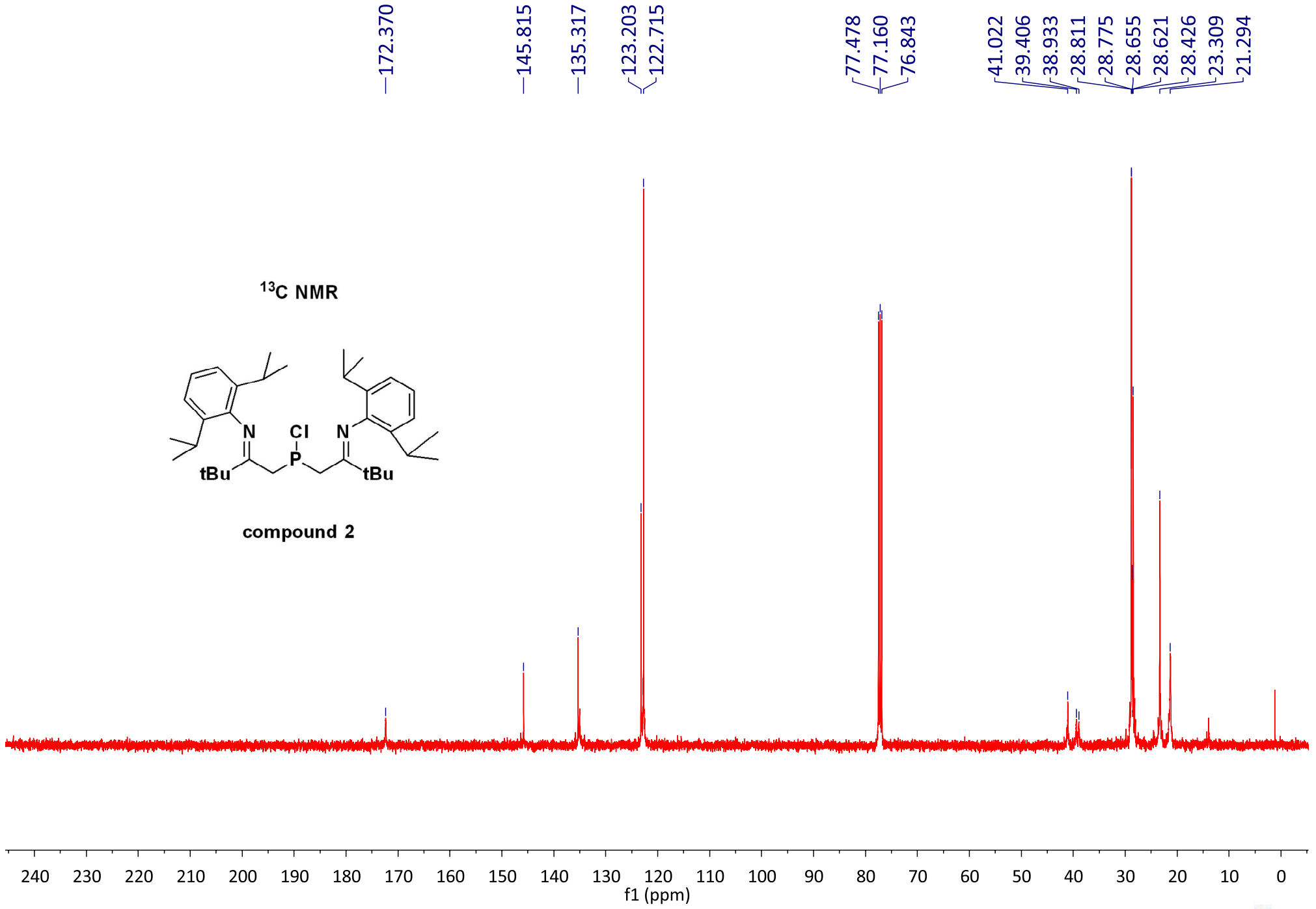
200
150
100
50
0
−50
−100
−150
−200
f1 (ppm)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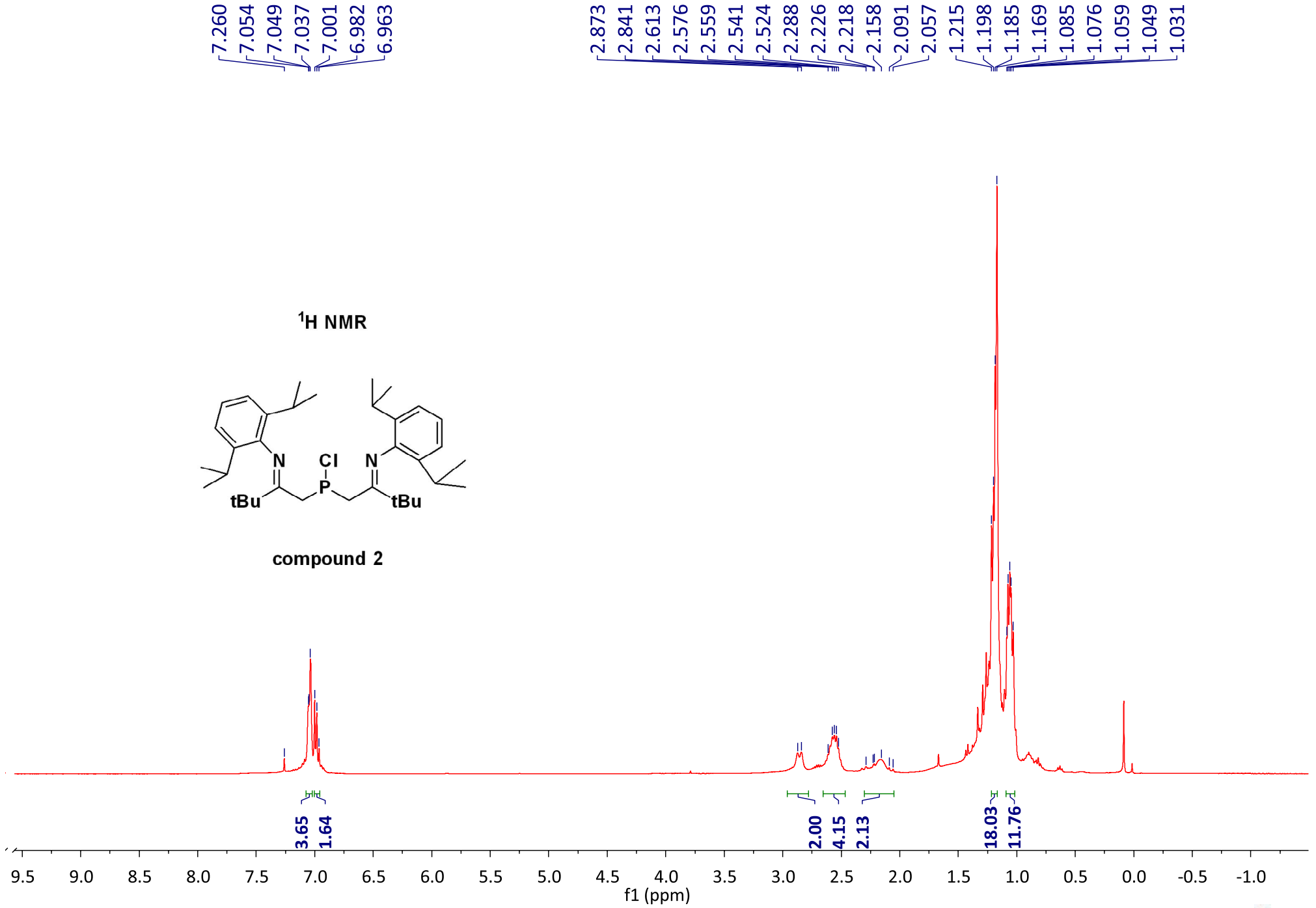
145.815
135.317
123.203
122.715
77.478
77.160
76.843
41.022
39.406
38.933
28.811
28.775
28.655
28.621
28.426
23.309
21.294
13C NMR
N
Cl
N
P
tBu
tBu
compound 2
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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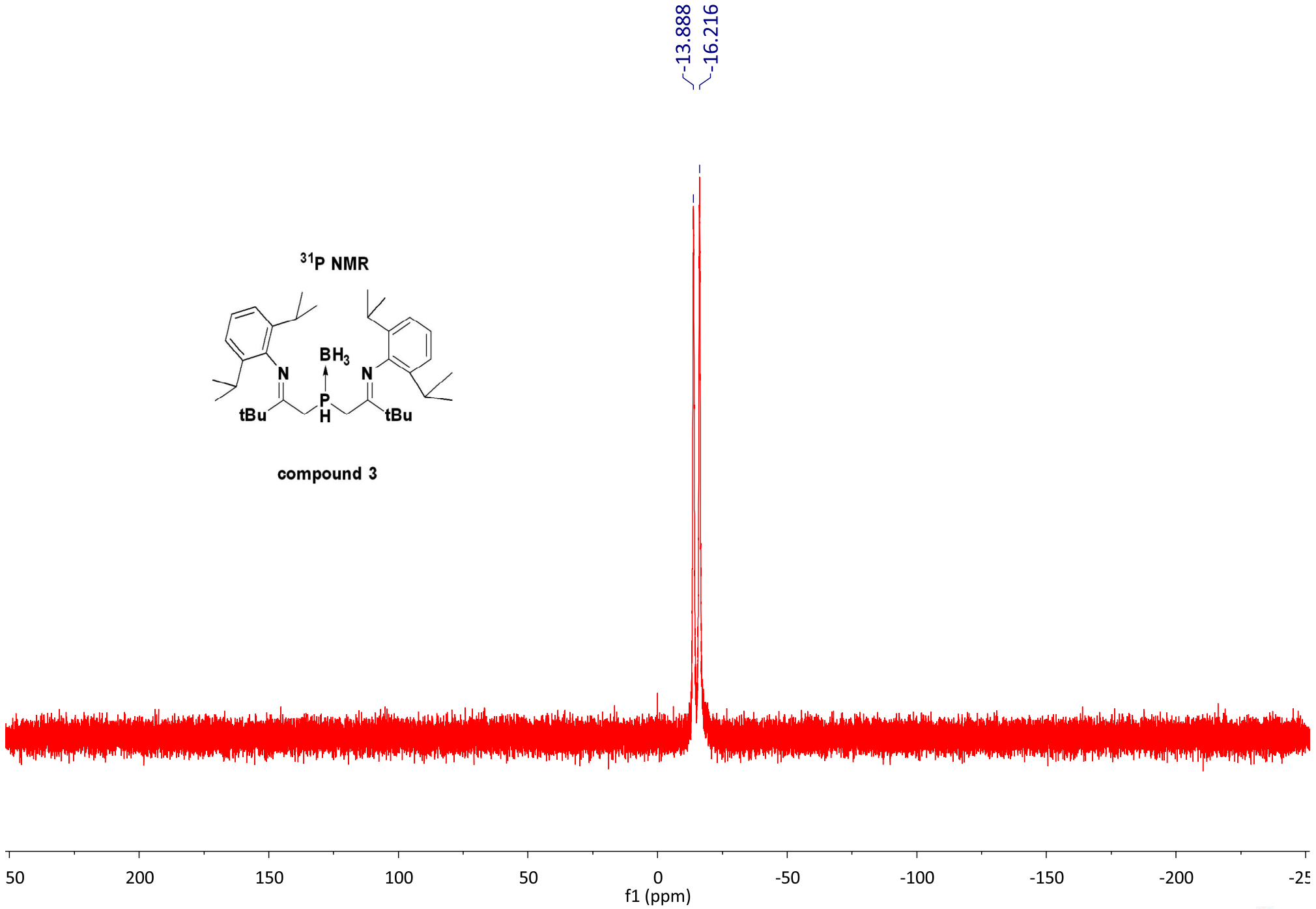
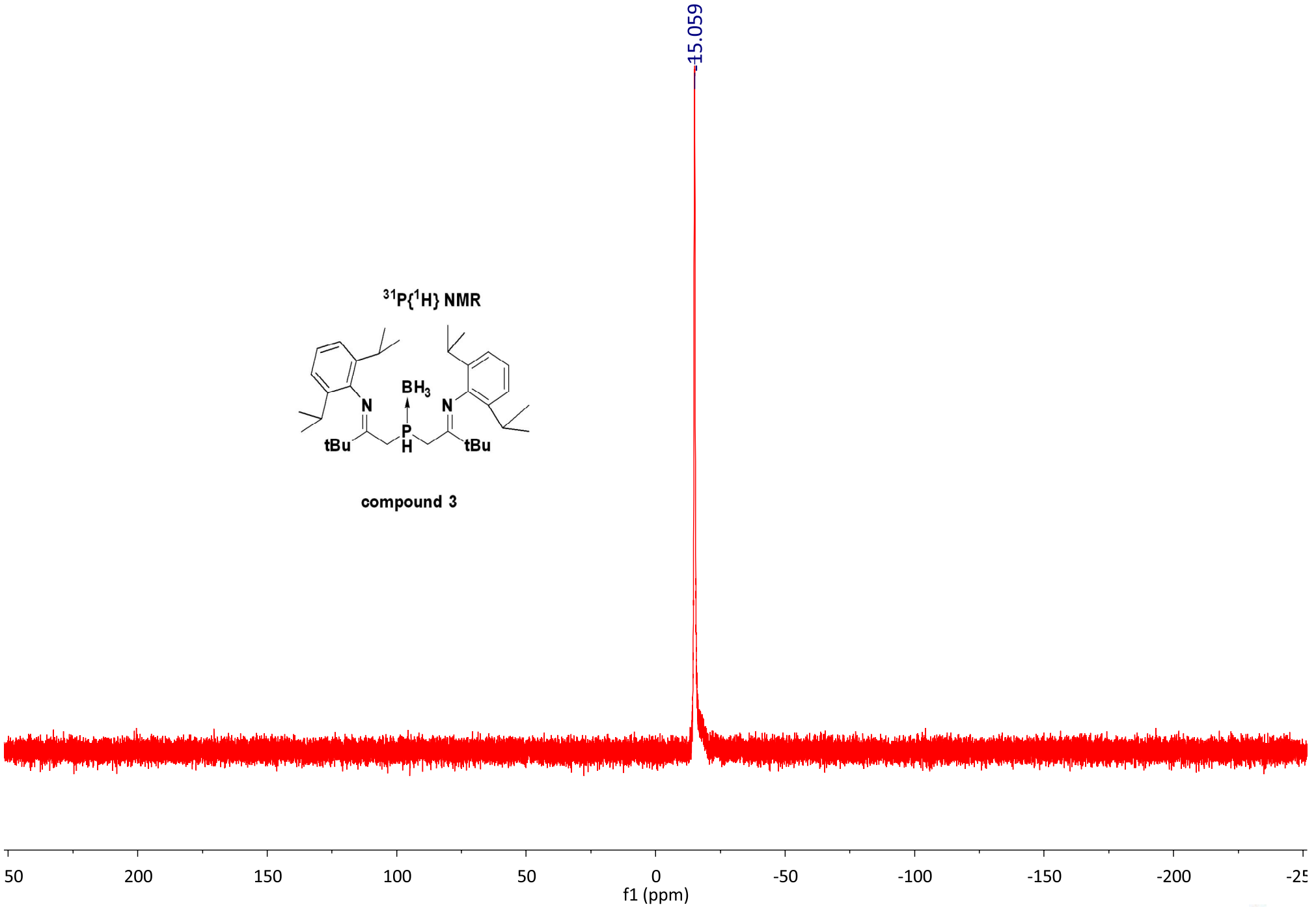
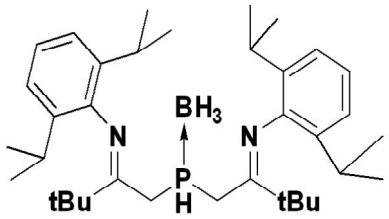
7.054
7.049
7.037
7.001
6.982
6.963
2.873
2.841
2.613
2.576
2.559
2.541
2.524
2.288
2.226
2.218
2.158
2.091
2.057
1.215
1.198
1.185
1.169
1.085
1.076
1.059
1.049
1.031
^{1}H NMR
N
Cl
N
P
tBu
tBu
compound 2
3.65
1.64
2.00
4.15
2.13
18.03
11.76
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

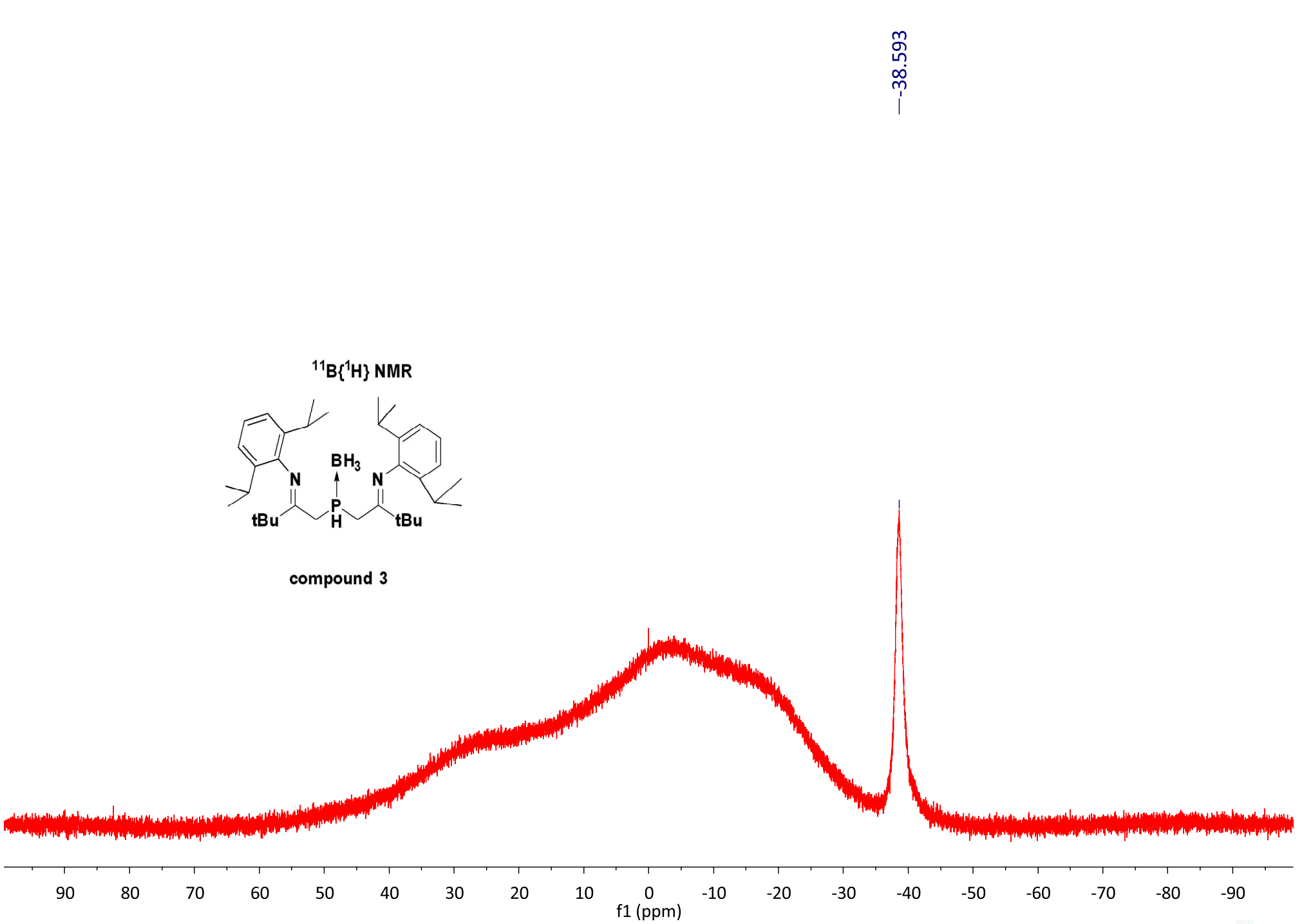

-13.888
-16.216
31P NMR
BH3
N
N
P
H
tBu
tBu
compound 3
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)

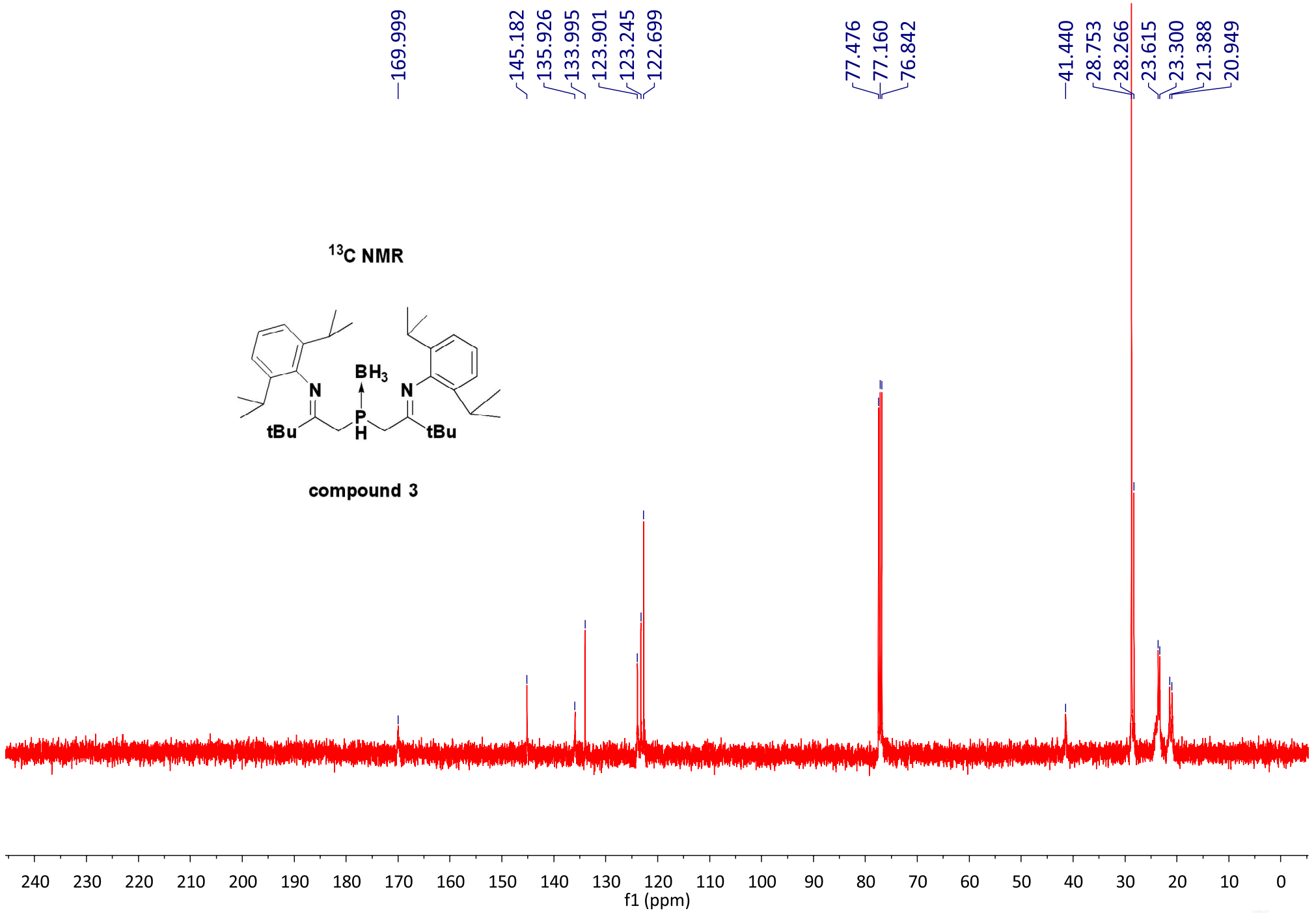

-15.059
$^{31}P\{^{1}H\}$ NMR
BH3
N
N
P
H
tBu
tBu
compound 3
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)

^{11}B NMR



compound 3


-38.593
$^{11}B\{^{1}H\}$ NMR
BH3
N
N
P
H
tBu
tBu
compound 3
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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135.926
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123.901
123.245
122.699
77.476
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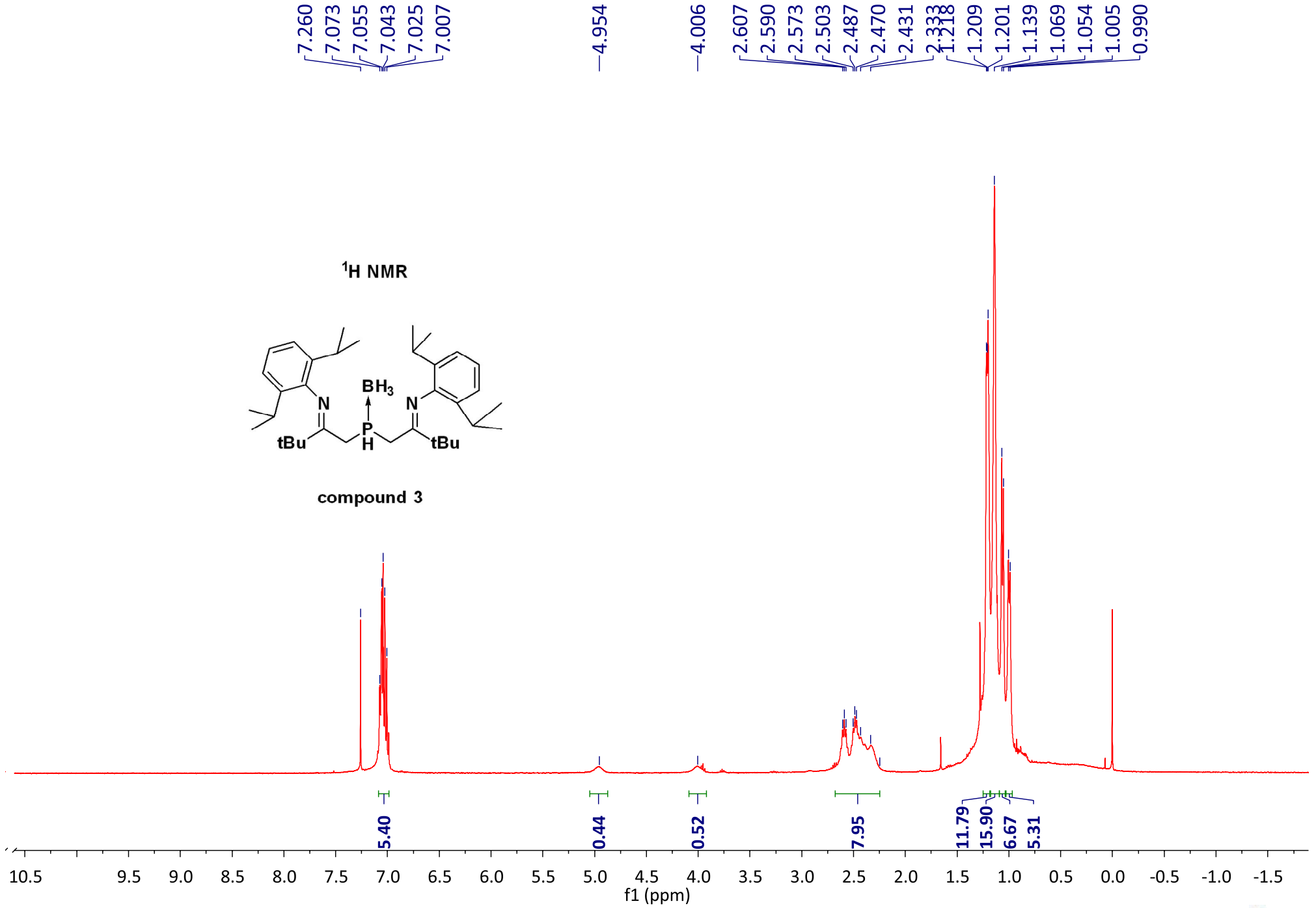
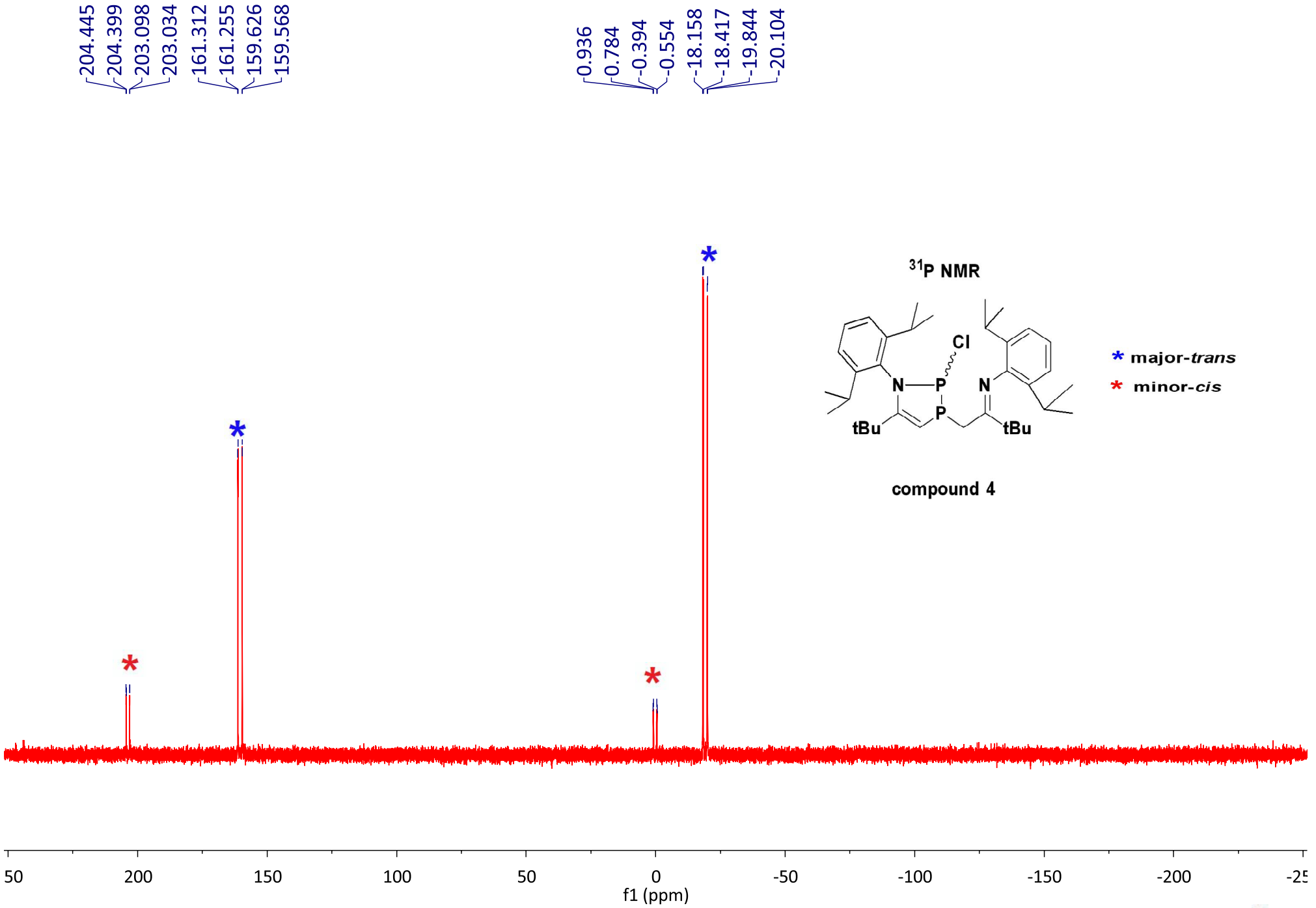
76.842
41.440
28.753
28.266
23.615
23.300
21.388
20.949
13C NMR
BH3
N
N
P
H
tBu
tBu
compound 3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.260
7.073
7.055
7.043
7.025
7.007
4.954
4.006
2.607
2.590
2.573
2.503
2.487
2.470
2.431
2.333
1.218
1.209
1.201
1.139
1.069
1.054
1.005
0.990
^{1}H NMR
BH$_3$
N
N
P
H
tBu
tBu
compound 3
5.40
0.44
0.52
7.95
11.79
15.90
6.67
5.31
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)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161.255
159.626
159.568
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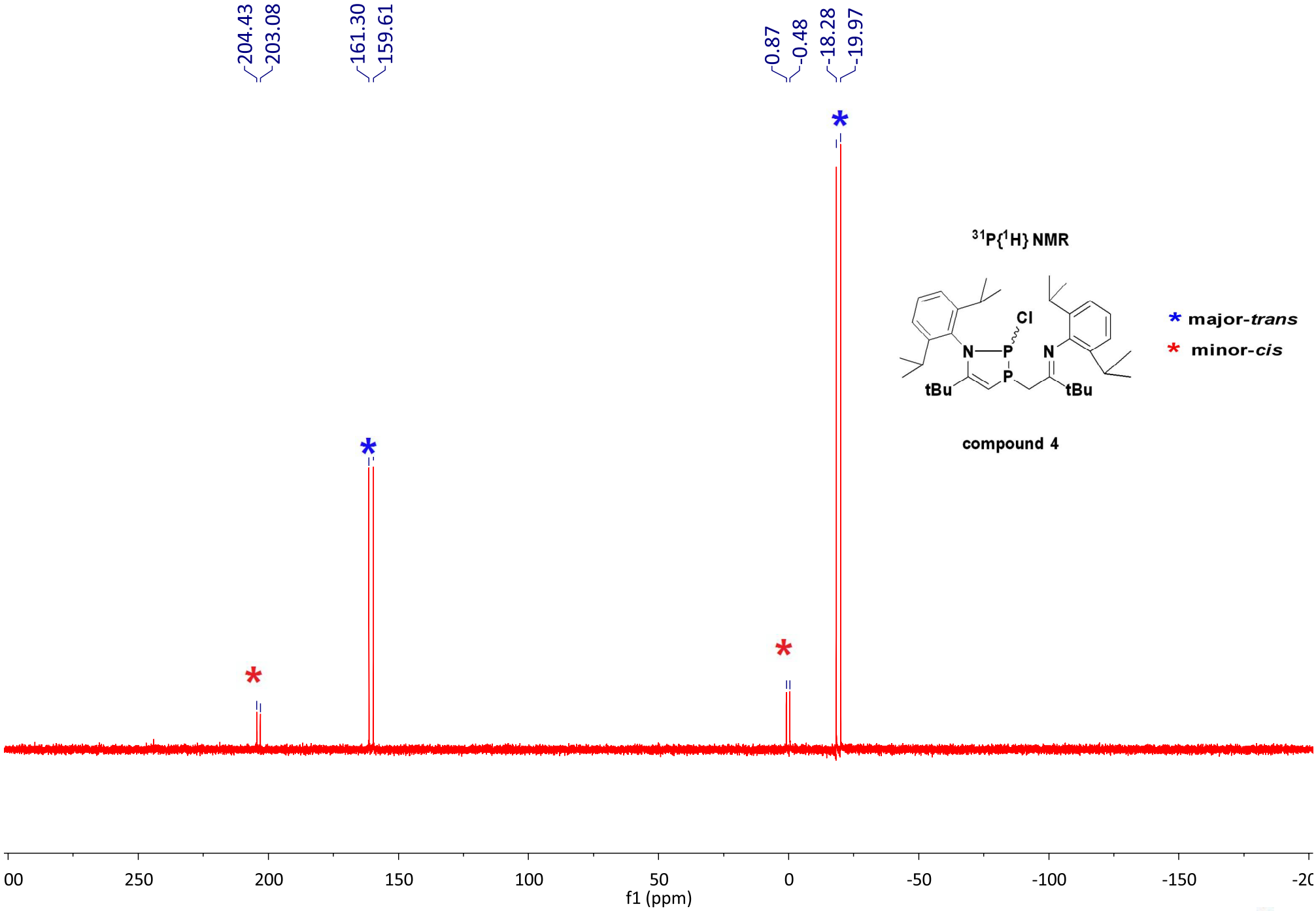
0.784
-0.394
-0.554
-18.158
-18.417
-19.844
-20.104
31P NMR
Cl
N
P
P
N
tBu
tBu
* major-trans
* minor-cis
compound 4
50
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)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159.61
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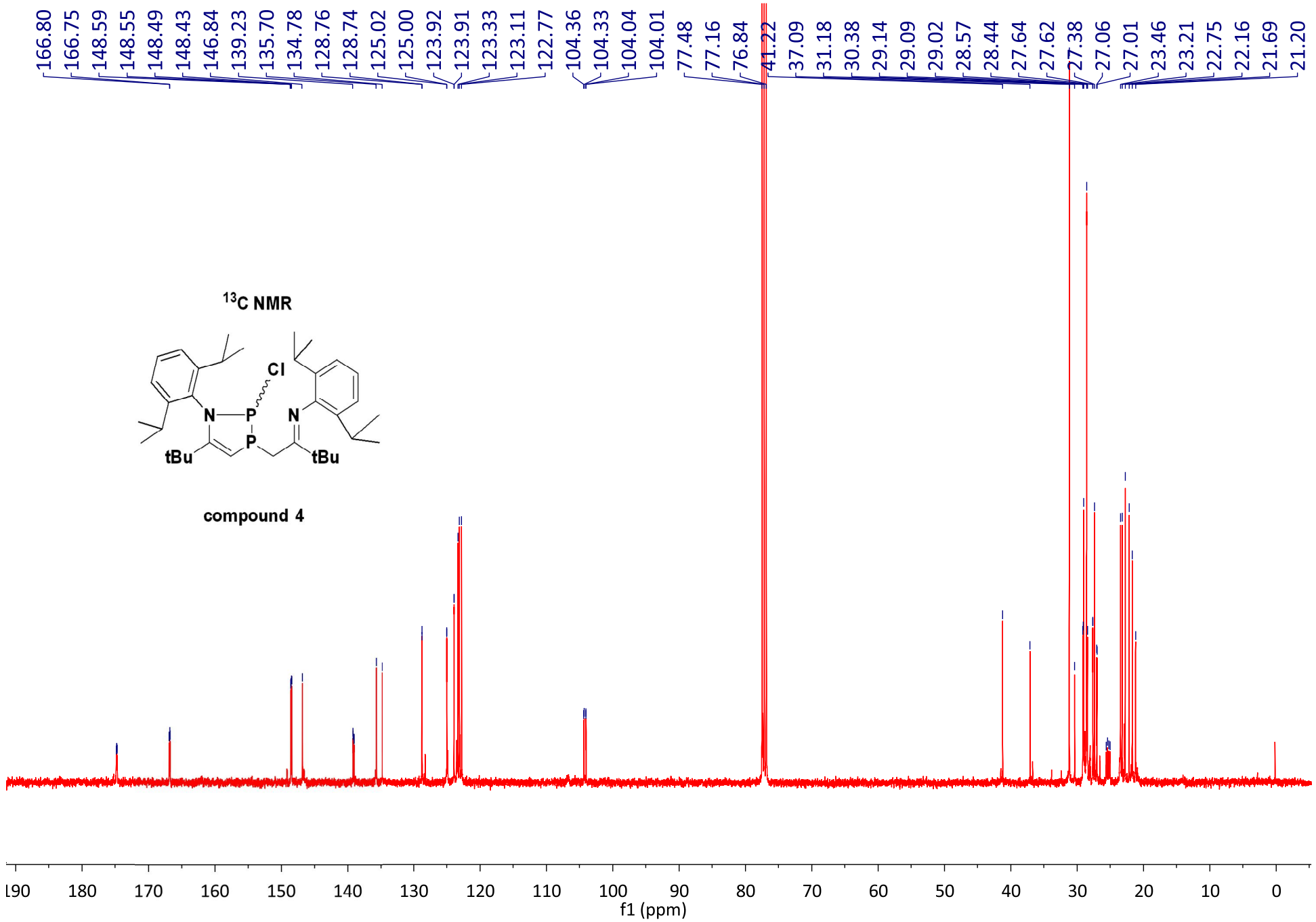
31P{1H} NMR
Cl
N
P
P
N
tBu
tBu
compound 4
* major-trans
* minor-cis
00
250
200
150
100
50
0
-50
-100
-150
-20
f1 (ppm)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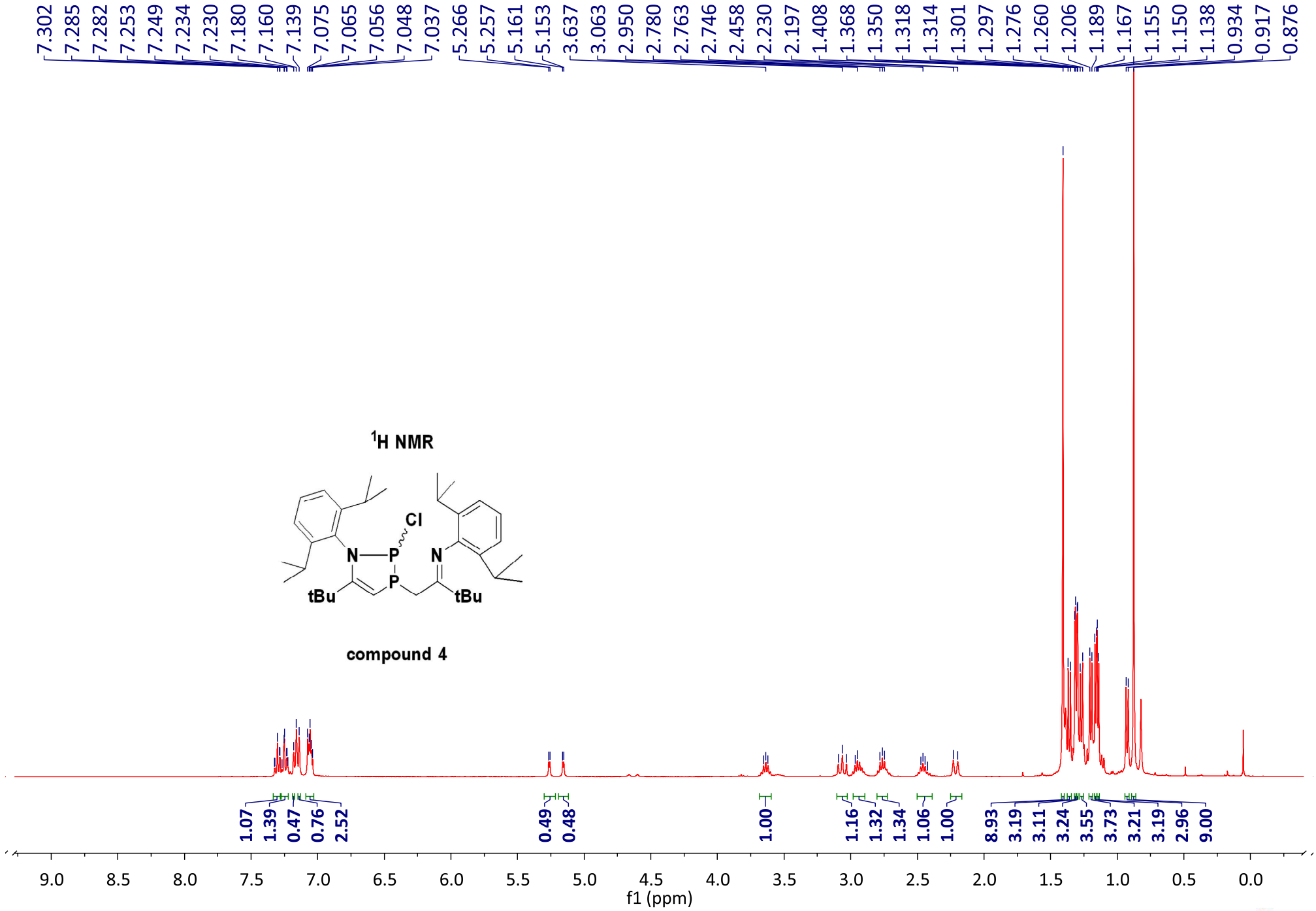
134.78
128.76
128.74
125.02
125.00
123.92
123.91
123.33
123.11
122.77
104.36
104.33
104.04
104.01
77.48
77.16
76.84
41.22
37.09
31.18
30.38
29.14
29.09
29.02
28.57
28.44
27.64
27.62
27.38
27.06
27.01
23.46
23.21
22.75
22.16
21.69
21.20
13C NMR
Cl
N
P
N
P
tBu
tBu
compound 4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.056
7.048
7.037
5.266
5.257
5.161
5.153
3.637
3.063
2.950
2.780
2.763
2.746
2.458
2.230
2.197
1.408
1.368
1.350
1.318
1.314
1.301
1.297
1.276
1.260
1.206
1.189
1.167
1.155
1.150
1.138
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0.917
0.876
1H NMR
Cl
N
P
N
P
tBu
tBu
compound 4
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1.39
0.47
0.76
2.52
0.49
0.48
1.00
1.16
1.32
1.34
1.06
1.00
8.93
3.19
3.11
3.24
3.55
3.73
3.21
3.19
2.96
9.00
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8.0
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7.0
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6.0
5.5
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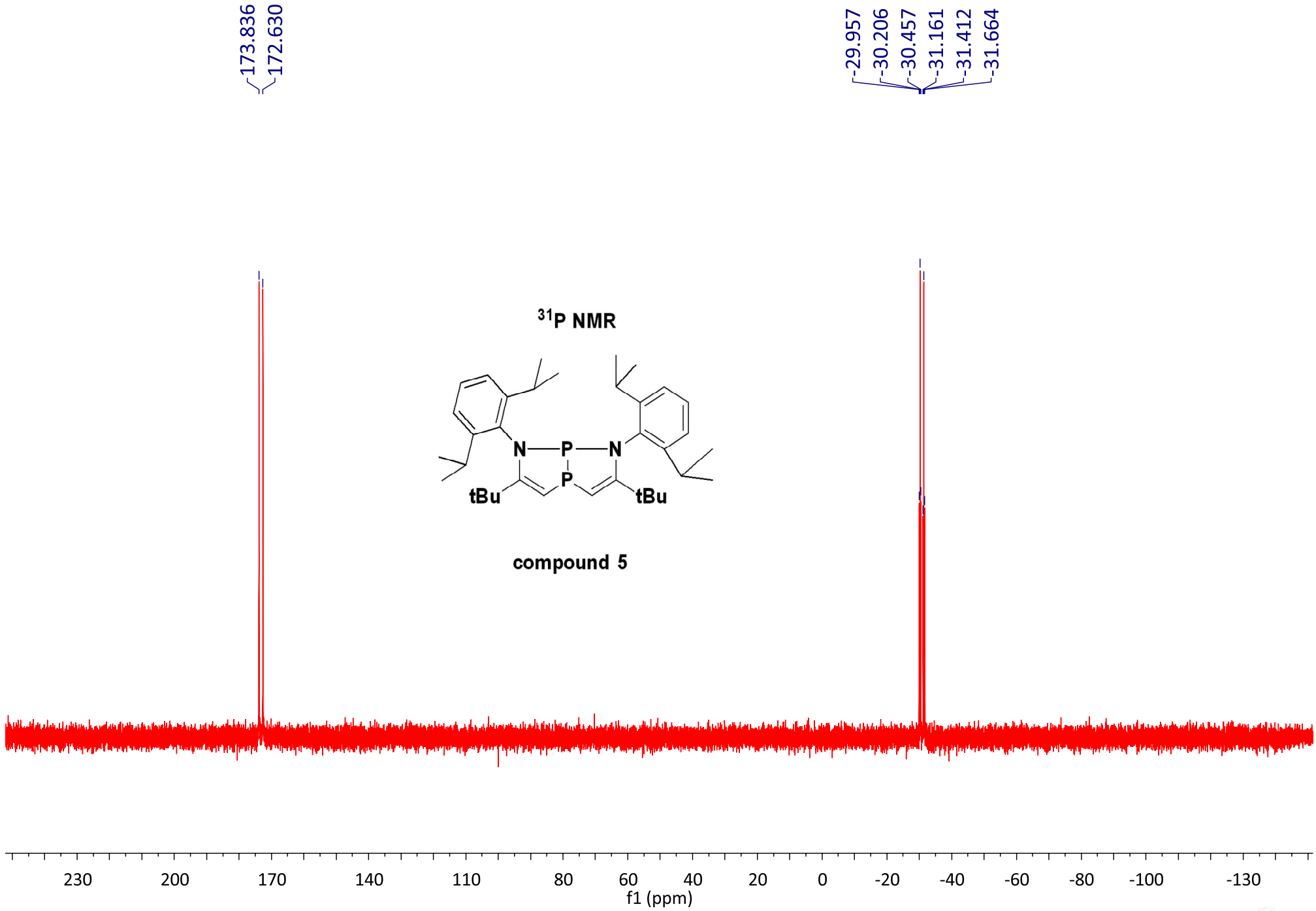
f1 (ppm)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172.630
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-30.457
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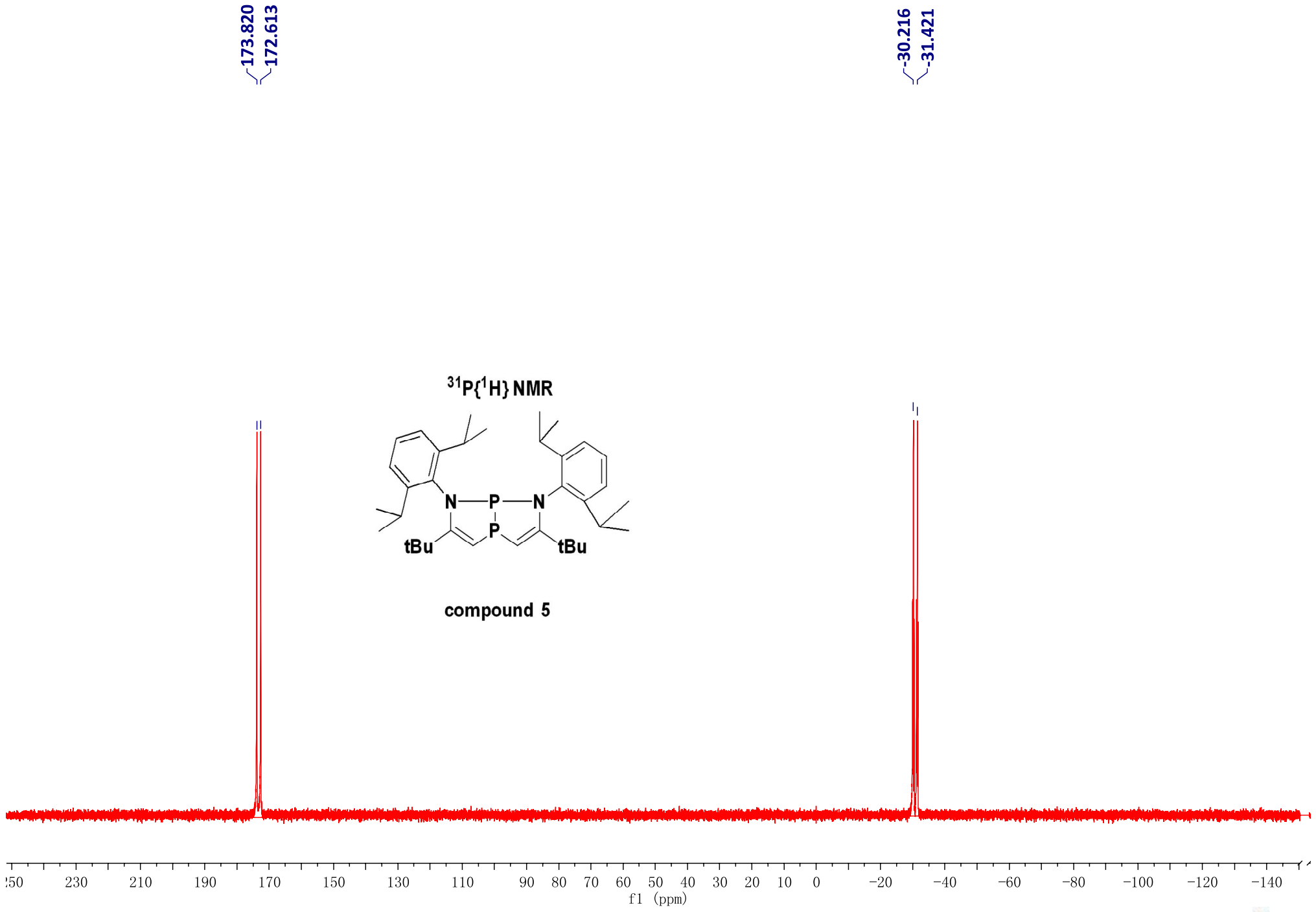
-31.412
-31.664
31P NMR
N
P
N
P
tBu
tBu
compound 5
230
200
170
140
110
80
60
40
20
0
-20
-40
-60
-80
-100
-130
f1 (ppm)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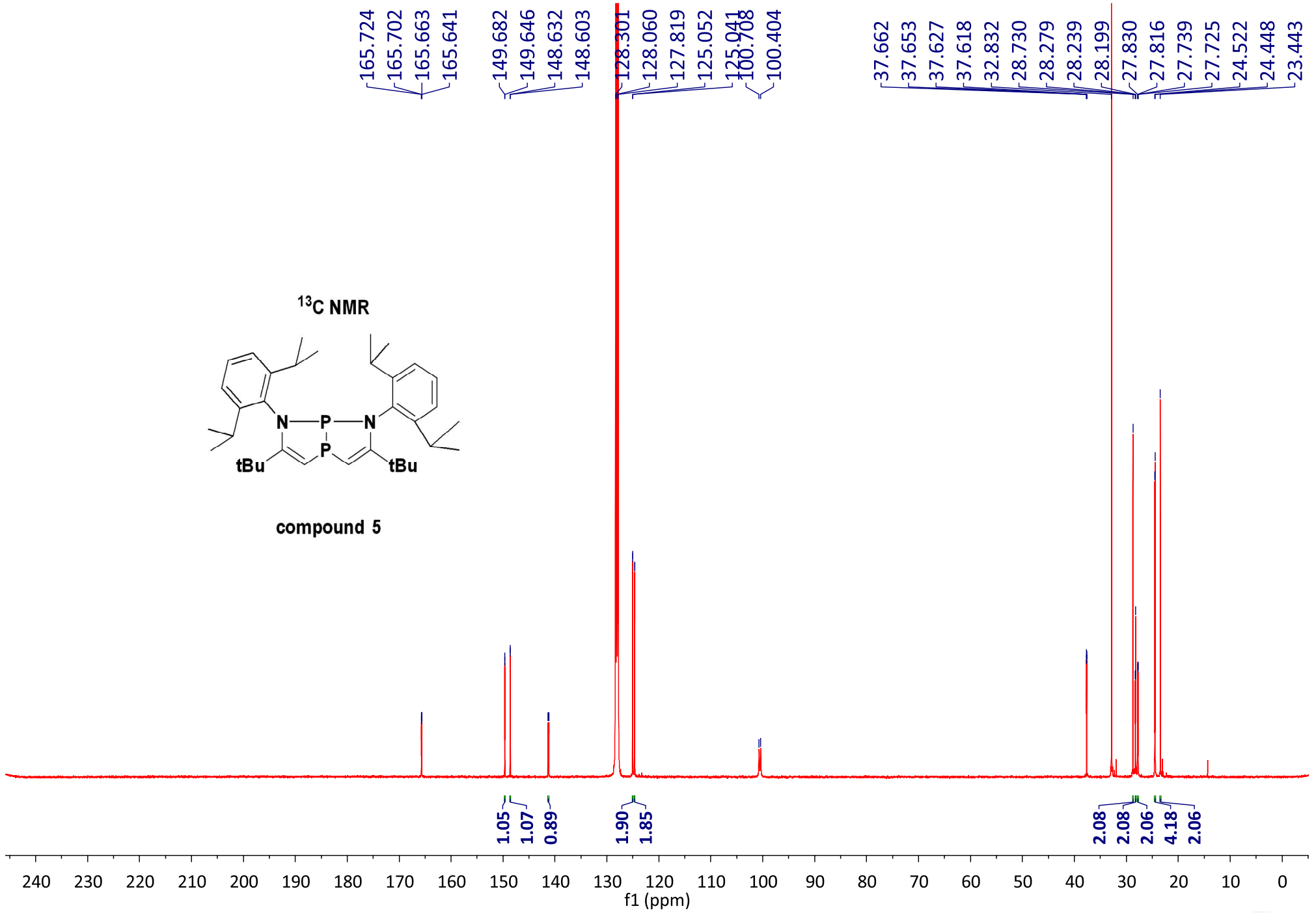
N
P
N
P
tBu
tBu
compound 5
f1 (ppm)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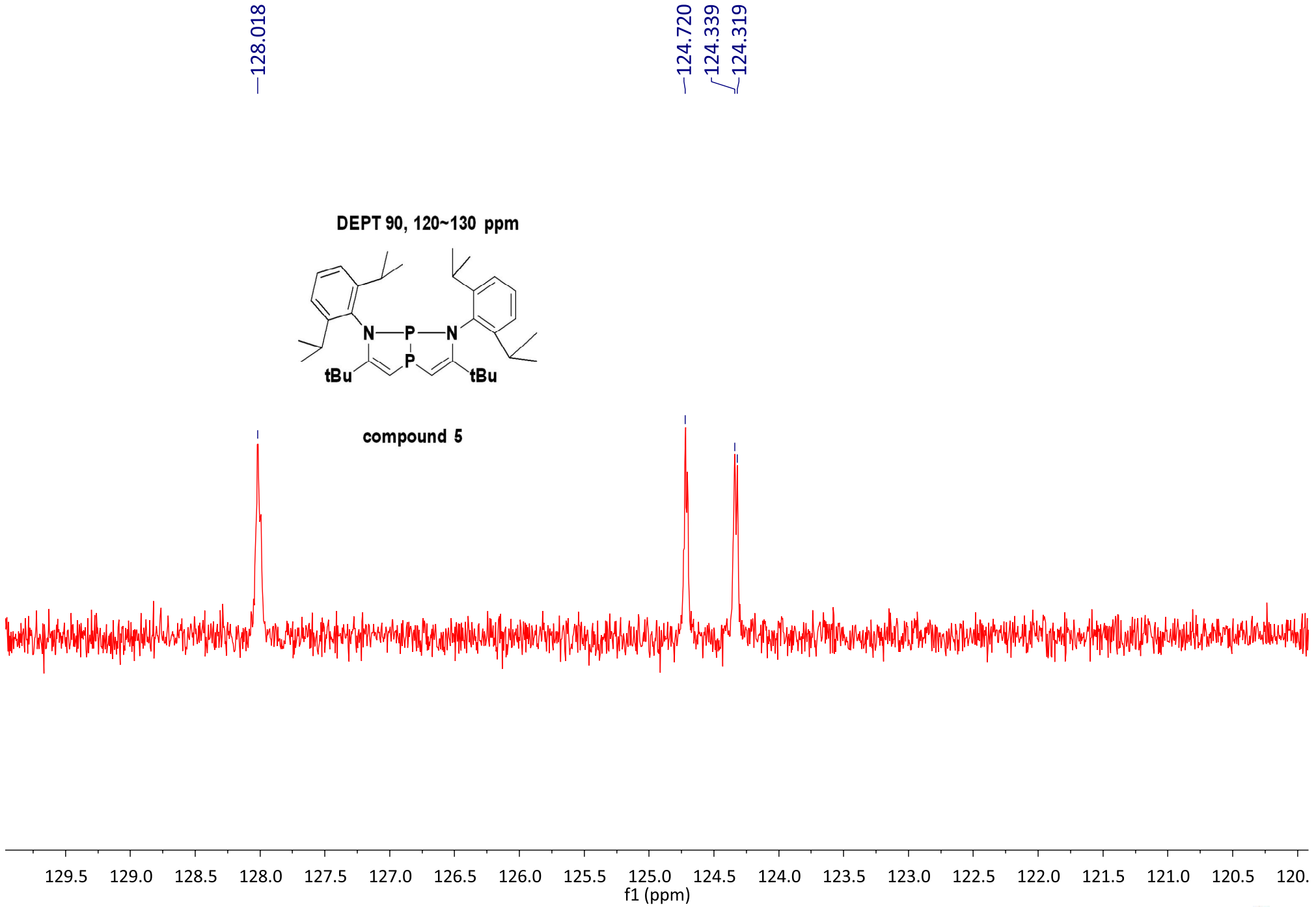
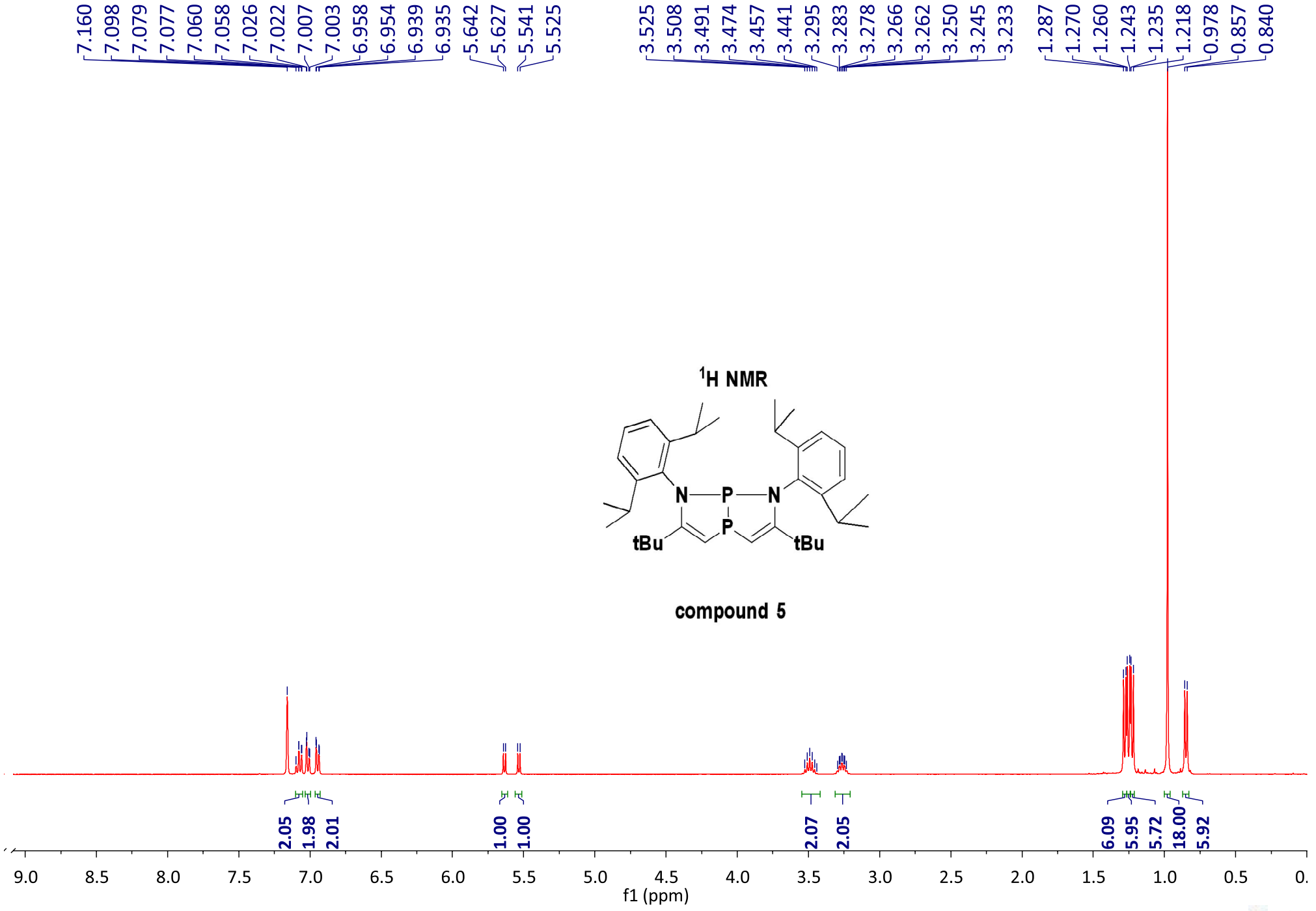
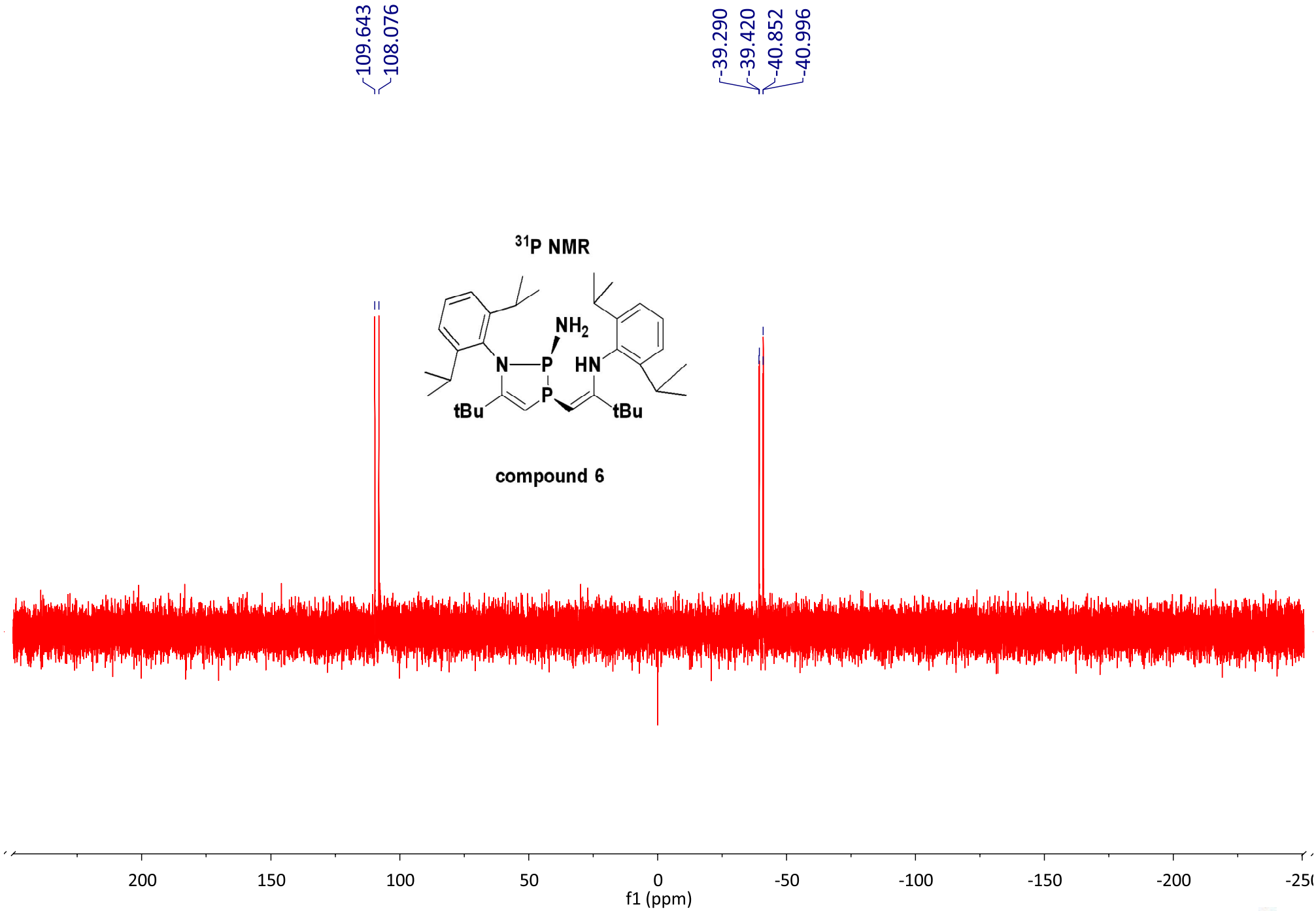
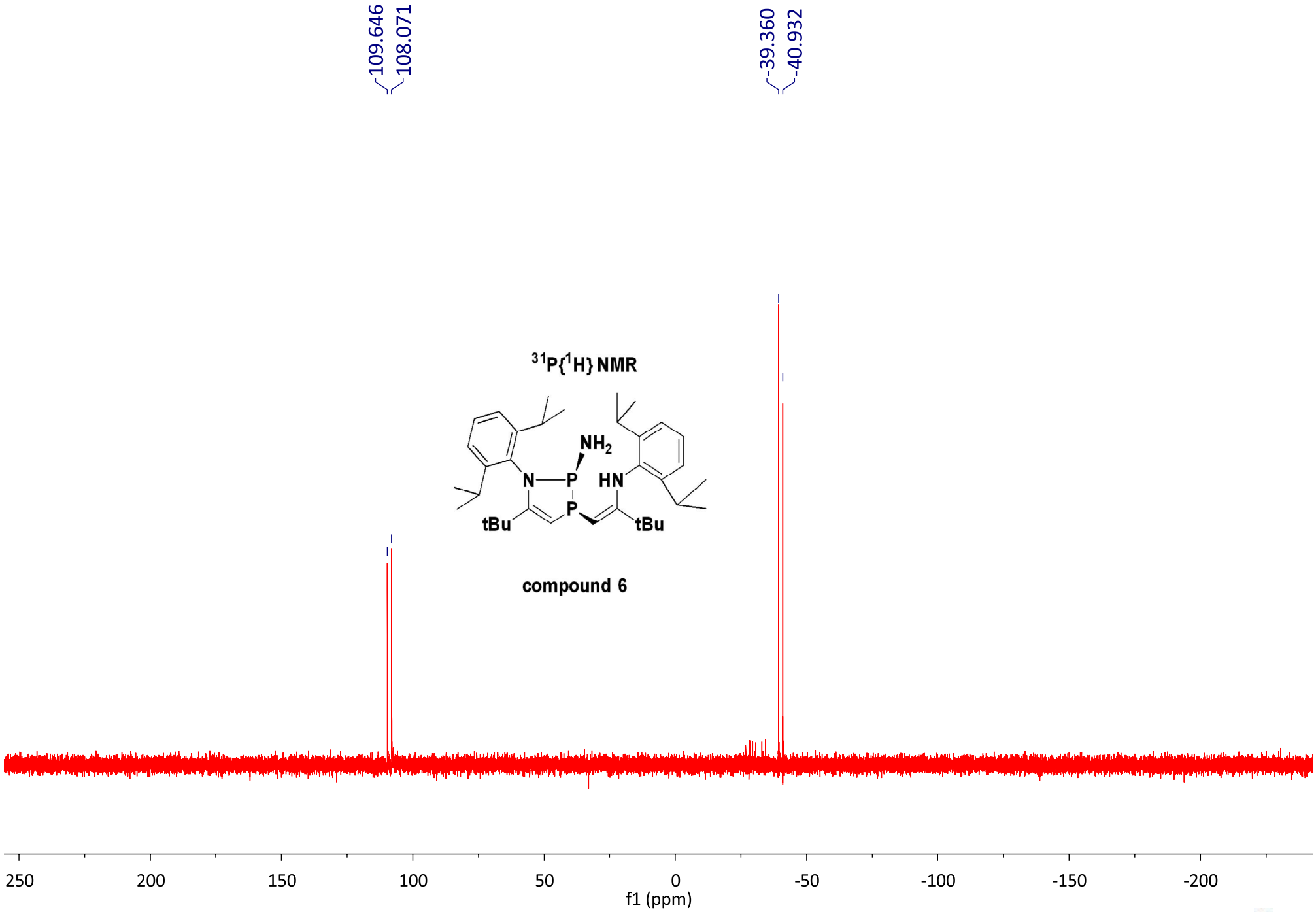
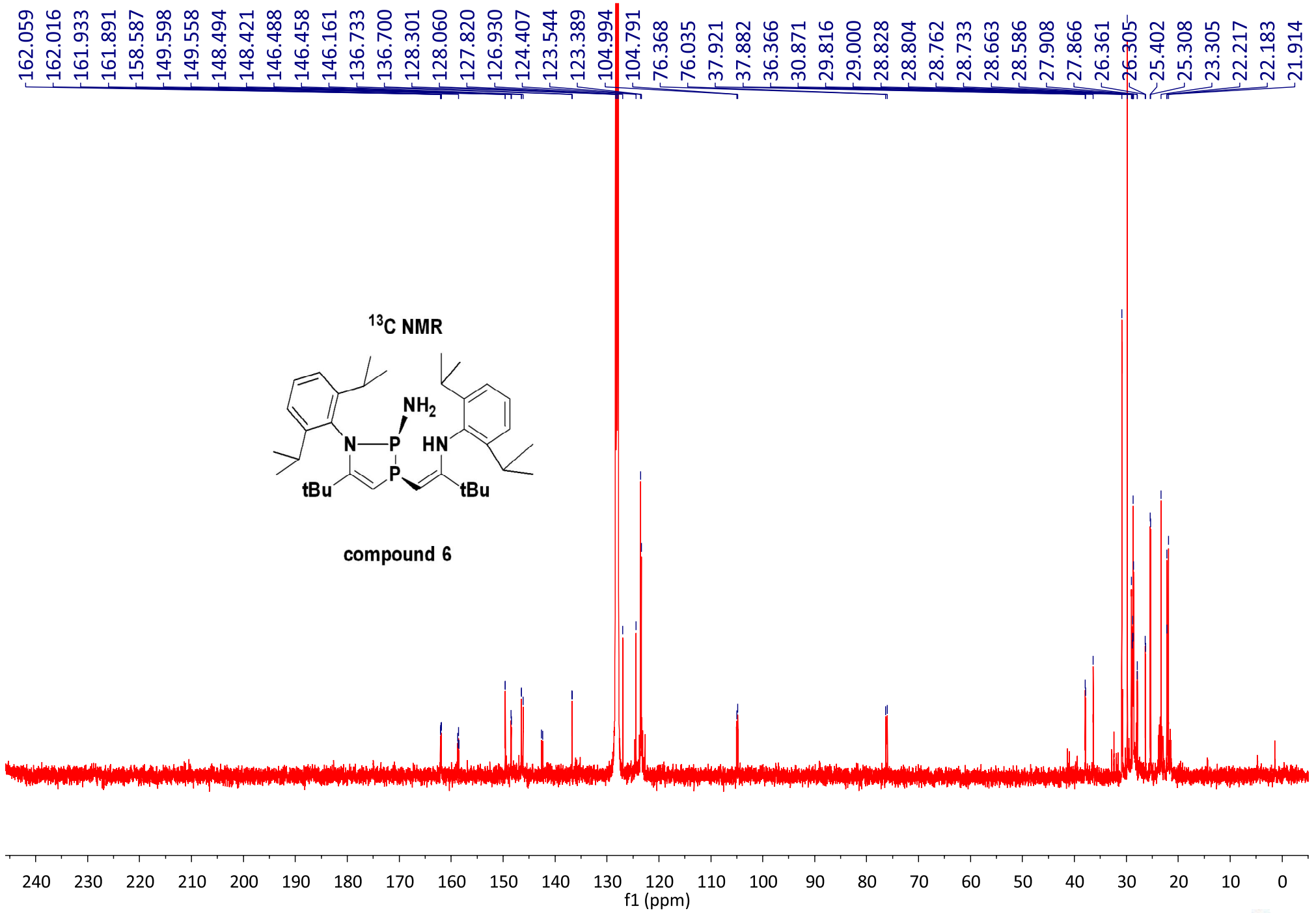
125.041
100.708
100.404
37.662
37.653
37.627
37.618
32.832
28.730
28.279
28.239
28.199
27.830
27.816
27.739
27.725
24.522
24.448
23.443
13C NMR
N
P
N
P
tBu
tBu
compound 5
1.05
1.07
0.89
1.90
1.85
2.08
2.08
2.06
4.18
2.06
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

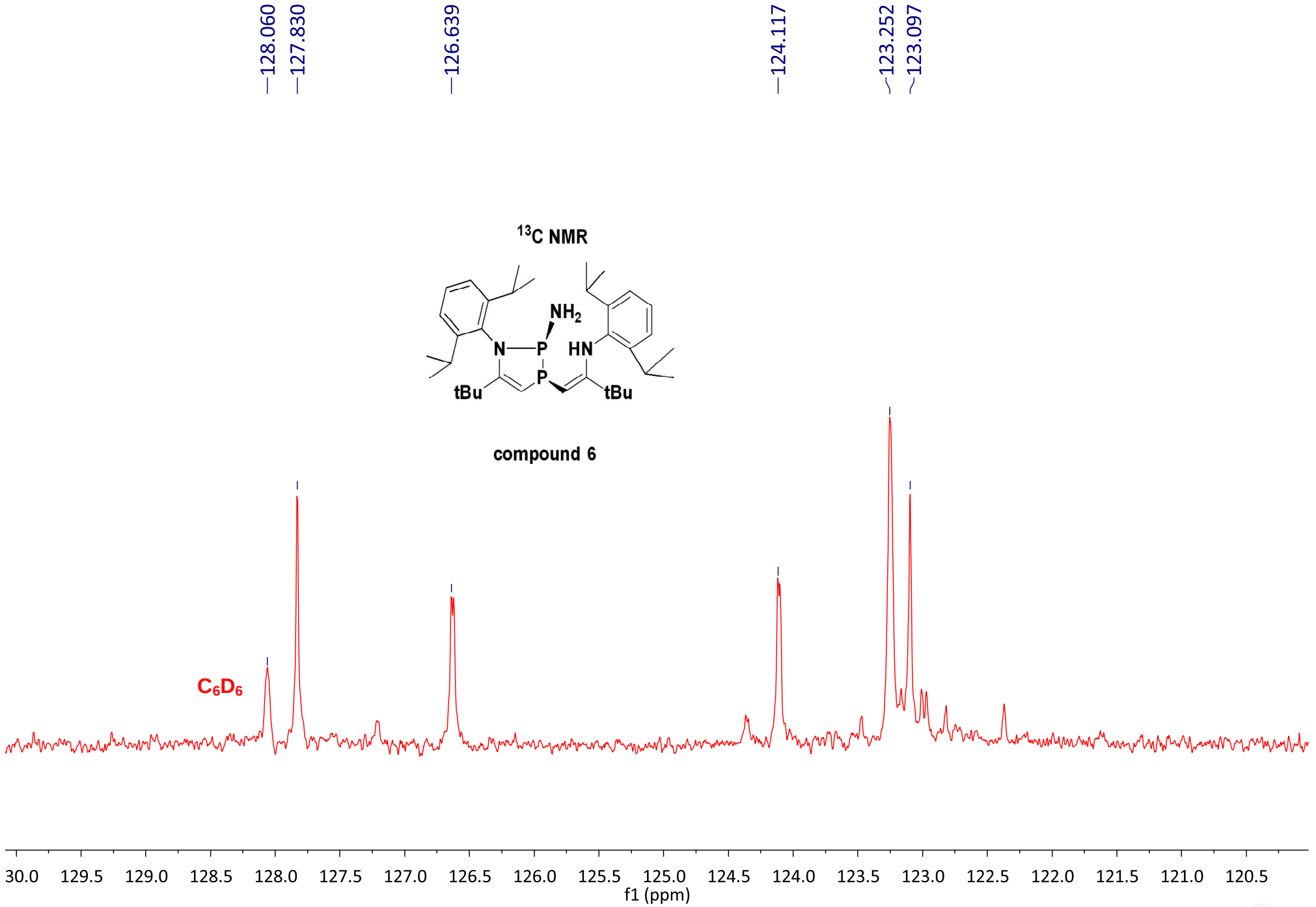

128.018
124.720
124.339
124.319
DEPT 90, 120~130 ppm
N
P
N
P
tBu
tBu
compound 5
129.5
129.0
128.5
128.0
127.5
127.0
126.5
126.0
125.5
125.0
124.5
124.0
123.5
123.0
122.5
122.0
121.5
121.0
120.5
120.
f1 (ppm)

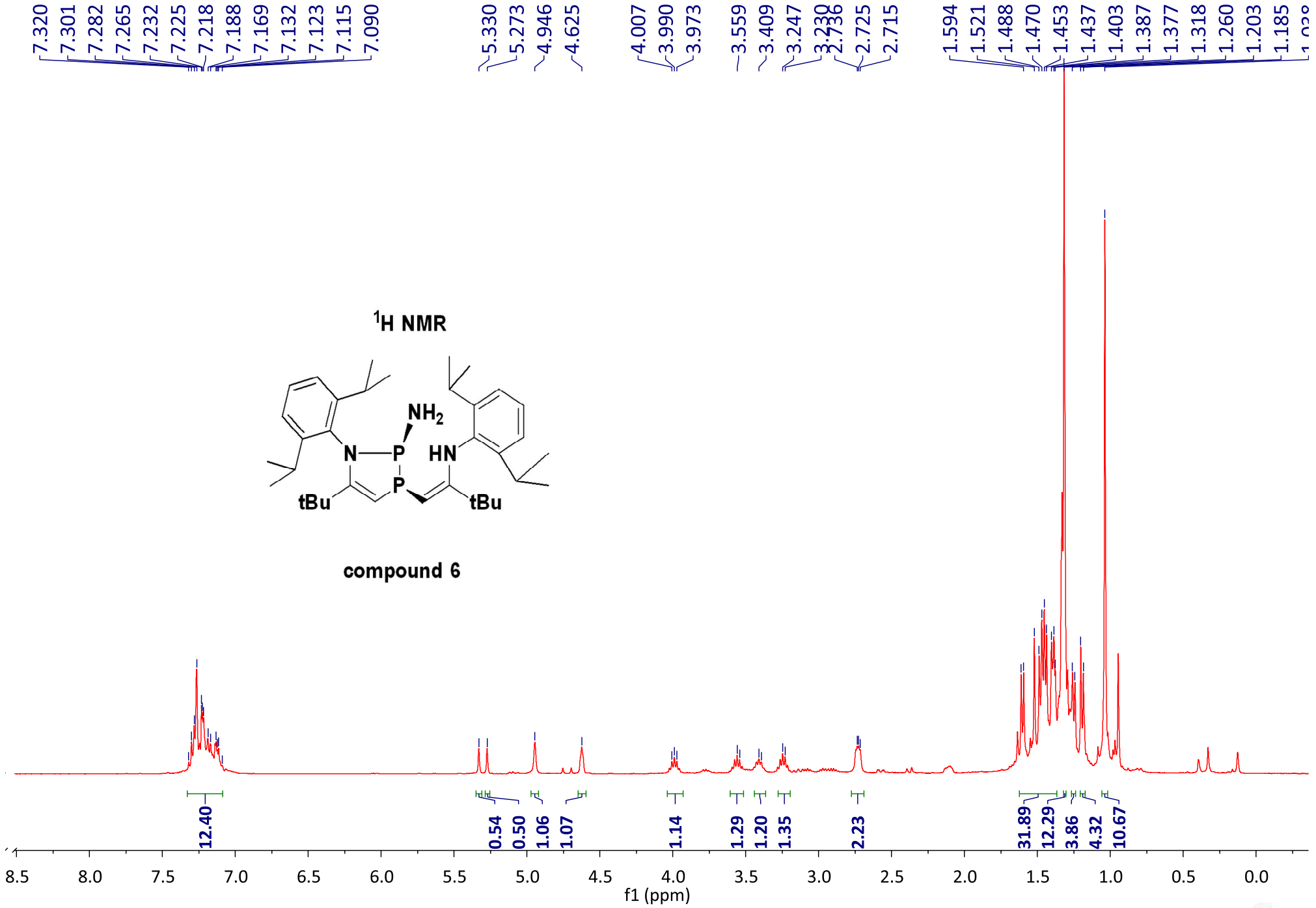

7.160
7.098
7.079
7.077
7.060
7.058
7.026
7.022
7.007
7.003
6.958
6.954
6.939
6.935
5.642
5.627
5.541
5.525
3.525
3.508
3.491
3.474
3.457
3.441
3.295
3.283
3.278
3.266
3.262
3.250
3.245
3.233
1.287
1.270
1.260
1.243
1.235
1.218
0.978
0.857
0.840
1H NMR
N
P
N
P
tBu
tBu
compound 5
2.05
1.98
2.01
1.00
1.00
2.07
2.05
6.09
5.95
5.72
18.00
5.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

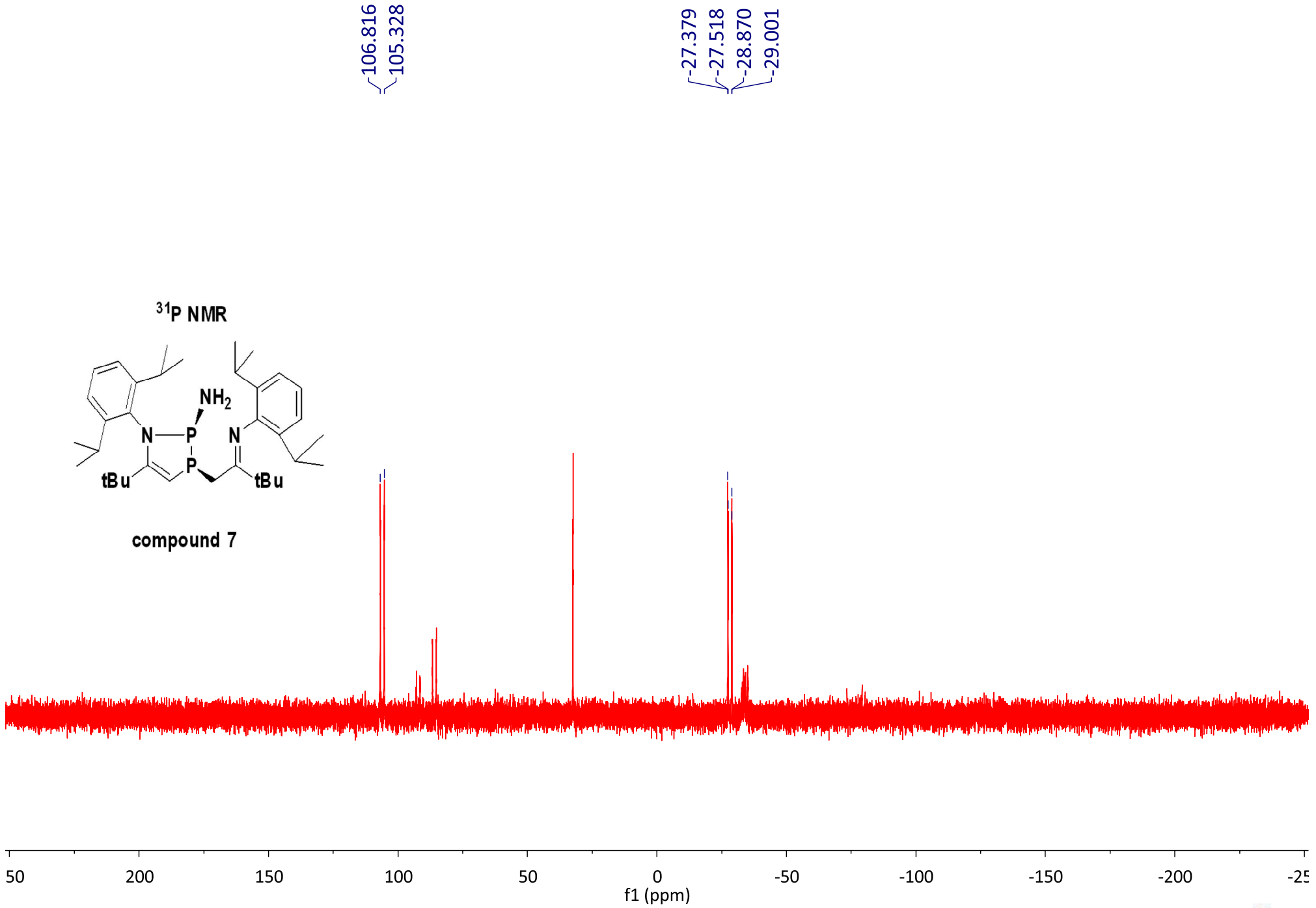

109.643
108.076
39.290
39.420
40.852
40.996
31P NMR
NH2
N
P
HN
P
tBu
tBu
compound 6
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)

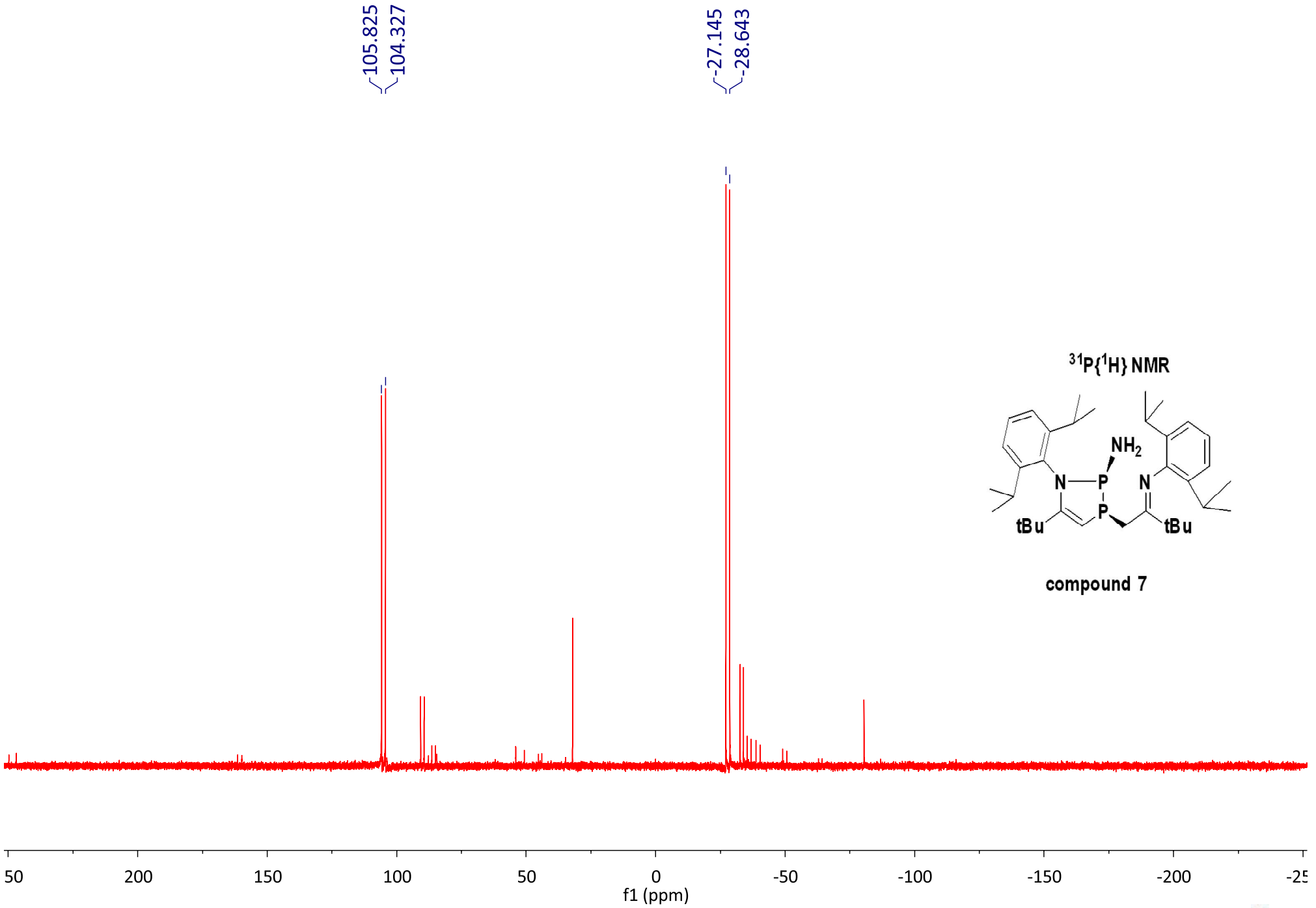

109.646
108.071
-39.360
-40.932
31P{1H} NMR
NH2
N
P
HN
P
tBu
tBu
compound 6
250
200
150
100
50
0
-50
-100
-150
-200
f1 (ppm)

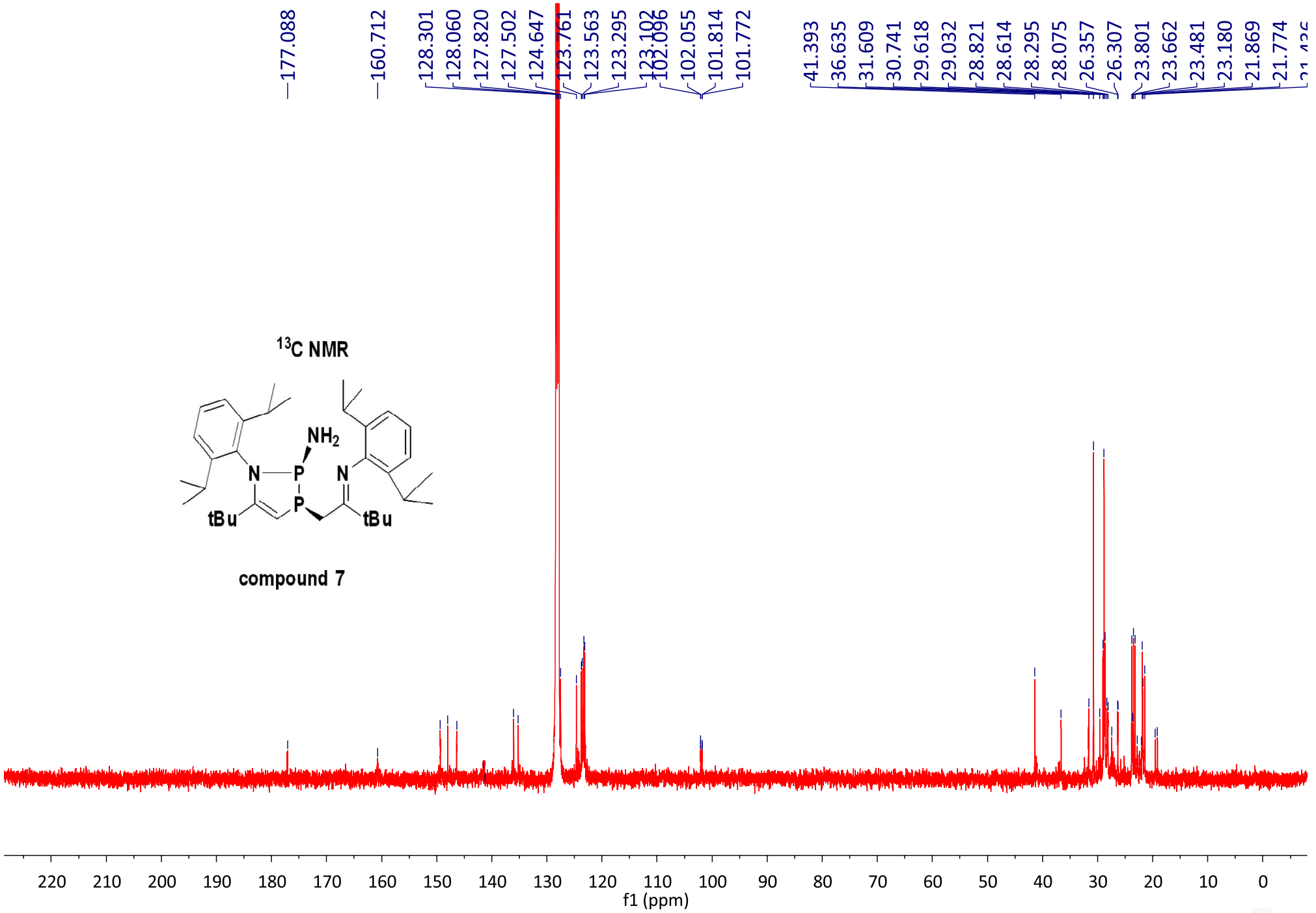

162.059
162.016
161.933
161.891
158.587
149.598
149.558
148.494
148.421
146.488
146.458
146.161
136.733
136.700
128.301
128.060
127.820
126.930
124.407
123.544
123.389
104.994
104.791
76.368
76.035
37.921
37.882
36.366
30.871
29.816
29.000
28.828
28.804
28.762
28.733
28.663
28.586
27.908
27.866
26.361
26.305
25.402
25.308
23.305
22.217
22.183
21.914
13C NMR
NH2
N
P
HN
P
tBu
tBu
compound 6
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


128.060
127.830
126.639
124.117
123.252
123.097
13C NMR
NH2
N
P
HN
P
tBu
tBu
compound 6
C6D6
30.0
129.5
129.0
128.5
128.0
127.5
127.0
126.5
126.0
125.5
125.0
124.5
124.0
123.5
123.0
122.5
122.0
121.5
121.0
120.5
f1 (ppm)


7.320
7.301
7.282
7.265
7.232
7.225
7.218
7.188
7.169
7.132
7.123
7.115
7.090
5.330
5.273
4.946
4.625
4.007
3.990
3.973
3.559
3.409
3.247
3.230
2.736
2.725
2.715
1.594
1.521
1.488
1.470
1.453
1.437
1.403
1.387
1.377
1.318
1.260
1.203
1.185
^{1}H NMR
NH$_2$
N
P
HN
P
tBu
tBu
compound 6
12.40
0.54
0.50
1.06
1.07
1.14
1.29
1.20
1.35
2.23
31.89
12.29
3.86
4.32
10.67
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


106.816
105.328
27.379
27.518
28.870
29.001
31P NMR
NH2
N
P
N
P
tBu
tBu
compound 7
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)

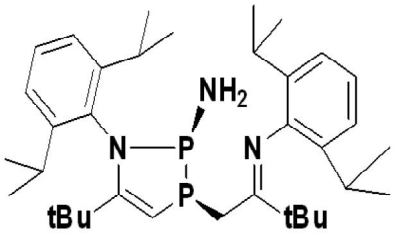

105.825
104.327
-27.145
-28.643
31P{1H} NMR
NH2
N
P
N
P
tBu
tBu
compound 7
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)


177.088
160.712
128.301
128.060
127.820
127.502
124.647
123.761
123.563
123.295
123.102
123.096
102.096
102.055
101.814
101.772
41.393
36.635
31.609
30.741
29.618
29.032
28.821
28.614
28.295
28.075
26.357
26.307
23.801
23.662
23.481
23.180
21.869
21.774
13C NMR
NH2
N
P
N
P
tBu
tBu
compound 7
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

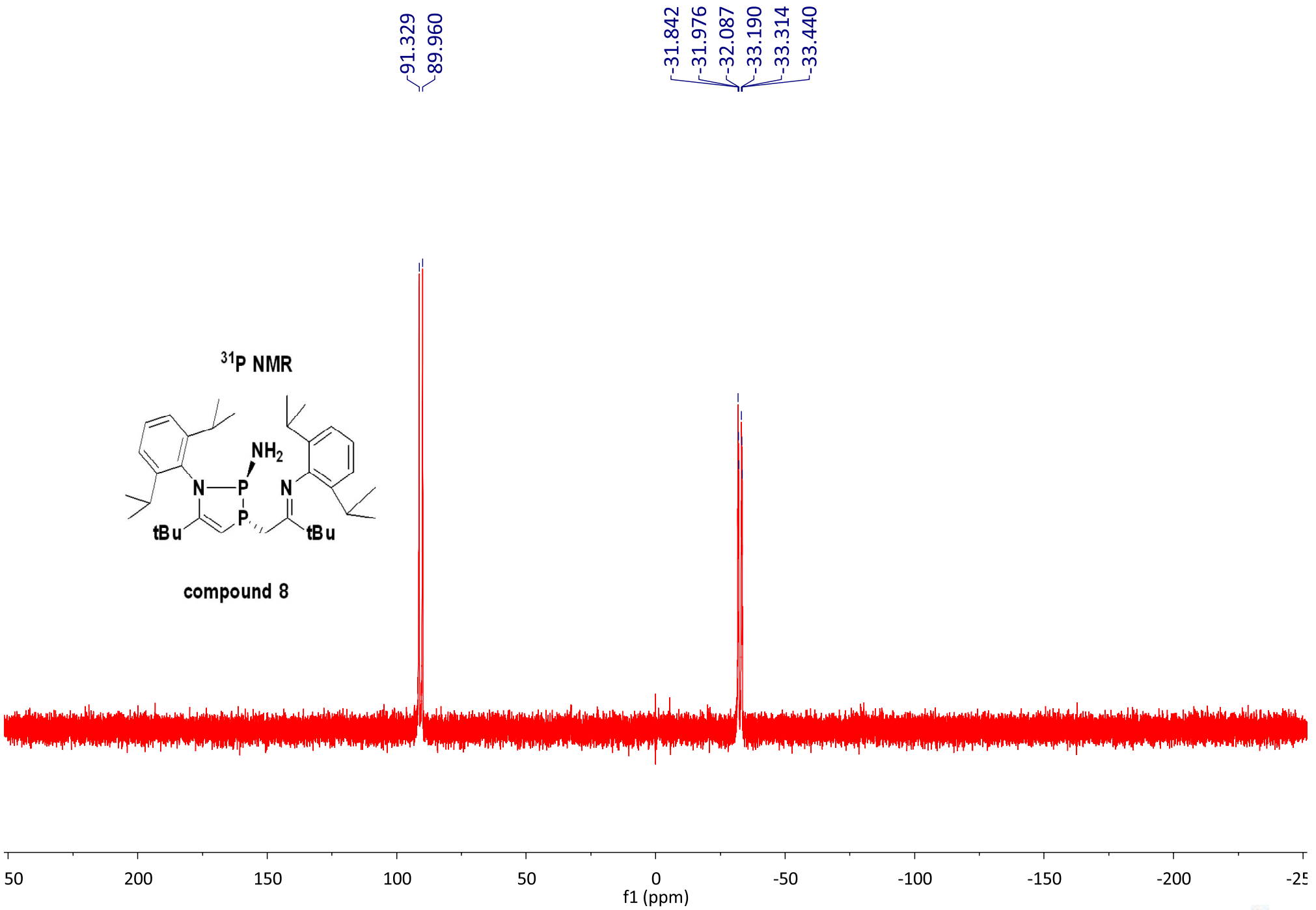
S#772224

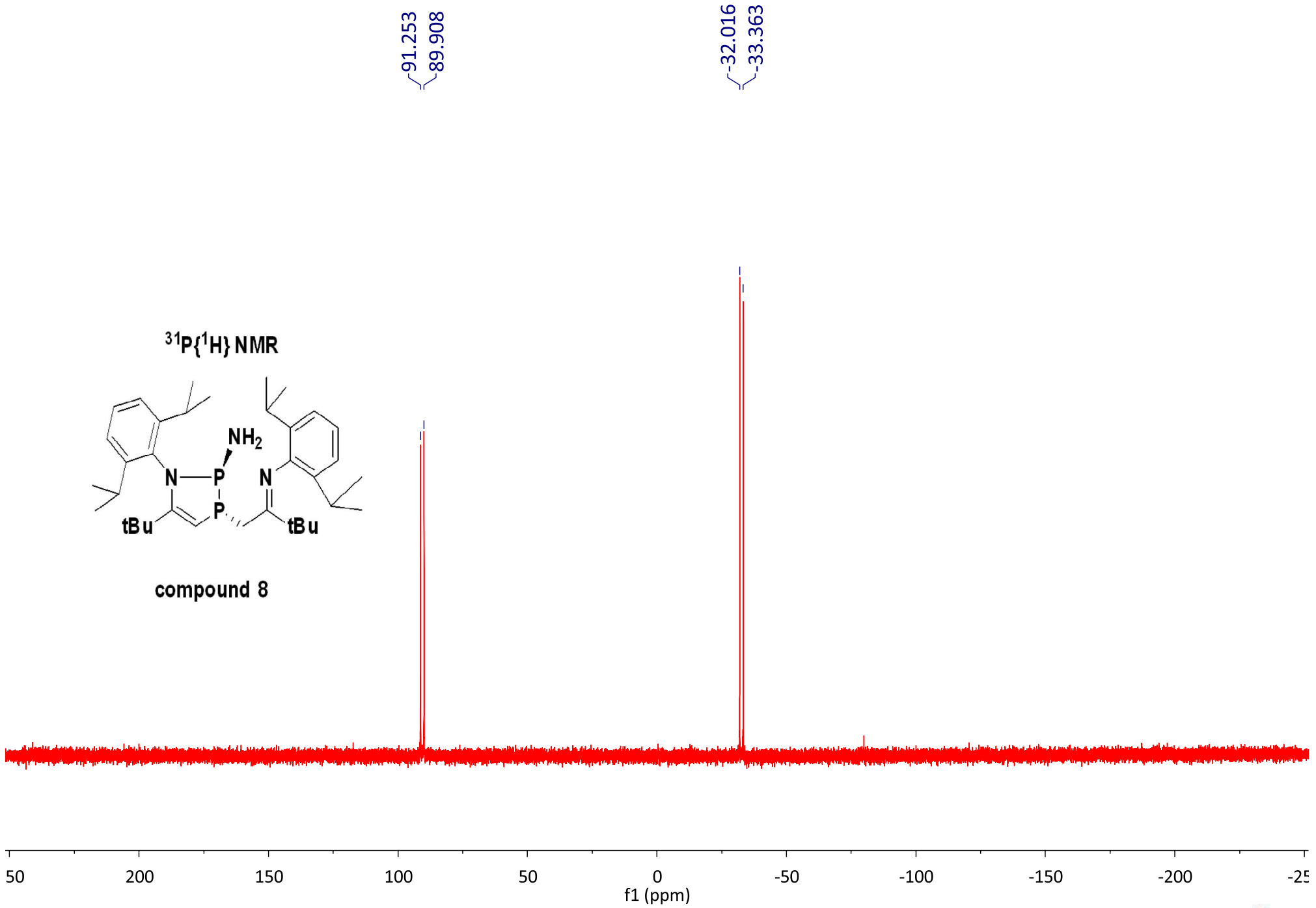
7.115 7.099 7.055 7.044 7.015 6.996 6.986 6.977 6.967 6.948 6.937 6.925 4.589 4.532 3.625 3.607 3.329 3.082 3.065 3.048 2.976 2.971 2.944 2.928 2.910 2.893 2.431 2.421 2.398 2.388 1.955 1.946 1.930 1.920 1.356 1.292 1.286 1.275 1.241 1.229 1.225 1.211 1.193 1.188 1.171 0.781

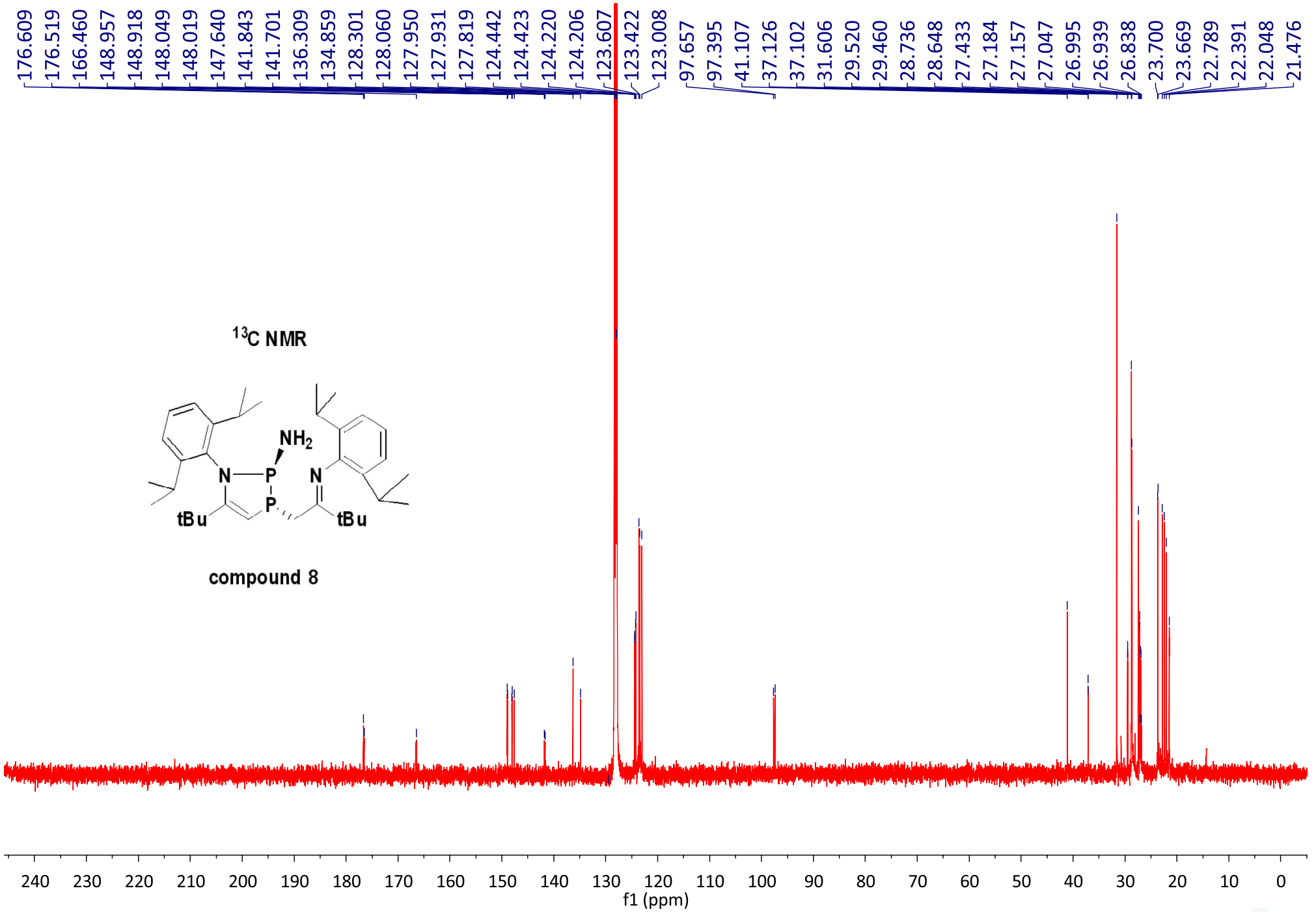
^{1}H NMR

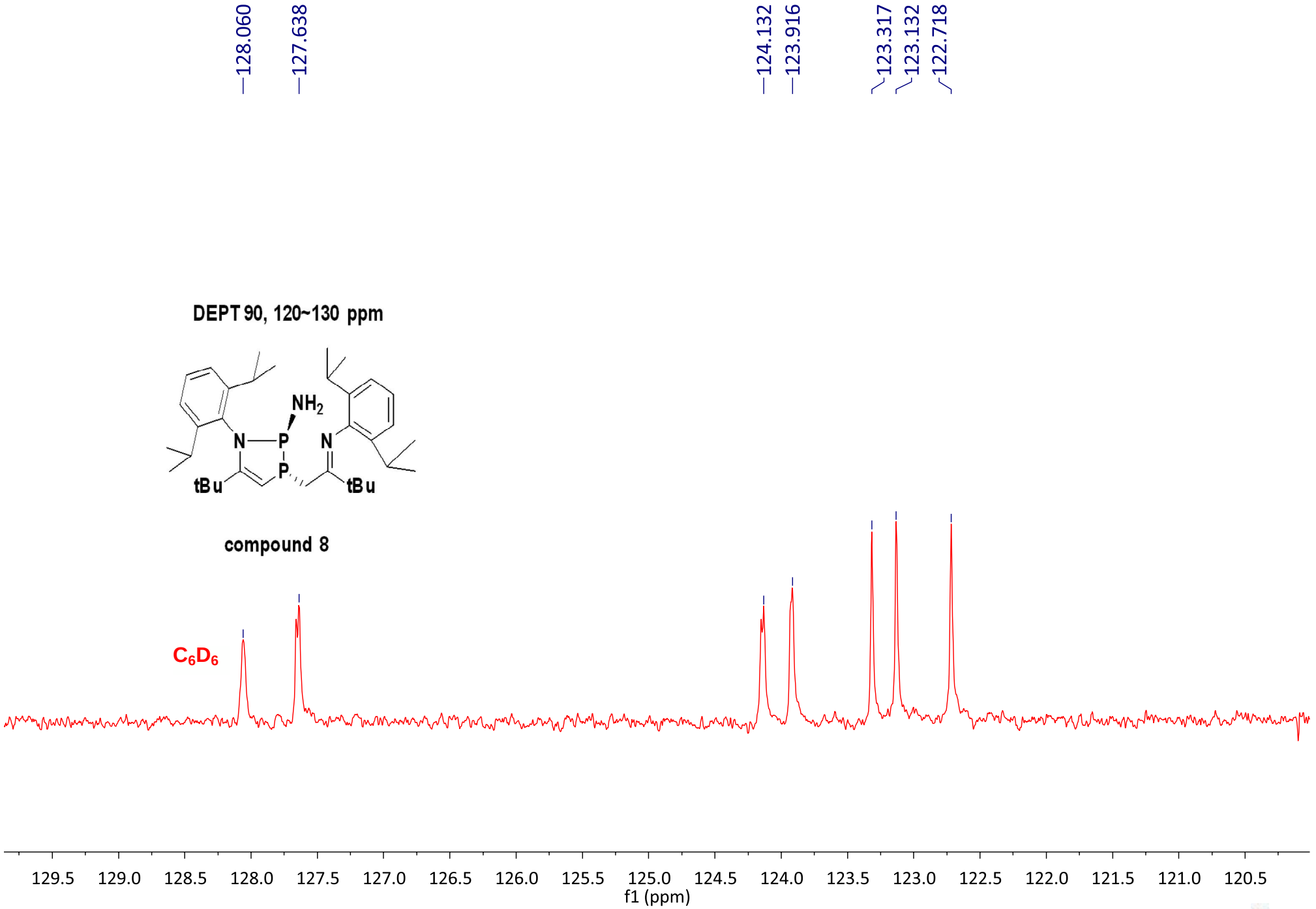


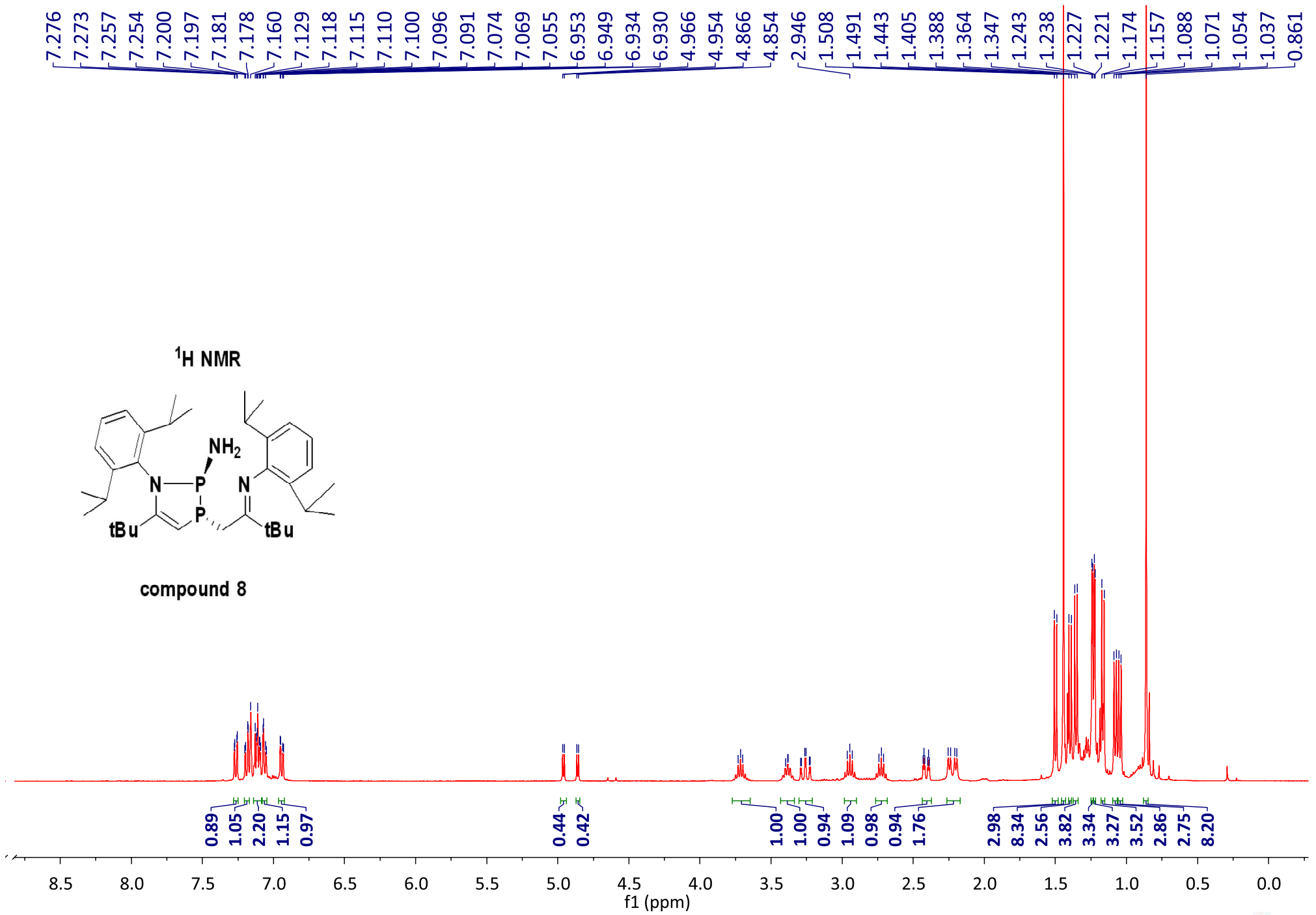
compound 7


91.329
89.960
31.842
31.976
32.087
33.190
33.314
33.440
31P NMR
NH2
N
P
P
N
tBu
tBu
compound 8
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)


91.253
89.908
-32.016
-33.363
31P{1H} NMR
NH2
N
P
N
P
tBu
tBu
compound 8
50
200
150
100
50
0
-50
-100
-150
-200
-25
f1 (ppm)


176.609
176.519
166.460
148.957
148.918
148.049
148.019
147.640
141.843
141.701
136.309
134.859
128.301
128.060
127.950
127.931
127.819
124.442
124.423
124.220
124.206
123.607
123.422
123.008
97.657
97.395
41.107
37.126
37.102
31.606
29.520
29.460
28.736
28.648
27.433
27.184
27.157
27.047
26.995
26.939
26.838
23.700
23.669
22.789
22.391
22.048
21.476
13C NMR
NH2
N
P
P
N
tBu
tBu
compound 8
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


128.060
127.638
124.132
123.916
123.317
123.132
122.718
DEPT 90, 120~130 ppm
NH2
N
P
N
P
tBu
tBu
compound 8
C6D6
129.5
129.0
128.5
128.0
127.5
127.0
126.5
126.0
125.5
125.0
124.5
124.0
123.5
123.0
122.5
122.0
121.5
121.0
120.5
f1 (ppm)


7.276
7.273
7.257
7.254
7.200
7.197
7.181
7.178
7.160
7.129
7.118
7.115
7.110
7.100
7.096
7.091
7.074
7.069
7.055
6.953
6.949
6.934
6.930
4.966
4.954
4.866
4.854
2.946
1.508
1.491
1.443
1.405
1.388
1.364
1.347
1.243
1.238
1.227
1.221
1.174
1.157
1.088
1.071
1.054
1.037
0.861
^{1}H NMR
NH$_2$
N
P
N
P
tBu
tBu
compound 8
0.89
1.05
2.20
1.15
0.97
0.44
0.42
1.00
1.00
0.94
1.09
0.98
0.94
1.76
2.98
8.34
2.56
3.82
3.34
3.27
3.52
2.86
2.75
8.20
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)