Supplementary Information

A metal and a metalloid Lewis acid bridged by a μ_2-phosphinidene

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1 General methods

All reactions were performed under dried and deoxygenated argon atmosphere using Schlenk or glovebox techniques. The used argon (>99.998%) was purified by a system of three columns (deoxygenation by a BTS copper catalyst (BASF PuriStar® R3-15S) at ca. 100 °C, removing moisture with silica gel, phosphorus pentoxide desiccant with indicator (Sicapent®) and calcium chloride). Glassware, spatulae, cannulae as well as filter papers were dried in a compartment dryer at 110 °C for at least one hour. Additionally, the glassware was heated with a heat gun (up to 550 °C) under active vacuum (<0.02 mbar) and filled with argon three times. Sterile syringes were purged with argon three times before use. The solvents were dried by standard procedures[1] by refluxing over proper desiccants under an argon atmosphere (*n*-pentane and toluene over sodium wire (Ø = 2 mm); diethyl ether stabilized with 3,5-di-*tert*-butyl-4-hydroxytoluene (BHT) and tetrahydrofuran over benzophenone and sodium wire; dichloromethane over calcium hydride) for several days and distilled before use. Alternatively, diethyl ether and toluene were dried using a MBraun SPS-800 solvent purification system. For filtration stainless steel cannulae (Ø = 1 mm and 2 mm) with Whatman® glass microfiber filters (grade GF/B) were used if not stated otherwise. After use, devices made of stainless steel were cleaned with acetone, water and diluted hydrochloric acid and glassware by storage in a concentrated solution of potassium hydroxide in isopropanol for at least two days and in diluted hydrochloric acid for one day. Afterwards, the glassware was washed with water and soap, acetone and petroleum ether 40/65. All joints were greased with OKS 1112 grease or with PTFE paste (Carl Roth). Vacuum was applied by a rotary vane pump (vacuubrand RZ6) enabling pressures $<10^{-2}$ mbar.

NMR spectra were recorded on a Bruker Avance I 300 MHz, Bruker Avance I 400 MHz, Bruker Avance I 500 MHz or Bruker Avance III HD Ascend 500 MHz spectrometer at the NMR department of the University of Bonn and subsequently analysed by the program *Mestrenova 14.2*. The calibration of the ^{1}H and ^{13}C NMR spectra was done via the solvent residual signals relative to tetramethylsilane (<1% in $CDCl_3$) (C_6D_6: $\delta(^{1}H)$ = 7.16 ppm and $\delta(^{13}C)$ = 128.06 ppm, CD_2Cl_2: $\delta(^{1}H)$ = 5.32 ppm and $\delta(^{13}C)$ = 53.84 ppm).[2] ^{11}B NMR spectra were measured relative to $BF_3{\cdot}OEt_2$ in $CDCl_3$ as external reference by using the ^{2}H frequency of the deuterated solvent (lock frequency) and the frequency ratio value $\Xi(^{11}B)$ = 32.083974%, and ^{31}P NMR spectra relative to 85% H_3PO_4 in water using the ^{2}H frequency of the deuterated solvent (lock frequency) and the frequency ratio value $\Xi(^{31}P)$ = 40.480742%.[3] All lock frequencies were calibrated internally against the ^{1}H signals of solutions of tetramethylsilane with a volume fraction of $\Phi \leq 1\%$ in the corresponding deuterated solvent. The used deuterated solvents were purified by distillation over proper desiccants (C_6D_6 and THF-d_8 over a potassium mirror, CD_2Cl_2 over CaH_2, and CD_3CN over CaH_2 and P_2O_5) , trap-to-trap recondensation and degassing by three freeze-pump-thaw cycles. The purified solvent was stored over 3 Å or 4 Å molecular sieves. The chemical shift (δ) is given in parts per million (ppm) and the coupling constant ($^{n}J_{X,Y}$) in Hertz (Hz) as absolute values

neglecting the sign where *n* is the number of bonds between the coupling nuclei X and Y. For assigning the multiplicity following abbreviations were used: s = singlet, d = doublet, ddd = doublet of doublets of doublets, m = multiplet, sat = satellites and br = broad. For ^{1}H NMR spectra additionally the number of nuclei is given accordingly which is determined via integration. The ^{1}H and ^{13}C NMR signals of compounds were assigned by a combination of COSY, HSQC and HMBC experiments to unequivocally assign protons and carbon resonances if necessary. All measurements were performed at ambient temperature (298 K) if not stated otherwise.

Mass spectra using electrospray ionisation (ESI) or atmospheric pressure chemical ionisation (APCI) were recorded on a Thermo Fisher Scientific Orbitrap XL spectrometer with an HPLC autosampler using acetonitrile or dichloromethane as solvents. The solutions were prepared in a glovebox using dried, recondensed and degassed solvents. Only selected data are given for detected ions. The peaks are given in mass-to-charge ratio (*m/z*) while only the isotopomer with the highest relative abundance is represented. Additionally, the relative intensities of the peaks are given in parentheses and the proposed molecule fragments in square brackets if not stated otherwise. High resolution mass spectra (HRMS) that were obtained using ESI or APCI were recorded in a single measurement and, hence, no standard deviations for were obtained.

ATR-IR spectra of solids were recorded in the spectral range of 4000–400 cm^{-1} on a Bruker Alpha FTIR spectrometer with a single-reflection ATR measurement attachment (Platinum-ATR Diamond) or a Shimadzu IRSpirit FTIR spectrometer with a single-reflection ATR measurement attachment (QATR-S) in a glovebox at ambient temperature. For apodization the Happ-Genzel function was used. All analyses were performed using the programs *EZ OMNIC 7.3* of Fisher Scientific, *OPUS* of Bruker and *LabSolutions IR 2.26* of Shimadzu. Only selected wavenumbers of the absorption bands are given using reciprocal centimetres (cm^{-1}). The intensities of the bands are marked as very strong (vs), strong (s), medium (m) or weak (w).

Melting points were measured using an SRS DigiMelt device or a Büchi melting point determination device according to Dr. Tottoli. The samples were flame-sealed in a glass capillary (Ø = 0.1 mm) *in vacuo* (<0.02 mbar) and heated quickly (ca. 5 K/min) for a rough determination of the melting point or decomposition temperature. Afterwards, a heating rate of approximately 2 K/min was used until the sample melted or decomposed. The thermally treated samples were cooled to ambient temperature and studied by ^{1}H and/or ^{31}P NMR spectroscopy to confirm whether decomposition had occurred. No internal or external temperature corrections were performed.

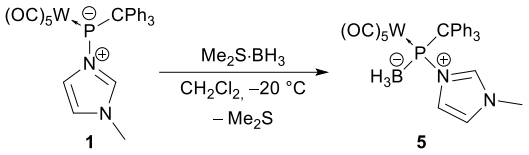
UV/vis spectra were measured using the spectrometer UV-1650PC of Shimadzu with a double-beam optics photometric system and a maximum wavelength range of 190.0 to 1100 nm, a spectra band width of 2 nm and a wavelength accuracy of ±0.5 nm with an automatic wavelength correction. To

avoid the measurement of the lamp interchange of the 50 W halogen lamp (340.8 nm) all spectra were measured between 350 to 700 nm. Before the measurement of the analyte solution, an automatic baseline correction was performed (baseline stability: ±0.001 abs./hour). A silicon photodiode was used as detector with a photometric range of −0.5 to 3.999 abs. with an accuracy of ±0.004 abs. at 1.0 abs. (±0.002 abs. at 0.5 abs.). The used cuvettes (Hellma precision cells 110-QS) (46 mm × 12.5 mm × 12.5 mm) were made of quartz glass (Suprasil® quartz, Heraeus) with two polished windows. The used cuvettes had a spectral range of 200 to 2500 nm, a light pathlength of 10 mm and a chamber volume of 3.5 μL. For the *in situ* measurements an aliquot of the reaction mixture was taken in the glovebox and diluted by the same solvent which was used in the experiment until only a light colour was visible. The diluted analyte solution was then added to the cuvettes, closed with a PTFE stopper and quickly transported to the spectrometer outside of the glovebox, and the measurement was started immediately. The determination of the extinction coefficient was not possible for the *in situ* measurements due to the involvement of air sensitive compounds and the variable amount of analyte in the reaction mixture.

Single crystal X-ray diffraction analyses were performed on a Bruker D8 Venture diffractometer, equipped with a low-temperature device (Oxford Cryostream 800 series) at 100(2) K by using graphite monochromated Mo-K_α radiation (λ = 0.71073 Å). Intensities were measured by fine-slicing Φ and ω scans and corrected background, polarization and Lorentz effects. A semi-empirical absorption correction was applied for the data sets following Blessing's method.[4] The structure was solved by direct methods and refined anisotropically by the least-squares procedure implemented in ShelX program system.[5] All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were included isotropically refined using a riding model at the bound carbon atoms. The program *Olex2 1.5*[6] of *OlexSys* was used for analyses and the ellipsoid representations of the molecular structures with the probability level set to 50%. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication numbers 2320467 (**5**) and 2320468 (**6**) which can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

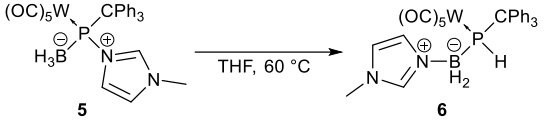
2 Experimental procedures and characterisation

Synthesis of complex 5



0.03 mL (0.32 mmol, 1.3 eq.) of borane dimethylsulfide was added dropwise to a solution of 0.165 g (0.24 mmol, 1.0 eq.) of complex **1**[7] in 3.0 mL of dichloromethane at −20 °C. The solution was stirred for 70 minutes at −20 °C and then warmed up to ambient temperature within 3 minutes. Afterwards, 8.0 mL of *n*-pentane were added to the formed colourless turbid solution under formation of a colourless precipitate. The colourless solution was filtered off using a filter cannula (Ø = 1 mm) with a Whatman® 595 filter paper. The colourless solid residue was washed two times with 4 mL of *n*-pentane at ambient temperature and then dried *in vacuo* for 45 minutes. Yield: 0.149 g (0.21 mmol, 89%). Mp 173 °C (dec.). IR (ATR Diamond): ν_{max} / cm^{-1} = 1910 (vs) (CO), 1974 (w) (CO), 2064 (m) (CO), 2402 (w) (BH), 3155 (w) (CH). ^{1}H NMR (400.13 MHz, CD_2Cl_2, 298 K): δ / ppm = 8.13 (s, 1H; Im), 7.81 (br s, 2H; *ortho*-C*H*), 7.62 (br s, 2H; *ortho*-C*H*), 7.44–7.12 (m, 9H; CPh_3), 6.93–6.92 (m, 1H; Im), 6.85 (s, 1H; Im), 6.45 (br s, 2H; *ortho*-C*H*), 3.73 (s, 3H; NCH_3), 1.78–1.00 (br m, 3H; BH_3). ^{11}B{^{1}H} NMR (128.38 MHz, CD_2Cl_2, 298 K): δ / ppm = −24.9 (s). ^{11}B NMR (128.38 MHz, CD_2Cl_2, 298 K): δ / ppm = −24.9 (br s). ^{13}C{^{1}H} NMR (100.63 MHz, CD_2Cl_2, 298 K): δ / ppm = 201.4 (d, $^{2}J_{P,C}$ = 23.3 Hz; *trans*-*C*O), 198.7 (d_{sat}, $^{1}J_{P,C}$ = 127.5 Hz, $^{2}J_{P,C}$ = 4.7 Hz; *cis*-*C*O), 146.8 (s; *ipso*-*C*), 140.5 (s; Im), 132.1 (br s; *ortho*-*C*H), 131.5 (d, $J_{P,C}$ = 4.9 Hz; Ph), 128.5 (br s; *ortho*-*C*H), 128.2 (s; Ph), 127.9 (d, $J_{P,C}$ = 1.2 Hz; Ph), 127.6 (br s; *ortho*-*C*H), 126.4 (d, $J_{P,C}$ = 1.6 Hz; Im), 122.4 (s; Ph), 121.4 (s; Im), 64.7 (d, $^{1}J_{P,C}$ = 12.0 Hz; *C*CPh_3), 36.6 (s; *C*H_3). ^{31}P{^{1}H} NMR (162.00 MHz, CD_2Cl_2, 298 K): δ / ppm = 163.5 (s). ^{31}P NMR (162.00 MHz, CD_2Cl_2, 298 K): δ / ppm = 163.5 (s). MS (APCI pos., selected data): *m/z* (%) = 693.094 (100) [*M*−H]$^{+}$, 555.052 (48) [*M*−H−2CO−*N*-MeIm]$^{+}$, 371.184 (80) [*M*−W(CO)$_5$+H]$^{+}$ 243.117 (85) [CPh_3]$^{+}$. MS (ESI pos., selected data): *m/z* (%) = 691.076 (97) [*M*−3H]$^{+}$. HRMS (APCI pos.): *m/z* calcd for [$C_{28}H_{23}BN_2O_5PW$]$^{+}$: 693.0950; found: 693.0944. HRMS (ESI pos.): *m/z* calcd for [$C_{28}H_{21}BN_2O_5PW$]$^{+}$: 691.0795; found: 691.0767.

Synthesis of complex 6



5 6

A solution of 0.121 g (0.17 mmol, 1.0 eq.) of the compound **5** in THF was stirred for 22 hours at 60 °C. All volatiles of the pale yellow solution were removed *in vacuo* at 60 °C and further dried under the same conditions for 45 minutes. The obtained pale yellow solid was redissolved in 15 mL of diethyl ether. 40 mL of *n*-pentane were added to the pale yellow solution at ambient temperature. The solution was stirred for 45 minutes at −80 °C to form a pale yellow fine suspension. The pale yellow solution was filtered off using a filter cannula (Ø = 1 mm) with a Whatman® 595 filter paper at −80 °C. The pale yellow solid residue was washed two times with *n*-pentane at −80 °C and then dried *in vacuo* for 21.5 hours at ambient temperature. Yield: 0.090 g (0.13 mmol, 75%). Mp 166 °C. IR (ATR Diamond): ν_{max} / cm^{-1} = 1895 (vs) (CO), 1979 (w) (CO), 1993 (w) (CO), 2062 (m) (CO), 2386 (w) (BH), 3010 (w) (CH), 3154 (w) (CH). ^{1}H NMR (500.04 MHz, CD_3CN, 298 K): δ / ppm = 7.36–7.33 (m, 6H; CPh_3), 7.28–7.21 (m, 9H; CPh_3), 6.94–6.92 (m, 1H; Im), 6.65–6.63 (m, 1H; Im), 6.60 (s, 1H; Im), 5.38 (ddd, $^{1}J_{P,H}$ = 289.11 Hz, $^{3}J_{H,H}$ = 6.48 Hz, $^{3}J_{H,H}$ = 1.77 Hz, 1H; P*H*), 3.51 (s, 3H; NCH_3), 2.95 (br d, $^{2}J_{P,H}$ = 57.3 Hz, 2H; BH_2). ^{11}B{^{1}H} NMR (128.38 MHz, THF-d_8, 298 K): δ / ppm = −13.3 (s). ^{11}B NMR (128.38 MHz, THF-d_8, 298 K): δ / ppm = −13.4 (s). ^{13}C{^{1}H} NMR (125.75 MHz, CD_3CN, 298 K): δ / ppm = 201.7 (d, $^{2}J_{P,C}$ = 17.8 Hz; *trans*-*C*O), 199.1 (d_{sat}, $^{1}J_{W,C}$ = 125.9 Hz, $^{2}J_{P,C}$ = 5.5 Hz; *cis*-*C*O), 147.1 (s; *ipso*-*C*), 139.0 (d, $J_{P,C}$ = 3.10 Hz; Im), 131.6 (d, $J_{P,C}$ = 4.9 Hz; Ph), 128.6 (s; Ph), 127.5 (d, $J_{P,C}$ = 2.0 Hz; Ph), 127.1 (d, $J_{P,C}$ = 1.6 Hz; Im), 123.0 (s; Im), 57.9 (d, $^{1}J_{P,C}$ = 8.7 Hz; *C*Ph_3), 35.4 (s; *C*H_3). ^{15}N{^{1}H} NMR (50.68 MHz, CD_3CN, 298 K): δ / ppm = −182.8 (s; P-*N*), −212.5 (s; *N*-CH_3). ^{31}P{^{1}H} NMR (162.00 MHz, THF-d_8, 298 K): δ / ppm = −38.3 (br s). ^{31}P NMR (162.00 MHz, THF-d_8, 298 K): δ / ppm = −38.3 (br d, $^{1}J_{P,H}$ = 289.3 Hz). MS (APCI pos., selected data): *m/z* (%) = 693.095 (74) [*M*−H]$^+$, 555.052 (44) [*M*−H−2CO−*N*-MeIm]$^+$, 371.184 (19) [*M*−W(CO)$_5$+H]$^+$, 243.117 (100) [CPh_3]$^+$. MS (ESI pos., selected data): *m/z* (%) = 371.182 (100) [*M*−W(CO)$_5$+H]$^+$, 243.116 (54) [CPh_3]$^+$. HRMS (APCI pos.): *m/z* calcd for [$C_{28}H_{23}BN_2O_5PW$]$^+$: 693.0952; found: 693.0950.

Generation of complex 3

Via [W(CO)$_5$(NCMe)]: 9.3 mg (0.03 mmol, 1.7 eq.) of [W(CO)$_5$(NCMe)] were added to a solution of 10.3 mg (0.02 mmol, 1.0 eq.) of compound **1** in 0.5 mL of benzene-d_6. The solution was stirred for 6 h at ambient temperature to form a deep violet solution. Content in reaction mixture: 4% (by ^{31}P{^{1}H} NMR integration). ^{31}P{^{1}H} NMR (121.59 MHz, C_6D_6, 298 K): δ / ppm = 811.2 (s). UV/vis (THF): λ_{max} = 540 nm.

Via $[W(CO)_5(thf)]$: 0.5 mL (0.04 mmol, 2.8 eq.) of a freshly prepared $[W(CO)_5(thf)]$ solution (c = 83 mM in THF) were added to a solution of 10.3 mg (0.02 mmol, 1.0 eq.) of compound **1** in THF. The solution was stirred at ambient temperature for 6.5 h to obtain a deep violet solution. Content in reaction mixture 46% (by $^{31}P\{^1H\}$ NMR integration). $^{31}P\{^1H\}$ NMR (121.51 MHz, THF, 298 K): δ / ppm = 791.4 (s_{sat}, $^1J_{W,P}$ = 185.2 Hz).

Generation of complex 4

24.5 mg (0.05 mmol, 3.4 eq.) of $B(C_6F_5)_3$ were added to a solution of 9.5 mg (0.01 mmol, 1.0 eq.) of compound **1** in 0.5 mL of benzene-d_6. The solution was stirred for 6.5 h to obtain a turquoise-blue solution. Content in reaction mixture: 24% (by $^{31}P\{^1H\}$ NMR integration). $^{31}P\{^1H\}$ NMR (121.51 MHz, C_6D_6, 298 K): δ / ppm = 1040.3 (s_{sat}, $^1J_{W,P}$ = 180.1 Hz). UV/vis (C_6H_6): λ_{max} = 603 nm.

3 NMR spectra

Compound 5

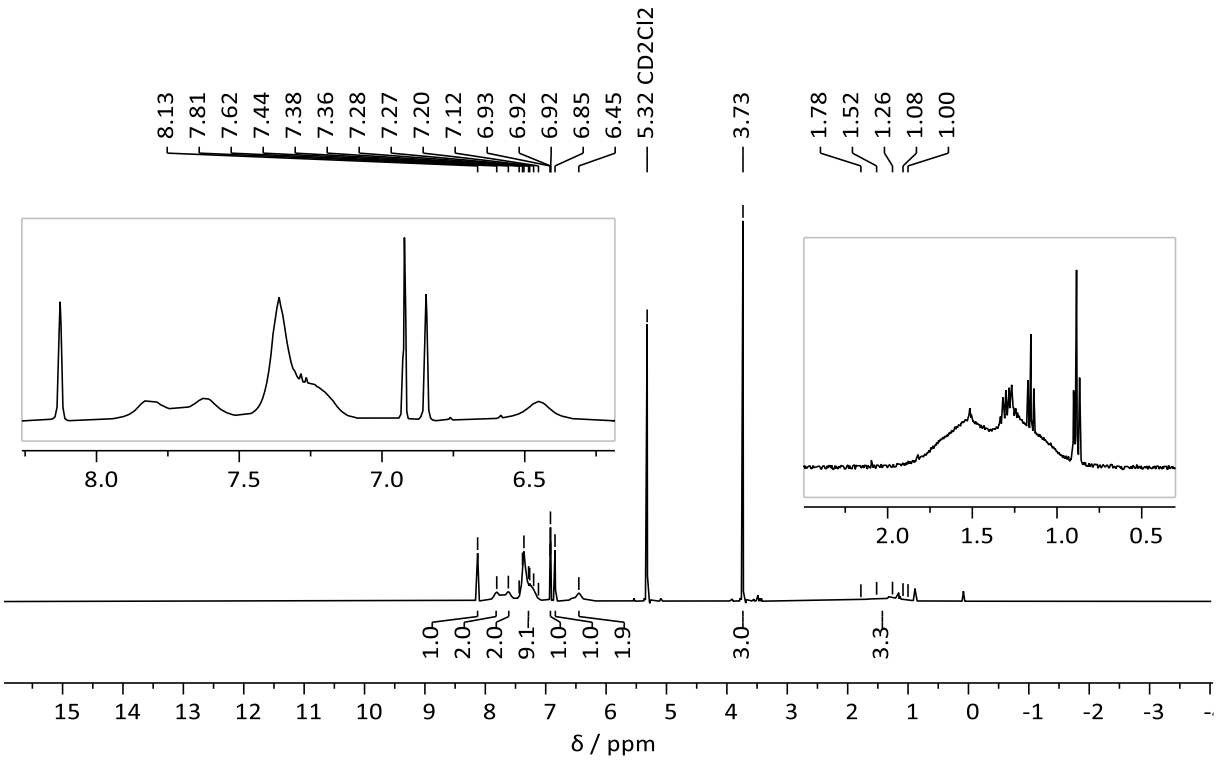


Fig. S1 ^{1}H NMR spectrum (400.13 MHz, CD_2Cl_2, 298 K) of compound **5**.

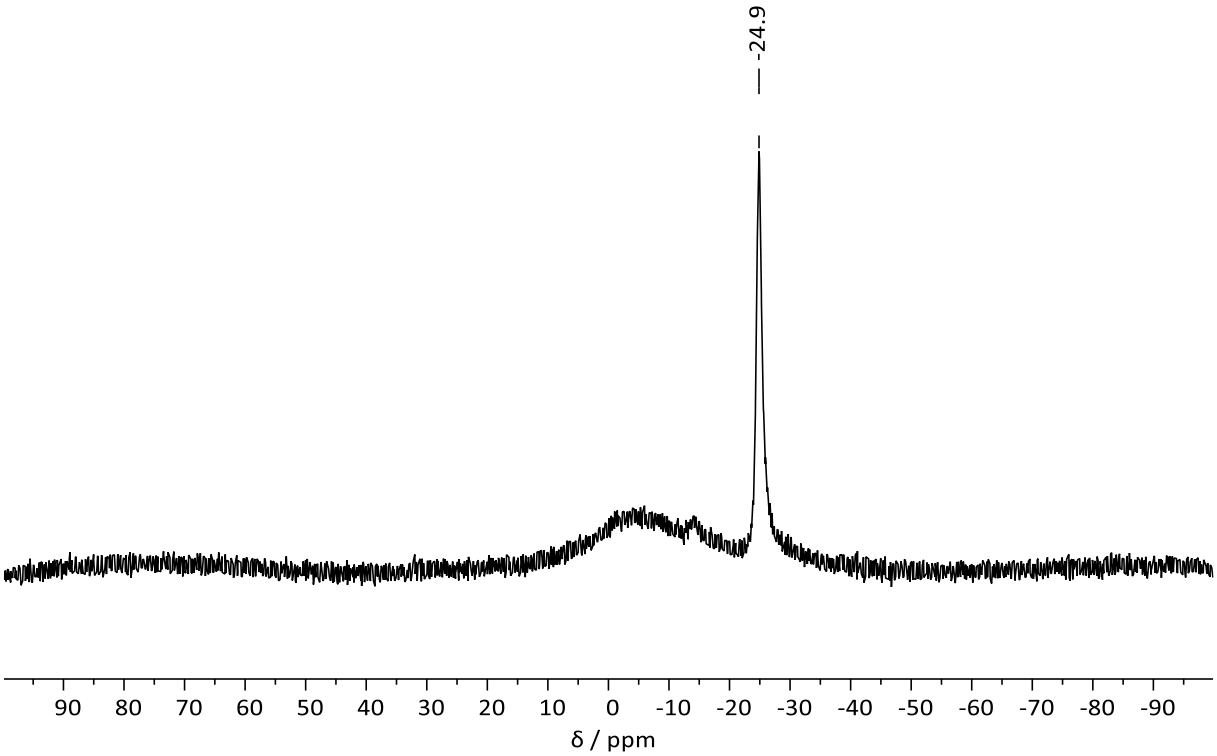


Fig. S2 $^{11}B\{^{1}H\}$ NMR spectrum (128.38 MHz, CD_2Cl_2, 298 K) of compound **5**.

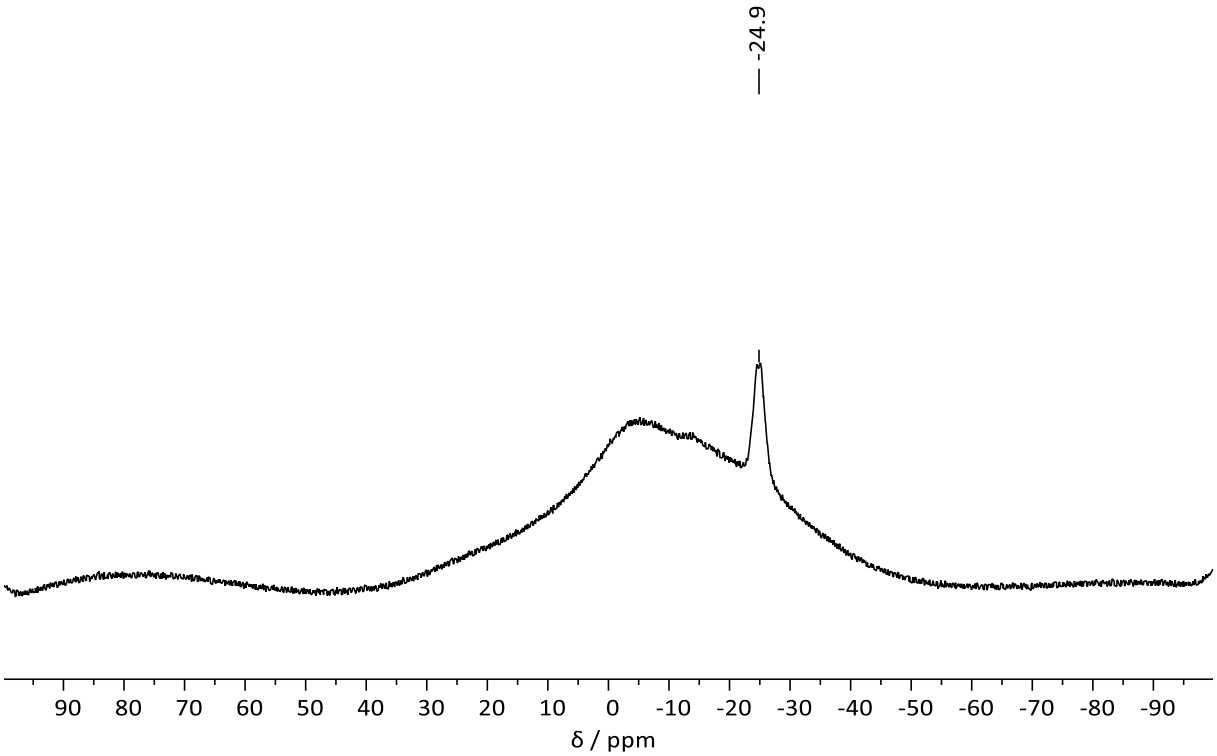


Fig. S3 ^{11}B NMR spectrum (128.38 MHz, CD_2Cl_2, 298 K) of compound **5**.

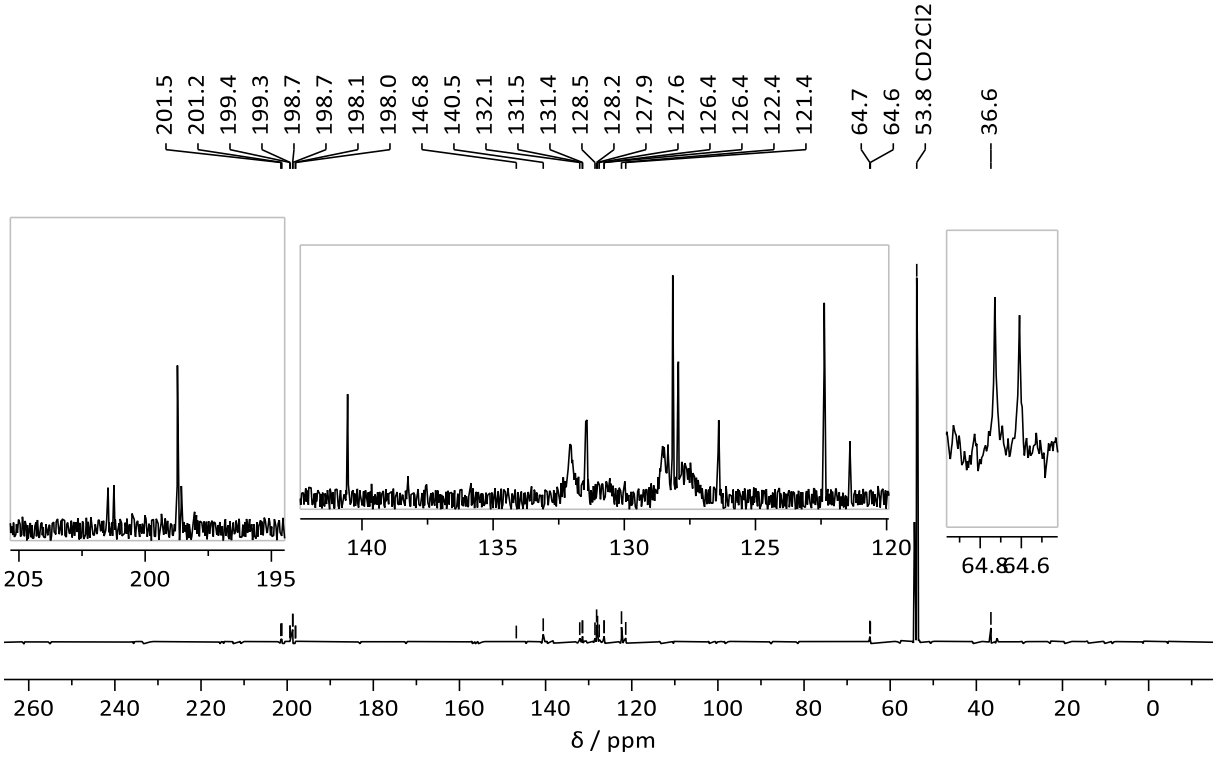


Fig. S4 $^{13}C\{^1H\}$ NMR spectrum (100.63 MHz, CD_2Cl_2, 298 K) of compound **5**.

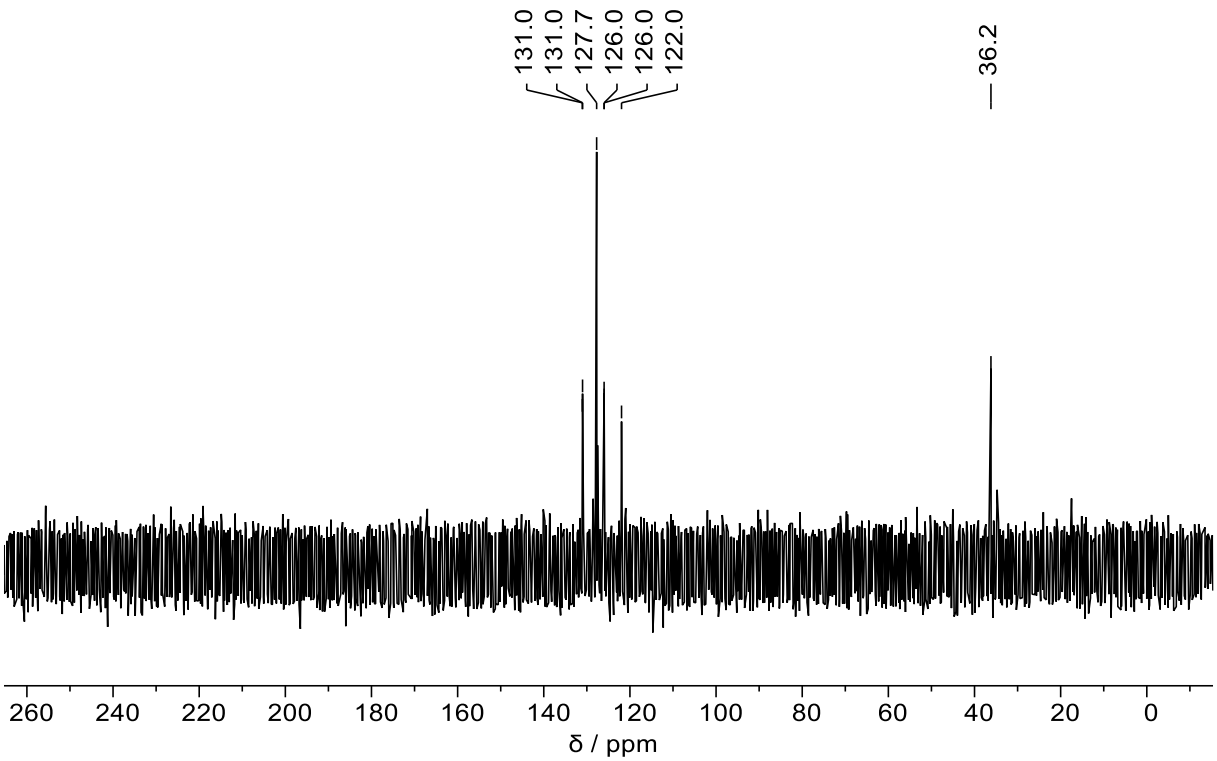


Fig. S5 $^{13}C\{^{1}H\}$ DEPT135 NMR spectrum (100.63 MHz, CD_2Cl_2, 298 K) of compound **5**.

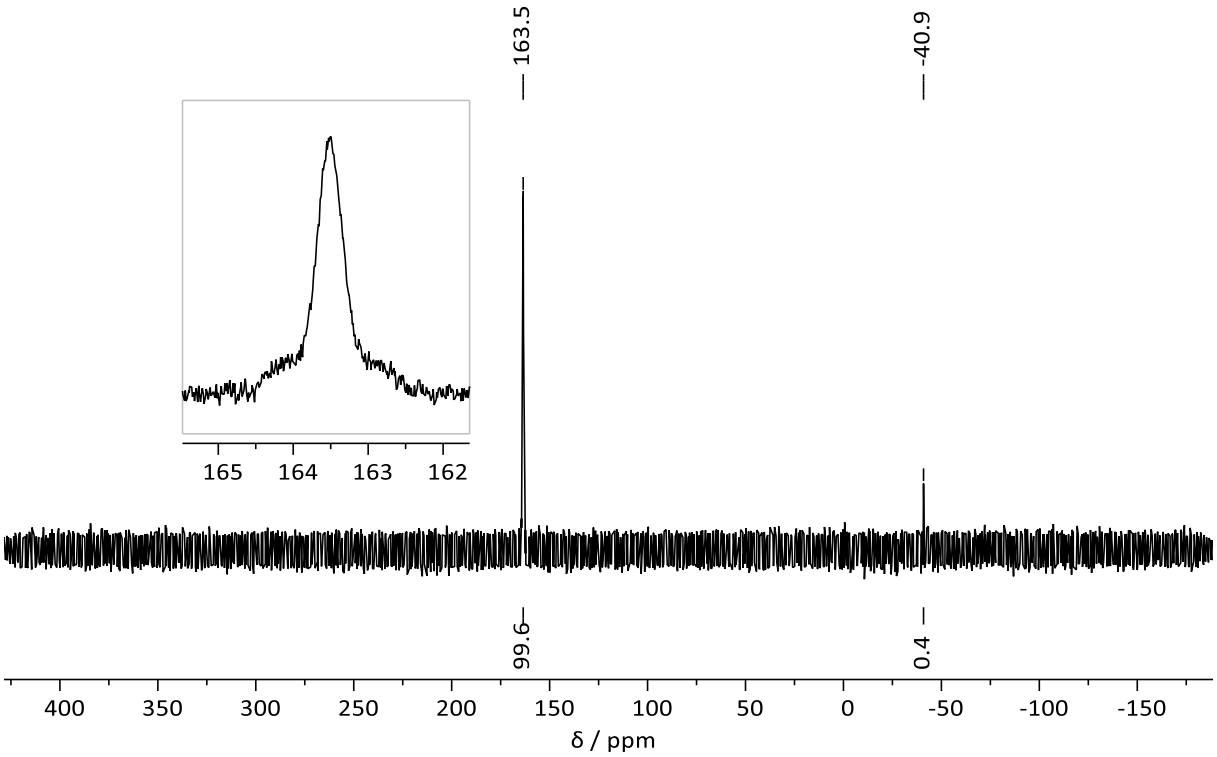


Fig. S6 $^{31}P\{^{1}H\}$ NMR spectrum (162.00 MHz, CD_2Cl_2, 298 K) of compound **5**.

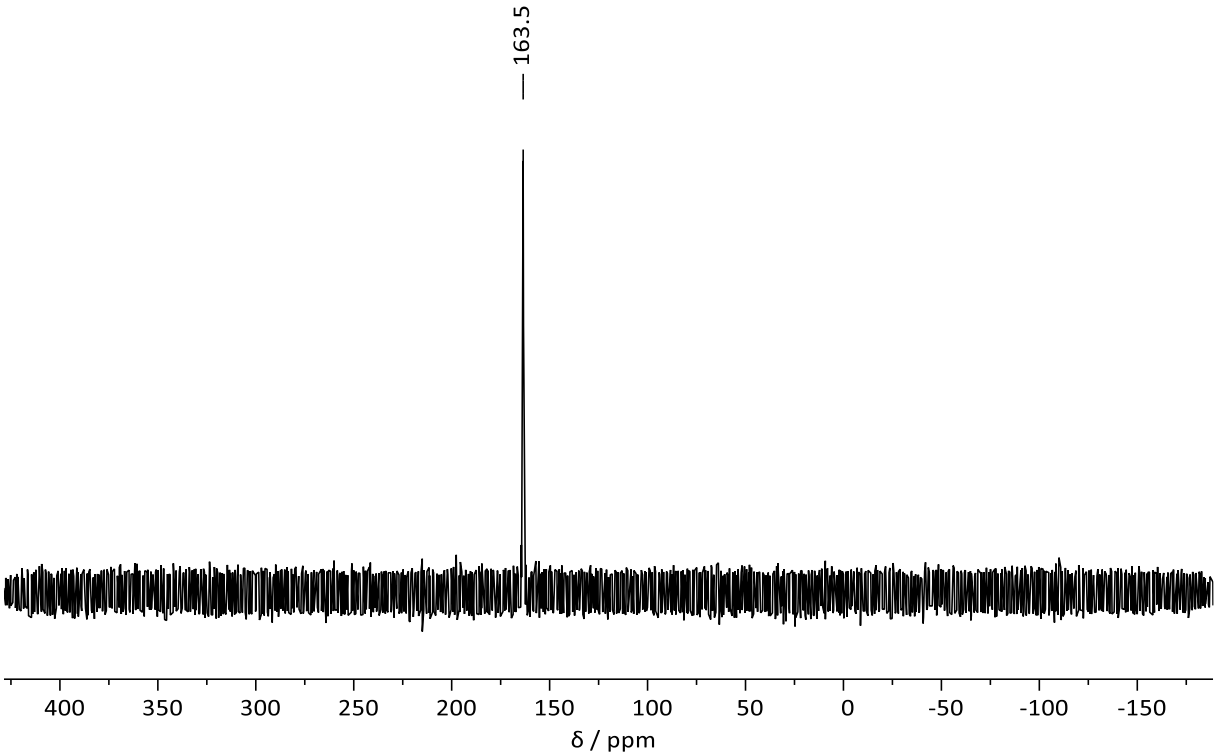


Fig. S7 ^{31}P NMR spectrum (162.00 MHz, CD_2Cl_2, 298 K) of compound **5**.

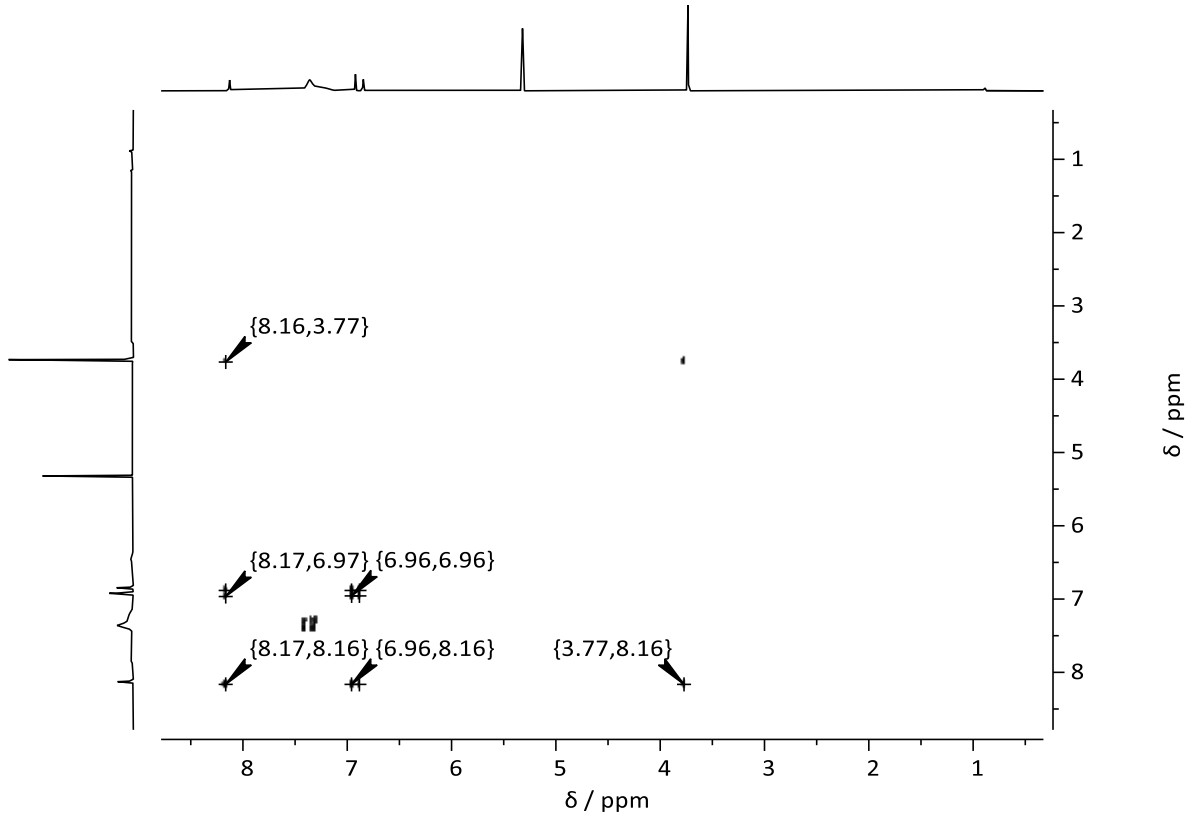


Fig. S8 ^{1}H,^{1}H COSY NMR spectrum (400.13 MHz, 400.13 MHz, CD_2Cl_2, 298 K) of compound **5**.

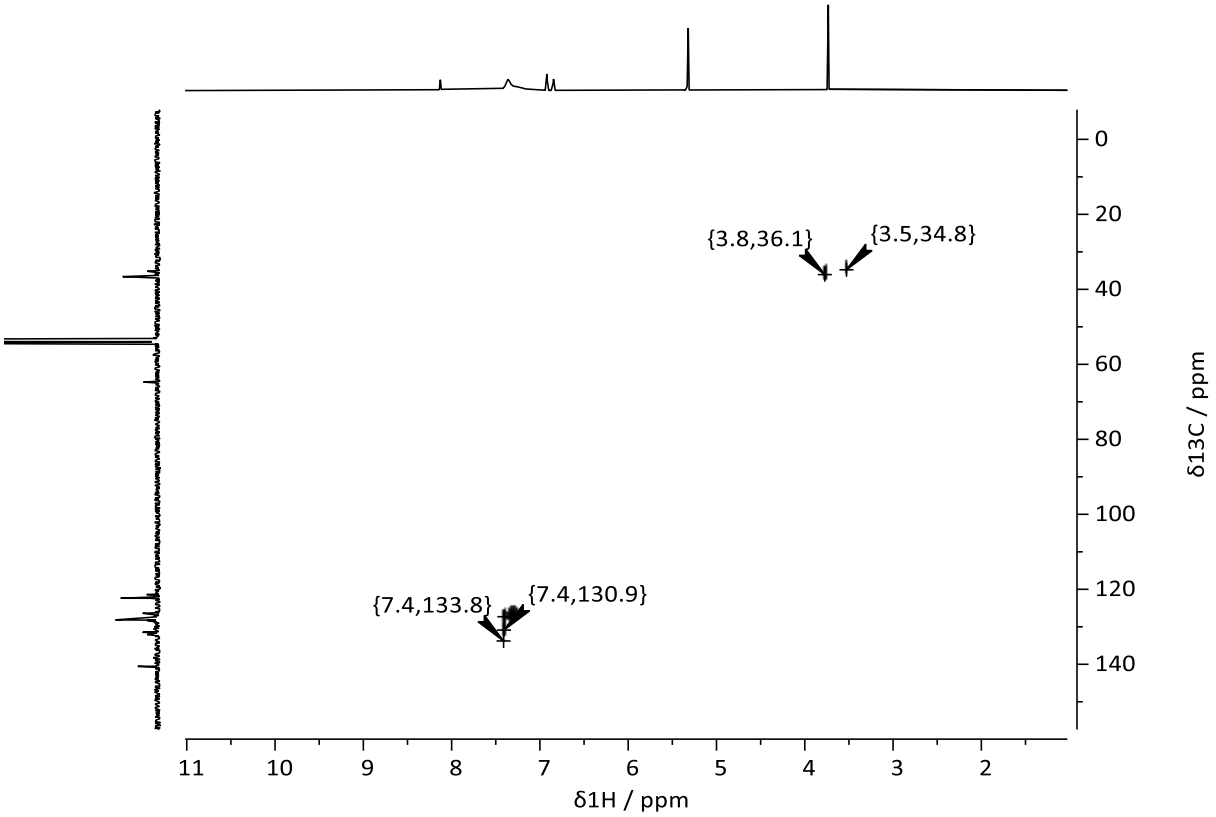


Fig. S9 $^{1}H,^{13}C$ HSQC NMR spectrum (400.13 MHz, 100.62 MHz, CD_2Cl_2, 298 K) of compound **5**.

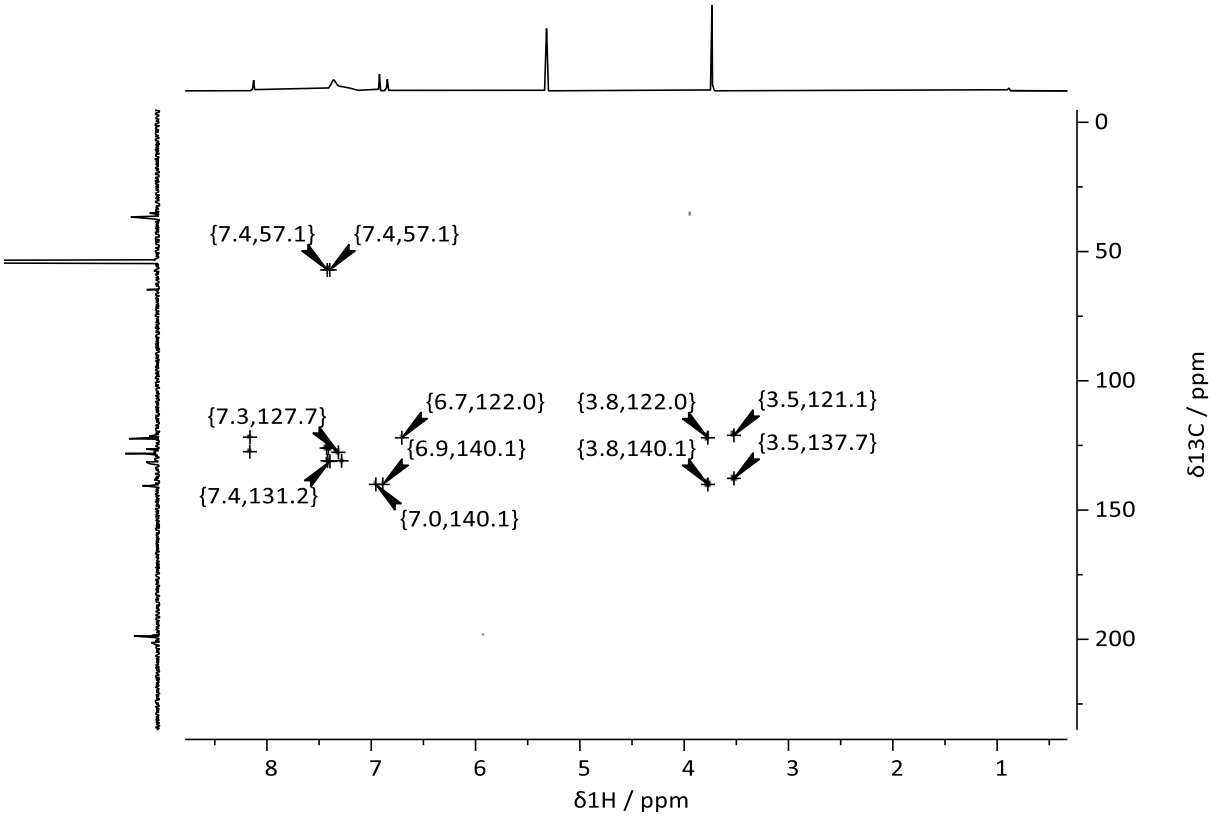


Fig. S10 $^{1}H,^{13}C$ HMBC NMR spectrum (400.13 MHz, 100.62 MHz, CD_2Cl_2, 298 K) of compound **5**.

Compound 6

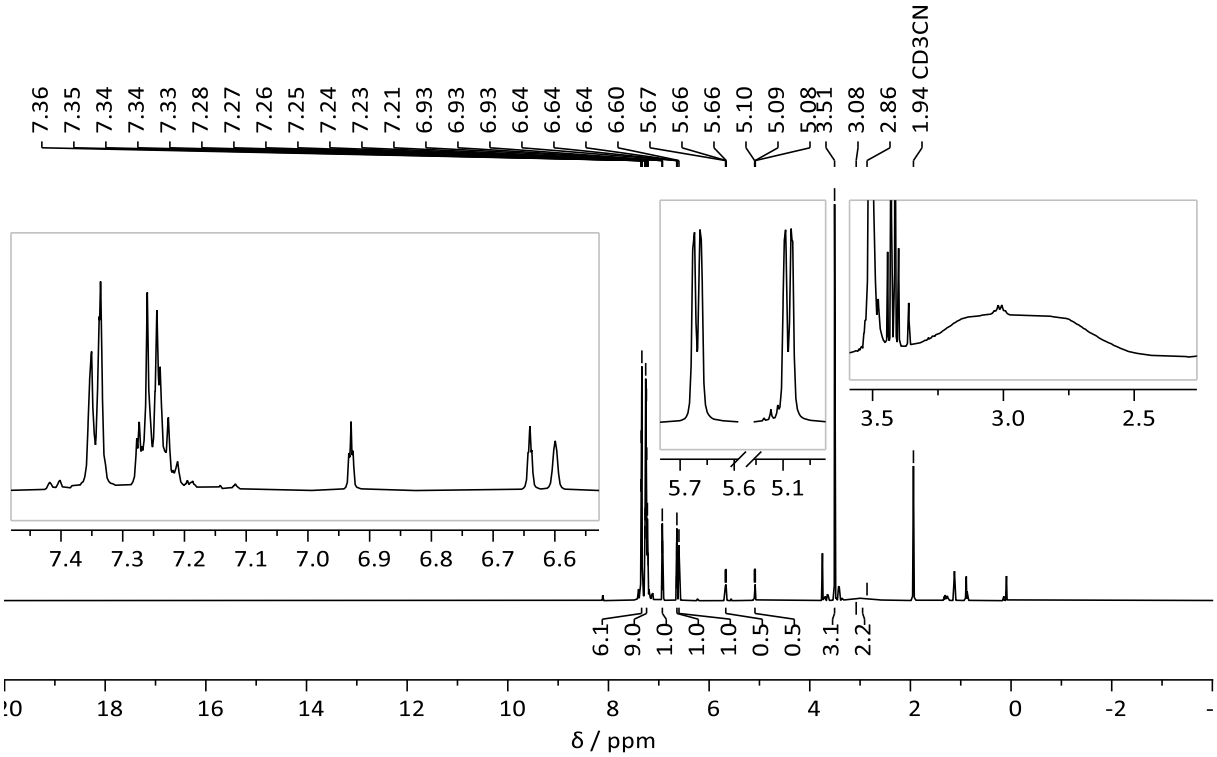


Fig. S11 ^{1}H NMR spectrum (500.04 MHz, CD_3CN, 298 K) of compound **6**.

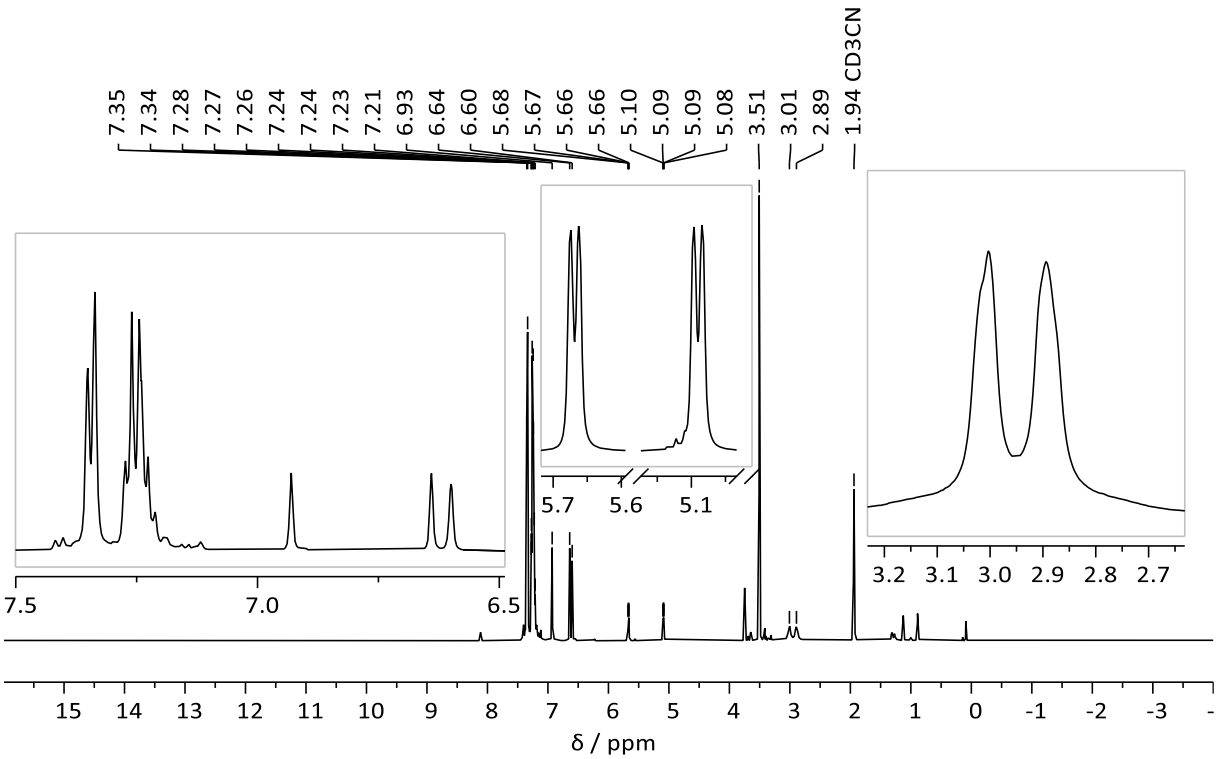


Fig. S12 ^{1}H{^{11}B} NMR spectrum (500.04 MHz, CD_3CN, 298 K) of compound **6**.

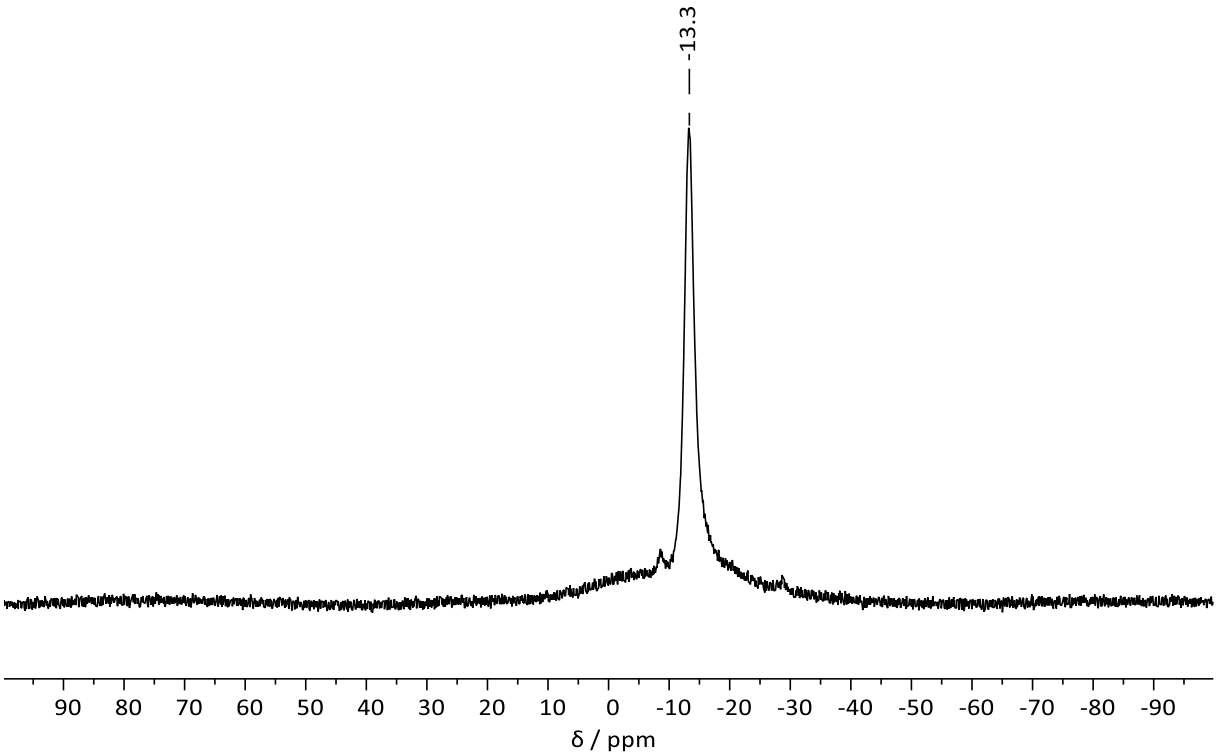


Fig. S13 $^{11}B\{^{1}H\}$ NMR spectrum (128.38 MHz, THF-d_8, 298 K) of compound **6**.

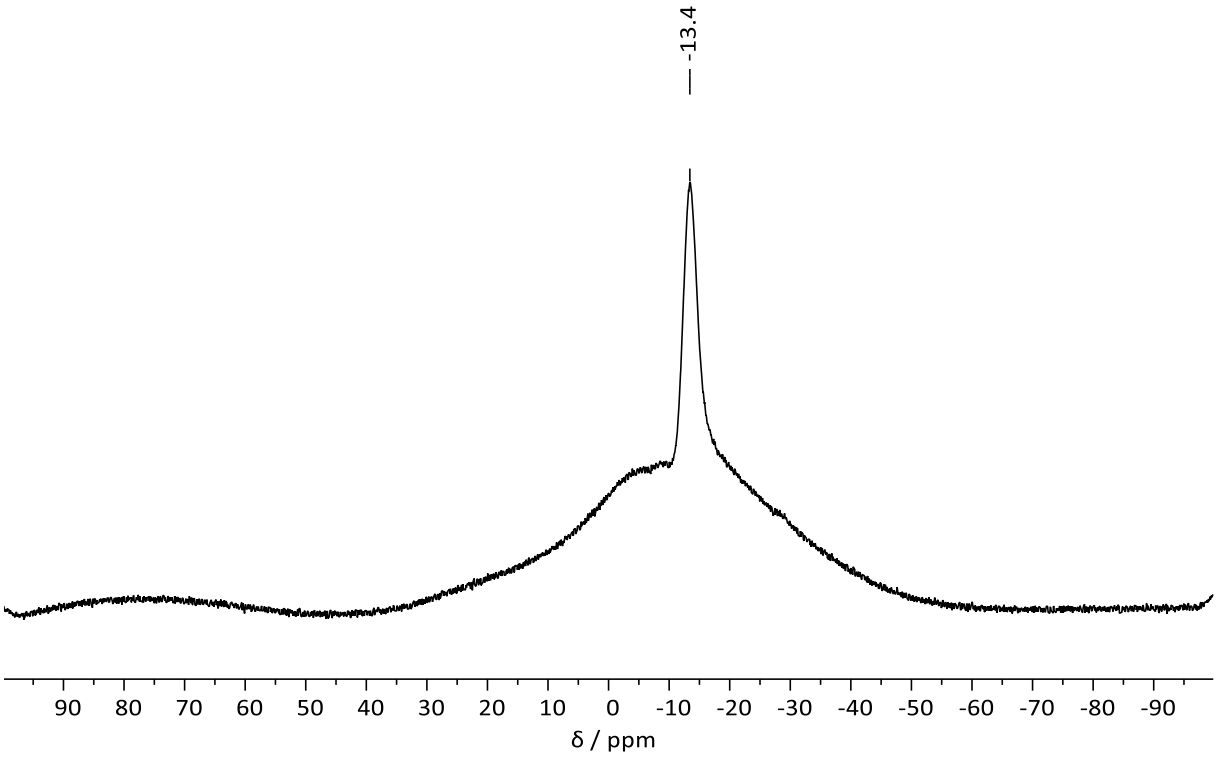


Fig. S14 ^{11}B NMR spectrum (128.38 MHz, THF-d_8, 298 K) of compound **6**.

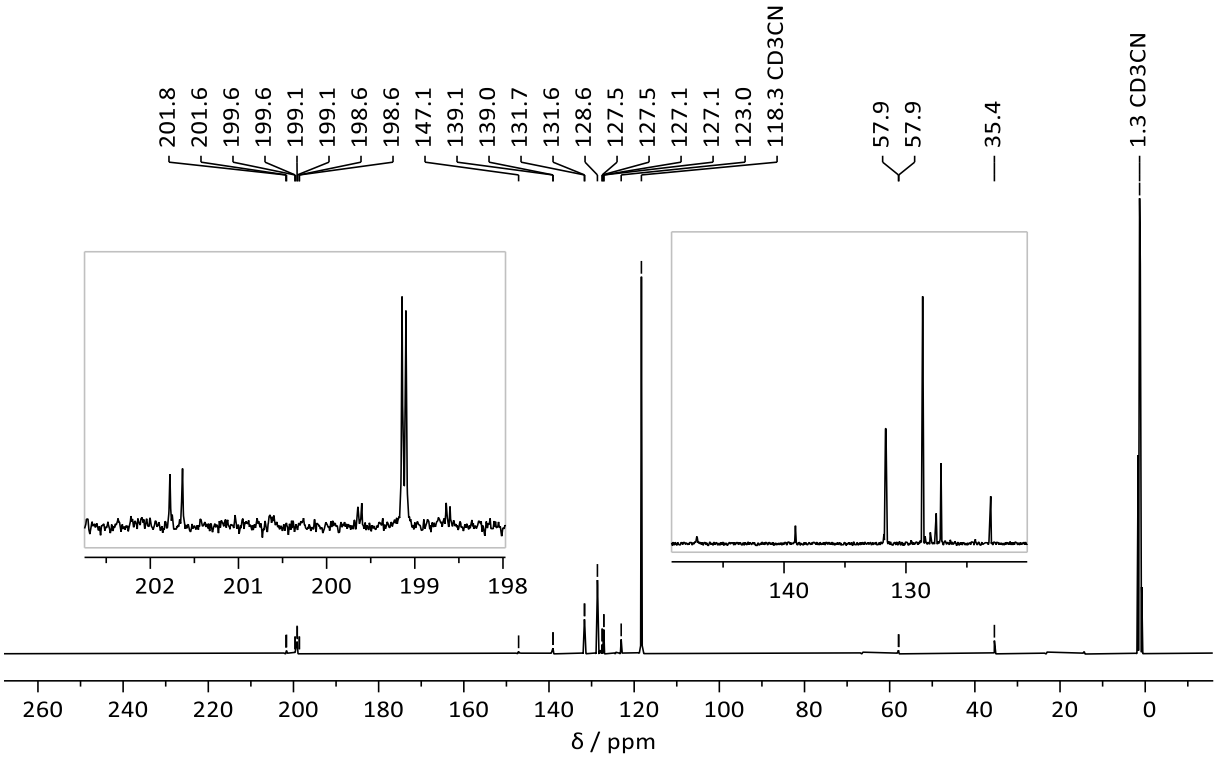


Fig. S15 $^{13}C\{^{1}H\}$ NMR spectrum (125.75 MHz, CD_3CN, 298 K) of compound **6**.

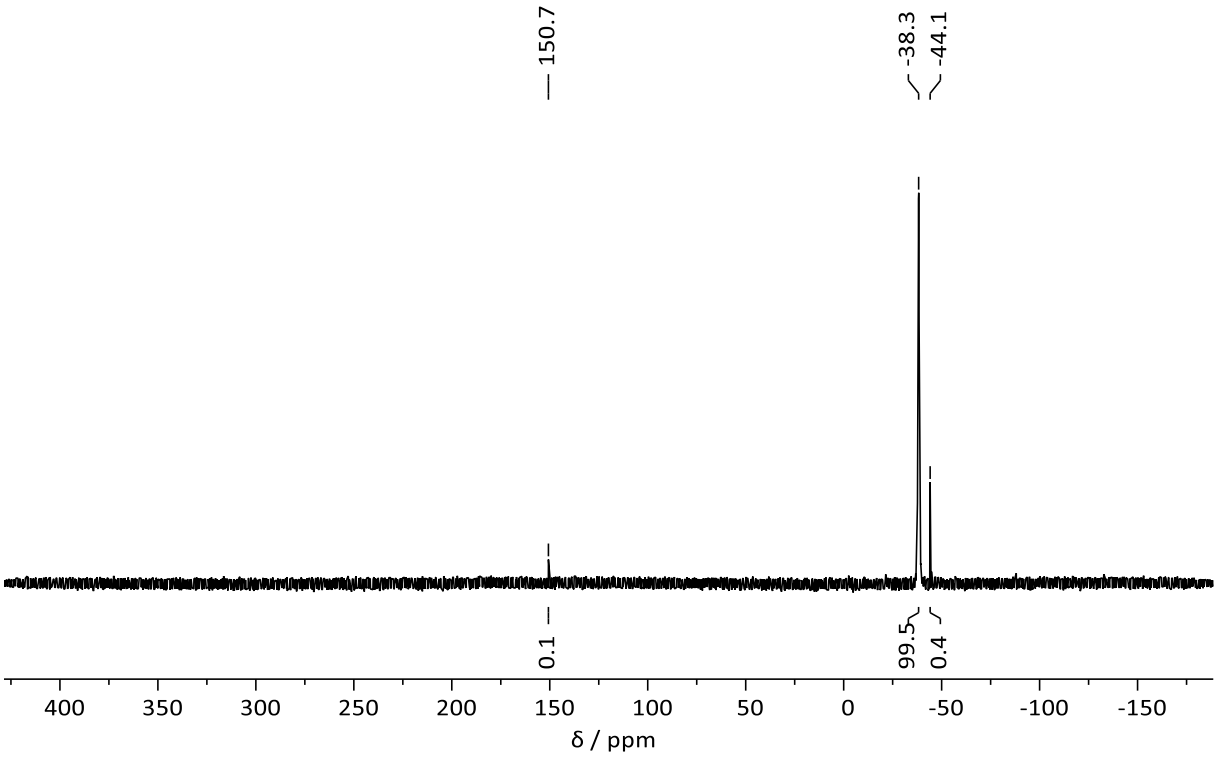


Fig. S16 $^{31}P\{^{1}H\}$ NMR spectrum (162.00 MHz, THF-d_8, 298 K) of compound **6**.

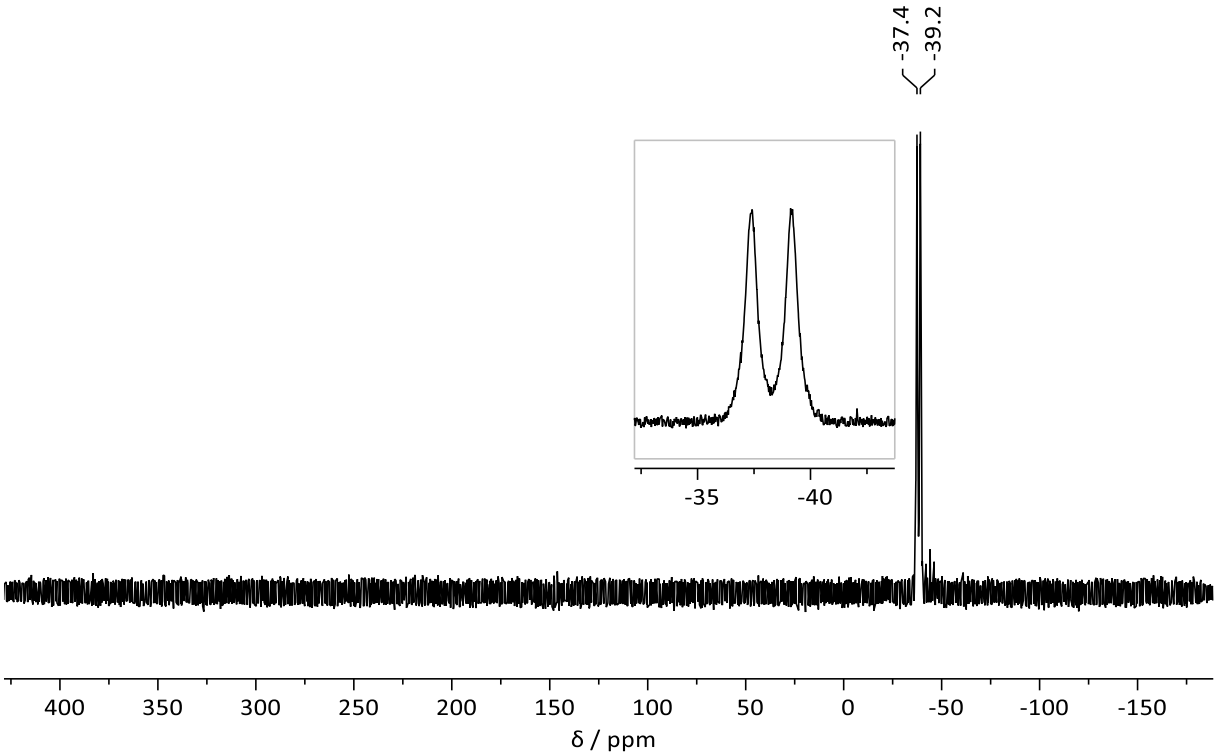


Fig. S17 ^{31}P NMR spectrum (162.00 MHz, THF-d_8, 298 K) of compound **6**.

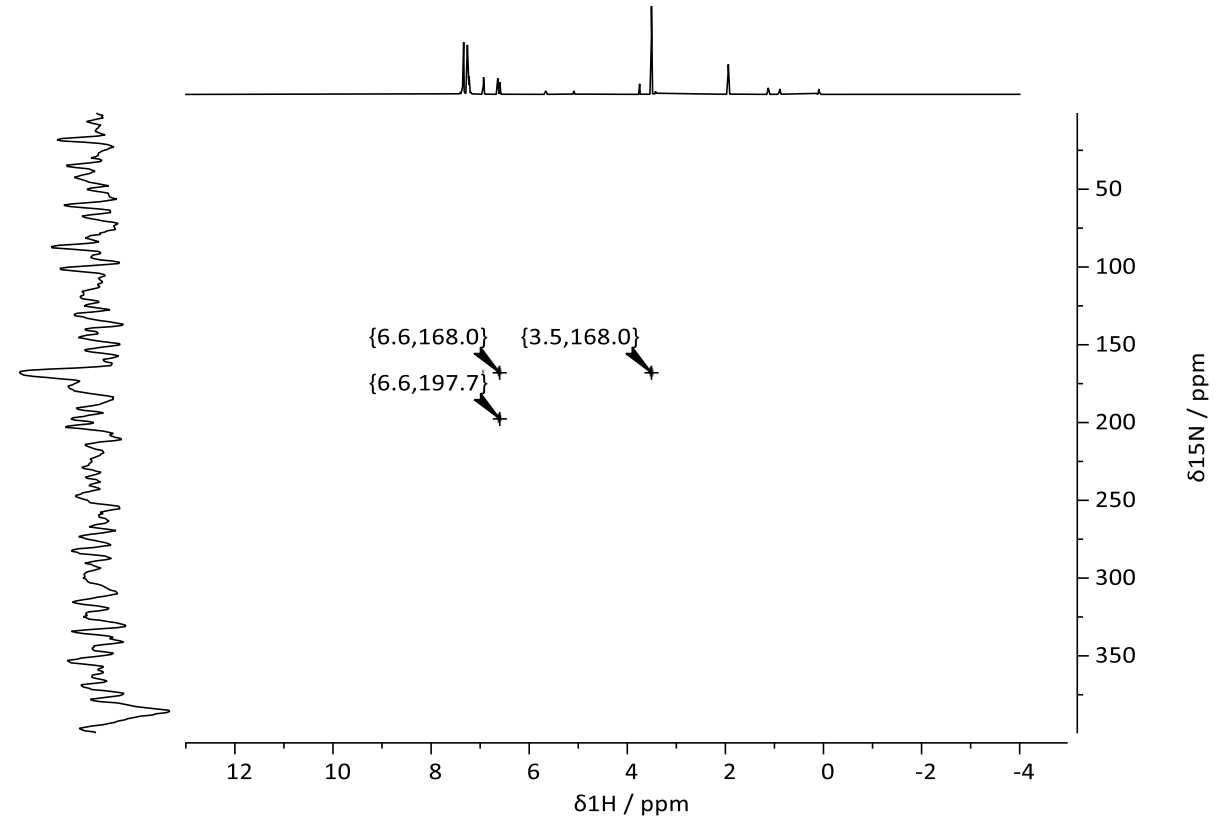


Fig. S18 ^{1}H,^{15}N HMBC NMR spectrum (500.04 MHz, 50.68 MHz, CD_3CN, 298 K) of compound **6**.

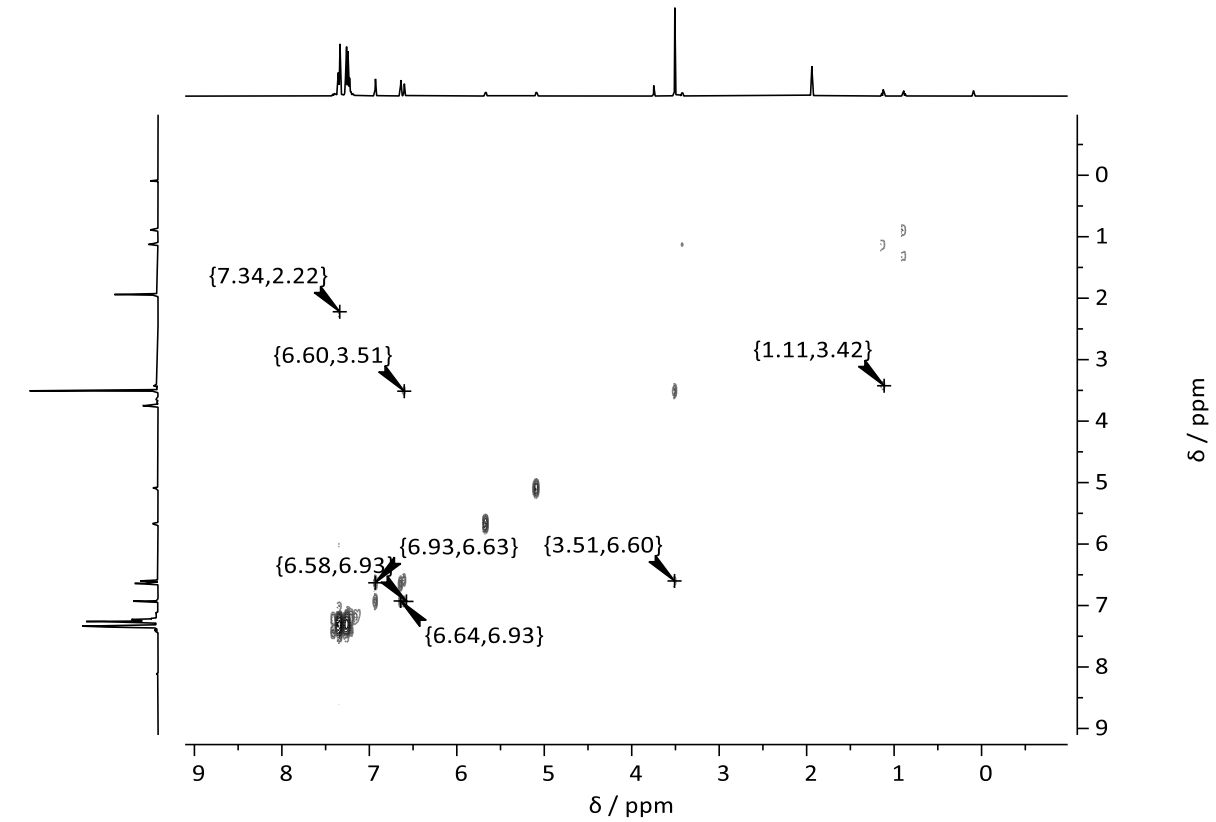


Fig. S19 ^{1}H,^{1}H COSY NMR spectrum (500.04 MHz, 500.04 MHz, CD_3CN, 298 K) of compound **6**.

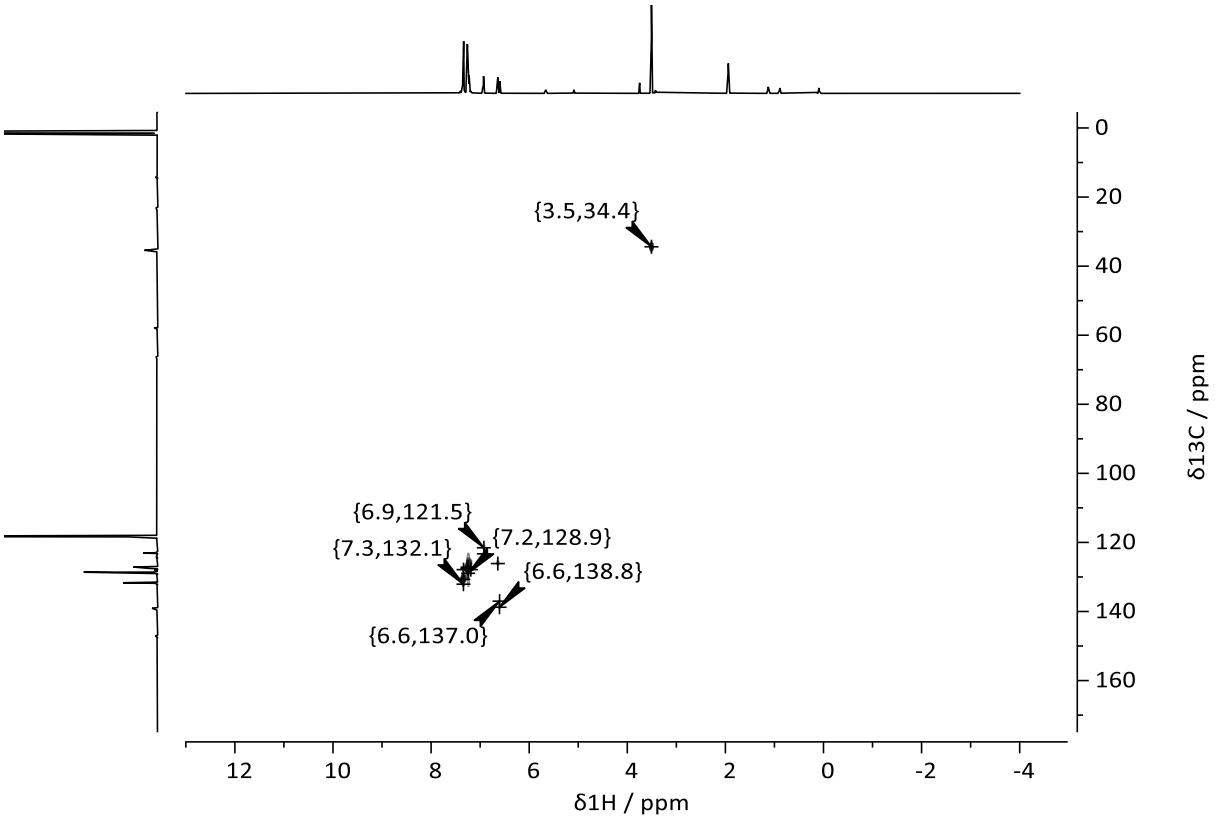


Fig. S20 ^{1}H,^{13}C HSQC NMR spectrum (500.04 MHz, 125.75 MHz, CD_3CN, 298 K) of compound **6**.

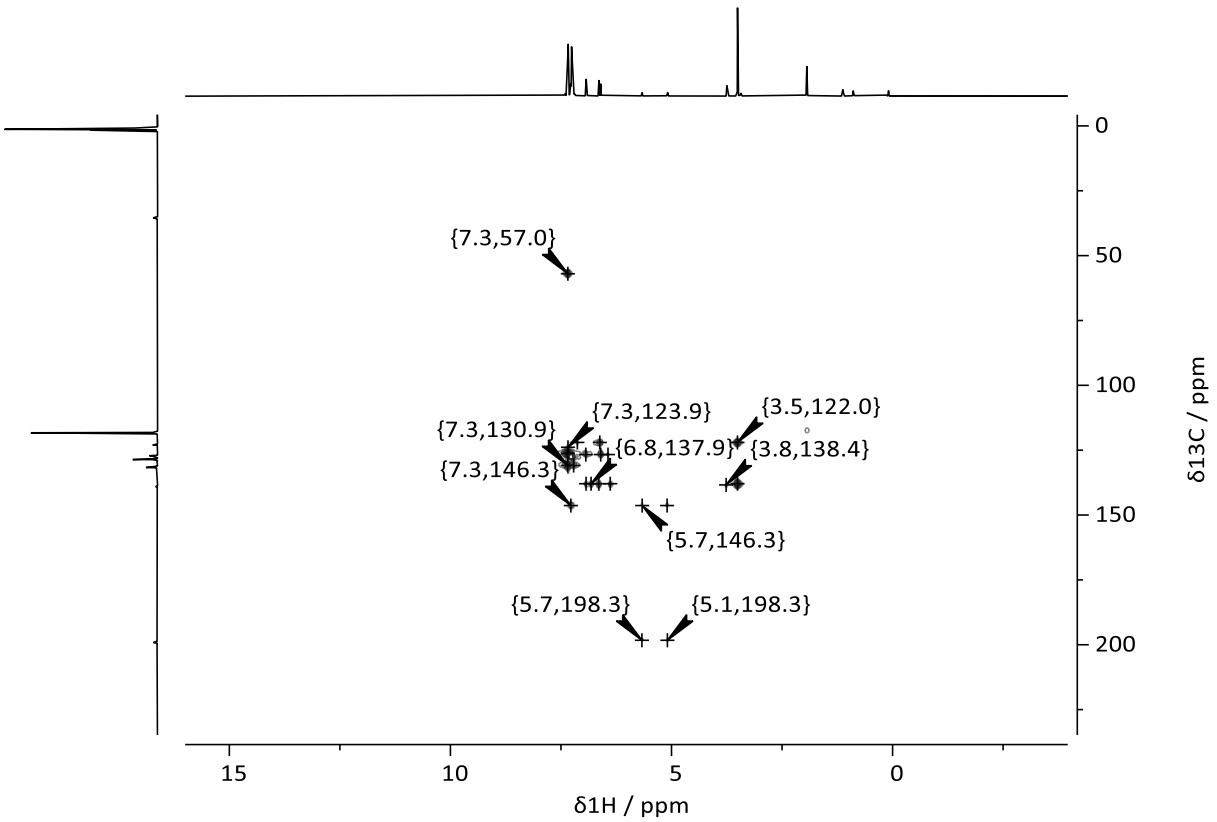


Fig. S21 $^{1}H,^{13}C$ HMBC NMR spectrum (500.04 MHz, 125.75 MHz, CD_3CN, 298 K) of compound **6**.

Reaction mixture of compound 1 with $[W(CO)_5(NCMe)]$ to obtain compound 3

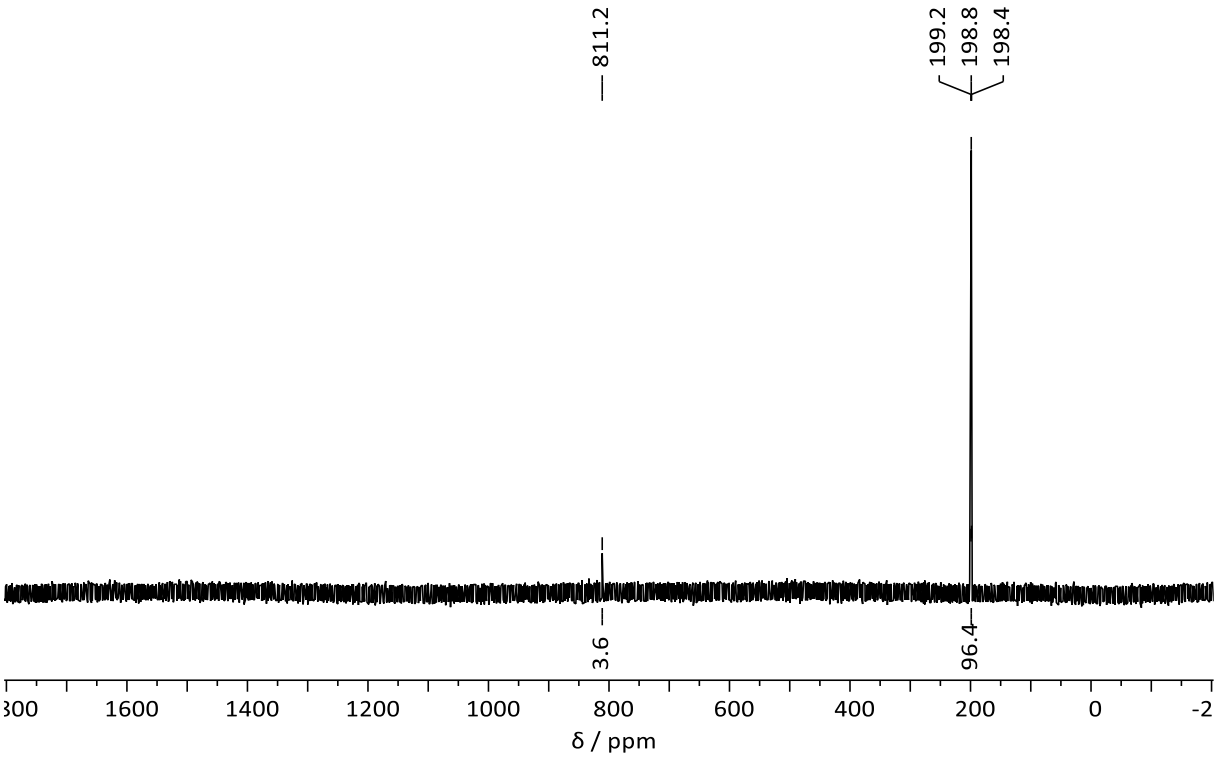


Fig. S22 $^{31}P\{^{1}H\}$ NMR spectrum (121.59 MHz, C_6D_6, 298 K) of the reaction mixture of compound **1** with $[W(CO)_5(NCMe)]$ containing compound **3** after 6 h.

Reaction mixture of compound 1 with $[W(CO)_5(thf)]$ to obtain compound 3

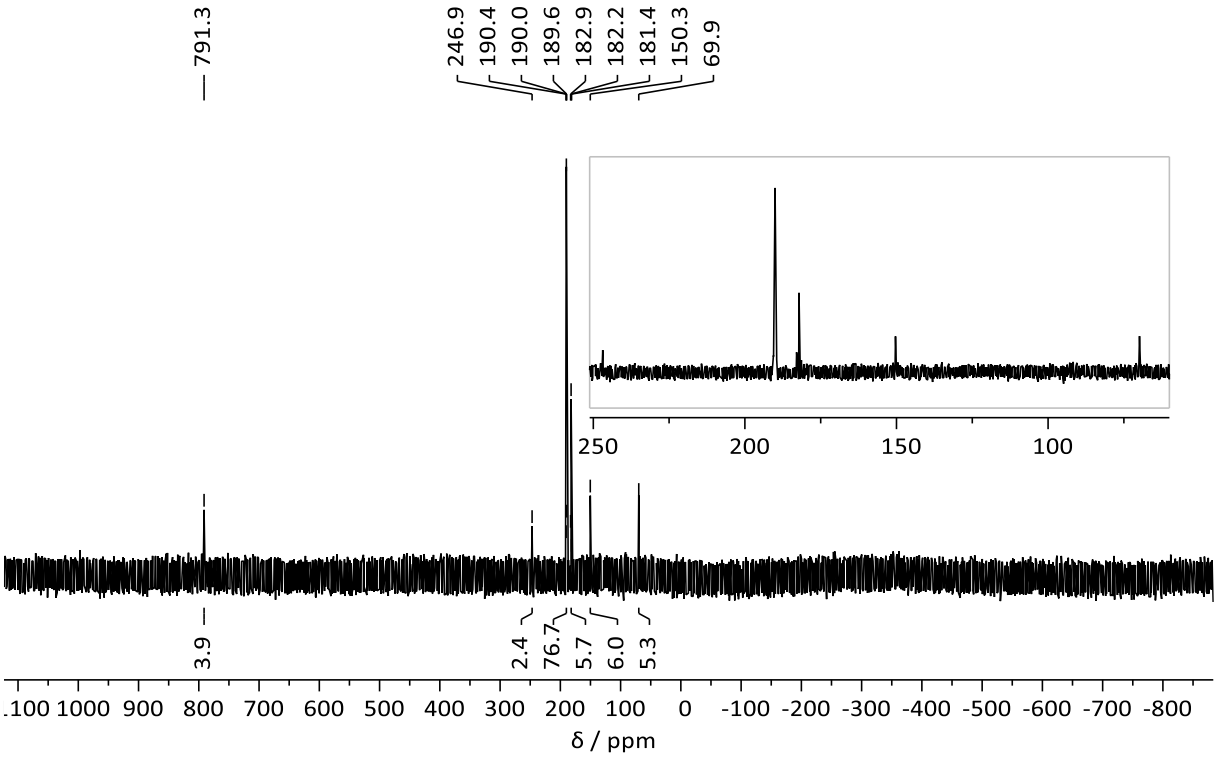


Fig. S23 $^{31}P\{^1H\}$ NMR spectrum (121.51 MHz, THF, 298 K) of the reaction mixture of compound **1** with $[W(CO)_5(thf)]$ containing compound **3** after 3.5 h.

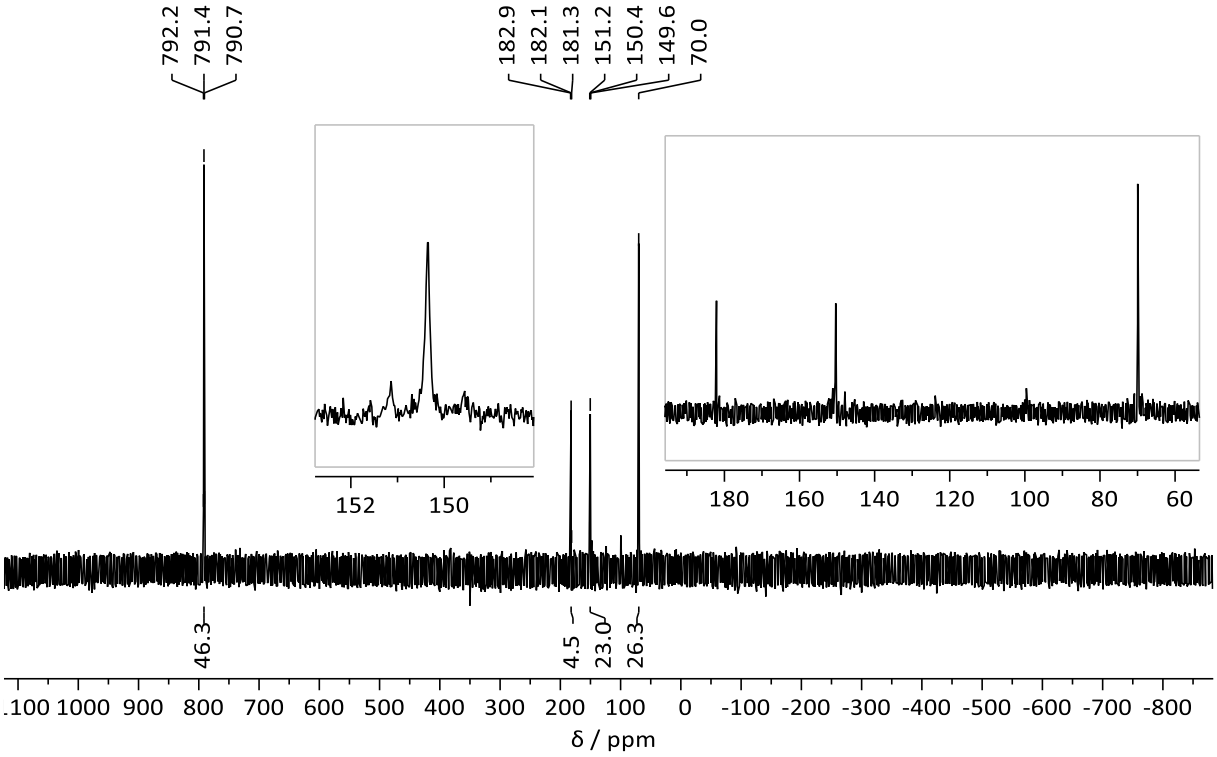


Fig. S24 $^{31}P\{^1H\}$ NMR spectrum (121.51 MHz, THF, 298 K) of the reaction mixture of compound **1** with $[W(CO)_5(thf)]$ containing compound **3** after 6.5 h.

Reaction mixture of compound 1 with $B(C_6F_5)_3$ to obtain compound 4

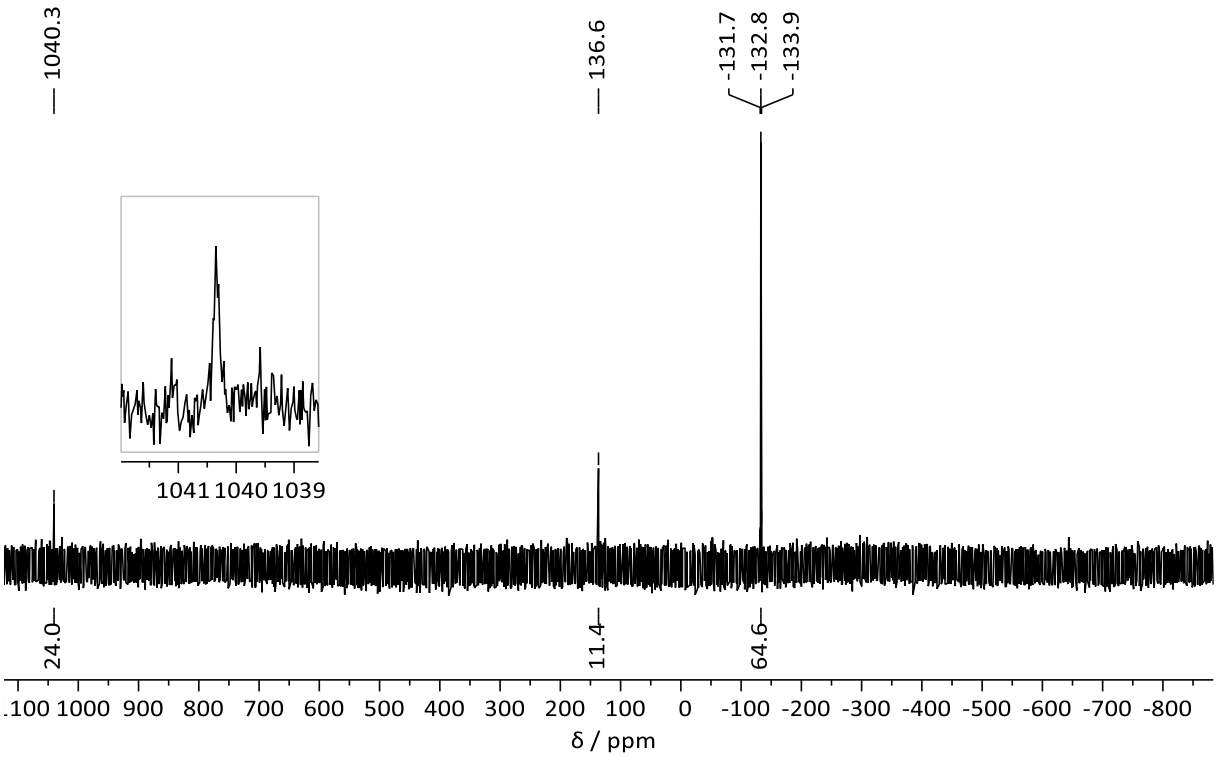


Fig. S25 $^{31}P\{^1H\}$ NMR spectrum (121.57 MHz, C_6D_6, 298 K) of the reaction mixture of compound **1** with $B(C_6F_5)_3$ containing compound **4** after 6.5 h.

4 *in situ* UV/vis spectra

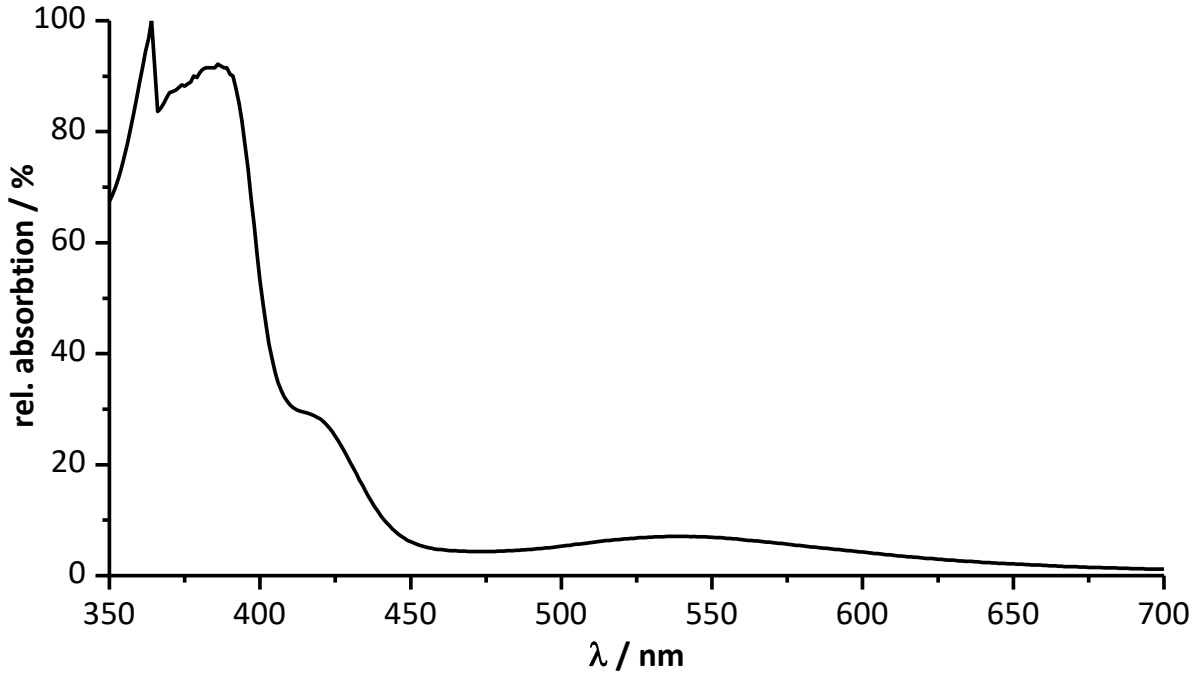


Fig. S26 *in situ* UV/vis spectrum of the reaction mixture of compound **1** with $[W(CO)_5(NCMe)]$ in THF after stirring for 4 h at ambient temperature with a normalized absorption scale.

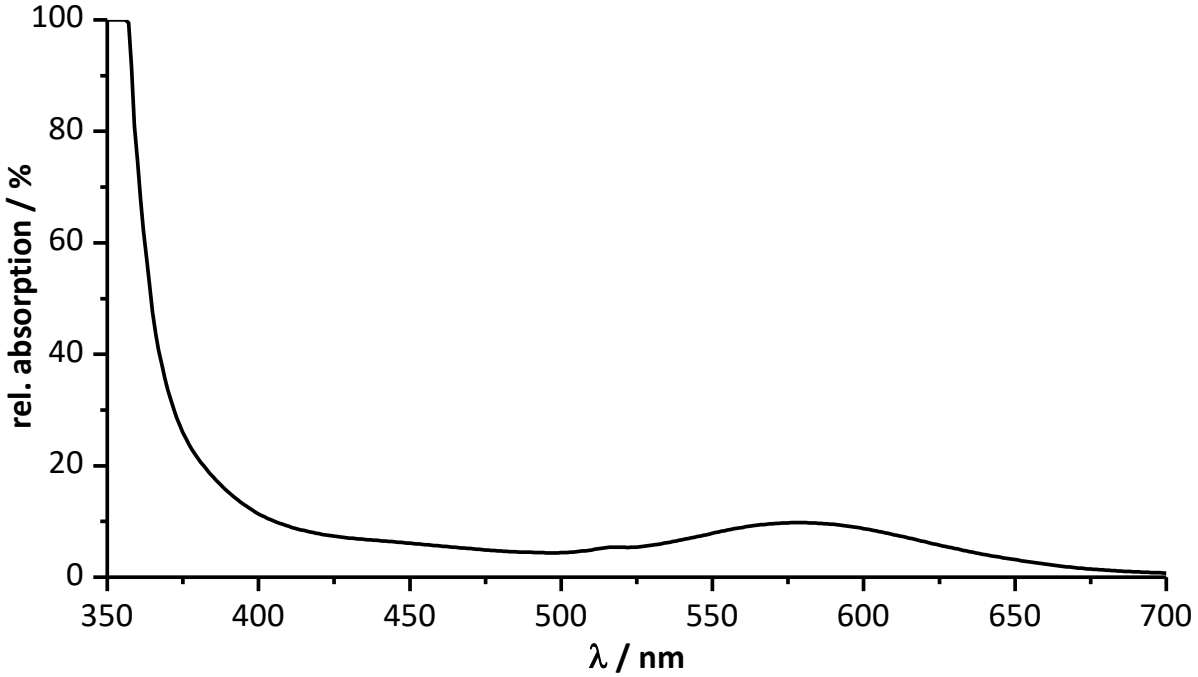


Fig. S27 *in situ* UV/vis spectrum of the reaction mixture of compound **1** with $B(C_6F_5)_3$ in benzene after stirring for 30 minutes at ambient temperature with a normalized absorption scale.

5 X-ray diffraction studies

Compound 5

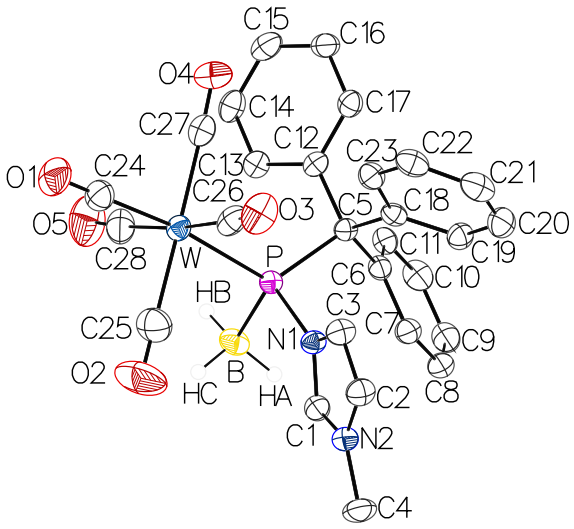


Fig. S28 Molecular structures of **5** in the single crystal lattice at 100(2) K. Thermal ellipsoids are set at 50% probability level. Solvent molecules and hydrogen atoms were omitted for clarity except for those bound to boron atoms. Suitable single crystals were obtained as clear colourless blocks by cooling a concentrated solution of **5** in CD_2Cl_2 at −30 °C. CCDC 2320467.

Table S1 Crystal data and structure refinements for **5**.

Identification code	GSTR793, DB-630 // GXraymo_7114_om_4
Crystal habitus	clear colourless block
Device type	Bruker D8 Venture
Empirical formula	$C_{30}H_{28}BCl_4N_2O_5PW$
Moiety formula	$C_{28}H_{24}BN_2O_5PW$, 2 (CH_2Cl_2)
Formula weight / g/mol	863.97
T / K	100.0
Crystal system	triclinic
Space group	$P\bar{1}$
a / Å	11.0075(6)
b / Å	12.3330(7)
c / Å	12.9754(7)
α / °	85.521(2)
β / °	73.945(2)
γ / °	81.084(2)
V / Å^3	1671.17(16)
Z	2
ρ_{calc} / g/cm^3	1.717
μ / mm^{-1}	3.865
F(000)	848.0
Crystal size / mm^3	0.6 × 0.48 × 0.44
Absorption correction	empirical
Min. and max. transmission	0.338087 and 0.746427

Radiation	Mo-K_α (λ = 0.71073 Å)
2Θ range for data collection / °	5.884 to 58.498
Completeness to Θ	0.995
Index ranges	−14 ≤ *h* ≤ 15, −16 ≤ *k* ≤ 16, 0 ≤ *l* ≤ 17
Reflections collected	9067
Independent reflections	9067 (R_{int} = 0.0618, R_σ = 0.0252)
Data / restraints / parameters	9067 / 3 / 411
Goodness-of-fit on F^2	1.111
Final *R* indexes ($I \geq 2\sigma(I)$)	R_1 = 0.0199, ωR_2 = 0.0471
Final *R* indexes (all data)	R_1 = 0.0219, ωR_2 = 0.0483
Largest diff. peak and hole / e/Å^3	1.10 and −0.77

Table S2 Bond lengths for **5**.

Atom	Atom	Length / Å	Atom	Atom	Length / Å
W	P	2.5688(5)	C6	C7	1.405(3)
W	C24	1.994(2)	C6	C11	1.398(3)
W	C25	2.059(2)	C7	C8	1.391(3)
W	C26	2.033(2)	C8	C9	1.391(3)
W	C27	2.046(2)	C9	C10	1.386(3)
W	C28	2.063(2)	C10	C11	1.396(3)
P	N1	1.8138(16)	C12	C13	1.400(3)
P	C5	1.9540(19)	C12	C17	1.400(3)
P	B	1.959(2)	C13	C14	1.391(3)
O1	C24	1.148(3)	C14	C15	1.391(3)
O2	C25	1.133(3)	C15	C16	1.383(3)
O3	C26	1.141(3)	C16	C17	1.395(3)
O4	C27	1.137(3)	C18	C19	1.395(3)
O5	C28	1.138(3)	C18	C23	1.406(3)
N1	C1	1.346(2)	C19	C20	1.399(3)
N1	C3	1.389(2)	C20	C21	1.383(3)
N2	C1	1.324(3)	C21	C22	1.391(3)
N2	C2	1.384(3)	C22	C23	1.386(3)
N2	C4	1.466(2)	Cl1	C29	1.757(3)
C2	C3	1.357(3)	Cl2	C29	1.754(3)
C5	C6	1.540(3)	Cl3	C30	1.764(2)
C5	C12	1.540(2)	Cl4	C30	1.754(2)
C5	C18	1.540(3)			

Table S3 Bond angles for **5**.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
C24	W	P	172.79(6)	C18	C5	C6	112.55(15)
C24	W	C25	90.24(9)	C18	C5	C12	110.02(14)
C24	W	C26	87.53(9)	C7	C6	C5	120.86(16)
C24	W	C27	88.09(8)	C11	C6	C5	121.89(16)
C24	W	C28	88.45(9)	C11	C6	C7	117.24(17)
C25	W	P	84.05(7)	C8	C7	C6	121.67(18)
C25	W	C28	93.76(10)	C7	C8	C9	120.14(18)
C26	W	P	96.87(6)	C10	C9	C8	119.12(18)
C26	W	C25	90.24(9)	C9	C10	C11	120.68(19)
C26	W	C27	88.41(8)	C10	C11	C6	121.14(18)
C26	W	C28	174.34(8)	C13	C12	C5	120.91(16)
C27	W	P	97.72(6)	C17	C12	C5	120.82(17)
C27	W	C25	177.90(8)	C17	C12	C13	117.98(17)
C27	W	C28	87.47(8)	C14	C13	C12	121.12(18)
C28	W	P	87.54(6)	C15	C14	C13	120.20(19)
N1	P	W	107.17(5)	C16	C15	C14	119.34(18)
N1	P	C5	101.73(8)	C15	C16	C17	120.70(18)
N1	P	B	100.26(9)	C16	C17	C12	120.66(18)
C5	P	W	121.14(6)	C19	C18	C5	123.47(17)
C5	P	B	111.77(9)	C19	C18	C23	117.15(17)
B	P	W	111.89(7)	C23	C18	C5	119.37(17)
C1	N1	P	124.34(13)	C18	C19	C20	121.19(19)
C1	N1	C3	107.21(16)	C21	C20	C19	120.6(2)
C3	N1	P	128.07(13)	C20	C21	C22	119.02(19)
C1	N2	C2	108.74(16)	C23	C22	C21	120.33(19)
C1	N2	C4	126.56(17)	C22	C23	C18	121.58(19)
C2	N2	C4	124.68(17)	O1	C24	W	178.9(2)
N2	C1	N1	109.48(17)	O2	C25	W	178.1(2)
C3	C2	N2	106.78(17)	O3	C26	W	176.02(18)
C2	C3	N1	107.79(17)	O4	C27	W	175.58(17)
C6	C5	P	109.45(12)	O5	C28	W	175.0(2)
C6	C5	C12	109.55(14)	Cl2	C29	Cl1	112.35(14)
C12	C5	P	106.38(12)	Cl4	C30	Cl3	111.90(13)
C18	C5	P	108.70(12)				

Table S4 Torsion angles for **5**.

A	B	C	D	Angle / °	A	B	C	D	Angle / °
W	P	N1	C1	119.77(15)	C6	C7	C8	C9	−0.5(3)
W	P	N1	C3	−52.26(17)	C7	C6	C11	C10	−0.5(3)
P	N1	C1	N2	−173.41(13)	C7	C8	C9	C10	−0.1(3)
P	N1	C3	C2	173.17(14)	C8	C9	C10	C11	0.3(3)
P	C5	C6	C7	−60.2(2)	C9	C10	C11	C6	0.0(3)
P	C5	C6	C11	121.10(17)	C11	C6	C7	C8	0.8(3)
P	C5	C12	C13	−42.3(2)	C12	C5	C6	C7	−176.53(17)
P	C5	C12	C17	143.96(15)	C12	C5	C6	C11	4.8(2)
P	C5	C18	C19	118.38(17)	C12	C5	C18	C19	−125.50(19)
P	C5	C18	C23	−62.97(19)	C12	C5	C18	C23	53.1(2)
N2	C2	C3	N1	−0.1(2)	C12	C13	C14	C15	0.3(3)
C1	N1	C3	C2	0.0(2)	C13	C12	C17	C16	0.8(3)
C1	N2	C2	C3	0.1(2)	C13	C14	C15	C16	0.1(3)
C2	N2	C1	N1	−0.1(2)	C14	C15	C16	C17	−0.1(3)
C3	N1	C1	N2	0.0(2)	C15	C16	C17	C12	−0.4(3)
C4	N2	C1	N1	−178.51(18)	C17	C12	C13	C14	−0.8(3)
C4	N2	C2	C3	178.57(19)	C18	C5	C6	C7	60.7(2)
C5	P	N1	C1	−112.13(16)	C18	C5	C6	C11	−117.92(19)
C5	P	N1	C3	75.84(18)	C18	C5	C12	C13	−159.88(17)
C5	C6	C7	C8	−177.94(18)	C18	C5	C12	C17	26.4(2)
C5	C6	C11	C10	178.18(17)	C18	C19	C20	C21	−0.2(3)
C5	C12	C13	C14	−174.65(17)	C19	C18	C23	C22	−3.6(3)
C5	C12	C17	C16	174.71(17)	C19	C20	C21	C22	−1.9(3)
C5	C18	C19	C20	−178.43(17)	C20	C21	C22	C23	1.2(3)
C5	C18	C23	C22	177.68(17)	C21	C22	C23	C18	1.6(3)
C6	C5	C12	C13	75.9(2)	C23	C18	C19	C20	2.9(3)
C6	C5	C12	C17	−97.83(19)	B	P	N1	C1	2.87(18)
C6	C5	C18	C19	−3.0(2)	B	P	N1	C3	−169.17(17)
C6	C5	C18	C23	175.62(16)					

Compound 6

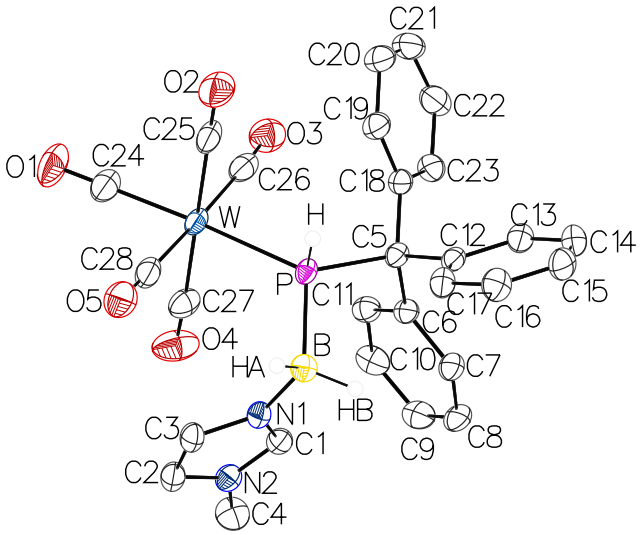


Fig. S29 Molecular structures of **6** in the single crystal lattice at 100(2) K. Thermal ellipsoids are set at 50% probability level. Solvent molecules and hydrogen atoms were omitted for clarity except for those bound to phosphorus and boron atoms. Suitable single crystals were obtained as clear colourless blocks by cooling a concentrated solution of **6** in THF at −30 °C. CCDC 2320468.

Table S5 Crystal data and structure refinements for **6**.

Identification code	GSTR804, DB-636 // GXraymo_7283f
Crystal habitus	clear yellow block
Device type	Bruker D8 Venture
Empirical formula	$C_{32}H_{32}BN_2O_6PW$
Moiety formula	$C_{28}H_{24}BN_2O_5PW$, C_4H_8O
Formula weight / g/mol	766.22
T / K	100.0
Crystal system	triclinic
Space group	$P\bar{1}$
a / Å	9.5360(6)
b / Å	12.7052(8)
c / Å	13.0180(7)
α / °	86.357(2)
β / °	80.306(2)
γ / °	85.980(2)
V / Å^3	1548.73(16)
Z	2
ρ_{calc} / g/cm^3	1.643
μ / mm^{-1}	3.828
F(000)	760.0
Crystal size / mm^3	0.4 × 0.28 × 0.24
Absorption correction	multi-scan
Min. and max. transmission	0.4882 and 0.7461
Radiation	Mo-K$_\alpha$ (λ = 0.71073 Å)
2Θ range for data collection / °	4.342 to 55.998

Completeness to Θ	0.985
Index ranges	$-12 \le h \le 12$, $-16 \le k \le 16$, $-17 \le l \le 17$
Reflections collected	50193
Independent reflections	7393 (R_{int} = 0.0381, R_σ = 0.0296)
Data / restraints / parameters	7393 / 0 / 398
Goodness-of-fit on F^2	1.050
Final R indexes ($I \ge 2\sigma(I)$)	R_1 = 0.0154, ωR_2 = 0.0359
Final R indexes (all data)	R_1 = 0.0159, ωR_2 = 0.0361
Largest diff. peak and hole / e/Å^3	0.63 and −1.05

Table S6 Bond lengths for **6**.

Atom	Atom	Length / Å	Atom	Atom	Length / Å
W	P	2.5650(4)	C6	C7	1.397(2)
W	C24	1.9943(16)	C6	C11	1.4048(19)
W	C25	2.0465(16)	C7	C8	1.397(2)
W	C26	2.0377(17)	C8	C9	1.388(2)
W	C27	2.0510(16)	C9	C10	1.394(2)
W	C28	2.0509(17)	C10	C11	1.390(2)
P	C5	1.9179(14)	C12	C13	1.402(2)
P	B	1.9904(16)	C12	C17	1.395(2)
O1	C24	1.149(2)	C13	C14	1.388(2)
O2	C25	1.132(2)	C14	C15	1.390(2)
O3	C26	1.147(2)	C15	C16	1.383(2)
O4	C27	1.137(2)	C16	C17	1.3970(19)
O5	C28	1.142(2)	C18	C19	1.400(2)
N1	C1	1.3261(19)	C18	C23	1.398(2)
N1	C3	1.3853(18)	C19	C20	1.394(2)
N1	B	1.5586(19)	C20	C21	1.390(3)
N2	C1	1.3328(18)	C21	C22	1.384(3)
N2	C2	1.3757(19)	C22	C23	1.397(2)
N2	C4	1.4565(19)	O6	C29	1.428(2)
C2	C3	1.357(2)	O6	C32	1.425(2)
C5	C6	1.5379(19)	C29	C30	1.532(2)
C5	C12	1.5487(18)	C30	C31	1.542(2)
C5	C18	1.5387(19)	C31	C32	1.524(2)

Table S7 Bond angles for **6**.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
C24	W	P	173.51(5)	C7	C6	C11	117.67(13)
C24	W	C25	90.56(6)	C11	C6	C5	119.86(12)
C24	W	C26	89.31(6)	C8	C7	C6	120.99(14)
C24	W	C27	88.44(6)	C9	C8	C7	120.69(14)
C24	W	C28	89.92(6)	C8	C9	C10	119.01(14)
C25	W	P	87.84(4)	C11	C10	C9	120.33(14)
C25	W	C27	177.15(6)	C10	C11	C6	121.30(14)
C25	W	C28	90.27(6)	C13	C12	C5	117.91(12)
C26	W	P	96.91(4)	C17	C12	C5	124.65(13)
C26	W	C25	87.80(6)	C17	C12	C13	117.44(13)
C26	W	C27	89.53(6)	C14	C13	C12	121.51(14)
C26	W	C28	177.91(6)	C13	C14	C15	120.19(14)
C27	W	P	93.45(4)	C16	C15	C14	119.24(14)
C28	W	P	83.80(4)	C15	C16	C17	120.52(14)
C28	W	C27	92.40(6)	C12	C17	C16	121.11(14)
C5	P	W	123.10(4)	C19	C18	C5	119.55(13)
C5	P	B	107.48(6)	C23	C18	C5	122.31(13)
B	P	W	118.20(5)	C23	C18	C19	118.00(14)
C1	N1	C3	107.09(12)	C20	C19	C18	121.05(15)
C1	N1	B	124.91(12)	C21	C20	C19	120.06(15)
C3	N1	B	128.00(12)	C22	C21	C20	119.60(15)
C1	N2	C2	108.47(12)	C21	C22	C23	120.33(15)
C1	N2	C4	125.11(13)	C22	C23	C18	120.85(15)
C2	N2	C4	126.42(13)	O1	C24	W	179.56(15)
N1	C1	N2	109.88(13)	O2	C25	W	178.79(15)
C3	C2	N2	106.40(12)	O3	C26	W	176.80(13)
C2	C3	N1	108.15(13)	O4	C27	W	175.47(13)
C6	C5	P	104.42(9)	O5	C28	W	178.36(14)
C6	C5	C12	111.54(11)	N1	B	P	111.31(9)
C6	C5	C18	112.47(11)	C32	O6	C29	104.68(13)
C12	C5	P	112.25(9)	O6	C29	C30	105.52(13)
C18	C5	P	109.58(9)	C29	C30	C31	103.61(13)
C18	C5	C12	106.68(11)	C32	C31	C30	103.54(13)
C7	C6	C5	122.41(12)	O6	C32	C31	105.69(14)

6 Computational Methods

Quantum chemical calculations were performed with ORCA (v. 4.2.1).[8] All geometry optimizations were run in redundant internal coordinates with tight convergence criteria, also computed using Grimme's fast PBEh-3c composite approach.[9] In all optimizations and energy evaluations, the 2010 Grimme's semiempirical atom-pair-wise correction (DFT-D3 methods), taking into account the major part of the contribution of dispersion forces to the energy, was included.[10] Harmonic frequency calculations verified the nature of the computed species as minima or TS (transition state) structures, featuring none or only one negative eigenvalues, respectively. Moreover, all TS structures were confirmed by intrinsic reaction coordinate (IRC) calculations. From these geometries, all reported electronic data were corrected for the Gibbs energy term at the optimization level and obtained by means of single-point (SP) calculations using the double-hybrid-meta-GGA functional PWPB95[11] with Grimme's D3 correction (PWPB95-D3) as well as the more polarized Ahlrichs' segmented def2-QZVPP[12] basis set. The frontier molecular orbitals (FMOs) energies were obtained at the same PWPB95-D3/def2-QZVPP level, although the Kohn-Sham isosurfaces were drawn at the optimization level (Figure 3). AIM wavefunction analyses were performed with the B3LYP[13] functional and the def2-TZVPP[12] basis set and using Aimall.[14] Solvent effects (tetrahydrofuran, dichloromethane, toluene or benzene) were included using the Conductor-like Polarizable Continuum Model (CPCM).[15] Isotropic values (σ_{Iso}) for the ^{31}P NMR magnetic shielding tensor were computed using the Gauge Including Atomic Orbital (GIAO) method,[16] using the PBE0[17] functional and the def2-TZVP basis set.[12] The expected chemical shifts δ^P were estimated through a linear equation $\delta^P = 241.6491 - 0.8664 \cdot \sigma_{Iso}$, which in turn was obtained from a linear regression ($R^2 = 0.9968$) of seventeen reference compounds spanning a wide range of chemical shifts, from δ^P −525.0 (P_4) to 598.6 ppm (Tsi-P=P-Tsi, Tsi referring to the trisyl (or tris(trimethylsilyl)methyl) substituent), as reported elsewhere.[7,18]

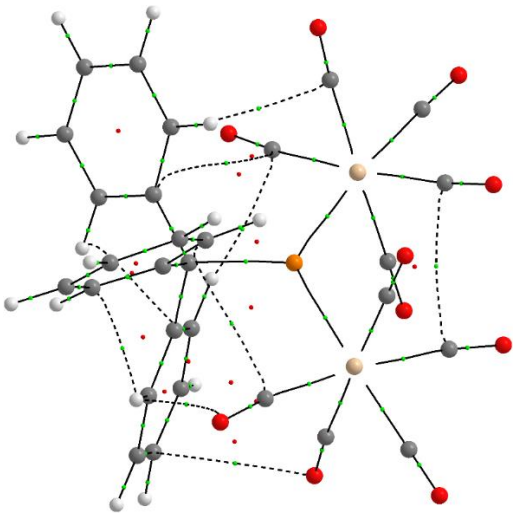


Fig. S30 Computed [CPCMtol/B3LYP/def2-TZVP(ecp)] structure for **2** showing bond and ring critical points (small green and red spheres, respectively) as well as bond paths (non-covalent interactions shown by dashed lines).

Full PES for the reaction of 1' with $H_3B{\cdot}SMe_2$

Besides the main path described in the main text (Scheme 4), the alternative S_N1-type mechanism is disfavoured and requires initial rather endergonic barrierless elimination of *N*-MeIm and P-insertion of the phosphinidene complex **7'** into the B-H bond of the $H_3B{\cdot}SMe_2$ reagent affording **8'**, from which dimethyl sulphide is replaced at the boron centre by *N*-MeIm in a typical S_N2 reaction (Scheme S114). Phosphinidene **7'** can also react with the *N*-MeIm·SMe_2 adduct, which is exergonically produced from *N*-MeIm and SMe_2 ($\Delta\Delta G$ = -10.29 kcal/mol) over a moderately low barrier ($\Delta\Delta G^{‡}$ = 24.40 kcal/mol). This reaction can take place through the imidazole N3 atom giving the highly unstable product **14'** or through C2 affording **9'**, the latter readily undergoing B-to-P hydride transfer to give **10'**. Upon cleavage of the C-P bond, the ion pair **11'** or its B···H bound derivative **12'** are formed, both allowing the low-barrier formation of the final model complex **6'** (Scheme S114). Intermediate **9'** can also lead to the slightly less stable P-decomplexed bicyclic phosphonium borate **13'**. Finally, the final phosphino-borane N-MeIm complex adduct **6'** could undergo a very unfavoured N-to-C [1,2]-boron shift to the less stable isomer **15'** (Scheme S114).

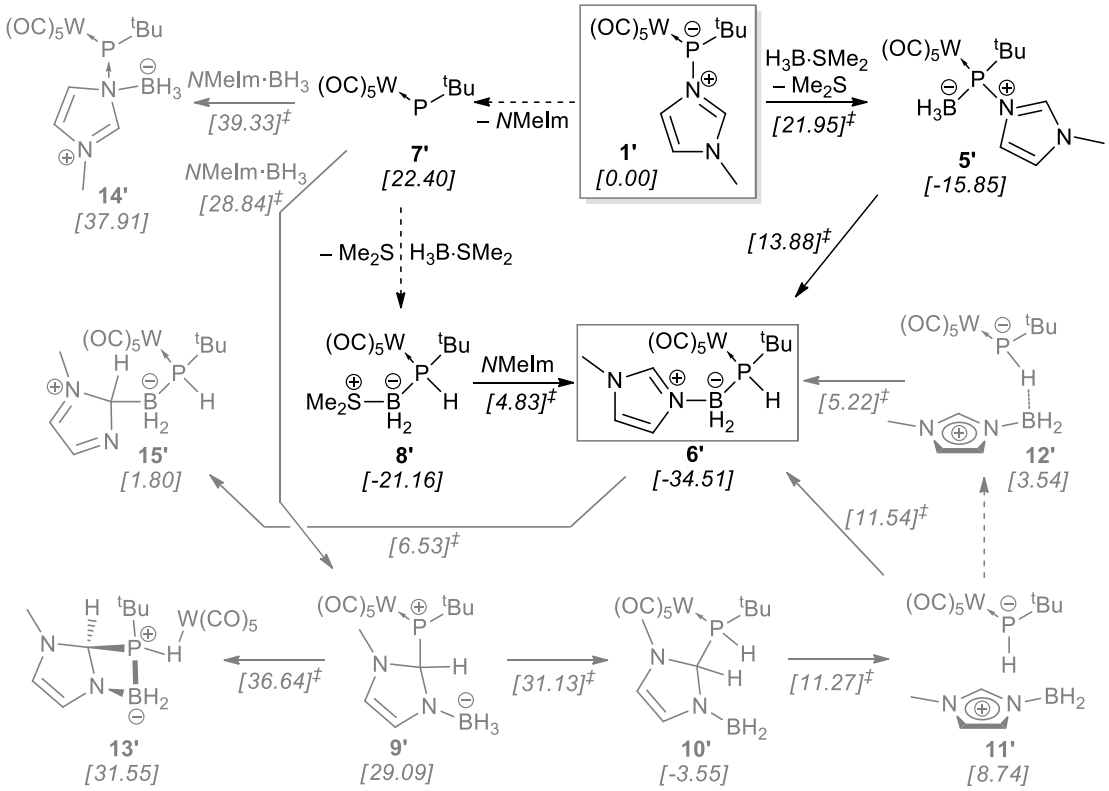


Fig. S31 Proposed full potential energy surface for the formation of rearranged model product **6'** from phosphinidene adduct complex **1'**. In square brackets the computed [$CPCM_{THF}$/PWPB95-D3/def2-QZVPP//$CPCM_{THF}$/PBEh-3c] relative Gibbs free energies (kcal/mol) for ground and transition states (the latter indicated by the ‡ superscript). Dashed arrows indicate barrierless processes.

7 Calculated structures

Cartesian coordinates (in Å) and energies (in hartrees) for all computed species. Geometries, zero-point energy correction (ZPE) and Gibbs energy correction (G_{corr}) at the optimization level (*vide supra*), whereas electronic energies are computed at the CPCM(THF)/PWPB95-D3/def2-QZVPP(ecp) level, unless otherwise stated. Solvents different from THF are indicated in square brackets.

$BH_3{\cdot}SMe_2$

E = -504.5986302725 au
ZPE = 0.11030038 au
G_{corr} = 0.08078862 au

B	-0.163242	0.010727	-0.067181	H	0.355633	-1.460100	-2.646604
H	0.784942	0.358920	-0.732224	H	-0.316088	-2.734767	-1.603098
H	-0.727905	0.923431	0.487893	C	-1.677616	0.614541	-2.521224
H	0.078798	-0.908852	0.678238	H	-2.168631	1.447946	-2.024470
S	-1.484240	-0.699434	-1.307203	H	-0.702803	0.928256	-2.888183
C	-0.559768	-1.908625	-2.266824	H	-2.301138	0.262818	-3.339916
H	-1.177694	-2.271827	-3.084768				

Me_2S

E = -477.9619654310 au
ZPE = 0.07799832 au
G_{corr} = 0.05101430 au

S	-1.313958	-0.740359	-1.294333	C	-1.768562	0.567799	-2.452700
C	-0.531705	-1.899277	-2.436647	H	-2.265510	1.353454	-1.886403
H	-1.234218	-2.239621	-3.196510	H	-0.888752	0.991085	-2.935897
H	0.334801	-1.451370	-2.921660	H	-2.455998	0.200033	-3.213546
H	-0.200032	-2.760475	-1.859401				

N-MeIm

E = -265.4765447343 au
ZPE = 0.10213822 au
G_{corr} = 0.07436292 au

N	-2.174600	-1.716837	-1.350332	H	-6.307446	-1.001496	-1.237650
C	-3.232665	-1.623170	-0.586596	H	-5.647616	0.464765	-0.493151
N	-4.217880	-0.907713	-1.168267	H	-5.591311	-1.072648	0.375476
C	-3.753830	-0.516530	-2.391787	H	-3.344771	-2.053089	0.397856
C	-2.489986	-1.026759	-2.484540	H	-4.347111	0.073283	-3.070568
C	-5.513798	-0.609544	-0.604597	H	-1.797750	-0.931954	-3.306945

N-MeIm·BH_3

E = -292.1303685677 au
ZPE = 0.13527106 au
G_{corr} = 0.10489198 au

N	-2.198192	-1.702818	-1.357216	C	-2.493290	-1.016749	-2.502374
C	-3.250382	-1.623077	-0.570265	C	-5.514354	-0.610180	-0.602928
N	-4.212901	-0.913271	-1.161732	H	-6.297706	-1.002541	-1.246550
C	-3.751721	-0.519344	-2.388679	H	-5.636411	0.465196	-0.499468

H	-5.598128	-1.071355	0.376421
H	-3.330402	-2.064067	0.409004
H	-4.346158	0.069891	-3.065413
H	-1.789118	-0.933377	-3.311902
B	-0.844453	-2.456952	-1.032892
H	-0.953098	-2.934074	0.079623
H	-0.680585	-3.326681	-1.867342
H	0.063360	-1.648514	-1.075370

(BH_3·SMe_2+*N*MeIm→*N*MeIm·BH_3+SMe_2)‡

E = -770.0545922799 au
ZPE = 0.21230421 au
G_{corr} = 0.17345094 au
ν = -321.07 cm^{-1}

B	0.207259	0.224572	0.027255
H	-0.035804	-0.043128	1.172165
H	1.267527	-0.075841	-0.444973
H	-0.567985	0.876762	-0.615916
S	-0.810863	-1.879304	-0.668890
C	-2.367349	-1.757323	0.228279
H	-2.860456	-2.726316	0.283549
H	-2.196183	-1.368524	1.231140
H	-3.007120	-1.064692	-0.314707
C	0.092729	-2.996884	0.415893
H	1.088275	-3.128562	-0.002909
H	0.182344	-2.566301	1.412295
H	-0.399607	-3.966233	0.471944
N	1.148231	2.257546	0.762172
C	0.798135	3.433523	0.308743
N	1.504133	4.421416	0.892939
C	2.361627	3.830982	1.778419
C	2.126025	2.489414	1.683038
C	1.380997	5.837394	0.631925
H	2.318883	6.240783	0.255444
H	1.103079	6.371179	1.538476
H	0.608871	5.996100	-0.115928
H	0.042861	3.622622	-0.438788
H	3.046136	4.401733	2.383494
H	2.603416	1.687237	2.223158

1 [toluene]

E = -1976.904309879727 au
ZPE = 0.42390259 au (B3LYP-D3/def2TZVP(ecp))
G_{corr} = 0.36180286 au (B3LYP-D3/def2TZVP(ecp))

P	-0.013401	0.290879	0.125654
W	-0.046488	2.826749	-0.562418
C	0.239583	4.726180	-1.165015
O	0.413394	5.815584	-1.503595
C	-1.563946	2.577854	-1.943941
O	-2.394397	2.471341	-2.724224
C	-1.421731	3.564388	0.766726
O	-2.164301	4.055157	1.496338
C	1.416496	2.987512	0.868742
O	2.220535	3.052296	1.687242
C	1.356142	2.249451	-1.965954
O	2.139288	1.968346	-2.754304
C	-1.645993	-0.792315	-0.217705
C	-1.643294	-1.850268	0.885261
C	-2.544120	-1.851608	1.949352
C	-0.645737	-2.836907	0.880507
C	-2.441054	-2.782501	2.981420
H	-3.341774	-1.125575	1.982662
C	-0.547662	-3.773289	1.898816
H	0.066947	-2.861788	0.068085
C	-1.441811	-3.745769	2.966506
H	-3.156891	-2.753741	3.793633
H	0.232162	-4.524046	1.860507
H	-1.367238	-4.473572	3.764557
C	-2.944123	0.016209	-0.280385
C	-3.854646	-0.134742	-1.329245
C	-3.272754	0.935795	0.718170
C	-5.032332	0.604589	-1.378834
H	-3.645786	-0.822604	-2.133565
C	-4.445287	1.675231	0.678462
H	-2.601467	1.079287	1.546238
C	-5.335921	1.515843	-0.377502
H	-5.707326	0.469129	-2.214630
H	-4.653480	2.386850	1.467023
H	-6.247039	2.098815	-0.420453
C	-1.388526	-1.446390	-1.584162
C	-0.715956	-0.771779	-2.601794
C	-1.910864	-2.708989	-1.877216
C	-0.548158	-1.338545	-3.860262
H	-0.324835	0.219526	-2.428292
C	-1.753656	-3.279621	-3.134270
H	-2.456562	-3.251264	-1.117617
C	-1.065855	-2.598530	-4.133119
H	-0.015604	-0.788328	-4.625500
H	-2.173400	-4.257995	-3.332605
H	-0.939432	-3.042826	-5.112156
N	0.012983	0.284447	1.971630
C	0.688110	-0.658070	2.632772
N	0.551728	-0.474855	3.945887
C	-0.234147	0.645400	4.146866
C	-0.561510	1.118087	2.918210
C	1.114780	-1.324614	4.986901
H	0.309084	-1.788809	5.552890
H	1.737580	-0.727823	5.650689
H	1.717844	-2.096764	4.517570
H	1.253718	-1.446020	2.173810

H	-0.475827	1.001876	5.132088	H	-1.130380	1.984256	2.648801

1'

E = -1398.3979673186 au
ZPE = 0.27432915 au
G_{corr} = 0.22196562 au

P	-0.602680	0.592384	0.363179	C	-5.256187	2.936176	-0.049588
C	-0.256281	0.438475	2.213456	H	-5.414412	3.626411	-0.873965
C	0.486996	-0.895349	2.337273	H	-5.759798	3.307685	0.838812
H	0.747308	-1.080835	3.382498	H	-5.666017	1.966242	-0.312917
H	-0.124964	-1.730638	1.992845	H	-3.531351	0.712877	-0.144468
H	1.417574	-0.907895	1.768327	H	-3.324005	4.822955	0.714244
C	0.591801	1.551776	2.816595	H	-0.823299	3.721289	0.965956
H	0.107787	2.526500	2.740431	W	1.329351	1.544095	-1.116217
H	0.764036	1.362696	3.880649	C	2.675018	2.163268	-2.456631
H	1.565555	1.621889	2.332818	O	3.440773	2.526709	-3.237694
C	-1.578324	0.330575	2.974756	C	1.665806	3.229864	-0.006445
H	-1.385356	0.061788	4.017134	O	1.892891	4.182770	0.588535
H	-2.128170	1.273240	2.985725	C	2.826857	0.610541	-0.070540
H	-2.228773	-0.436264	2.549755	O	3.695628	0.114220	0.485543
N	-1.863710	1.919744	0.417080	C	1.028330	-0.175118	-2.211265
C	-3.132526	1.676452	0.125109	O	0.869617	-1.128184	-2.820254
N	-3.836144	2.798017	0.211417	C	-0.164355	2.500541	-2.149325
C	-2.986852	3.809672	0.578995	O	-1.001616	3.034771	-2.716833
C	-1.755802	3.258296	0.702946				

3 [toluene]

E = -2341.760140558626 au
ZPE = 0.36438046 au (B3LYP-D3/def2TZVP(ecp))
G_{corr} = 0.29456188 au (B3LYP-D3/def2TZVP(ecp))

P	-0.090175	-0.081456	-0.085413	C	-1.422782	2.410680	4.358414
C	0.094999	-0.039375	1.850926	C	-2.563495	2.850293	3.693357
C	1.599666	0.234189	1.928365	C	-2.848397	2.350738	2.429739
C	2.144503	1.449137	2.349886	C	-1.981781	1.445393	1.829441
C	3.519881	1.644059	2.380375	H	0.299208	1.148343	4.299471
C	4.386067	0.640925	1.962551	H	-1.202852	2.770187	5.355597
C	3.861008	-0.559961	1.501719	H	-3.229992	3.561823	4.163292
C	2.487489	-0.759077	1.486882	H	-3.743444	2.661285	1.906314
H	1.500404	2.251203	2.669639	H	-2.236126	1.057909	0.852139
H	3.912228	2.591923	2.725872	W	0.328497	2.080250	-1.232364
H	5.456384	0.798910	1.981675	C	-1.709153	2.218274	-1.573049
H	4.517460	-1.347919	1.156136	O	-2.834279	2.277419	-1.762464
H	2.102731	-1.709499	1.150679	C	0.176268	3.274899	0.455767
C	-0.307375	-1.343931	2.547941	O	0.128017	4.039567	1.303501
C	0.529153	-2.002711	3.447944	C	2.384753	1.894123	-0.973369
C	0.095712	-3.138162	4.125520	O	3.516737	1.784601	-0.909813
C	-1.184080	-3.634694	3.920394	C	0.594299	1.140014	-3.041732
C	-2.040121	-2.966750	3.050023	O	0.794477	0.702732	-4.080298
C	-1.606541	-1.829387	2.387023	C	0.633012	3.823547	-2.270743
H	1.527498	-1.636005	3.631999	O	0.800026	4.796414	-2.850520
H	0.767785	-3.633945	4.814400	W	-0.460421	-2.224467	-1.235372
H	-1.517329	-4.523444	4.440472	C	0.341177	-3.447104	0.234404
H	-3.048170	-3.327200	2.890636	O	0.764208	-4.198879	0.981892
H	-2.297432	-1.295339	1.751966	C	-2.346481	-2.669462	-0.486775
C	-0.812162	1.029871	2.463206	O	-3.393002	-2.949192	-0.128341
C	-0.565013	1.501912	3.754387	C	-1.420153	-1.167039	-2.727166

O	-2.008506	-0.629161	-3.545176	C	-0.594399	-3.893316	-2.435460
C	1.417165	-1.866358	-2.040006	O	-0.648360	-4.808381	-3.118743
O	2.452918	-1.663817	-2.473196				

4 [benzene]

E = -3916.490330557042 au (opt B3LYP-D3/def2TZVP(ecp))
ZPE = 0.47842463 au (B3LYP-D3/def2TZVP(ecp))
G_{corr} = 0.39624814 au (B3LYP-D3/def2TZVP(ecp))

P	0.079587	-0.126512	-0.034024	C	3.335147	-0.507838	0.235544
C	-0.389804	0.184782	1.843721	O	4.026549	-1.229365	0.773006
C	0.870310	-0.336001	2.556155	C	2.297568	-0.475343	-2.463300
C	1.766170	0.504908	3.216990	O	2.578112	-1.133555	-3.351029
C	2.885095	-0.005327	3.864771	C	3.918837	1.604295	-1.616139
C	3.140940	-1.369652	3.867509	O	4.885745	2.031085	-2.038243
C	2.268986	-2.219798	3.199521	B	-1.048894	-1.533299	-1.055586
C	1.158897	-1.703991	2.550811	C	-0.668149	-2.830957	-0.145844
H	1.592862	1.566793	3.252072	C	0.608666	-3.392778	-0.184734
H	3.555932	0.675380	4.373313	C	0.996419	-4.493796	0.553599
H	4.011708	-1.764478	4.374405	C	0.088311	-5.084868	1.415753
H	2.453523	-3.286093	3.179063	C	-1.191399	-4.564552	1.502657
H	0.488579	-2.380669	2.054714	C	-1.544388	-3.466287	0.732969
C	-1.680455	-0.502338	2.340235	F	1.560028	-2.852996	-0.969666
C	-1.699507	-1.484384	3.331513	F	2.242351	-4.970570	0.468500
C	-2.899499	-1.988647	3.822250	F	0.446301	-6.130486	2.158944
C	-4.112121	-1.517382	3.343928	F	-2.078490	-5.125459	2.328458
C	-4.110020	-0.509844	2.387035	F	-2.805873	-3.049007	0.872062
C	-2.912345	-0.003479	1.910652	C	-2.626090	-1.173972	-1.216432
H	-0.785163	-1.858022	3.760179	C	-3.166417	0.099036	-1.173196
H	-2.874871	-2.753312	4.588137	C	-4.489477	0.389580	-1.462999
H	-5.044930	-1.914606	3.723051	C	-5.338733	-0.630531	-1.849003
H	-5.043261	-0.099975	2.021874	C	-4.838638	-1.919124	-1.950191
H	-2.937393	0.832144	1.233588	C	-3.509559	-2.157625	-1.651518
C	-0.613292	1.687885	2.097219	F	-2.398118	1.157222	-0.827663
C	-0.810222	2.084879	3.425074	F	-4.947764	1.643570	-1.370043
C	-1.060457	3.407449	3.748286	F	-6.617143	-0.376273	-2.133498
C	-1.142166	4.371685	2.746334	F	-5.640052	-2.912822	-2.348404
C	-0.981333	3.987571	1.425372	F	-3.071034	-3.417579	-1.823912
C	-0.721879	2.657057	1.108756	C	-0.555868	-1.634379	-2.614327
H	-0.774453	1.346243	4.214386	C	-0.264569	-2.820837	-3.285711
H	-1.201545	3.685634	4.785025	C	0.029045	-2.883765	-4.639773
H	-1.341677	5.405639	2.996752	C	0.013879	-1.732770	-5.406000
H	-1.061401	4.716189	0.628893	C	-0.316889	-0.534753	-4.799956
H	-0.620982	2.395950	0.068757	C	-0.599401	-0.518611	-3.446687
W	2.146751	0.824565	-0.850378	F	-0.268562	-4.006509	-2.653605
C	1.156717	2.261795	-1.999047	F	0.320238	-4.054848	-5.214399
O	0.664300	3.089095	-2.602777	F	0.302270	-1.779114	-6.706051
C	2.348215	2.227135	0.656372	F	-0.355108	0.592551	-5.518995
O	2.581377	3.056253	1.404588	F	-0.946274	0.680342	-2.938733

(**1'**→**5'**)‡

E = -1902.9830201490 au
ZPE = 0.38455619 au
G_{corr} = 0.32416144 au
ν = -305.28 cm^{-1}

P	0.114669	0.011294	-0.130400	C	1.980013	-0.032922	0.136680

C	2.372738	1.446582	0.195823
H	3.451894	1.539197	0.342785
H	2.112977	1.966705	-0.727479
H	1.890130	1.972237	1.020758
C	2.441577	-0.737182	1.407053
H	2.177940	-1.795963	1.410585
H	3.530671	-0.678186	1.498655
H	2.010474	-0.281555	2.298217
C	2.653405	-0.666789	-1.081114
H	3.736820	-0.531035	-1.018993
H	2.469626	-1.740840	-1.143018
H	2.312774	-0.209717	-2.012013
N	-0.146736	-1.726728	-0.643740
C	-0.483005	-2.025853	-1.889374
N	-0.651699	-3.336843	-2.004844
C	-0.411704	-3.910272	-0.782328
C	-0.099596	-2.901440	0.066027
C	-1.040367	-4.042328	-3.210814
H	-2.001579	-4.527557	-3.062922
H	-0.290004	-4.787964	-3.459509
H	-1.120592	-3.332841	-4.028436
H	-0.601008	-1.305404	-2.682123
H	-0.488320	-4.971581	-0.619032
H	0.146295	-2.937852	1.110709
W	-1.403485	0.348000	1.959879
C	-2.753798	0.653642	3.398398
O	-3.547512	0.811484	4.219702
C	-0.613736	-1.187701	3.053178
O	-0.194667	-2.030842	3.707342
C	-0.110539	1.626249	2.908493
O	0.582923	2.340756	3.473522
C	-2.198583	1.944984	0.918515
O	-2.664828	2.843802	0.391432
C	-2.675796	-0.941352	0.994362
O	-3.373744	-1.663010	0.445876
B	-0.710849	1.383398	-2.409825
H	-0.394497	2.383894	-1.832405
H	0.110189	0.801494	-3.068531
H	-1.760642	0.851929	-2.160692
H	-3.526742	2.543921	-2.739509
C	-3.076936	3.262598	-3.422831
S	-1.665693	2.524116	-4.261410
H	-2.710342	4.111177	-2.849341
H	-3.815396	3.610993	-4.142571
C	-2.466387	1.130853	-5.072285
H	-2.940379	0.486890	-4.332470
H	-3.204215	1.474271	-5.795179
H	-1.695904	0.566620	-5.593863

5‘

E = -1425.0618224374 au
ZPE = 0.30699807 au
G_{corr} = 0.25367733 au

P	0.005965	0.113547	-0.004356
C	0.013463	0.001806	1.872884
C	1.491163	-0.004282	2.275435
H	1.566071	0.018442	3.364925
H	2.001945	-0.898341	1.920458
H	2.034077	0.862893	1.897063
C	-0.685775	1.197254	2.512589
H	-1.742281	1.255660	2.246450
H	-0.635627	1.109398	3.600698
H	-0.214352	2.140736	2.238443
C	-0.640776	-1.293862	2.350189
H	-0.481219	-1.400179	3.425879
H	-1.719429	-1.299150	2.186591
H	-0.212879	-2.171153	1.864939
N	-1.687230	-0.452853	-0.336337
C	-1.989859	-1.656028	-0.807751
N	-3.302417	-1.754666	-0.950088
C	-3.874395	-0.572944	-0.553103
C	-2.862703	0.240749	-0.172383
C	-4.016243	-2.912237	-1.457475
H	-4.552978	-2.643983	-2.363353
H	-4.717857	-3.267458	-0.707762
H	-3.303448	-3.698928	-1.682856
H	-1.276274	-2.428179	-1.041506
H	-4.937723	-0.409282	-0.580101
H	-2.898509	1.250902	0.190808
W	0.308054	2.391287	-1.162506
C	0.574962	4.061708	-2.238747
O	0.722010	5.012749	-2.866421
C	-1.203225	3.340086	-0.162951
O	-2.032924	3.919956	0.372584
C	1.634004	3.103620	0.236500
O	2.373023	3.540531	0.990742
C	1.883569	1.542940	-2.197830
O	2.763271	1.134495	-2.796070
C	-1.010100	1.684098	-2.572881
O	-1.742644	1.286341	-3.353540
B	1.062384	-1.348070	-0.732179
H	2.213939	-1.011380	-0.567371
H	0.818981	-2.395024	-0.166016
H	0.797111	-1.398698	-1.916649

(**5‘**→**6‘**)‡

E = -1425.0101507493 au
ZPE = 0.30294434 au
G_{corr} = 0.24937939 au
ν = -305.28 cm^{-1}

P	0.586397	0.006987	0.138302
C	0.479543	0.027705	2.018330
C	1.880982	0.318468	2.561649
H	1.834850	0.421919	3.648495
H	2.579983	-0.486764	2.332620
H	2.295066	1.245857	2.163072
C	-0.465361	1.149467	2.443748
H	-1.474076	0.994529	2.068456
H	-0.512941	1.180028	3.534593
H	-0.120953	2.127351	2.106397
C	-0.025446	-1.305987	2.558044
H	-0.122790	-1.241451	3.644593
H	-1.000946	-1.558894	2.143778
H	0.661436	-2.123061	2.339774
N	-2.328432	-0.381420	0.023360
C	-2.549035	-1.230718	-0.947965
N	-3.864524	-1.439514	-1.147504
C	-4.531887	-0.667188	-0.238984
C	-3.564949	-0.021244	0.476120
C	-4.457971	-2.300953	-2.144609
H	-5.049793	-1.720931	-2.849888
H	-5.095205	-3.046668	-1.674047
H	-3.668952	-2.812043	-2.689515
H	-1.798760	-1.727786	-1.545689
H	-5.607428	-0.645361	-0.182248
H	-3.697902	0.678059	1.286356
W	0.539370	2.114333	-1.317334
C	0.502060	3.701947	-2.534089
O	0.483653	4.609929	-3.238443
C	-1.269886	2.694672	-0.517157
O	-2.270715	3.055732	-0.105845
C	1.545235	3.238856	0.077466
O	2.107333	3.895944	0.824846
C	2.332097	1.520207	-2.123732
O	3.327393	1.187476	-2.574187
C	-0.464837	1.013203	-2.735085
O	-1.018507	0.415305	-3.534444
B	0.710025	-1.703939	-0.556187
H	1.957047	-0.548672	0.016049
H	0.696985	-2.675663	0.125271
H	0.964967	-1.767215	-1.717420

6'

E = -1425.0923653315 au
ZPE = 0.30843458 au
G_{corr} = 0.25447001 au

P	0.100183	-0.042704	0.185659
C	0.010731	0.258861	2.039114
C	1.391103	0.643620	2.565100
H	1.342634	0.825135	3.641677
H	2.127474	-0.144212	2.401529
H	1.772950	1.550006	2.095888
C	-0.983224	1.392157	2.289423
H	-1.988972	1.119803	1.964377
H	-1.030516	1.619258	3.357716
H	-0.705985	2.309641	1.771113
C	-0.479864	-0.998661	2.754510
H	-0.607467	-0.790378	3.820267
H	-1.441484	-1.337778	2.365248
H	0.224021	-1.824826	2.660469
N	2.258587	-1.982709	-0.339901
C	2.986487	-1.923325	-1.439759
N	4.275636	-2.053575	-1.138126
C	4.382606	-2.202068	0.217952
C	3.118649	-2.163161	0.709377
C	5.377725	-2.006718	-2.077884
H	5.989345	-2.899007	-1.975440
H	5.986821	-1.125330	-1.893534
H	4.983352	-1.961680	-3.088314
H	2.601857	-1.810498	-2.438907
H	5.331042	-2.326922	0.710916
H	2.769800	-2.267803	1.721806
W	0.987951	1.877725	-1.318867
C	1.613960	3.252188	-2.628129
O	1.968402	4.033977	-3.395290
C	-0.981782	2.414582	-1.571224
O	-2.079953	2.705295	-1.685876
C	1.162832	3.324905	0.127280
O	1.286168	4.186556	0.869699
C	2.915326	1.312312	-0.907274
O	3.998520	1.035463	-0.660845
C	0.848434	0.566233	-2.891249
O	0.784389	-0.120125	-3.804274
B	0.703125	-1.871295	-0.268772
H	0.255312	-2.066590	-1.375219
H	0.284125	-2.676149	0.526257
H	-1.279840	-0.220189	-0.053580

7'

E = -1132.8596592581 au
ZPE = 0.16829023 au
G_{corr} = 0.12153372 au

P	-0.465712	0.483009	0.364403
C	-0.126008	0.355497	2.207852
C	0.534500	-1.033513	2.347992
H	0.623243	-1.272496	3.412603
H	-0.063778	-1.821948	1.884462
H	1.533957	-1.058112	1.914027

C	0.764135	1.434288	2.822725
H	0.319840	2.424638	2.714838
H	0.885813	1.243476	3.893700
H	1.757126	1.454869	2.378604
C	-1.486756	0.343856	2.925089
H	-1.339169	0.173908	3.996210
H	-2.006592	1.297167	2.807217
H	-2.135194	-0.444112	2.539447
W	1.214305	1.495812	-1.046389
C	2.524867	2.324637	-2.448266
O	3.247370	2.780405	-3.205602
C	1.345868	3.232748	0.085044
O	1.438638	4.190241	0.698897
C	2.796761	0.748829	0.056247
O	3.675376	0.340778	0.662899
C	1.125939	-0.235194	-2.195389
O	1.069474	-1.179751	-2.832540
C	-0.389892	2.225402	-2.144523
O	-1.273834	2.610988	-2.754867

8'

E = -1637.5554985189 au
ZPE = 0.28303342 au
G_{corr} = 0.23011308 au

P	0.100183	-0.042704	0.185659
C	0.010731	0.258861	2.039114
C	1.391103	0.643620	2.565100
H	1.342634	0.825135	3.641677
H	2.127474	-0.144212	2.401529
H	1.772950	1.550006	2.095888
C	-0.983224	1.392157	2.289423
H	-1.988972	1.119803	1.964377
H	-1.030516	1.619258	3.357716
H	-0.705985	2.309641	1.771113
C	-0.479864	-0.998661	2.754510
H	-0.607467	-0.790378	3.820267
H	-1.441484	-1.337778	2.365248
H	0.224021	-1.824826	2.660469
N	2.258587	-1.982709	-0.339901
C	2.986487	-1.923325	-1.439759
N	4.275636	-2.053575	-1.138126
C	4.382606	-2.202068	0.217952
C	3.118649	-2.163161	0.709377
C	5.377725	-2.006718	-2.077884
H	5.989345	-2.899007	-1.975440
H	5.986821	-1.125330	-1.893534
H	4.983352	-1.961680	-3.088314
H	2.601857	-1.810498	-2.438907
H	5.331042	-2.326922	0.710916
H	2.769800	-2.267803	1.721806
W	0.987951	1.877725	-1.318867
C	1.613960	3.252188	-2.628129
O	1.968402	4.033977	-3.395290
C	-0.981782	2.414582	-1.571224
O	-2.079953	2.705295	-1.685876
C	1.162832	3.324905	0.127280
O	1.286168	4.186556	0.869699
C	2.915326	1.312312	-0.907274
O	3.998520	1.035463	-0.660845
C	0.848434	0.566233	-2.891249
O	0.784389	-0.120125	-3.804274
B	0.703125	-1.871295	-0.268772
H	0.255312	-2.066590	-1.375219
H	0.284125	-2.676149	0.526257
H	-1.279840	-0.220189	-0.053580

(**8'**→**6'**)‡

E = -1903.0102401361 au
ZPE = 0.38562048 au
G_{corr} = 0.32409685 au
ν = -337.45 cm^{-1}

P	-0.003611	-0.126805	0.297716
C	0.474197	0.184218	2.090700
C	1.971244	0.432577	2.242679
H	2.192532	0.729586	3.270730
H	2.565780	-0.455215	2.032589
H	2.326771	1.225339	1.585407
C	-0.292957	1.426955	2.545638
H	-1.372774	1.286673	2.469983
H	-0.059577	1.643631	3.591100
H	-0.030292	2.309859	1.962377
C	0.050819	-1.007935	2.946755
H	0.266757	-0.806426	3.999398
H	-1.019509	-1.205993	2.861874
H	0.577871	-1.920017	2.667982
W	0.427098	1.708917	-1.479336
C	0.575159	3.044208	-2.958298
O	0.644080	3.806687	-3.818265
C	-1.354388	2.530936	-0.864472
O	-2.343156	2.982961	-0.513758
C	1.446260	3.024934	-0.279437
O	2.019707	3.801650	0.334836
C	2.219094	0.876130	-2.029162
O	3.226271	0.449601	-2.364128
C	-0.564845	0.453331	-2.771924
O	-1.104978	-0.213754	-3.525932
B	0.321718	-1.983148	-0.256261

H	0.309677	-2.878341	0.532377
H	-1.393445	-0.155682	0.515619
H	0.408466	-2.168998	-1.432002
S	2.774604	-1.956797	-0.167191
C	3.034303	-2.981552	-1.625676
H	4.060601	-3.342533	-1.655736
H	2.341648	-3.821510	-1.626247
H	2.847380	-2.368523	-2.503771
C	3.056869	-3.195176	1.111988
H	2.910192	-2.723986	2.081731
H	2.350935	-4.017456	1.008831
H	4.077283	-3.569566	1.055759
N	-1.945548	-2.414743	-0.597851
C	-2.392274	-2.860541	-1.744024
N	-3.694821	-3.192542	-1.670344
C	-4.102178	-2.941887	-0.389498
C	-3.003329	-2.460877	0.261345
C	-4.512679	-3.709873	-2.744264
H	-5.344507	-3.038931	-2.948236
H	-4.902318	-4.692929	-2.488262
H	-3.907627	-3.797527	-3.642393
H	-1.815530	-2.961374	-2.650258
H	-5.112070	-3.122750	-0.061389
H	-2.918886	-2.148355	1.290344

(**7'**→**9'**)‡

E = -1424.9888177124 au
ZPE = 0.30575145 au
G_{corr} = 0.25188025 au
ν = -170.67 cm^{-1}

P	0.147428	-0.002640	-0.008738
C	0.353567	-0.354722	1.834029
C	1.567705	0.509371	2.212645
H	1.889149	0.239631	3.221935
H	2.420754	0.344135	1.550451
H	1.337013	1.573661	2.217454
C	-0.812930	-0.029412	2.756099
H	-1.647702	-0.715307	2.609443
H	-0.502624	-0.131874	3.799752
H	-1.182248	0.985421	2.621323
C	0.751616	-1.823099	2.010724
H	1.013852	-2.015046	3.054769
H	-0.056613	-2.512874	1.759848
H	1.610005	-2.084728	1.392251
N	-1.363454	-1.740598	-1.746003
C	-1.647909	-1.367421	-0.468603
N	-2.788840	-0.611505	-0.512999
C	-3.093129	-0.376931	-1.787231
C	-2.193966	-1.104359	-2.557855
C	-3.491826	-0.071903	0.630392
H	-3.597281	-0.839982	1.390771
H	-4.478239	0.251454	0.314271
H	-2.943479	0.774377	1.038989
H	-1.453378	-2.027386	0.366832
H	-3.925029	0.234030	-2.093735
H	-2.141965	-1.192247	-3.629684
W	-0.325834	2.345432	-0.775934
C	-0.175516	4.178103	-1.623731
O	-0.062367	5.210979	-2.105489
C	-2.353236	2.599002	-1.064079
O	-3.451625	2.878904	-1.211169
C	-0.614010	3.164229	1.083885
O	-0.786982	3.673485	2.091909
C	1.709449	2.524949	-0.516726
O	2.829374	2.700912	-0.396695
C	-0.075921	1.510482	-2.649566
O	0.072805	1.079394	-3.693866
B	-0.201767	-2.728777	-2.163866
H	0.099716	-3.373801	-1.183619
H	-0.642949	-3.422601	-3.056828
H	0.731513	-2.058236	-2.554411

9'

E = -1424.9886403826 au
ZPE = 0.30629703 au
G_{corr} = 0.25210872 au

P	0.054772	-0.042519	0.022398
C	0.284794	-0.372970	1.869670
C	1.536042	0.450787	2.206717
H	1.856090	0.215959	3.224831
H	2.371933	0.223347	1.541708
H	1.349052	1.523654	2.164469
C	-0.838823	0.014399	2.822471
H	-1.701672	-0.644094	2.722672
H	-0.495576	-0.072737	3.857443
H	-1.174331	1.040067	2.675309
C	0.626044	-1.852741	2.063151
H	0.916211	-2.035871	3.101546
H	-0.221661	-2.510728	1.858825
H	1.450905	-2.163350	1.421716
N	-1.288241	-1.696714	-1.781391
C	-1.475745	-1.258245	-0.457712
N	-2.717911	-0.584134	-0.492171
C	-3.109119	-0.446050	-1.730456
C	-2.208209	-1.177505	-2.539130
C	-3.408382	-0.055554	0.664335
H	-3.510847	-0.839281	1.409758
H	-4.393561	0.281570	0.359746

H	-2.846984	0.776690	1.080351
H	-1.419859	-2.040607	0.297842
H	-3.989285	0.101980	-2.024579
H	-2.250261	-1.330416	-3.604882
W	-0.325213	2.364782	-0.816103
C	-0.202796	4.178449	-1.662192
O	-0.116271	5.215991	-2.149191
C	-2.347734	2.566676	-1.064100
O	-3.461082	2.803592	-1.203002
C	-0.563080	3.212112	1.038397
O	-0.710997	3.732509	2.045589
C	1.725649	2.481629	-0.598839
O	2.854624	2.609199	-0.502439
C	-0.134883	1.506918	-2.679627
O	-0.032751	1.056473	-3.723753
B	-0.098114	-2.612631	-2.242108
H	0.015446	-3.503534	-1.428327
H	-0.371316	-3.009389	-3.352973
H	0.896265	-1.915208	-2.239020

(**9'**→**10'**)‡

E = -1424.9840433059 au
ZPE = 0.30378668 au
G_{corr} = 0.25075411 au
ν = -458.10 cm^{-1}

P	-0.140698	-0.040111	0.045963
C	0.279365	-0.382226	1.842760
C	1.568972	0.396579	2.121688
H	1.919436	0.157518	3.128355
H	2.368164	0.130234	1.427251
H	1.423413	1.474808	2.075022
C	-0.812393	0.052282	2.817729
H	-1.708695	-0.561310	2.723927
H	-0.452672	-0.060135	3.844476
H	-1.101484	1.094017	2.681749
C	0.570761	-1.875448	2.016717
H	0.931587	-2.061623	3.031418
H	-0.314483	-2.498612	1.882140
H	1.334806	-2.222680	1.320711
N	-1.334968	-1.717168	-1.739402
C	-1.575339	-1.263577	-0.405290
N	-2.815005	-0.577985	-0.478342
C	-3.175045	-0.474099	-1.767413
C	-2.277291	-1.189117	-2.528782
C	-3.615523	-0.207365	0.664365
H	-3.679462	-1.046478	1.356923
H	-4.618275	0.037344	0.326328
H	-3.204769	0.652749	1.188810
H	-1.580133	-2.047571	0.356417
H	-4.048856	0.068469	-2.087488
H	-2.286549	-1.346720	-3.594103
W	-0.239761	2.310022	-0.867337
C	-0.116851	4.115769	-1.751157
O	-0.042012	5.143373	-2.255340
C	-2.284519	2.500654	-0.987021
O	-3.407886	2.702267	-1.043772
C	-0.344799	3.227966	0.967867
O	-0.416420	3.786914	1.961627
C	1.819323	2.317753	-0.756124
O	2.957843	2.365989	-0.711006
C	-0.175180	1.437329	-2.735659
O	-0.142696	1.002329	-3.789293
B	0.014543	-2.274158	-2.054438
H	0.308870	-3.227246	-1.367719
H	0.224620	-2.379813	-3.235895
H	0.713186	-1.328422	-1.469716

10'

E = -1425.0437736487 au
ZPE = 0.30768990 au
G_{corr} = 0.25522523 au

P	0.651402	-0.157914	0.010160
C	1.010529	-0.453395	1.823128
C	2.358770	0.211534	2.110169
H	2.627624	0.044892	3.155654
H	3.157992	-0.206422	1.495122
H	2.337459	1.288189	1.947377
C	-0.081229	0.166586	2.690018
H	-1.037693	-0.342132	2.570030
H	0.196188	0.086601	3.743309
H	-0.238002	1.222161	2.469510
C	1.130938	-1.950379	2.111845
H	1.438981	-2.094034	3.150068
H	0.188011	-2.483212	1.987124
H	1.877984	-2.429604	1.477188
N	-0.617315	-1.726464	-1.850527
C	-0.787492	-1.289651	-0.461160
N	-2.052180	-0.576539	-0.422951
C	-2.471772	-0.468628	-1.759188
C	-1.648090	-1.105212	-2.582460
C	-3.054048	-1.064239	0.507807
H	-3.368803	-2.093424	0.300676
H	-3.929860	-0.419389	0.455082
H	-2.679006	-1.017595	1.528197
H	-0.795160	-2.148532	0.212680
H	-3.363914	0.084057	-2.008589
H	-1.682041	-1.187692	-3.655792

W	0.643069	2.195614	-0.969130
C	0.721004	3.982040	-1.876437
O	0.773732	4.998253	-2.408621
C	-1.408996	2.383068	-0.807862
O	-2.526106	2.593912	-0.711595
C	0.790026	3.198901	0.814512
O	0.874610	3.822271	1.769365
C	2.687971	2.053498	-1.045741
O	3.827937	1.984667	-1.077072
C	0.521998	1.341806	-2.840955
O	0.494612	0.936359	-3.907515
B	0.344445	-2.608986	-2.332236
H	1.112885	-3.111097	-1.569106
H	0.372469	-2.846126	-3.500681
H	1.690180	-0.945017	-0.528452

(**10'**→**11'**)‡

E = -1425.0169523139 au
ZPE = 0.30551003 au
G_{corr} = 0.25202621 au
ν = -35.50 cm^{-1}

P	0.579099	-0.109992	0.288681
C	1.056380	-0.195778	2.115544
C	2.422466	0.417680	2.403630
H	2.679811	0.308622	3.462769
H	3.208082	-0.065911	1.820633
H	2.442886	1.481616	2.168032
C	-0.015883	0.523778	2.929222
H	-1.000533	0.073651	2.786251
H	0.214536	0.474241	3.997309
H	-0.094429	1.577185	2.659533
C	1.075385	-1.674086	2.511617
H	1.310823	-1.786840	3.574819
H	0.108196	-2.148866	2.333836
H	1.827172	-2.230059	1.947763
N	-1.090697	-1.778135	-2.500044
C	-1.240866	-2.032640	-1.182326
N	-2.398234	-1.546503	-0.785439
C	-2.988736	-0.874474	-1.840983
C	-2.186307	-1.025402	-2.907040
C	-2.832538	-1.499669	0.590990
H	-2.606335	-2.440623	1.083542
H	-3.902631	-1.323754	0.627012
H	-2.296337	-0.692439	1.092908
H	-0.593440	-2.663615	-0.602049
H	-3.928102	-0.361380	-1.733418
H	-2.288570	-0.673882	-3.918326
W	0.858699	2.227707	-0.887143
C	1.024251	3.888661	-1.975229
O	1.130167	4.840972	-2.621098
C	-1.189514	2.254266	-0.906454
O	-2.334904	2.236653	-0.885738
C	0.851922	3.393750	0.805410
O	0.862643	4.090173	1.714733
C	2.884352	1.961401	-0.693603
O	4.007694	1.776526	-0.578694
C	0.924086	1.094935	-2.578925
O	0.987115	0.445033	-3.524913
B	0.006401	-2.233196	-3.320618
H	0.890406	-2.812039	-2.784689
H	-0.059125	-2.052806	-4.487957
H	1.694609	-0.844761	-0.199546

11'

E = -1425.0189246255 au
ZPE = 0.30591790 au
G_{corr} = 0.24995982 au

P	0.099475	-0.120174	0.594817
C	0.446244	0.049731	2.444713
C	1.715132	0.835962	2.755164
H	1.889648	0.880890	3.835646
H	2.590944	0.372067	2.297951
H	1.657385	1.860343	2.388822
C	-0.761569	0.721734	3.092933
H	-1.676864	0.150469	2.921465
H	-0.622954	0.804492	4.174843
H	-0.926077	1.727464	2.704823
C	0.588701	-1.366263	3.009043
H	0.752729	-1.336693	4.091197
H	-0.306390	-1.962973	2.823514
H	1.435970	-1.891227	2.562974
N	-1.969826	-1.593188	-2.812630
C	-1.994487	-1.763818	-1.481231
N	-3.131108	-1.306196	-1.012109
C	-3.884598	-0.812076	-2.060298
C	-3.160846	-0.988581	-3.181028
C	-3.508896	-1.305662	0.389564
H	-4.037154	-2.223385	0.633958
H	-4.149848	-0.451871	0.583573
H	-2.600049	-1.218519	0.982846
H	-1.201650	-2.183886	-0.884721
H	-4.858568	-0.381371	-1.908566
H	-3.377586	-0.736666	-4.204047
W	0.161665	2.142722	-0.774850
C	0.208977	3.740572	-1.964744
O	0.247985	4.656642	-2.667461
C	-1.877360	2.044804	-0.727660

O	-3.019910	1.961767	-0.665064
C	0.101796	3.450927	0.818673
O	0.067428	4.237181	1.649324
C	2.199865	1.967242	-0.574262
O	3.325885	1.821297	-0.438435
C	0.228896	0.974113	-2.428779
O	0.269431	0.337108	-3.390050
B	-0.848094	-1.939441	-3.672713
H	0.075419	-2.483312	-3.170189
H	-0.973232	-1.765683	-4.836168
H	1.346617	-0.714039	0.256109

(**11'**→**6'**)‡

E = -1425.0162018357 au
ZPE = 0.30552250 au
G_{corr} = 0.25170287 au
ν = -57.07 cm^{-1}

P	-0.440408	-0.665726	0.247793
C	-0.299928	0.217695	1.916192
C	1.178837	0.532148	2.151379
H	1.321401	1.045089	3.108183
H	1.783178	-0.377868	2.184354
H	1.586998	1.172808	1.367494
C	-1.085277	1.523089	1.983515
H	-2.152234	1.362122	1.838499
H	-0.952846	2.007255	2.957290
H	-0.752179	2.225402	1.217193
C	-0.779894	-0.745297	2.998945
H	-0.662408	-0.303341	3.992770
H	-1.832482	-1.001678	2.873991
H	-0.212108	-1.678861	2.980493
N	1.997767	-3.281235	0.565327
C	1.469839	-3.276461	-0.668804
N	0.591118	-4.242173	-0.764399
C	0.492709	-4.882393	0.460105
C	1.368158	-4.281744	1.285347
C	-0.157430	-4.600505	-1.955198
H	-1.221275	-4.488416	-1.770423
H	0.058308	-5.632804	-2.216498
H	0.139170	-3.953621	-2.773484
H	1.753891	-2.605427	-1.460741
H	-0.179596	-5.706812	0.619285
H	1.605998	-4.475962	2.316336
W	-2.939288	-0.983632	-0.578231
C	-4.716213	-1.294100	-1.418727
O	-5.740435	-1.469422	-1.926386
C	-2.813210	1.005762	-1.072290
O	-2.693769	2.116767	-1.319436
C	-2.051423	-1.467914	-2.357921
O	-1.573289	-1.730337	-3.367063
C	-2.762611	-2.882198	0.142181
O	-2.633245	-3.932654	0.588401
C	-3.936117	-0.495873	1.144913
O	-4.557730	-0.240134	2.073952
B	2.944879	-2.300356	1.047275
H	-0.008962	0.439885	-0.537689
H	3.285195	-2.373030	2.178832
H	3.359072	-1.505756	0.274528

12'

E = -1425.0284755813 au
ZPE = 0.30604678 au
G_{corr} = 0.25121681 au

0.25121681

P	1.180780	0.028740	-0.053714
C	1.048361	-0.317088	1.798719
C	2.208865	0.460906	2.425181
H	2.242581	0.270684	3.501160
H	3.171111	0.156574	2.007901
H	2.111590	1.537504	2.286957
C	-0.275058	0.102664	2.424512
H	-1.115638	-0.432312	1.977054
H	-0.279608	-0.119876	3.495883
H	-0.463305	1.168640	2.307499
C	1.274889	-1.810398	2.041188
H	1.309146	-2.016089	3.115175
H	0.472635	-2.416040	1.618278
H	2.214321	-2.151271	1.604133
N	-1.941763	-1.385488	-1.370160
C	-2.904323	-1.577726	-0.477073
N	-4.045414	-1.102590	-0.947303
C	-3.818233	-0.581846	-2.196744
C	-2.501950	-0.759479	-2.456077
C	-5.319254	-1.104161	-0.252906
H	-6.063114	-1.621041	-0.852703
H	-5.640080	-0.081284	-0.074693
H	-5.207233	-1.615562	0.697739
H	-2.780333	-2.051377	0.482570
H	-4.602211	-0.138291	-2.785302
H	-1.927005	-0.506808	-3.328765
W	0.375141	2.398174	-0.797835
C	-0.167372	4.160749	-1.566251
O	-0.488780	5.170329	-2.019797
C	-1.558807	1.894293	-0.343373
O	-2.631626	1.617752	-0.053381
C	0.526032	3.339618	1.019470
O	0.592366	3.933064	1.996064

C	2.368985	2.788117	-1.113714
O	3.480660	2.998555	-1.274320
C	0.234075	1.610911	-2.686952
O	0.167072	1.223353	-3.762075
B	-0.475781	-1.767649	-1.195375
H	-0.305194	-2.724233	-0.504214
H	0.154843	-1.654117	-2.198451
H	-0.098244	-0.733397	-0.331358

(**12'→6'**)‡

E = -1425.0277897509 au
ZPE = 0.30591436 au
G_{corr} = 0.25322195 au
ν = -169.93 cm^{-1}

P	0.935280	0.106950	-0.095528
C	0.765735	-0.214620	1.761432
C	2.077785	0.283700	2.371748
H	2.070412	0.124762	3.453078
H	2.938862	-0.250048	1.964575
H	2.236385	1.348614	2.199754
C	-0.419999	0.503766	2.394644
H	-1.366614	0.166251	1.966970
H	-0.455942	0.307596	3.470680
H	-0.364163	1.582764	2.257463
C	0.645821	-1.715831	2.020763
H	0.679191	-1.911396	3.096431
H	-0.296095	-2.121042	1.648498
H	1.455363	-2.275805	1.551089
N	-1.944090	-1.334497	-1.301214
C	-2.787362	-1.969543	-0.500257
N	-4.031358	-1.633789	-0.809377
C	-3.993006	-0.743958	-1.853184
C	-2.686263	-0.559533	-2.156241
C	-5.233563	-2.131874	-0.167295
H	-5.844683	-2.663026	-0.891989
H	-5.798186	-1.301391	0.247620
H	-4.955645	-2.810460	0.632819
H	-2.509606	-2.658123	0.280396
H	-4.885967	-0.328489	-2.286798
H	-2.230184	0.050313	-2.916181
W	0.695684	2.613513	-0.876414
C	0.560346	4.452549	-1.625132
O	0.474857	5.514862	-2.066333
C	-1.305910	2.524861	-0.432147
O	-2.418713	2.451355	-0.177005
C	1.071536	3.492354	0.940462
O	1.276007	4.053698	1.916696
C	2.718638	2.527841	-1.229582
O	3.844180	2.467759	-1.417870
C	0.327046	1.899702	-2.763654
O	0.119323	1.558269	-3.836431
B	-0.397958	-1.431856	-1.246929
H	-0.050477	-2.430746	-0.699797
H	0.077601	-1.150558	-2.303449
H	-0.471141	-0.202391	-0.365368

(**9'→13'**)‡

E = -1424.9758030270 au
ZPE = 0.30547683 au
G_{corr} = 0.25129288 au
ν = -168.58 cm^{-1}

P	-0.060892	-0.695351	0.293321
C	0.080854	-0.471176	2.141591
C	1.447441	0.173427	2.384905
H	1.590305	0.325905	3.457387
H	2.267349	-0.453158	2.029693
H	1.531598	1.148857	1.902211
C	-1.028218	0.450234	2.640006
H	-2.013443	0.012949	2.487787
H	-0.899502	0.624614	3.710804
H	-1.007616	1.420645	2.142966
C	0.000047	-1.832394	2.830668
H	0.116037	-1.703575	3.910422
H	-0.962391	-2.311508	2.652513
H	0.788263	-2.506729	2.492526
N	-1.989734	-0.673482	-1.363978
C	-1.588966	-1.644625	-0.323350
N	-2.696002	-1.778277	0.585281
C	-3.500241	-0.643948	0.315113
C	-3.080189	-0.013665	-0.782433
C	-3.393504	-3.054453	0.564755
H	-3.831450	-3.295884	-0.410746
H	-4.195928	-3.031861	1.301183
H	-2.709645	-3.853244	0.848744
H	-1.268561	-2.605403	-0.728784
H	-4.347569	-0.409103	0.940502
H	-3.479154	0.884896	-1.227840
W	0.240642	2.615864	-2.333009
C	1.336662	4.222587	-2.681081
O	1.965951	5.164142	-2.885179
C	-1.387051	3.589317	-3.142027
O	-2.266710	4.157288	-3.593121
C	-0.241341	3.345915	-0.471480
O	-0.489673	3.770633	0.558058
C	1.879565	1.668733	-1.521658
O	2.797389	1.162486	-1.072260
C	0.726913	1.864852	-4.192707

O	1.012428	1.466815	-5.221726
B	-0.786065	0.044814	-1.779880
H	0.064630	-0.541578	-2.377766
H	-1.072778	1.230302	-2.018270
H	0.973677	-1.633359	0.093805

13'

E = -1424.9838856280 au
ZPE = 0.30572879 au
G_{corr} = 0.25126647 au

P	0.125485	-1.258981	0.378241
C	-0.025671	-0.531241	2.066736
C	1.376093	-0.054316	2.456488
H	1.336079	0.399905	3.448795
H	2.094727	-0.874226	2.497082
H	1.759255	0.699428	1.766112
C	-0.996658	0.647749	2.039769
H	-2.000649	0.340410	1.753288
H	-1.047572	1.085465	3.038833
H	-0.671935	1.431127	1.354464
C	-0.515197	-1.614707	3.026871
H	-0.557200	-1.207802	4.039736
H	-1.516219	-1.957171	2.764753
H	0.152055	-2.477798	3.045493
N	-1.382796	-0.808707	-1.491535
C	-1.473985	-1.830325	-0.441433
N	-2.727596	-1.634122	0.240271
C	-3.385585	-0.603047	-0.471869
C	-2.599808	-0.115920	-1.430742
C	-3.472012	-2.833213	0.553203
H	-3.714189	-3.430505	-0.335123
H	-4.402983	-2.565138	1.050111
H	-2.902898	-3.458087	1.241118
H	-1.357485	-2.863879	-0.797477
H	-4.378058	-0.292758	-0.185679
H	-2.815406	0.694865	-2.107884
W	0.272061	2.583002	-1.946182
C	0.501819	4.351012	-2.800121
O	0.629458	5.385713	-3.289198
C	-1.560026	3.192799	-1.233903
O	-2.561234	3.577572	-0.843753
C	1.162505	3.312940	-0.243224
O	1.662173	3.741428	0.689600
C	2.125888	2.004405	-2.637728
O	3.156771	1.710554	-3.026715
C	-0.595485	1.862115	-3.672098
O	-1.066619	1.488168	-4.641292
B	0.002343	-0.171722	-1.298514
H	0.875560	-0.441643	-2.076020
H	-0.037769	1.012510	-0.852605
H	1.055889	-2.303354	0.529077

(**7'**→**14'**)‡

E = -1424.9737670081 au
ZPE = 0.30619920 au
G_{corr} = 0.25354442 au
ν = -170.67 cm^{-1}

P	0.480319	0.079640	-0.257338
C	0.995026	-0.428476	1.475235
C	2.145766	0.559659	1.749726
H	2.672595	0.224410	2.646672
H	2.884517	0.575470	0.943045
H	1.816460	1.578341	1.927613
C	-0.085859	-0.317756	2.540721
H	-0.853412	-1.079983	2.398212
H	0.341956	-0.475044	3.534644
H	-0.569585	0.658381	2.534880
C	1.616434	-1.827155	1.481523
H	2.065711	-2.018989	2.460205
H	0.885284	-2.604419	1.290372
H	2.402575	-1.915298	0.730686
N	-1.297180	-1.358368	-0.734665
C	-2.476389	-0.909117	-0.265928
N	-3.246847	-0.505867	-1.248438
C	-2.554914	-0.678582	-2.440652
C	-1.362444	-1.202914	-2.117888
C	-4.619585	-0.048144	-1.153054
H	-5.261689	-0.739369	-1.693492
H	-4.712273	0.944409	-1.585335
H	-4.922573	-0.019199	-0.112131
H	-2.766898	-0.935300	0.771718
H	-2.987489	-0.413674	-3.389820
H	-0.539504	-1.499200	-2.744799
W	-0.389743	2.472369	-0.449185
C	-0.801209	4.391656	-0.922703
O	-1.031809	5.476792	-1.209382
C	-2.319001	2.237627	0.185767
O	-3.375995	2.177963	0.623074
C	-0.068228	3.120129	1.474444
O	0.054550	3.571003	2.517052
C	1.593931	2.848621	-0.889766
O	2.686571	3.088140	-1.108081
C	-0.775068	2.051018	-2.428078
O	-0.978175	1.918562	-3.544201
B	-1.052371	-2.967911	-0.269161
H	-1.149202	-2.992976	0.933955
H	-1.955055	-3.571253	-0.809592

H	0.033928	-3.272693	-0.688911

14'

E = -1424.9765759007 au
ZPE = 0.30678700 au
G_{corr} = 0.25410097 au

P	0.451726	0.019372	-0.304162
C	0.954805	-0.488254	1.441479
C	2.052341	0.531823	1.781157
H	2.548051	0.215967	2.702256
H	2.823601	0.581863	1.007925
H	1.672021	1.536271	1.945818
C	-0.146031	-0.437749	2.493386
H	-0.864491	-1.248185	2.362391
H	0.281231	-0.556228	3.493162
H	-0.687011	0.508605	2.473688
C	1.630211	-1.863423	1.438364
H	2.045877	-2.066764	2.429738
H	0.941655	-2.666194	1.196800
H	2.450893	-1.897559	0.720628
N	-1.154949	-1.067774	-0.711935
C	-2.348811	-0.746595	-0.131370
N	-3.261927	-0.545015	-1.036636
C	-2.682641	-0.682893	-2.296695
C	-1.396405	-0.990686	-2.098127
C	-4.677310	-0.318099	-0.801220
H	-5.230477	-1.202076	-1.107787
H	-5.007805	0.537423	-1.381566
H	-4.842948	-0.132491	0.254409
H	-2.514157	-0.701783	0.932808
H	-3.257606	-0.565315	-3.198817
H	-0.607467	-1.191227	-2.802552
W	-0.307525	2.525011	-0.559080
C	-0.575046	4.446252	-1.031302
O	-0.717254	5.552680	-1.315549
C	-2.331144	2.411992	-0.325404
O	-3.465195	2.467966	-0.161504
C	-0.272320	3.066860	1.419899
O	-0.303763	3.439361	2.501347
C	1.723551	2.853904	-0.721814
O	2.837034	3.086868	-0.813879
C	-0.447226	2.074572	-2.562113
O	-0.536490	1.875076	-3.683808
B	-1.067861	-2.833292	-0.380424
H	-1.099279	-2.931838	0.815262
H	-2.055505	-3.259816	-0.928719
H	-0.031228	-3.146110	-0.899109

(**6'**→**15'**)‡

E = -1425.0242454238 au
ZPE = 0.30541621 au
G_{corr} = 0.25176665 au
ν = -115.61 cm^{-1}

P	0.370230	0.095951	0.031330
C	0.184494	0.243419	1.894415
C	1.341111	1.052606	2.475212
H	1.227731	1.126039	3.559568
H	2.304581	0.593156	2.263144
H	1.367653	2.067816	2.079594
C	-1.140019	0.961021	2.158412
H	-1.992372	0.370010	1.819108
H	-1.259964	1.131698	3.231042
H	-1.192664	1.932200	1.665652
C	0.144066	-1.141093	2.536282
H	-0.061467	-1.042509	3.605398
H	-0.638949	-1.767882	2.105652
H	1.091736	-1.667362	2.428304
N	3.388974	-0.738826	0.387716
C	3.443111	-1.244977	-0.838500
N	4.007641	-2.478948	-0.831372
C	4.282478	-2.781907	0.457298
C	3.891996	-1.696093	1.201162
C	4.166832	-3.340669	-1.982383
H	3.300868	-3.990574	-2.095131
H	5.059489	-3.948046	-1.863924
H	4.274176	-2.732863	-2.876496
H	3.311352	-0.682965	-1.750790
H	4.714770	-3.725610	0.746403
H	3.944323	-1.570791	2.270678
W	0.811862	2.208186	-1.402339
C	1.131528	3.760939	-2.618311
O	1.312608	4.647827	-3.328380
C	-1.164098	2.119265	-1.953716
O	-2.266567	2.064328	-2.246922
C	0.316520	3.574662	0.050875
O	0.050498	4.395410	0.801016
C	2.768910	2.274226	-0.758800

O	3.854056	2.363327	-0.417060
C	1.306772	0.982248	-2.971143
O	1.584458	0.344538	-3.879077
B	1.270354	-1.532536	-0.489509
H	1.132128	-1.760999	-1.655659
H	1.380292	-2.451125	0.259189
H	-0.924905	-0.389590	-0.271125

15'

E = -1425.0336472295 au
ZPE = 0.30688649 au
G_{corr} = 0.25363102 au

P	0.427203	0.041279	0.040122
C	0.168606	0.293234	1.885972
C	1.286125	1.161614	2.457457
H	1.147984	1.277552	3.535700
H	2.266390	0.716450	2.289293
H	1.289802	2.160285	2.020126
C	-1.183019	0.979133	2.082364
H	-2.006401	0.345534	1.747985
H	-1.340340	1.195856	3.142203
H	-1.252223	1.923094	1.541995
C	0.152614	-1.056798	2.599713
H	-0.081356	-0.910103	3.657863
H	-0.599949	-1.728552	2.183019
H	1.117483	-1.558120	2.536464
N	3.585744	-0.998656	0.916586
C	3.153239	-1.240271	-0.381976
N	3.830087	-2.431775	-0.803506
C	4.474510	-2.921102	0.207585
C	4.308557	-2.001213	1.290666
C	3.698043	-3.016430	-2.120807
H	2.712846	-3.465882	-2.220859
H	4.465349	-3.770919	-2.260098
H	3.809820	-2.238066	-2.870585
H	3.316392	-0.410281	-1.071097
H	5.012303	-3.856138	0.172170
H	4.725990	-2.106326	2.280997
W	0.882170	2.126313	-1.444400
C	1.230259	3.634455	-2.708507
O	1.428689	4.495510	-3.446576
C	-1.028788	1.870716	-2.158195
O	-2.095928	1.717124	-2.534694
C	0.174619	3.527788	-0.119563
O	-0.202027	4.368276	0.558714
C	2.745944	2.320381	-0.607120
O	3.781820	2.444210	-0.138188
C	1.602729	0.861547	-2.891321
O	2.013151	0.204553	-3.733405
B	1.476922	-1.557182	-0.388686
H	1.182325	-1.813672	-1.534862
H	1.269626	-2.486221	0.354268
H	-0.850716	-0.473692	-0.270007

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