Supporting Information

General and Chemoselective Reduction of Phosphine Oxides by an Enhanced Oxophilic Competition Mechanism

Mengyao You, Ziwei Zhang, Chao Chen, Zhichao Mei, Xinxin Zhang, Jiang Bai, Haiyang Huang,* Qiang Xiao*

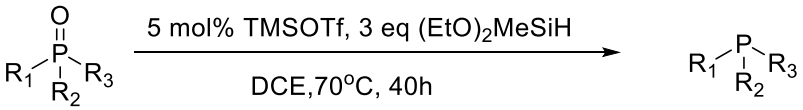
Jiangxi Provincial Key Laboratory of Organic Functional Molecules; Institute of Organic Chemistry, Jiangxi Science and Technology Normal University. Nanchang 330013, China

huanghaiyang1209@163.com ; xiaoqiang@tsinghua.org.cn

1. Materials and Instruments

All reactions were routinely performed under an atmosphere of air by using standard Schlenk tube and dry deoxygenated solvents. Dry DCE were purchased from J&K Scientific Ltd. Silica gel (200 - 300 mesh) purchased from Qingdao Hai Yang Chemical Industry Co. Ltd. was used for chromatographic separations. NMR spectra (400 MHz/100 MHz) were recorded on an Advance DPX spectrometer (Bruker, Billerica, MA, USA) at room temperature with Chloroform-d as solvent. Tetramethylsilane (TMS) was used as an internal reference. High resolution mass spectrometry (HRMS) data were measured with an AB Sciex TOF 4600 instrument (Billerica, MA, USA). ..**2r** was synthesized according to the method described in Reference 1. **2t** was synthesized according to the method described in Reference 2. 2w was synthesized according to the method described in Reference 3. 2x was synthesized according to the method described in Reference 4. **2ab, 2ac, 2ad, 2ae, 2af, 2ag** were synthesized according to the method described in Reference 5. **2ag** was synthesized according to the method described in Reference 6. **2al** was synthesized according to the method described in Reference 7. **2aj** was synthesized according to the method described in Reference 8. **2ak** was synthesized according to the method described in Reference 9. **2ai, 2ao** were synthesized according to the method described in Reference 10. **2aq, 2ar** were synthesized according to the method described in Reference 11. **2as, 2ar, 2at, 2ax, 2ay** were synthesized according to the method described in Reference 12. The other phosphine oxides were purchased from commercial companies.

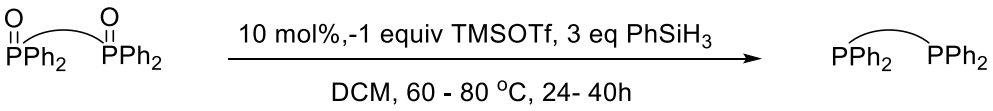
2. General procedure for the preparation of Phophines



General procedure A using TMSOTf as catalyst and $(EtO)_2SiH$ as reducing agent (**GP A**). Phosphine oxides (1.0mmol),) were added in a 10 mL Schlenk tube. The tube was sealed with a Teflon tape, and then placed in Ar atmosphere and evacuated/backed three times with Ar. Under the Ar atmosphere, TMSOTf (5 mol%), $(EtO)_2SiH$ (3 eq) and DCE (3.0 mL) were added and stirred for 40 h at 70 ^oC. After required reaction time the mixture was cooled down to room temperature and then ethyl acetate (10 mL) and water (10 mL) were added. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL × 3). All combined organic solutions were dried with anhydrous Na_2SO_4 and purified by flash chromatography (PE : DCM=5 : 1) to afford the corresponding product. Phosphine oxides **2a-2q** were prepared according to this method.

General procedure B using TMSOTf as catalyst and $PhSiH_3$ reducing agent **(GP B**). Phosphine oxides (1.0mmol),) were added in a 10mL Schlenk tube. The tube was sealed with a Teflon tape, and then placed in Ar atmosphere and evacuated/backed

three times with Ar. Under the Ar atmosphere, TMSOTf (5 mol%), $PhSiH_3$ (3 eq) and DCE (3.0 mL) were added and stirred for 40 h at 70 ^oC. After required reaction time the mixture was cooled down to room temperature and then ethyl acetate (10 mL) and water (10 mL) were added. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL × 3). All combined organic solutions were dried with anhydrous Na_2SO_4 and purified by flash chromatography (PE : DCM=5 : 1) to afford the corresponding product . Phosphine oxides **2r-2ao** were prepared according to this method.



General procedure C using TMSOTf as the catalyst, more $PhSiH_3$ reducing agent for longer time **(GP C**). Phosphine oxides (1.0mmol),) were added in a 10mL Schlenk tube. The tube was sealed with a Teflon tape, and then placed in Ar atmosphere and evacuate backed three times with Ar. Under the Ar atmosphere, TMSOTf (10 mol% - 1eq), $PhSiH_3$ (5 eq) and DCE (3.0 mL) were added and stirred for 40 h at 70 ^oC. After required reaction time the mixture was cooled down to room temperature and then ethyl acetate (10 mL) and water (10 mL) were added. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL × 3). All combined organic solutions were dried with anhydrous Na_2SO_4 and purified by flash chromatography (PE : DCM=5 : 1) to afford the corresponding product. Phosphine oxides **2ap-2bh** were prepared according to this method.

3. The hectogram-scale preparation of triphenylphosphine.

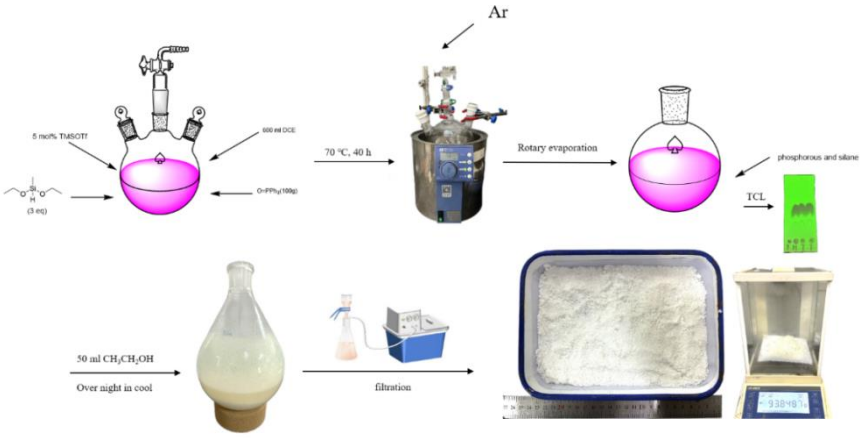


Fig. S1. the hundred gram-scale reaction process (schematic plot).

Phosphine oxides **1a** (100 g) were added in a 2000 mL three-necked flask. The tube was sealed with a Teflon tape, and then placed in Ar atmosphere and evacuated/backed three times with Ar. Under the Ar atmosphere, TMSOTf (5 mol%),

$(EtO)_2SiH$ (3 eq) and DCE (600 mL) were added at 70℃ for 40 h. The mixture was subjected to rotary evaporation to remove the dichloroethane (DCE) solvent. Following this, 50 mL of ethanol was added to the residue. The resulting solution was then cooled to -20 ℃ and allowed to stand overnight to facilitate the crystallization and subsequent separation of triphenylphosphine. The desired product was obtained by filtering the mixture under reduced pressure, effectively separating the triphenylphosphine from the product **2a** (93.8g , 99%).

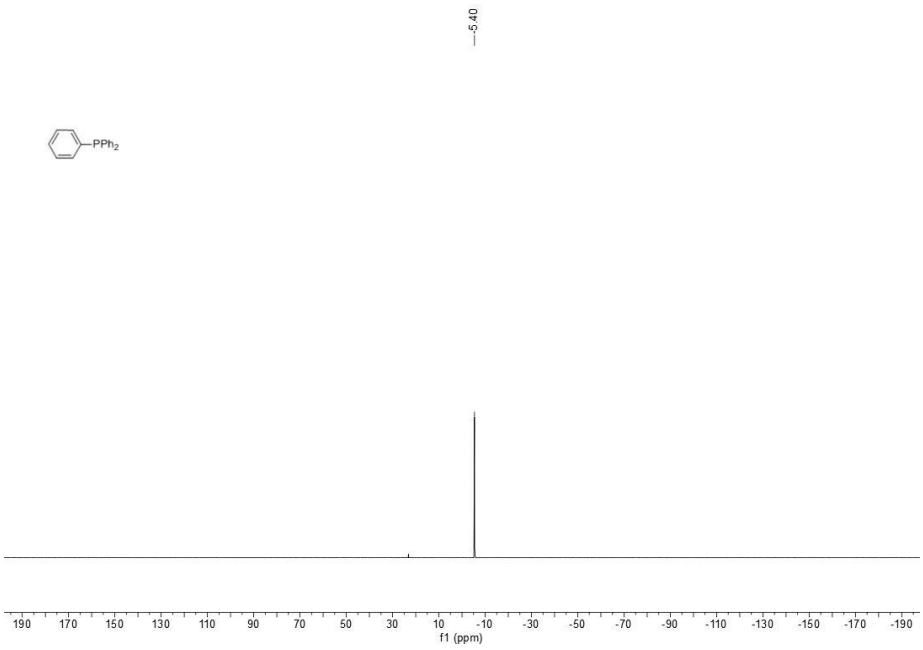


Fig. S2. ^{31}P NMR of intermediate **2a** separated by simple filtration

4. The Track Experiments (^{31}P-NMR)

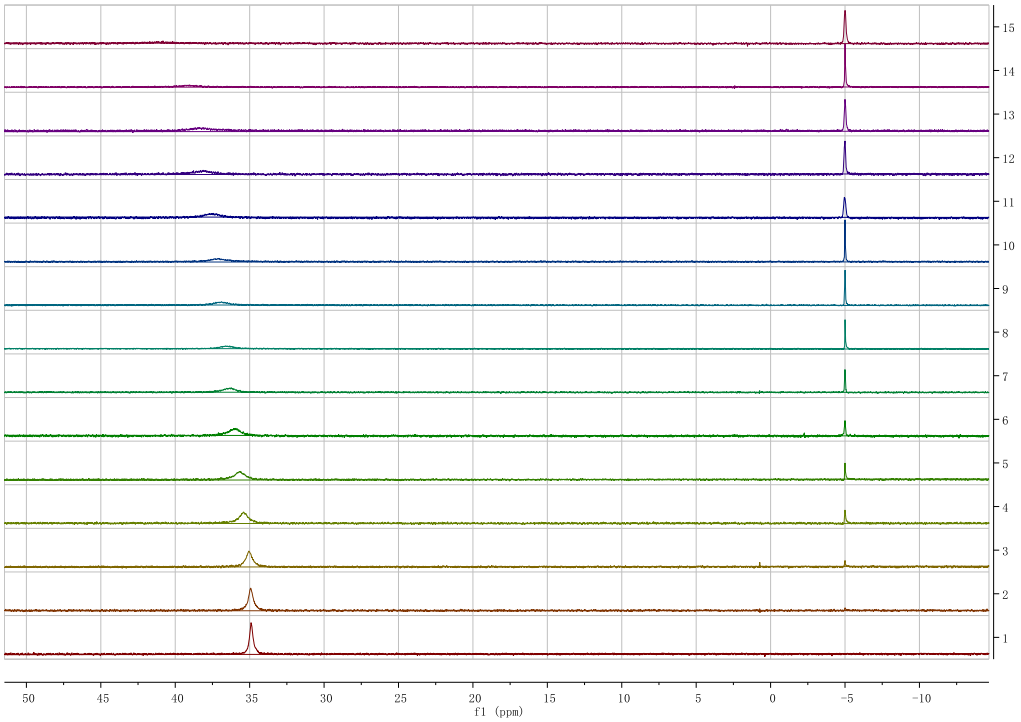


Fig. S3. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 50 ^{o}C (Test every two hours).

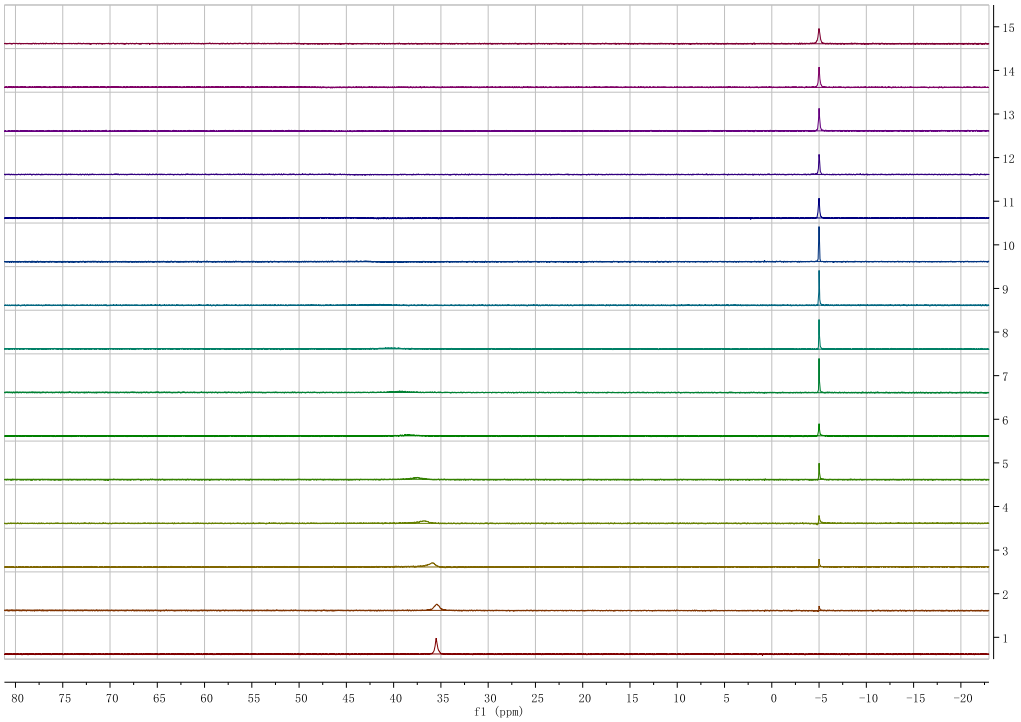


Fig. S4. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

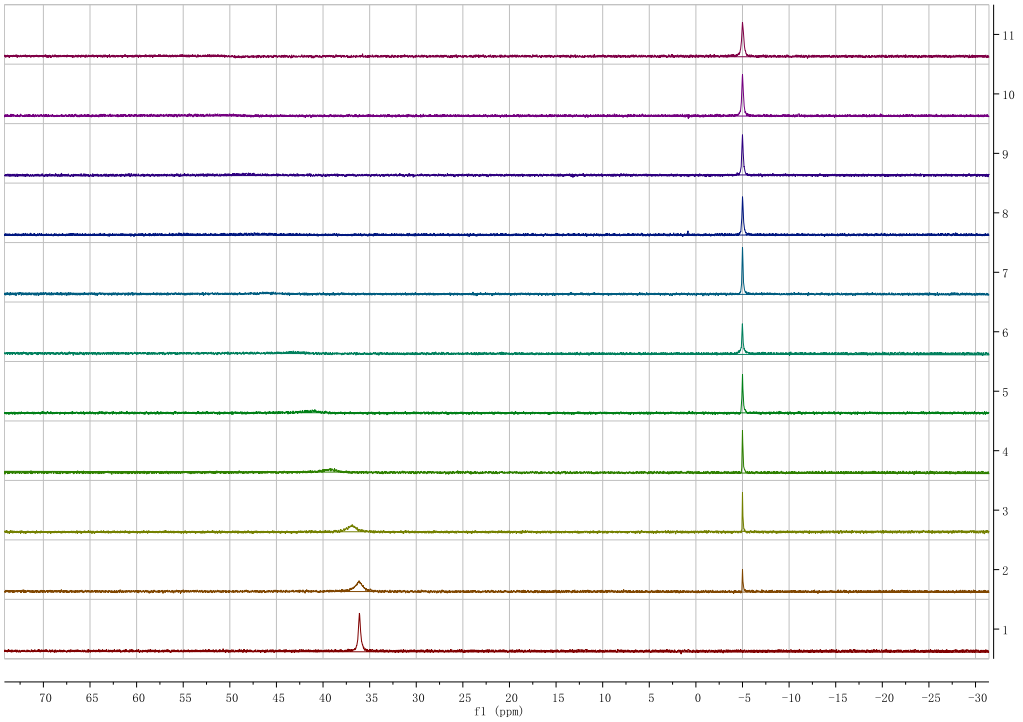


Fig. S5. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 70 ^{o}C (Test every two hours).

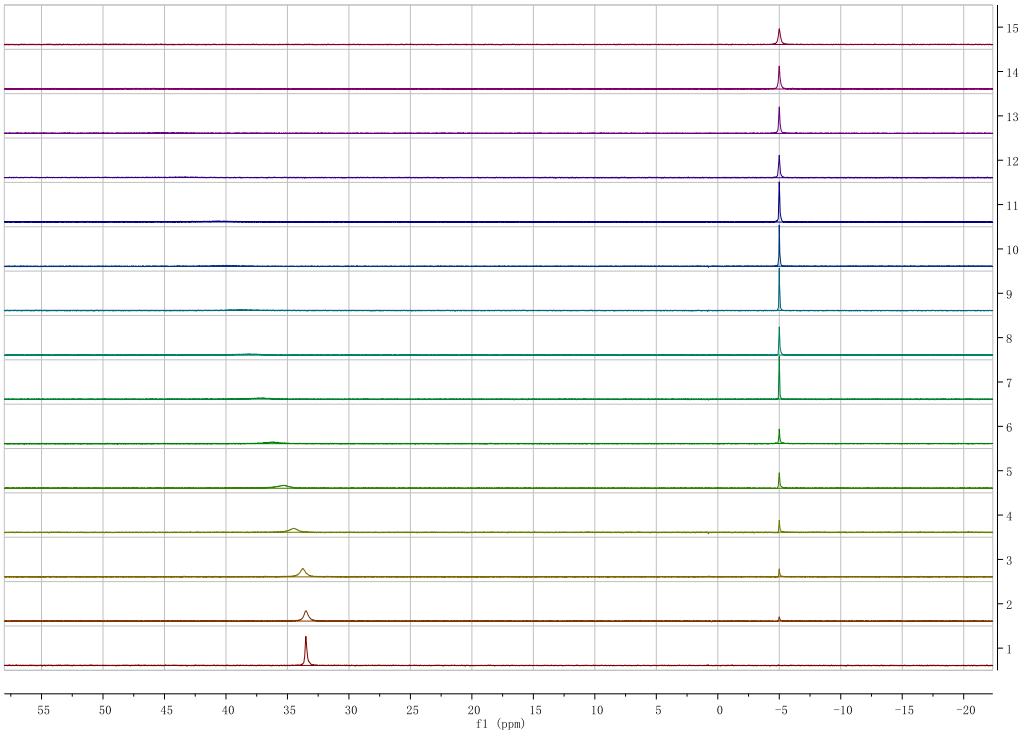


Fig. S6. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (5 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

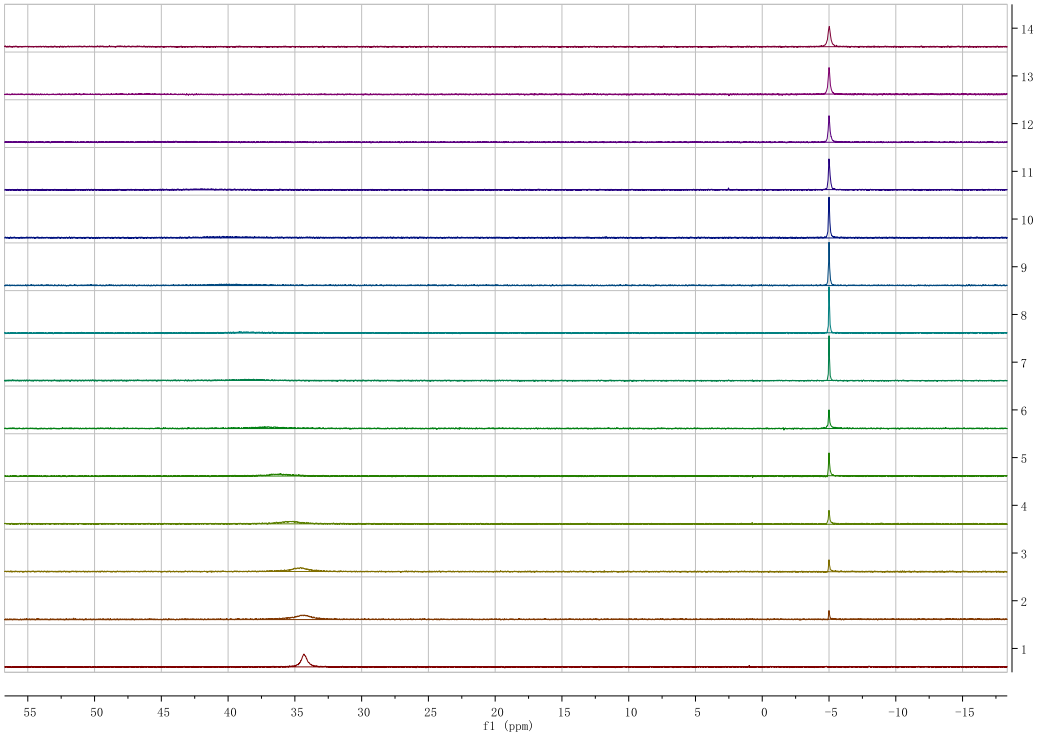


Fig. S7. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (10 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

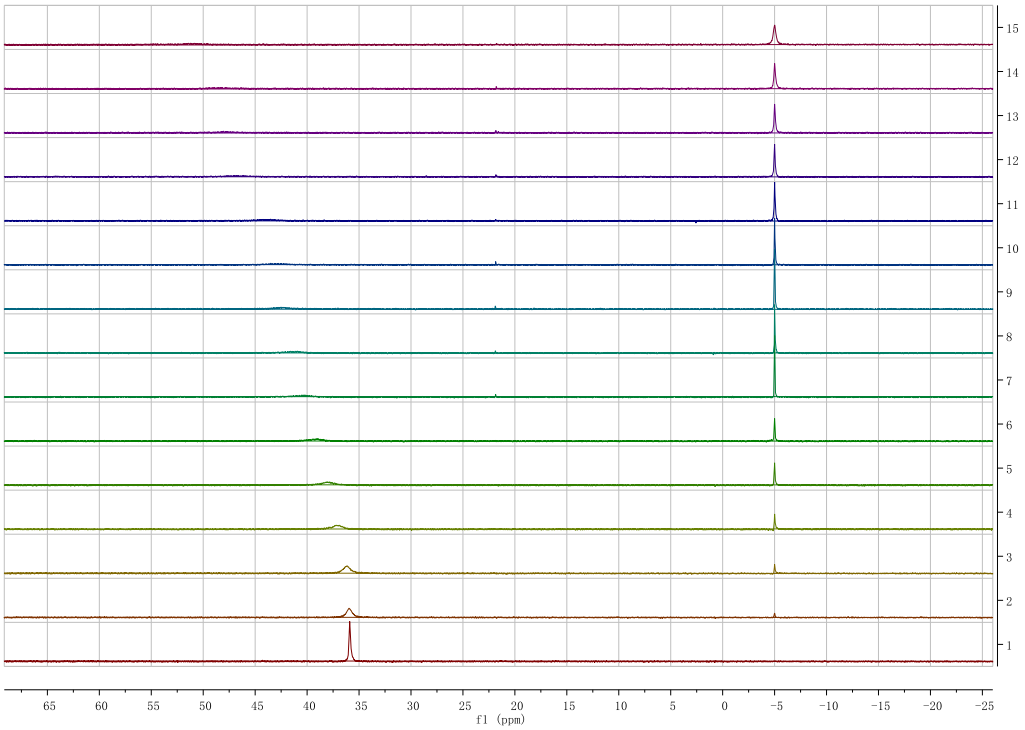


Fig. S8. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2 eq.) in the presence of TMSOTf (15 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

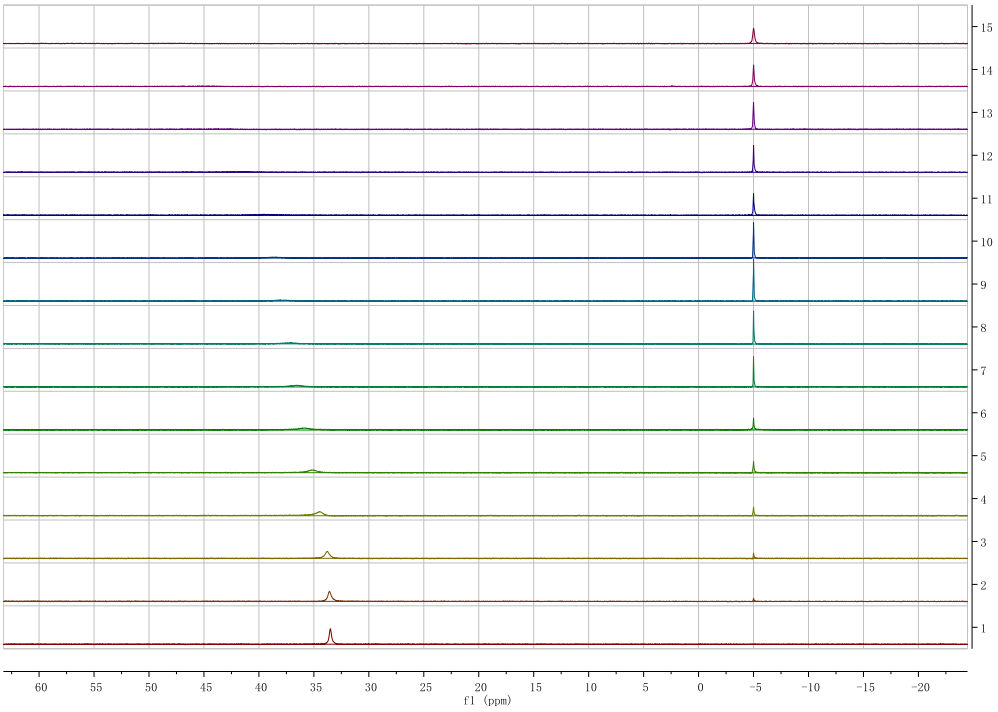


Fig. S9. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (1.5 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

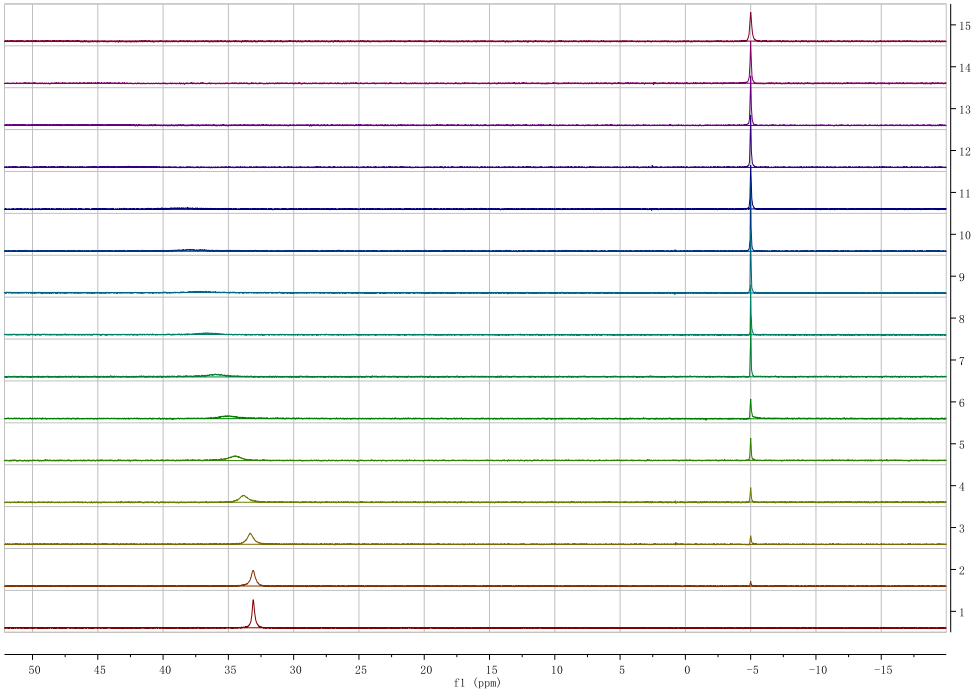


Fig. S10. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (1.8 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

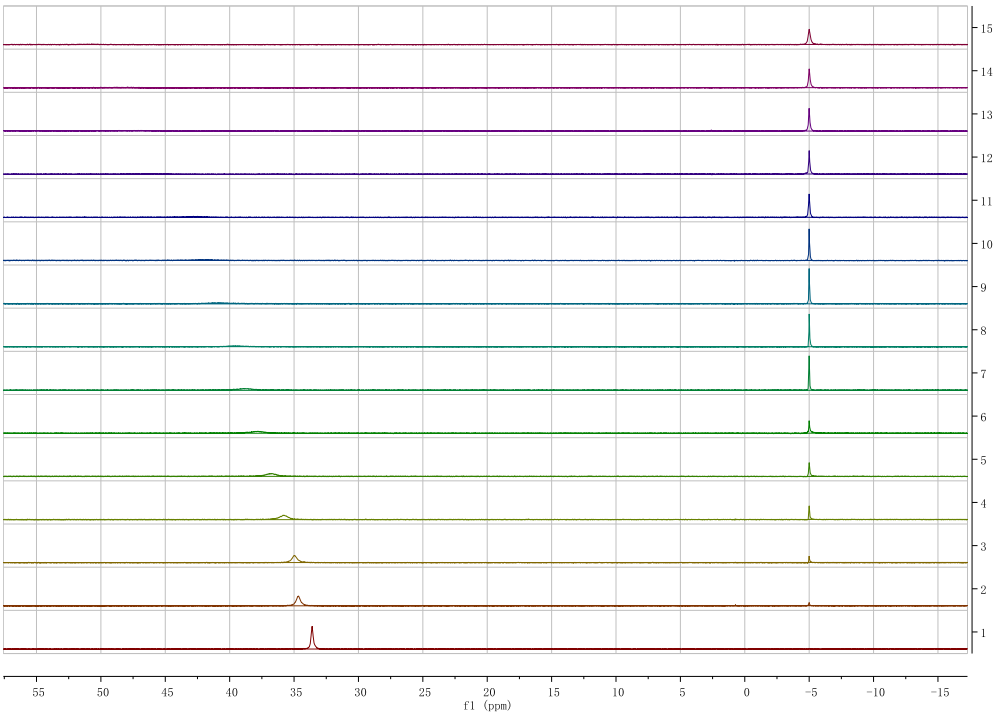


Fig. S11. ^{31}P NMR tracing of triphenylphosphine oxide with $Me(EtO)_2SiH$ (2.5 eq.) in the presence of TMSOTf (8 mol%) as catalyst in the DCE solvent in 60 ^{o}C (Test every two hours).

5. Computation of reaction mechanism

Computational Methods: All density functional theory calculations were carried out with the Gaussian 16 programs.[13] The geometry optimizations, Intrinsic reaction coordinate (IRC), and frequency analyses of the reactants, transition states, and products were performed using the B3LYP-D3 method at the 6-31G(d,p) level.[14-18] Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima. The single-point energy calculations were performed at the M06-2X-D3/def-TZVP/SMD(DCE) level of theory for solution-phase. The corrections of Gibbs free energy calculations (at the 6-31G(d,p) level) were added to the single-point energies (at the M06-2X-D3/def-TZVP/SMD(DCE)) to obtain the Gibbs free energy in solution.

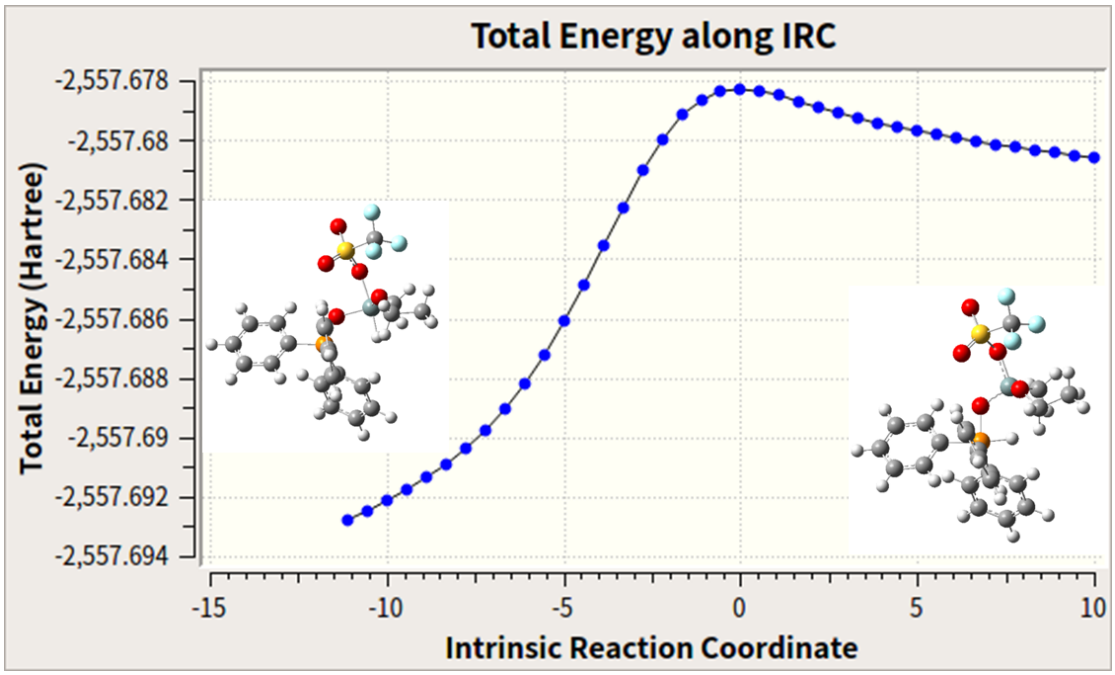


Fig. S12. The main geometries calculated at the B3LYP-D3/6-31G(d,p) level.

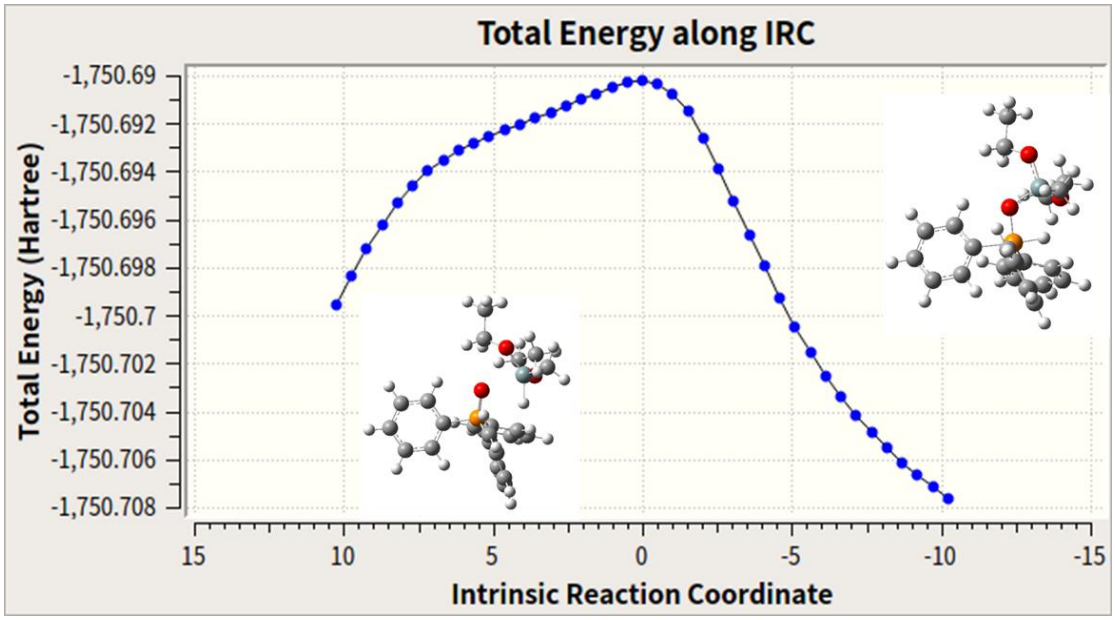


Fig. S13. The IRC plots of **Ts-1** calculated at the B3LYP-D3/6-31G(d,p) level.

Table S1. Thermal Free Energies with thermal correction (Hartree/Particle).

Intermediates or transition states	Thermal correction to Gibbs Free Energy (B3LYP-D3/6-31G(d,p)	Single-point energies (M06-2X-D3/def-TZVP/SMD(DCE))	Thermal Free Energies with thermal correction
1a	0.232677	-1111.4909636	-1111.258287
2a	0.227686	-1036.2330636	-1036.005378
$^{-}$OTf	-0.005179	-961.6112298	-961.6164088
$Me(EtO)_2SiH$	0.148908	-638.9406096	-638.7917016
$Me(EtO)_2SiOH$	0.153123	-714.2379765	-714.0848535
$Me(EtO)_3Si$	0.204754	-792.8336153	-792.6288613
IM1	0.160176	-1599.8475195	-1599.687344
IM2	0.102955	-1445.9533233	-1445.850368
IM3	0.359268	-2557.4648223	-2557.105554
IM3′	0.340418	-1595.8468471	-1595.506429
IM1-1	0.405308	-1750.4257458	-1750.020438
IM2′	0.398528	-1749.7432243	-1749.344696
IM3-3	0.400297	-1750.4392965	-1750.039000
IM4	0.359906	-2557.4377532	-2557.077847
IM4′	0.358416	-2557.4607933	-2557.102377
IM5	0.108764	-1521.2482529	-1521.139489
TS1	0.360242	-2557.4360604	-2557.075818
TS1′	0.339630	-1595.74323	-1595.403600
TS1″	0.578487	-2388.6287034	-2388.050216
TS1‴	0.834816	-3500.1732856	-3499.338470
TS1-1	0.407656	-1750.4079785	-1750.000323
TS2	0.358416	-2557.4575771	-2557.099161

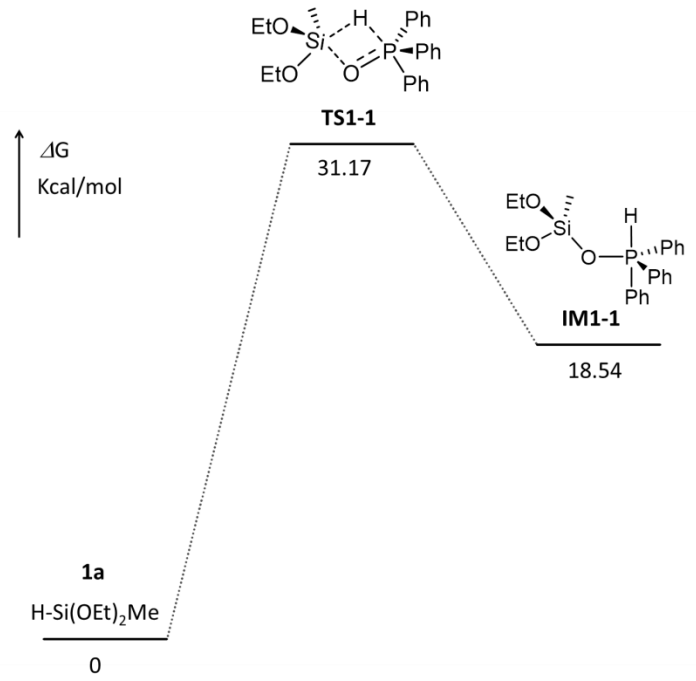
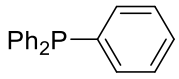
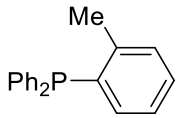


Fig. S14. Free energy profile for the uncatalyzed reduction of $O=PPh_3$ by $H\text{-}Si(OEt)_2Me$.

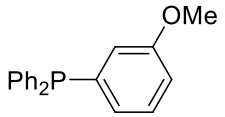
6. The analytical and spectral characterization data of compounds **2**.



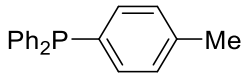
2a: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2a** was afforded (95%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.32;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, J = 5.8 Hz, 15H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.24 (d, $J_{P\text{-}C}$ = 12.1Hz,3C), 133.79 (d, $J_{P\text{-}C}$=19.2Hz, 6CH), 128.75 (s, 3CH), 128.54 (d, $J_{P\text{-}C}$ = 7.1 Hz, 6CH). HRMS Calcd. For $C_{18}H_{16}P^+$ $[M + H^+]^+$, 263.0992. Found: 263.0996.



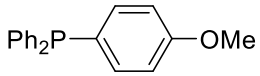
2b: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2b** was afforded (96%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -13.32; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.22 (m, 12H), 7.13 (t, J = 7.5 Hz, 1H), 6.82 (dd, J = 7.0, 4.5 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.25 (d, $J_{P\text{-}C}$ = 25.3 Hz, C), 136.35 (d, $J_{P\text{-}C}$ = 10.1 Hz, 2C), 136.04 (d, $J_{P\text{-}C}$ = 11.7 Hz, C), 134.05 (d, $J_{P\text{-}C}$ = 19.8 Hz, 4CH), 132.79(s, CH), 130.11 (d, $J_{P\text{-}C}$ = 5.1, CH), 128.77(s, 2CH), 128.72(s, CH), 128.59 (d, $J_{P\text{-}C}$ = 7.1 Hz, 4CH), 126.04(s, CH), 21.25 (d, $J_{P\text{-}C}$ = 21.0 Hz, CH_3). HRMS Calcd. For $C_{16}H_{18}P^+$ $[M + H^+]^+$, 277.1101. Found: 277.1102



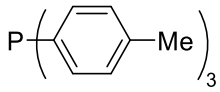
2c: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2c** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -4.63; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 2.4 Hz, 10H), 7.18 – 7.14 (m, 1H), 6.86 – 6.73 (m, 3H), 3.64 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.56 (d, $J_{P\text{-}C}$ = 8.4 Hz, C), 138.79 (d, $J_{P\text{-}C}$ = 11.3 Hz, C), 137.08 (d, $J_{P\text{-}C}$ = 10.8 Hz, 2C), 133.79 (d, $J_{P\text{-}C}$ = 19.6 Hz, 4CH), 129.51 (d, $J_{P\text{-}C}$ = 7.7 Hz, CH), 128.78(s,2CH), 128.51 (d, $J_{P\text{-}C}$ = 7.0 Hz, 4CH), 126.07 (d, $J_{P\text{-}C}$ = 18.9 Hz, CH), 119.01 (d, $J_{P\text{-}C}$ = 21.2Hz,CH), 114.35 (s, CH), 55.16 (s, CH_3). HRMS Calcd. For $C_{19}H_{18}OP^+$ $[M + H^+]^+$, 293.1050. Found: 293.1051.



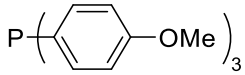
2d: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2d** was afforded (91%); ^{31}PNMR (162MHz,$CDCl_3$) δ 6.18;1HNMR (400MHz,CDCl3) δ7.29-7.30 (d,*J*=4.0Hz,10H),7.20-7.23 (t,*J*=8.0Hz,2H),7.12-7.14 (d,*J*=8.0Hz,2H); ^{13}CNMR (101 MHz, Chloroform-*d*) δ 138.90 (s, C), 137.67 (d, $J_{P\text{-}C}$ = 10.8 Hz, 3C), 134.34 – 133.24 (m, 6CH), 129.46 (d, $J_{P\text{-}C}$ = 7.3 Hz, 2CH), 128.88 – 127.67 (m, 6CH), 21.41 (s, CH_3). HRMS Calcd. For $C_{16}H_{18}P^+$ $[M + H^+]^+$, 277.1103. Found: 277.1102.



2e: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2e** was afforded (83%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.99; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.09 (m, 12H), 6.81 (d, *J* = 8.0 Hz, 3H), 3.72 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.43 (s, C), 137.94 (d, $J_{P\text{-}C}$ = 10.1Hz, 2C), 135.65 (d, $J_{P\text{-}C}$ = 22.2 Hz, 2CH), 133.46 (d, $J_{P\text{-}C}$ = 19.2 Hz, 4CH), 128.46 (d, $J_{P\text{-}C}$ = 9.1 Hz, 4CH), 127.67 (d, $J_{P\text{-}C}$ =13.1 Hz, C), 114.29 (d, $J_{P\text{-}C}$ = 8.1 Hz, 2CH), 55.21 (s, CH_3). HRMS Calcd. For $C_{19}H_{18}OP^+$ $[M + H^+]^+$, 293.1052. Found: 293.1055.

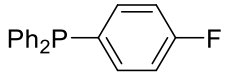


2f: Reaction condition as GP A for preparation of compounds **2a** (1.0 mmol), the white solid **2f** was afforded (96%); ^{31}PNMR (162MHz,$CDCl_3$) δ7.83; ^{1}HNMR (400MHz, $CDCl_3$) δ7.18-7.22 (t, *J*=8.0Hz, 6H), δ7.11-7.18 (d, *J*=4.0Hz); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.56 (s, 3C), 134.26 (d, $J_{P\text{-}C}$ = 9.1 Hz, 3C), 133.72 (d, $J_{P\text{-}C}$ = 19.2 Hz, 6CH), 129.33 (d, $J_{P\text{-}C}$ = 7.1 Hz, 6CH), 21.36 (s, $3CH_3$). HRMS Calcd. For $C_{21}H_{22}P^+$ $[M + H^+]^+$, 305.1421. Found:305.1418

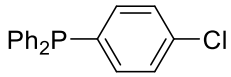


2g: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the

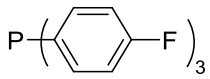
white solid **2g** was afforded (85%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -10.19;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.13 (m, 6H), 6.91 (d, *J* = 8.0 Hz, 6H), 3.83 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.15 (s, 3C), 134.98 (d, J_{P-C}= 20.7 Hz, 6CH), 128.84 (d, J_{P-C}= 7.1 Hz, 3C), 114.18 (d, J_{P-C} = 7.7 Hz, 6CH), 55.21 (s, $3CH_3$). HRMS Calcd. For $C_{21}H_{22}O_3P^+$ $[M + H^+]^+$, 353.1261. Found: 353.1258.



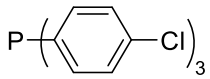
2h: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2h** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.61; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.28 (m, 12H), 7.05 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.42 (d, J_{C-F} = 249.0 Hz, C), 137.18 (d, J_{P-C} = 10.7 Hz, 2C), 135.83 (dd, J_{P-C} = 21.2, J_{F-C} = 8.0 Hz, 2CH), 133.59 (d, J_{P-C} = 19.5 Hz, 4CH), 132.67 (dd, J_{P-C} = 11.1, J_{F-C} =3.6 Hz, C), 128.84 (s, 2CH), 128.60 (d, J_{P-C} = 6.9 Hz, 4CH), 115.74 (dd, J_{F-C} = 20.9, J_{P-C} = 7.7 Hz, 2CH). HRMS Calcd. For $C_{18}H_{15}FP^+$ $[M + H^+]^+$, 281.0850. Found: 281.0858.



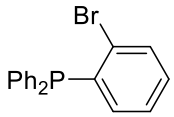
2i: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2i** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.43; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.23 (m, 6H), 7.23 – 7.18 (m, 6H), 7.16 – 7.10 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 136.75 (d, J_{P-C} = 10.8 Hz,2C), 135.99 (d, J_{P-C} = 12.4 Hz, C), 135.06 (s, C), 135.03 (d, *J*p-c = 20.2 Hz, 2CH), 133.72 (d, J_{P-C}= 19.7 Hz, 4CH), 128.98 (s, 2CH), 128.77 (d, J_{P-C} = 7.0 Hz, 2CH), 128.66 (d, J_{P-C}= 7.0 Hz, 4CH). HRMS Calcd. For $C_{18}H_{15}ClP^+$ $[M + H^+]^+$, 298.0482. Found: 281.0481.



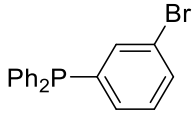
2j: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2j** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ-9.00; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.22 - 7.27 (m,,6H), 7.02-7.06 (t, *J*=8.0Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.48 (d, J_{F-C} = 249.5 Hz, 3C), 135.48 (dd, J_{P-C} = 21.2, J_{F-C} = 8.0 Hz, 6CH), 132.54 (dd, J_{P-C} = 11.0, J_{F-C} =3.3 Hz, 3C), 115.94 (dd, J_{F-C} = 21.0, J_{P-C} =7.6 Hz, 6CH). HRMS Calcd. For $C_{18}H_{13}F_3P^+$ $[M + H^+]^+$, 317.0662. Found: 317.0659.



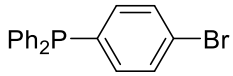
2k: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2k** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ-8.48; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 7.6 Hz, 6H), 7.19 (t, *J* = 7.8 Hz, 6H) ^{13}C NMR (101 MHz, Chloroform-*d*) δ 135.59 (s, 3C), 134.87 (d, J_{P-C} = 20.5 Hz, 6CH), 134.84 (s, 3C), 129.03 (d, J_{P-C} = 7.2 Hz,, 6CH). HRMS Calcd. For $C_{18}H_{13}Cl_3P^+$ $[M + H^+]^+$, 365.9712. Found: 365.9709



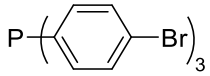
2l: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2l** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.05; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (m, 1H), 7.4 –7.23 (m, 10H), 7.20 – 7.15 (m, 2H), 6.75 (m, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.97 (d, $J_{P\text{-}C}$ = 12.1 Hz, C), 135.87 (d, $J_{P\text{-}C}$ = 11.1 Hz, 2C), 134.50(s, CH), 134.06 (d, $J_{P\text{-}C}$ = 20.3 Hz, 4CH), 133.01 (d, $J_{P\text{-}C}$ = 2.3 Hz, CH), 130.16(s, CH), 129.85(s, C), 129.05 (s, 2CH), 128.69 (d, $J_{P\text{-}C}$ = 7.2 Hz, 4CH), 127.43(s, CH). HRMS Calcd. For $C_{18}H_{15}BrP^{+}$ $[M + H^{+}]^{+}$, 341.9998. Found: 341.9993.



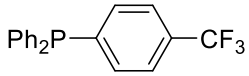
2m: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2m** was afforded (92%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.41; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 8.0 Hz, 2H), 7.38 – 7.23 (m, 10H), 7.15 (t, *J* = 8.0 Hz, 2H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 136.66(s, C), 136.55(s, 2C), 135.33(s, CH), 135.13(s, CH), 133.71 (d, $J_{P\text{-}C}$= 20.2Hz, 4CH), 131.70(s, CH), 131.63(s, CH), 128.98(s, 2CH), 128.64 (d, $J_{P\text{-}C}$ = 7.1 Hz, 4CH), 123.38(s, C). HRMS Calcd. For $C_{18}H_{15}BrP^{+}$ $[M + H^{+}]^{+}$, 341.9996. Found: 341.9995.



2n: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2n** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.44; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.45 (m, 2H), 7.37 – 7.27 (m, 10H), 7.16 (dd, *J* = 8.4, 7.0Hz, 2H); ^{13}C NMR (101MHz, Chloroform-*d*) δ 136.63 (s, C), 136.52 (s, C), 135.22 (d, $J_{P\text{-}C}$ = 20.0 Hz, 2CH), 133.71 (d, $J_{P\text{-}C}$ = 19.7 Hz, 4CH), 131.66 (d, $J_{P\text{-}C}$ = 6.9 Hz, 2CH), 128.98 (s, 2CH), 128.64 (d, $J_{P\text{-}C}$ = 7.0 Hz,4CH), 123.39 (s, C). HRMS Calcd. For $C_{18}H_{15}BrP^{+}$ $[M + H^{+}]^{+}$, 341.9996. Found: 341.9994.

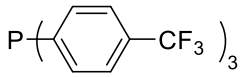


2o: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2o** was afforded (96%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -8.46;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.0 Hz, 6H), 7.04 (t, *J* = 8.0 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 135.37(s,3C), 135.12 (d, $J_{P\text{-}C}$ = 20.4 Hz,6CH), 133.45 (d, $J_{P\text{-}C}$ = 10.7 Hz, 3C), 131.99 (d, $J_{P\text{-}C}$ = 7.1 Hz,6CH). HRMS Calcd. For $C_{18}H_{13}Br_3P^{+}$ $[M + H^{+}]^{+}$, 499.8185. Found: 499.8184.

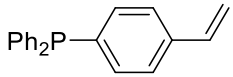


2p: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2p** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.34;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.0Hz, 2H), 7.47 – 7.27 (m, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.92 (d, $J_{P\text{-}C}$= 14.4 Hz, C), 136.08 (d, $J_{P\text{-}C}$ = 10.6

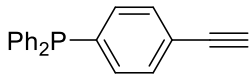
Hz, 2C), 133.96 (d, J_{P-C} = 20.0 Hz,4CH), 133.60 (d, J_{C-F} = 19.0 Hz, 2CH), 130.53 (q, J_{C-F} = 32.3 Hz, C), 129.25 (s, 2CH), 128.78 (d, J_{P-C}= 7.2 Hz,4CH), 125.13 (q, J_{C-F} = 7.4Hz, 2CH), 124.13 (q, $^{1}J_{C-F}$ = 272.3 Hz, C). HRMS Calcd. For $C_{19}H_{15}F_3P^+$ [M + H^+]$^+$, 331.0818. Found: 331.0817.



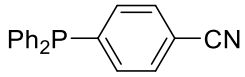
2q: Reaction condition as **GP A** for preparation of compounds **2a** (1.0 mmol), the white solid **2q** was afforded (91%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.02;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 7.8 Hz, 6H), 7.42 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.31 (d, J_{P-C} = 14.3 Hz, 3C), 133.98 (d, J_{P-C} = 20.2 Hz, 6CH), 131.60 (q, J_{C-F} = 32.7 Hz, 3C), 125.64 (q, J_{C-F} = 7.1Hz, 6CH), 123.84 (q, J_{C-F}=273.7, 3C). HRMS Calcd. For $C_{21}H_{13}F_9P^+$ [M + H^+]$^+$, 467.0566. Found: 467.0567.



2r[1]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2r** was afforded (82%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.83; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.07 (m, 14H), 6.70 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.76 (d, *J* = 17.6 Hz, 1H), 5.27 (d, *J* = 10.9 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.98(s, C), 137.20 (d, J_{P-C} = 10.9 Hz, 2C), 136.79 (d, J_{P-C} = 10.9 Hz, C), 136.42 (s, CH), 133.97 (d, J_{P-C} = 19.7 Hz, 2CH), 133.74 (d, J_{P-C}= 19.5 Hz,4 CH), 128.76 (s, 2CH), 128.54 (d, J_{P-C}= 6.9 Hz, 4CH), 126.31 (d, J_{P-C} = 7.1 Hz, 2CH), 114.67 (s, CH_2). HRMS Calcd. For $C_{20}H_{18}P^+$ [M + H^+]$^+$, 289.1101. Found: 289. 1100.

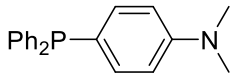


2s: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2s** was afforded (71%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.22; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.32 (m, 2H), 7.29 – 7.19 (m, 10H), 7.19 – 7.13 (m, 2H), 3.03 (s, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.79 (d, *J* = 12.1, C), 136.56 (d, *J* = 11.1 Hz, 2C), 133.84 (d, J_{P-C} = 19.7 Hz, 4CH), 133.37 (d, J_{P-C}= 19.3 Hz, 2CH), 132.01 (d, J_{P-C}= 6.8 Hz, 2CH), 128.98 (s, 2CH), 128.63 (d, J_{P-C}= 7.1 Hz, 4CH), 122.31 (s, C), 83.39 (s, C), 78.13 (s, CH). HRMS Calcd. For $C_{20}H_{16}P^+$ [M + H^+]$^+$, 287.0944. Found: 287. 0942.

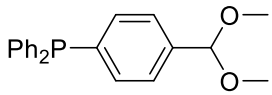


2t[2]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2t** was afforded (62%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -4.27;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 7.2 Hz, 1H), 7.36 – 7.19 (m, 8H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.16 (d, J_{P-C} = 16.8 Hz, C), 135.42 (d, J_{P-C} = 10.6 Hz, 2C), 134.06 (d, J_{P-C} = 20.3 Hz, 4CH), 133.52 (d, J_{P-C} = 18.6 Hz, 2CH), 131.72 (d, J_{P-C} = 6.0 Hz, 2CH), 129.51 (s, 2CH), 128.89 (d, J_{P-C} = 7.4 Hz, 4CH),

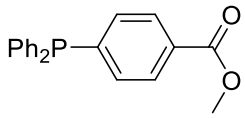
118.73 (s, C), 111.94 (s, C). HRMS Calcd. For $C_{19}H_{15}P^+$ [M + H^+]$^+$, 288.0897. Found: 288.0895.



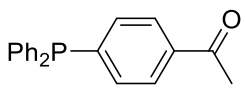
2u:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2u** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -7.11; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.15 (m, 12H), 6.76 (d, *J* = 8.4 Hz, 2H), 3.01 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.95 (s, C), 138.78 (d, J_{P-C} = 10.6 Hz, 2C), 135.61 (d, J_{P-C} = 21.7 Hz, 2CH), 133.35 (d, J_{P-C} = 18.8 Hz, 4CH), 128.33 (d, J_{P-C} = 6.6 Hz, 4CH), 128.20 (s, 2CH), 121.43 (d, J_{P-C} = 4.9 Hz, C), 112.37 (d, J_{P-C} = 8.4 Hz, 2CH), 40.23 (s. 2CH_3). HRMS Calcd. For $C_{20}H_{21}NP^+$ [M + H^+]$^+$, 306.1366. Found: 306.1365.



2v:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2v** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.85; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 7.1 Hz, 2H), 7.24 (s, 12H), 5.29 (s, 1H), 3.25 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.67 (s, C), 137.66 (d, J_{P-C} = 11.2 Hz, C), 137.10 (d, J_{P-C} = 10.8 Hz, 2C), 133.79 (d, J_{P-C} = 19.5 Hz, 4CH), 133.52 (s, 2CH), 128.80 (s, 2CH), 128.54 (d, J_{P-C} = 7.0 Hz, 4CH), 126.85 (d, J_{P-C} = 7.0 Hz, 2CH), 103.07 (s, CH), 52.91 (s, 2CH_3). HRMS Calcd. For $C_{21}H_{22}O_2P^+$ [M + H^+]$^+$, 337.1312. Found: 337.1311.

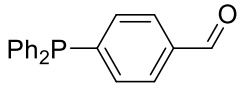


2w[3]:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2w** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.03; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.60 – 6.95 (m, 10H), 3.81 (s, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.89(s, C), 144.10 (d, J_{P-C}= 14.1 Hz, C), 136.22 (d, J_{P-C}= 10.7 Hz, 2C), 133.99 (d, J_{P-C}= 20.0 Hz, 4CH), 133.20 (d, J_{P-C}= 18.7 Hz, 2CH), 130.07(s, C), 129.32 (d, J_{P-C}= 6.5 Hz, 2CH), 129.17 (s, 2CH), 128.71 (d, J_{P-C}= 7.2 Hz, 4CH), 52.17 (s, CH_3). HRMS Calcd. For $C_{20}H_{18}O_2P^+$ [M + H^+]$^+$, 321.0999. Found: 321.0997.

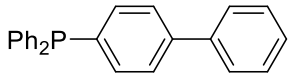


2x[4]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2x** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.03; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.60 – 6.95 (m, 10H), 3.81 (s, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.89 (s, C), 144.10 (d, J_{P-C}= 14.1 Hz, C), 136.22 (d, J_{P-C}= 10.7 Hz, 2C), 133.99 (d, J_{P-C}= 20.0 Hz, 4CH), 133.20 (d, J_{P-C}= 18.7 Hz, 2CH), 130.07 (s, C), 129.32 (d, J_{P-C}= 6.5 Hz, 2CH), 129.17 (s, 2CH),

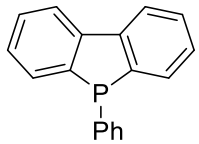
128.71 (d, J_{P-C}= 7.2 Hz, 4CH), 52.17 (s,CH_3). HRMS Calcd. For $C_{20}H_{18}OP^+$ [M + H^+]$^+$, 305.1017. Found: 305.1049.



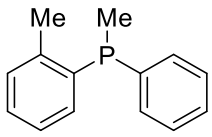
2y:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2y** was afforded (77%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -4.28; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.91 (s, 1H), 7.95 – 7.58 (m, 2H), 7.41 – 7.16 (m, 12H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.95 (s, CH), 146.55 (d, J_{P-C} = 15.6 Hz, C), 136.05 (s, C), 135.85 (d, J_{P-C}= 10.6 Hz, 2C), 134.09 (d, J_{P-C} = 20.2 Hz, 4CH), 133.57 (d, J_{P-C} = 18.5 Hz, 2CH), 129.36(s, 2CH), 129.31(s, 2CH), 128.81 (d, J_{P-C} = 7.4 Hz, 4CH). HRMS Calcd. For $C_{19}H_{16}OP^+$ [M + H^+]$^+$, 291.0894. Found: 291.0892.



2z:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2z** was afforded (76%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -6.07;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (t, *J* = 8.1 Hz, 4H), 7.43 – 7.22 (m, 15H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.51 (s, C), 140.56(s, C), 137.23 (d, J_{P-C} = 10.8 Hz, 2C), 136.13 (d, J_{P-C}= 10.9 Hz, C), 134.20 (d, J_{P-C} = 19.6 Hz, 2CH), 133.79 (d, J_{P-C}= 19.5 Hz, 4CH), 128.85 (s, 2CH), 128.79 (s, 2CH), 128.56 (d, J_{P-C}= 6.9 Hz, 4CH), 127.57 (s, CH), 127.19 (d, J_{P-C}= 7.1 Hz, 2CH), 127.10 (s, 2CH). HRMS Calcd. For $C_{24}H_{20}P^+$ [M + H^+]$^+$, 339.1257. Found: 339.1256.

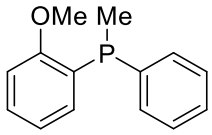


2aa:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2aa** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -10.09; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.63 – 7.56 (m, 2H), 7.35 (td, *J* = 7.7, 1.1 Hz, 2H), 7.26 – 7.16 (m, 4H), 7.16 – 7.07 (m, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.71 (d, J_{P-C}= 2.9 Hz, 2C), 142.62 (d, J_{P-C}= 2.7 Hz, 2C), 136.23 (d, J_{P-C}= 18.9 Hz, C), 132.72 (d, J_{P-C}= 20.1 Hz,2CH), 130.51 (d, J_{P-C} = 21.9 Hz, 2CH), 129.32 (s, CH), 128.72 (s, 2CH), 128.71 (d, J_{P-C}= 7.6 Hz, 2CH), 127.65 (d, J_{P-C}= 7.6 Hz, 2CH), 121.44 (s, 2CH). HRMS Calcd. For $C_{18}H_{14}P^+$ [M + H^+]$^+$, 261.0788. Found: 261.0787.

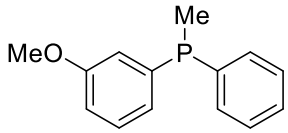


2ab[5]: Reaction condition **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ab** was afforded (91%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -36.28; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 6.73 (m, 9H), 2.31 (s, 3H), 1.50 (d, *J* = 4.0 Hz, 3H); ^{31}C NMR (101 MHz, Chloroform-*d*) δ 142.14 (d, J_{P-C}= 24.2 Hz, C), 140.00 (d, J_{P-C}= 11.7 Hz, C), 137.67 (d, J_{P-C}= 12.3 Hz, C), 132.22 (d, J_{P-C}= 18.7 Hz, 2CH),

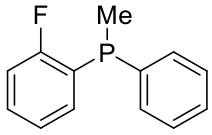
130.25 (s, CH), 130.09 (d, J_{P-C}= 4.4 Hz, CH), 128.50 (d, J_{P-C}= 6.8 Hz, 2CH), 128.40 (s, CH), 128.31 (s, CH), 126.03 (s, CH), 21.20 (d, J_{P-C}= 20.9 Hz, CH_3), 12.18 (d, J_{P-C}= 13.5 Hz, CH_3). HRMS Calcd. For $C_{14}H_{16}P^+$ $[M + H^+]^+$, 215.0944. Found: 215.0942.



2ac[5]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ac** was afforded (70%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -25.91; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.39 (td, *J* = 7.6, 2.6 Hz, 2H), 7.25 (t, *J* = 6.6 Hz, 4H), 7.07 – 6.95 (m, 1H), 6.84 (t, *J* = 7.4 Hz, 1H), 6.77 (dd, *J* = 8.2, 4.1 Hz, 1H), 3.70 (s, 3H), 1.54 (d, *J* = 3.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.00 (d, J_{P-C} = 12.9 Hz, C), 138.62 (d, J_{P-C} = 8.8 Hz, C), 132.54 (d, J_{P-C} = 19.3 Hz, 2CH), 131.64 (d, J_{P-C} = 3.7 Hz, C), 130.08 (s, CH), 128.56 (s, CH), 128.31 (d, J_{P-C} = 7.1 Hz, 2CH), 127.77 (d, J_{P-C} = 3.0 Hz, C), 120.97 (d, J_{P-C} = 3.7 Hz, CH), 110.32 (s, CH), 55.55 (s, CH_3), 10.96 (d, *J* = 11.0 Hz, CH_3). HRMS Calcd. For $C_{14}H_{16}OP^+$ $[M + H^+]^+$, 231.0894. Found: 231.0893.

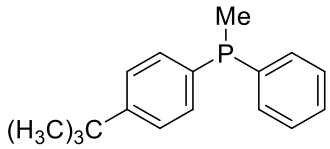


2ad[5]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ad** was afforded (73%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -25.95; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.30 (m, 2H), 7.25 (d, *J* = 6.6 Hz, 2H), 7.21 – 7.15 (m, 2H), 6.96 – 6.85 (m, 2H), 6.77 (dd, *J* = 8.1, 2.3 Hz, 1H), 3.70 (s, 3H), 1.54 (d, *J* = 3.5 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.42 (d, J_{P-C}= 7.9 Hz, C), 141.79 (d, J_{P-C}= 12.5 Hz, C), 132.17 (d, J_{P-C} = 18.6 Hz, C), 129.43 (d, J_{P-C} = 7.2 Hz, 2CH), 128.45 (d, J_{P-C}= 3.5 Hz, CH), 128.37 (s, CH), 124.34 (d, J_{P-C} = 17.8 Hz, CH), 117.61 (d, J_{P-C} = 20.1 Hz, CH), 113.82 (s, CH), 55.19 (s, CH_3), 12.44 (s, CH_3). HRMS Calcd. For $C_{14}H_{16}OP^+$ $[M + H^+]^+$, 231.0894. Found: 231.0893.

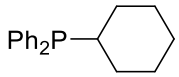


2ae[5]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ae** was afforded (89%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -25.89; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.42 (m, 2H), 7.32 (dd, *J* = 12.9, 2.8 Hz, 3H), 7.27 (dd, *J* = 10.6, 4.5 Hz, 1H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.05 (t, *J* = 8.0 Hz, 1H), 7.01 – 6.93 (m, 1H), 1.61 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.76 (dd, J_{C-F} = 248.5, J_{P-C} =7.1 Hz, C), 143.63 (dd, J_{P-C} = 15.2, J_{C-F} =5.0 Hz, C), 139.17 (d, J_{P-C} = 11.7 Hz, C), 132.37 (d, J_{P-C}= 19.1 Hz, 2CH), 129.93 (t, J_{P-C} = 7.5 Hz, CJ), 128.86(s, CH), 128.59 (d, *J* = 6.8 Hz, 2CH), 127.66 (dd, J_{P-C} = 19.6, J_{C-F} =2.8 Hz, CH), 118.29 (dd, J_{C-F} = 20.9, J_{P-C} =16.9 Hz, CH), 115.23 (d, J_{C-F} = 21.3 Hz, CH),

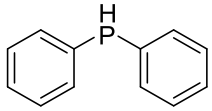
12.46 (d, $J_{P\text{-}C}$ = 14.0 Hz, CH_3). HRMS Calcd. For $C_{13}H_{13}FP^+$ $[M + H^+]^+$, 219.0694. Found: 219.0692.



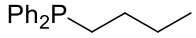
2af[5]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2af** was afforded (85%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -28.21;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 7.1 Hz, 2H), 7.35 (d, *J* = 4.1 Hz, 4H), 7.30 (t, *J* = 7.2 Hz, 3H), 1.61 (d, *J* = 3.1 Hz, 3H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.62(s, C), 140.43 (d, $J_{P\text{-}C}$ = 11.4 Hz, C), 136.34 (d, $J_{P\text{-}C}$ = 9.9 Hz, C), 132.15 (d, $J_{P\text{-}C}$ = 1.7 Hz, 2CH), 131.96 (d, $J_{P\text{-}C}$ = 1.01, 2CH), 128.37 (d, $J_{P\text{-}C}$ = 6.4 Hz , 2CH), 128.28 (s, CH), 125.47 (d, $J_{P\text{-}C}$ = 6.8 Hz, CH), 34.65 (s, C), 31.30 (s, $3CH_3$), 12.59 (d, $J_{P\text{-}C}$= 13.0 Hz, CH_3). HRMS Calcd. For $C_{17}H_{22}P^+$ $[M + H^+]^+$, 257.1414. Found: 257.1413.



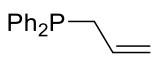
2ag[6]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ag** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -3.53;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59–7.43 (m, 4H), 7.42–7.30 (m, 6H), 2.26 (m, 1H), 1.8 –1.64 (m, 5H), 1.30 (m, 5H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.21 (d, $J_{P\text{-}C}$ = 13.9 Hz, 2C), 133.72 (d, $J_{P\text{-}C}$= 19.1 Hz,4CH), 128.64 (s,2CH), 128.33 (d, $J_{P\text{-}C}$= 7.0 Hz, 4CH), 35.52 (d, $J_{P\text{-}C}$ = 8.9 Hz, $2CH_2$), 29.68 (d, $J_{P\text{-}C}$ = 15.3 Hz, $2CH_2$), 26.88 (d, $3J_{P\text{-}C}$ = 11.3 Hz, $2CH_2$), 26.45 (d, $J_{P\text{-}C}$ = 1.0 Hz, CH_2). HRMS Calcd. For $C_{18}H_{22}P^+$ $[M + H^+]^+$, 269.1414. Found: 269.1413.



2ah: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ah** was afforded (98%); ^{31}P NMR (162 MHz,) δ -39.80. HRMS Calcd. For $C_{12}H_{12}P^+$ $[M + H^+]^+$, 187.0631. Found: 187.0631.

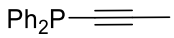


2al[7]: Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2al** was afforded (92%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ-15.95; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 (td, *J* = 7.5, 2.3 Hz, 4H), 7.24 (dd, *J* = 6.5, 3.9 Hz, 6H), 1.97 (t, *J* = 7.6 Hz, 2H), 1.35 (dt, *J* = 7.2, 3.7 Hz, 4H), 0.81 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.02 (d, $J_{P\text{-}C}$= 12.8 Hz, 2C), 132.73 (d, $J_{P\text{-}C}$= 18.3 Hz, 4CH), 128.45 (s, CH), 128.37 (d, $J_{P\text{-}C}$= 6.6 Hz, 4CH), 28.16 (d, $J_{P\text{-}C}$= 15.8 Hz, CH_2), 27.77 (d, $J_{P\text{-}C}$= 10.9 Hz, CH_2), 24.32 (d, $J_{P\text{-}C}$= 13.2 Hz, CH_2), 13.79 (s, CH_3). HRMS Calcd. For $C_{12}H_{12}P^+$ $[M + H^+]^+$, 243.1257. Found: 243.1256.

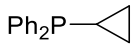


2aj[8]:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the

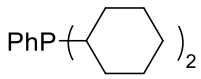
white solid **2aj** was afforded (63%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -7.11; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.48 (m, 4H), 7.41 (ddd, *J* = 7.5, 4.9, 2.3 Hz,6H), 6.74 (dt, *J* = 18.3, 11.9 Hz, 1H), 6.01 (ddd, *J* = 31.9, 11.6, 2.0 Hz,1H), 5.72 (ddd, *J* = 18.2, 14.1, 2.0 Hz, 1H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 137.69 (d, J_{P-C} = 9.7 Hz, CH_2), 136.86 (d, J_{P-C}= 13.6 Hz, 2C), 133.25 (d, J_{P-C}= 18.9 Hz, 4CH), 129.61 (d, J_{P-C} = 23.8 Hz, CH_2), 128.78(s, 2CH), 128.60 (d, J_{P-C}= 6.8 Hz, 4CH). HRMS Calcd. For $C_{15}H_{16}P^+$ $[M + H^+]^+$, 227.0944. Found: 227.0943.



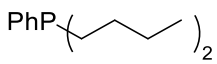
2ak[9]:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ak** was afforded (69%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -32.54; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (td, *J* = 8.2, 1.8 Hz, 4H), 7.23 (q, *J* = 4.9 Hz, 6H), 1.99 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 136.96 (d, J_{P-C} = 6.5 Hz,2C), 132.50 (d, J_{P-C} = 20.9 Hz, 4CH), 128.87 (s, 2CH), 128.53 (d, J_{P-C}= 7.5 Hz,4CH), 105.85 (d, J_{P-C} = 4.4 Hz, C), 75.18 (d, J_{p-c}= 1.5 Hz, C), 5.51 (s,CH_3). HRMS Calcd. For $C_{15}H_{14}P^+$ $[M + H^+]^+$, 225.0788. Found: 225.0787.



2ai[10]:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ai** was afforded (944%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ 3.11;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 (td, *J* = 7.4, 1.9 Hz, 4H), 7.29 –7.19 (m, 6H), 1.10 (m, 1H), 0.85 (m, 2H), 0.66–0.49 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.64 (d, J_{P-C} =9.6Hz, 2C), 132.54 (d, J_{P-C} =17.5Hz, 4CH), 128.45–128.34 (d, J_{P-C}=1.01Hz, 4CH), 128.30 (s, 2CH), 7.46 (d, J_{P-C} = 2.0 Hz, CH), 4.69 (d, J_{P-C} = 12.7 Hz, 2CH_2). HRMS Calcd. For $C_{15}H_{16}P^+$ $[M + H^+]^+$, 227.0944. Found: 227.0943.

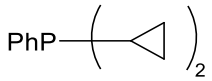


2ai:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ai** was afforded (80%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ 3.18; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 (dt, *J* = 6.8, 3.9 Hz, 2H), 7.36 (s, 3H), 2.02 – 1.74 (m, 6H), 1.66 (q, *J* = 13.3, 11.5 Hz, 6H), 1.37 – 1.28 (m, 2H), 1.28 – 1.08 (m, 6H), 1.02 (q, *J* = 12.1 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.72 (d, J_{P-C} = 18.9 Hz, 2CH), 131.84 (d, J_{P-C}= 12.6 Hz, C), 128.73 (s, C), 127.81 (d, J_{P-C} = 6.8 Hz, CH), 32.48 (d, J_{P-C}= 10.1 Hz,2CH), 30.02 (d, J_{P-C}= 16.7 Hz,2CH), 28.79 (d, J_{P-C}= 7.1 Hz, 2CH_2), 27.22 (d, J_{P-C} = 12.2 Hz, 2CH_2), 26.99 (d, J_{P-C}= 7.4 Hz, 2CH_2), 26.40 (s, 2CH_2). HRMS Calcd. For $C_{18}H_{28}P^+$ $[M + H^+]^+$, 275.1883. Found: 275.1882.

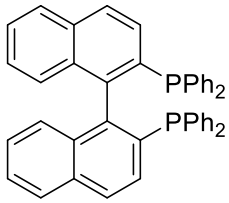


2an:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2an** was afforded (91%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -24.26;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (td, *J* = 7.3, 1.9 Hz, 2H), 7.25 – 7.15 (m, 3H), 1.55 (dt, *J* = 12.3, 5.2 Hz, 4H), 1.32 – 1.10 (m, 8H), 0.73 (t, *J* = 7.0 Hz,6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.08 (d, J_{P-C} = 5.9 Hz, C), 132.36 (d, J_{P-C} = 18.4 Hz,

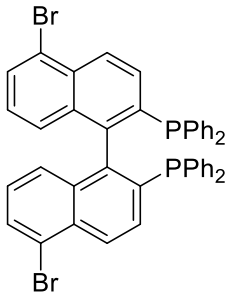
2CH), 128.56 (s, CH), 128.25 (d, J_{P-C} = 6.8 Hz, 2CH), 28.15 (d, J_{P-C} = 13.4 Hz, $2CH_2$), 27.94 (d, J_{P-C} = 10.6 Hz,$2CH_2$), 24.37 (d, J_{P-C} = 11.8 Hz, $2CH_2$), 13.79 (s, CH_3). HRMS Calcd. For $C_{14}H_{24}P^+$ $[M + H^+]^+$, 223.1570. Found: 223.1570.



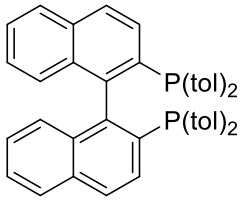
2ao[10]:Reaction condition as **GP B** for preparation of compounds **2a** (1.0 mmol), the white solid **2ao** was afforded (93%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ 10.79;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (m, 2H), 7.28 (m,2H), 7.24 – 7.18 (m, 1H), 0.95 – 0.83 (m, 2H), 0.76 (m, 4H), 0.50 (m, 4H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.51 (d, J_{P-C} = 9.2 Hz, C), 131.00 (d, J_{P-C} = 14.9 Hz, 2CH), 128.14 (d, J_{P-C} = 5.5 Hz, 2CH), 127.81 (s, CH), 7.32 (d, J_{P-C} = 1.7 Hz, 2CH), 3.92 (d, J_{P-C} = 11.1 Hz, $2CH_2$), 3.64 (d, J_{P-C} = 11.5 Hz, $2CH_2$). HRMS Calcd. For $C_{12}H_{16}P^+$ $[M + H^+]^+$, 191.0944. Found: 191.0943.



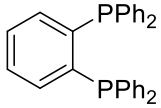
2ap:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2ap** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -15.55; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.5 Hz, 2H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.47 (dd, *J* = 8.5, 2.2 Hz, 2H), 7.42 – 7.33 (m, 2H), 7.28 (s, 1H), 7.15 (m, 19H), 6.94 (t, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ148.48 -125.80 (44C, aromatic carbons, observed complexity due to C-P splitting) HRMS Calcd. For $C_{44}H_{33}P_2^+$ $[M + H^+]^+$, 623.2012. Found: 623.2011.



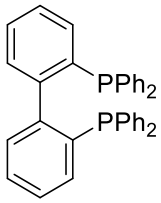
2aq[11]:Reaction condition as **GP C** for preparation of compounds of compounds **2a** (1.0 mmol), the white solid **2ar** was afforded (87%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ 27.46, -15.25;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.54 – 7.42 (m, 3H), 7.30 (dd, *J* = 8.5, 2.9 Hz, 1H), 7.28 – 7.17 (m, 5H), 7.13 (ddd, *J* = 15.9, 10.0, 4.8 Hz, 6H), 7.04 – 6.94 (m, 3H), 6.92 (d, *J* = 6.9 Hz, 2H), 6.84 (t, *J* = 7.3 Hz, 2H), 6.77 (t, *J* = 7.2 Hz, 1H), 6.71 (d, *J* = 8.3 Hz, 1H), 6.61 (t, *J* = 7.3 Hz, 1H), 6.53 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ144.99-125.55(44C, aromatic carbons, observed complexity due to C-P splitting). HRMS Calcd. For $C_{44}H_{31}Br_2P_2^+$ $[M + H^+]^+$,795.0211. Found: 795.0213.



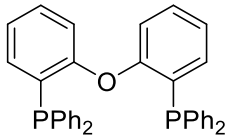
2ar[11]:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2as** was afforded (75%); ^{31}P NMR (162 MHz, Chloroform-d) δ -16.93; ^{1}H NMR (400 MHz, Chloroform-d) δ 7.87 (d, J = 8.5 Hz, 2H), 7.83 (d, J = 8.2 Hz, 2H), 7.47 (dd, J = 8.6, 2.3 Hz, 2H), 7.37 (ddd, J = 8.1, 6.8, 1.3 Hz, 2H), 7.08 – 6.90 (m, 18H), 6.86 (d, J = 8.5 Hz, 2H), 2.26 (d, J = 5.8 Hz, 12H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ145.35 -125.74 (44C, aromatic carbons, observed complexity due to C-P splitting) , 21.19. HRMS Calcd. For $C_{48}H_{41}P_2^+$ $[M + H^+]^+$, 679.2638. Found: 679.2636.



2as[12]:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2as** was afforded (97%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -13.84; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 – 7.05 (m, 22H), 7.01 – 6.94 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.79 (t, J_{P-C} = 10.3 Hz, 2C), 137.16 (t, J_{P-C} = 2.7 Hz, 4C), 134.14 (t, J_{P-C} = 3.1 Hz, 2CH), 133.93 (d, J_{P-C} = 20.2 Hz,8CH), 129.14(s, 2CH), 128.39(s, 4CH), 128.32 (t, J_{P-C} = 3.5 Hz, 8CH). HRMS Calcd. For $C_{32}H_{25}P_2^+$ $[M + H^+]^+$, 447.1386. Found: 447.1385.

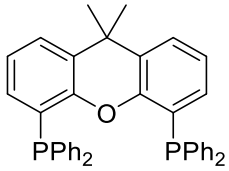


2at[12]:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2at** was afforded (85%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -10.10;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 7.7 Hz, 4H), 7.67 – 7.54 (m, 4H), 7.36 (td, *J* = 7.7, 1.1 Hz, 4H), 7.29 – 7.02 (m, 16H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.71 (d, J_{P-C} = 2.9 Hz, 2C), 142.62 (d, J_{P-C} = 2.6 Hz, 2C), 136.23 (d, J_{P-C} = 19.0 Hz, 4C), 132.73 (d, J_{P-C} = 20.1 Hz, 2CH), 130.51 (d, J_{P-C} = 21.9 Hz, 2CH), 129.32(s, 4CH), 128.72(s, 8CH), 128.72 (d, J_{P-C} = 7.6 Hz, 2CH), 127.65 (d, J_{P-C} = 7.6 Hz, 2CH), 121.44(s, 8CH). HRMS Calcd. For $C_{36}H_{29}P_2^+$ $[M + H^+]^+$, 523.1699. Found: 523.1698.

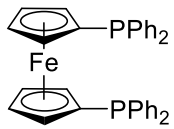


2au:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2au** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -16.86; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.17 (m, 22H), 6.99 (t, *J* = 7.4 Hz, 2H), 6.85 (m, 2H), 6.72 (dd, *J* = 8.0, 3.9 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ159.35

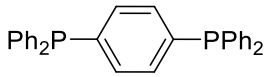
-118.07 (36C, aromatic carbons, observed complexity due to C-P splitting). HRMS Calcd. For $C_{36}H_{25}OP_2^+$ $[M + H^+]^+$, 539.1648. Found: 539.1647.



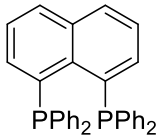
2av:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2av** was afforded (96%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -18.02; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.0 Hz, 2H), 7.20 (dd, *J* = 14.2, 6.8 Hz, 20H), 6.95 (d, *J* = 7.6 Hz, 2H), 6.54 (d, *J* = 7.4 Hz, 2H), 1.63 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.36 – 152.18 (m, 2C), 138.14 – 136.87 (m, 4C), 133.96 (t, J_{P-C} = 10.4 Hz, 8CH), 132.13(s, 2CH), 129.96(s, 2CH), 128.18 (dd, J_{P-C} = 6.2, 2.6 Hz, 8CH), 126.36(s, 4CH), 125.91 (dd, J_{P-C} = 11.1, 8.6 Hz, 2C), 123.37(s, 2CH), 34.49 (s, C), 31.87 (s, $2CH_3$). HRMS Calcd. For $C_{39}H_{33}OP_2^+$ $[M + H^+]^+$, 579.1961. Found: 579.1960.



2aw: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2aw** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -17.29; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (s, 30H), 4.28 (s, 5H), 4.02 (s, 5H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.91 (d, *J* = 9.9 Hz, 4C), 133.43 (d, *J* = 19.4 Hz, 8CH), 131.38 (d, *J* = 9.9 Hz, 2C), 128.48 (s, 4CH), 128.12 (d, *J* = 6.9 Hz, 8CH), 73.73 (d, *J* = 14.7 Hz, 4CH), 72.45 (d, *J* = 2.5 Hz, 4CH). HRMS Calcd. For $C_{34}H_{29}FeP_2^+$ $[M + H^+]^+$, 555.1049. Found: 555.1048.

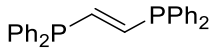


2ax[12]: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2aw** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -5.67; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (s, 20H), 7.31 – 7.23 (m, 4H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.03 (d, *J* = 12.2 Hz, 2C), 136.80 (d, *J* = 10.7 Hz, 4C), 133.89 (d, J_{P-C} = 20.0 Hz, 8CH), 133.52 (d, J_{P-C} = 6.2 Hz, 2CH), 133.33 (d, J_{P-C} = 6.2 Hz, 2CH), 128.90 (s, 4CH), 128.57 (d, J_{P-C} = 7.3 Hz, 8CH). HRMS Calcd. For $C_{30}H_{25}P_2^+$ $[M + H^+]^+$, 447.1386. Found: 447.1385.

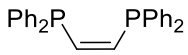


2ay[12]: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2a?** was afforded (75%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -14.69; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 6.3 Hz, 2H), 7.32 – 7.28 (m, 2H), 7.27 (d, *J* = 7.2 Hz, 2H), 7.21 – 7.15 (m,12H), 7.10 (m, 8H); ^{13}C NMR (101 MHz,

Chloroform-*d*) δ 140.12 (s, 4C), 137.88 (s, 2CH), 135.85 (t, J_{P-C} = 15.2 Hz, 2C), 134.64 – 134.31 (m, 2C), 133.77 (t, J_{P-C} = 21.1 Hz, 8CH), 131.46 (d, J_{P-C} = 9.3 Hz, 2C), 131.04 (s, 2CH), 128.19 (t, J_{P-C} = 3.4 Hz, 8CH), 127.81 (s, 4CH), 125.45 (s, 2CH). HRMS Calcd. For $C_{34}H_{27}P_2^+$ $[M + H^+]^+$, 497.1543. Found: 497.1542.

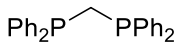


2az:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2az**[1] was afforded (47%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -7.59; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.28 (m, 8H), 7.27 – 7.22 (m, 12H), 6.65 (t, *J* = 4.04 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.00 – 141.33 (m, 2CH), 137.21 (dd, J_{P-C} = 5.8, 3.3 Hz, 4C), 133.70 – 132.98 (m, 8CH), 128.90 (s, 4CH), 128.60 (t, J_{P-C} = 3.5 Hz, 8CH). HRMS Calcd. For $C_{26}H_{23}P_2^+$ $[M + H^+]^+$, 397.1230. Found: 397.1229..

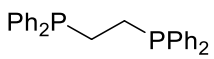


2az' :Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2az**[2] was afforded (40%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -23.20; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.33 (m, 8H), 7.31 (m, 12H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.56 (dd, *J* = 8.5, 7.0 Hz, 2CH), 138.62 (t, J_{P-C} = 3.4 Hz, 4C), 132.87 (t, J_{P-C} = 9.8 Hz, 8CH), 128.46 (s, 4CH), 128.41 (d, J_{P-C} = 2.9 Hz, 8CH). HRMS Calcd. For $C_{26}H_{23}P_2^+$ $[M + H^+]^+$, 397.1230. Found: 397.1228.

2ba: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2ba** was afforded (95%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -32.08; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (m, 8H), 7.47 – 7.29 (m, 12H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 135.77 (q, *J* = 4.9 Hz, 4C), 132.73 (d, *J* = 21.1 Hz, 8CH), 129.20(s, 4CH), 128.92 – 128.21 (m, 8CH), 107.60 – 106.26 (m, 2C). HRMS Calcd. For $C_{26}H_{21}P_2^+$ $[M + H^+]^+$, 395.1073. Found: 395.1072.

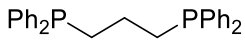


2bb: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2bc** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -22.40; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (dq, *J* = 6.5, 3.8 Hz, 8H), 7.30 (d, *J* = 3.0 Hz, 12H), 2.83 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.86 (t, J_{P-C} = 3.6 Hz, 4C), 132.87 (t, J_{P-C} = 10.3 Hz, 8CH), 128.73(s, 4CH), 128.42 (t, J_{P-C} = 3.5 Hz, 8CH), 28.10 (t, J_{P-C}= 22.9 Hz, CH_2). HRMS Calcd. For $C_{25}H_{23}P_2^+$ $[M + H^+]^+$, 385.1230. Found: 385.1229.

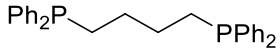


2bc: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2bd** was afforded (90%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -12.53; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 6.27 (m, 20H), 2.40 – 2.03 (m, 5H), 1.61 (dt, *J* = 15.4, 7.3 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.00 (t, J_{P-C}= 6.3 Hz, 4C), 132.78 (t, J_{P-C}= 9.3 Hz, 8CH), 128.74 (s, 4CH), 128.50 (t, J_{P-C}= 3.2 Hz, 8CH),

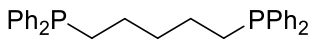
23.84 (d, J_{P-C} = 2.2 Hz, $2CH_2$). HRMS Calcd. For $C_{26}H_{25}P_2^+$ $[M + H^+]^+$, 399.1386. Found: 399.1386.



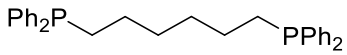
2bd:Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2be** was afforded (91%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -17.40; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 6.27 (m, 20H), 2.40 – 2.03 (m, 5H), 1.61 (dt, *J* = 15.4, 7.3 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.53 (d, J_{P-C} = 12.6 Hz, 4C), 132.73 (d, J_{P-C} = 18.4 Hz, 8CH), 128.55(s, 4CH), 128.42 (d, J_{P-C} = 6.8 Hz, 8CH), 29.64 (t, J_{P-C} = 12.2 Hz, $2CH_2$), 22.42 (t, J_{P-C} = 17.0 Hz, CH_2). HRMS Calcd. For $C_{27}H_{27}P_2^+$ $[M + H^+]^+$, 413.1543. Found: 413.1541.



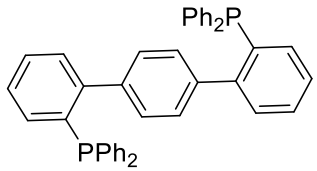
2be: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2bf** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -16.06; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.33 (m, 8H), 7.33 – 7.24 (m, 12H), 2.01 (t, *J* = 7.0 Hz, 4H), 1.59 – 1.27 (m, 4H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.73 (d, J_{P-C} = 12.9 Hz, 4C), 132.75 (d, J_{P-C} = 18.5 Hz, 8CH), 128.56(s,4CH), 128.43 (d, J_{P-C} = 6.9 Hz, 8CH), 27.76 (d, J_{P-C} = 11.3 Hz, $2CH_2$), 27.53 (d, J_{P-C} = 14.7 Hz, $2CH_2$). HRMS Calcd. For $C_{28}H_{29}P_2^+$ $[M + H^+]^+$, 427.1699. Found: 427.1698.



2bf: Reaction condition as **GP C** for preparation of compounds 2**a** (1.0 mmol), the white solid **2bg** was afforded (94%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -16.09; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.40 (td, *J* = 7.4, 3.2 Hz, 8H), 7.33 (d, *J* = 4.1 Hz, 12H), 2.05 – 1.89 (m, 4H), 1.61 – 1.49 (m, 2H), 1.49 – 1.36 (m, 4H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.85 (d, J_{P-C}= 12.6 Hz,4C), 132.72 (d, J_{P-C} = 18.3 Hz,8CH), 128.51 (s, 4CH), 128.40 (d, J_{P-C} = 6.6 Hz, 8CH), 32.61 (t, J_{P-C} = 12.9 Hz, CH), 27.83 (d, J_{P-C} = 11.1 Hz, 2CH), 25.54 (d, J_{P-C} = 16.1 Hz, 2CH). HRMS Calcd. For $C_{29}H_{31}P_2^+$ $[M + H^+]^+$, 441.1856. Found: 441.1855.



2bg: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2bh** was afforded (88%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -16.03; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.43 (td, *J* = 7.4, 3.3 Hz, 8H), 7.34 (q, *J* = 3.2, 2.1 Hz, 12H), 2.25 – 1.70 (m, 4H), 1.43 (d, *J* = 3.0 Hz, 8H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.79 (d, J_{P-C} = 12.2 Hz, 4C), 132.71 (d, J_{P-C} = 18.3 Hz, 8CH), 128.51 (s, 4CH), 128.39 (d, J_{P-C} = 6.6 Hz, 8CH), 30.80 (d, J_{P-C} = 12.8 Hz, $2CH_2$), 27.94 (d, J_{P-C}= 10.7 Hz, $2CH_2$), 25.83 (d, J_{P-C} = 15.9 Hz, $2CH_2$). HRMS Calcd. For $C_{30}H_{33}P_2^+$ $[M + H^+]^+$, 455.2012. Found: 455.2011.



2bh[12]: Reaction condition as **GP C** for preparation of compounds **2a** (1.0 mmol), the white solid **2bh** was afforded (82%); ^{31}P NMR (162 MHz, Chloroform-*d*) δ -13.08; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 4H), 7.22 – 7.11 (m, 22H), 6.99 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.07 (d, *J* = 28.2 Hz, 2C), 140.44 (d, *J* = 6.0 Hz, 2C), 137.78 (d, *J* = 12.3 Hz, 4C), 136.15 (d, *J* = 14.9 Hz, 2C), 134.04 (d, *J* = 20.0 Hz, 8CH), 134.03 (s, 2CH), 129.04 (d, *J* = 4.0 Hz, 4CH), 128.68 (s, 2CH), 128.45 (d, *J* = 3.0 Hz, 8CH), 128.37 (s, 2CH), 127.31 (s, 2CH). HRMS Calcd. For $C_{42}H_{33}P_2^+$ $[M + H^+]^+$, 599.2013. Found: 599.2012.

7. Reference

(1) R. Nishio, M. Sugiura and S. Kobayashi, *Org. Lett.*, **2005**, *7*, 4831−4834.

(2) Y. Li, S. Das, S. Zhou, K. Junge and M. Beller, *J. Am. Chem. Soc.*, **2012**, *134*, 9727−9732.

(3) S. Pucciarelli and S. Vincenzetti, *Int. J. Mol. Sci.*, **2019**, *20*, 1802.

(4) C. M. Whitaker, K. L. Kotta and R. J. McMahon, *J. Org. Chem.*, **1995**, *60*, 3499−3503.

(5) H. Adams, R. C. Collins, S. Jones and C. J. A. Warner, *Org. Lett.*, **2011**, *13*, 6576−6579.

(6) S. Booyens, A. Roodt and O. F. Wendt, *J. Org. Chem.*, **2007**, *692*, 5508−5511.

(7) H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda and T. Mita, *Nat. Commun.*, **2022**, *13*, 7034.

(8) S. Burck and D. Förster, *Chem. Commun.*, **2006**, *26*, 2810−2812.

(9) T. Wiegand and H. Eckert, *J. Am. Chem. Soc.*, **2012**, *134*, 4236−4249

(10) S. Jin and G. C. Haug, *ACS Catal.*, **2019**, *9*, 9764−9774.

(11) M. Alame, M. Jahjah, M. Berthod, M. Lemaire and C. de Bellefon, *J. Mol. Catal. A: Chem.*, **2007**, *268*, 205−212.

(12) D. Van Allen and D. Venkataraman, *J. Org. Chem.*, **2003**, *68*, 4590−4593.

(13) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16 Rev. A.03 (Gaussian Inc., **2016**)

(14) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623–11627.

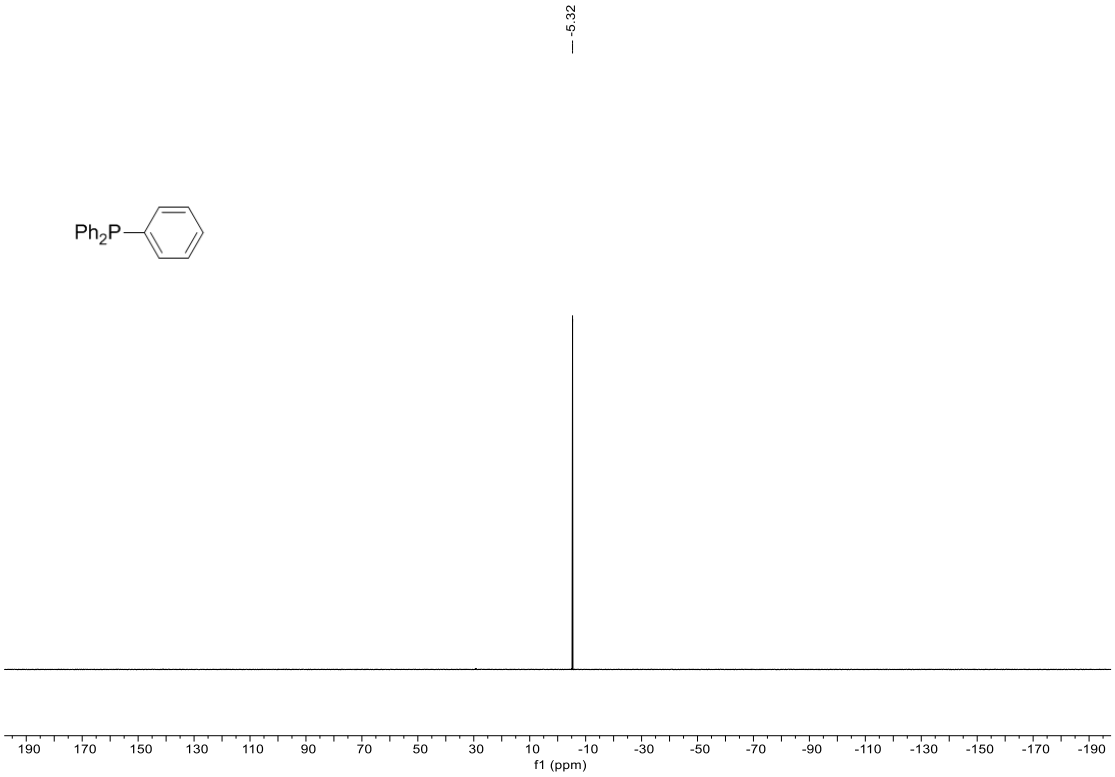
(15) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785–789.

(16) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*. **2010**, 132, 154104.

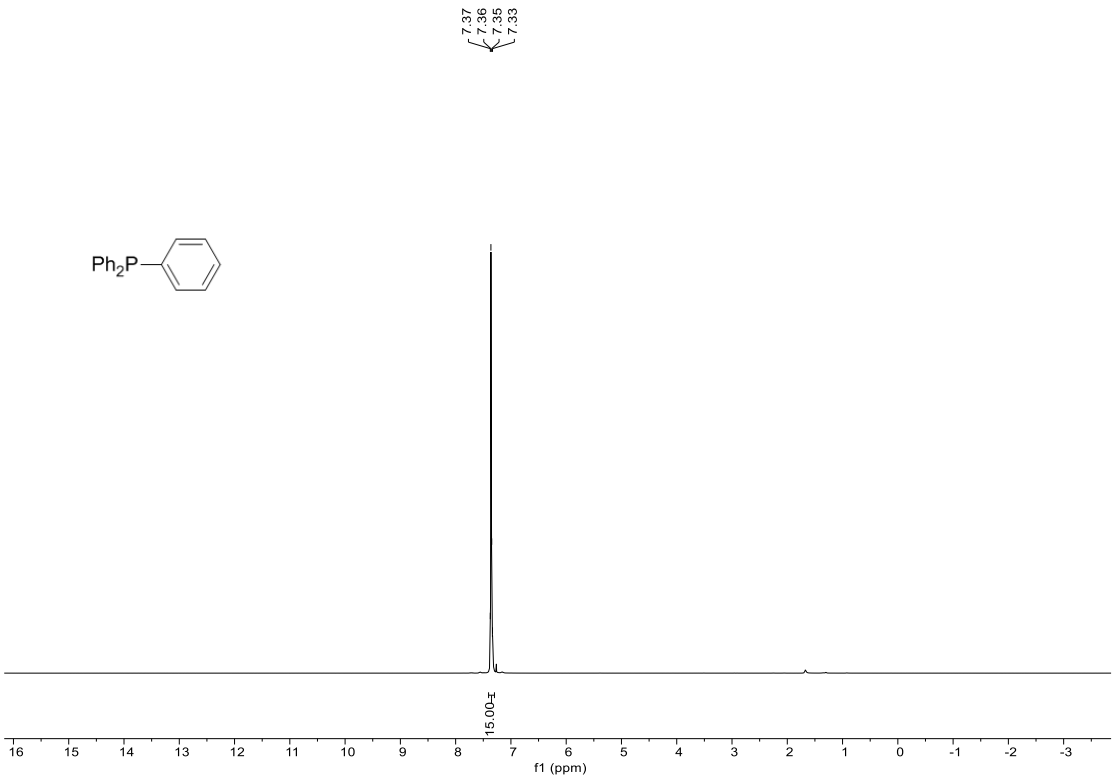
(17) S. Grimme, *J. Comput. Chem.* **2006**, *27*, 1787–1799.

(18) S. Grimme, *J. Comput. Chem.* **2004**, *25*, 1463–1473.

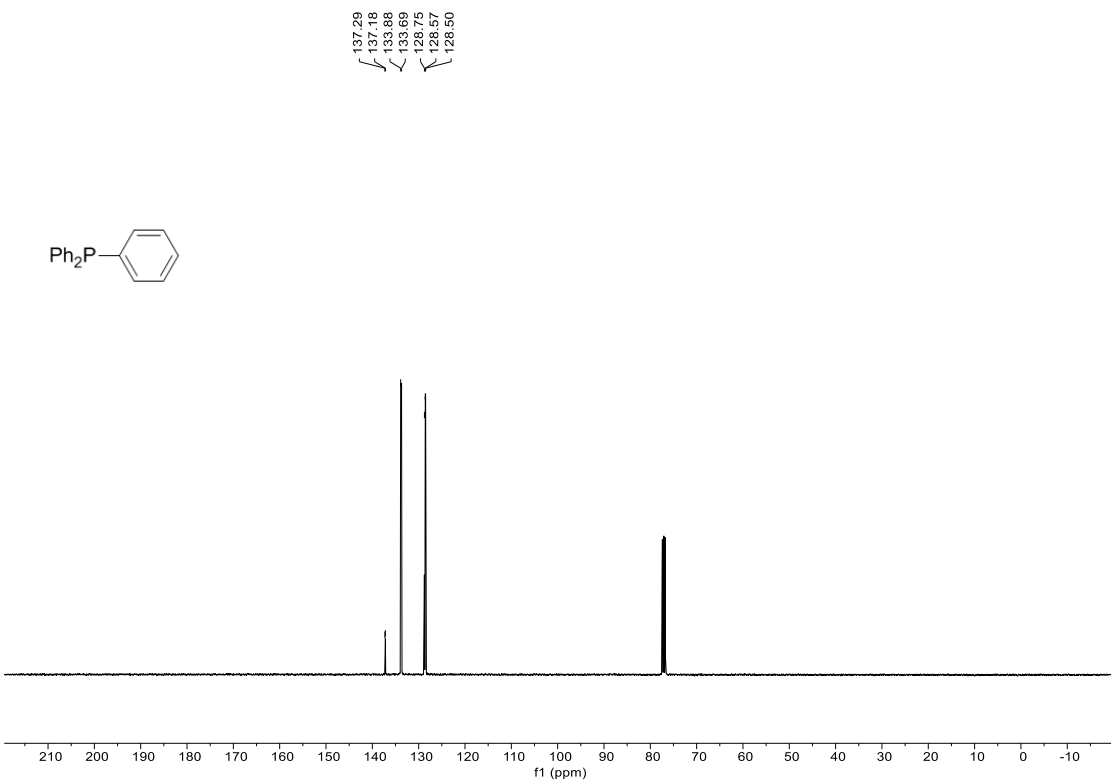
8. Copies of ^{31}P-NMR, ^{1}H-NMR, ^{13}C-NMR Spectra of compounds **2**.



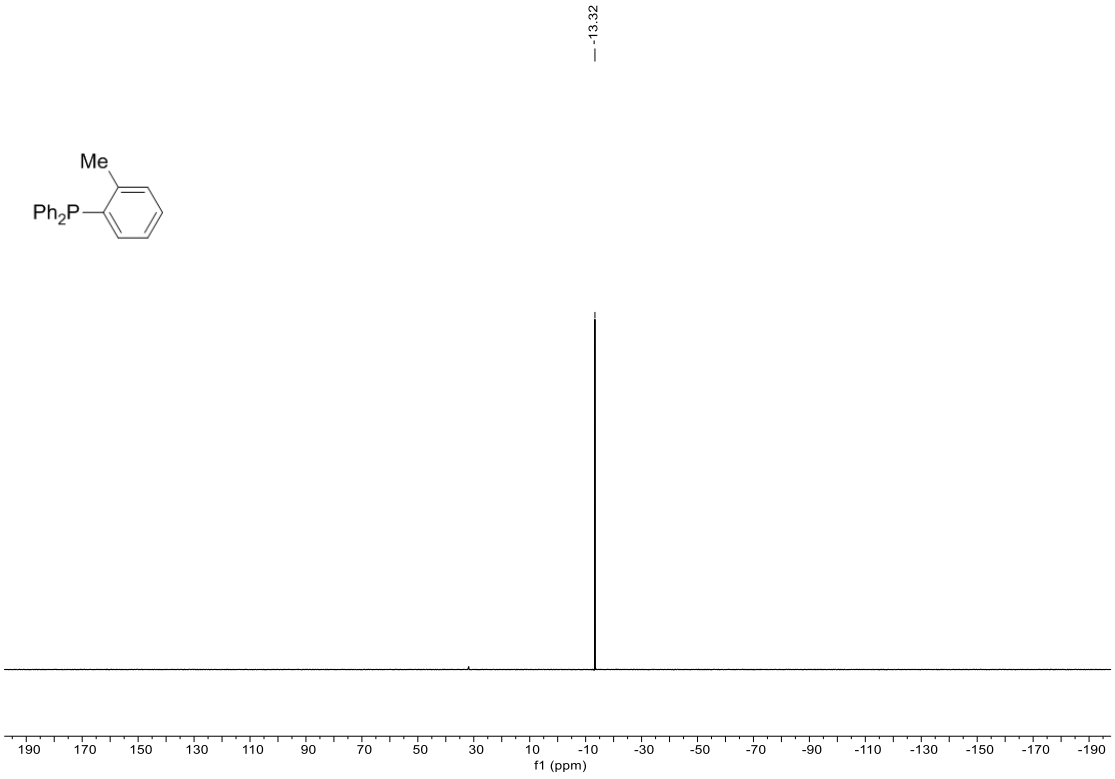
^{31}P NMR (162 MHz, $CDCl_3$) of **2a**



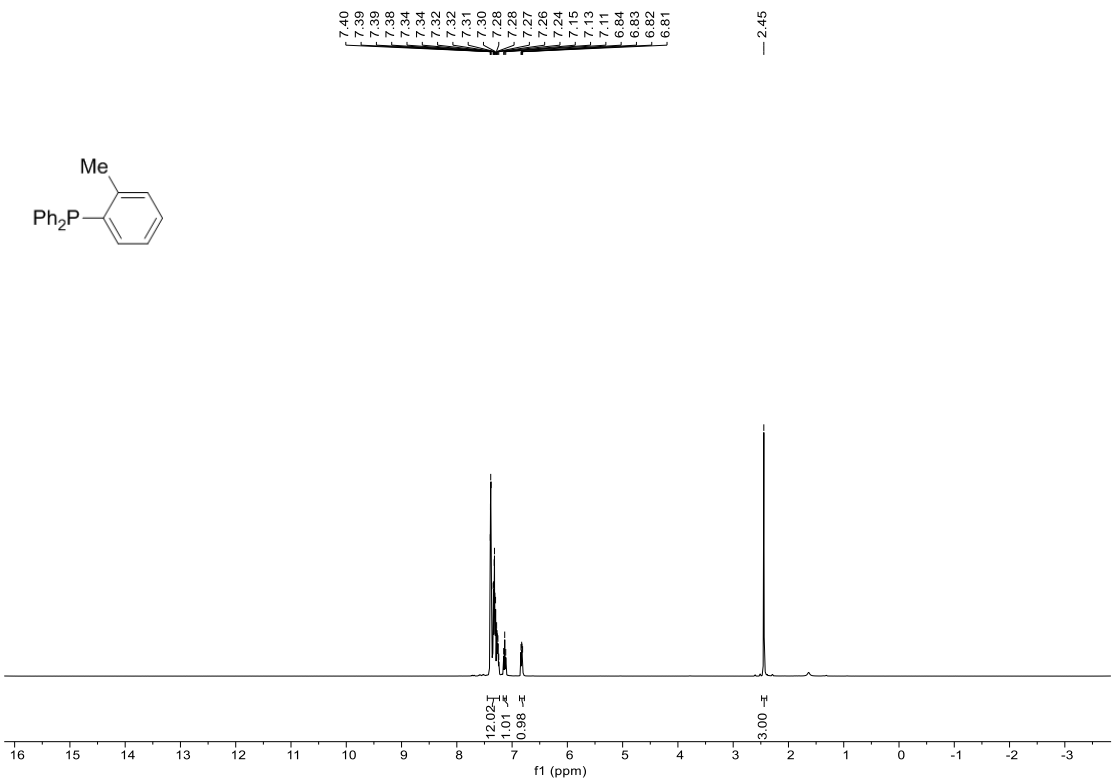
^{1}H NMR (400 MHz, $CDCl_3$) of **2a**



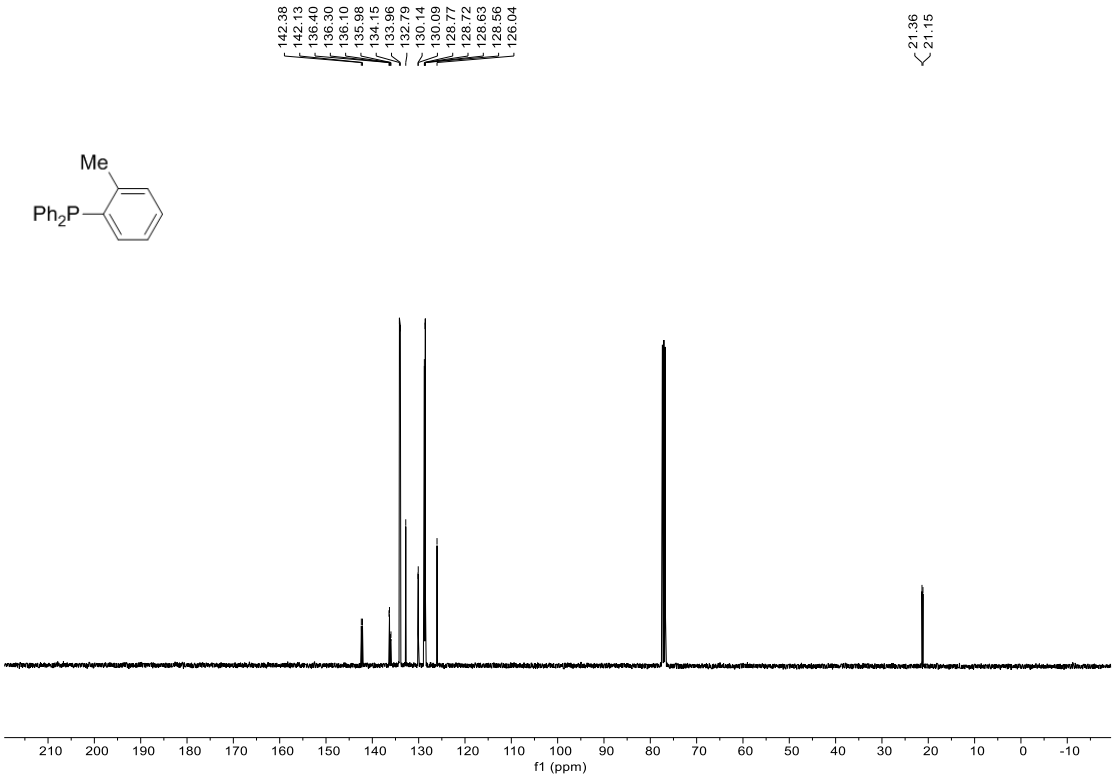
^{13}C NMR ((101 MHz, $CDCl_3$) of **2a**



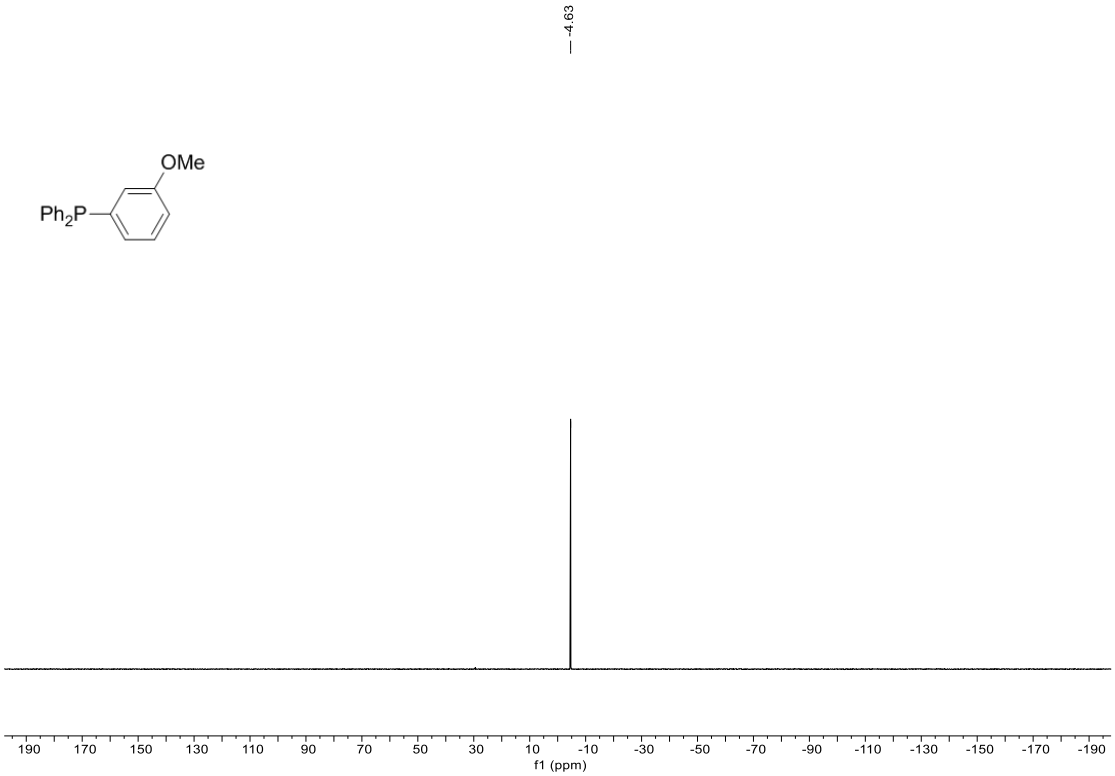
^{31}P NMR (162 MHz, $CDCl_3$) of **2b**



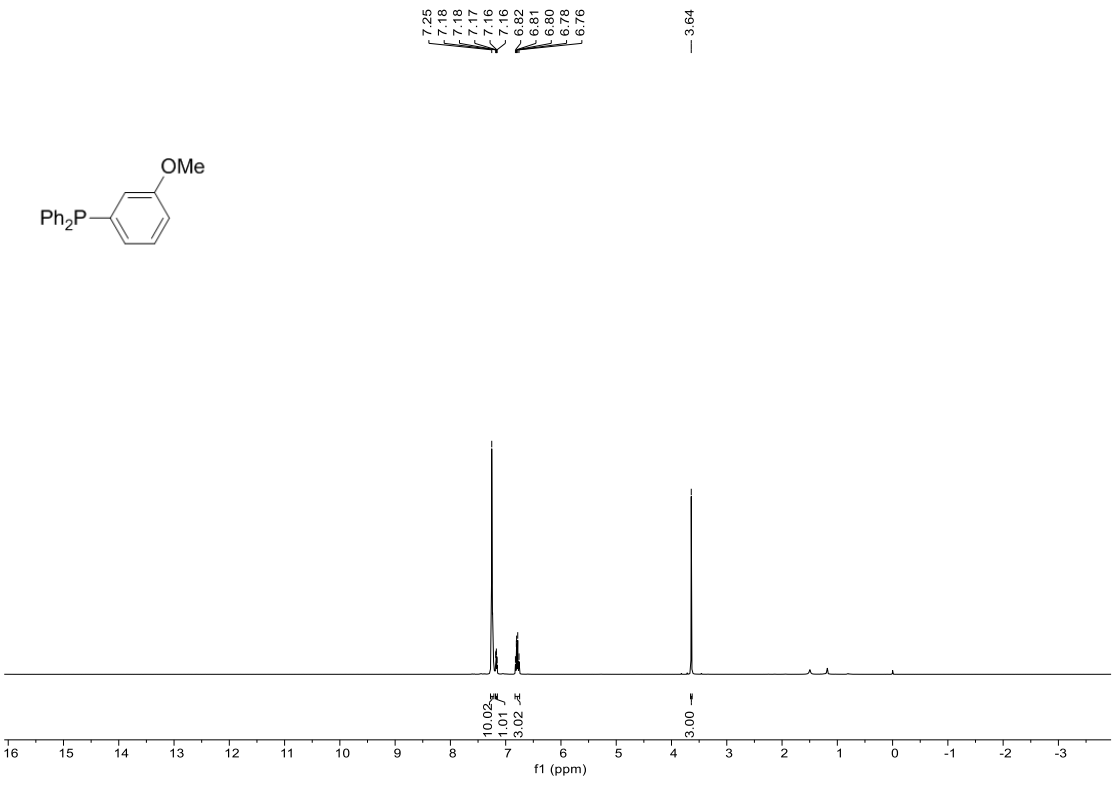
^{1}H NMR (400 MHz, $CDCl_3$) of **2b**



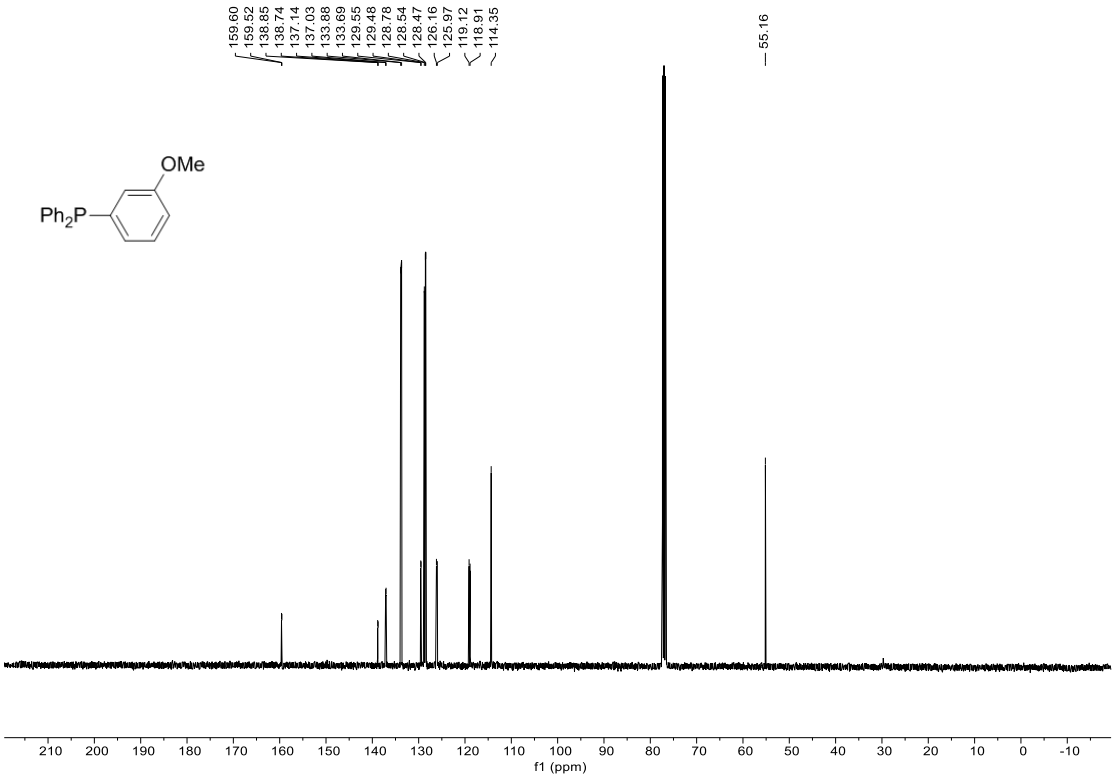
^{13}C NMR ((101 MHz, $CDCl_3$) of **2b**



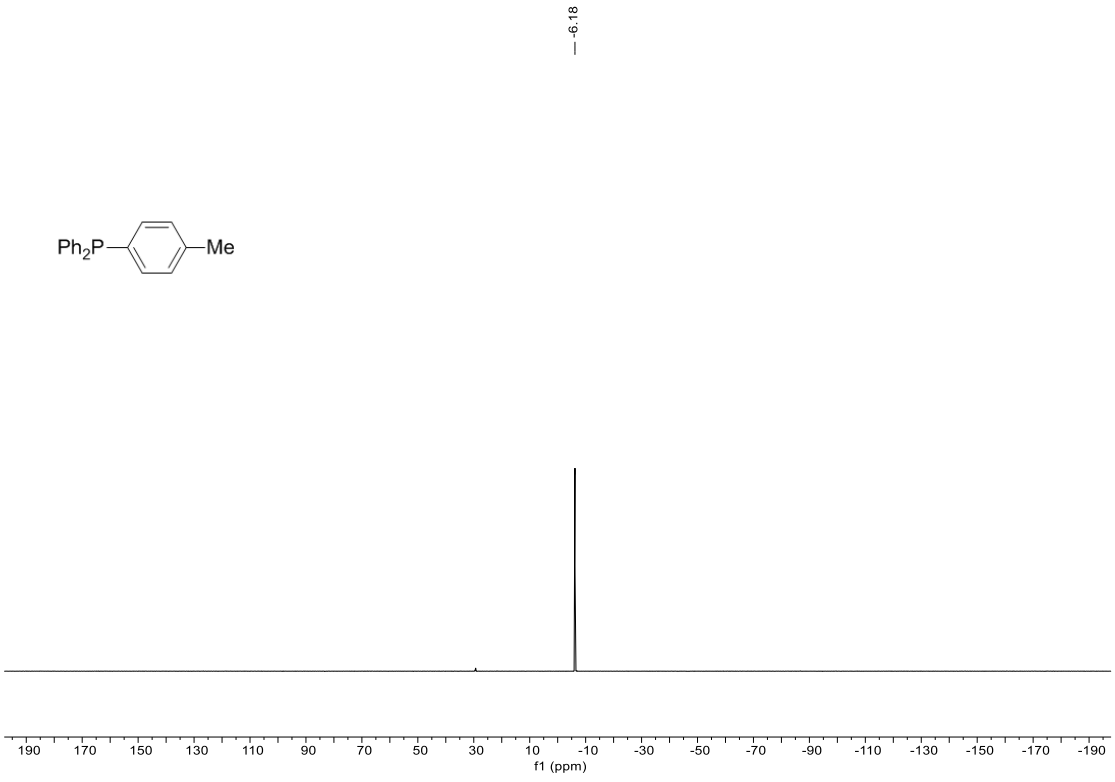
^{31}P NMR (162 MHz, $CDCl_3$) of **2c**



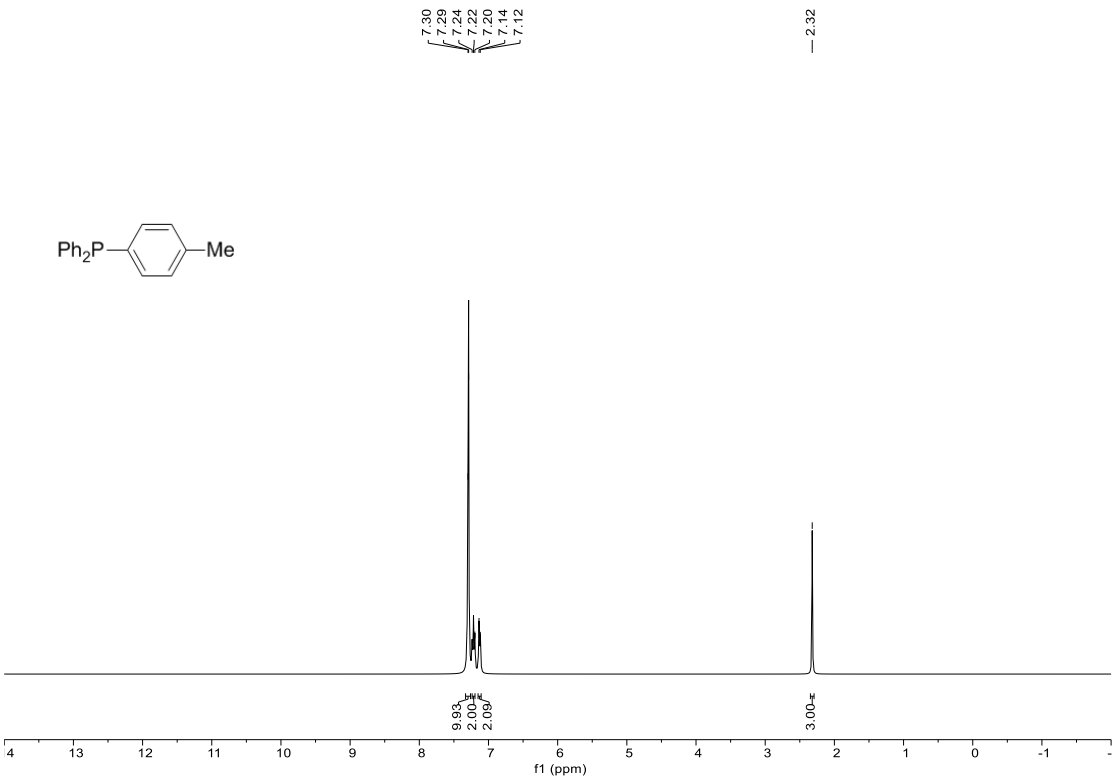
^{1}H NMR (400 MHz, $CDCl_3$) of **2c**



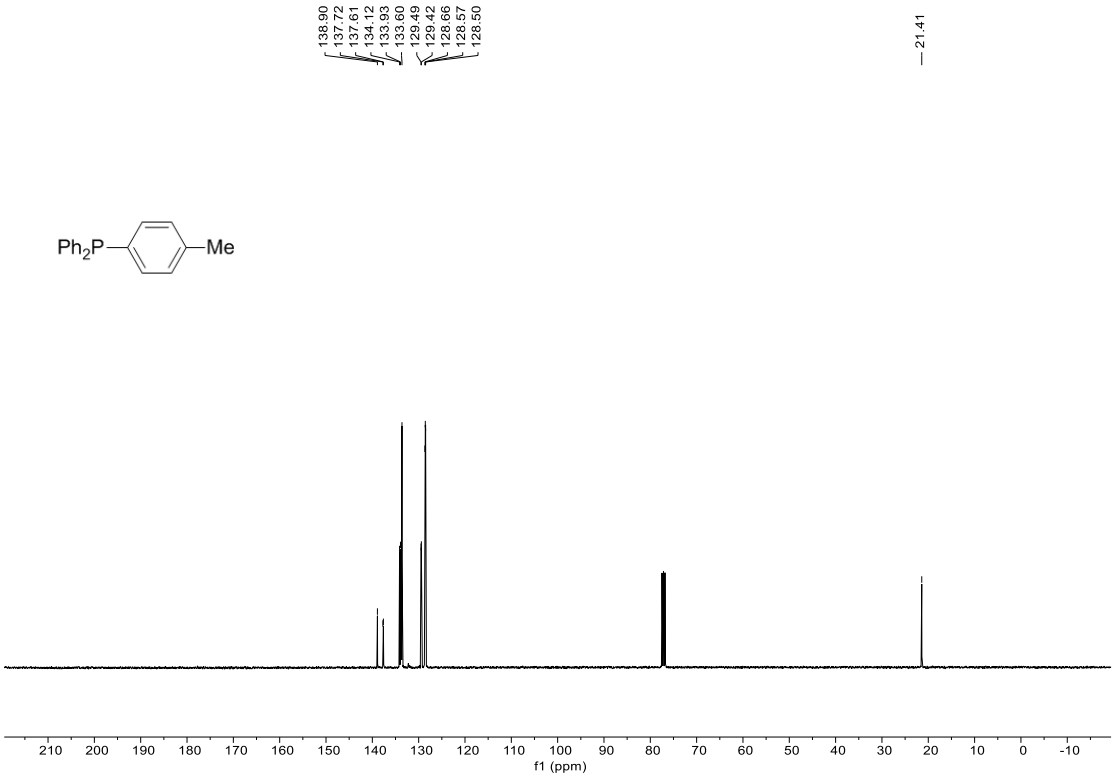
^{13}C NMR (101 MHz, $CDCl_3$) of **2c**



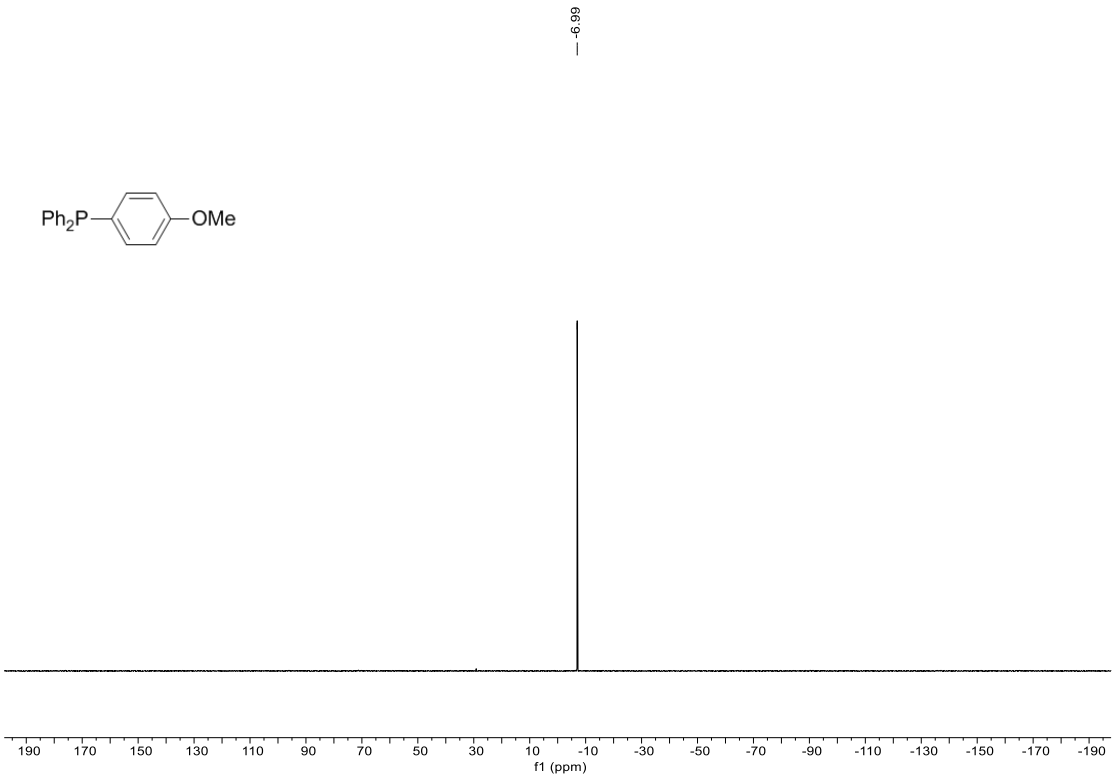
^{31}P NMR (162 MHz, $CDCl_3$) of **2d**



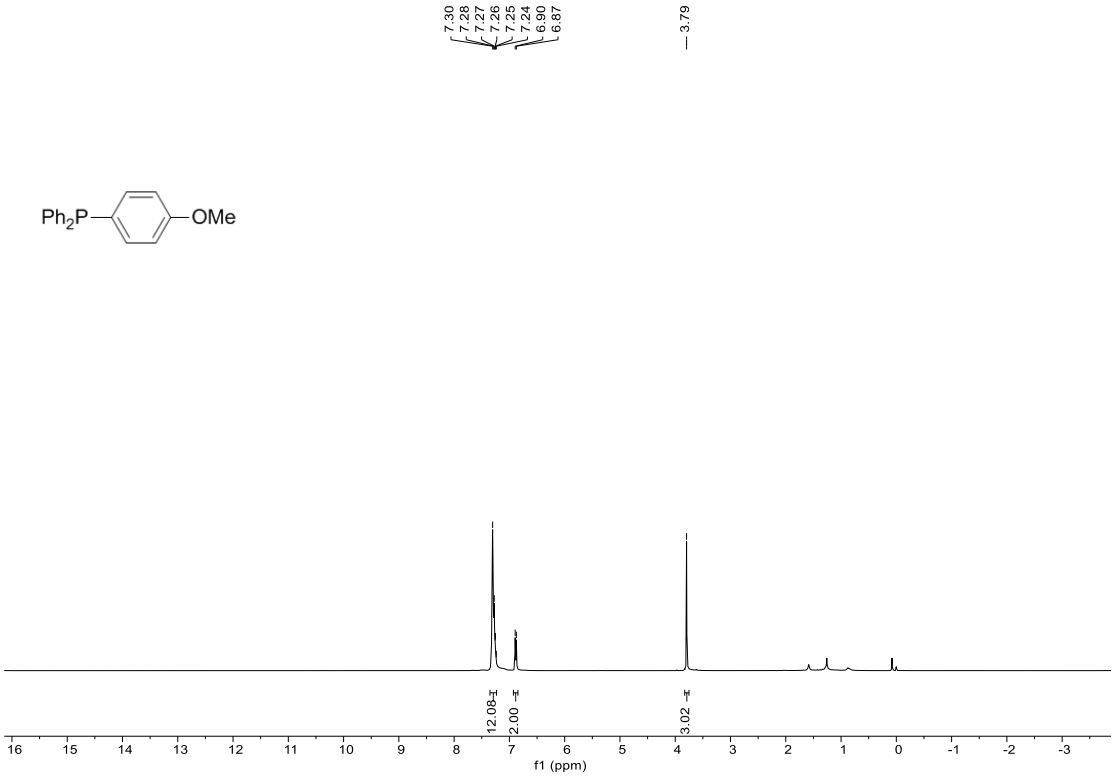
^{1}H NMR (400 MHz, $CDCl_3$) of **2d**



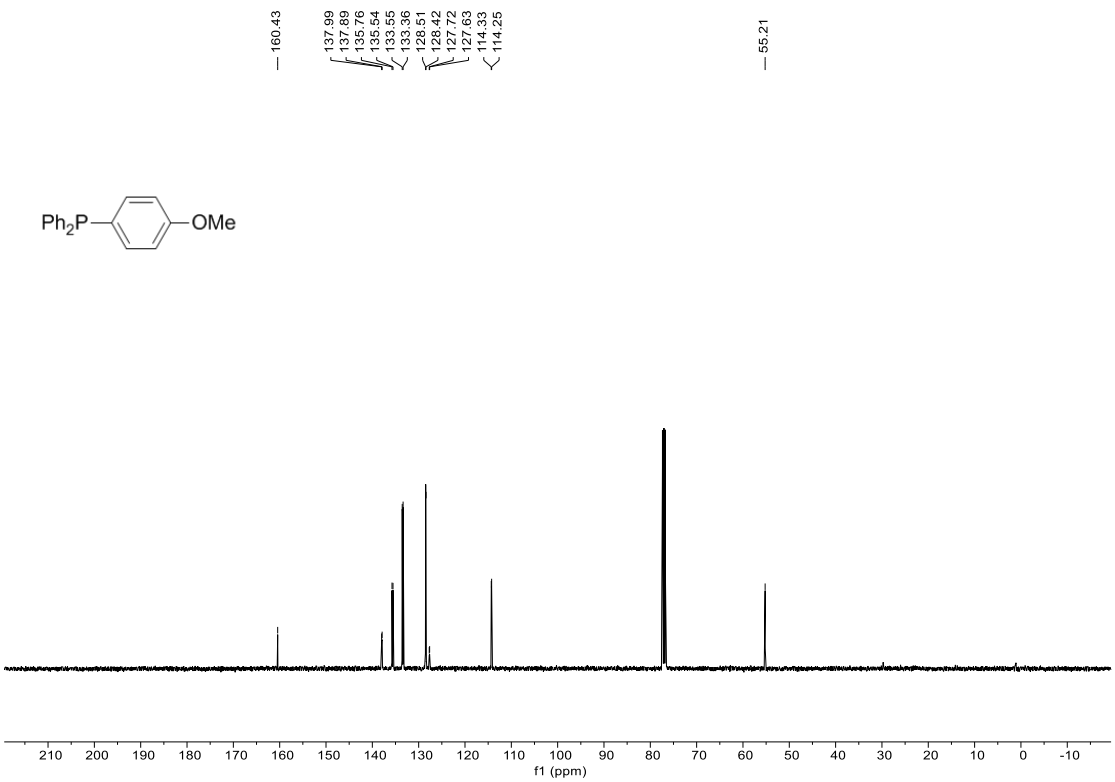
^{13}C NMR (101 MHz, $CDCl_3$) of **2d**



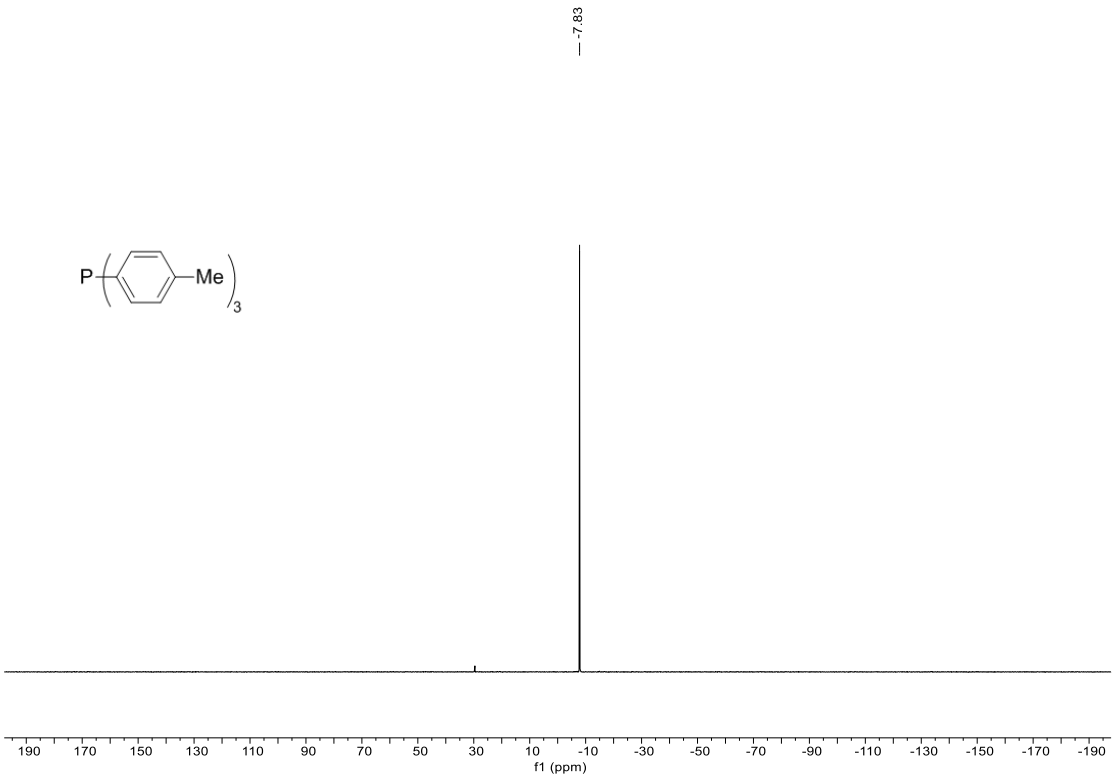
^{31}P NMR (162 MHz, $CDCl_3$) of 2**e**



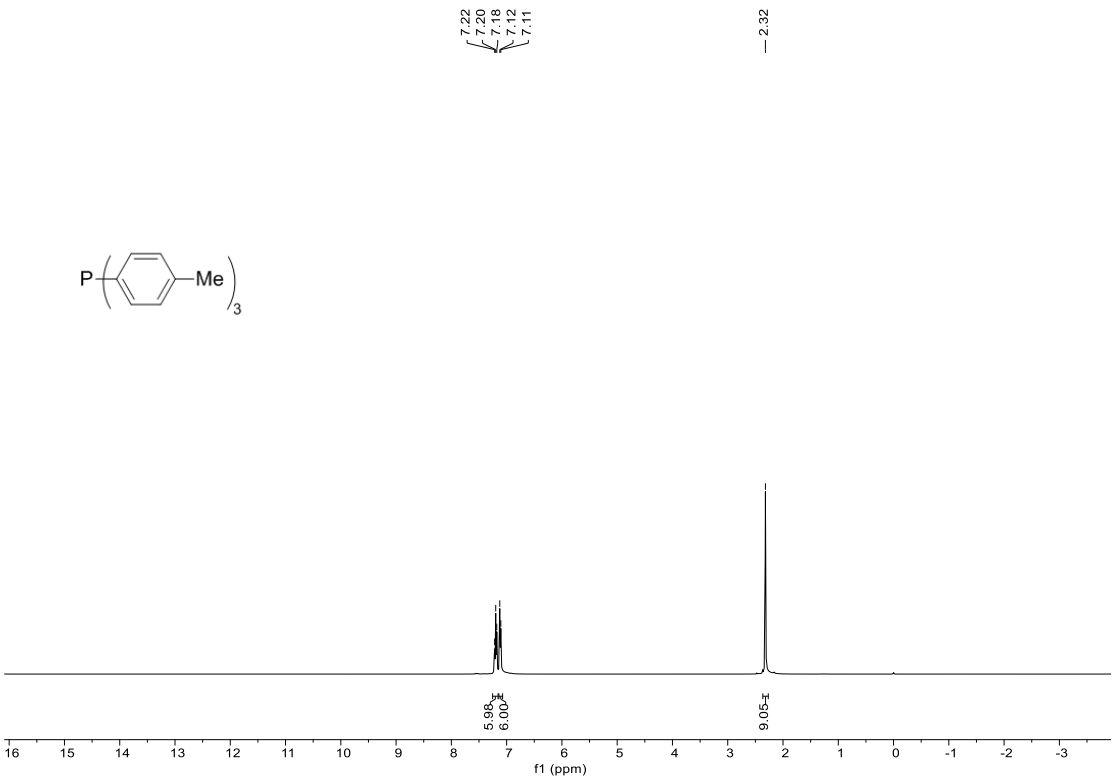
^{1}H NMR (400 MHz, $CDCl_3$) of **2e**



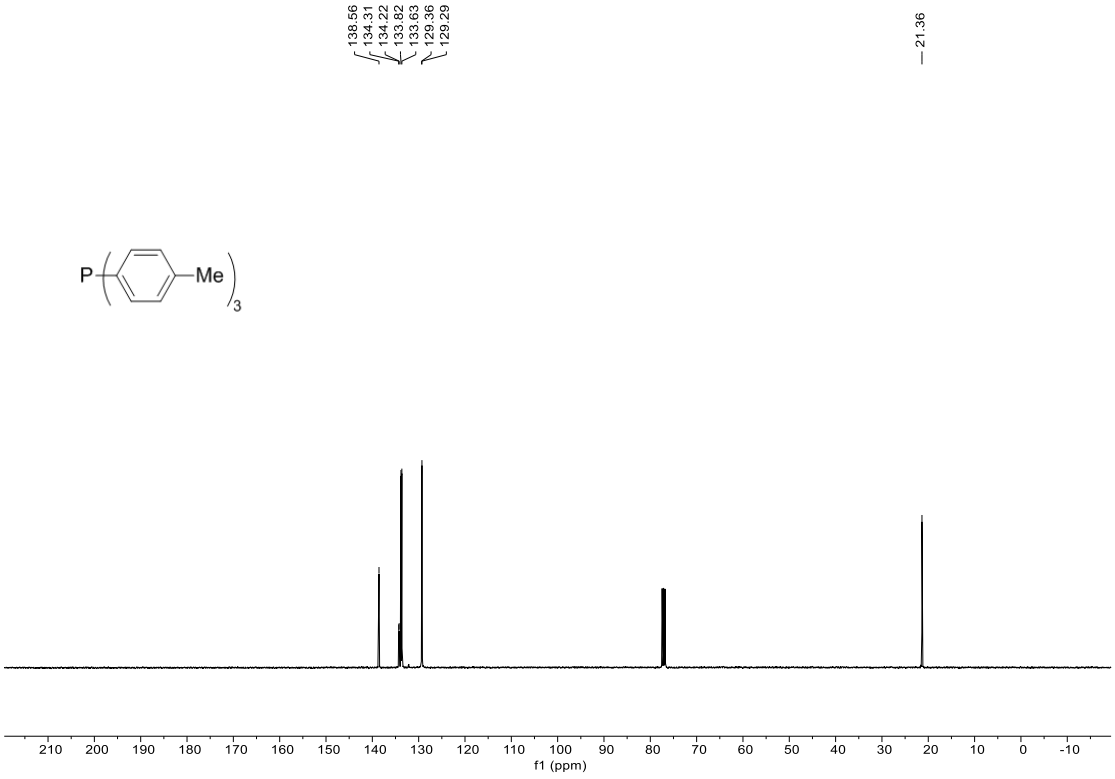
^{13}C NMR (101 MHz, $CDCl_3$) of **2e**



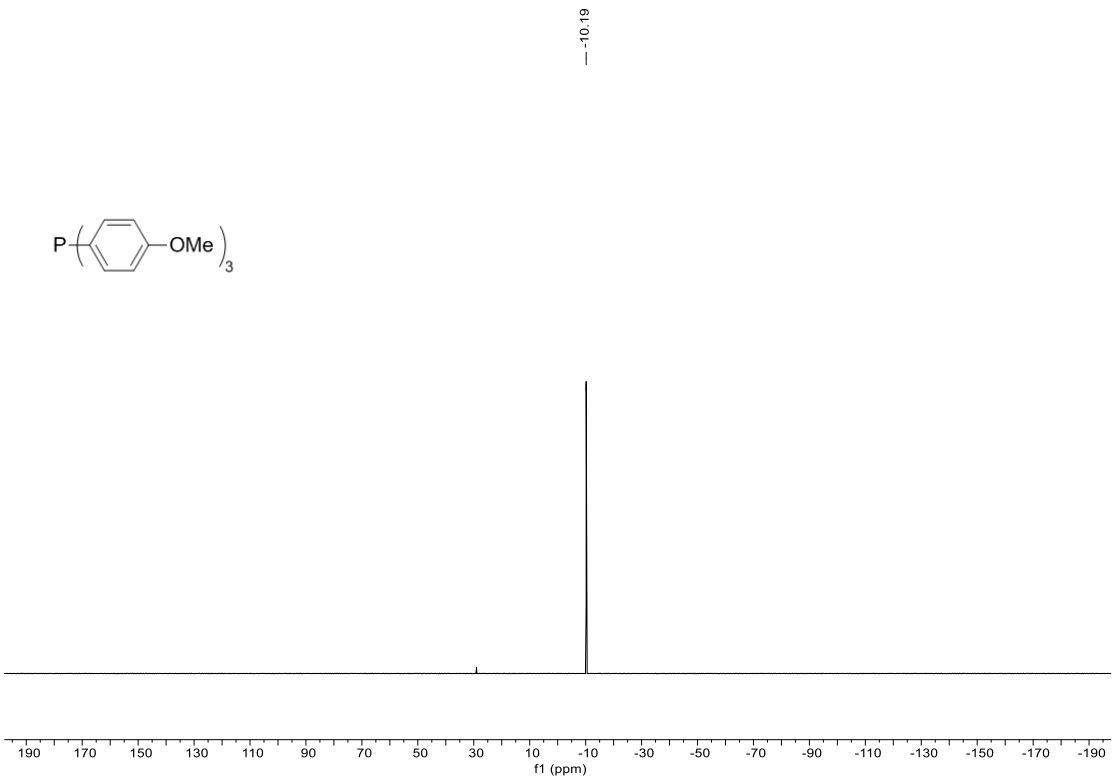
^{31}P NMR (162 MHz, $CDCl_3$) of **2f**



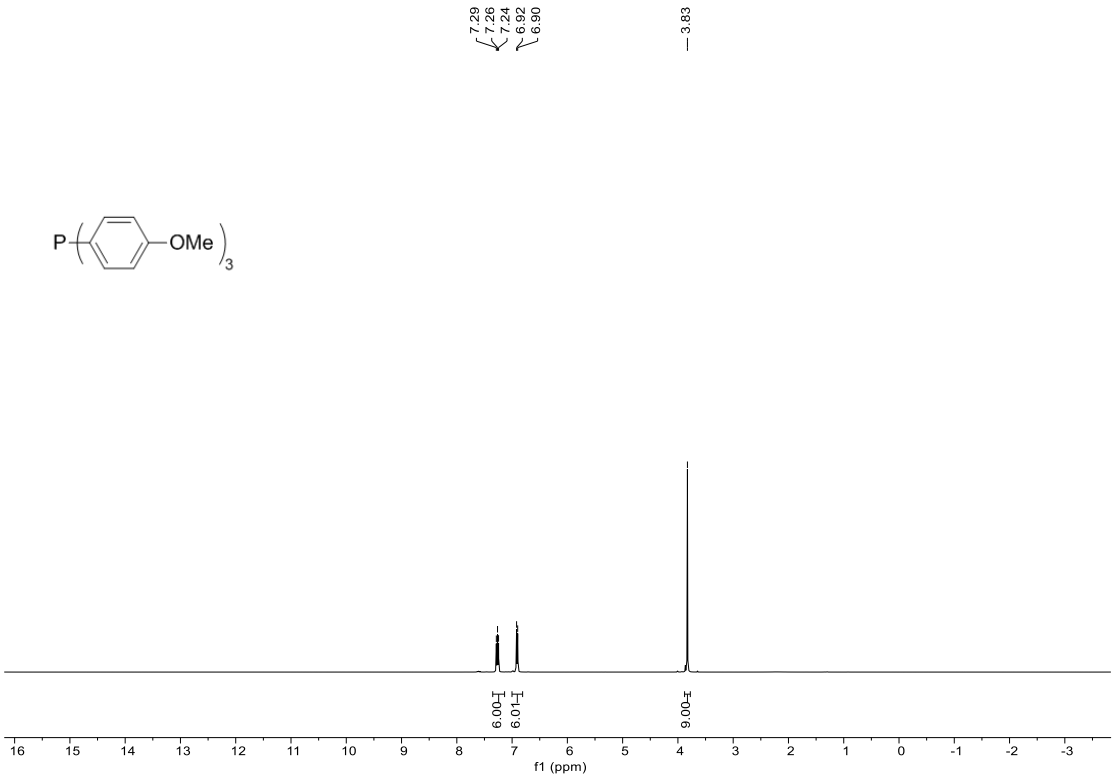
^{1}H NMR (400 MHz, $CDCl_3$) of **2f**



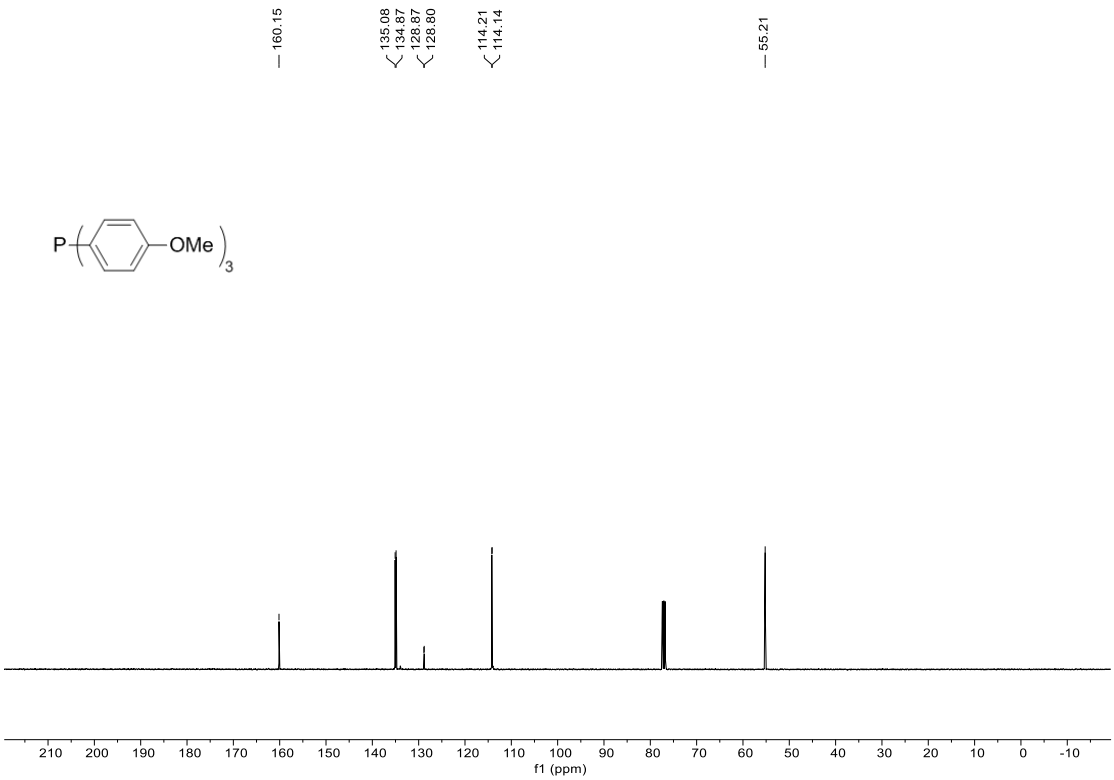
^{13}C NMR (101 MHz, $CDCl_3$) of **2f**



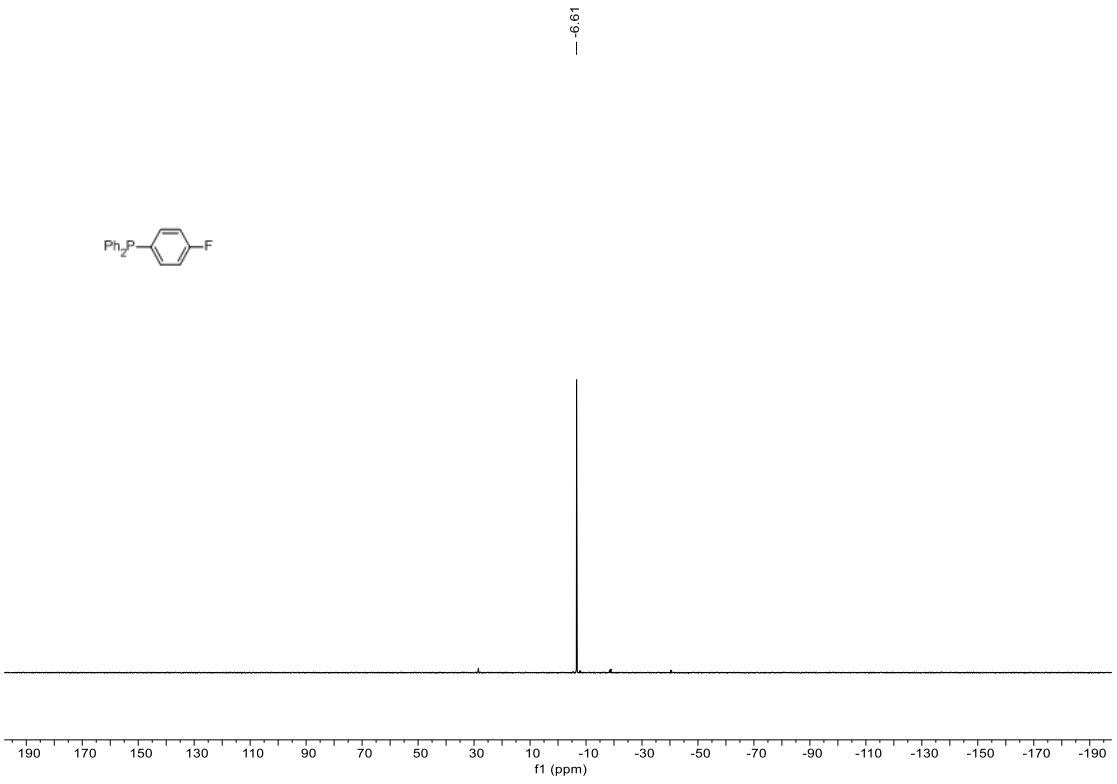
^{31}P NMR (162 MHz, $CDCl_3$) of **2g**



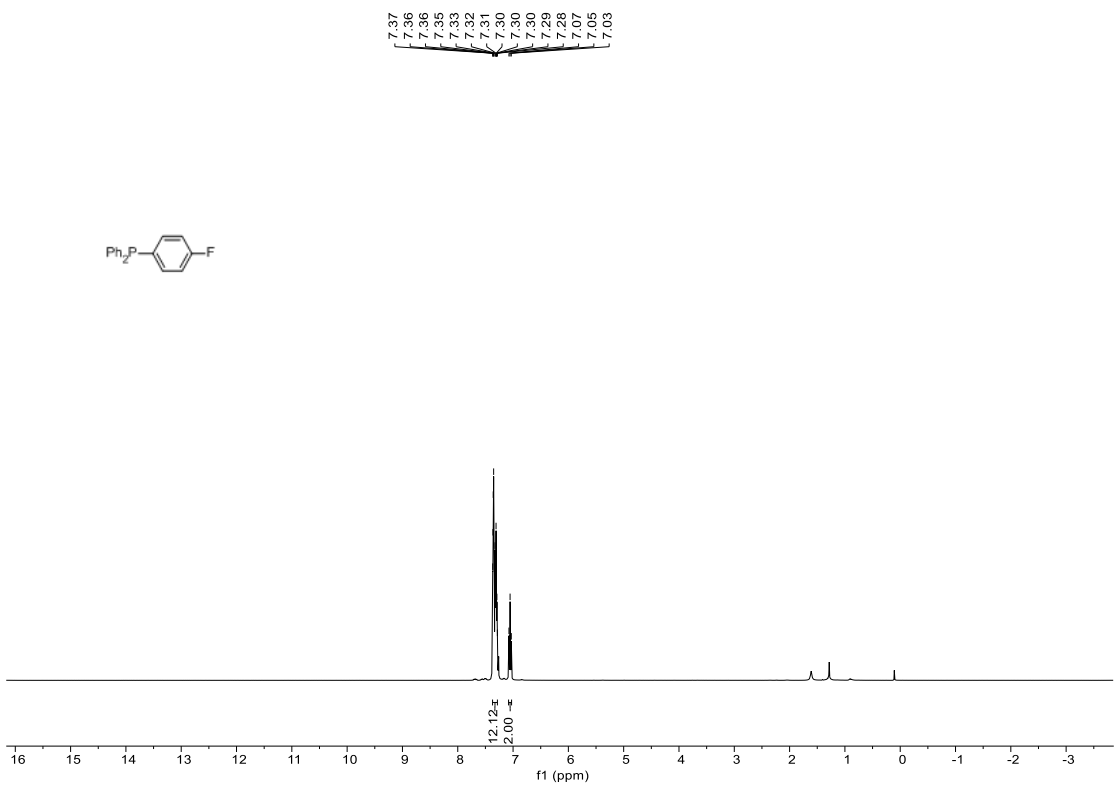
^{1}H NMR (400 MHz, $CDCl_3$) of **2g**



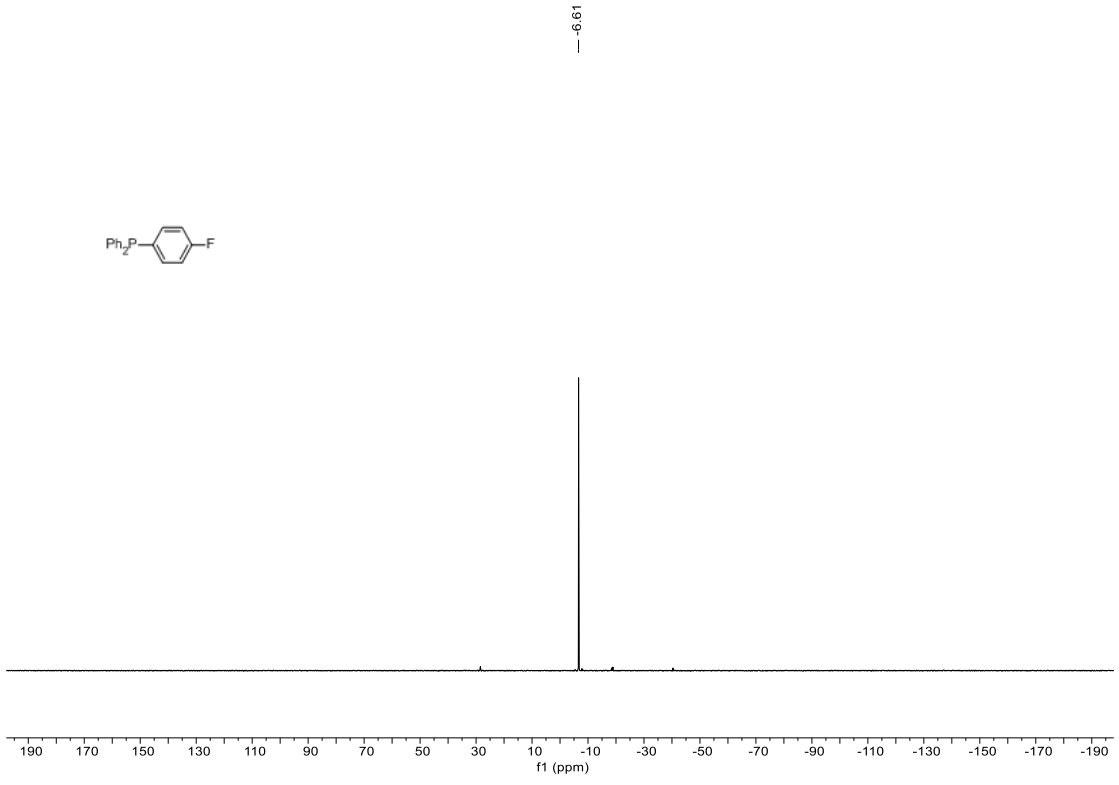
^{13}C NMR (101 MHz, $CDCl_3$) of **2g**



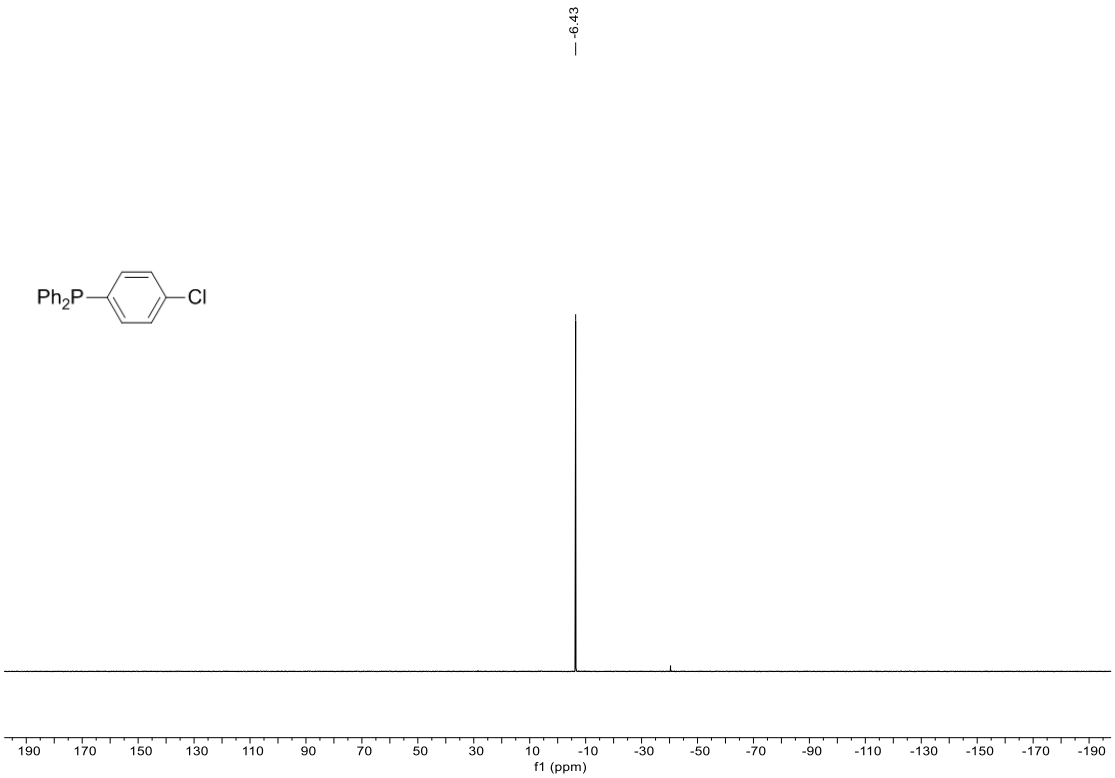
^{31}P NMR (162 MHz, $CDCl_3$) of **2h**



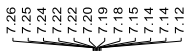
^{1}H NMR (400 MHz, $CDCl_3$) of **2h**

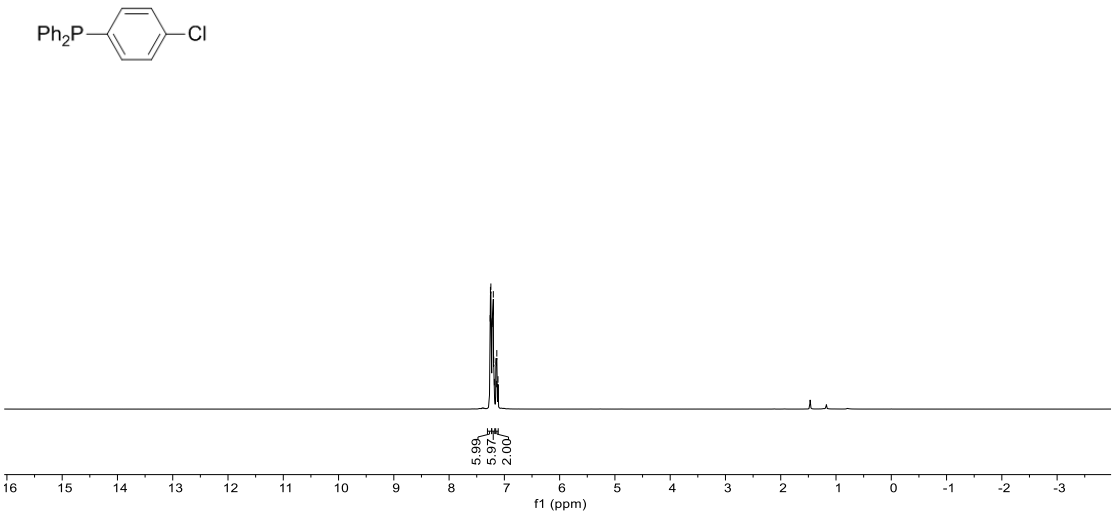


^{13}C NMR (101 MHz, $CDCl_3$) of **2h**

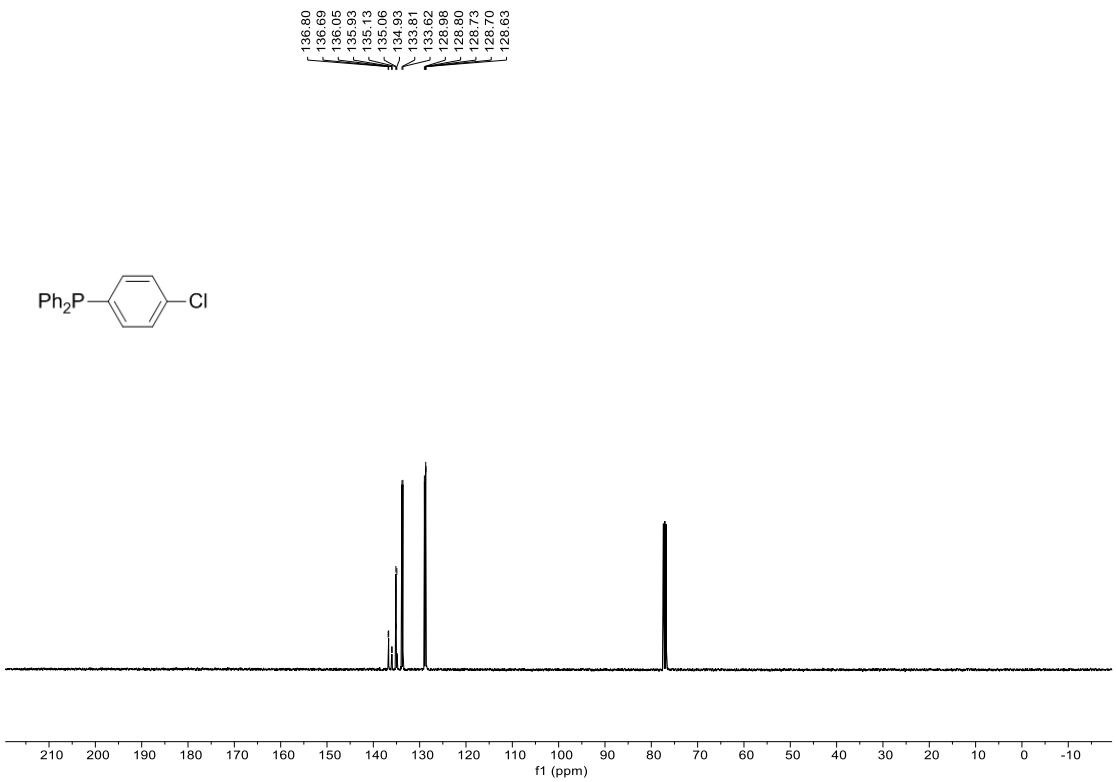


^{31}P NMR (162 MHz, $CDCl_3$) of **2i**

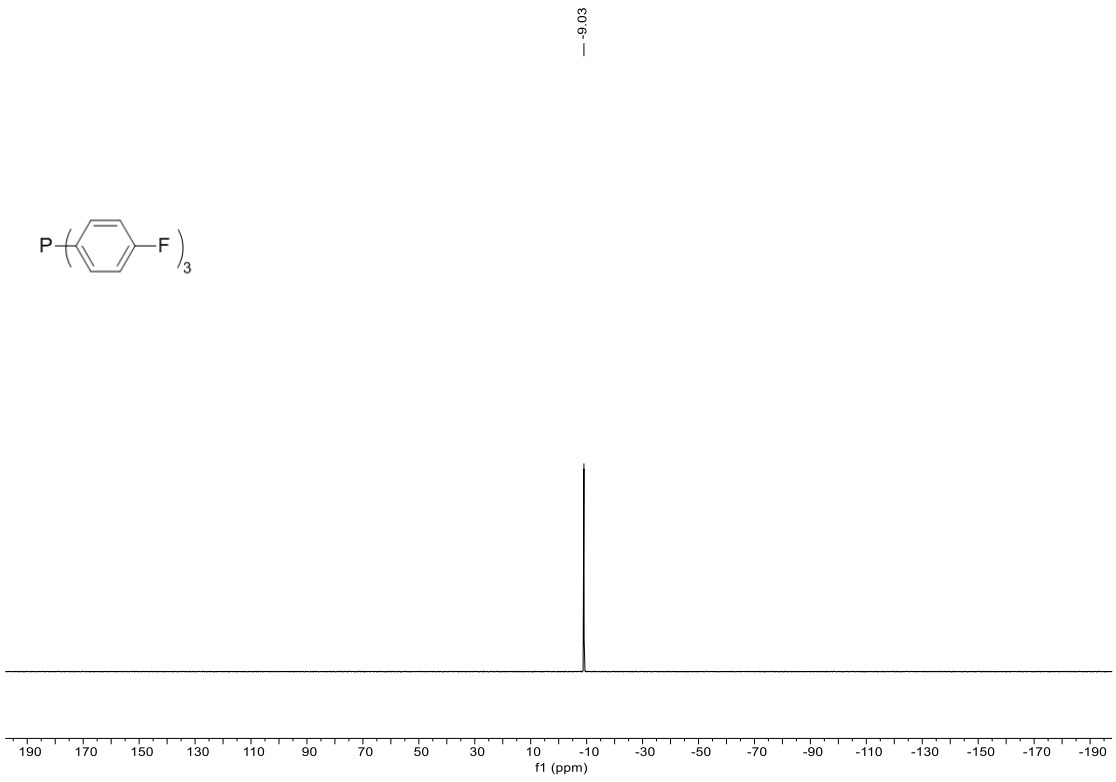




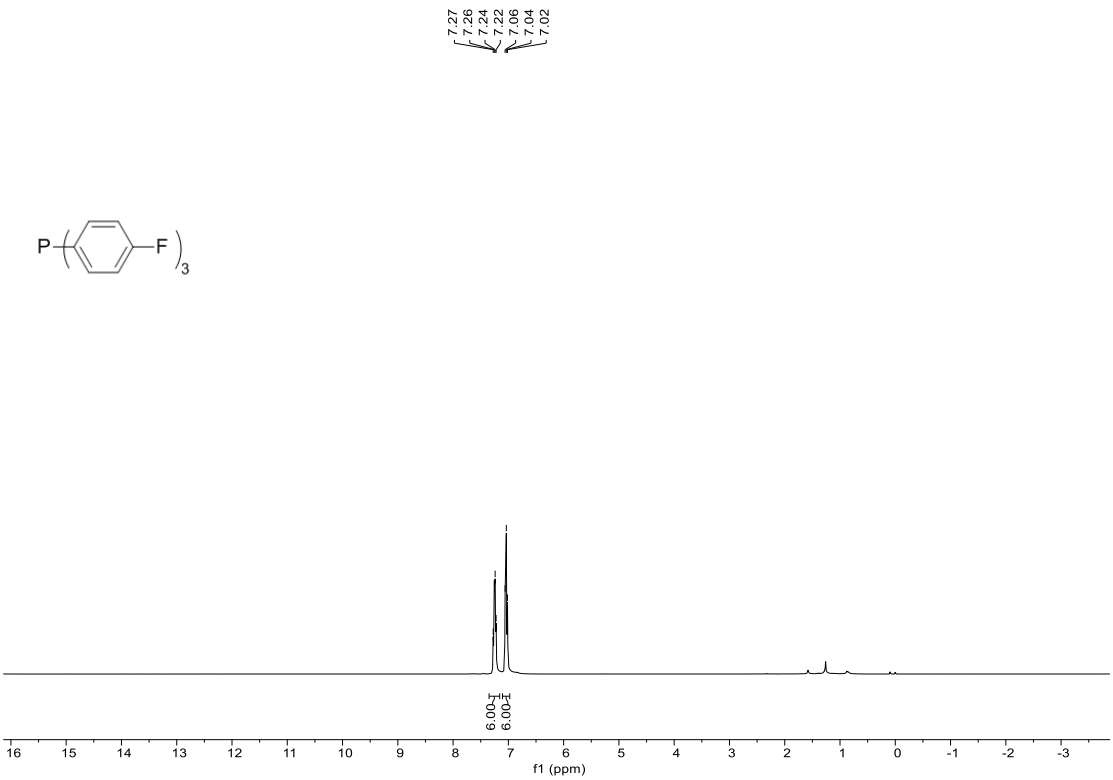
^{1}H NMR (400 MHz, $CDCl_3$) of **2i**



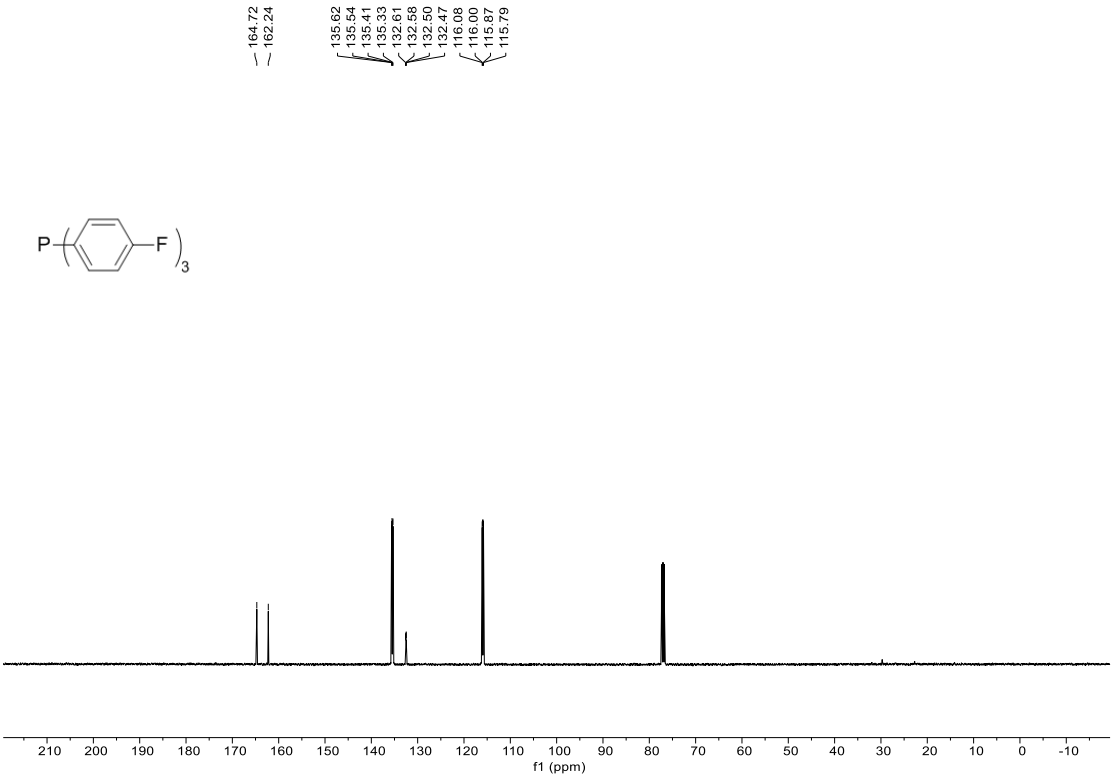
^{13}C NMR (101 MHz, $CDCl_3$) of **2i**



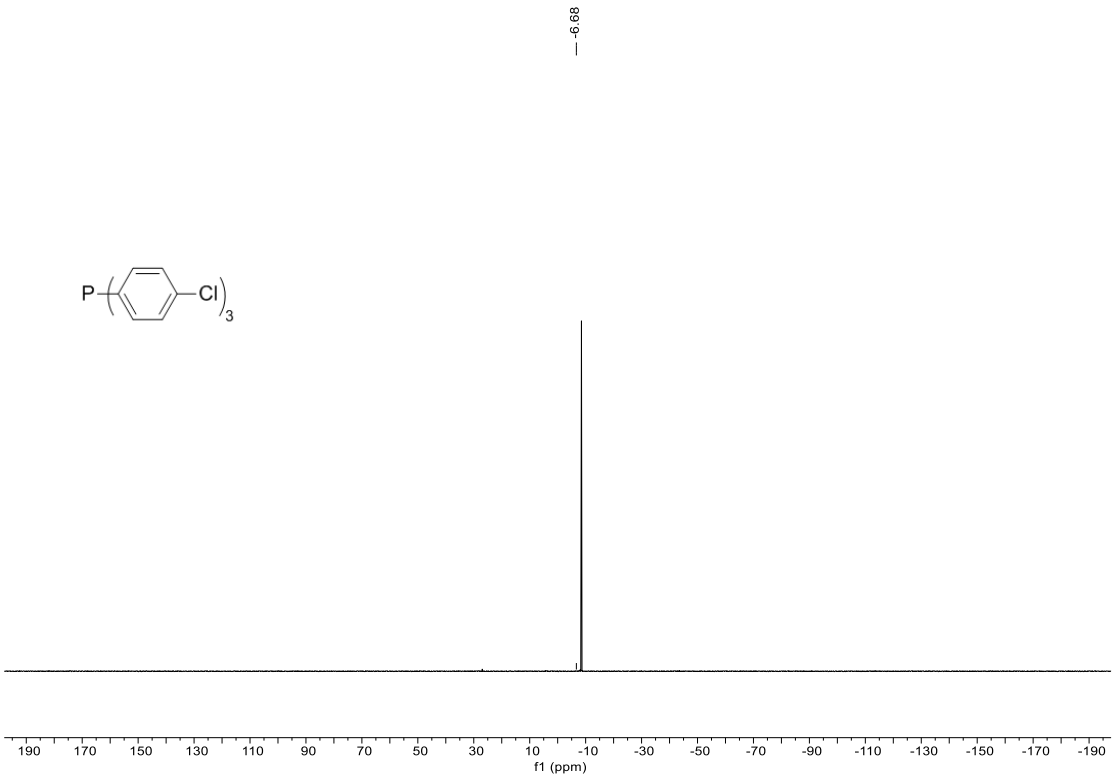
^{31}P NMR (162 MHz, $CDCl_3$) of **2j**



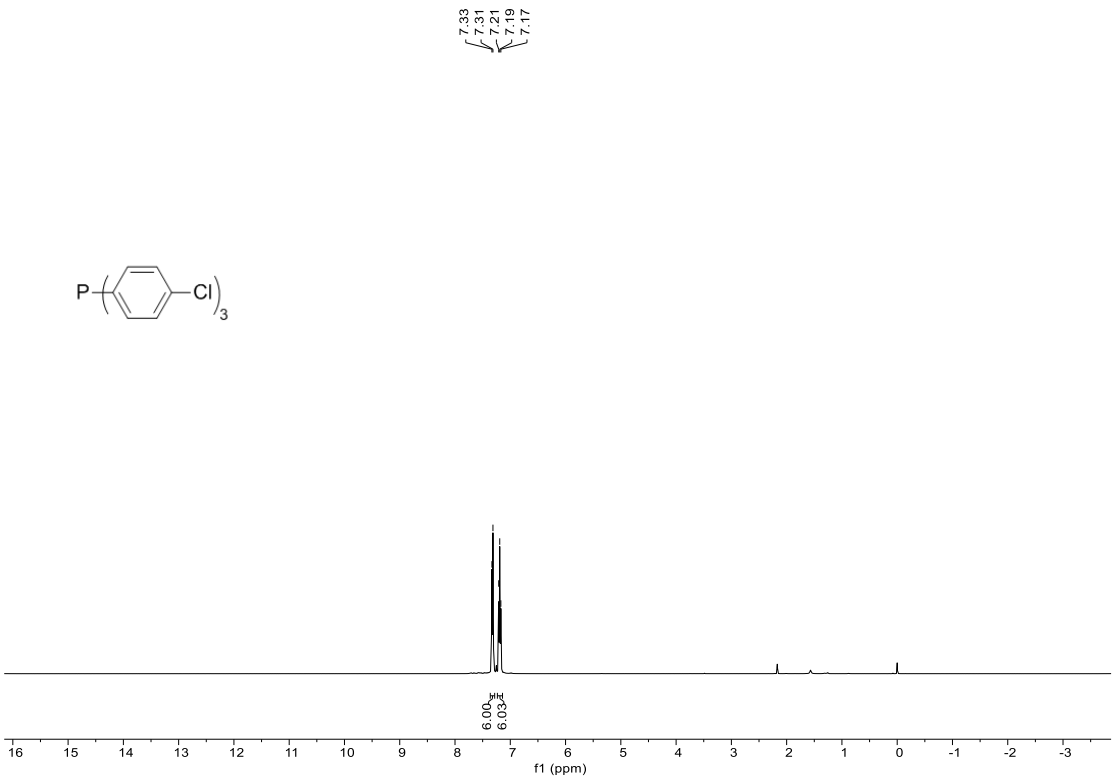
^{1}H NMR (400 MHz, $CDCl_3$) of **2j**



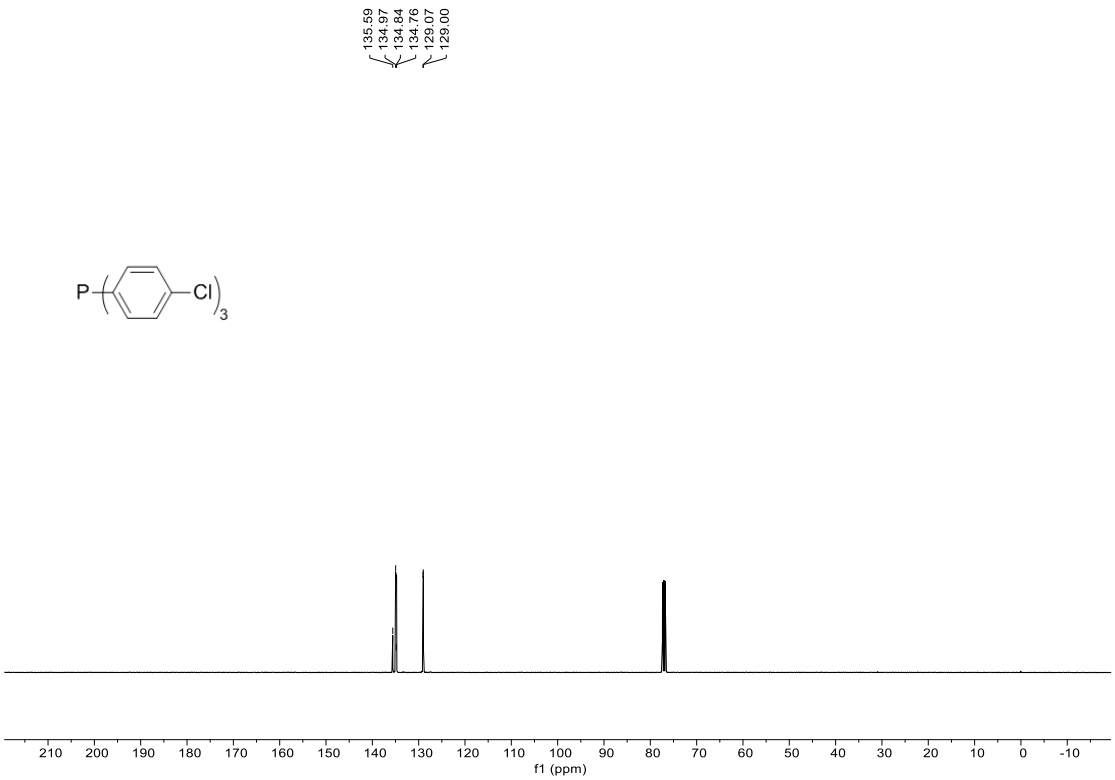
^{13}C NMR (101 MHz, $CDCl_3$) of **2j**



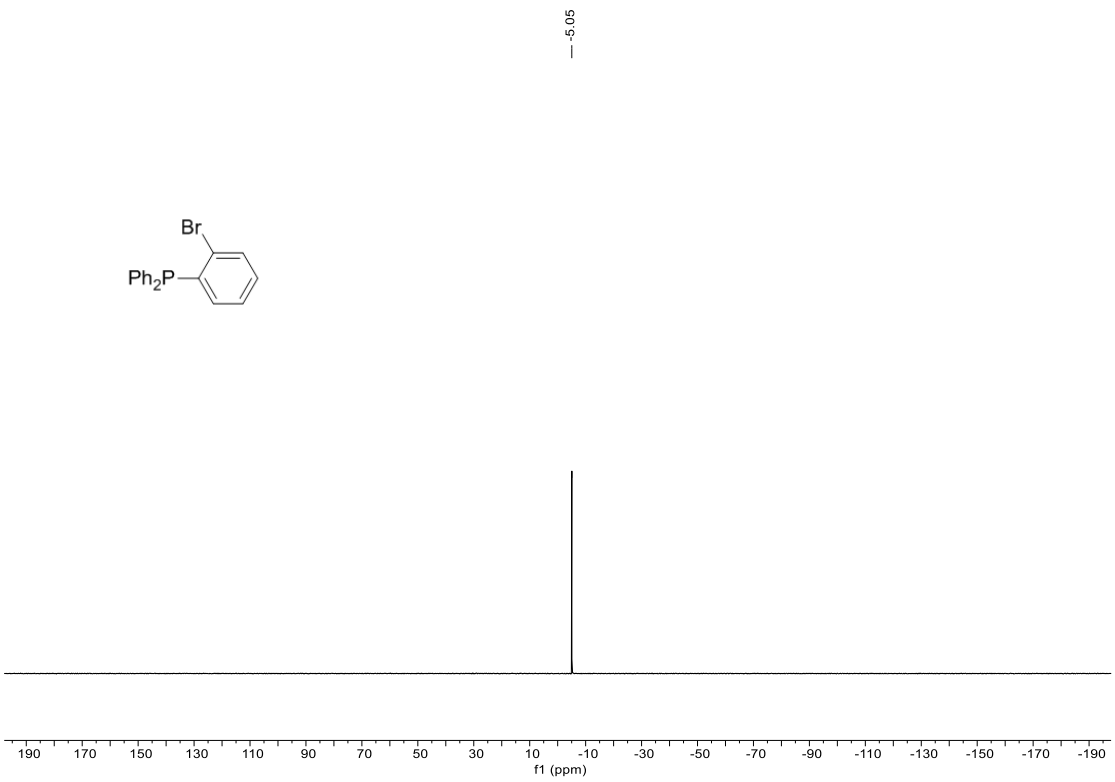
^{31}P NMR (162 MHz, $CDCl_3$) of **2k**



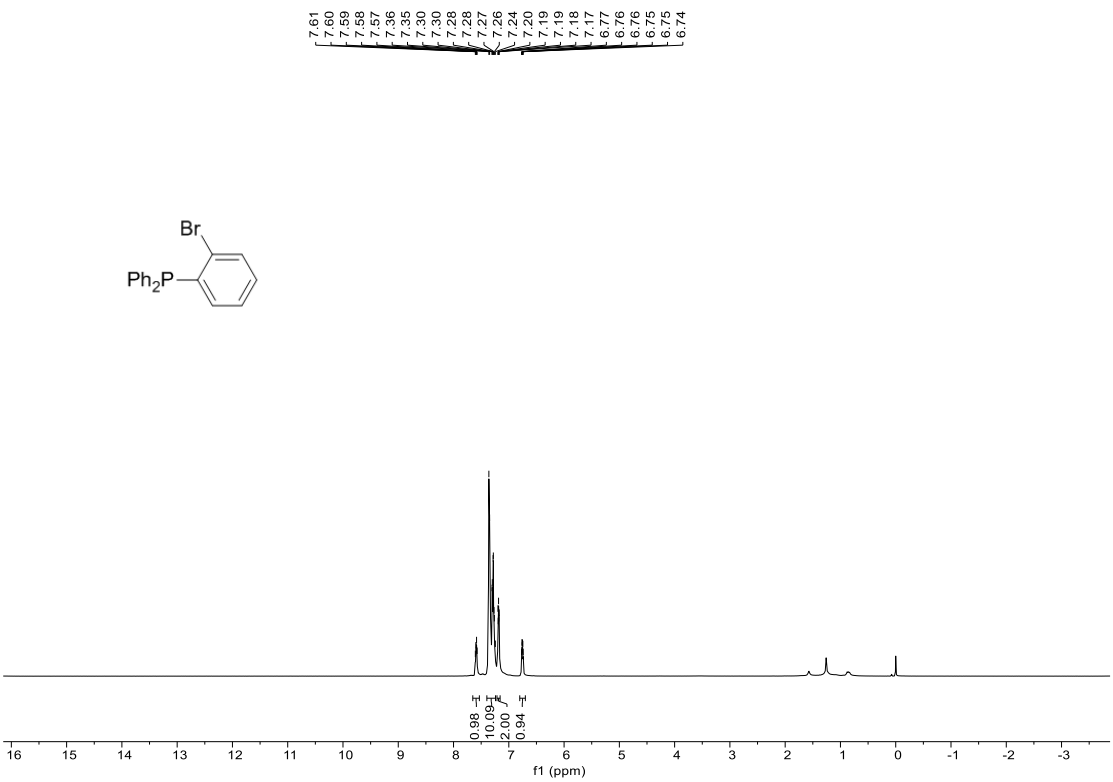
^{1}H NMR (400 MHz, $CDCl_3$) of **2k**



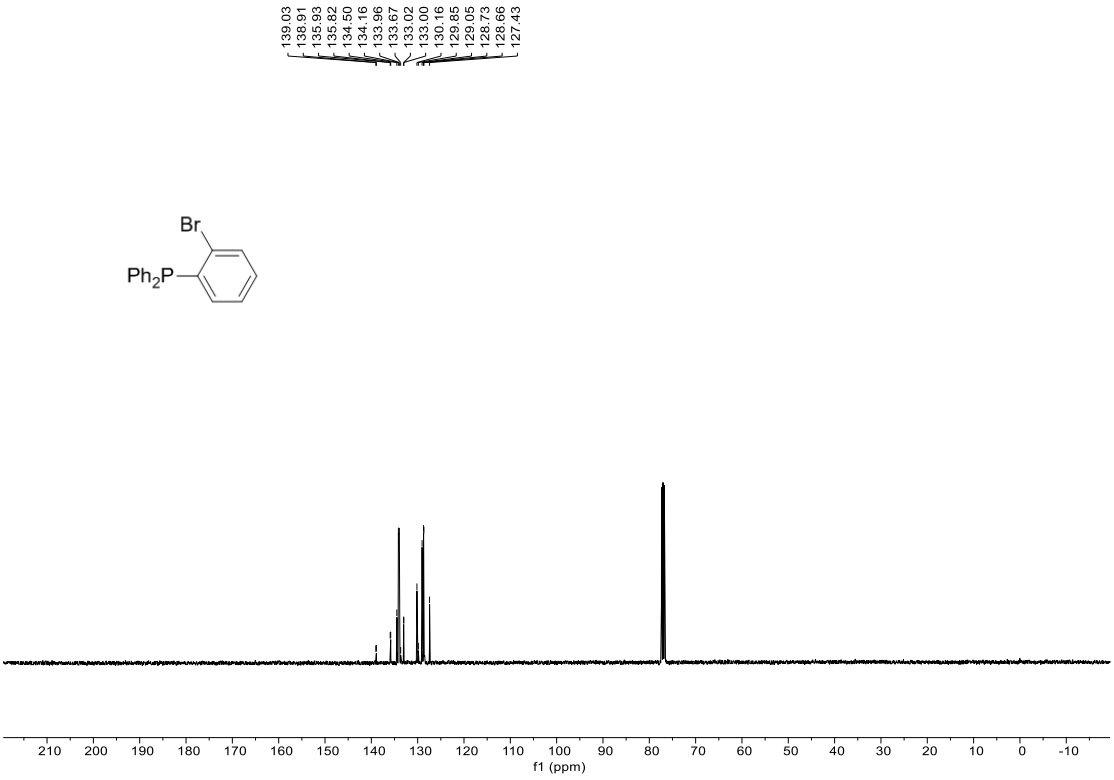
^{13}C NMR (101 MHz, $CDCl_3$) of **2k**



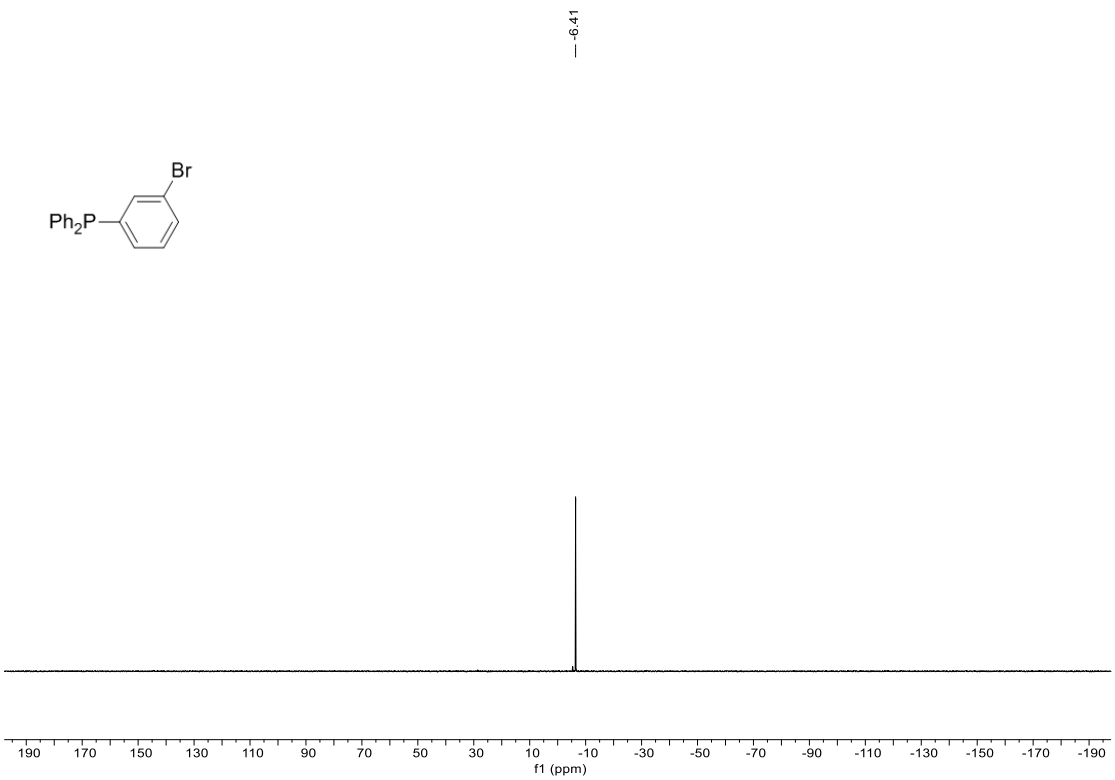
^{31}P NMR (162 MHz, $CDCl_3$) of **2l**



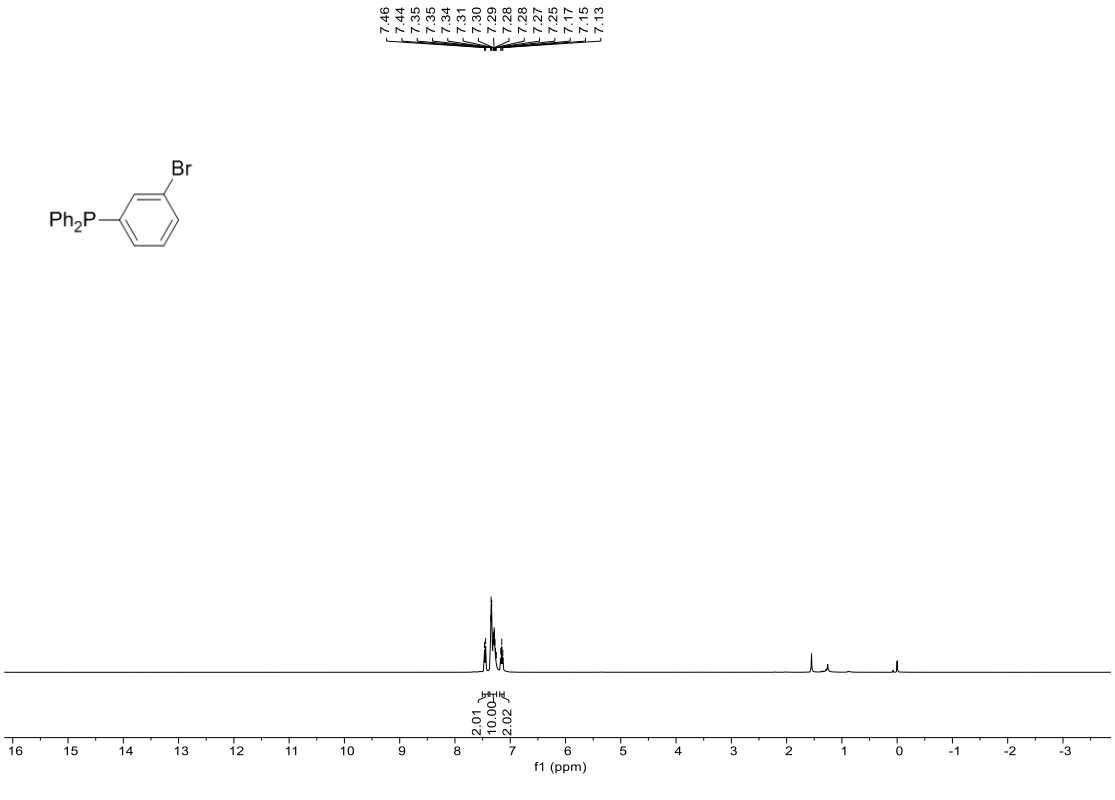
^{1}H NMR (400 MHz, $CDCl_3$) of **2l**



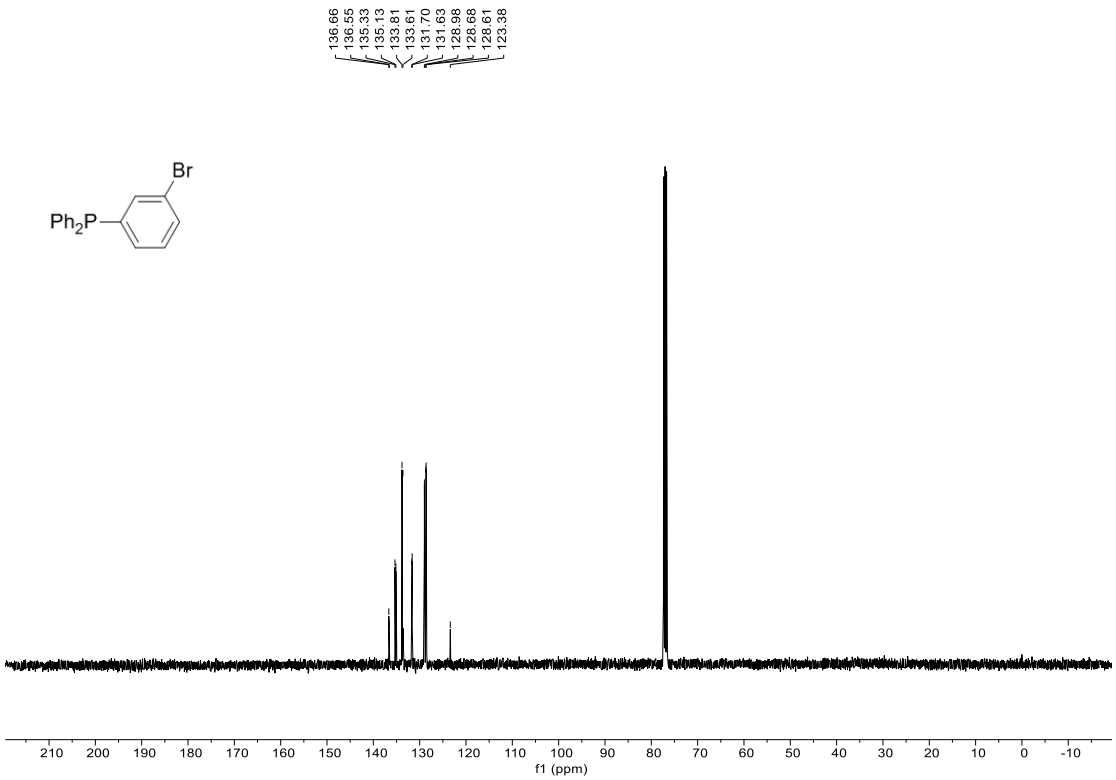
^{13}C NMR (101 MHz, $CDCl_3$) of **2l**



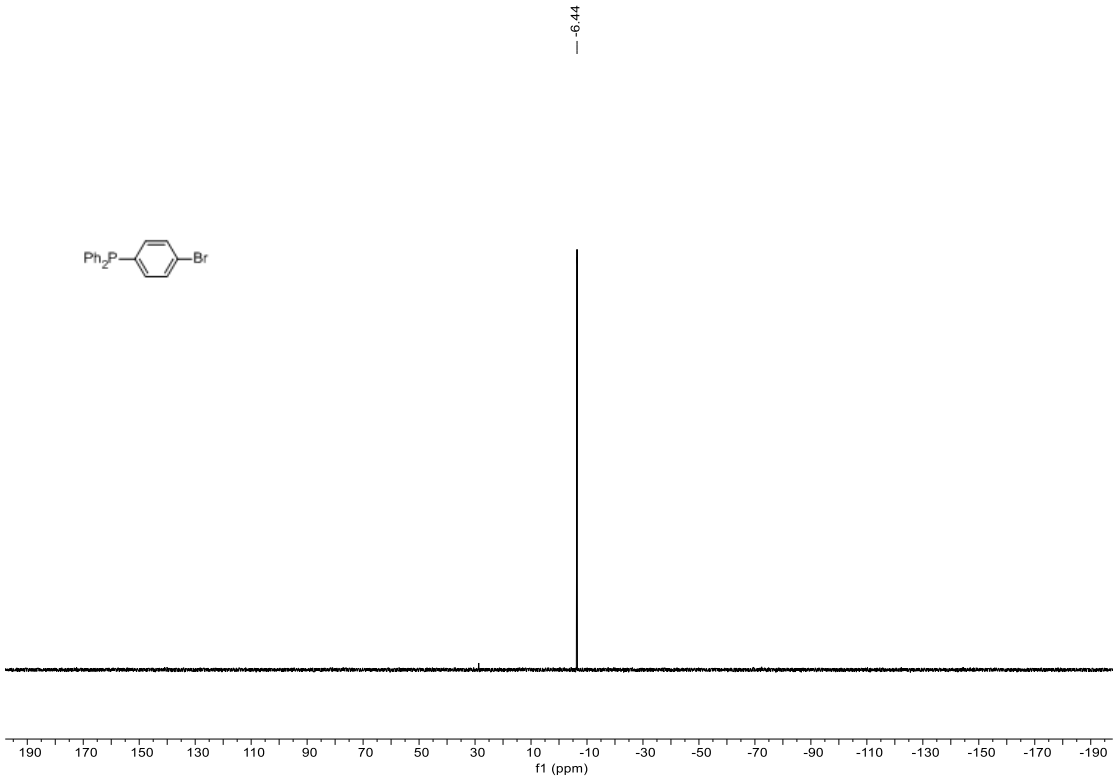
^{31}P NMR (162 MHz, $CDCl_3$) of **2m**



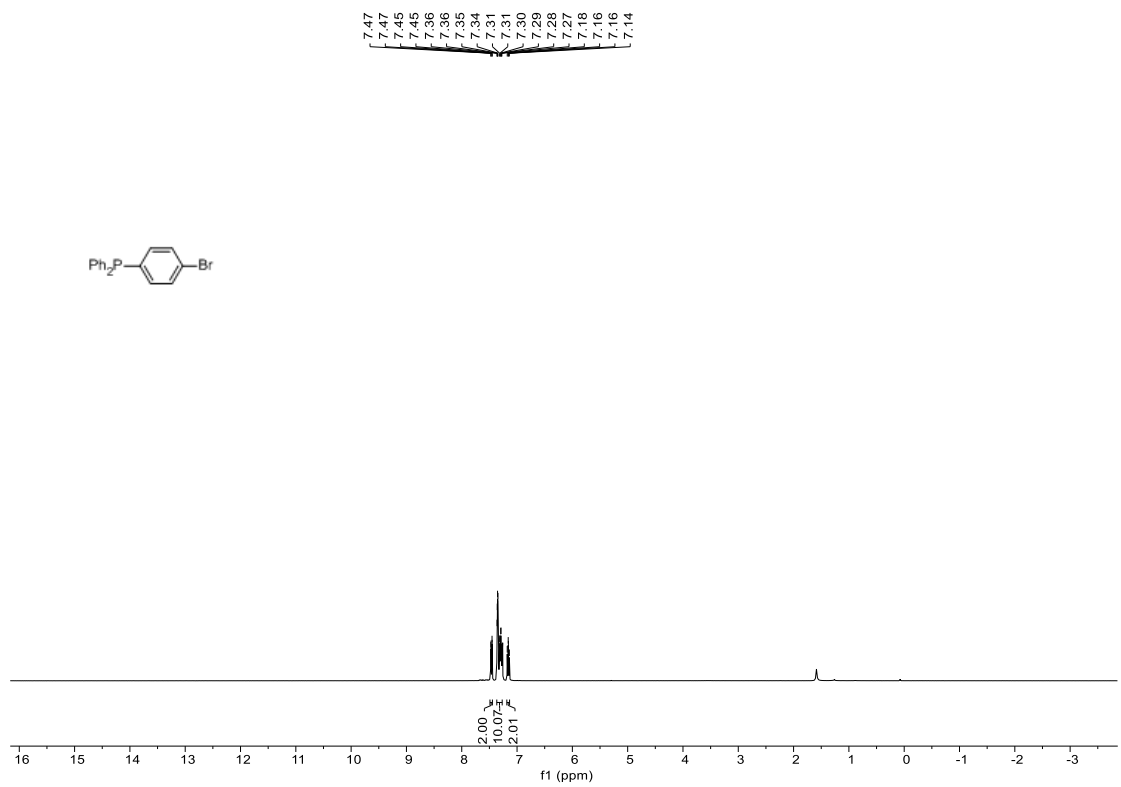
^{1}H NMR (400 MHz, $CDCl_3$) of **2m**



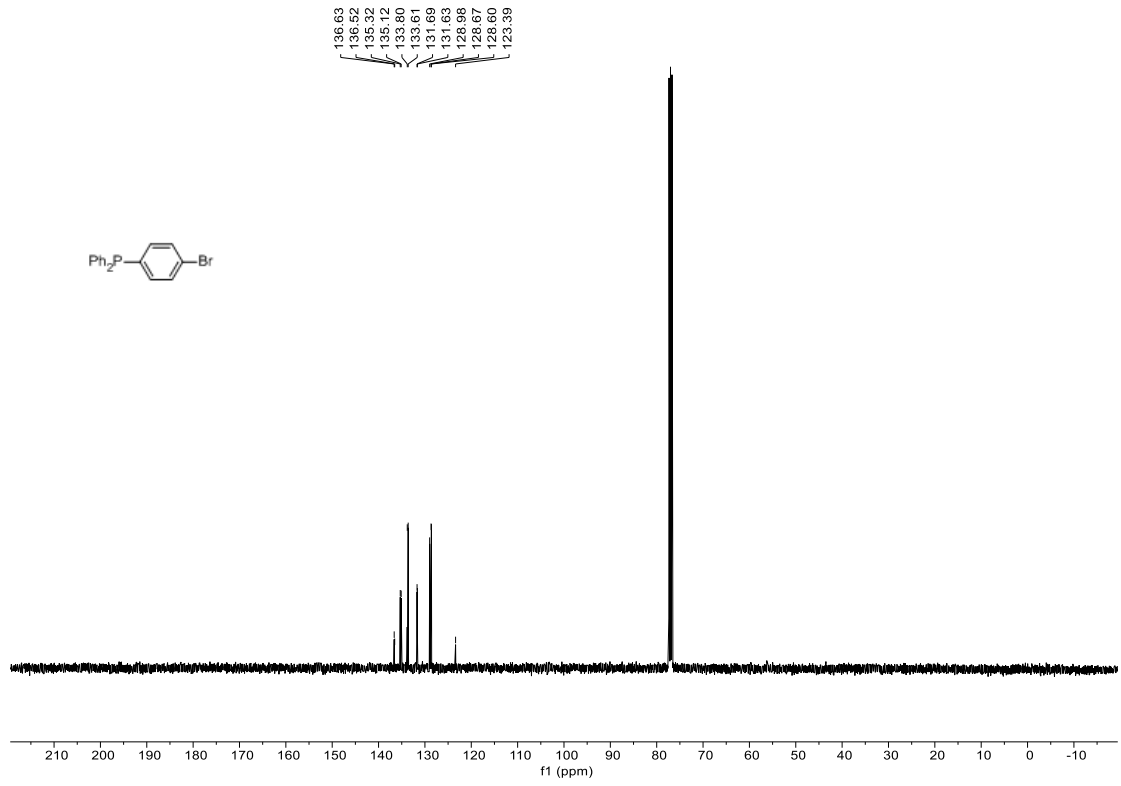
^{13}C NMR (101 MHz, $CDCl_3$) of **2m**



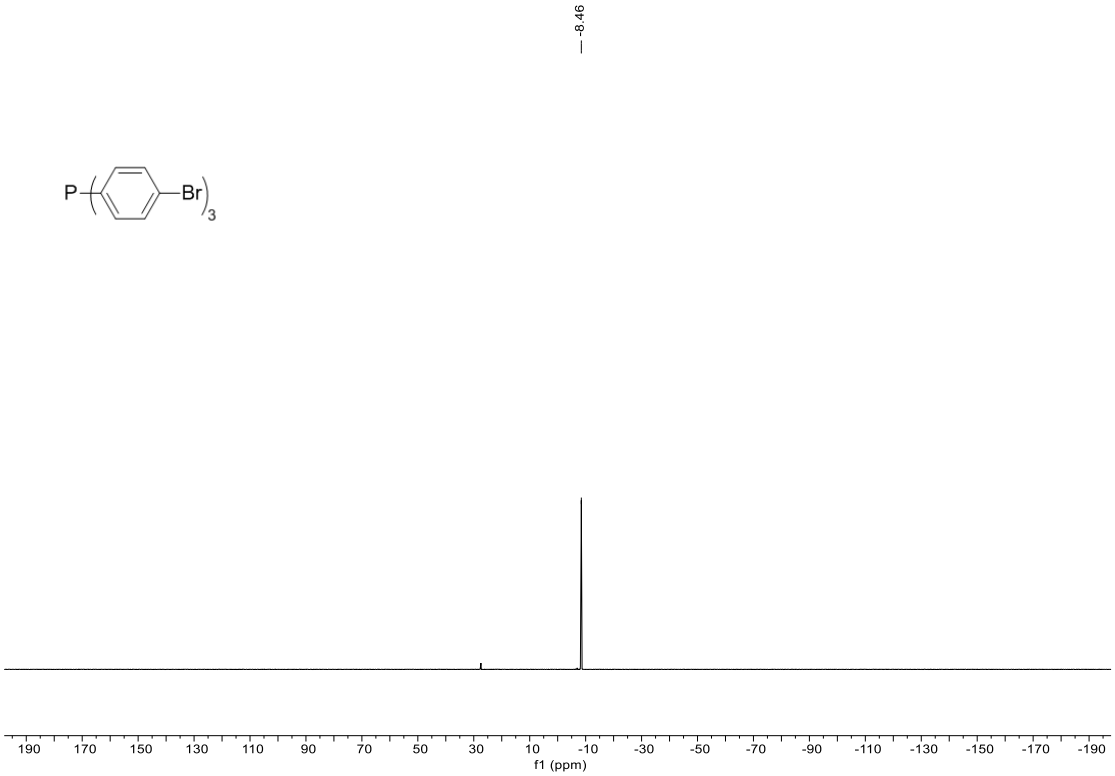
^{31}P NMR (162 MHz, $CDCl_3$) of **2n**



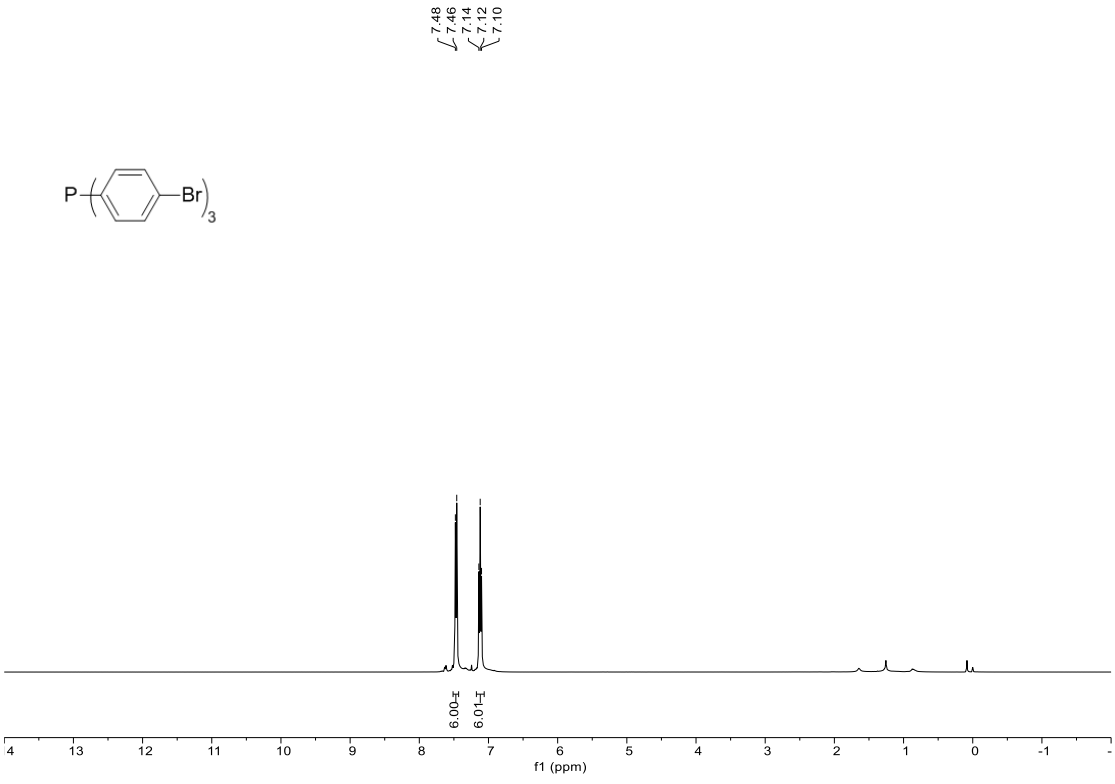
^{1}H NMR (400 MHz, $CDCl_3$) of **2n**



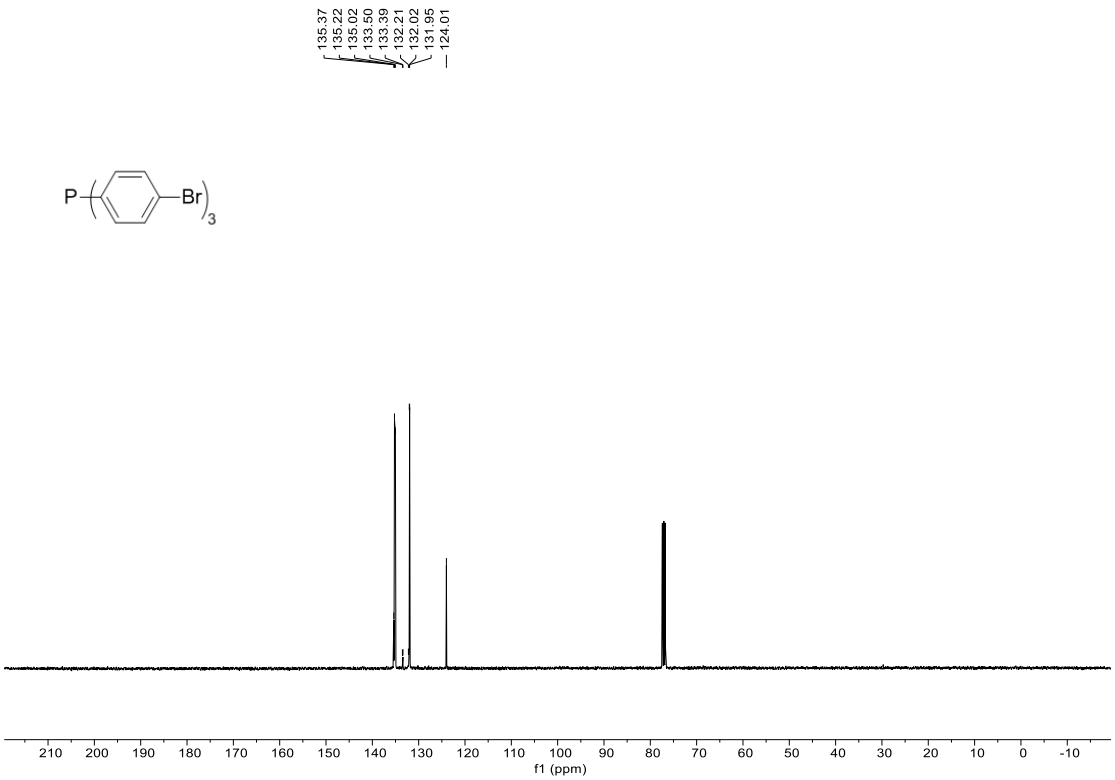
^{13}C NMR (101 MHz, $CDCl_3$) of **2n**



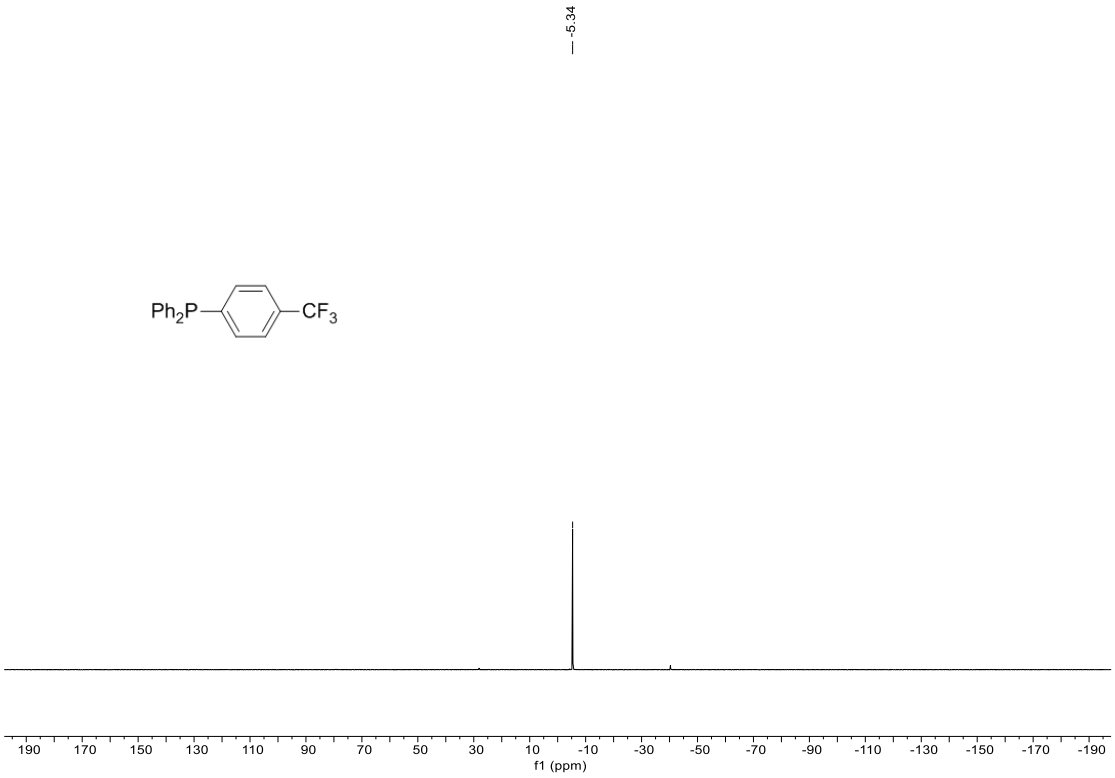
^{31}P NMR (162 MHz, $CDCl_3$) of **2o**



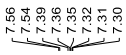
^{1}H NMR (400 MHz, $CDCl_3$) of **2o**

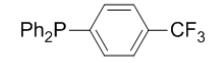


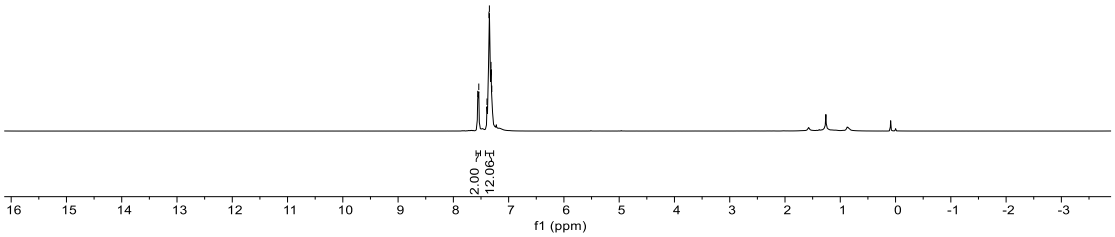
^{13}C NMR (101 MHz, $CDCl_3$) of **2o**



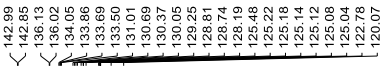
^{31}P NMR (162 MHz, $CDCl_3$) of **2p**

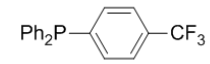


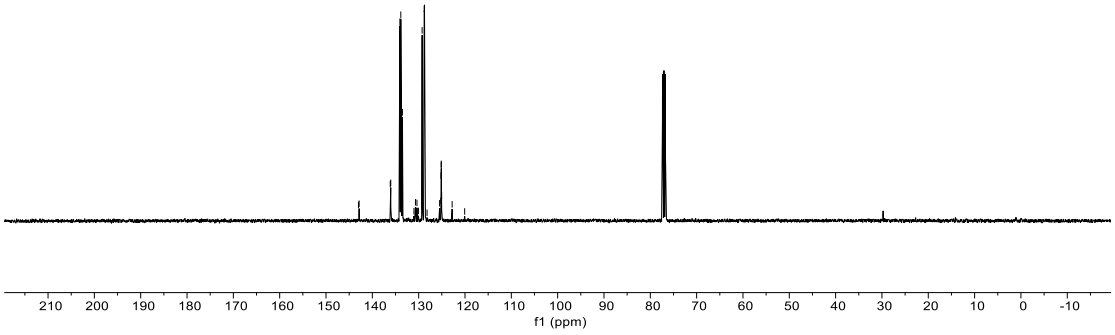




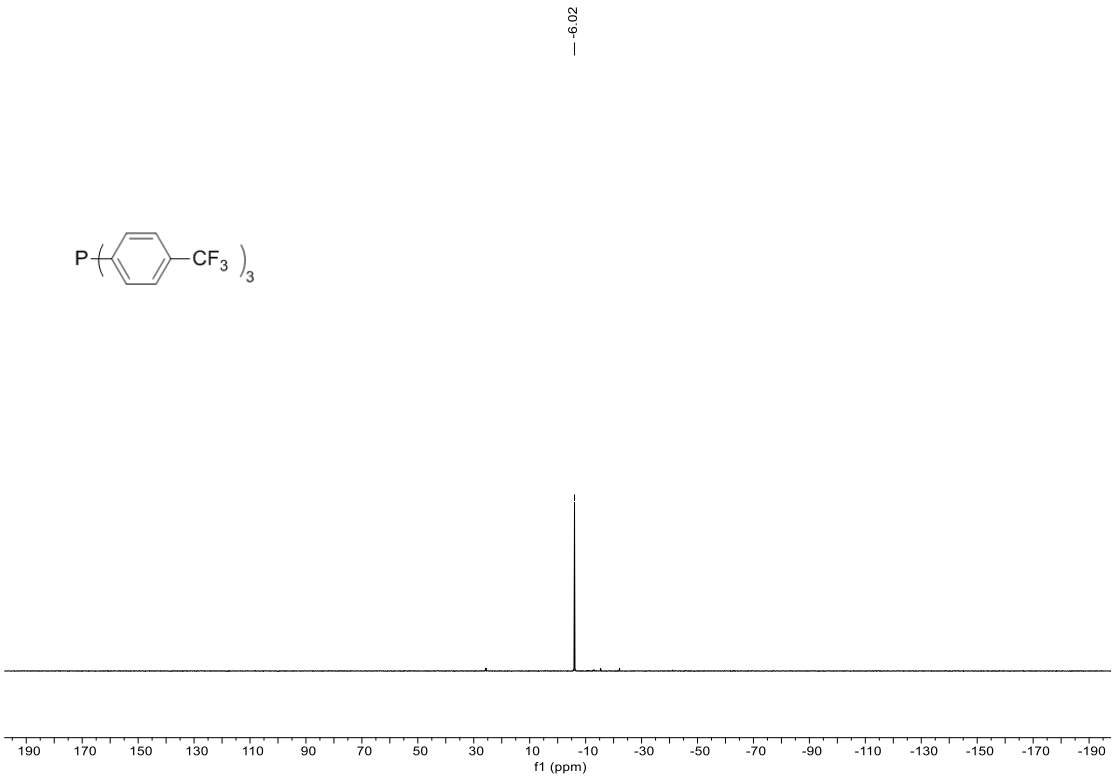
^{1}H NMR (400 MHz, $CDCl_3$) of **2p**



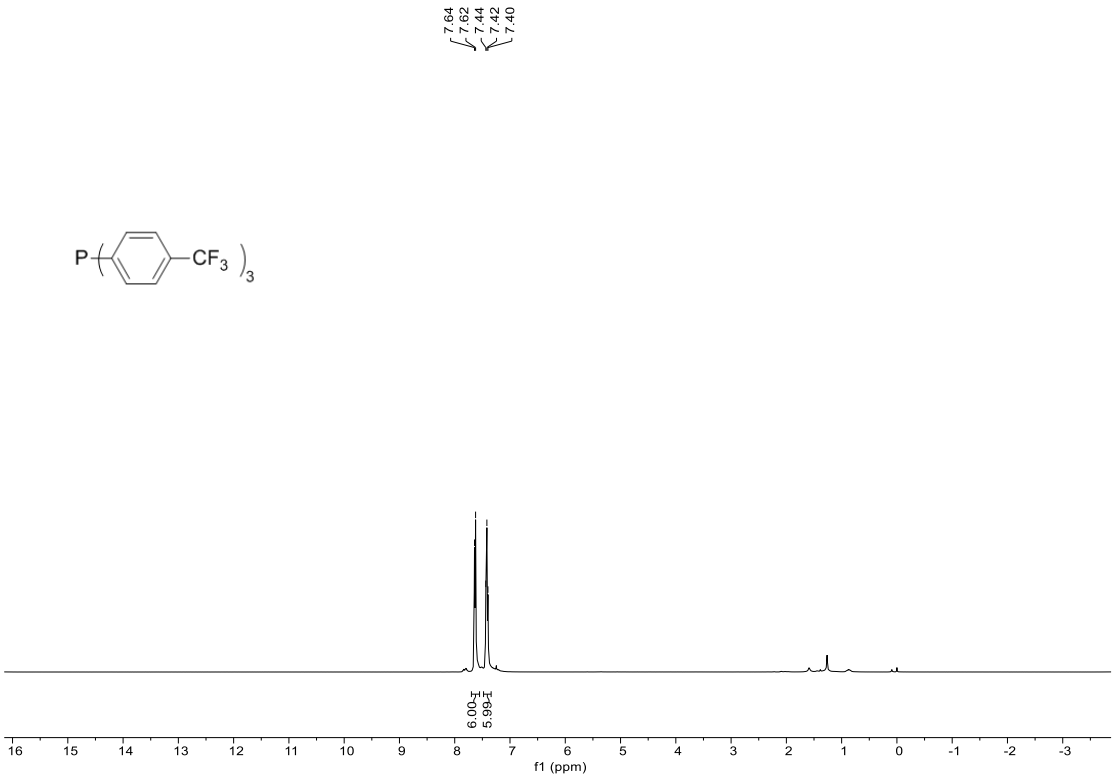




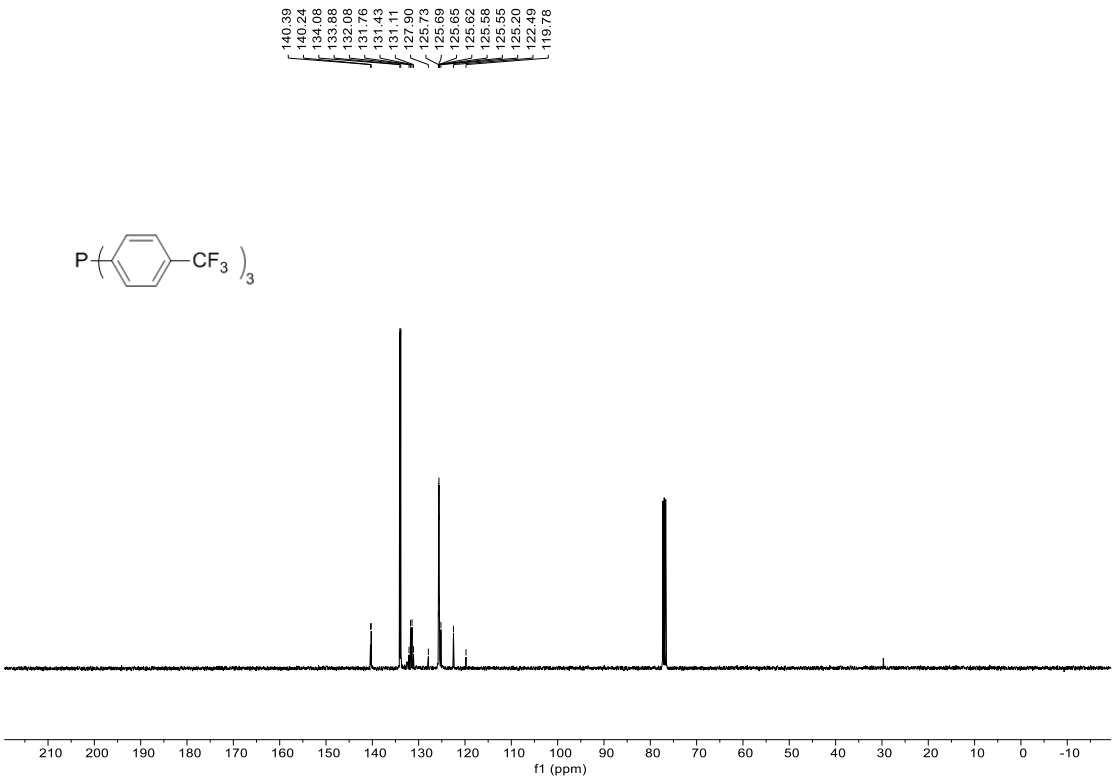
^{13}C NMR (101 MHz, $CDCl_3$) of **2p**



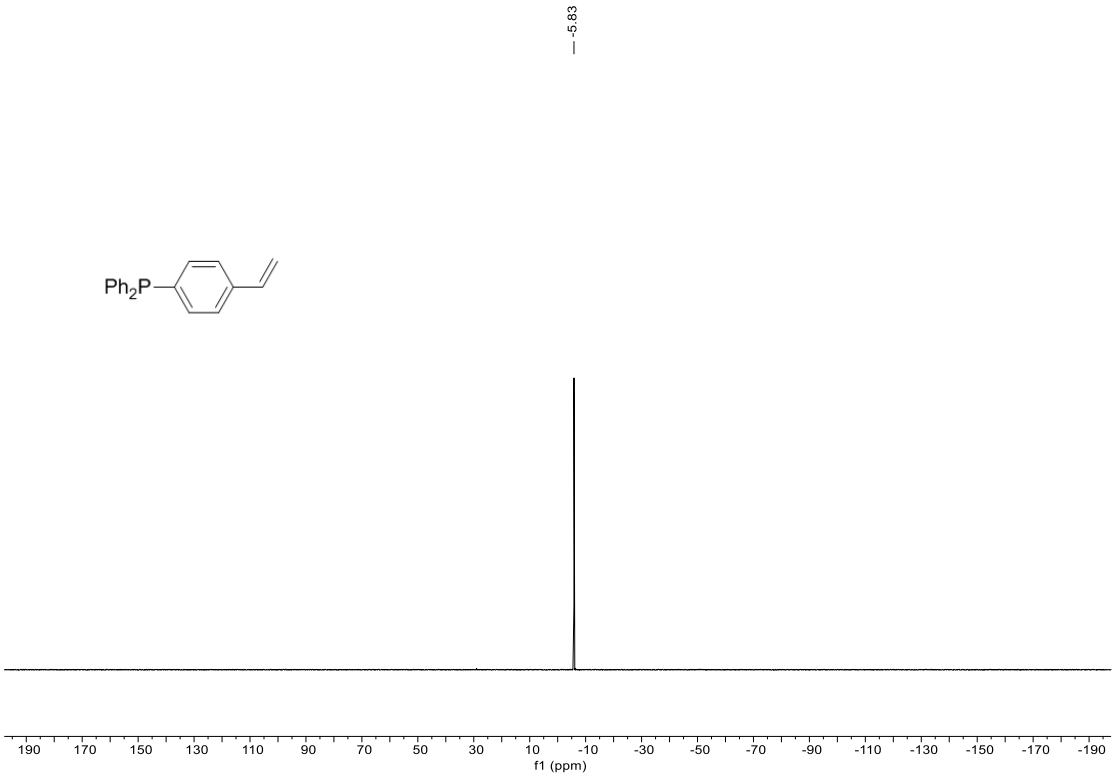
^{31}P NMR (162 MHz, $CDCl_3$) of **2q**



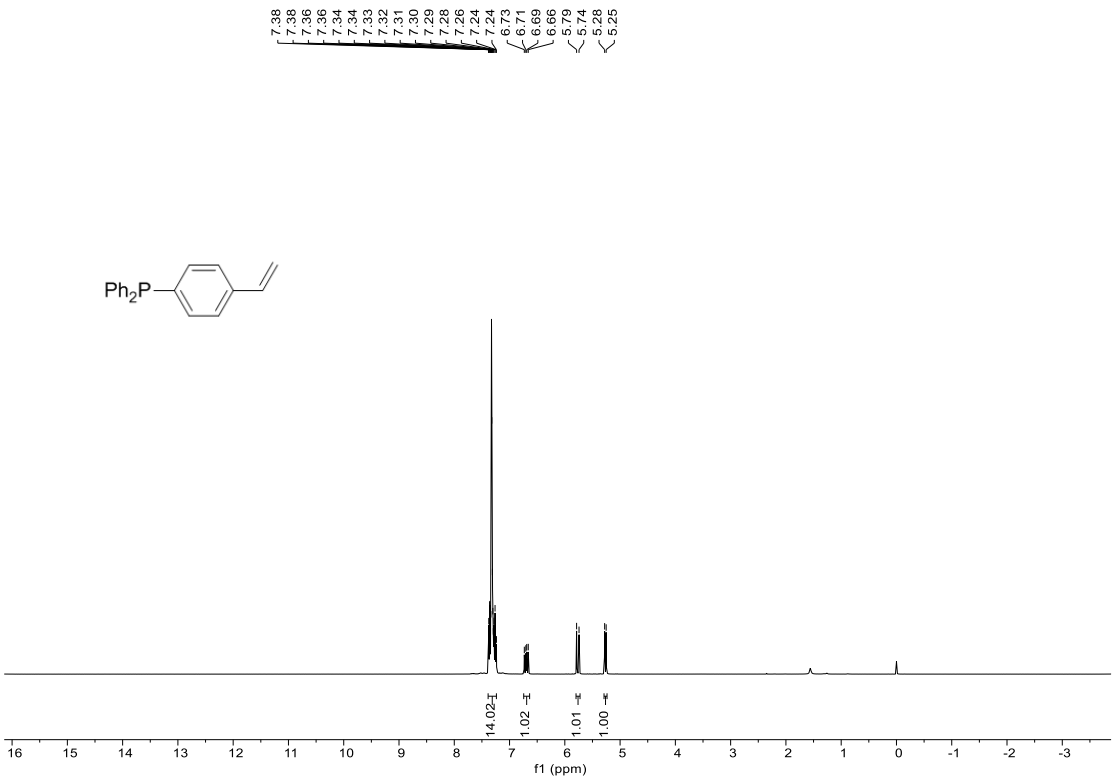
^{1}H NMR (400 MHz, $CDCl_3$) of **2q**



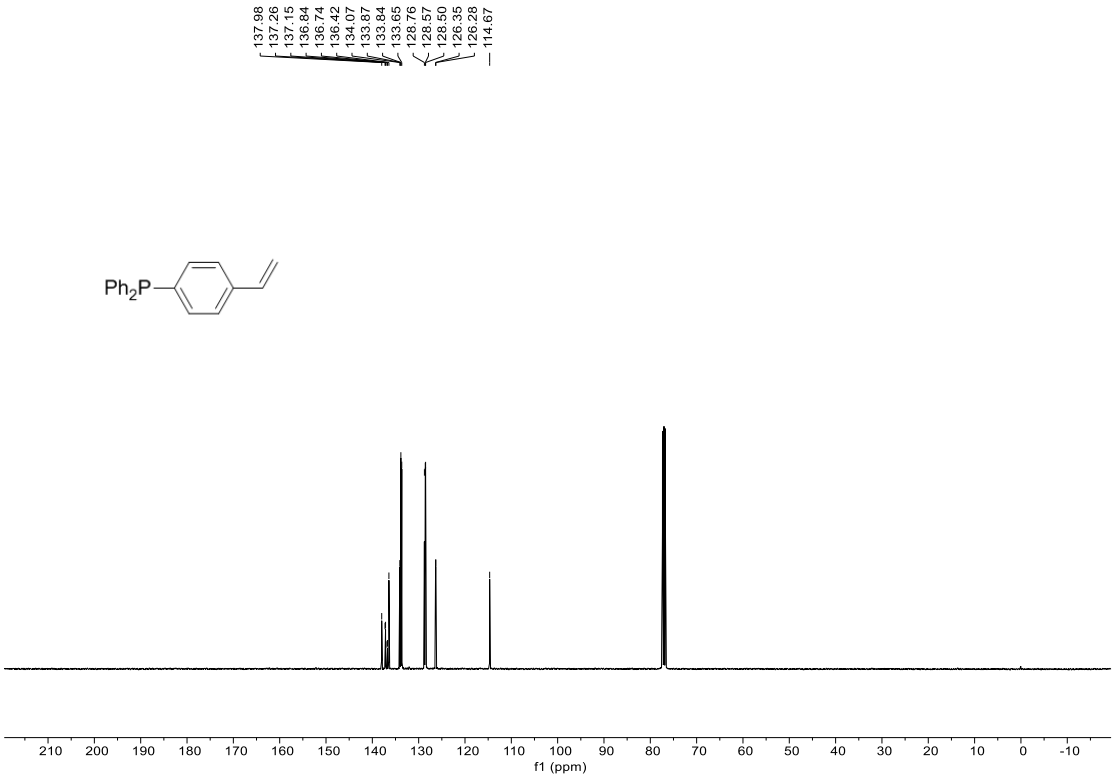
^{13}C NMR (101 MHz, $CDCl_3$) of **2q**



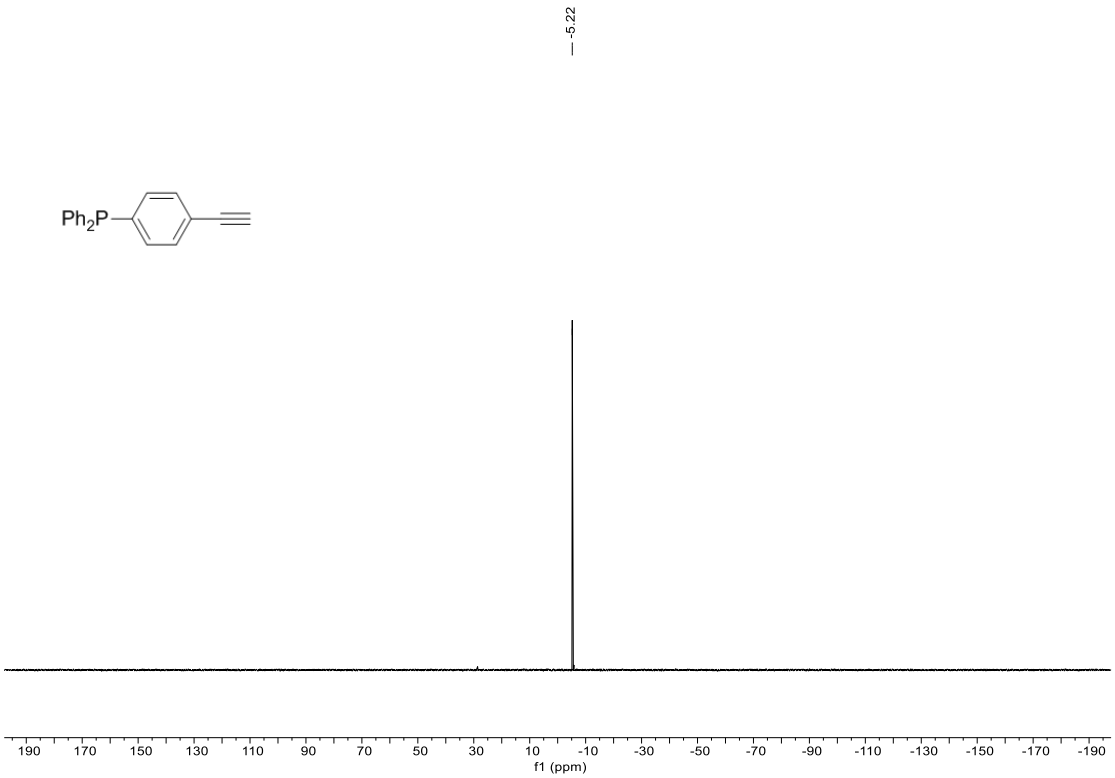
^{31}P NMR (162 MHz, $CDCl_3$) of **2r**



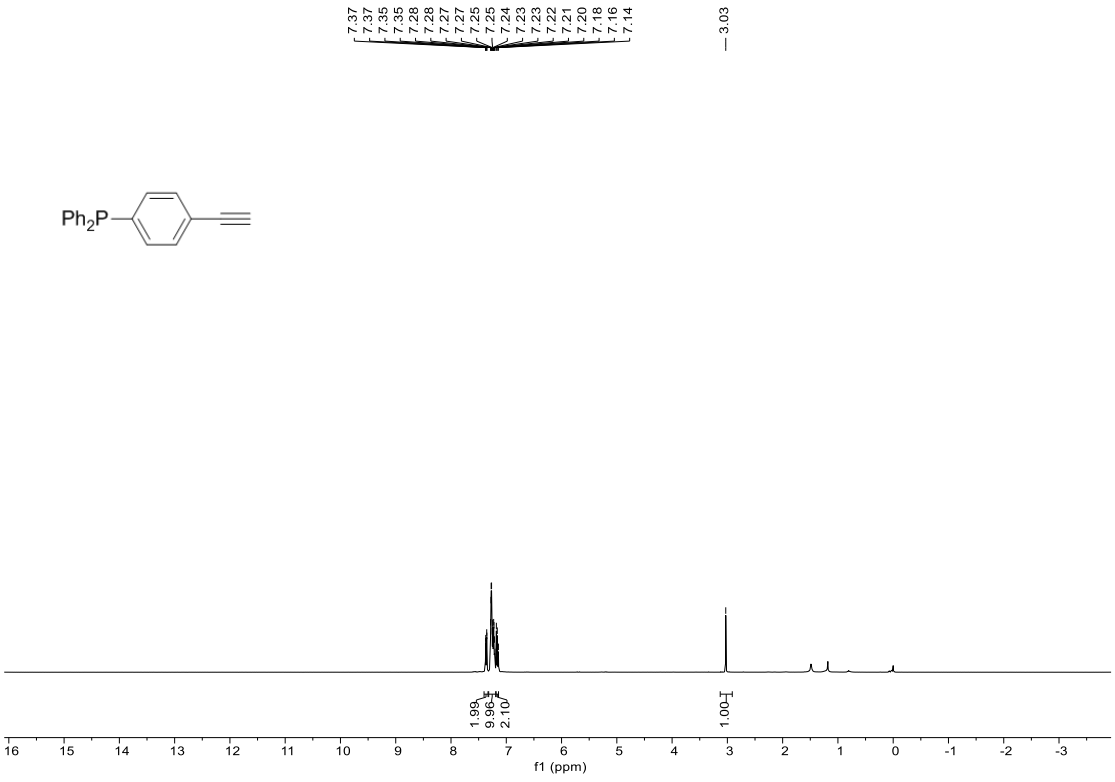
^{1}H NMR (400 MHz, $CDCl_3$) of **2r**



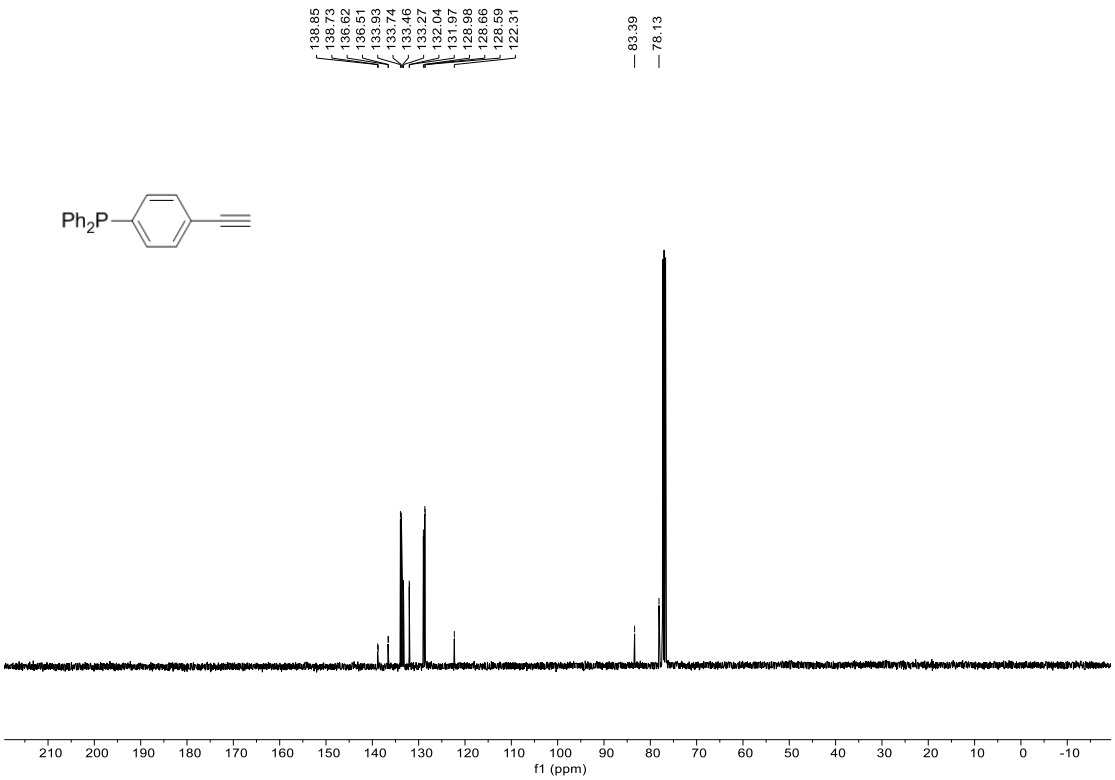
^{13}C NMR (101 MHz, $CDCl_3$) of **2r**



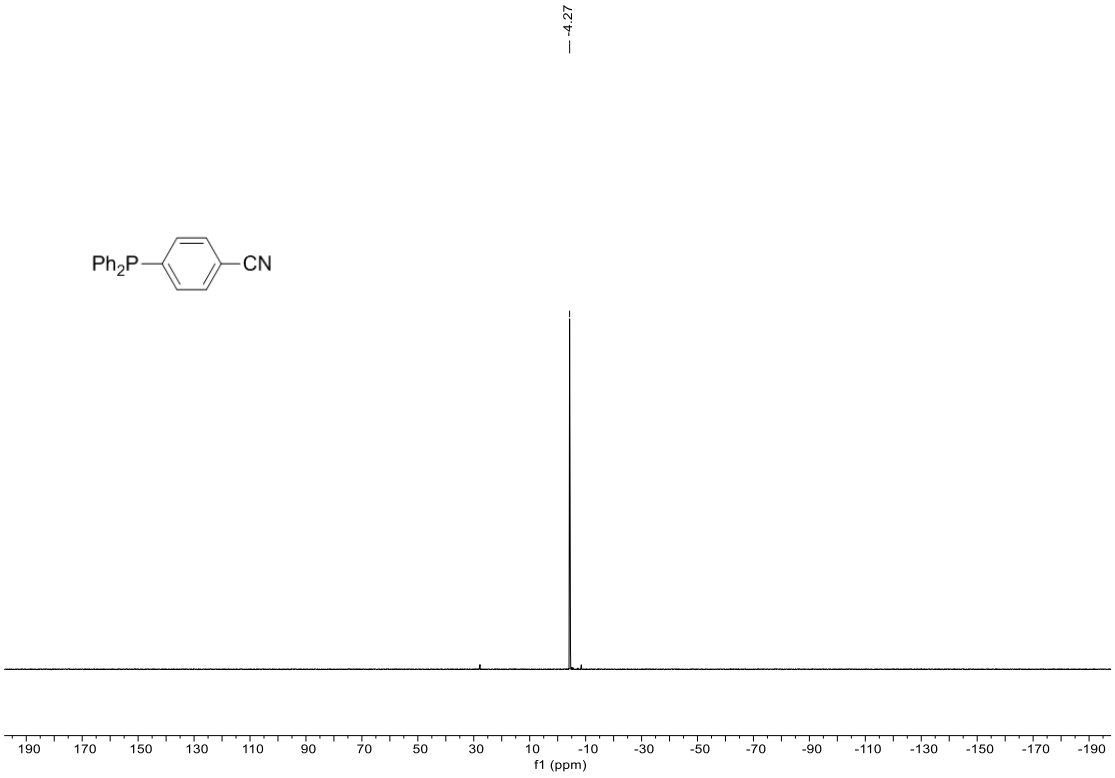
^{31}P NMR (162 MHz, $CDCl_3$) of **2s**



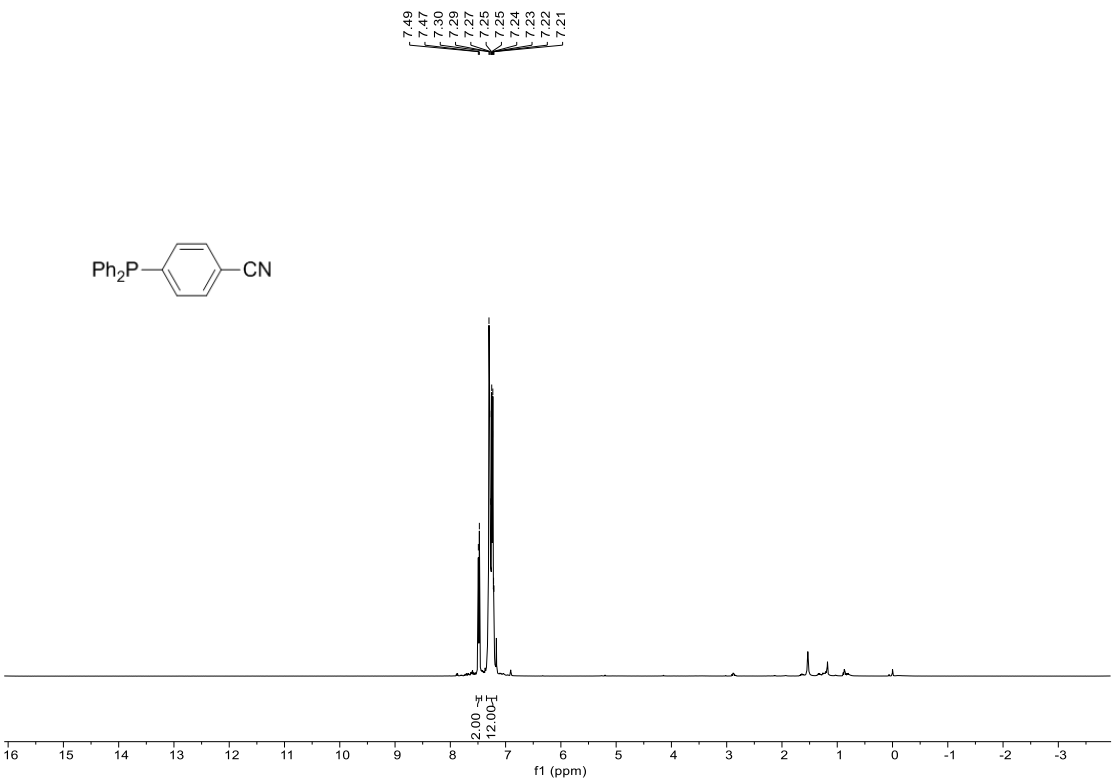
^{1}H NMR (400 MHz, $CDCl_3$) of **2s**



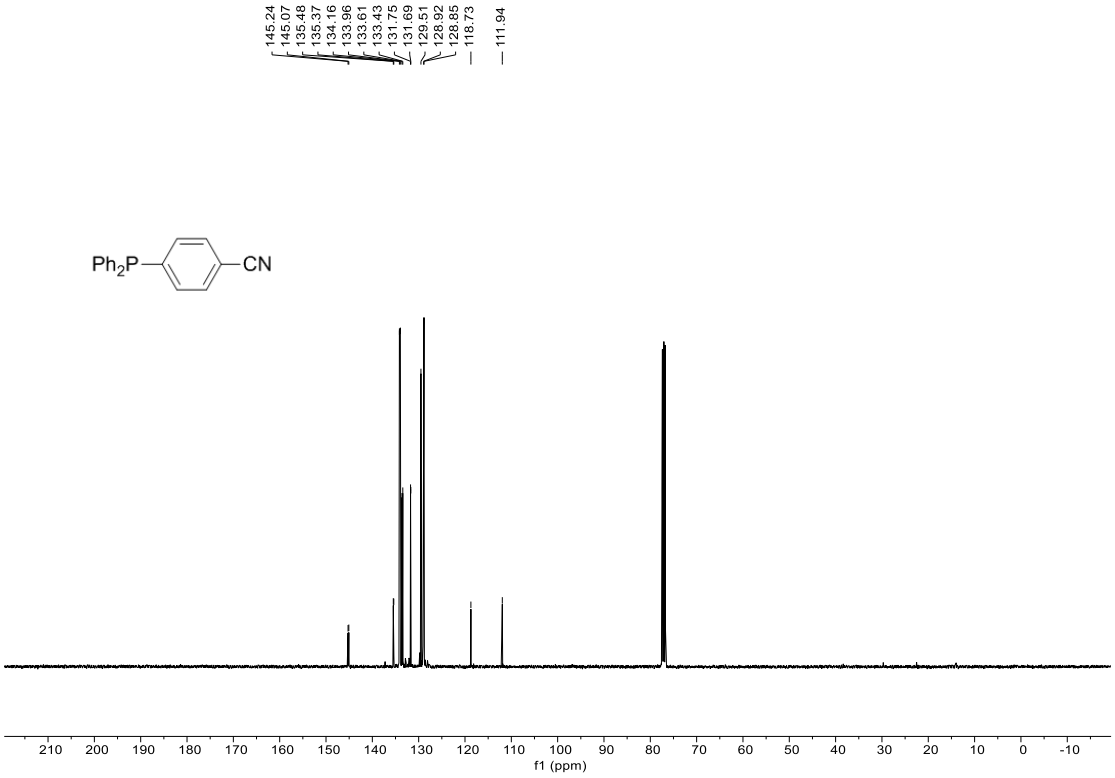
^{13}C NMR (101 MHz, $CDCl_3$) of **2s**



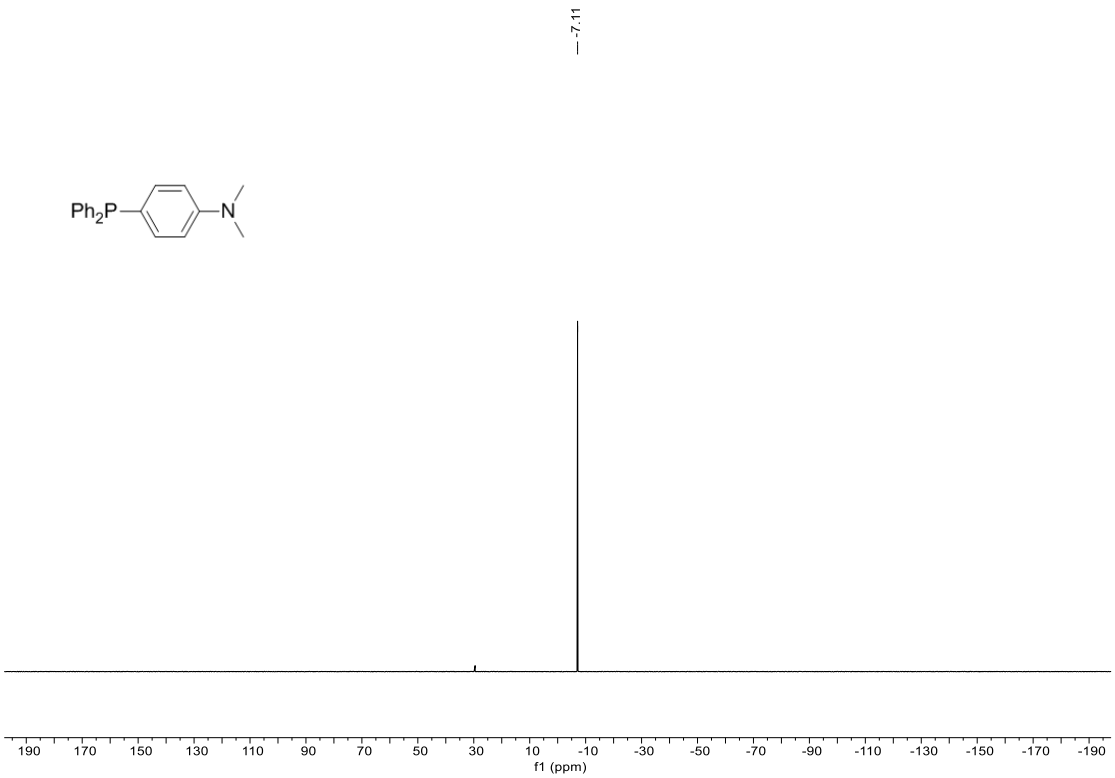
^{31}P NMR (162 MHz, $CDCl_3$) of **2t**



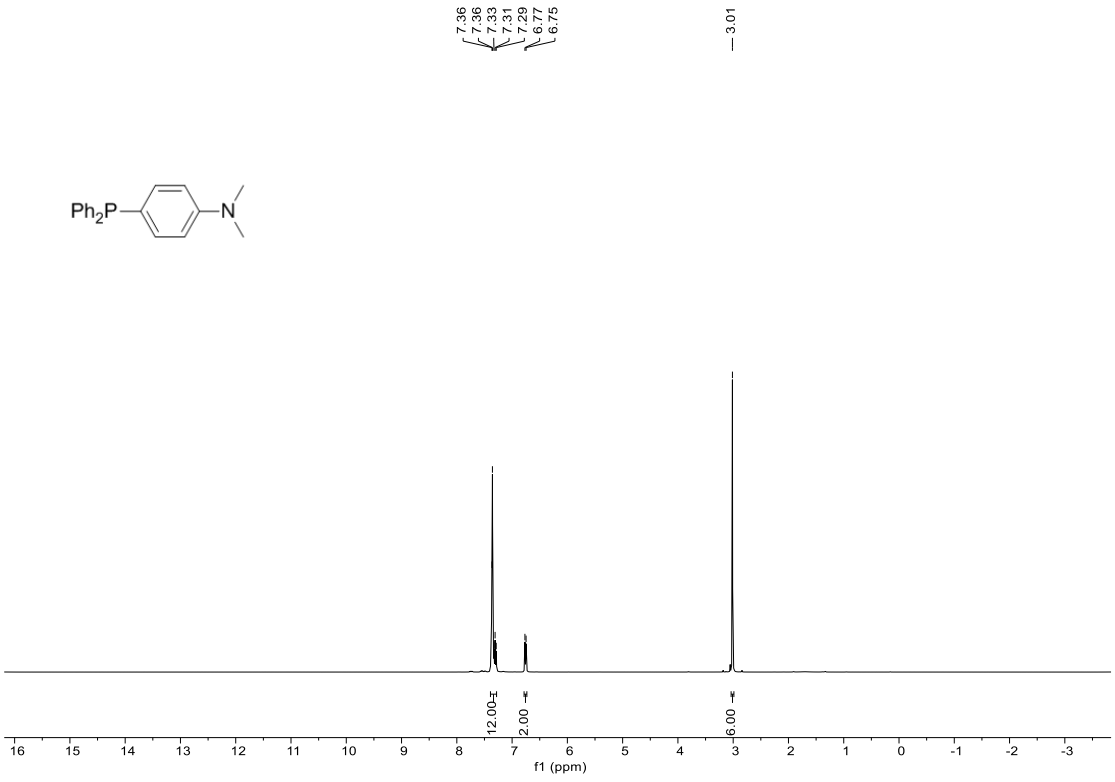
^{1}H NMR (400 MHz, $CDCl_3$) of **2t**



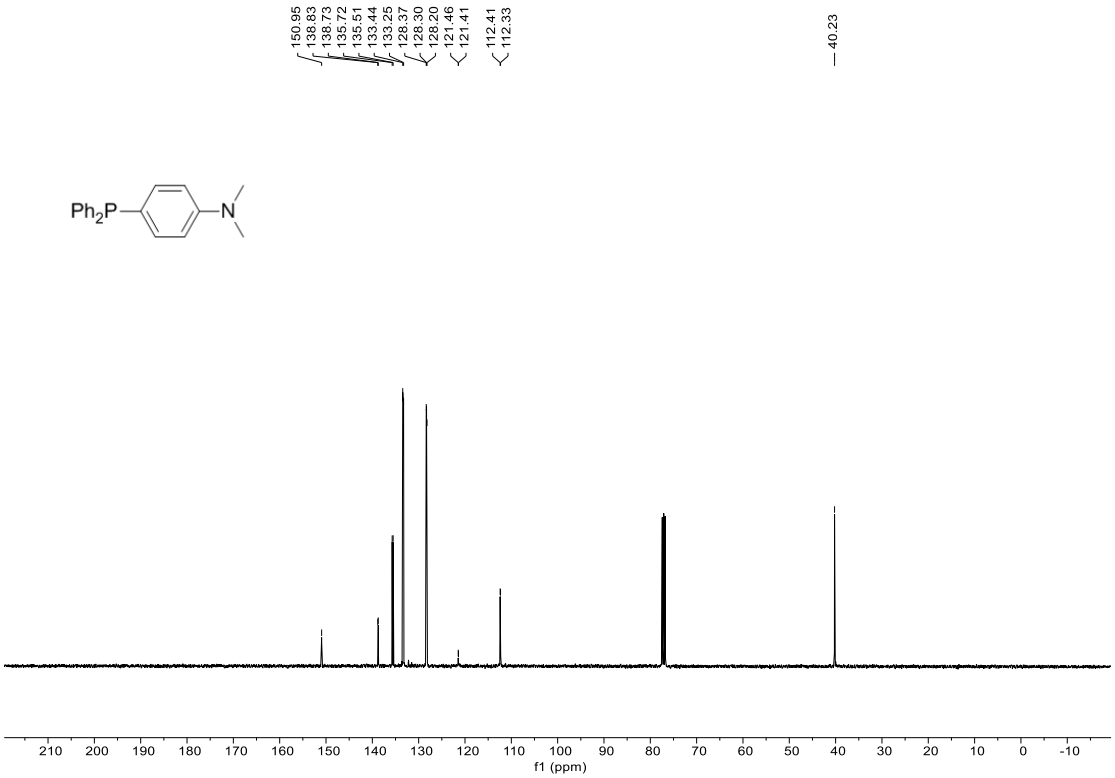
^{13}C NMR (101 MHz, $CDCl_3$) of **2t**



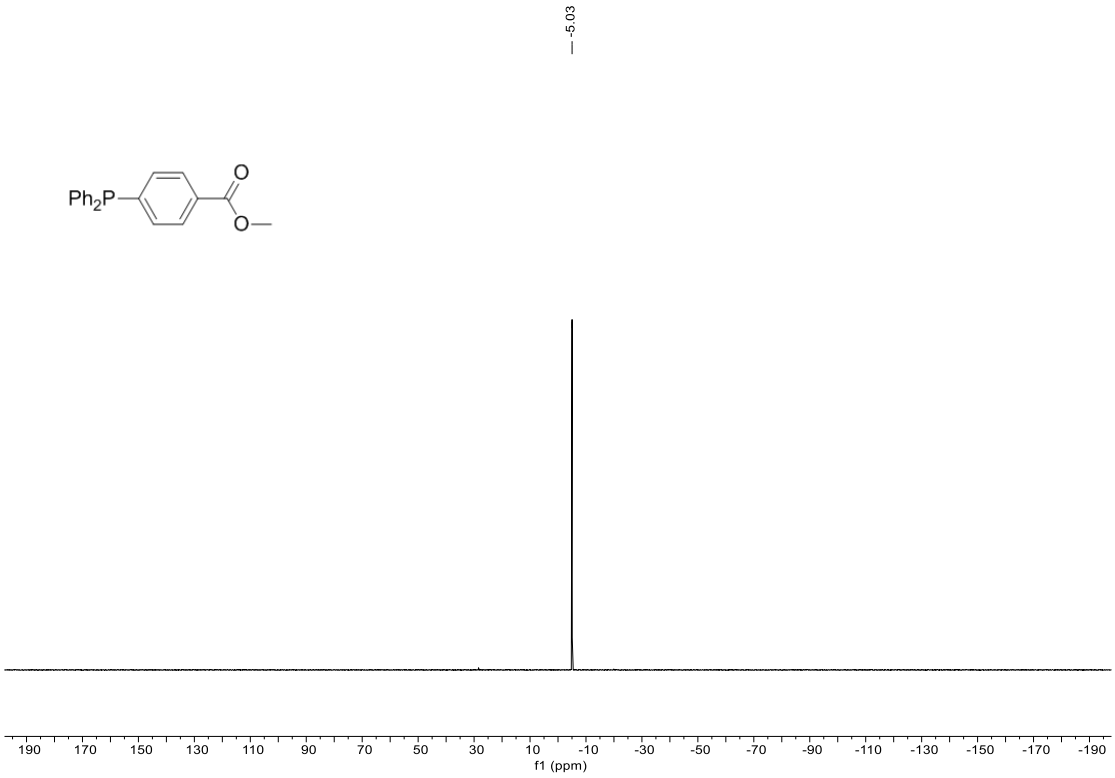
^{31}P NMR (162 MHz, $CDCl_3$) of **2u**



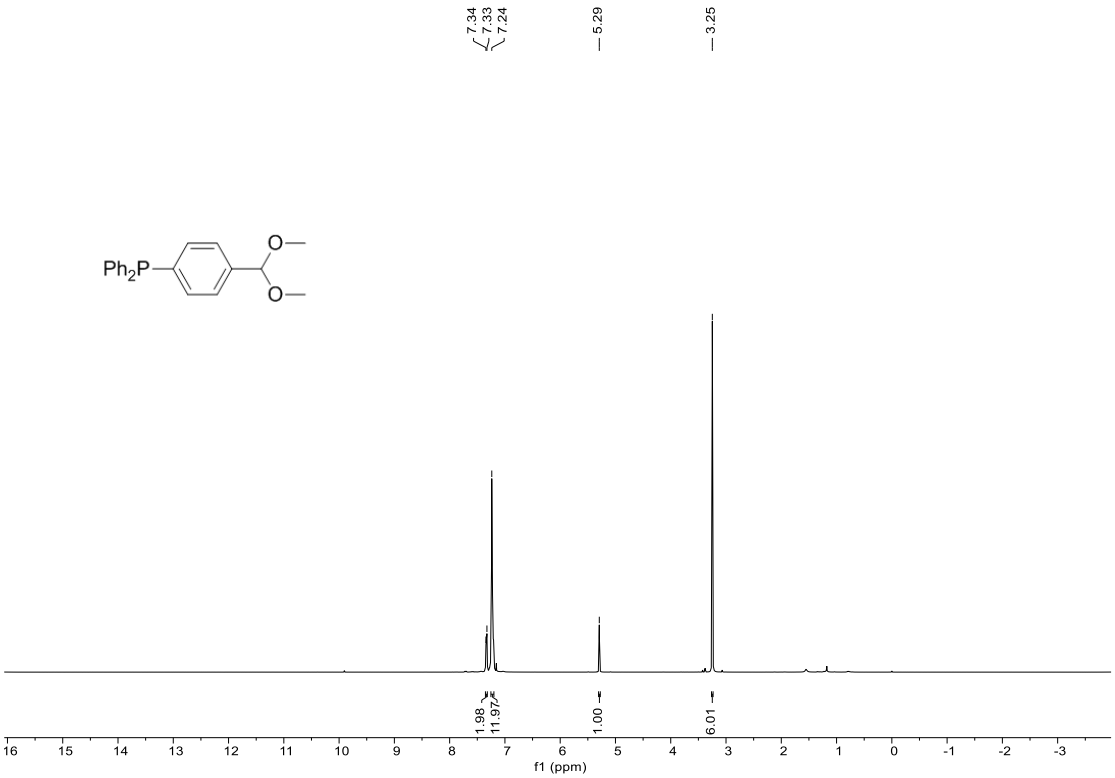
^{1}H NMR (400 MHz, $CDCl_3$) of **2u**



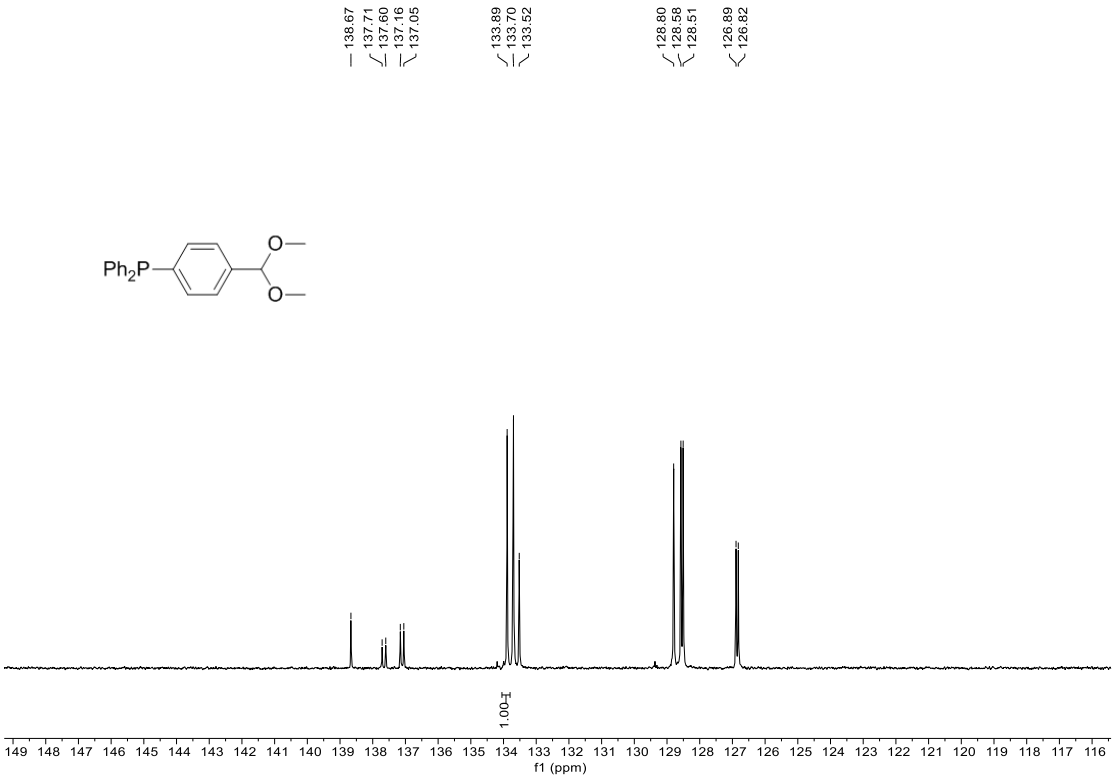
^{13}C NMR (101 MHz, $CDCl_3$) of **2u**



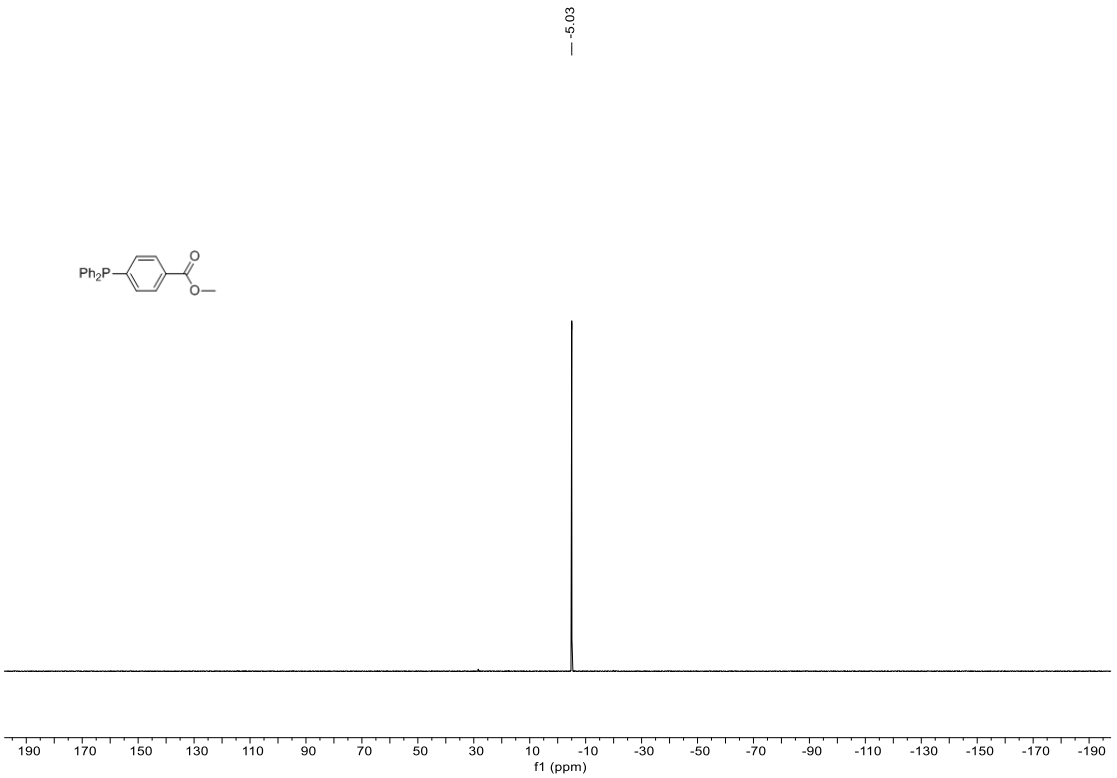
^{31}P NMR (162 MHz, $CDCl_3$) of **2v**



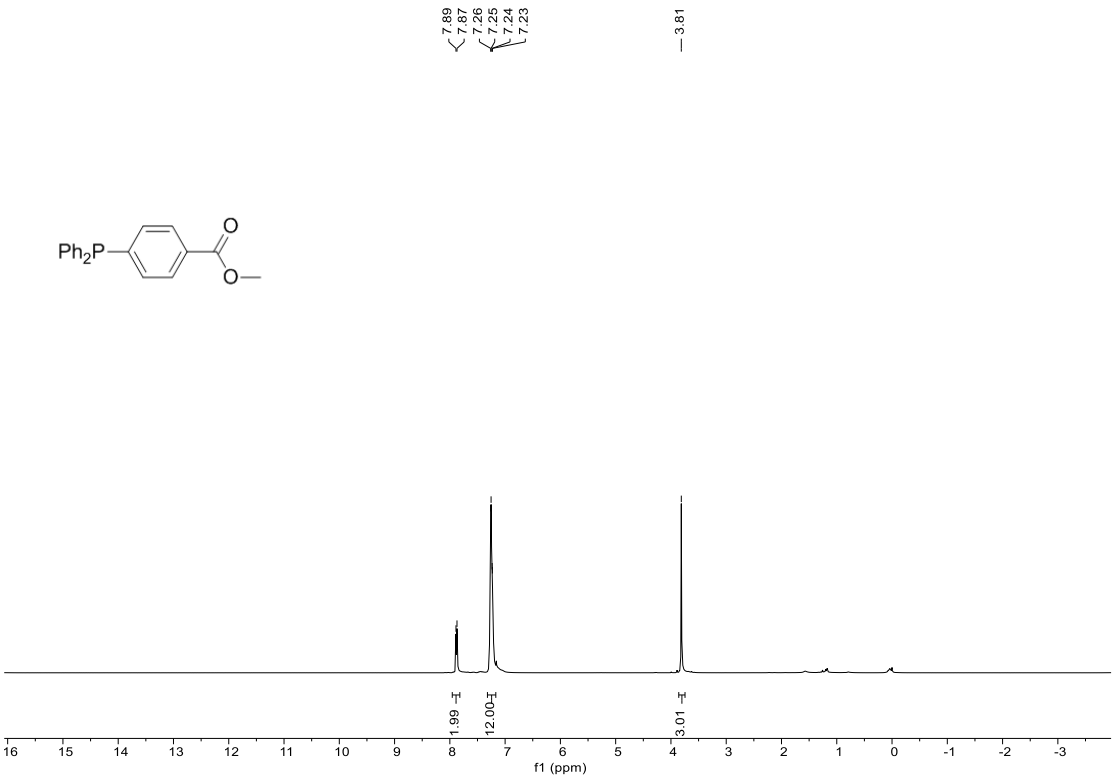
^{1}H NMR (400 MHz, $CDCl_3$) of **2v**



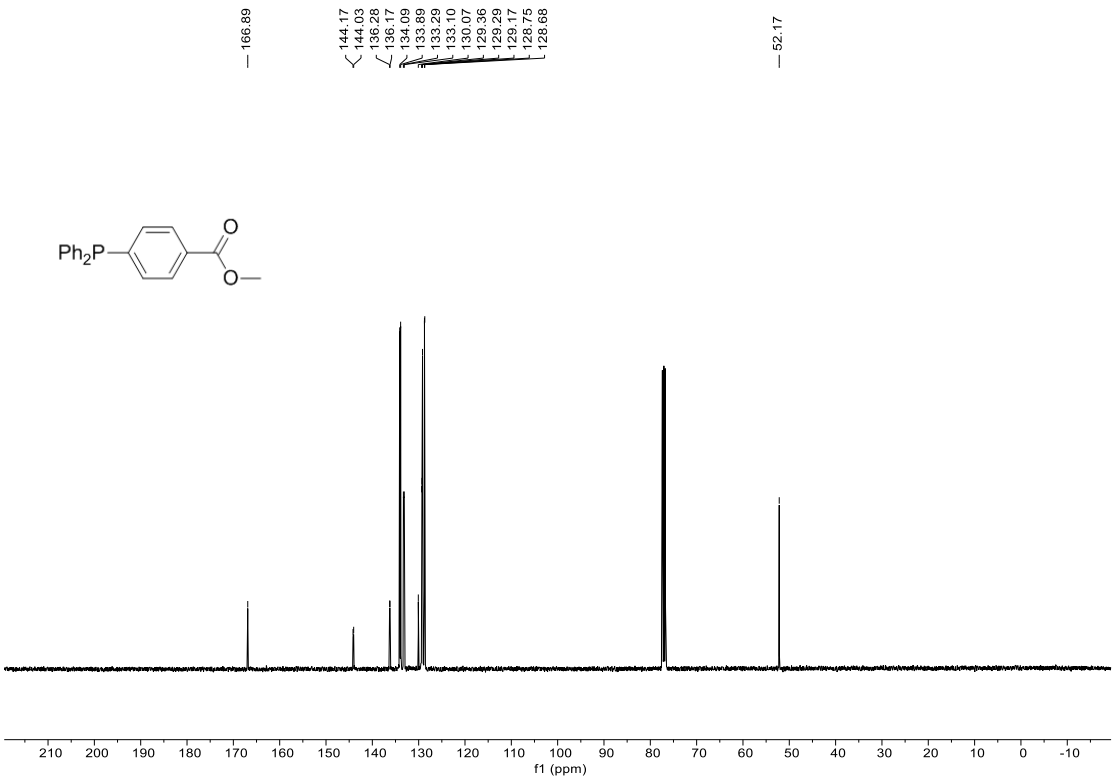
^{13}C NMR (101 MHz, $CDCl_3$) of **2v**



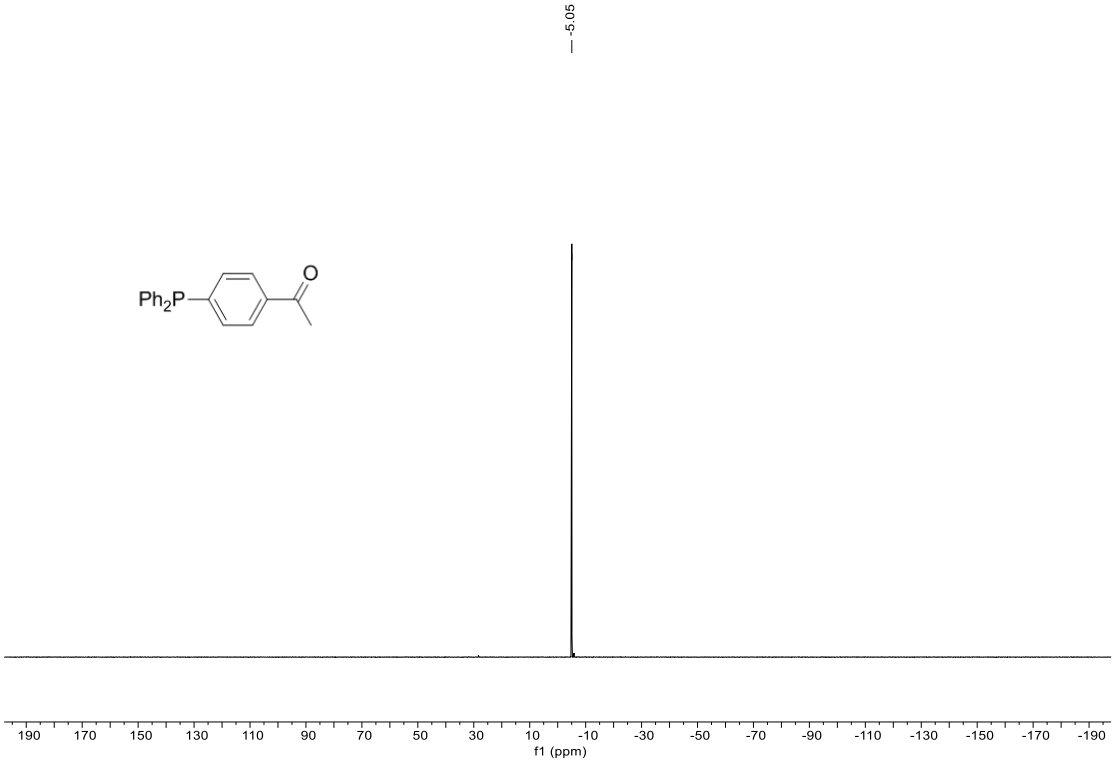
^{31}P NMR (162 MHz, $CDCl_3$) of **2w**



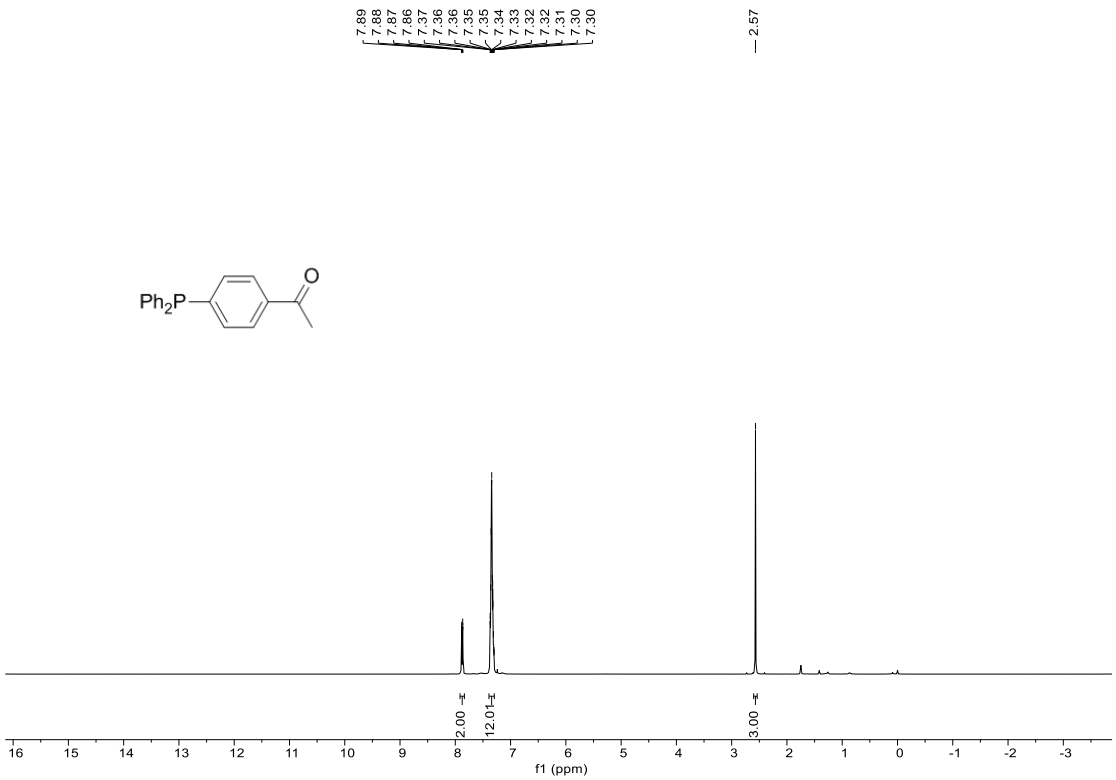
^{1}H NMR (400 MHz, $CDCl_3$) of **2w**



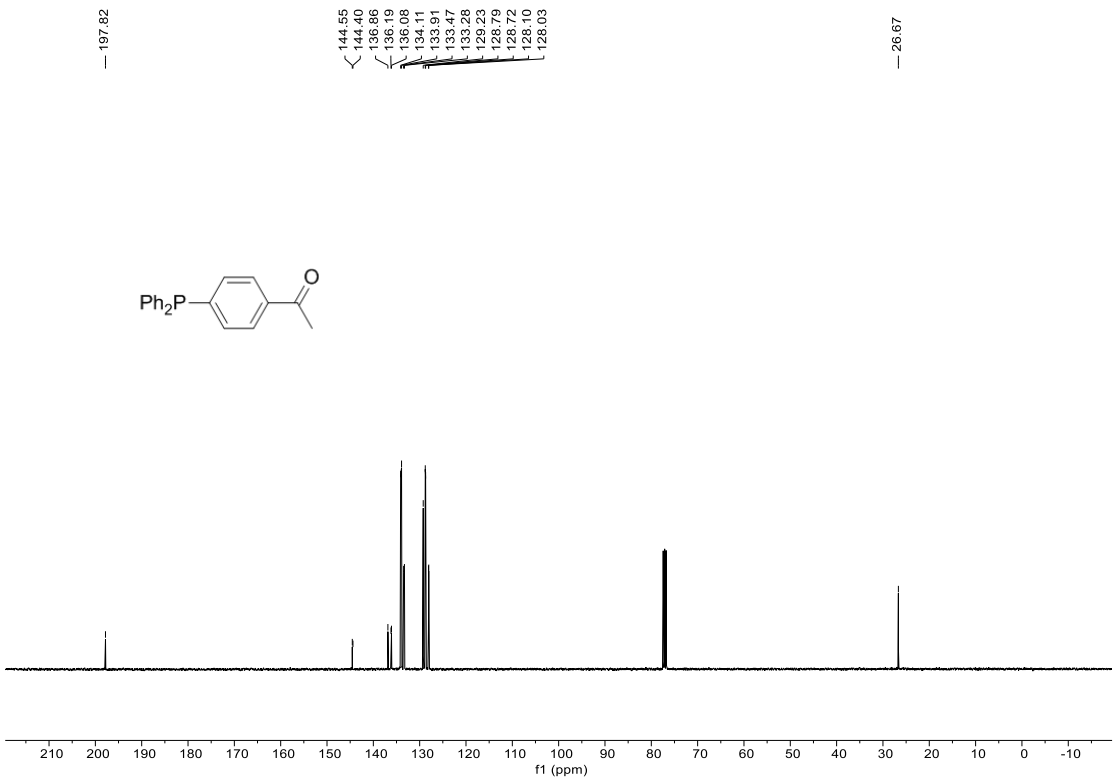
^{13}C NMR (101 MHz, $CDCl_3$) of **2w**



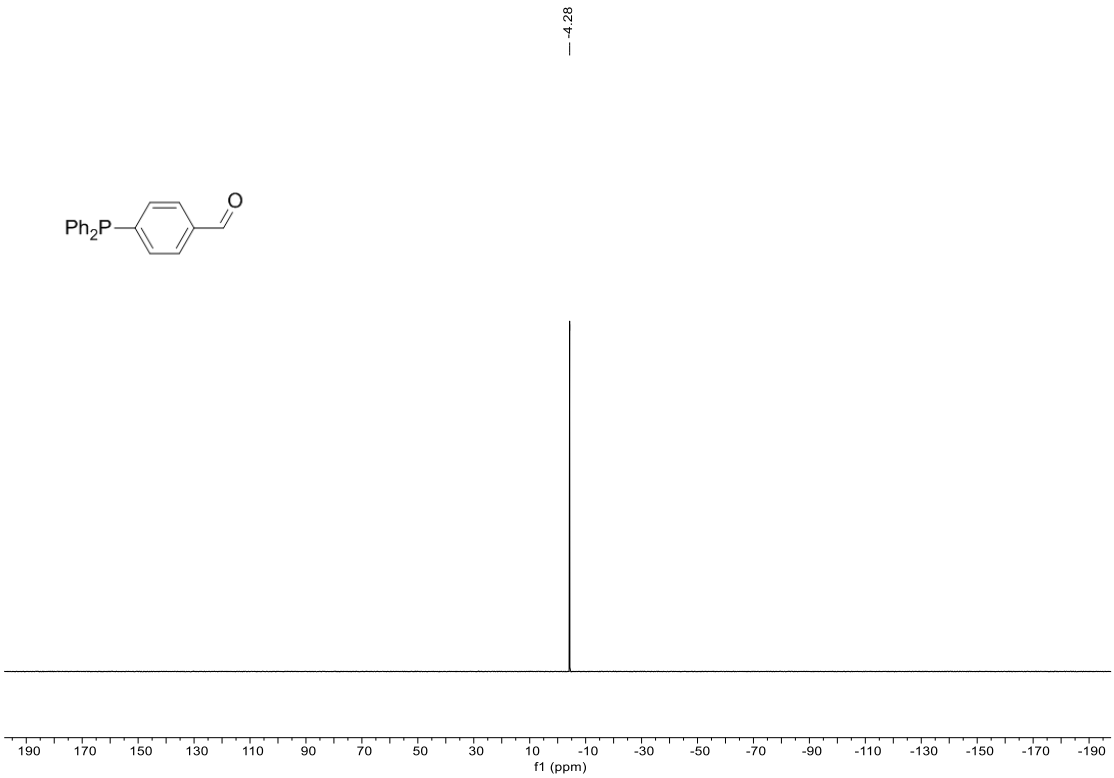
^{31}P NMR (162 MHz, $CDCl_3$) of **2x**



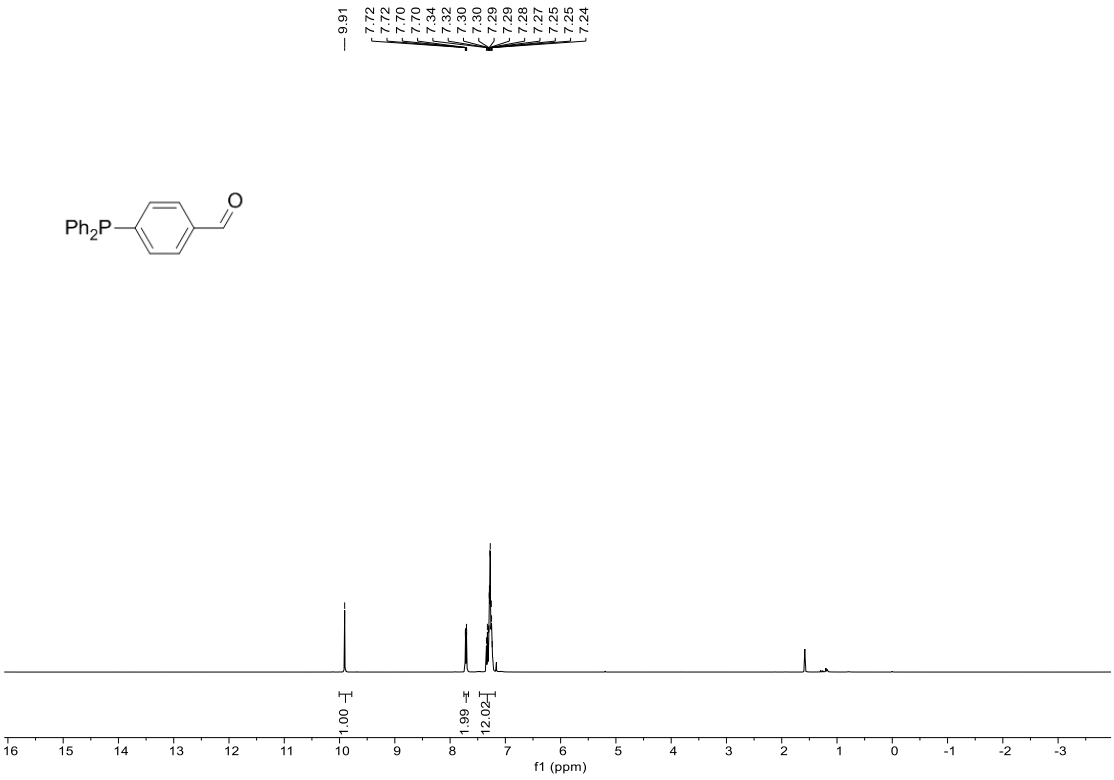
^{1}H NMR (400 MHz, $CDCl_3$) of **2x**



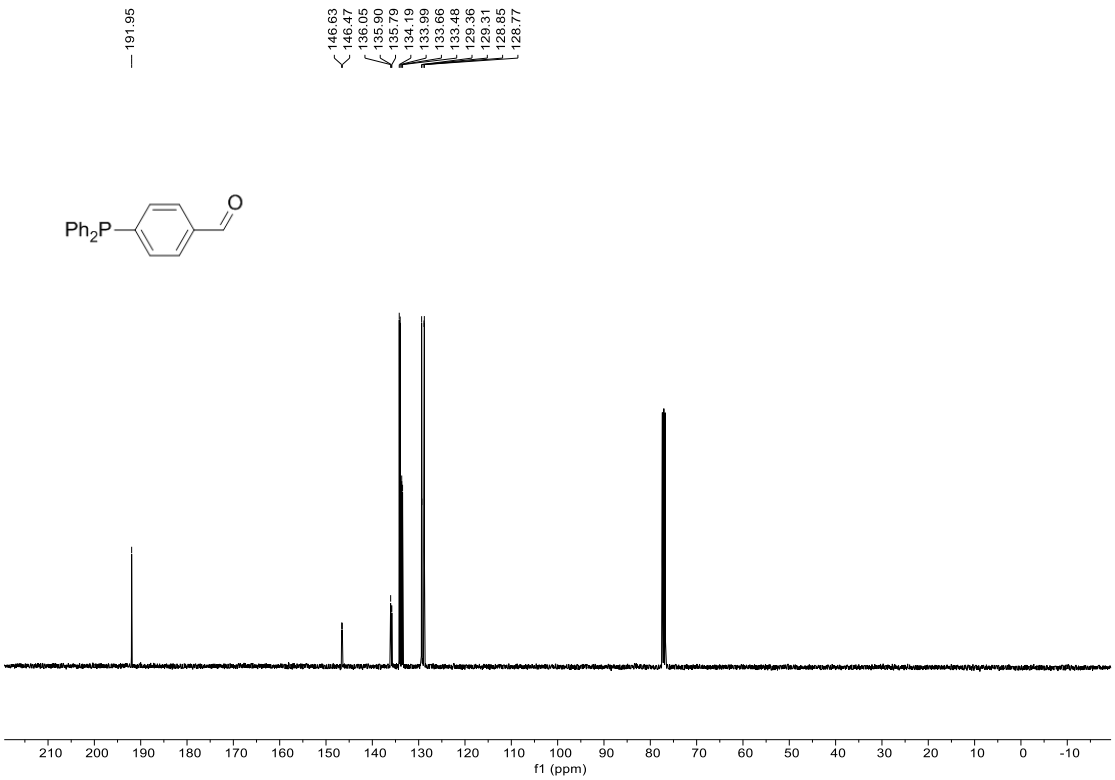
^{13}C NMR (101 MHz, $CDCl_3$) of **2x**



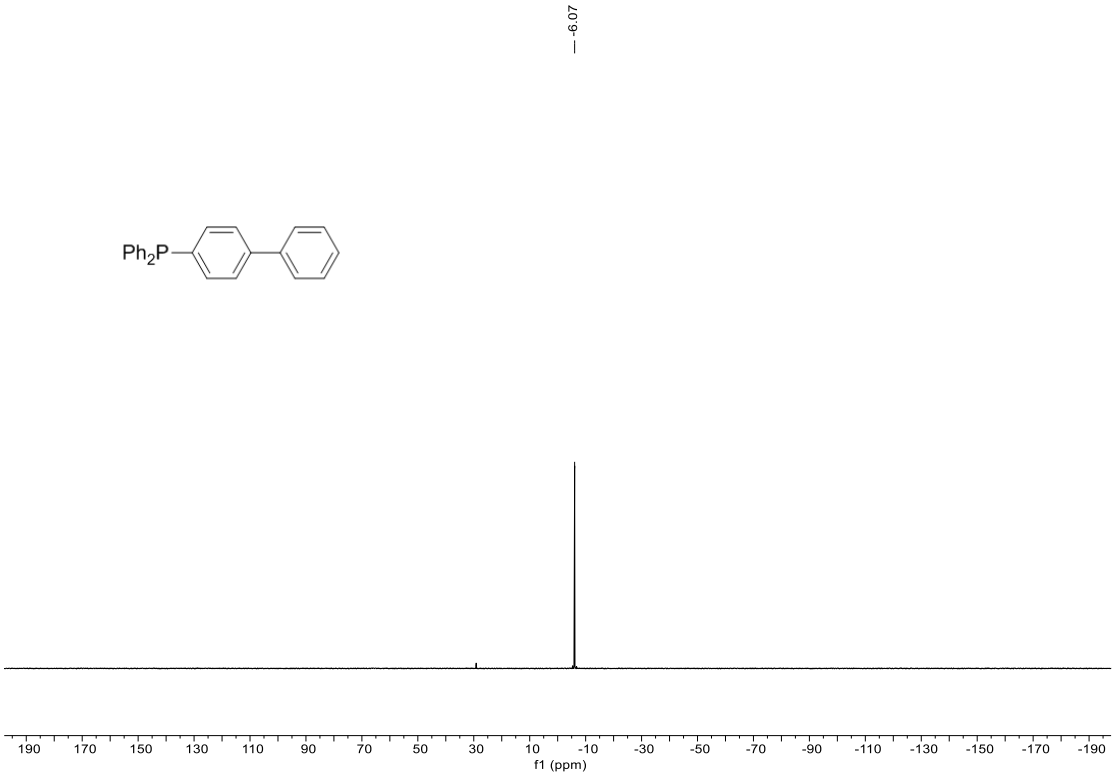
^{31}P NMR (162 MHz, $CDCl_3$) of **2y**



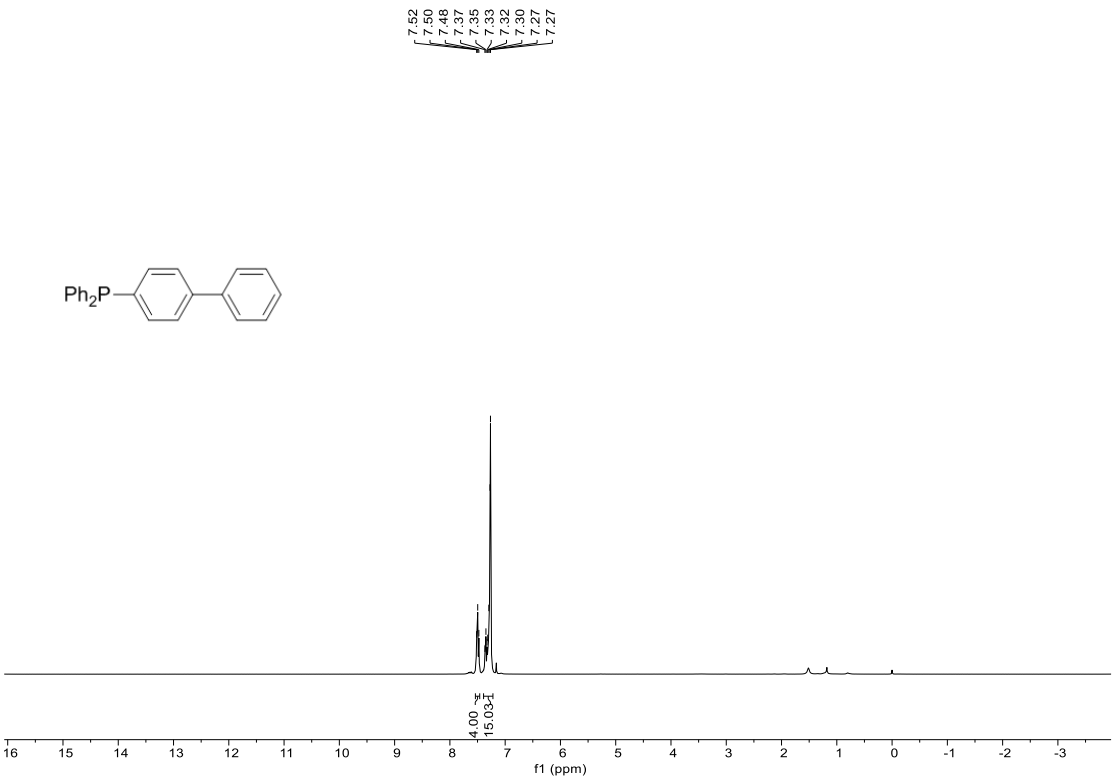
^{1}H NMR (400 MHz, $CDCl_3$) of **2y**



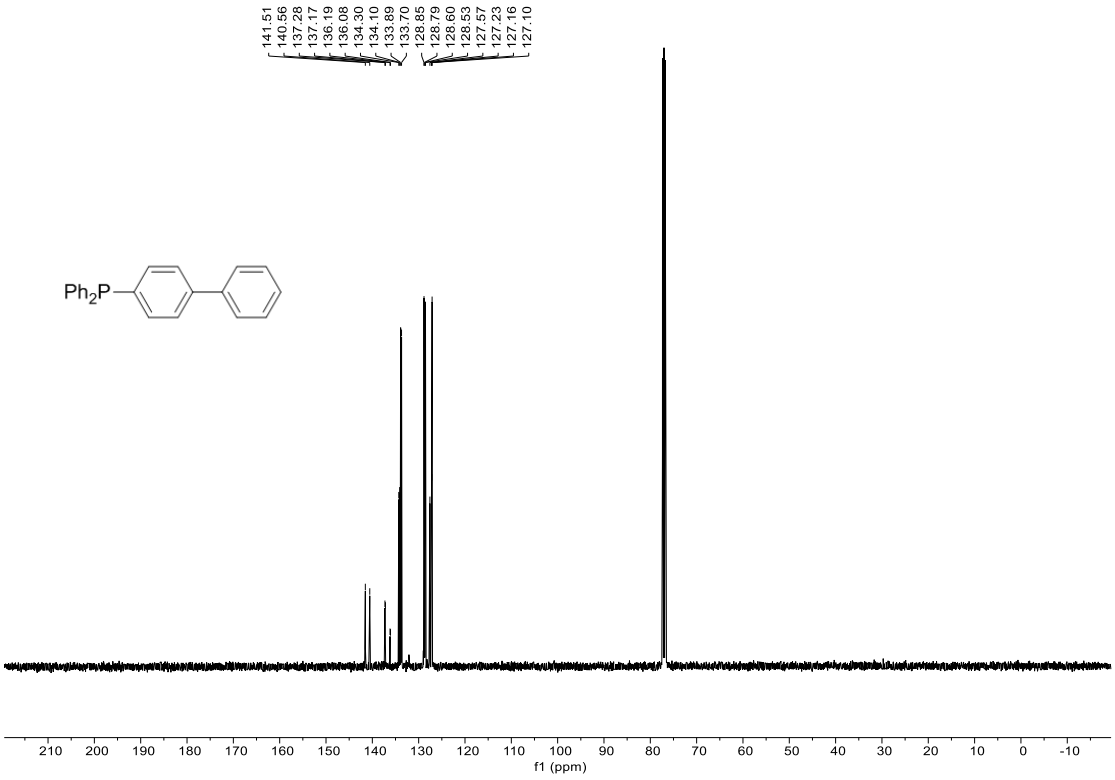
^{13}C NMR (101 MHz, $CDCl_3$) of **2y**



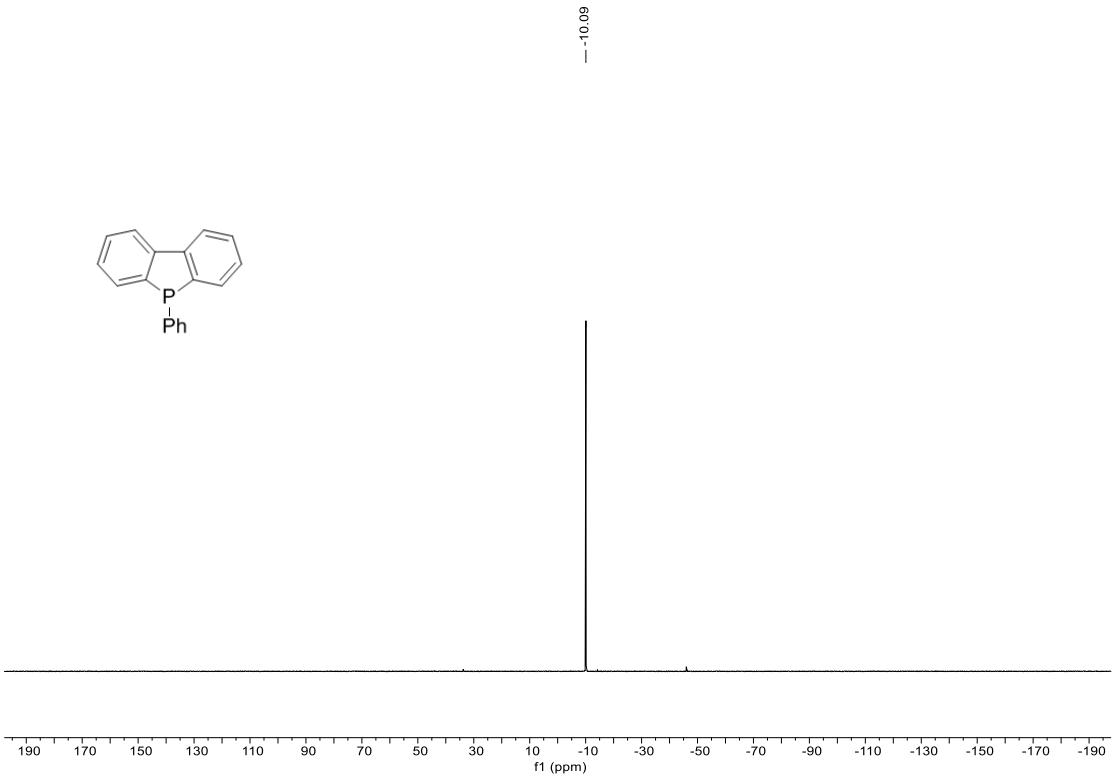
^{31}P NMR (162 MHz, $CDCl_3$) of **2z**



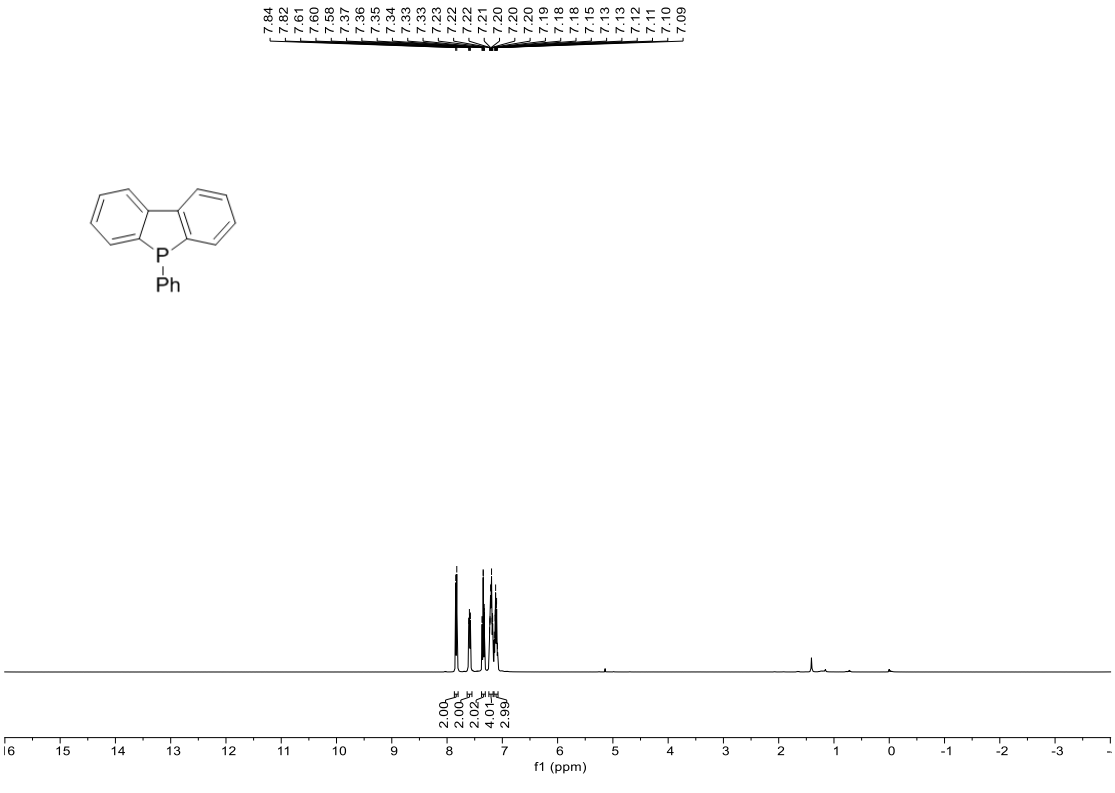
^{1}H NMR (400 MHz, $CDCl_3$) of **2z**



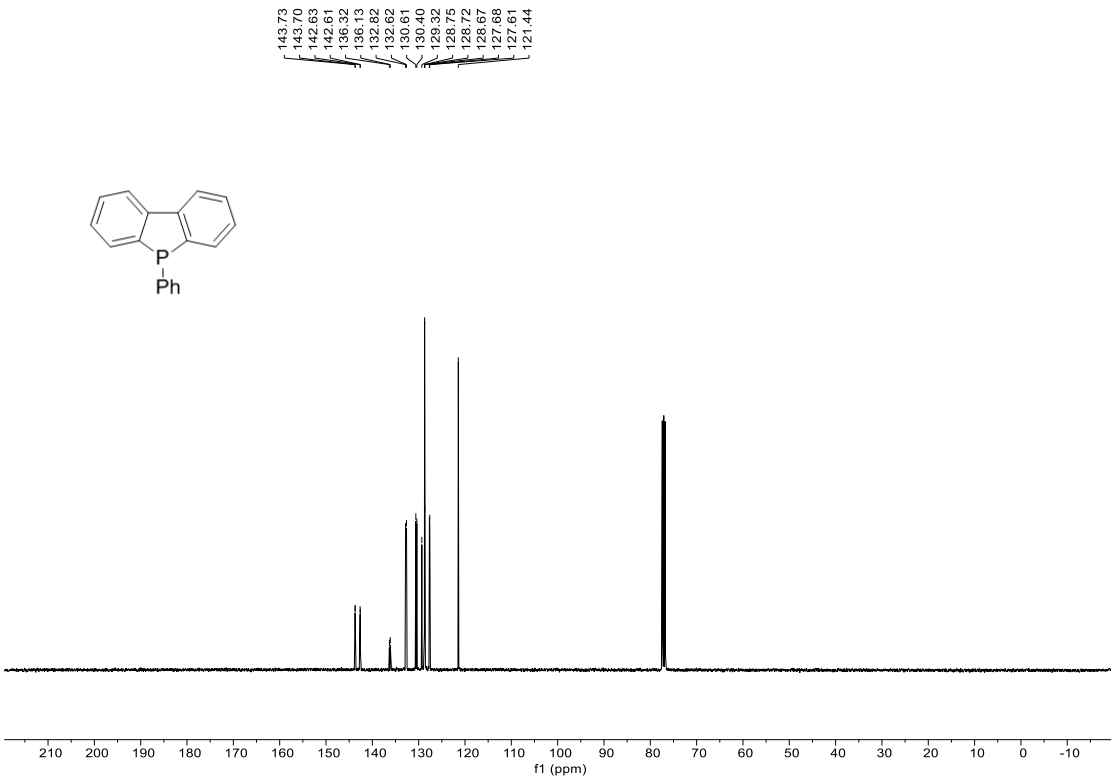
^{13}C NMR (101 MHz, $CDCl_3$) of **2z**



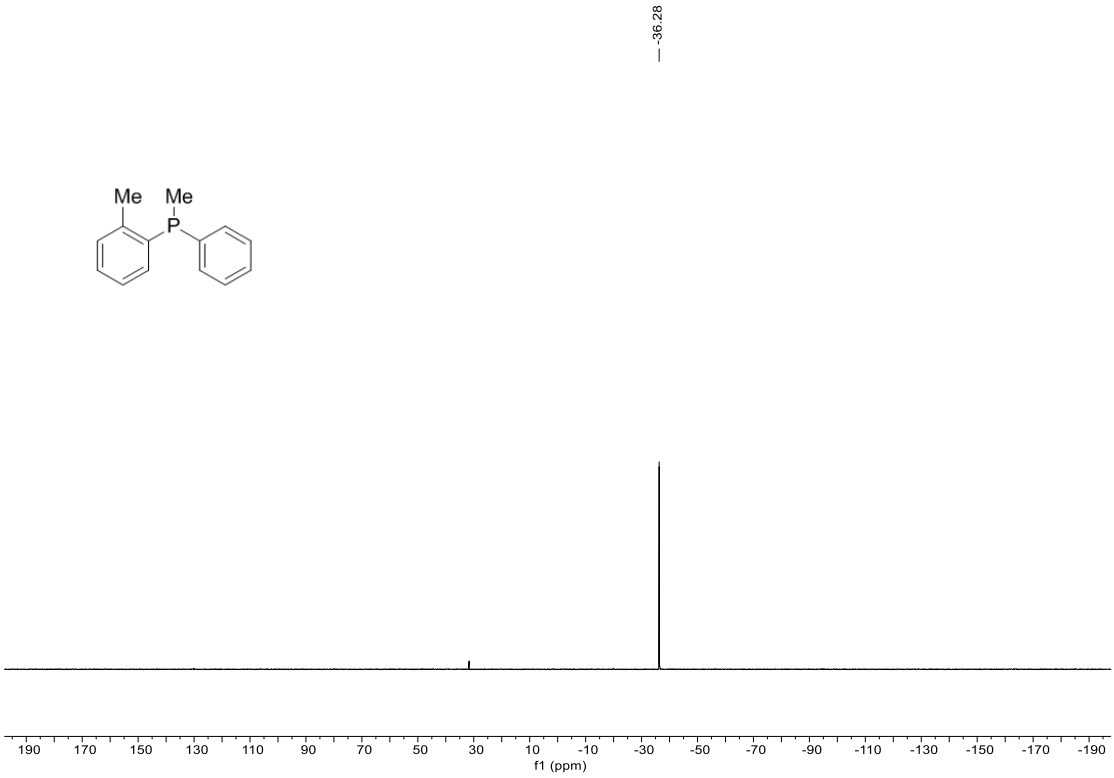
^{31}P NMR (162 MHz, $CDCl_3$) of **2aa**



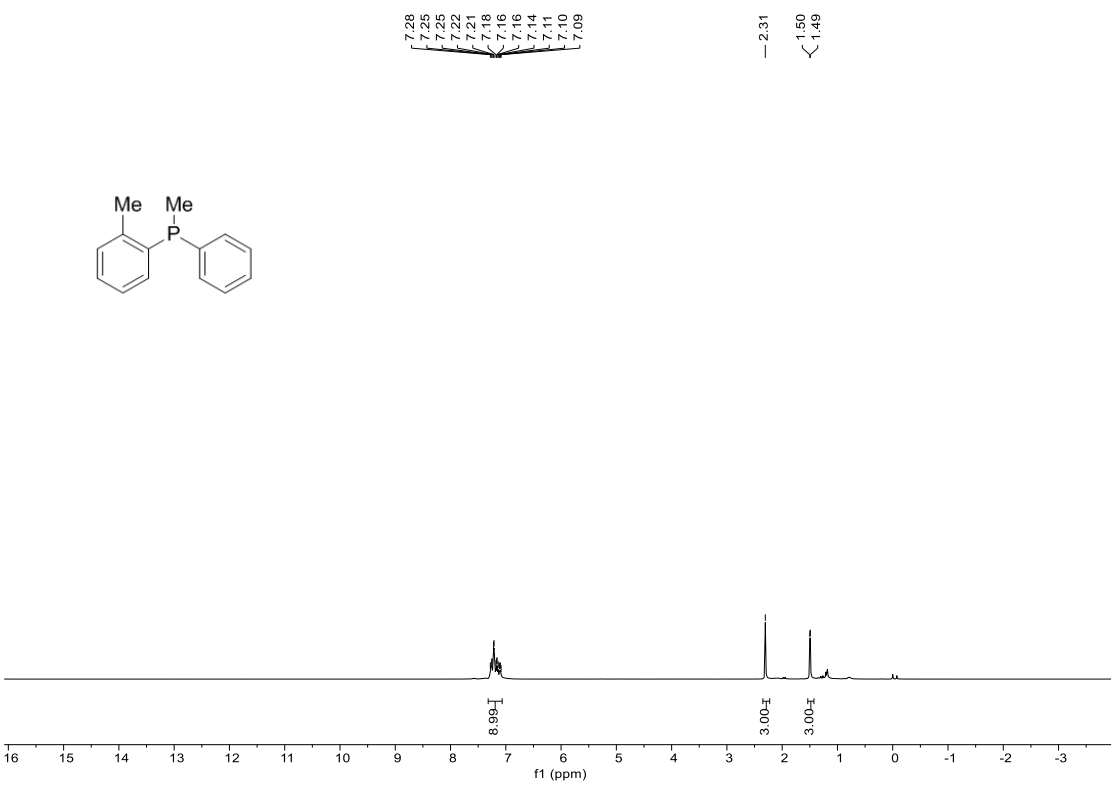
^{1}H NMR (400 MHz, $CDCl_3$) of **2aa**



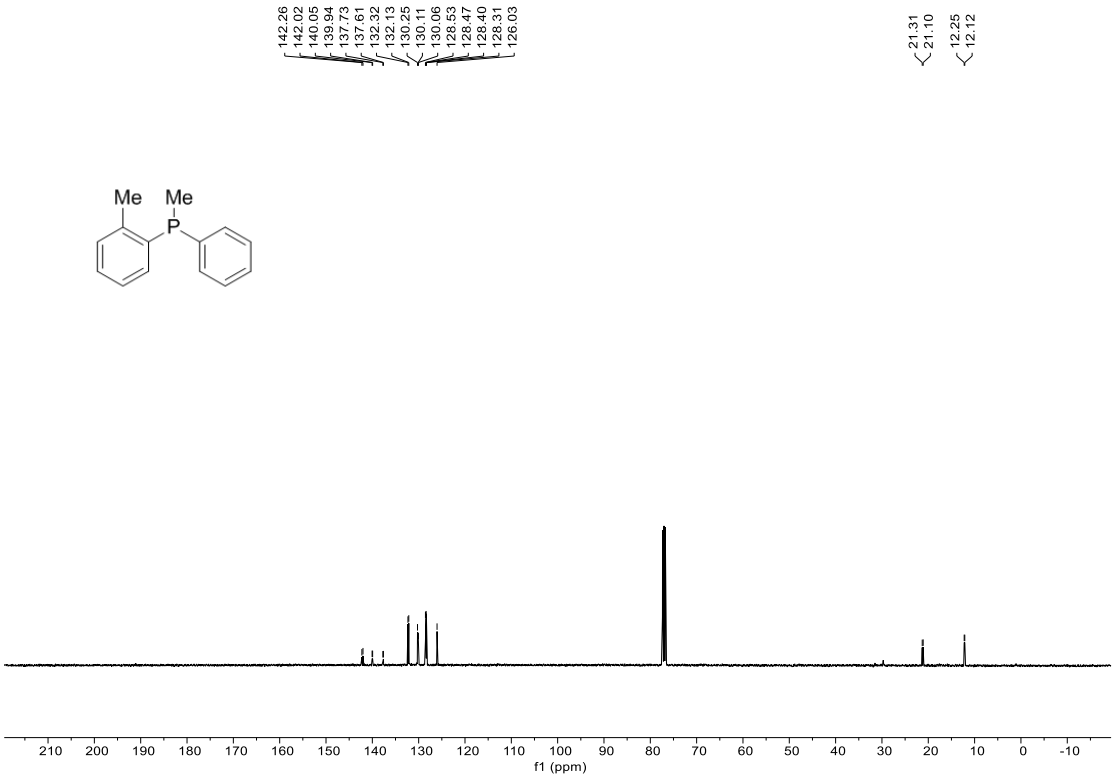
^{13}C NMR (101 MHz, $CDCl_3$) of **2aa**



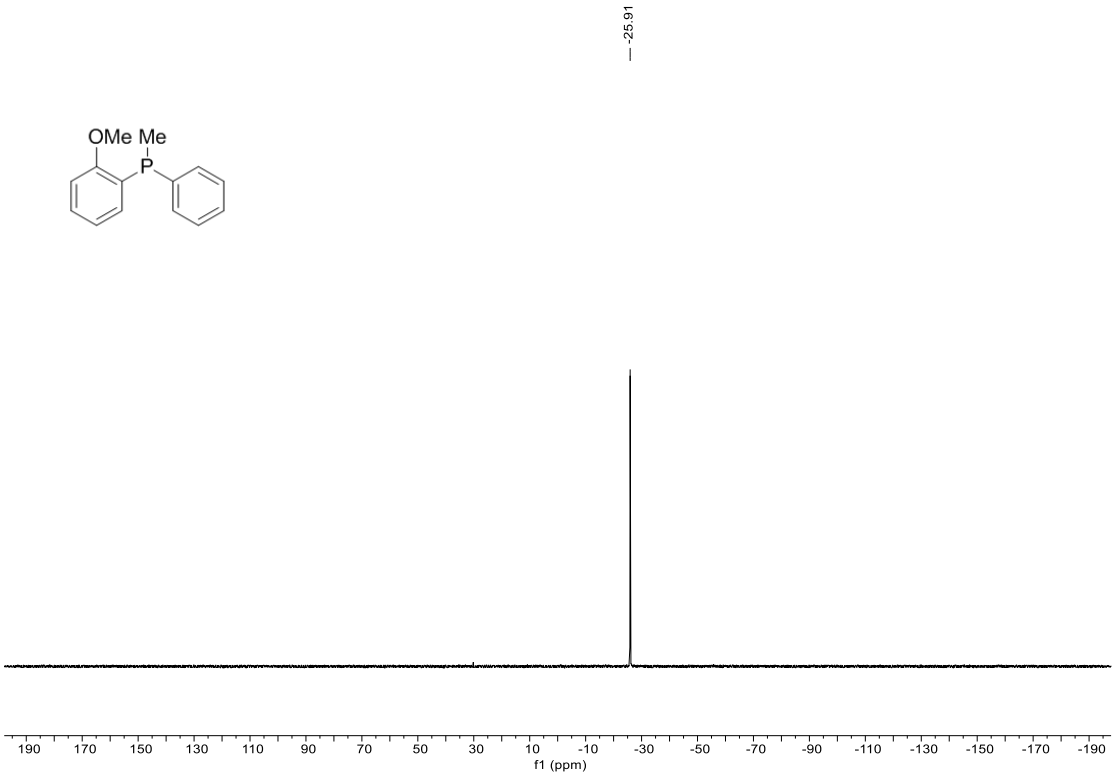
^{31}P NMR (162 MHz, $CDCl_3$) of **2ab**



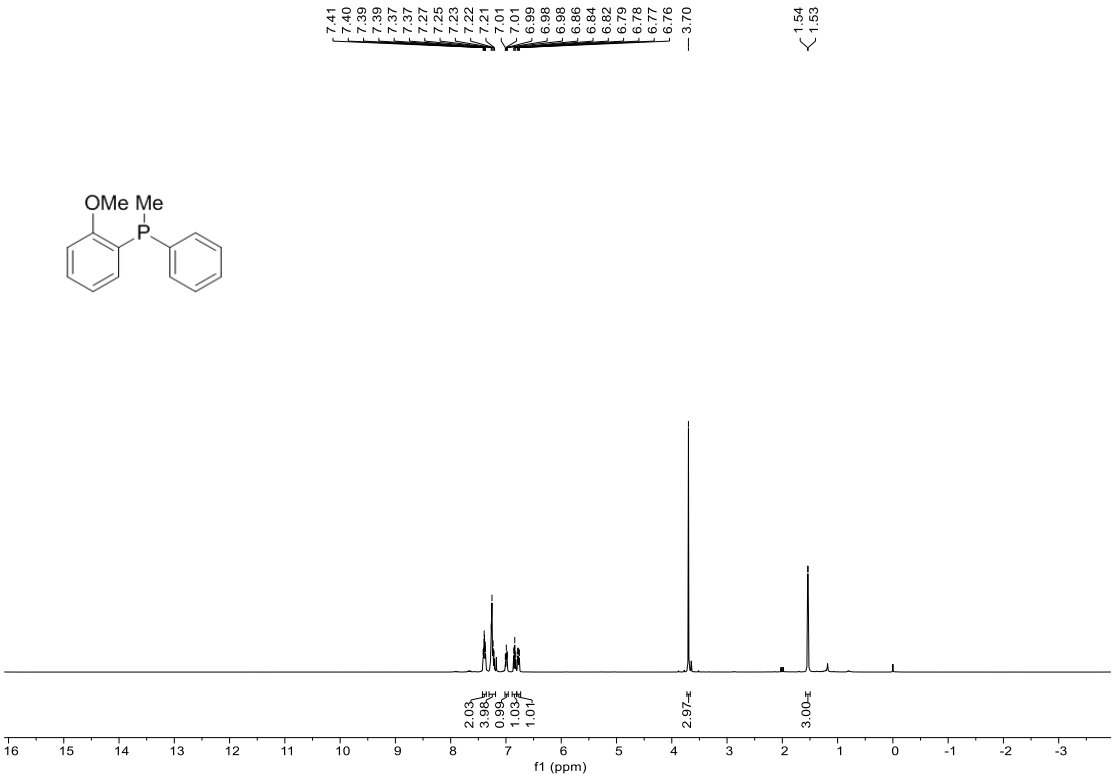
^{1}H NMR (400 MHz, $CDCl_3$) of **2ab**



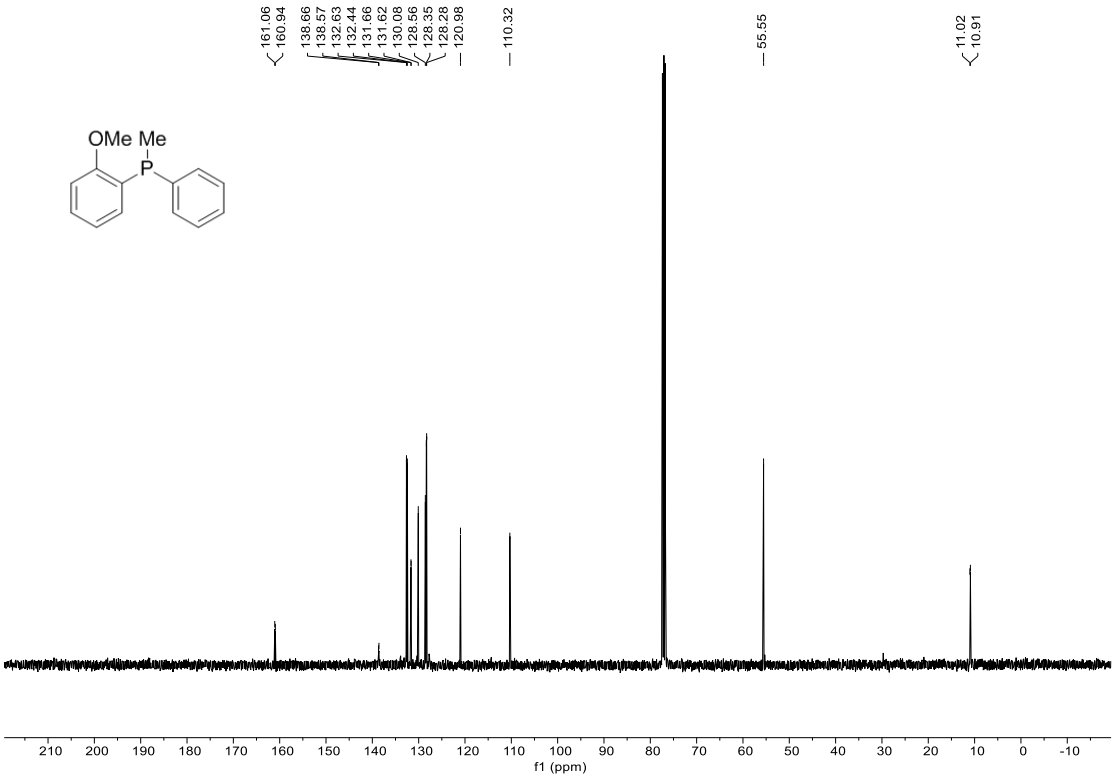
^{13}C NMR (101 MHz, $CDCl_3$) of **2ab**



^{31}P NMR (162 MHz, $CDCl_3$) of **2ac**

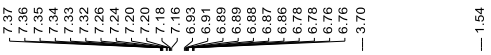


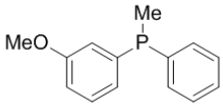
^{1}H NMR (400 MHz, $CDCl_3$) of **2ac**

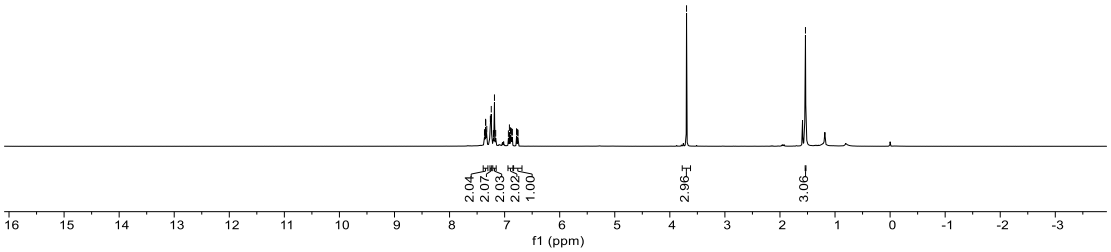


^{13}C NMR (101 MHz, $CDCl_3$) of **2ac**

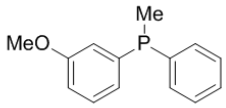
^{31}P NMR (162 MHz, $CDCl_3$) of **2ad**

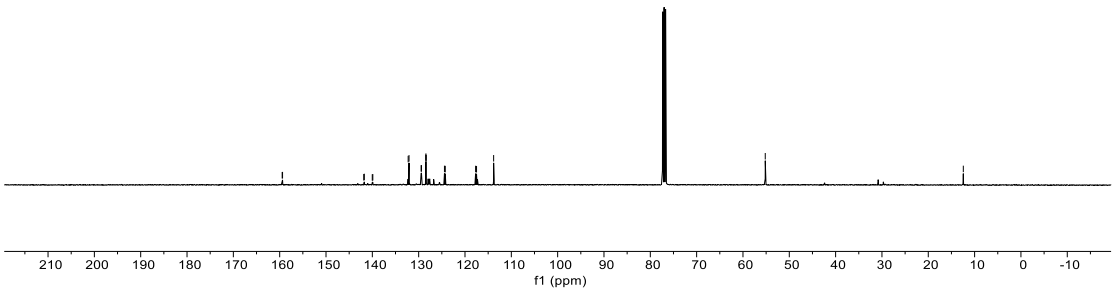




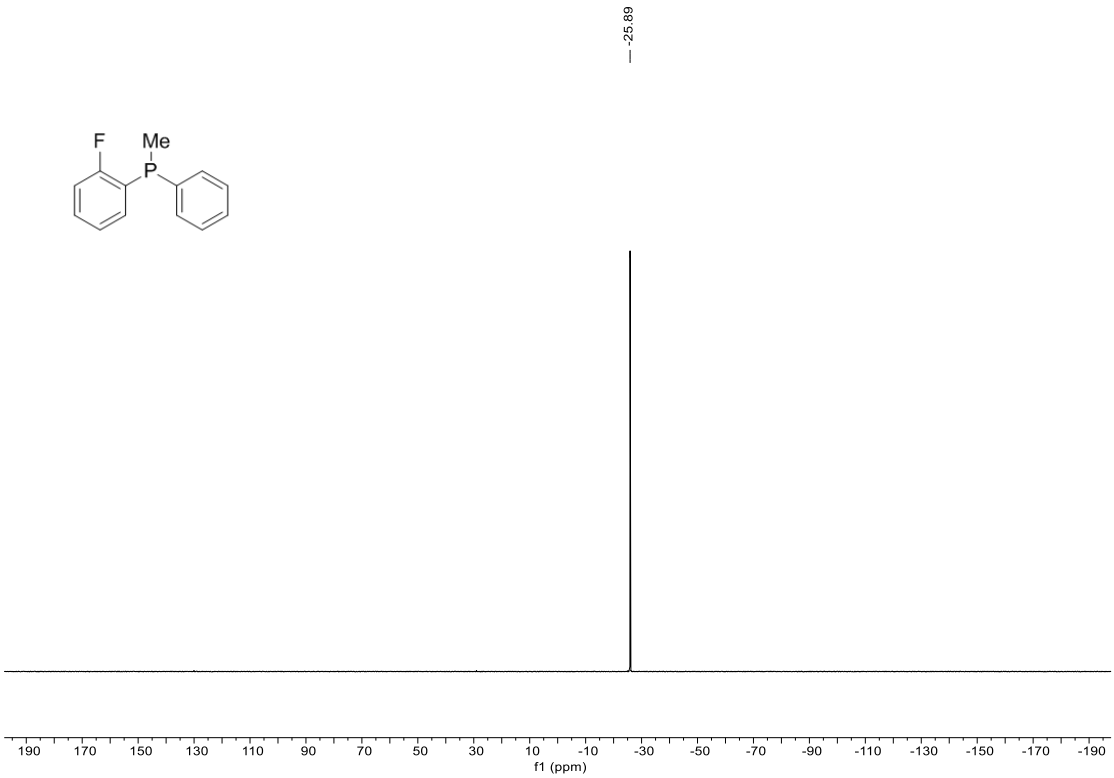


^{1}H NMR (400 MHz, $CDCl_3$) of **2ad**

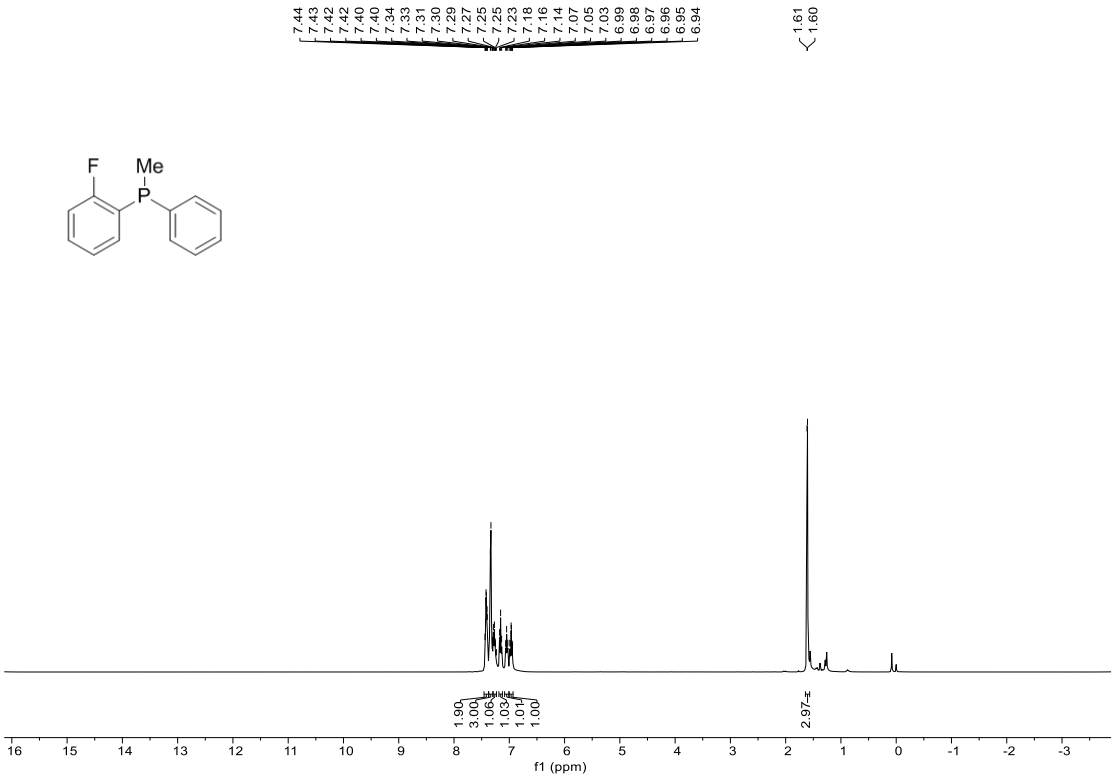




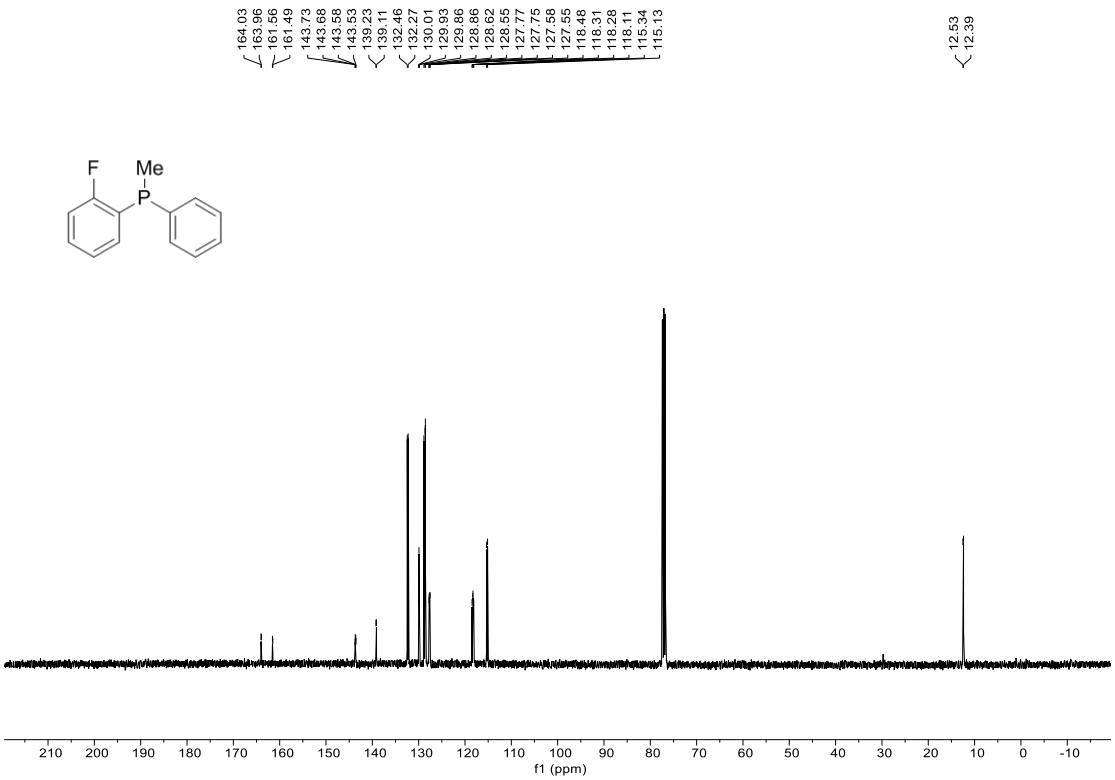
^{13}C NMR (101 MHz, $CDCl_3$) of **2ad**



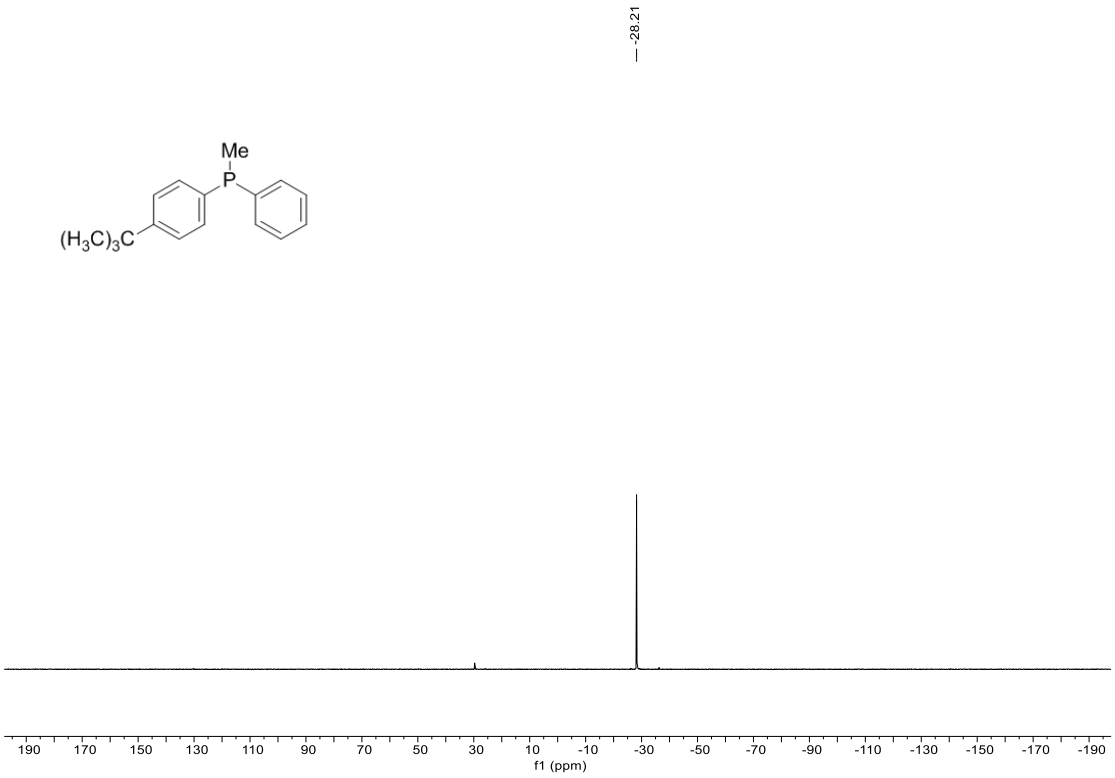
^{31}P NMR (162 MHz, $CDCl_3$) of **2ae**



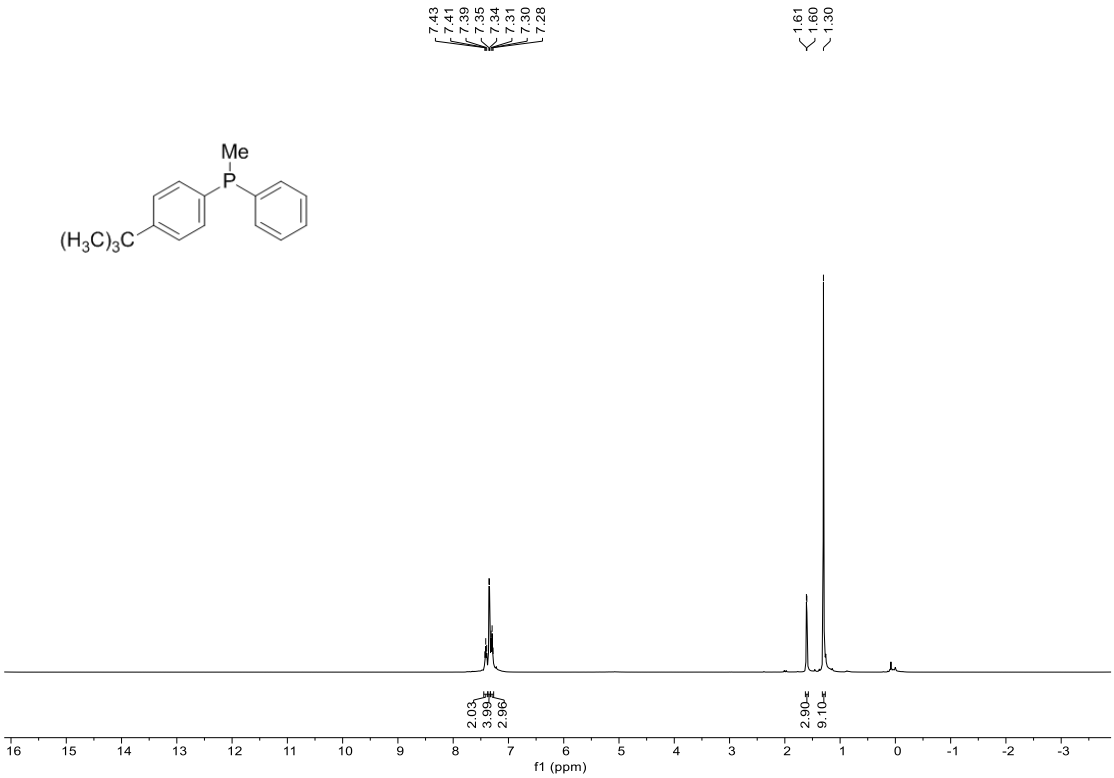
^{1}H NMR (400 MHz, $CDCl_3$) of **2ae**



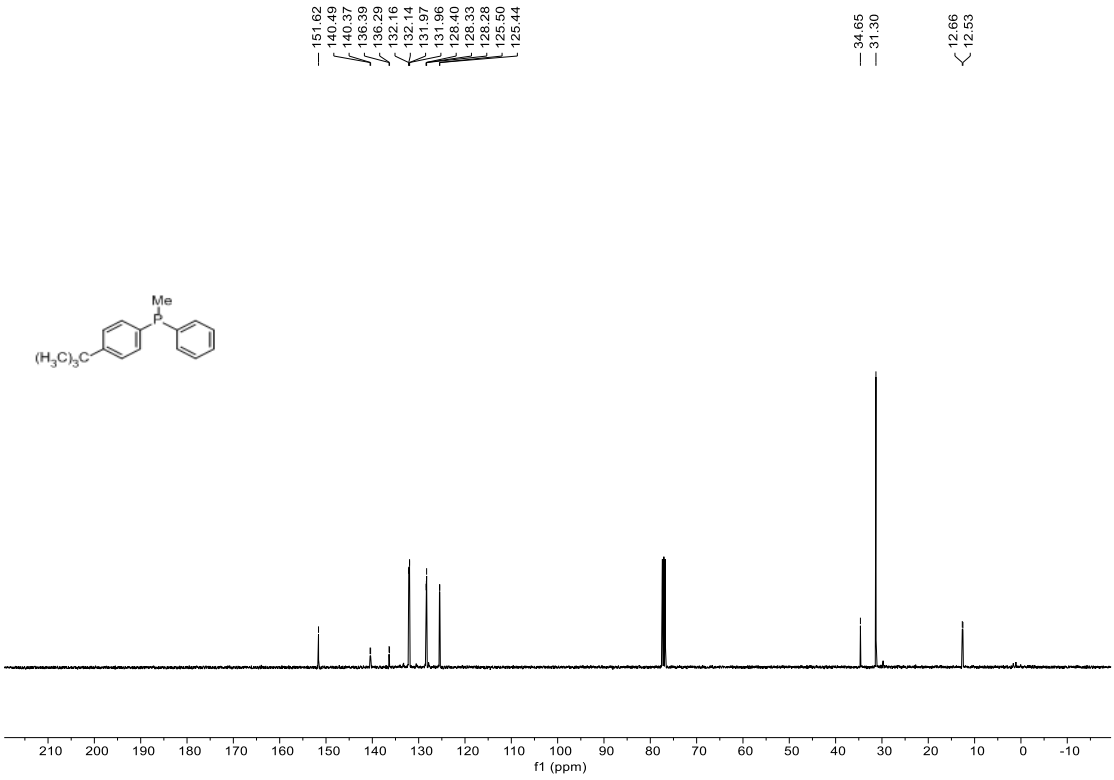
^{13}C NMR (101 MHz, $CDCl_3$) of **2ae**



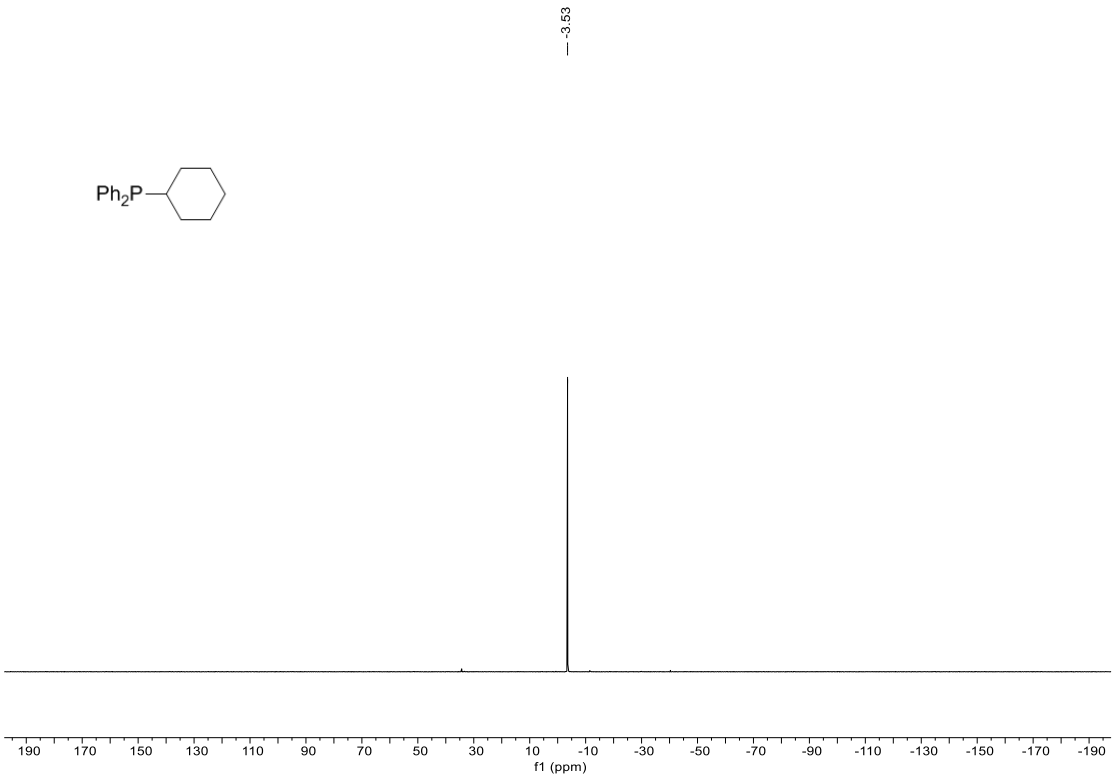
^{31}P NMR (162 MHz, $CDCl_3$) of **2af**



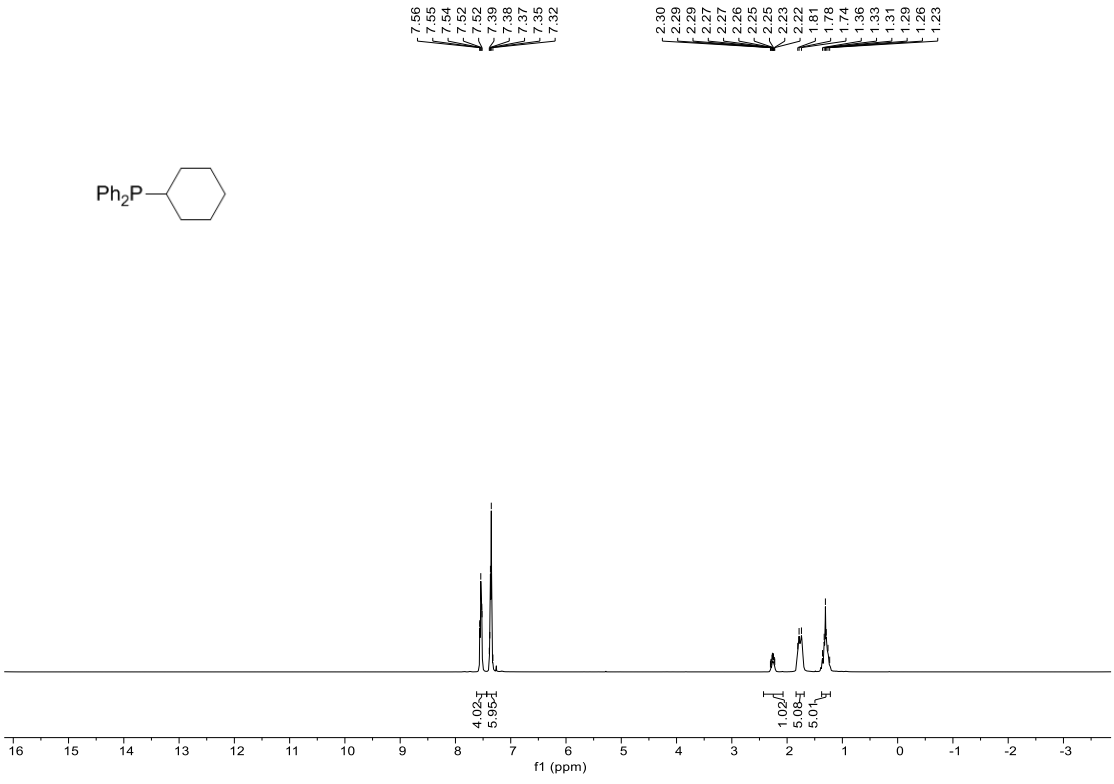
^{1}H NMR (400 MHz, $CDCl_3$) of **2af**



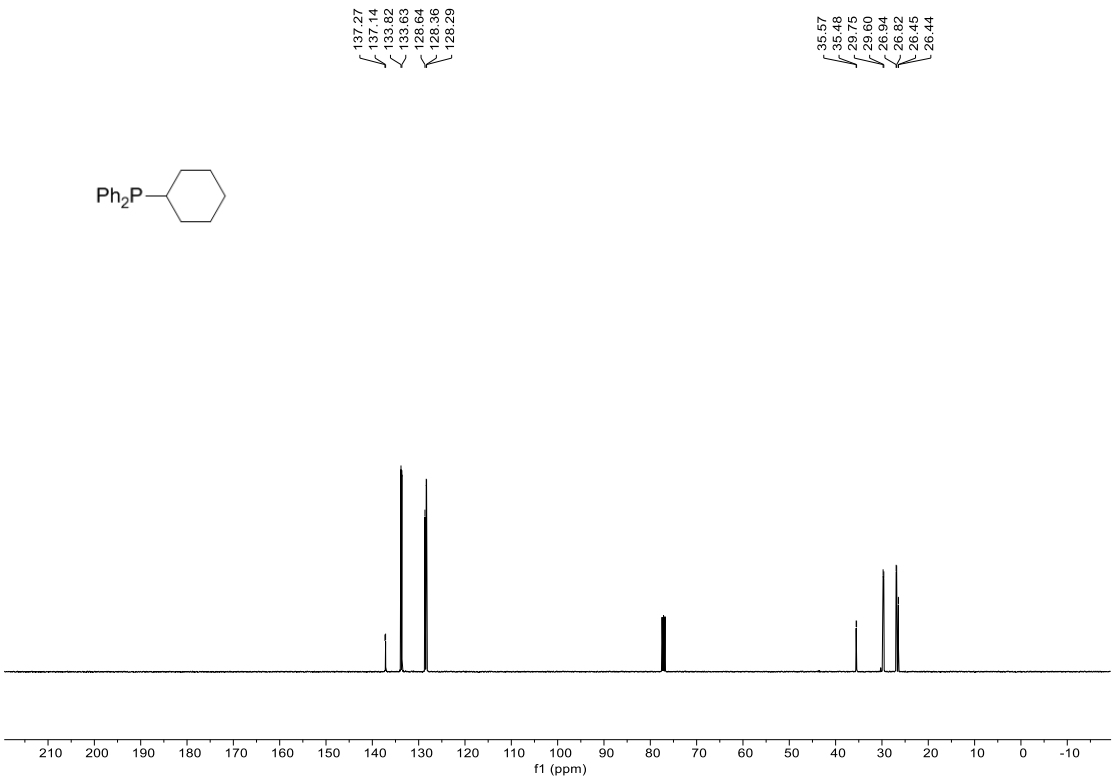
^{13}C NMR (101 MHz, $CDCl_3$) of **2af**



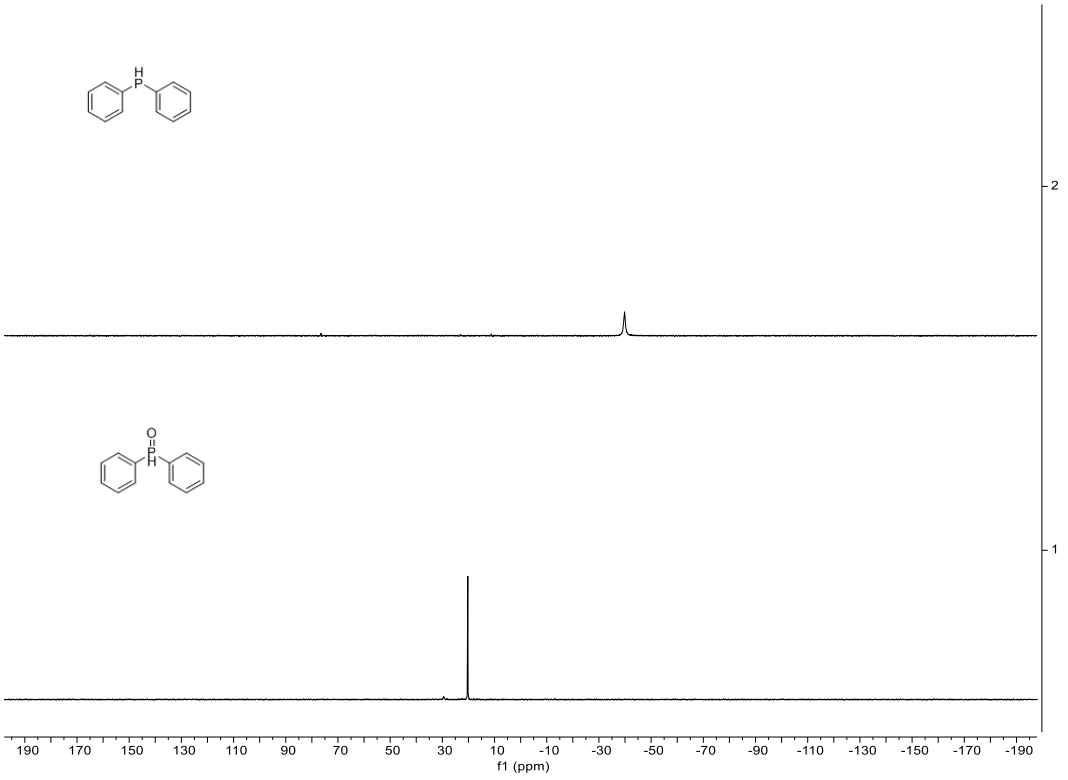
^{31}P NMR (162 MHz, $CDCl_3$) of **2ag**



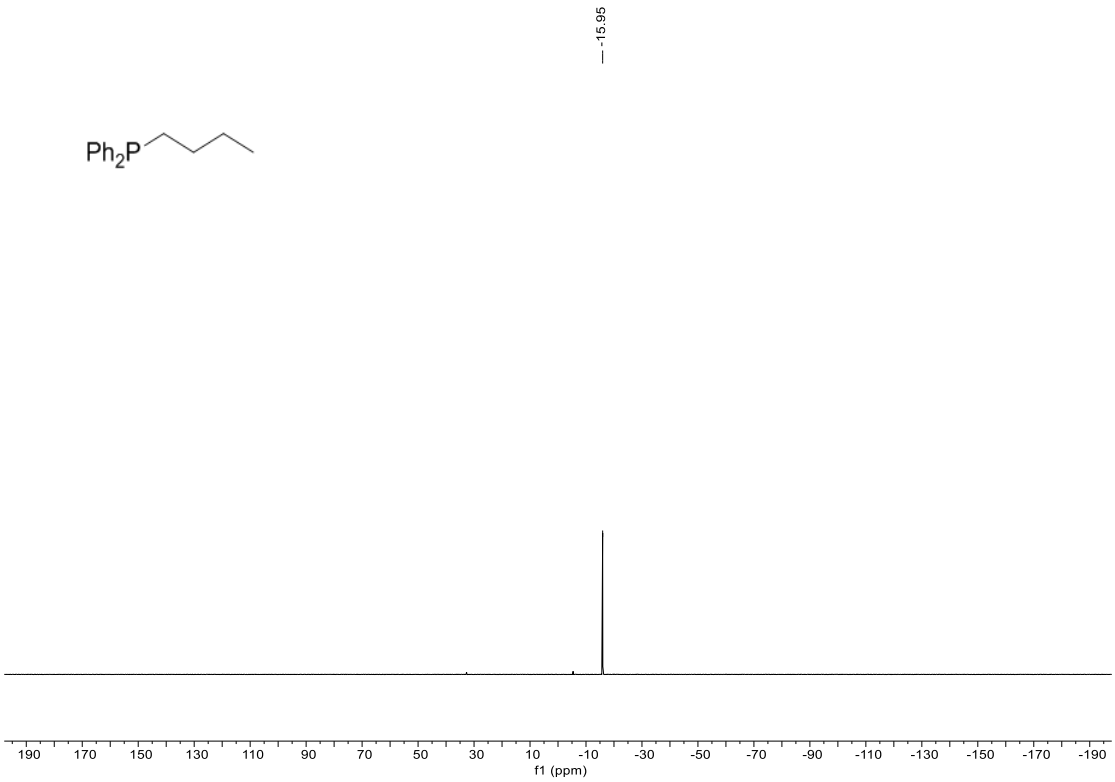
^{1}H NMR (400 MHz, $CDCl_3$) of **2ag**



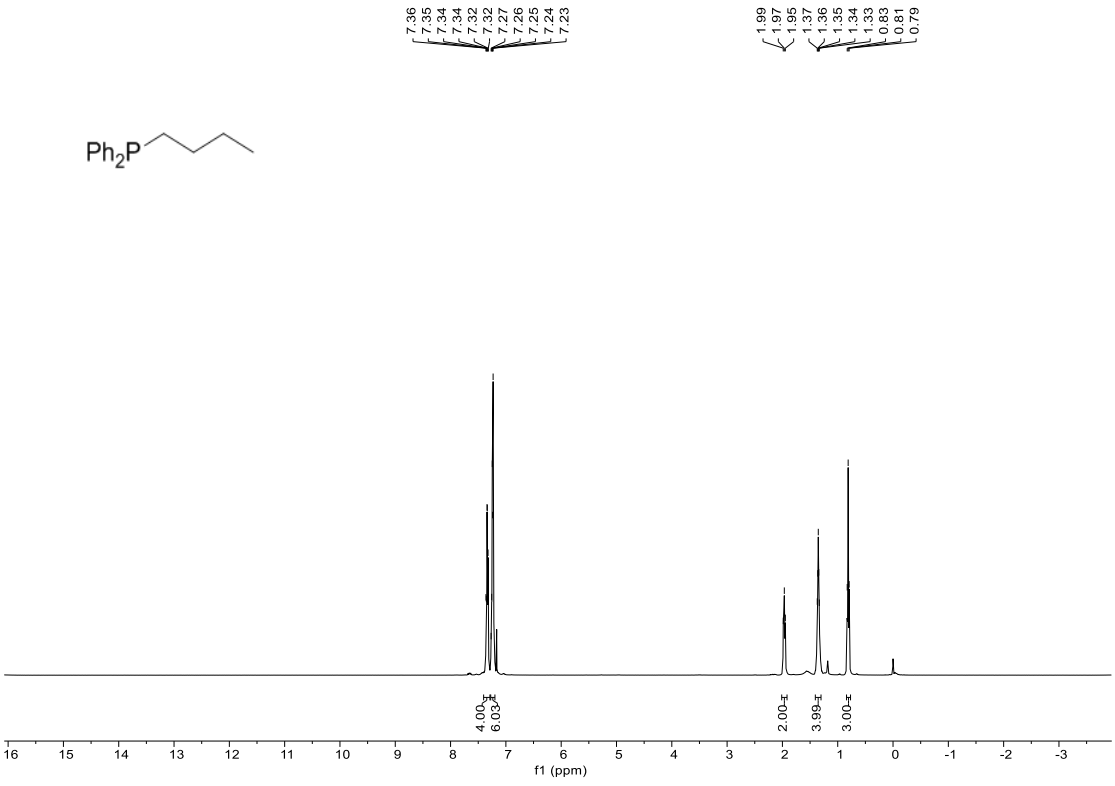
^{13}C NMR (101 MHz, $CDCl_3$) of **2ag**



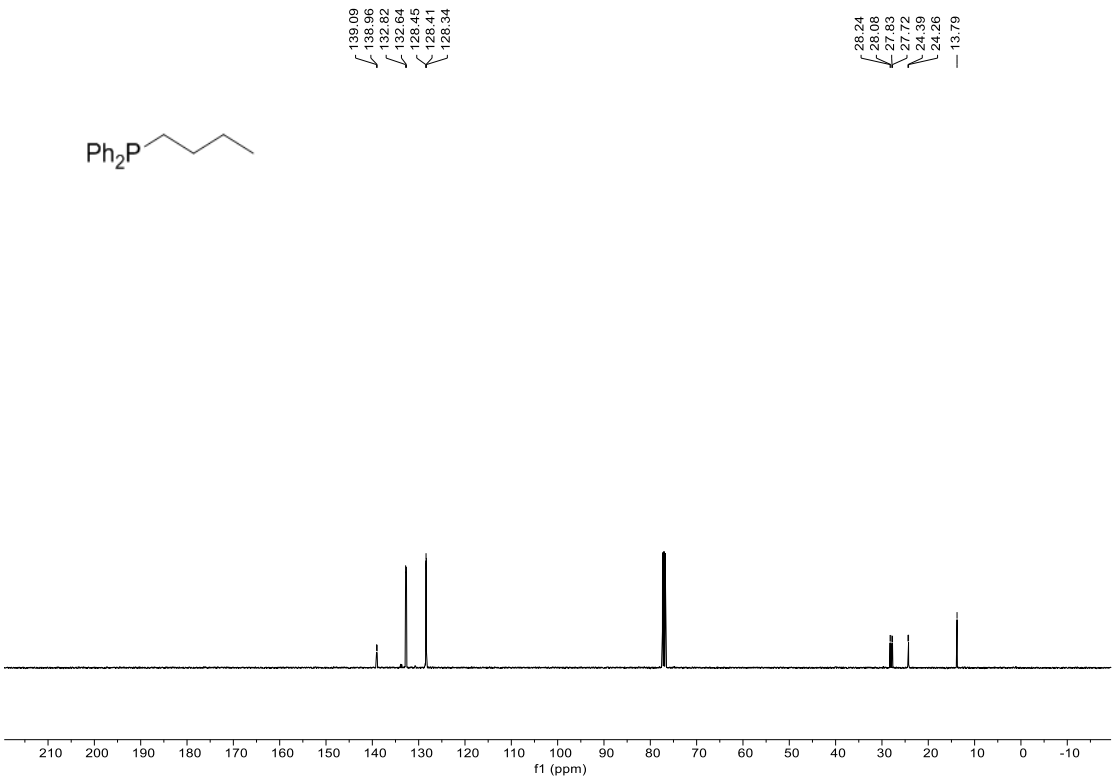
^{31}P NMR (162 MHz, $CDCl_3$) of **2ah**



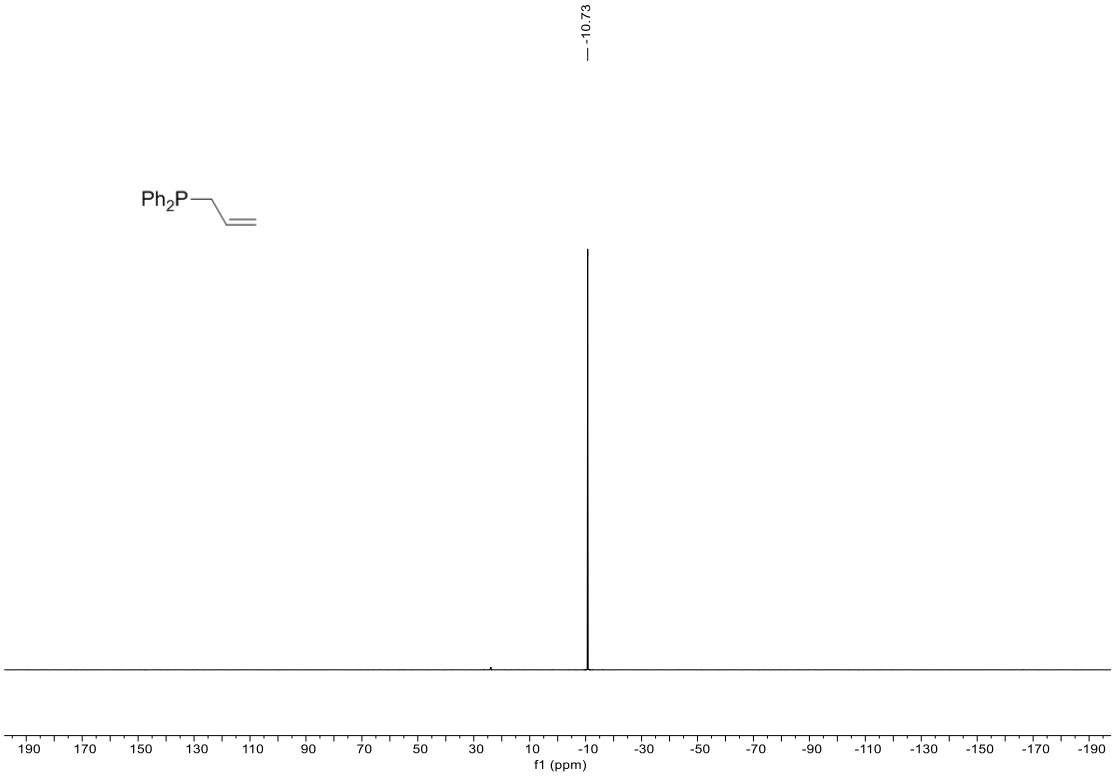
^{31}P NMR (162 MHz, $CDCl_3$) of **2ai**



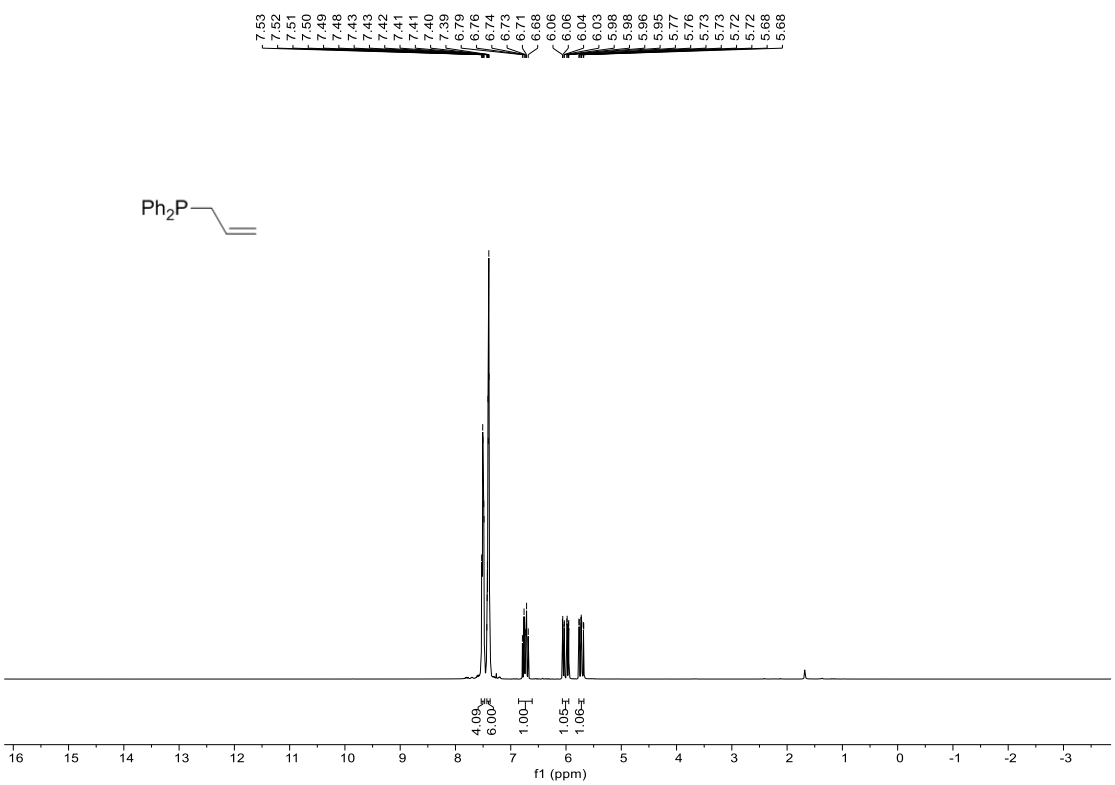
^{1}H NMR (400 MHz, $CDCl_3$) of **2ai**



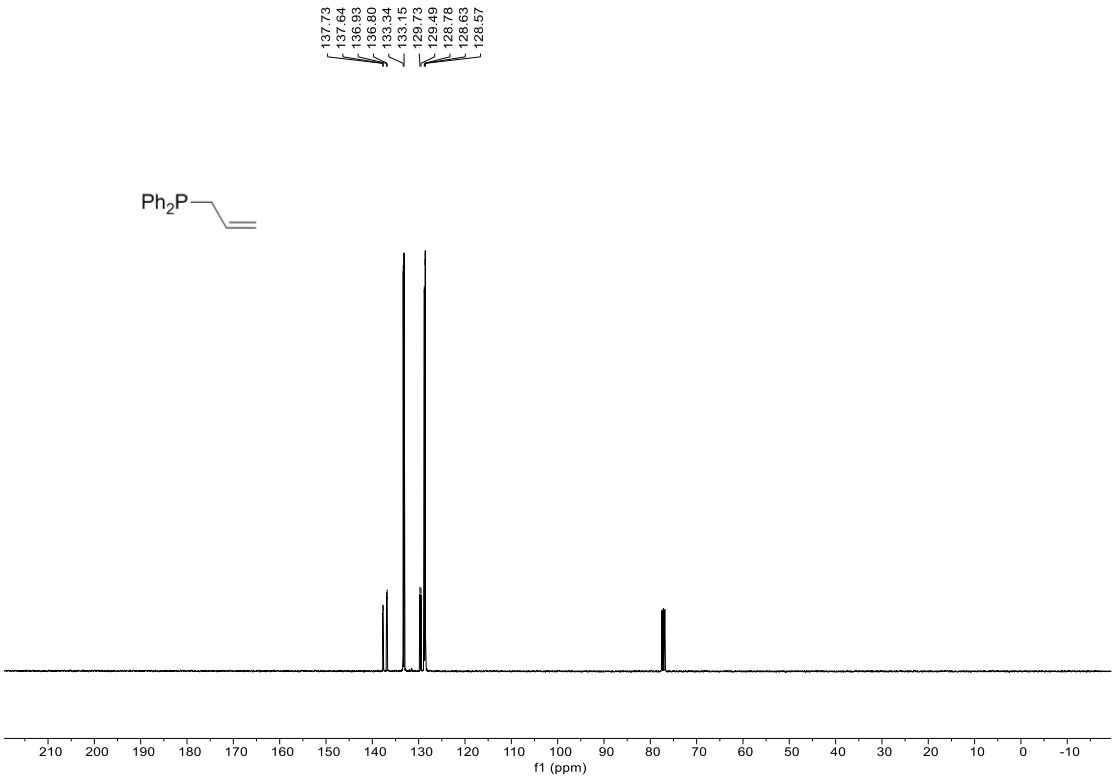
^{13}C NMR (101 MHz, $CDCl_3$) of **2ai**



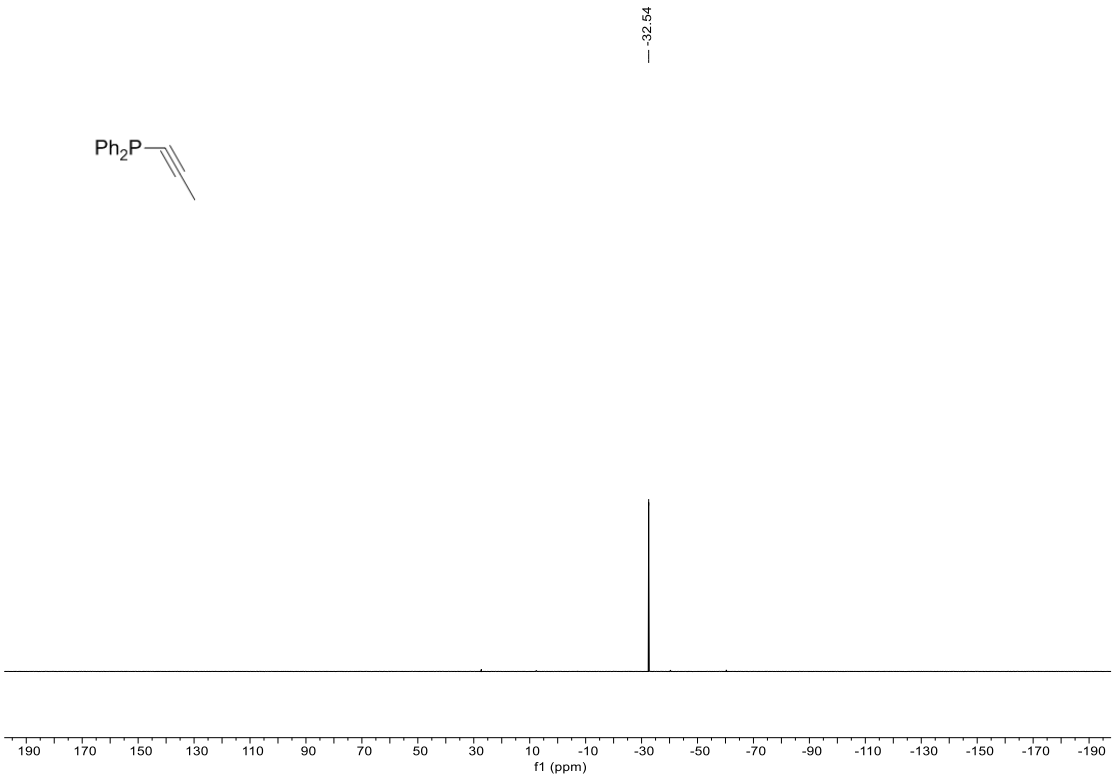
^{31}P NMR (162 MHz, $CDCl_3$) of **2aj**



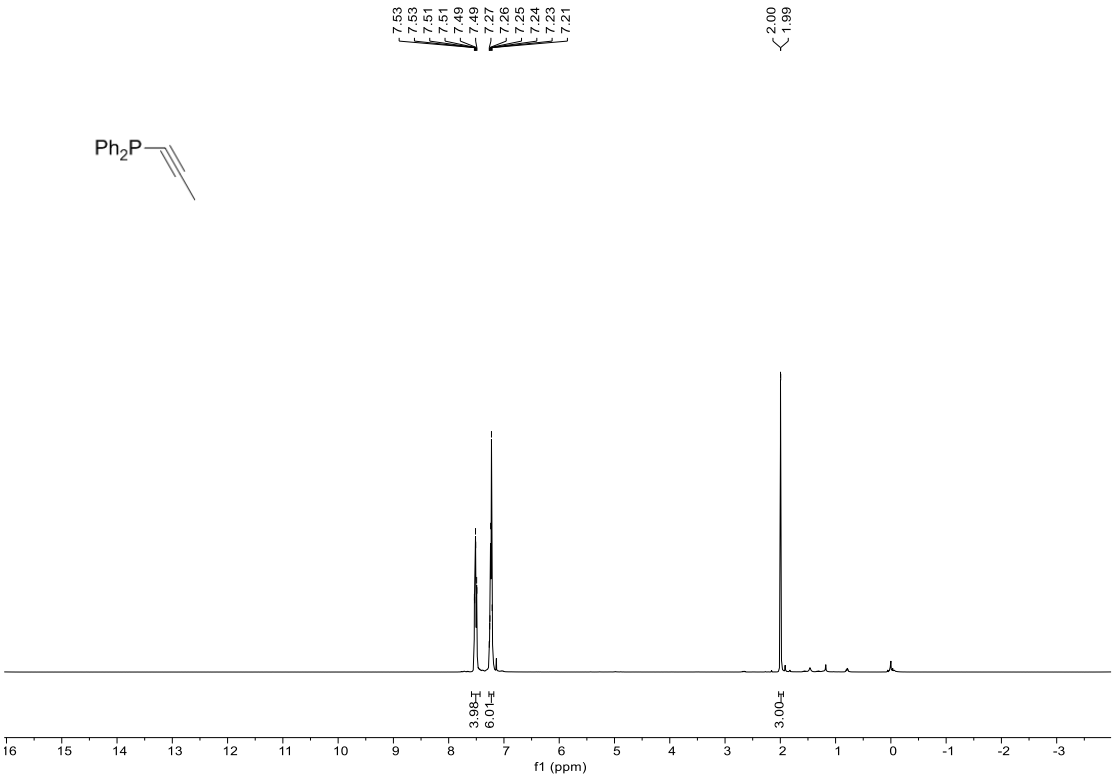
^{1}H NMR (400 MHz, $CDCl_3$) of **2aj**



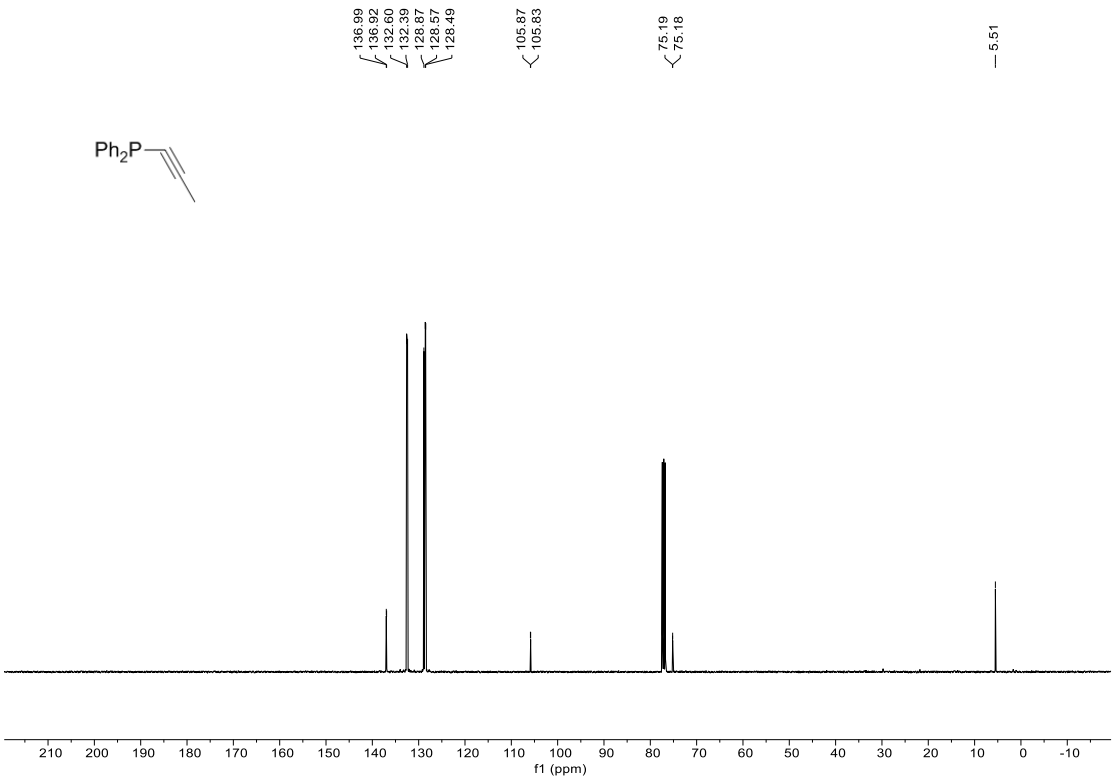
^{13}C NMR (101 MHz, $CDCl_3$) of **2aj**



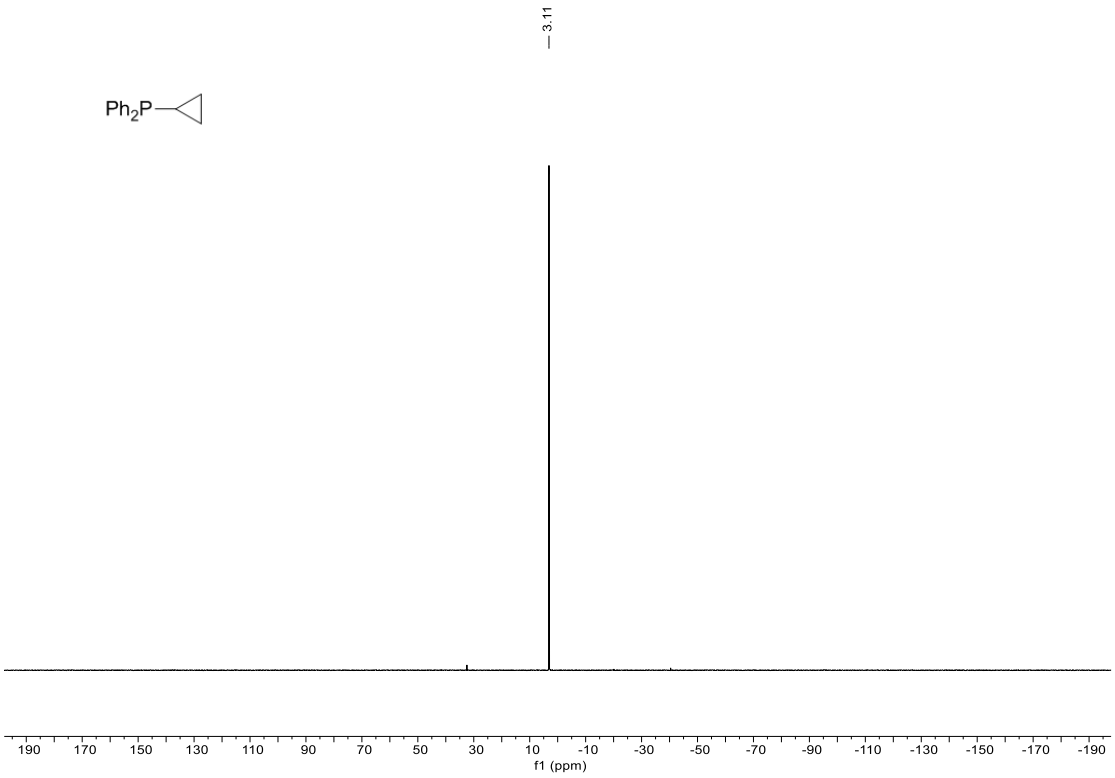
^{31}P NMR (162 MHz, $CDCl_3$) of **2ak**



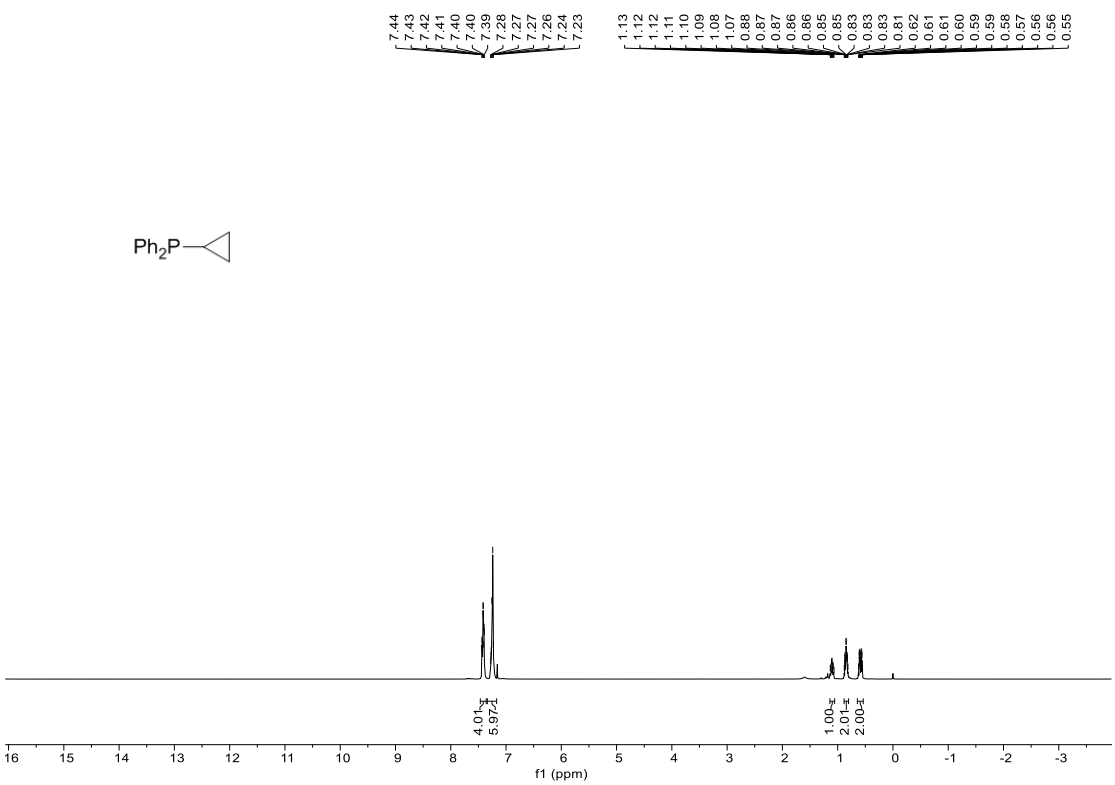
^{1}H NMR (400 MHz, $CDCl_3$) of **2ak**



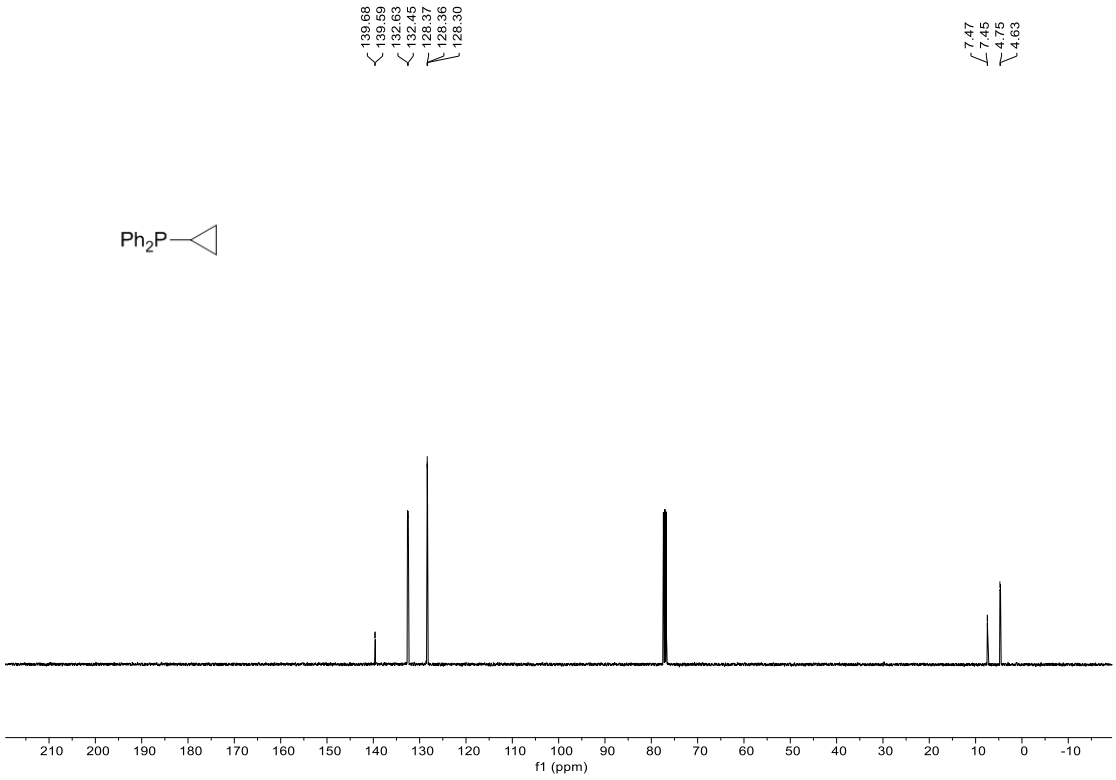
^{13}C NMR (101 MHz, $CDCl_3$) of **2ak**



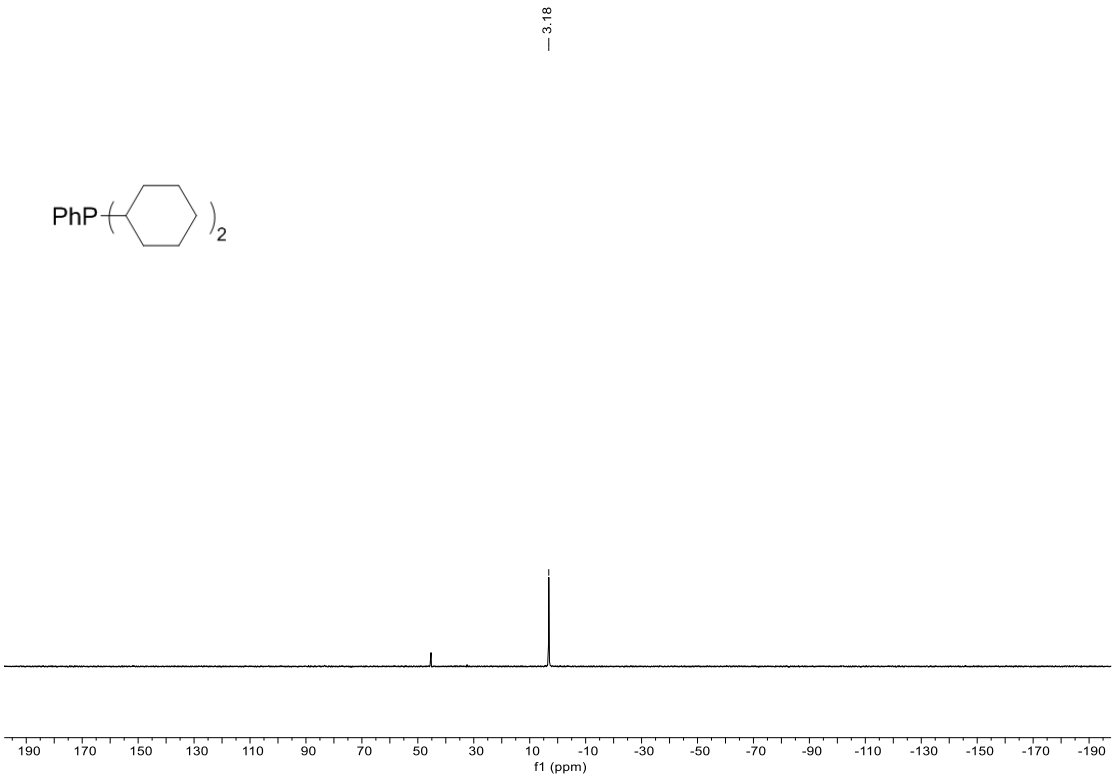
^{31}P NMR (162 MHz, $CDCl_3$) of **2al**



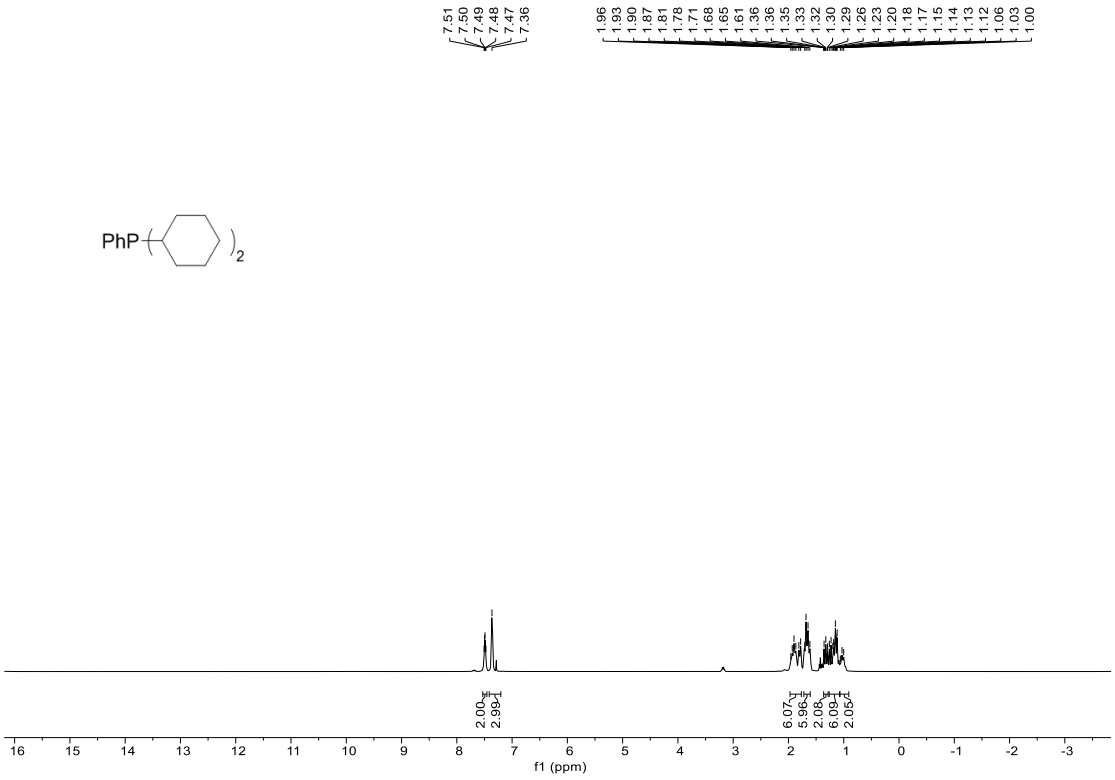
^{1}H NMR (400 MHz, $CDCl_3$) of **2al**



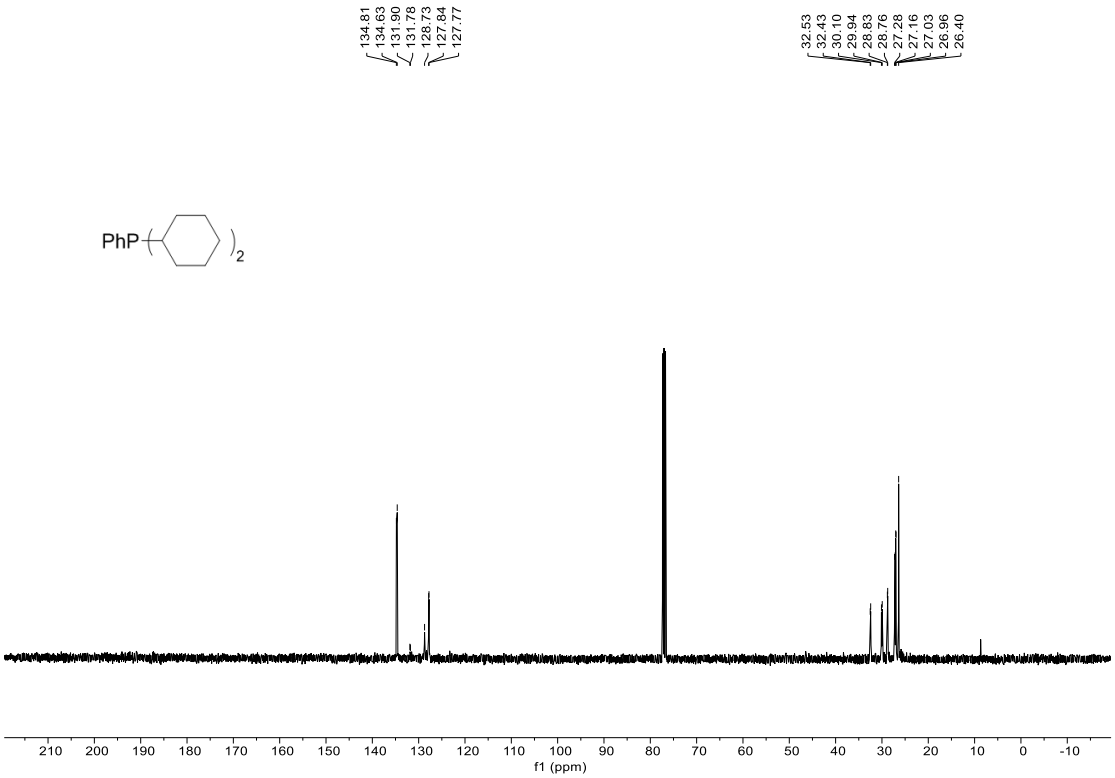
^{13}C NMR (101 MHz, $CDCl_3$) of **2al**



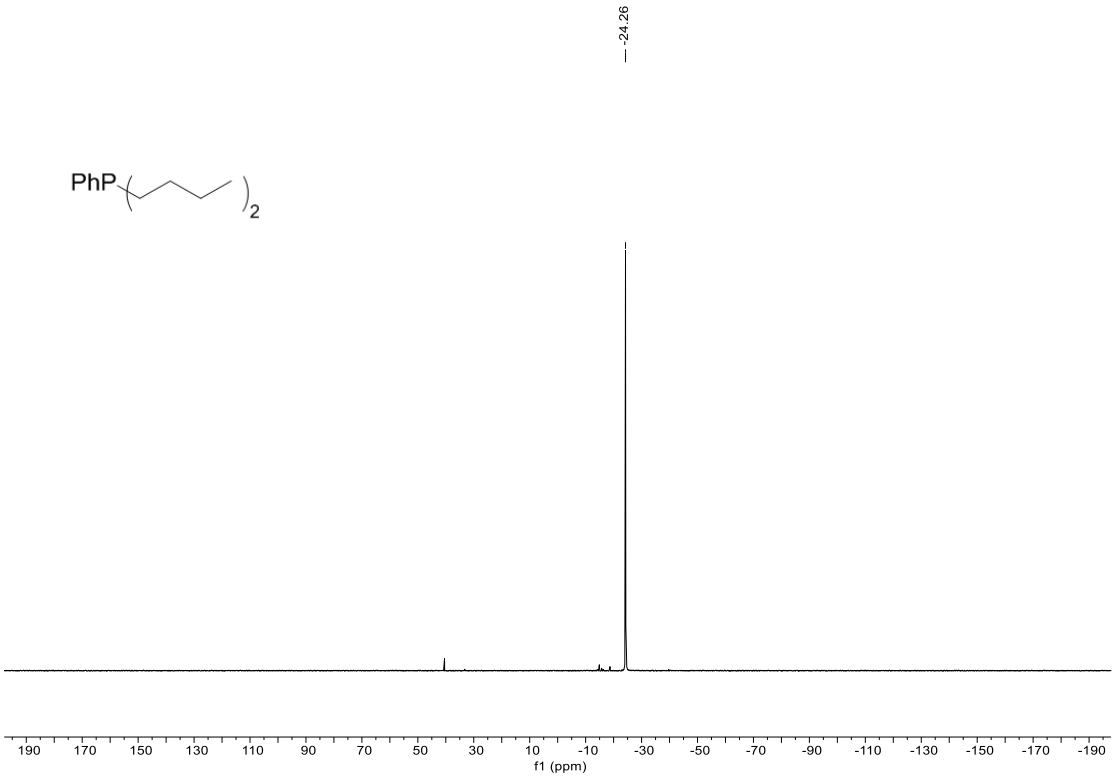
^{31}P NMR (162 MHz, $CDCl_3$) of **2am**



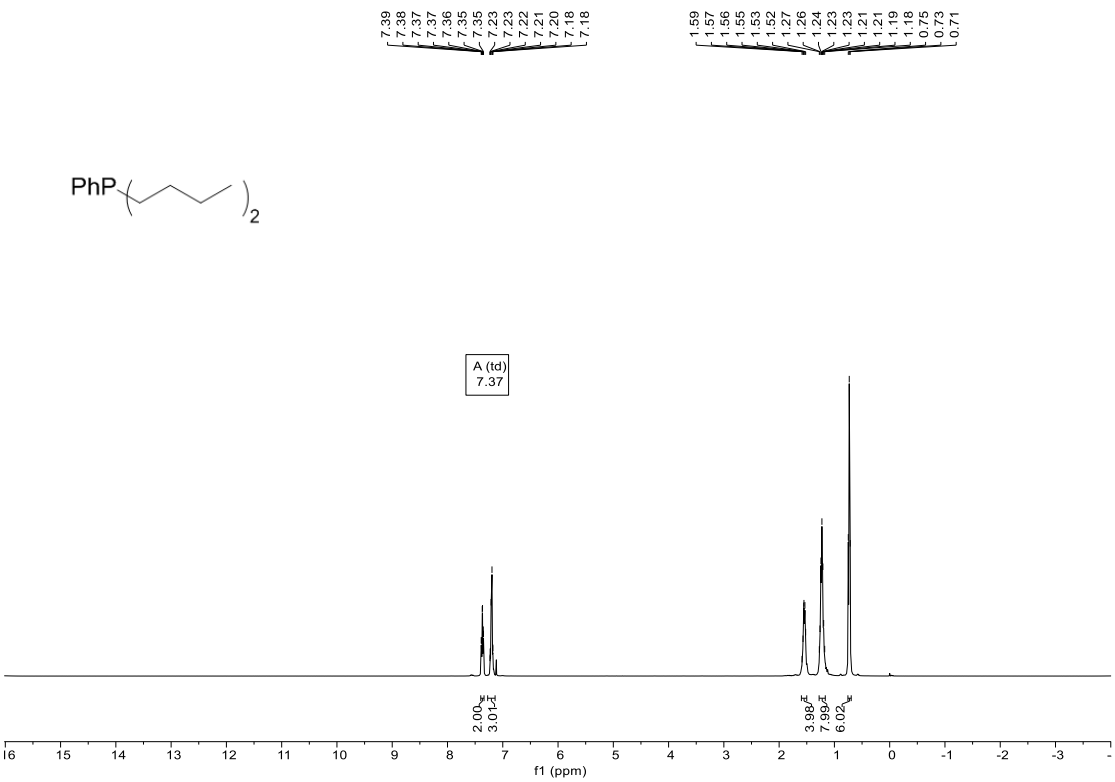
^{1}H NMR (400 MHz, $CDCl_3$) of **2am**



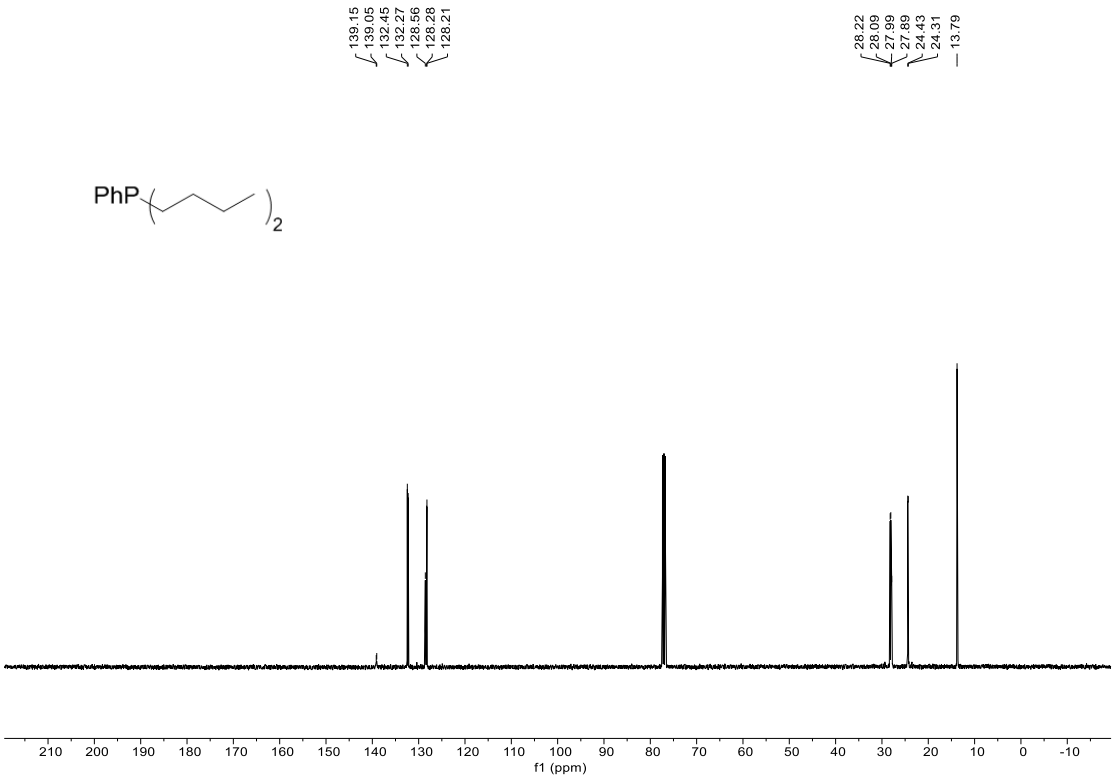
^{13}C NMR (101 MHz, $CDCl_3$) of **2am**



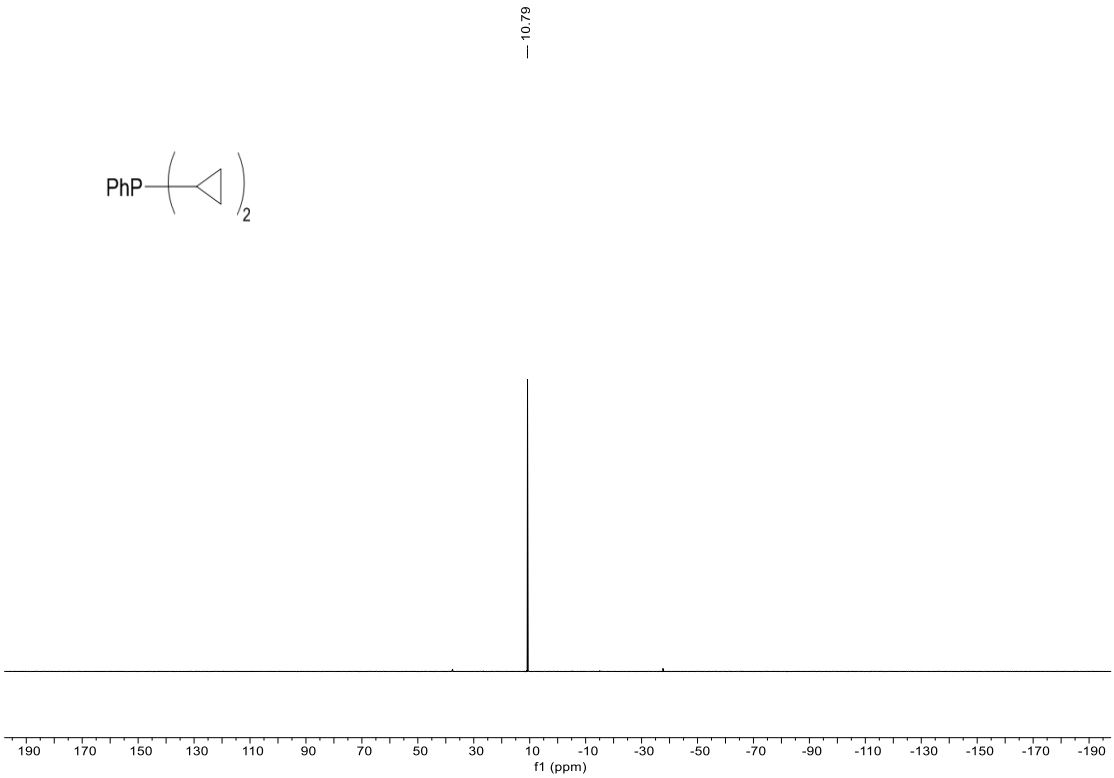
^{31}P NMR (162 MHz, $CDCl_3$) of **2an**



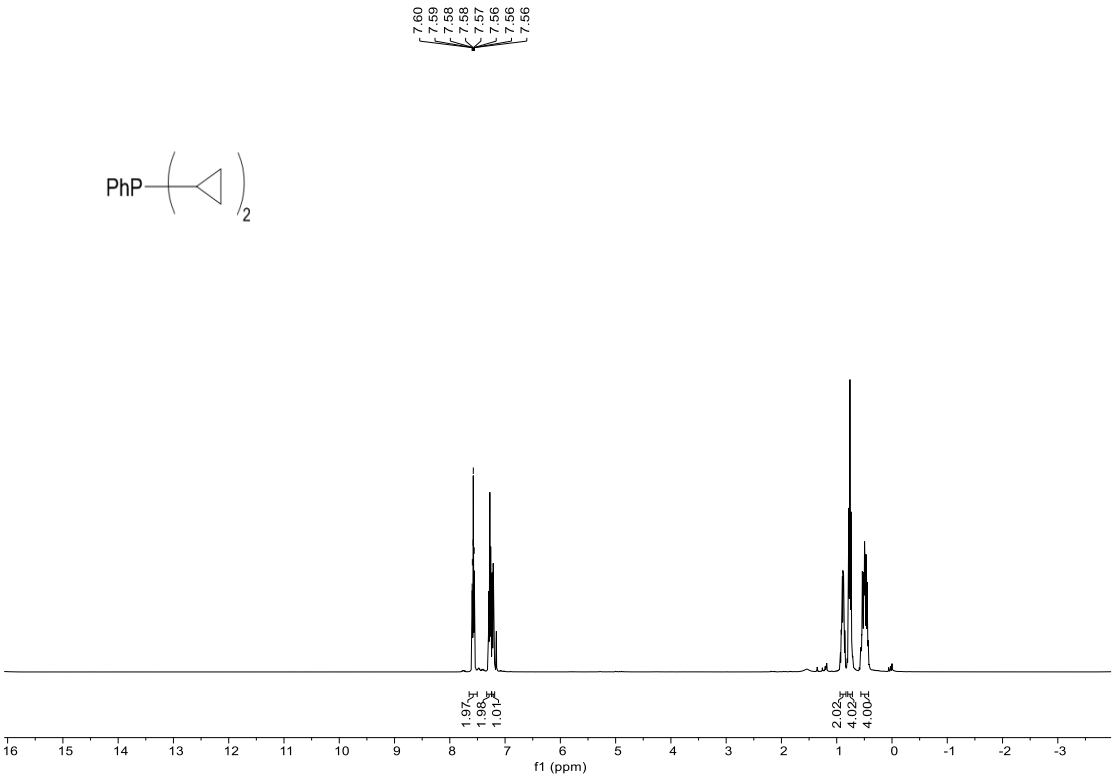
^{1}H NMR (400 MHz, $CDCl_3$) of **2an**



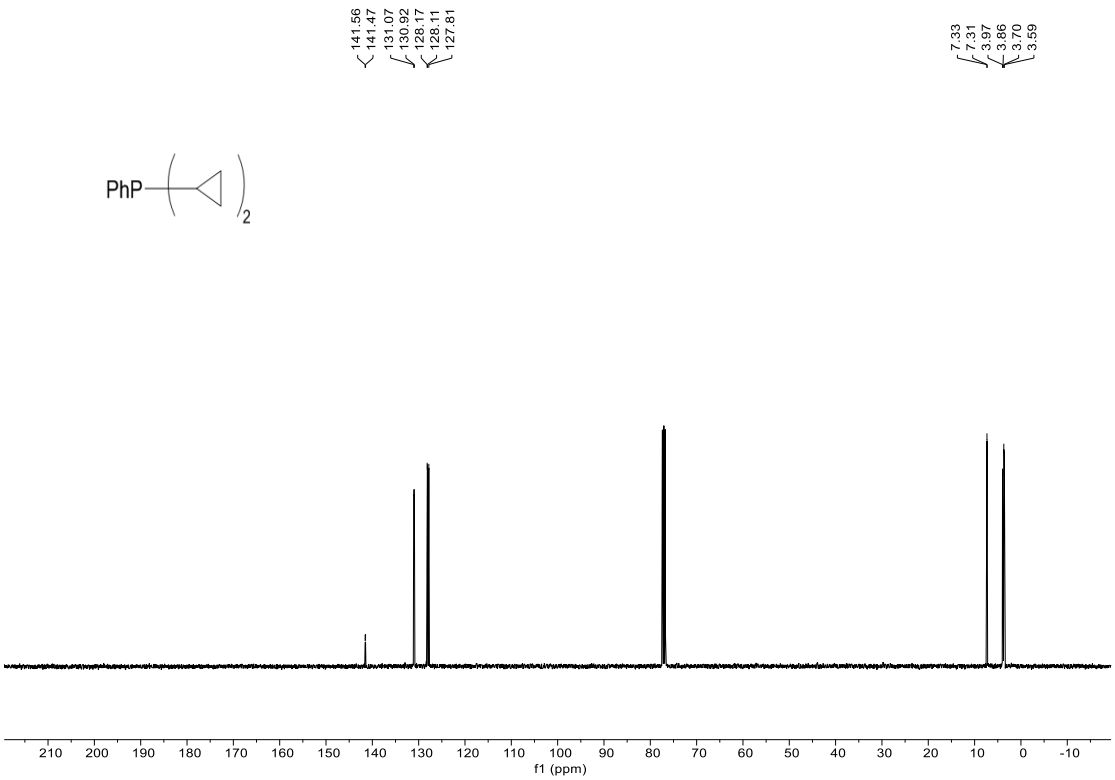
^{13}C NMR (101 MHz, $CDCl_3$) of **2an**



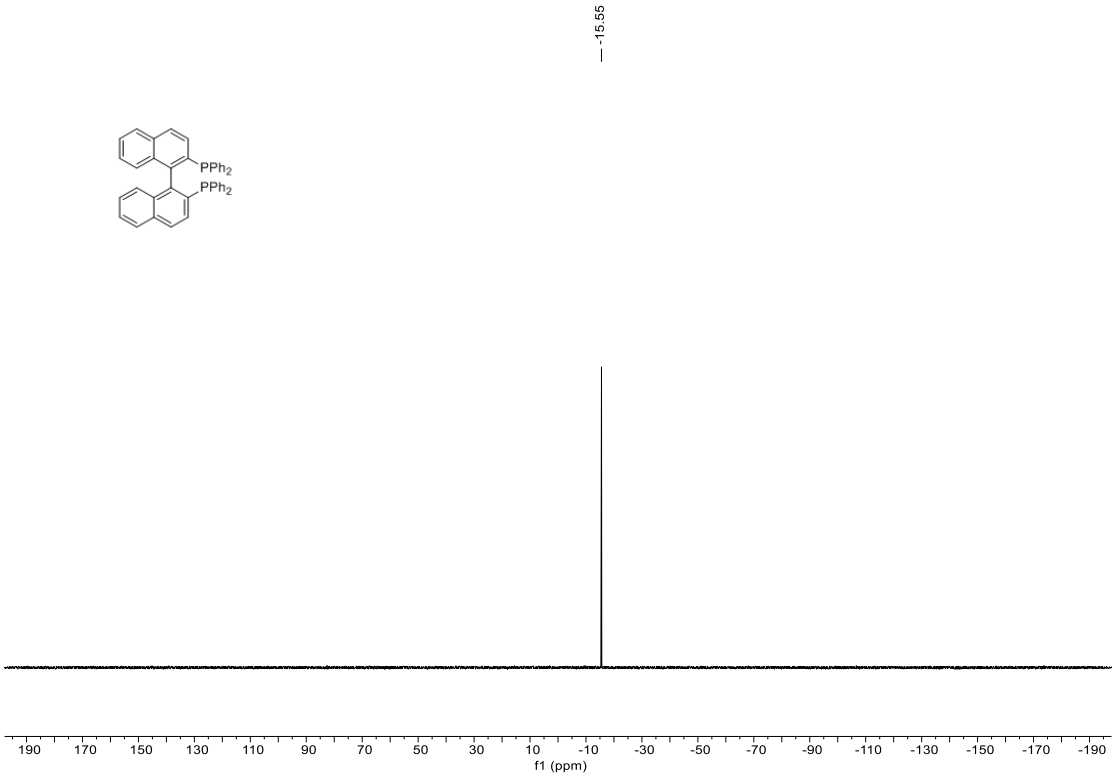
^{31}P NMR (162 MHz, $CDCl_3$) of **2ao**



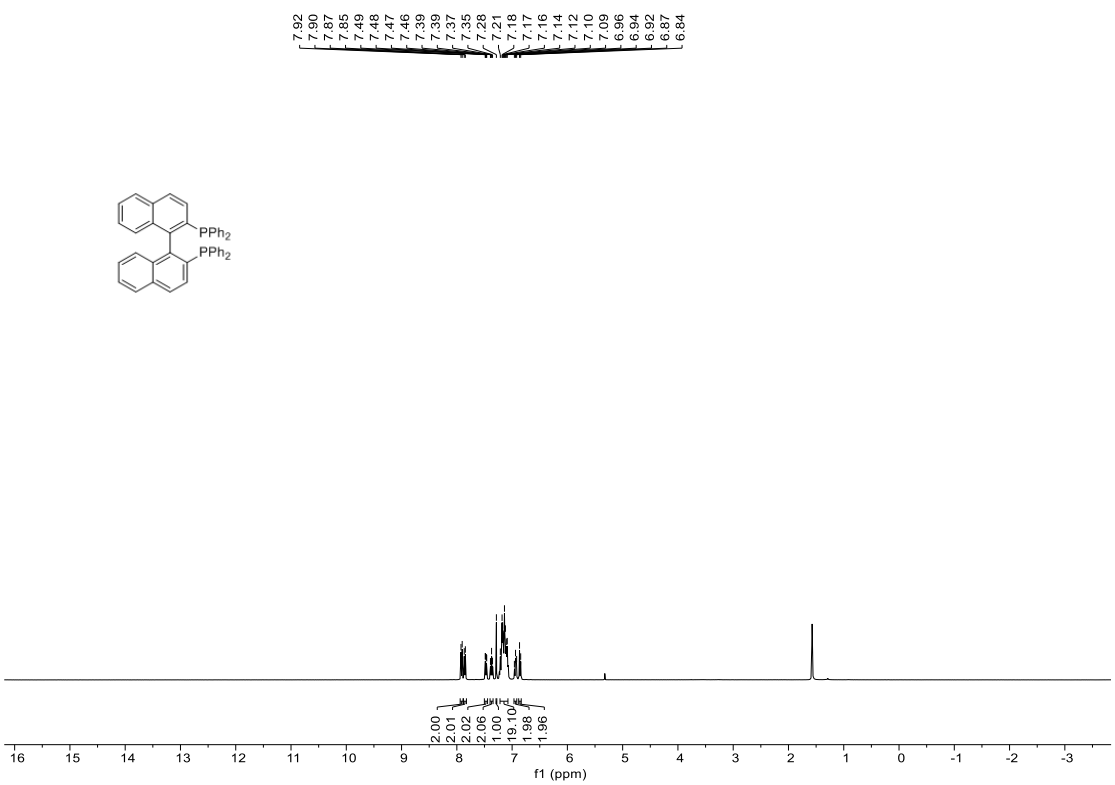
^{1}H NMR (400 MHz, $CDCl_3$) of **2ao**



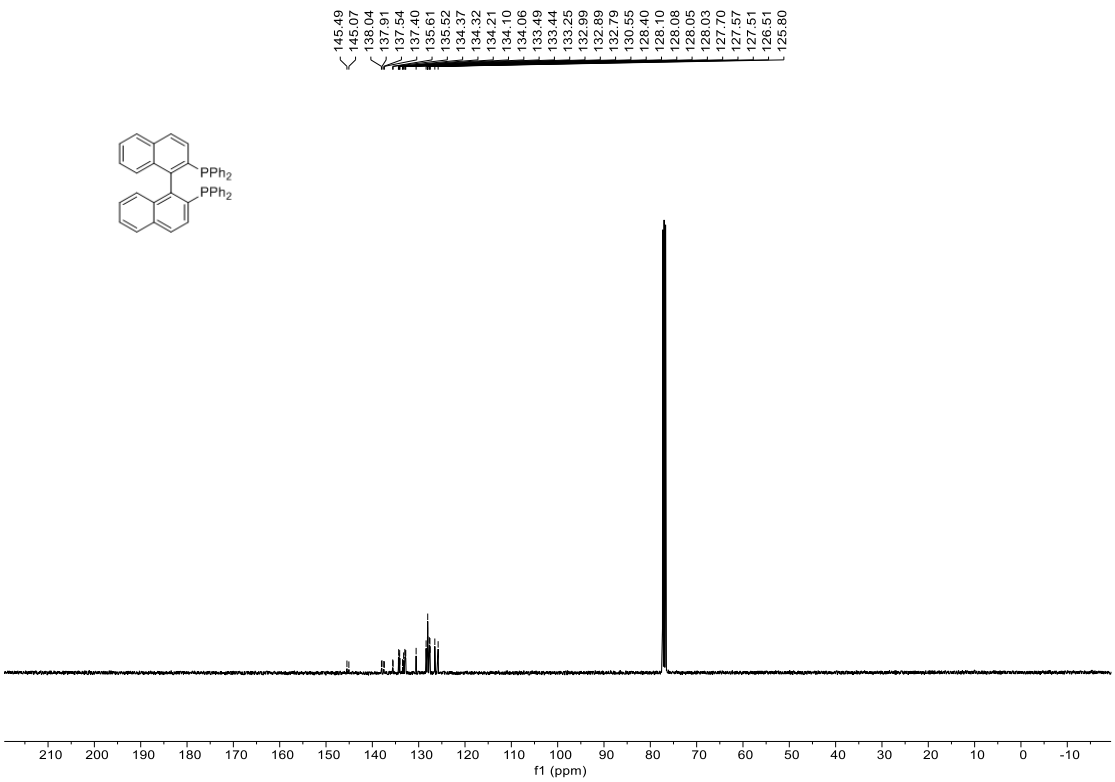
^{13}C NMR (101 MHz, $CDCl_3$) of **2ao**



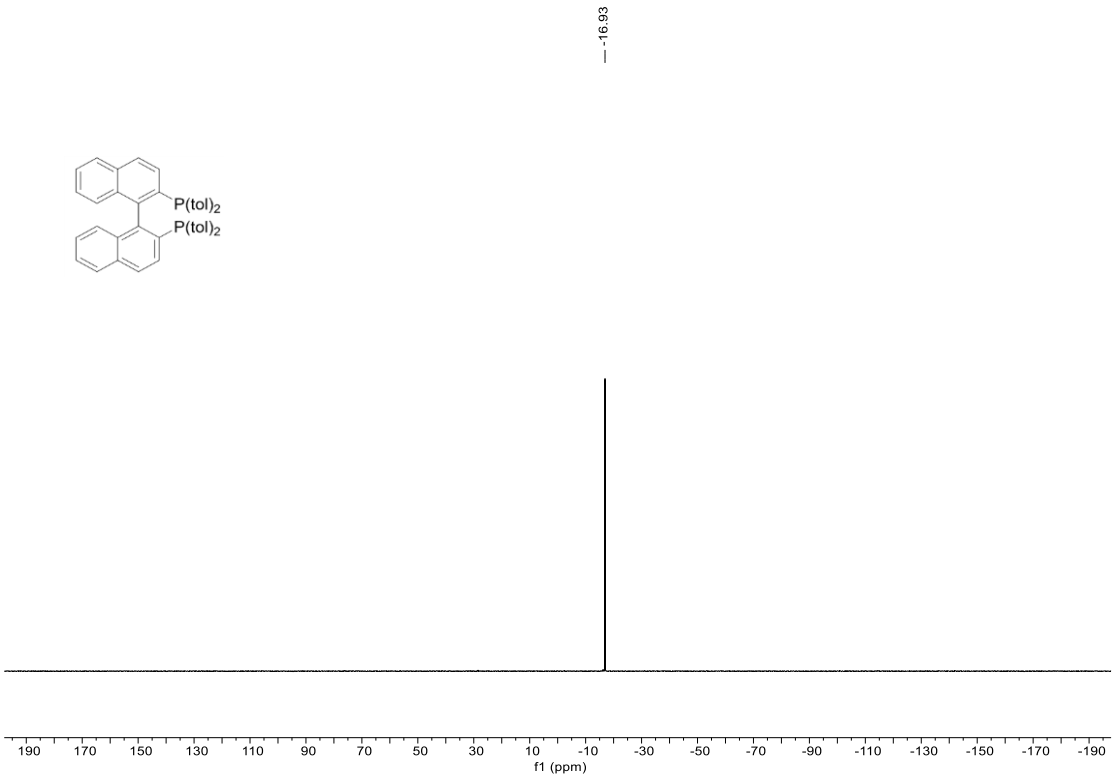
^{31}P NMR (162 MHz, $CDCl_3$) of **2ap**



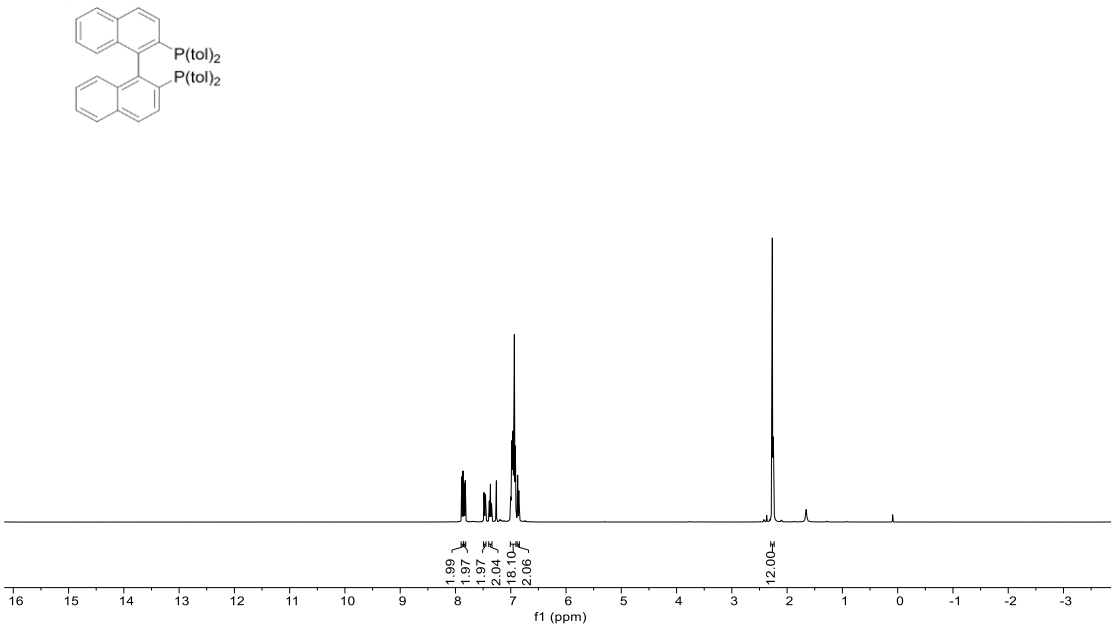
^{1}H NMR (400 MHz, $CDCl_3$) of **2ap**



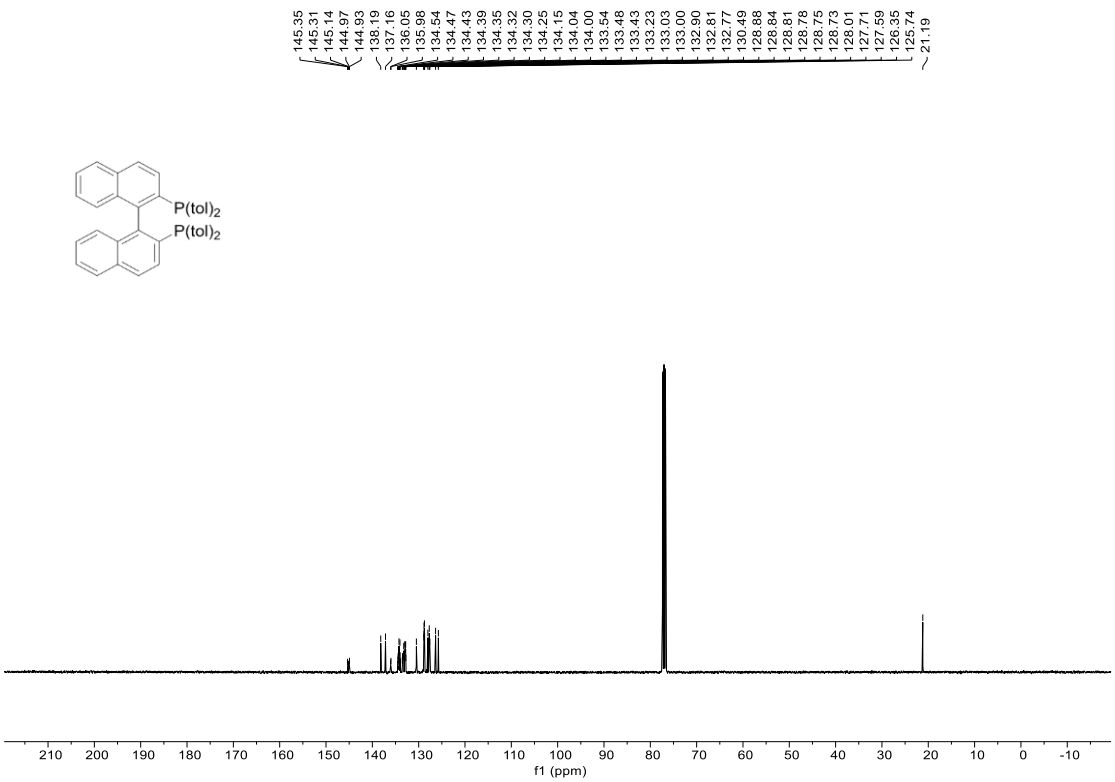
^{13}C NMR (101 MHz, $CDCl_3$) of **2ap**



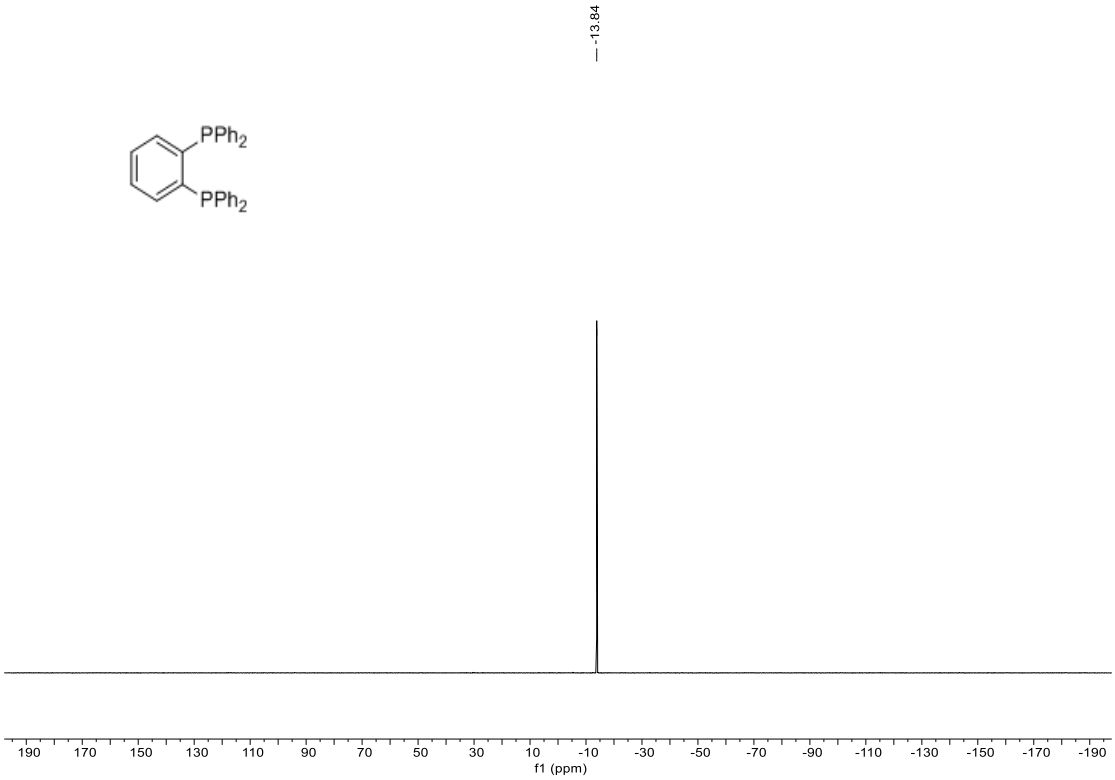
^{31}P NMR (162 MHz, $CDCl_3$) of **2ar**



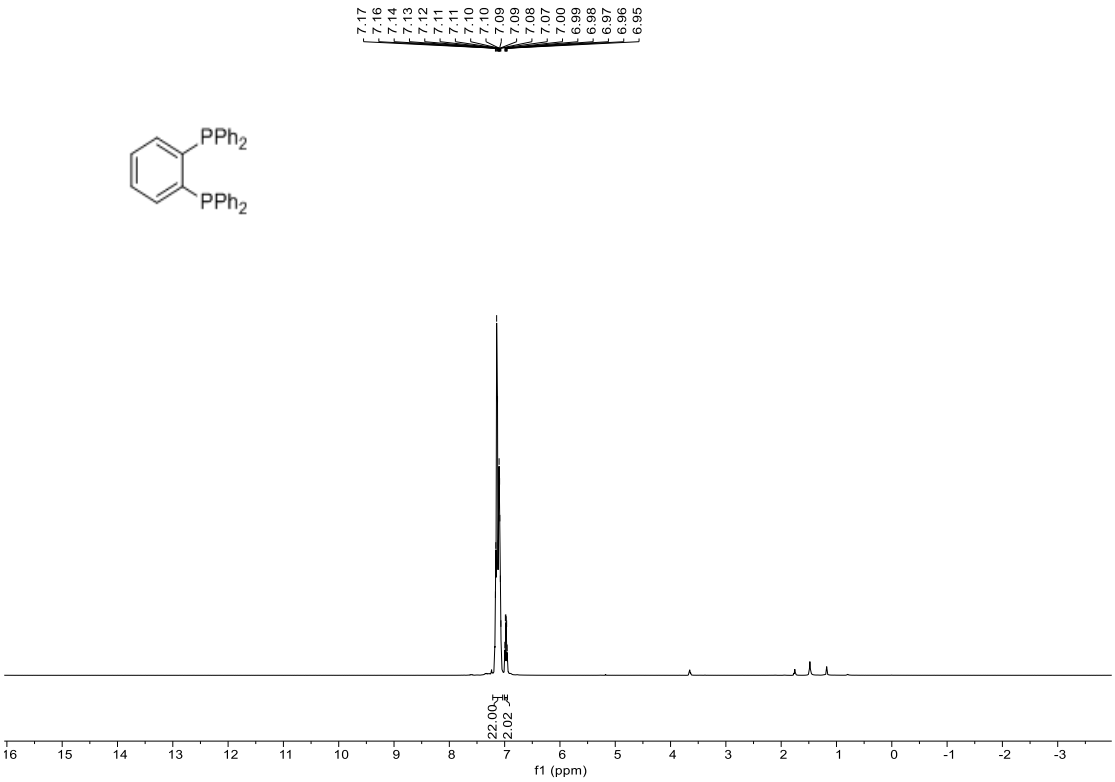
^{1}H NMR (400 MHz, $CDCl_3$) of **2ar**



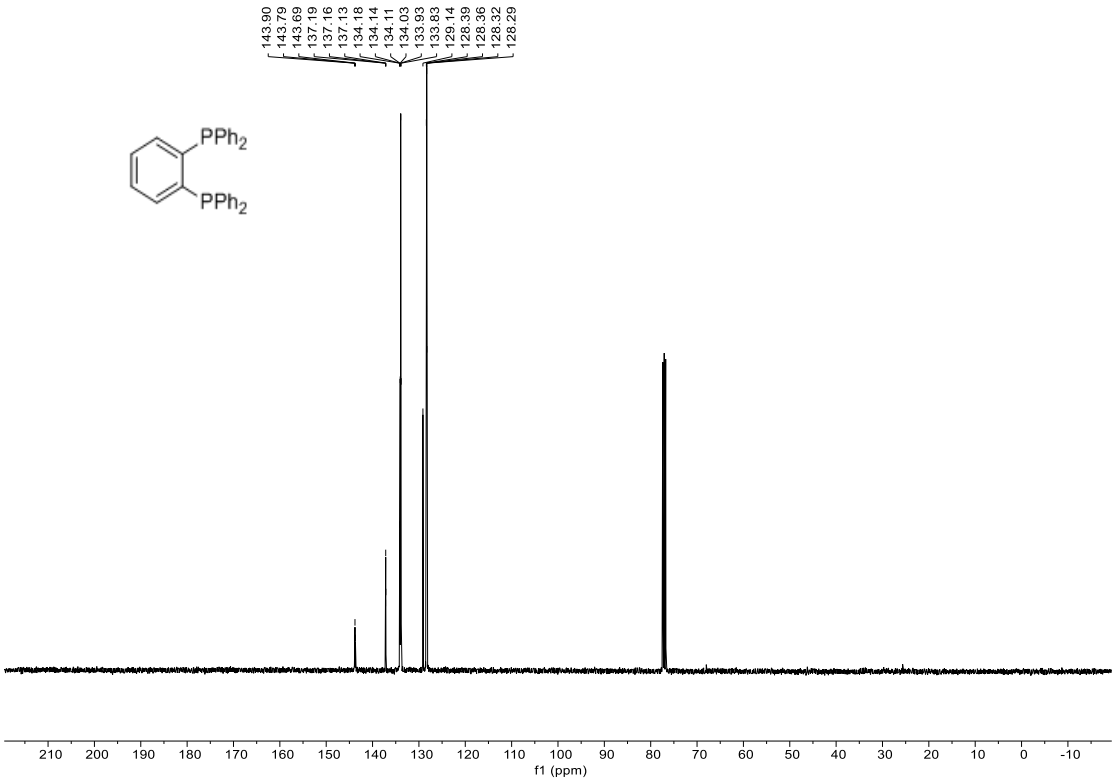
^{13}C NMR (101 MHz, $CDCl_3$) of **2ar**



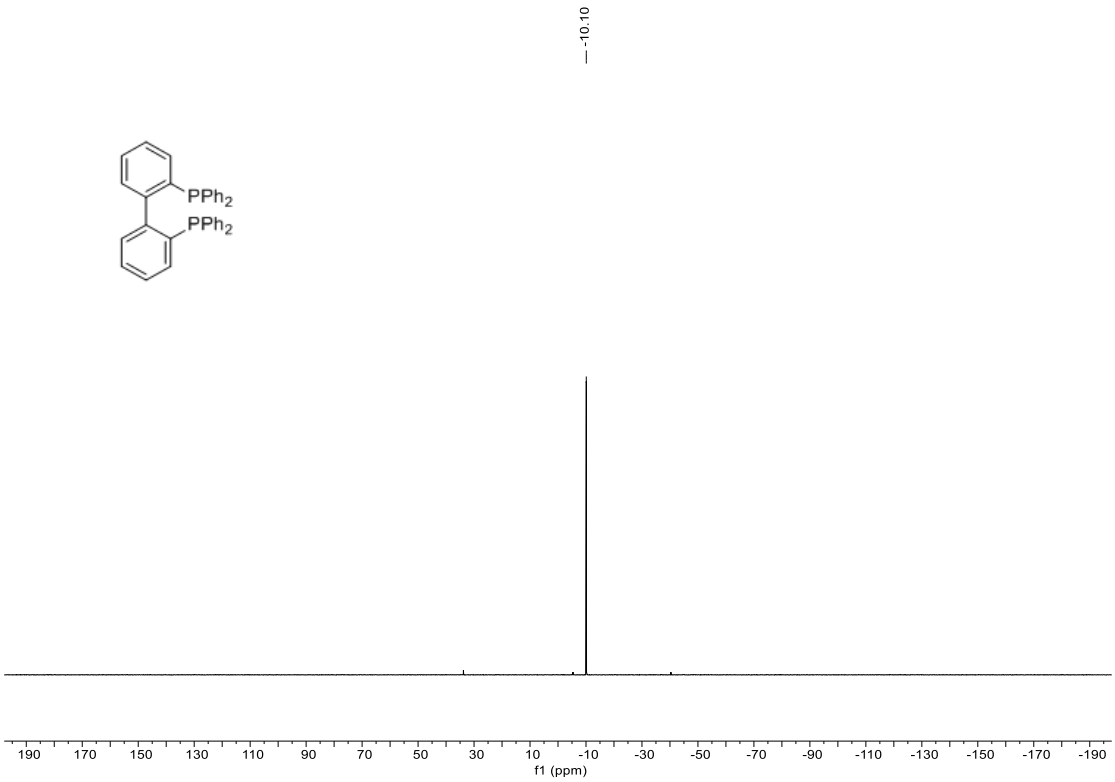
^{31}P NMR (162 MHz, $CDCl_3$) of **2as**



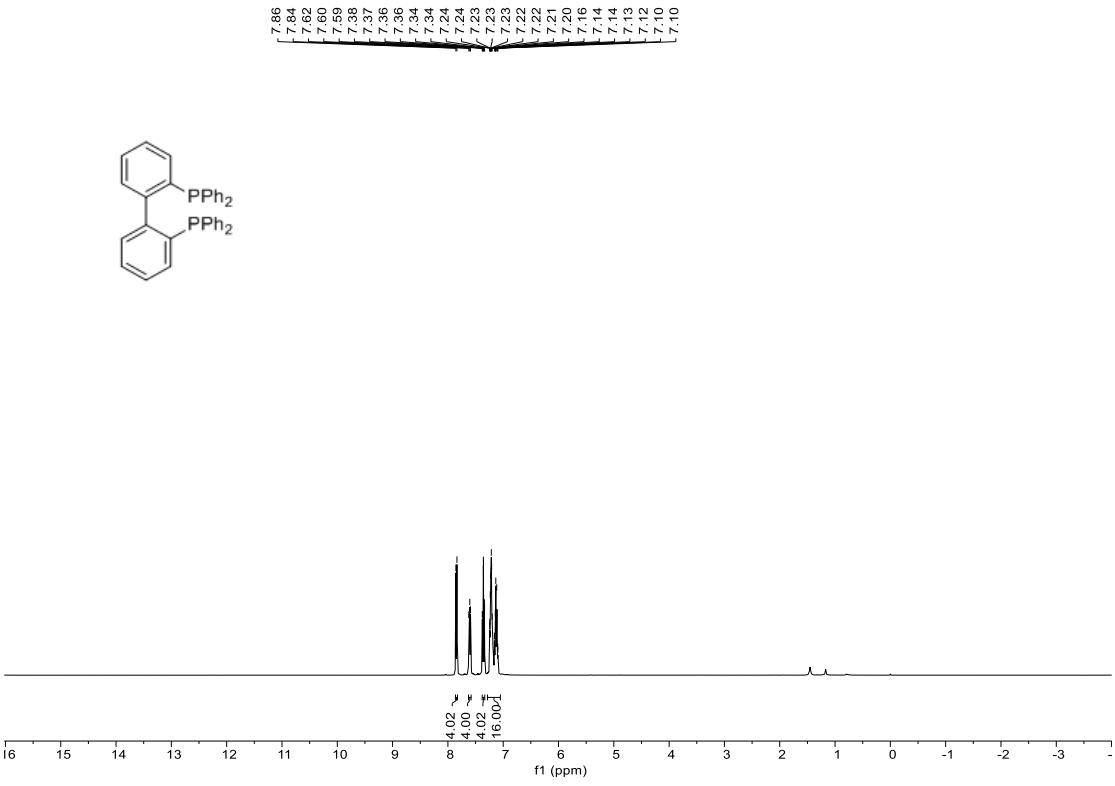
^{1}H NMR (400 MHz, $CDCl_3$) of **2as**



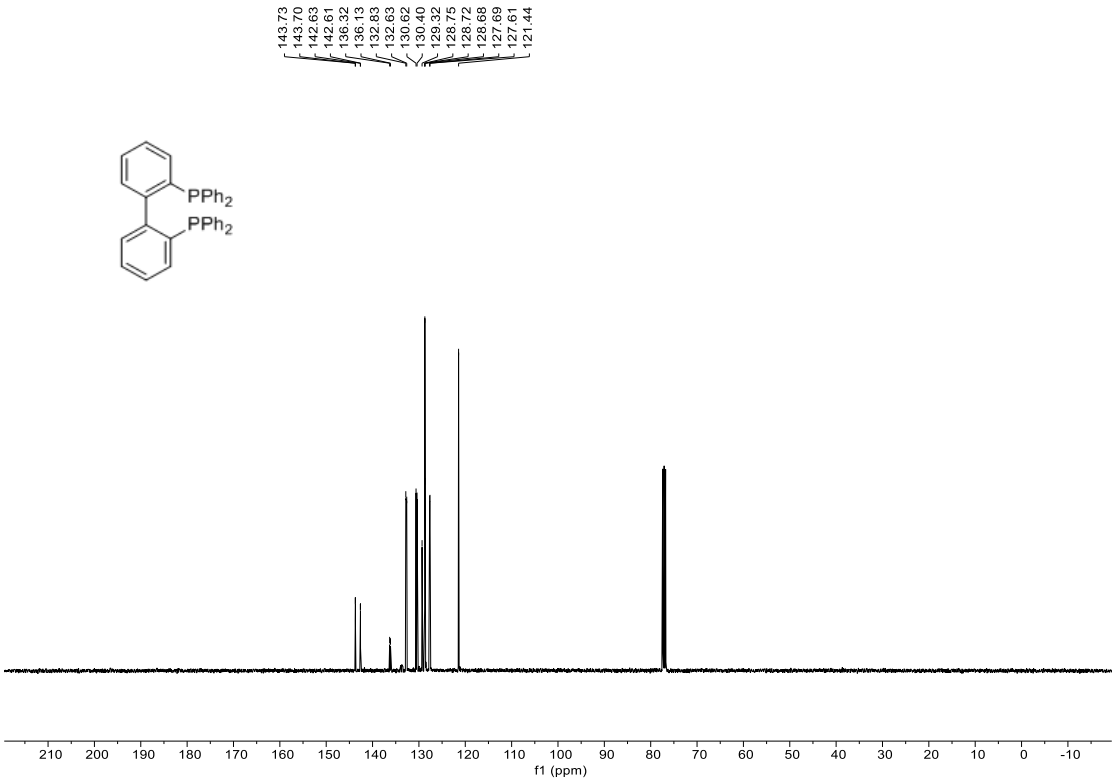
^{13}C NMR (101 MHz, $CDCl_3$) of **2as**



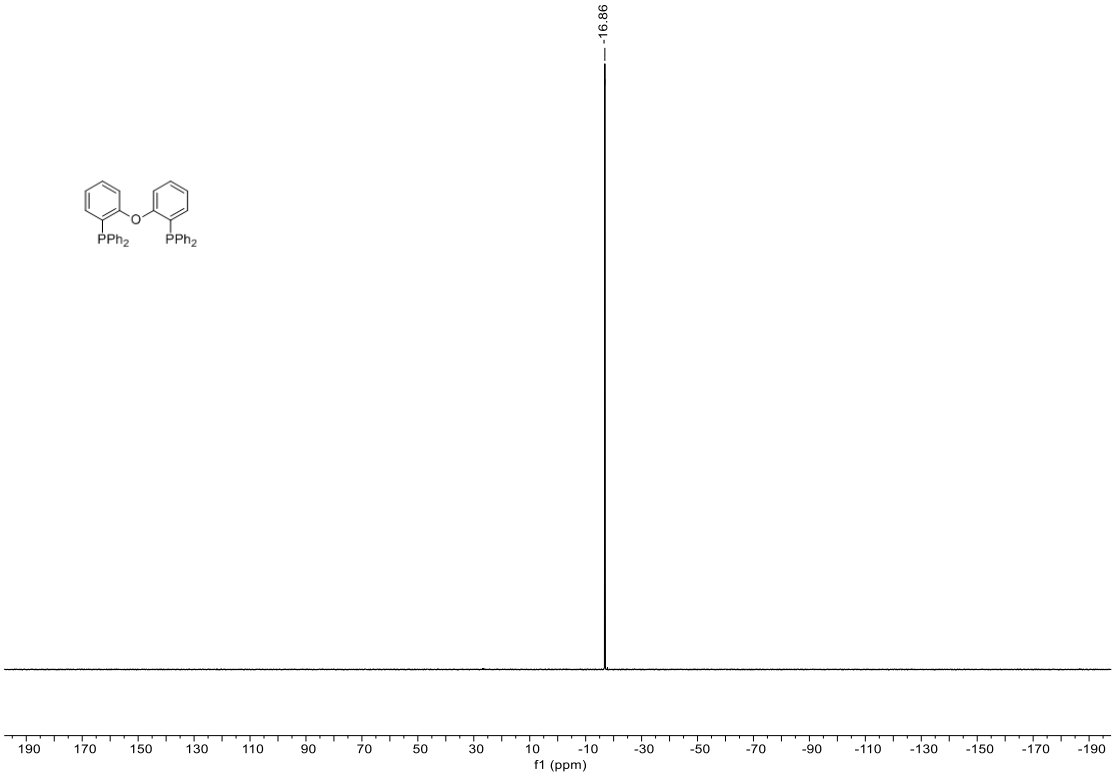
^{31}P NMR (162 MHz, $CDCl_3$) of **2at**



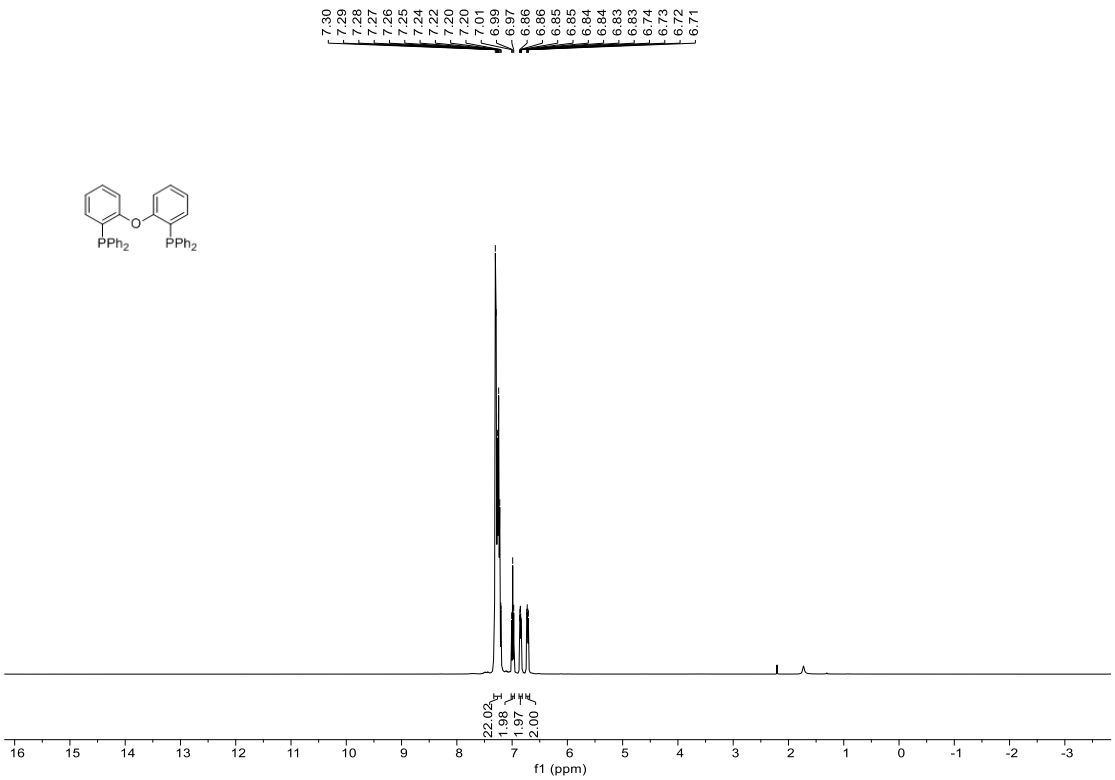
^{1}H NMR (400 MHz, $CDCl_3$) of **2at**



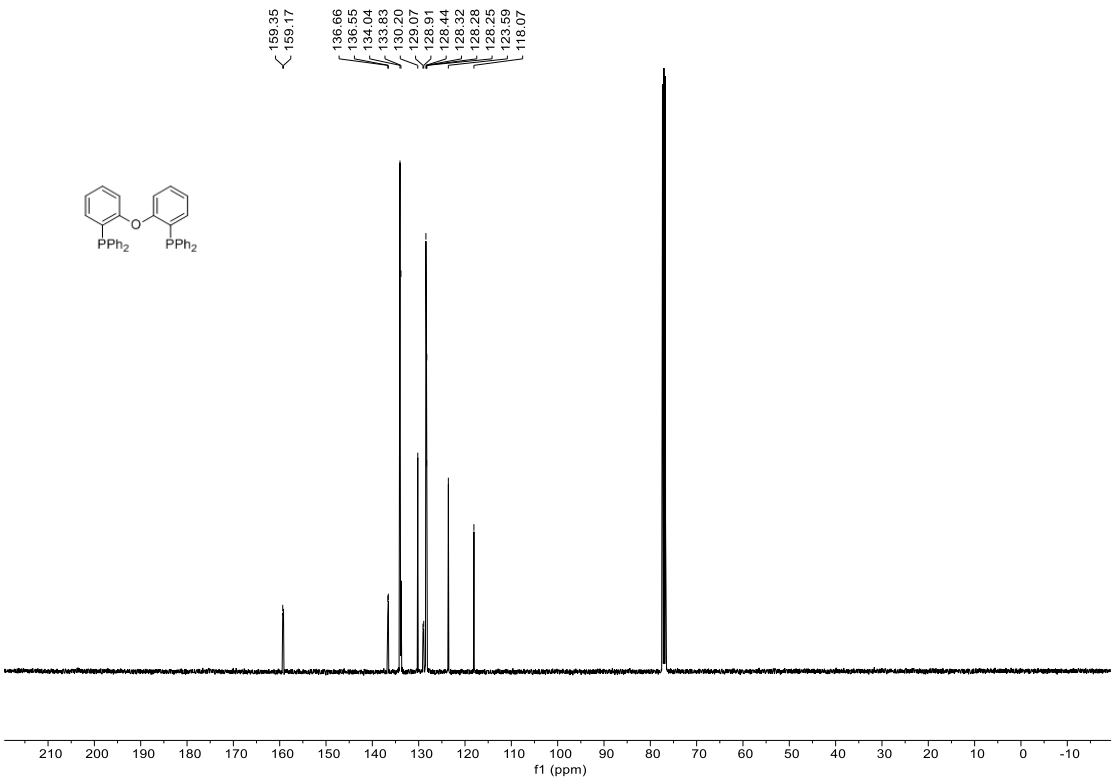
^{13}C NMR (101 MHz, $CDCl_3$) of **2at**



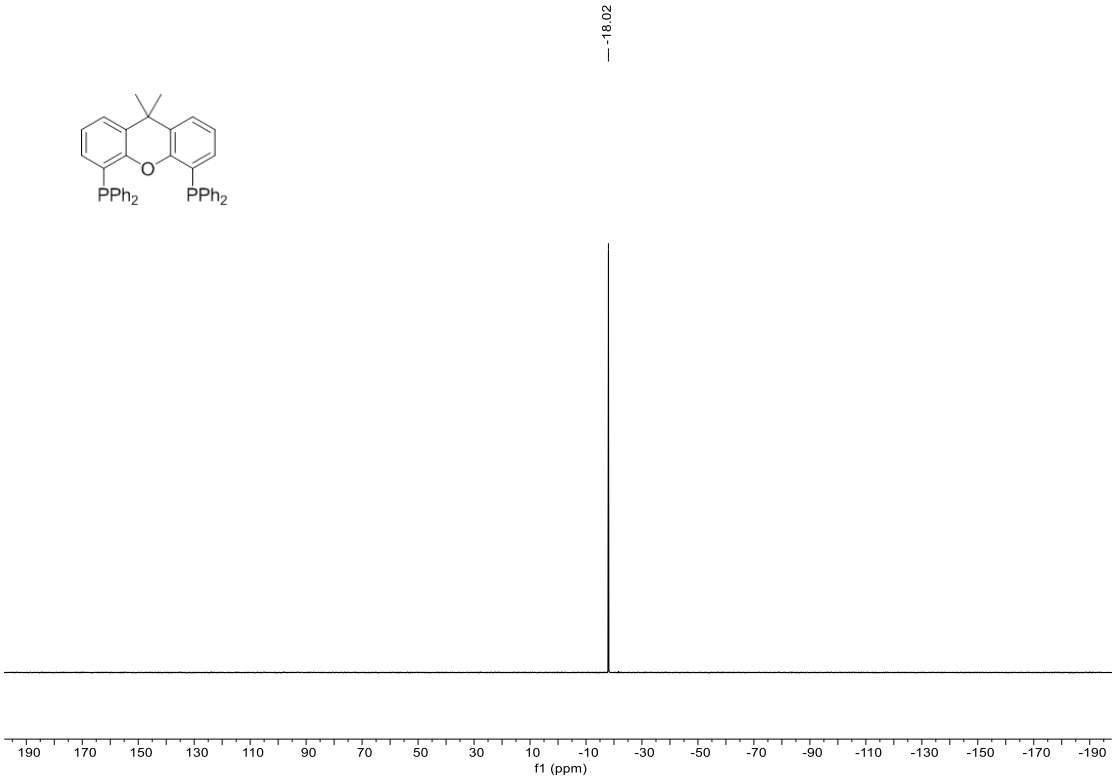
^{31}P NMR (162 MHz, $CDCl_3$) of **2au**



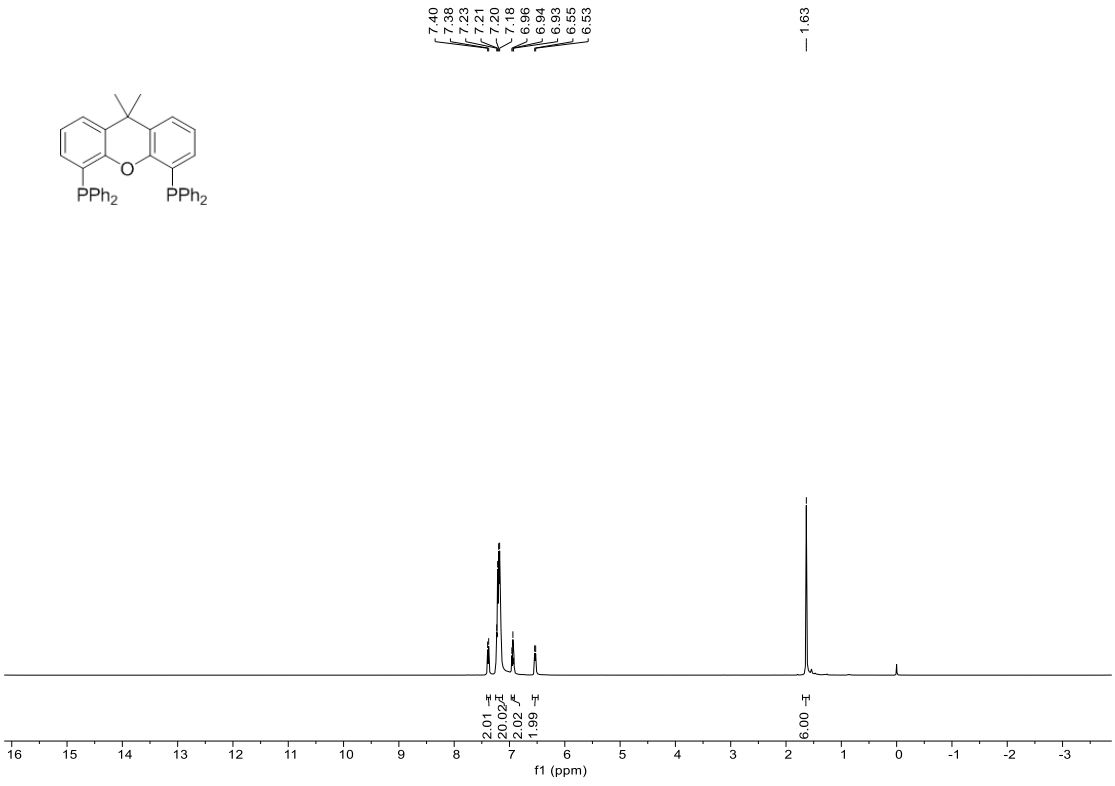
^{1}H NMR (400 MHz, $CDCl_3$) of **2au**



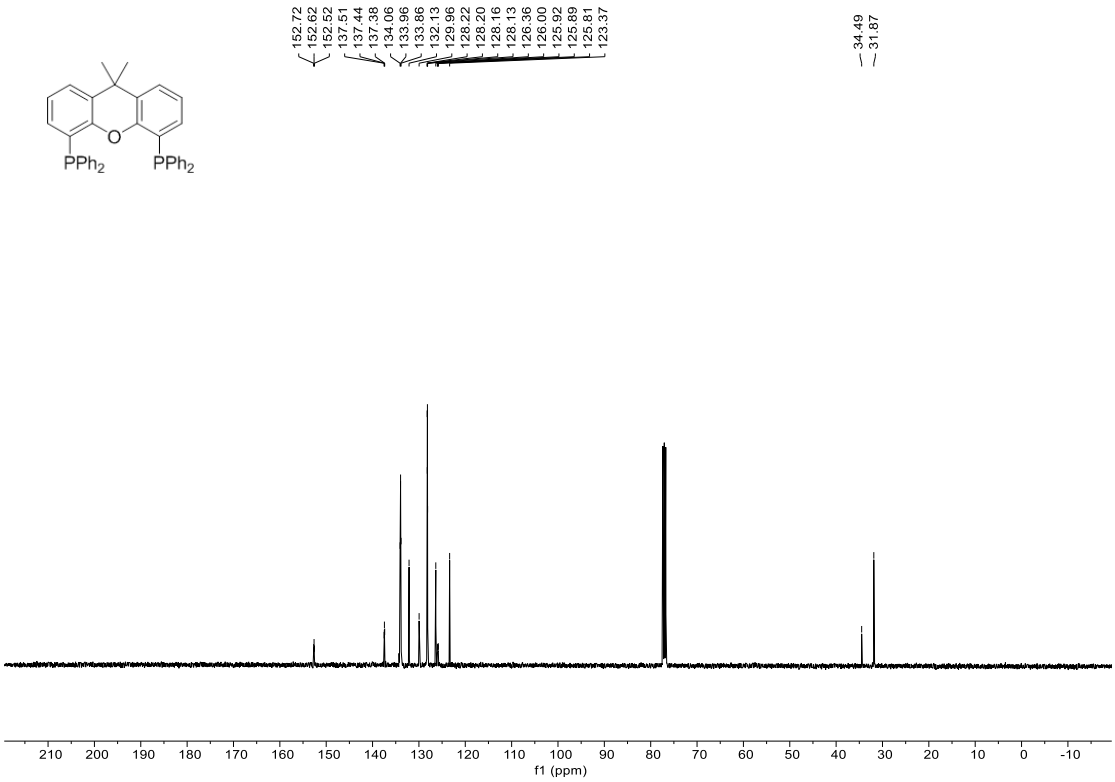
^{13}C NMR (101 MHz, $CDCl_3$) of **2au**



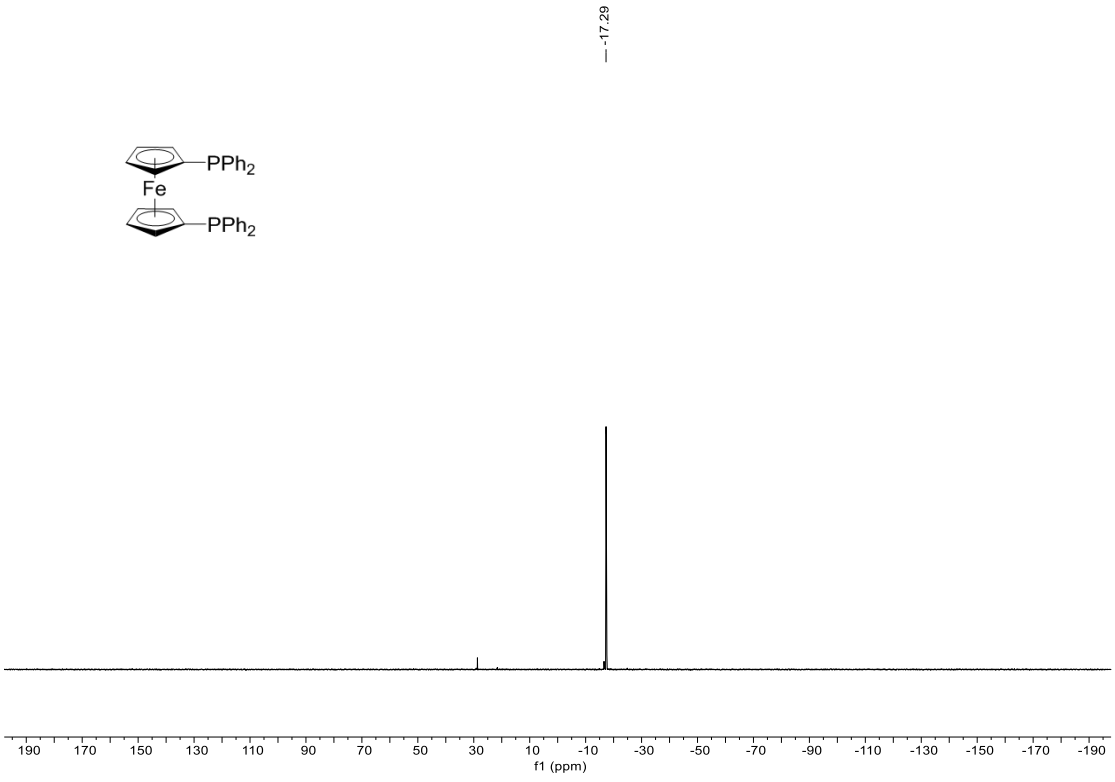
^{31}P NMR (162 MHz, $CDCl_3$) of **2av**



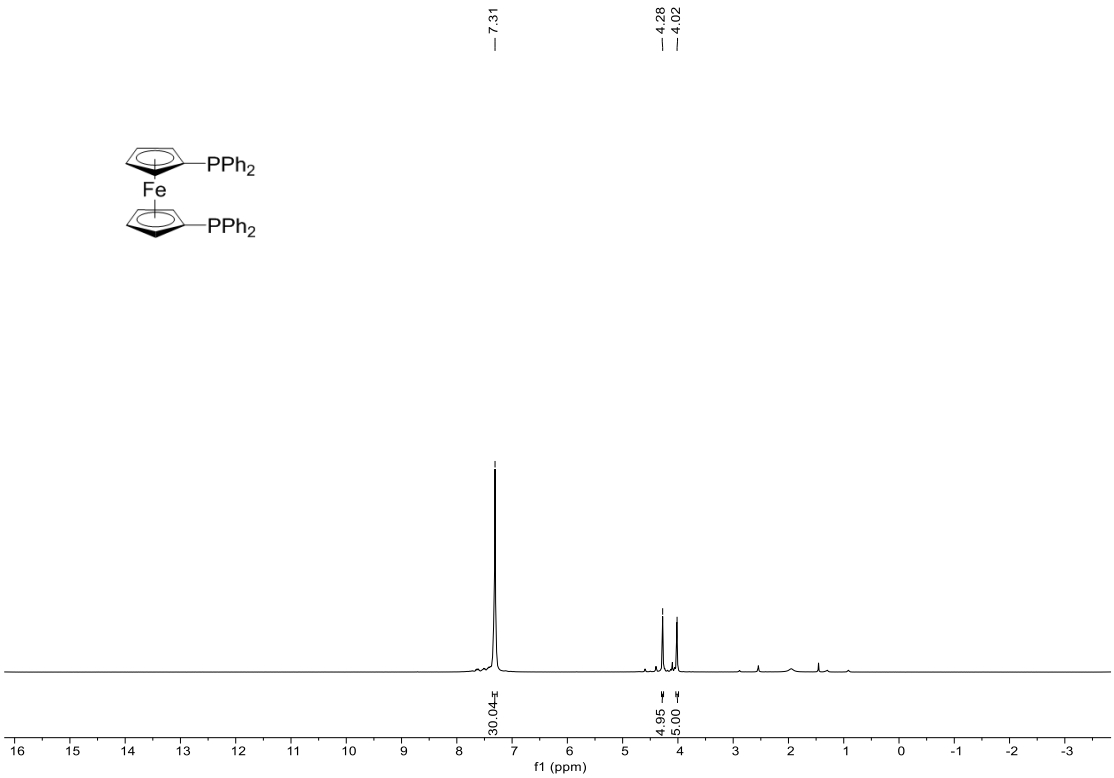
^{1}H NMR (400 MHz, $CDCl_3$) of **2av**



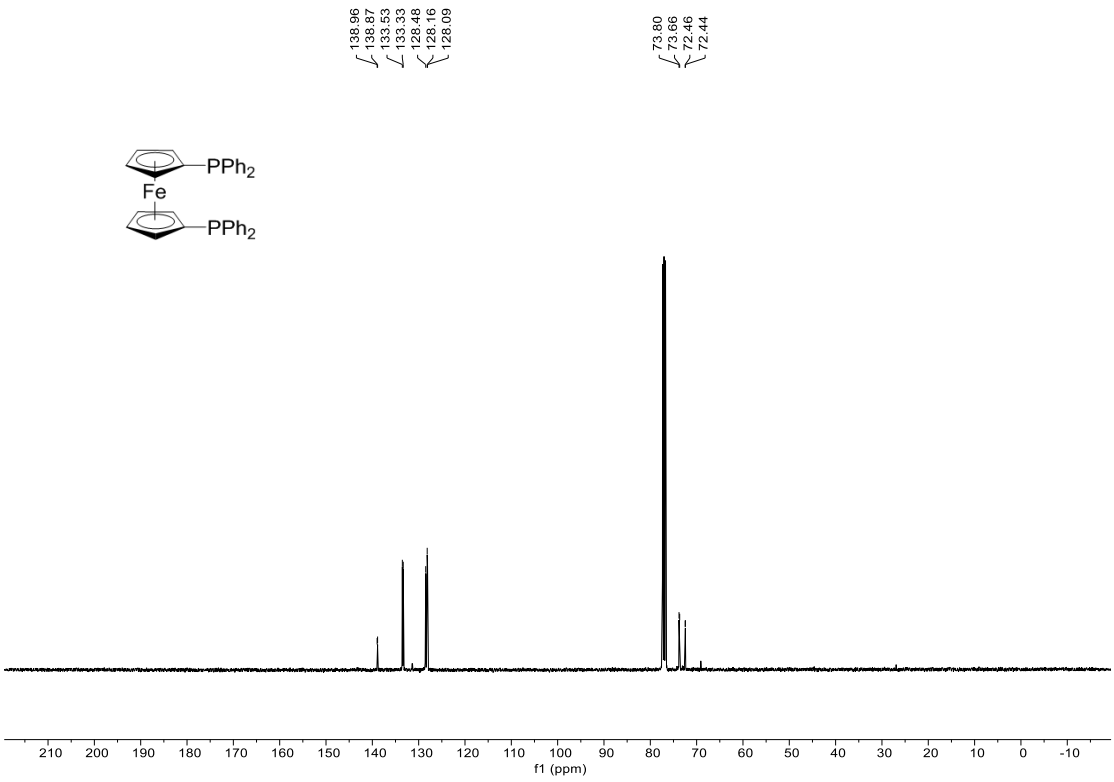
^{13}C NMR (101 MHz, $CDCl_3$) of 2**av**



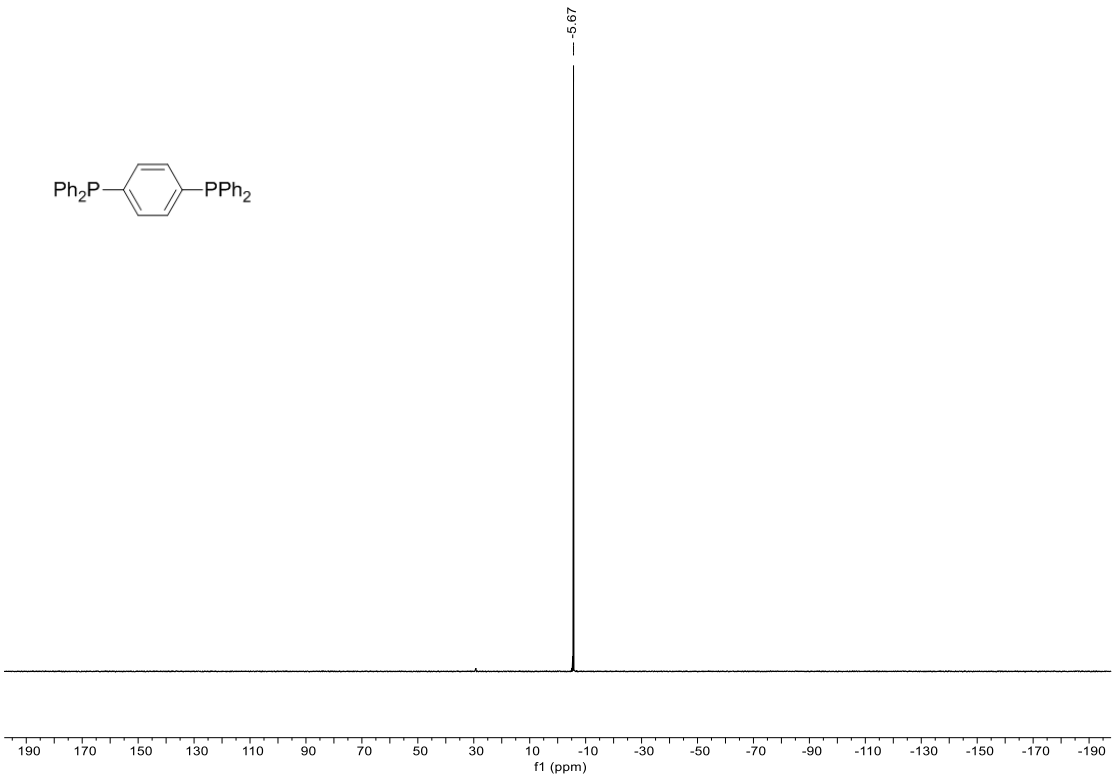
^{31}P NMR (162 MHz, $CDCl_3$) of **2aw**



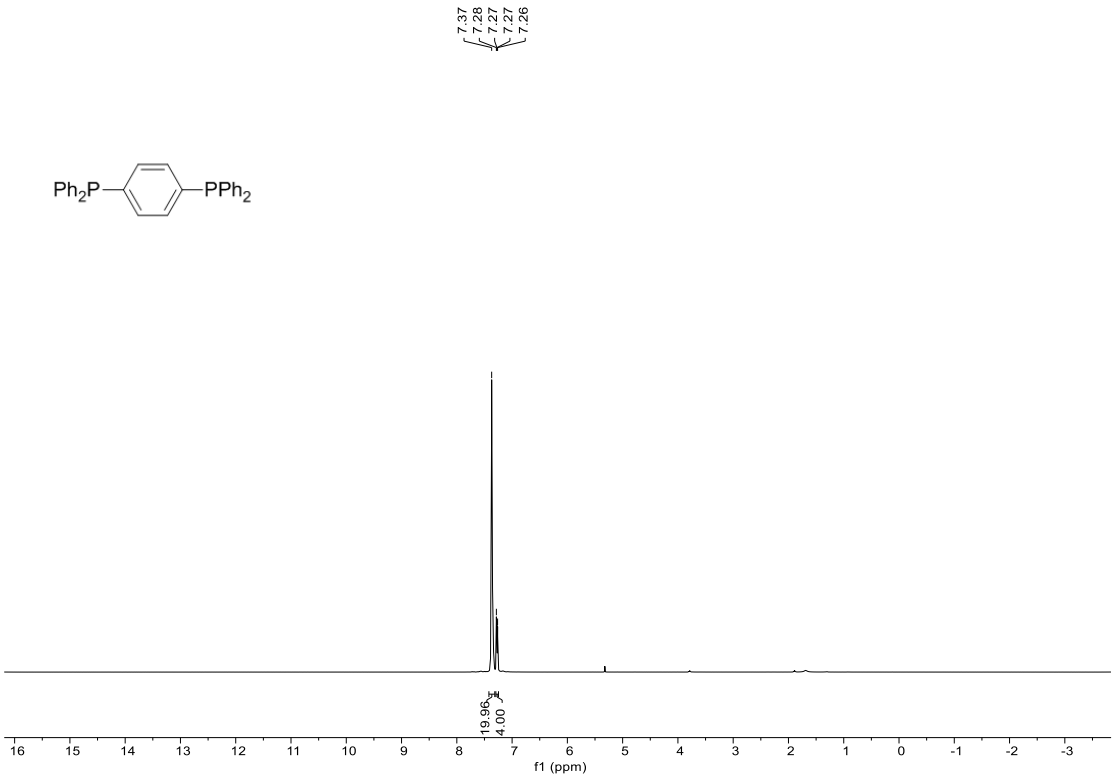
^{1}H NMR (400 MHz, $CDCl_3$) of **2aw**



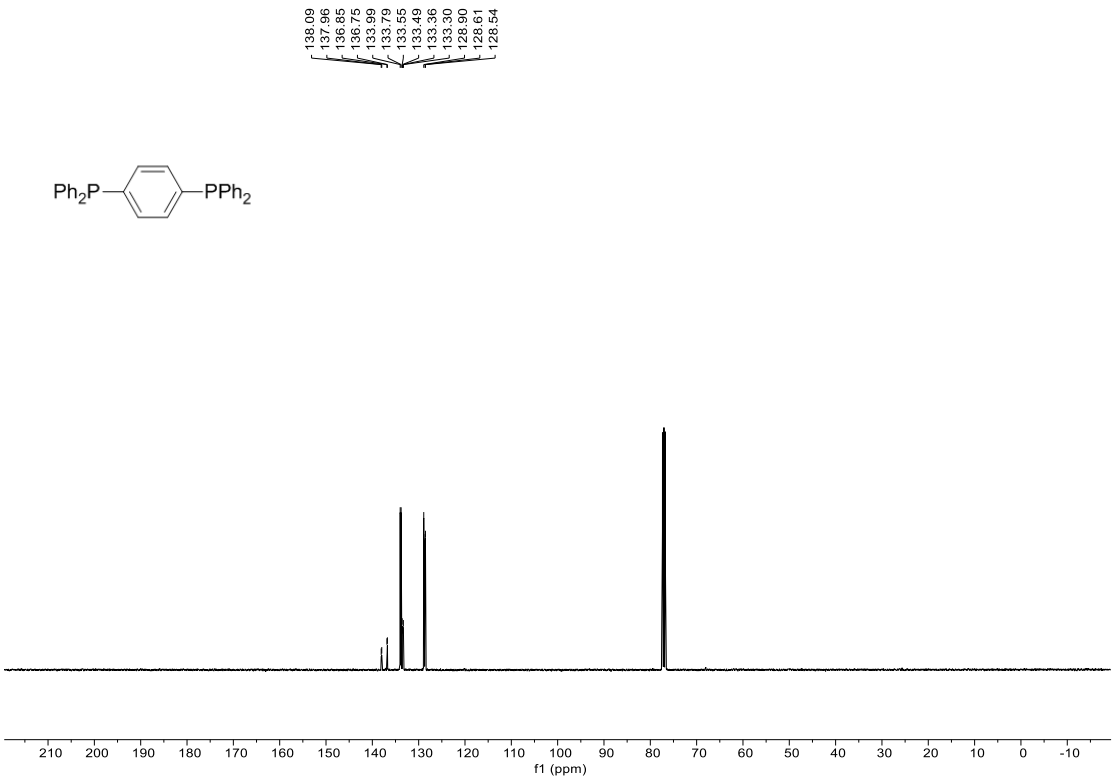
^{13}C NMR (101 MHz, $CDCl_3$) of **2aw**



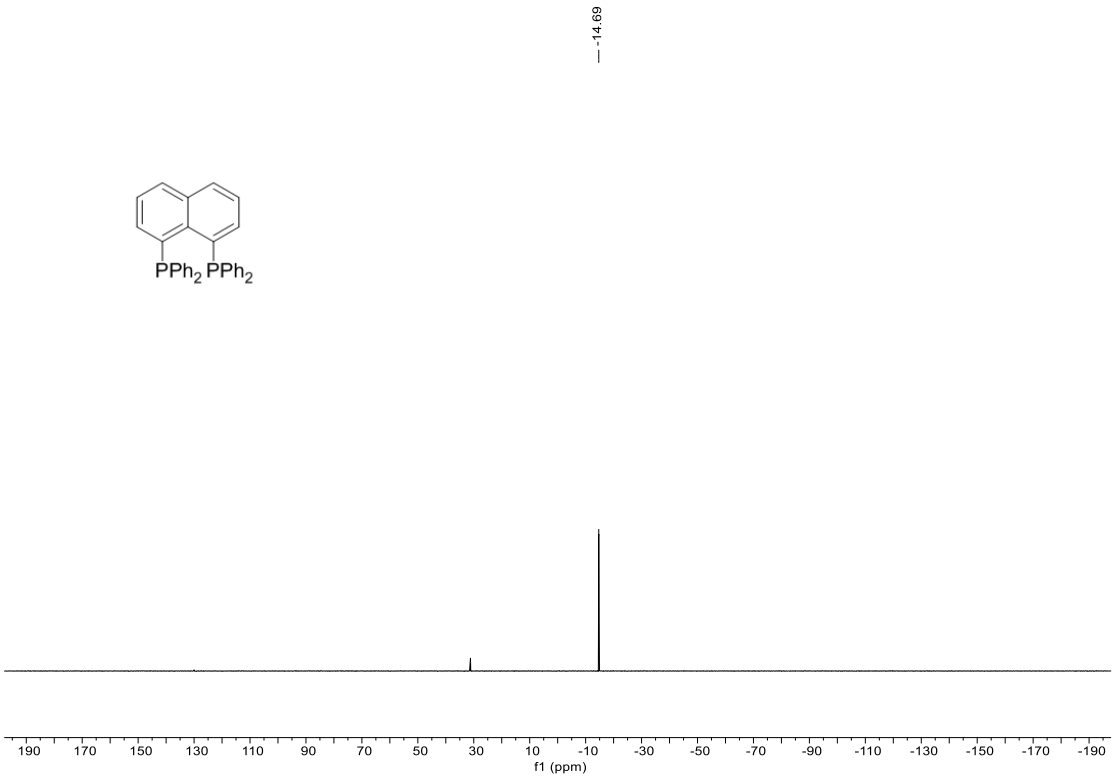
^{31}P NMR (162 MHz, $CDCl_3$) of **2ax**



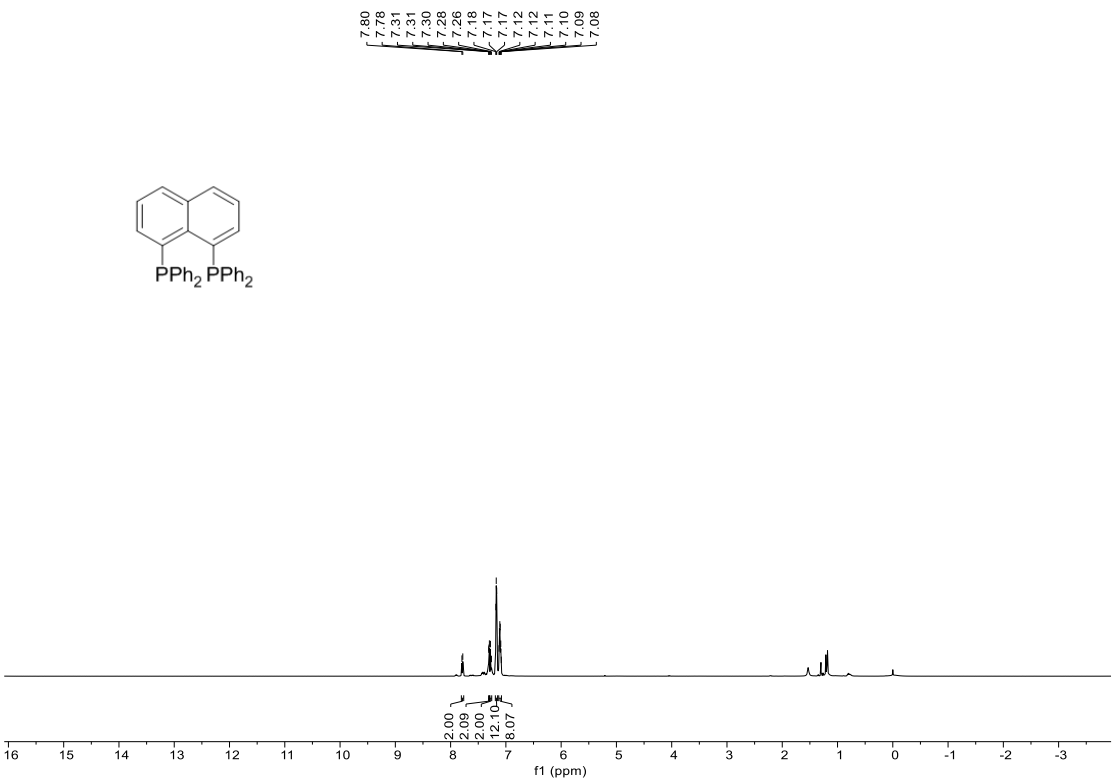
^{1}H NMR (400 MHz, $CDCl_3$) of **2ax**



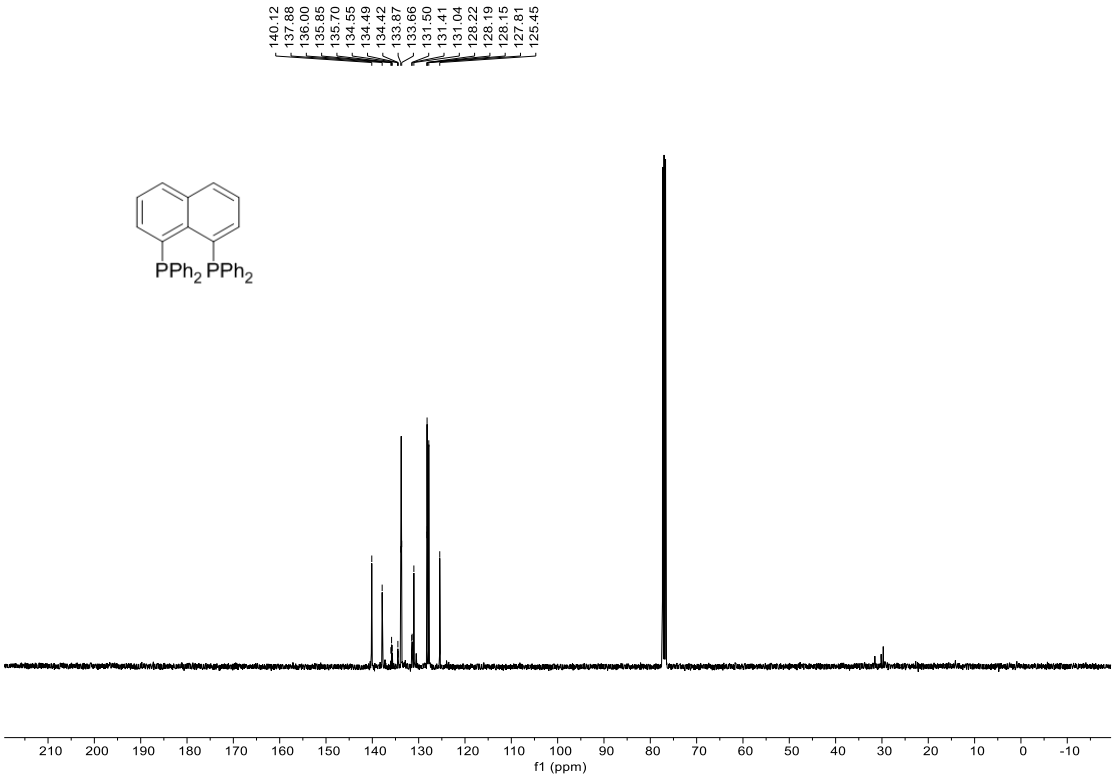
^{13}C NMR (101 MHz, $CDCl_3$) of **2ax**



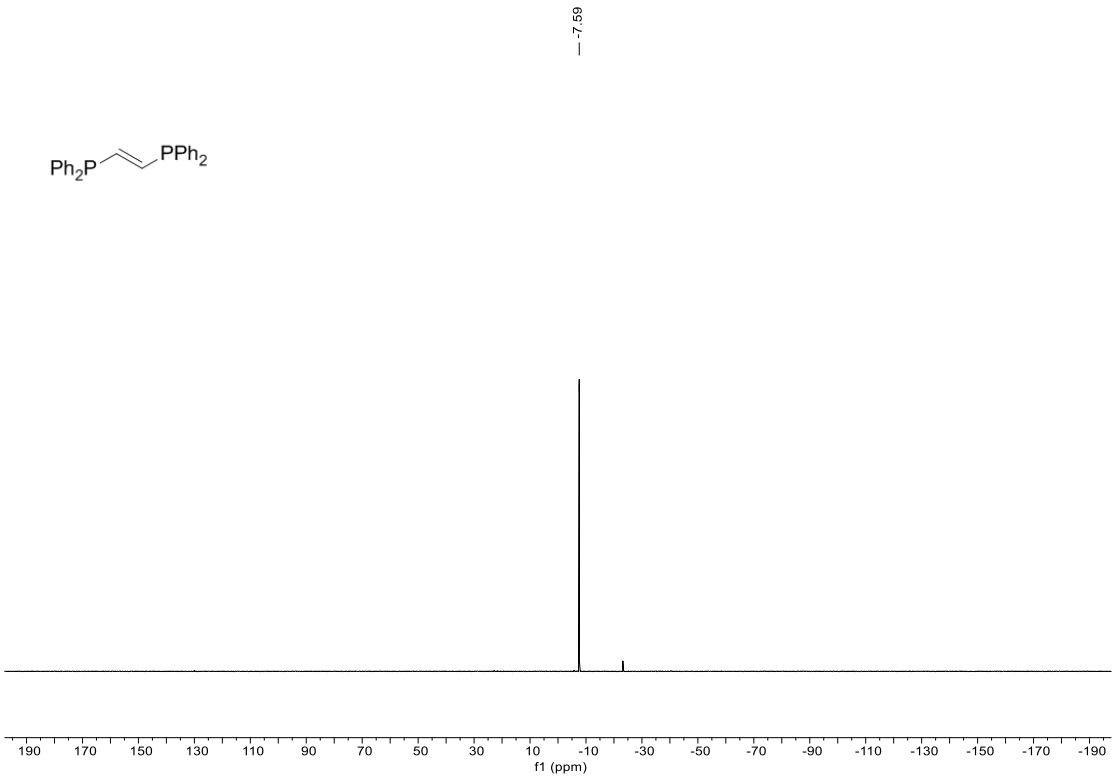
^{31}P NMR (162 MHz, $CDCl_3$) of **2ay**



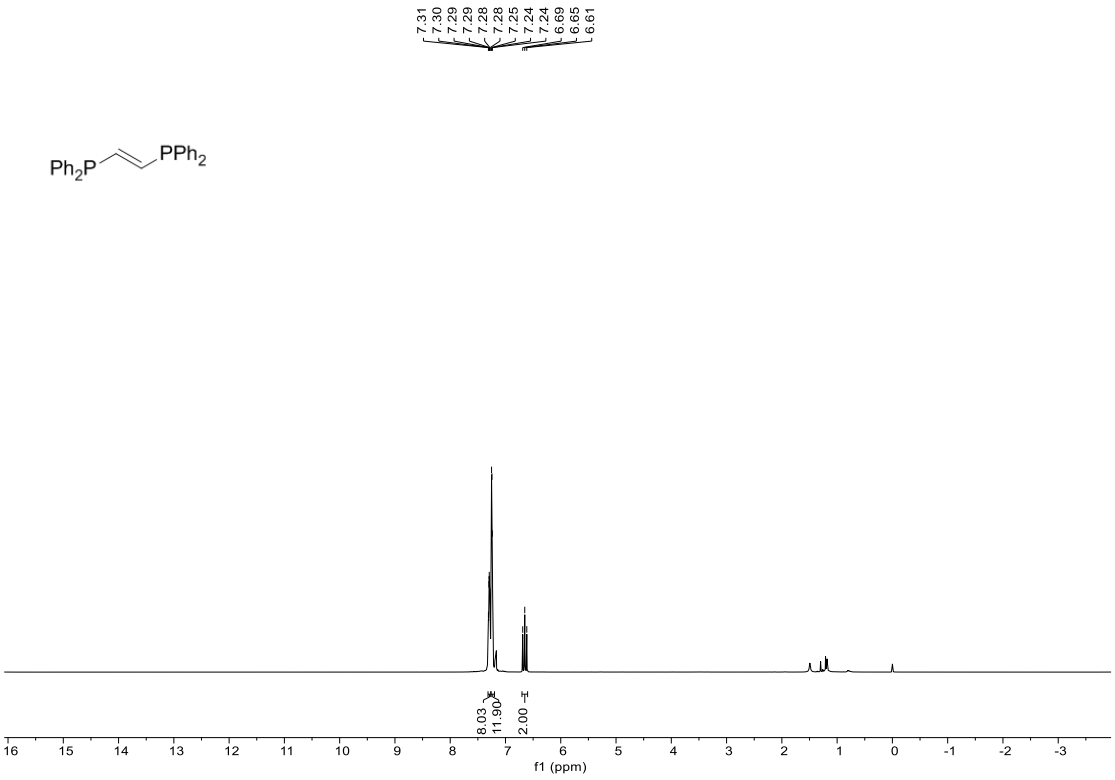
^{1}H NMR (400 MHz, $CDCl_3$) of **2ay**



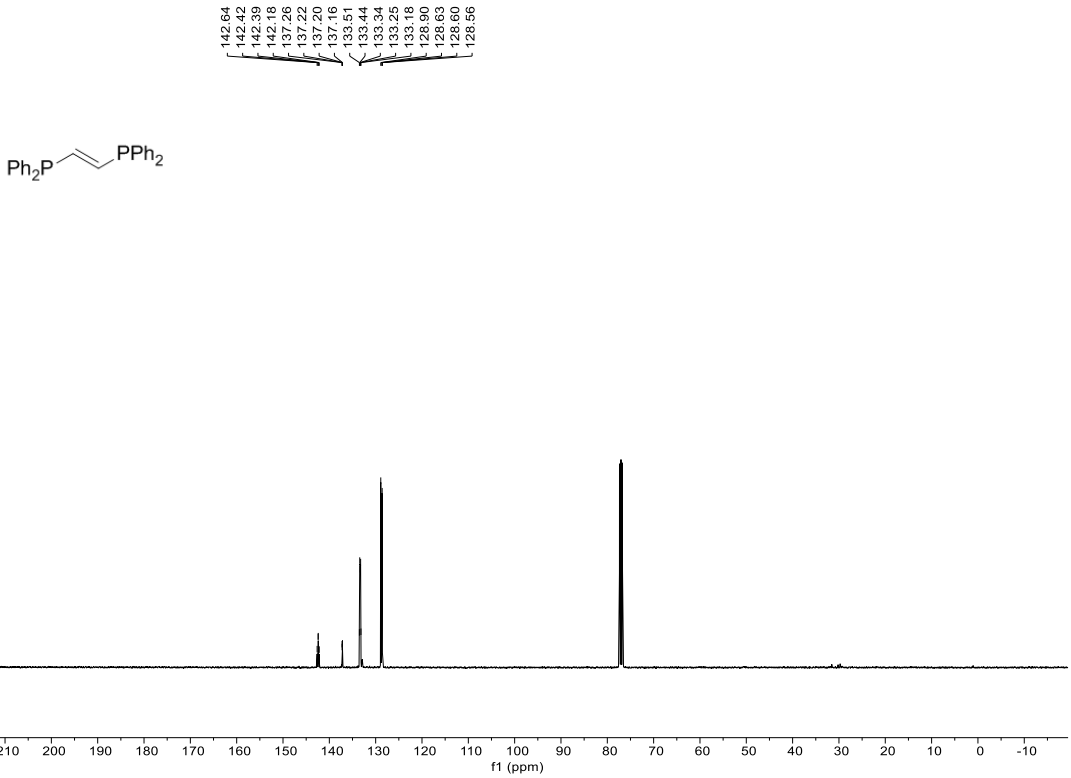
^{13}C NMR (101 MHz, $CDCl_3$) of **2ay**



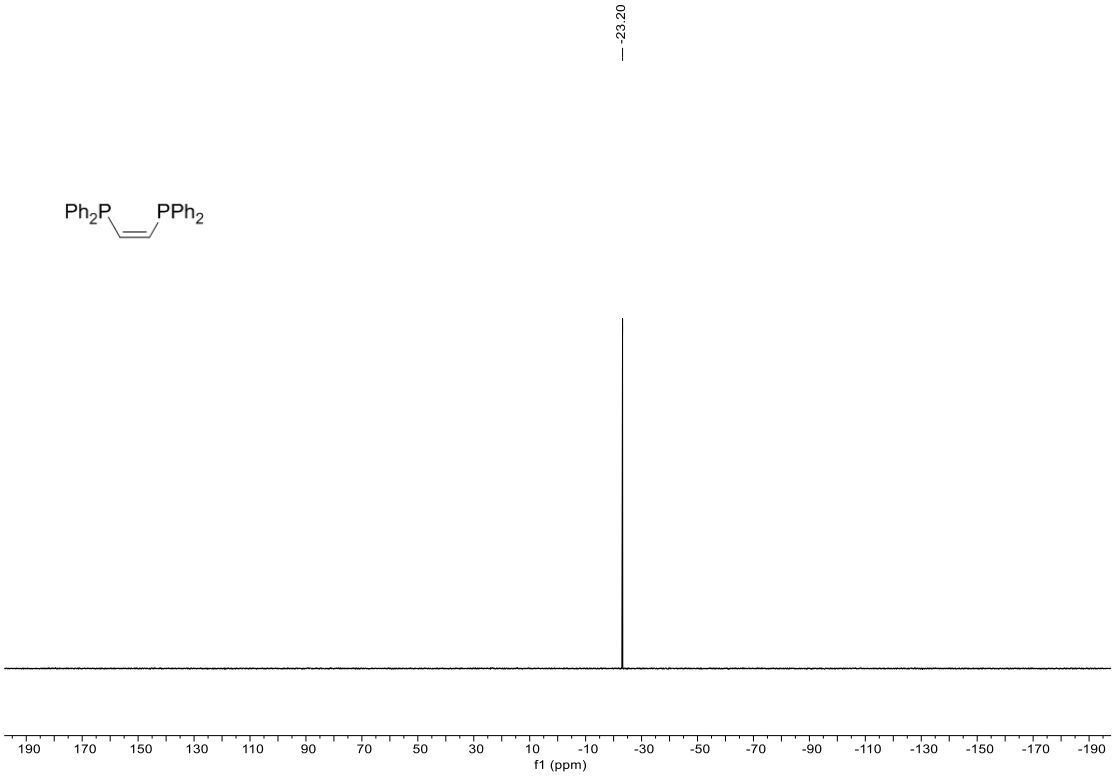
^{31}P NMR (162 MHz, $CDCl_3$) of **2az**[1]



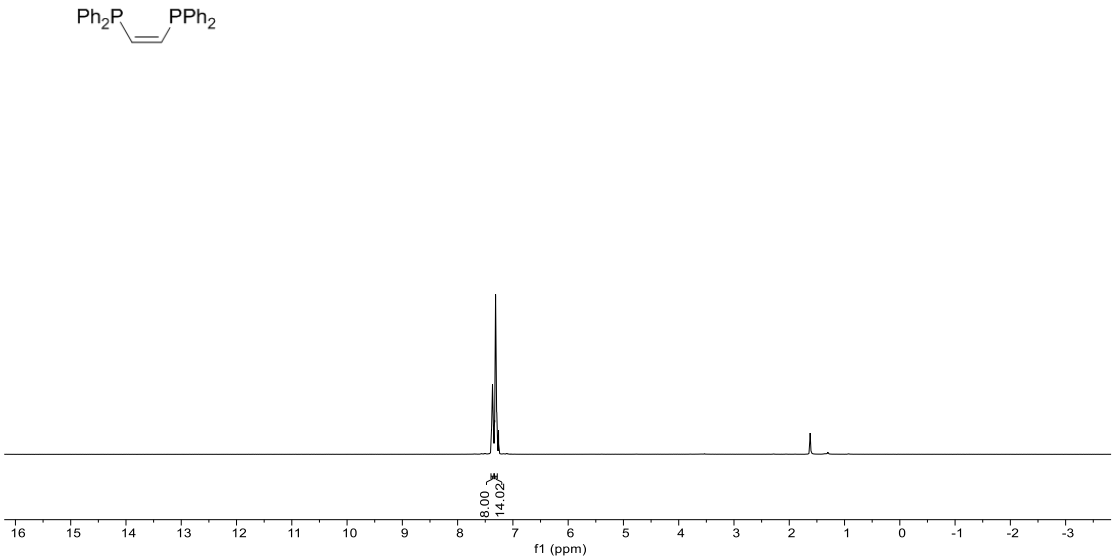
^{1}H NMR (400 MHz, $CDCl_3$) of **2az**[1]



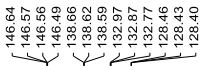
^{13}C NMR (101 MHz, $CDCl_3$) of **2az**[1]

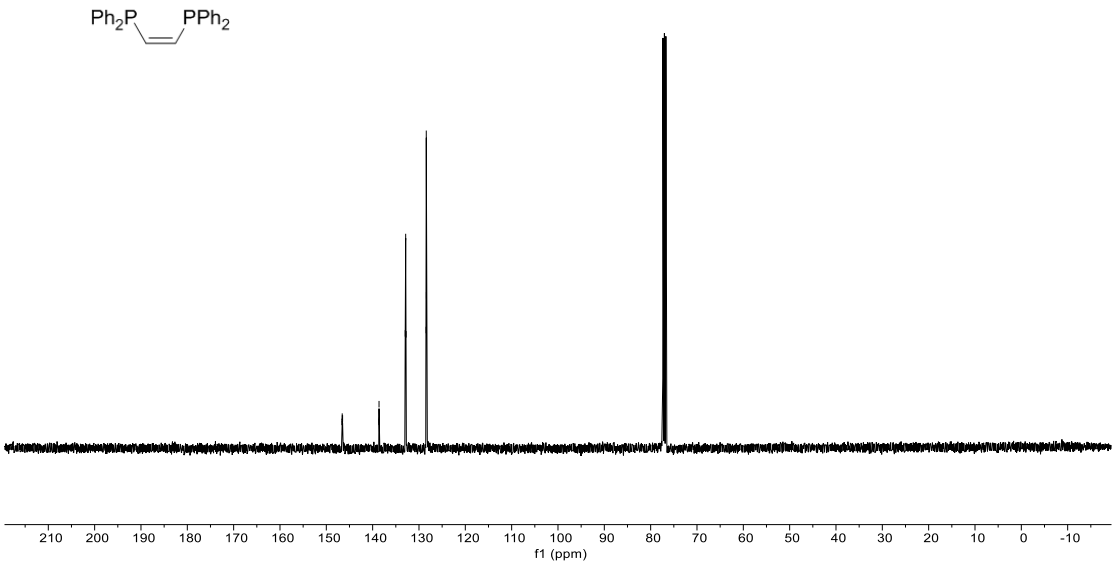


^{31}P NMR (162 MHz, $CDCl_3$) of **2az**[2]

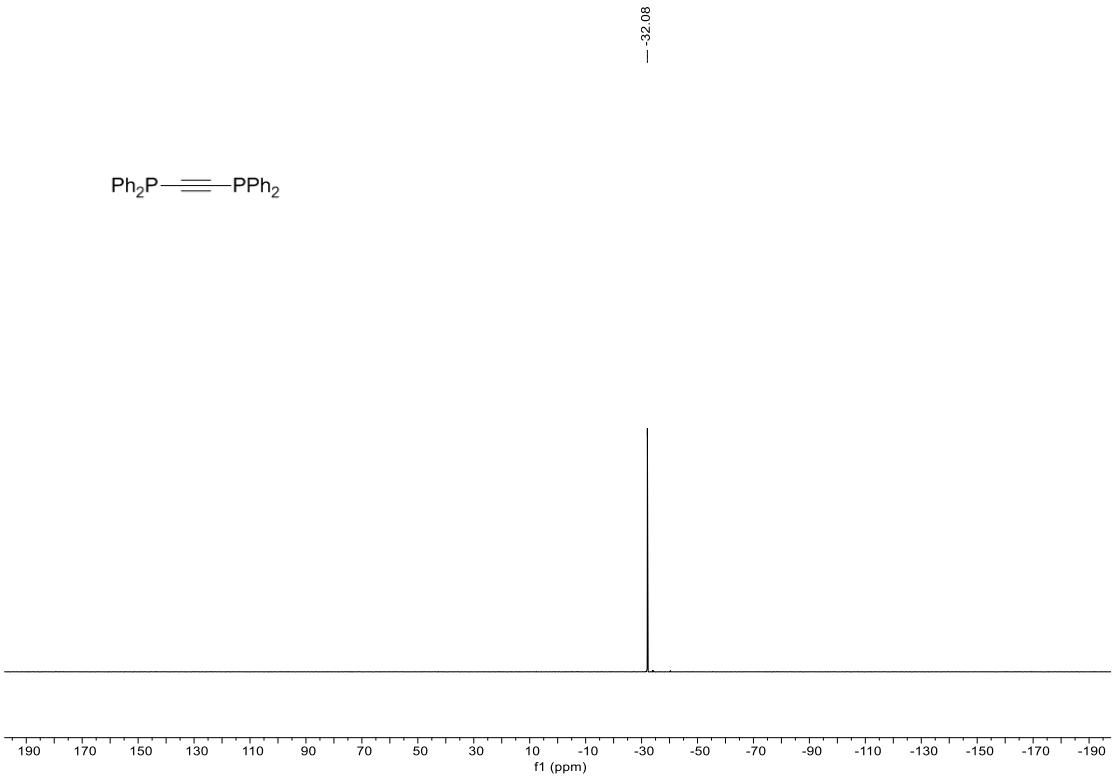


^{1}H NMR (400 MHz, $CDCl_3$) of **2ae**[2]

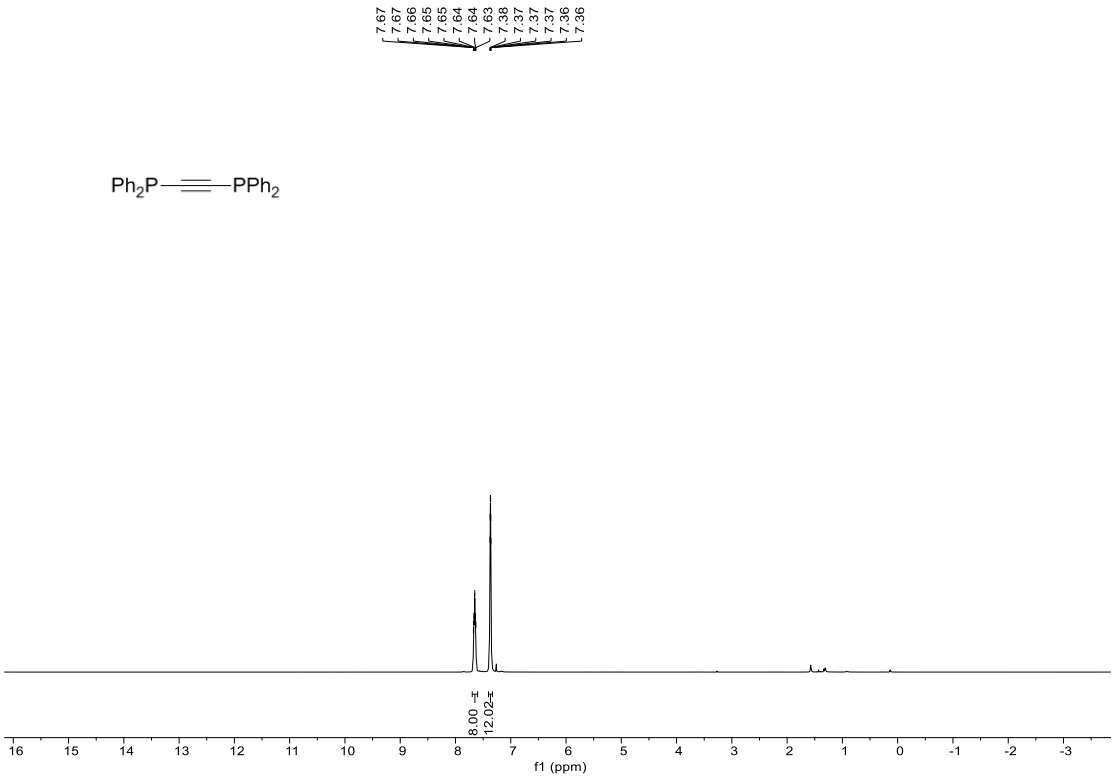




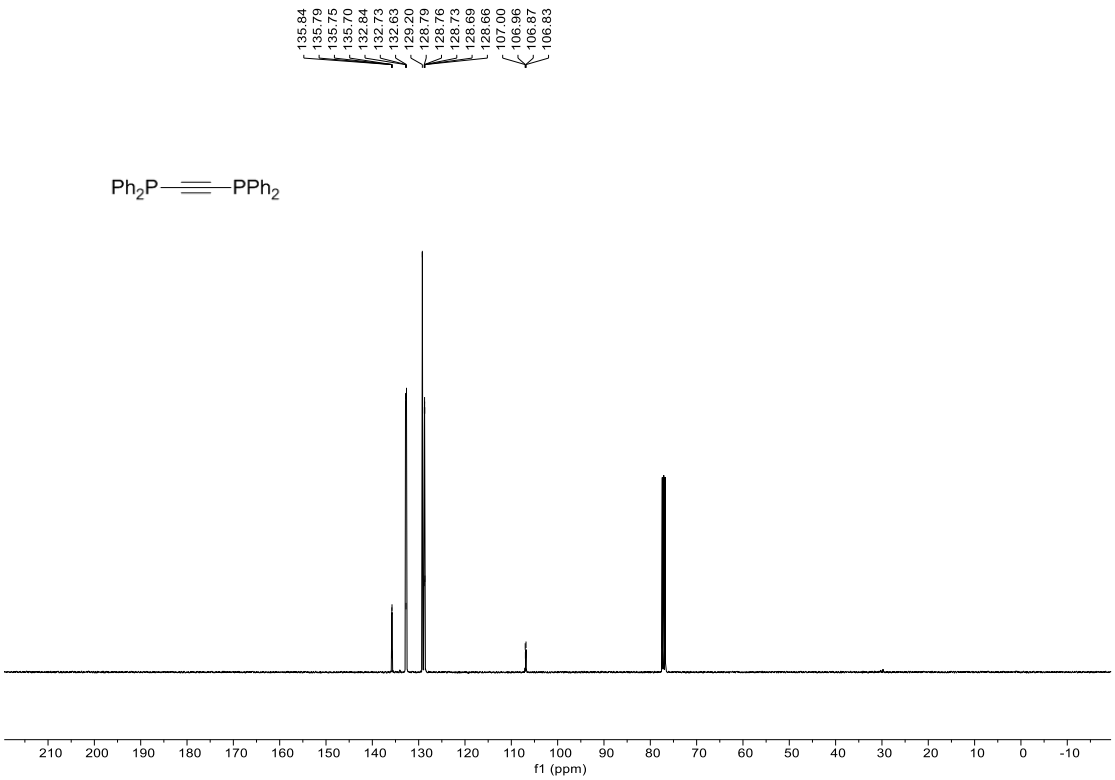
^{13}C NMR (101 MHz, $CDCl_3$) of **2ae**[2]



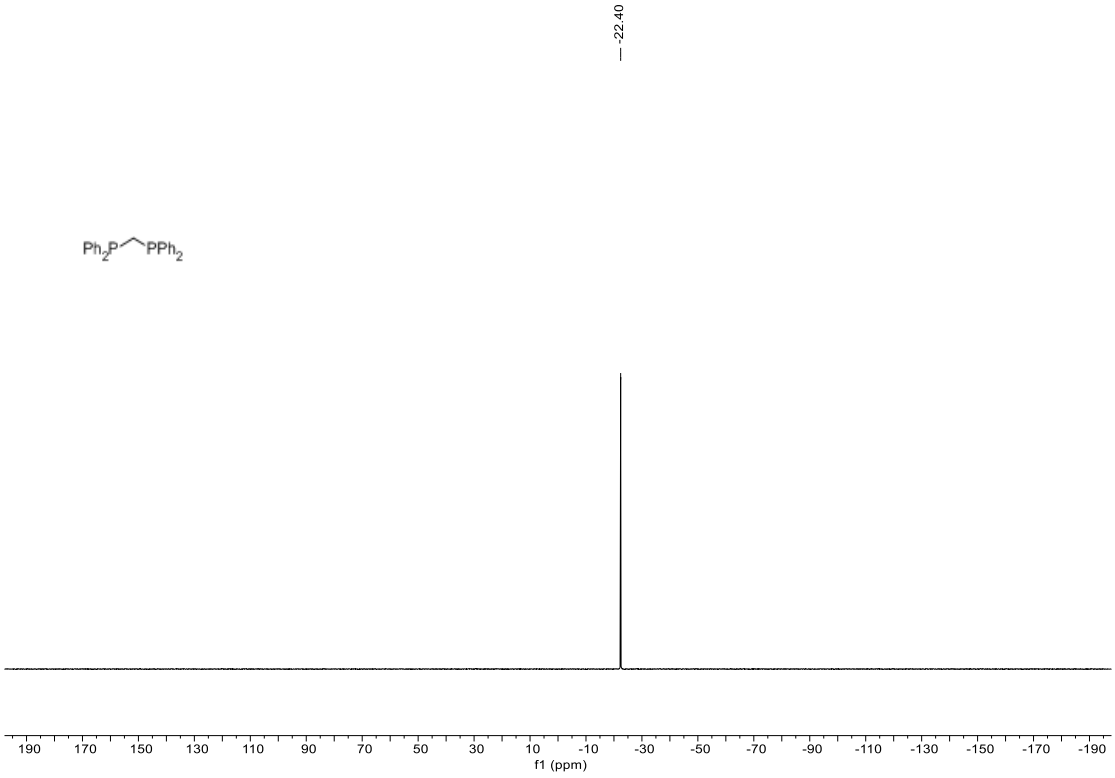
^{31}P NMR (162 MHz, $CDCl_3$) of **2 ba**



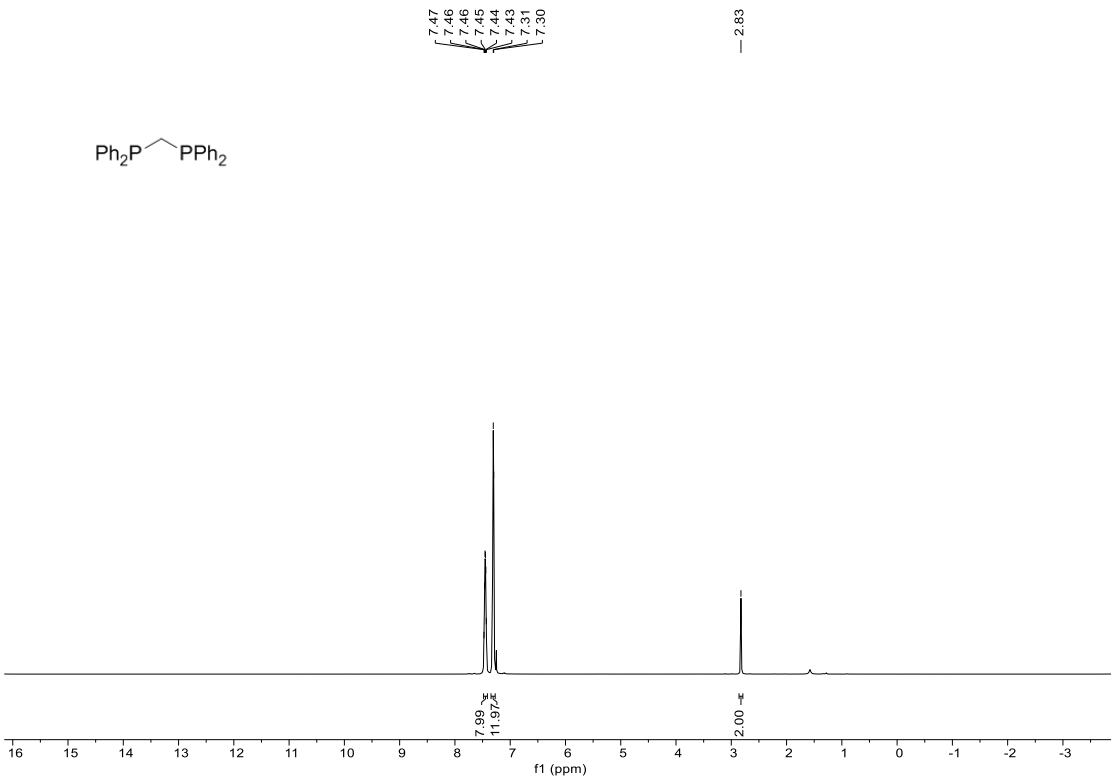
^{1}H NMR (400 MHz, $CDCl_3$) of **2 ba**



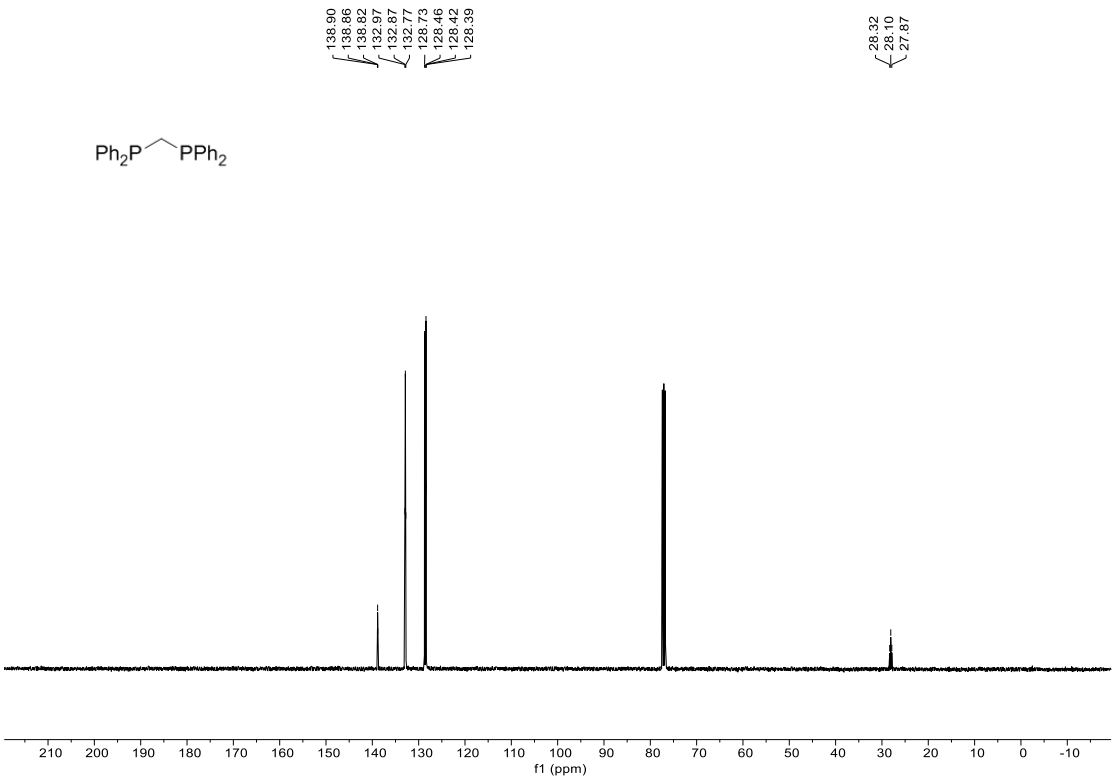
^{13}C NMR (101 MHz, $CDCl_3$) of **2 ba**



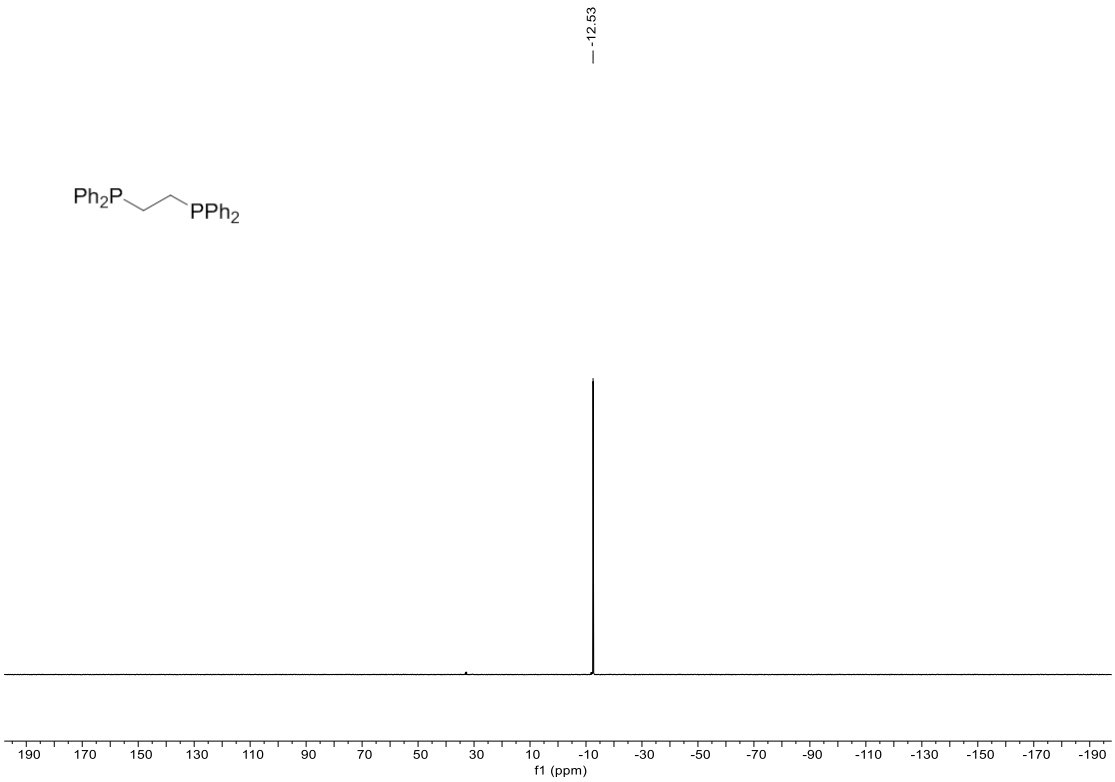
^{31}P NMR (162 MHz, $CDCl_3$) of **2bb**



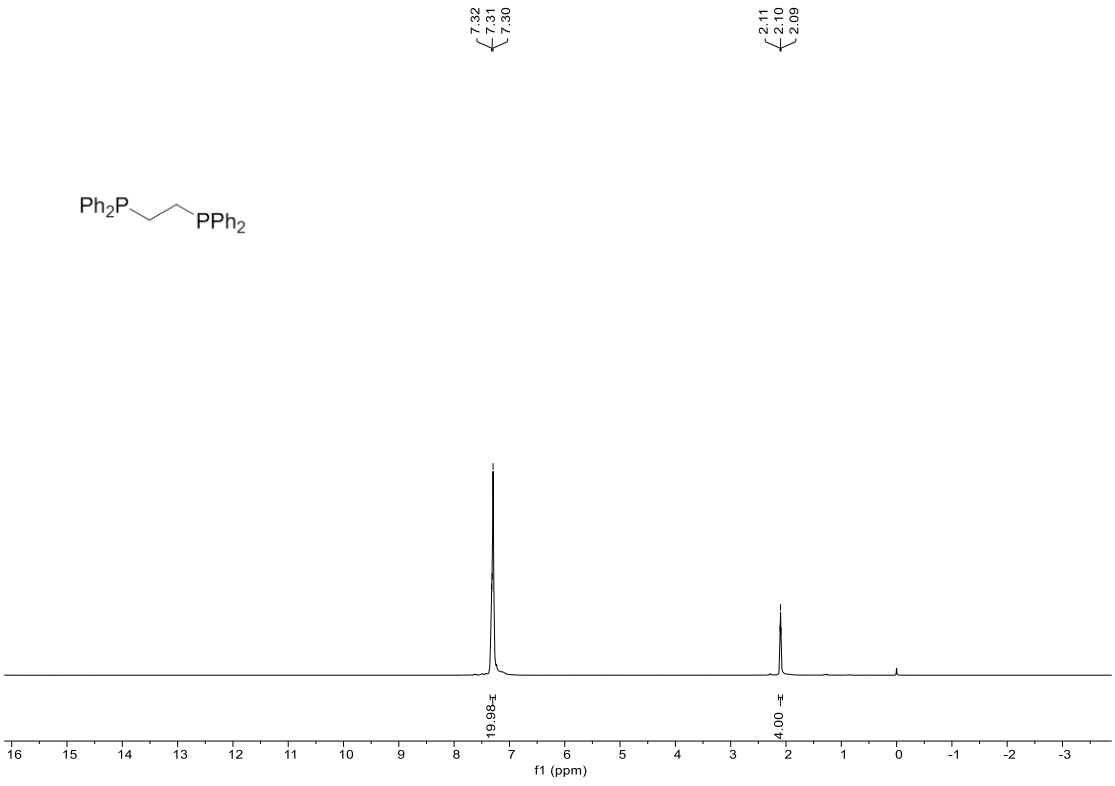
^{1}H NMR (400 MHz, $CDCl_3$) of **2bb**



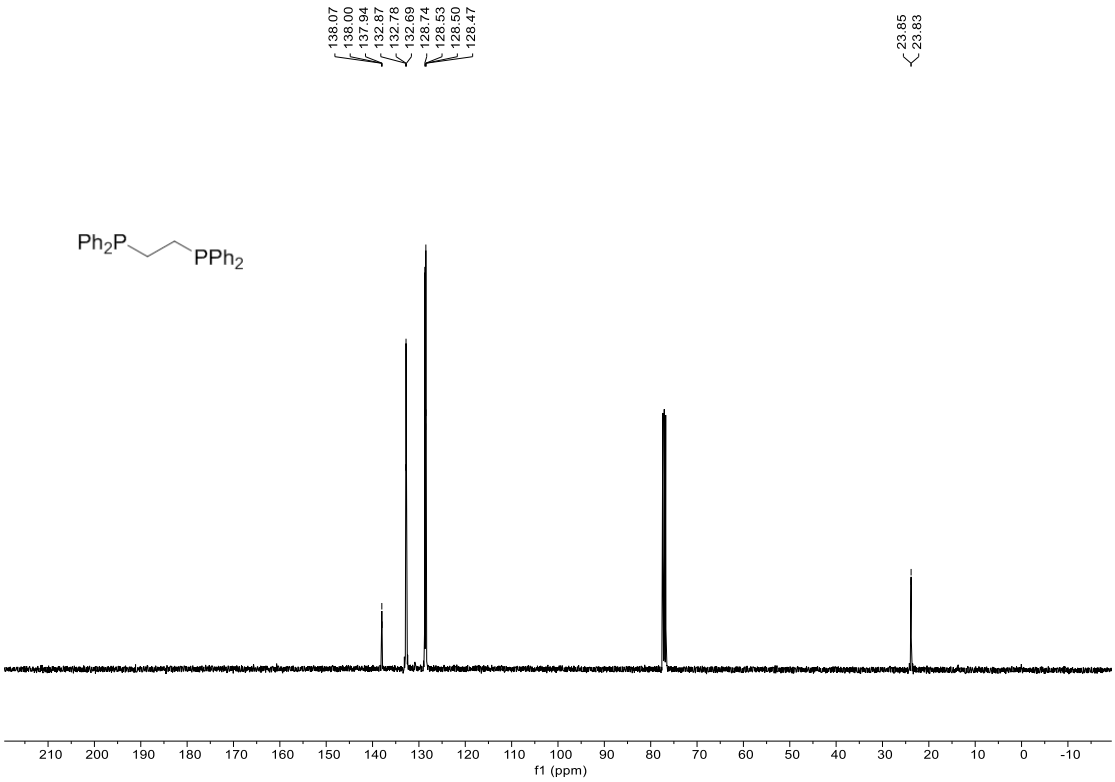
^{13}C NMR (101 MHz, $CDCl_3$) of **2bb**



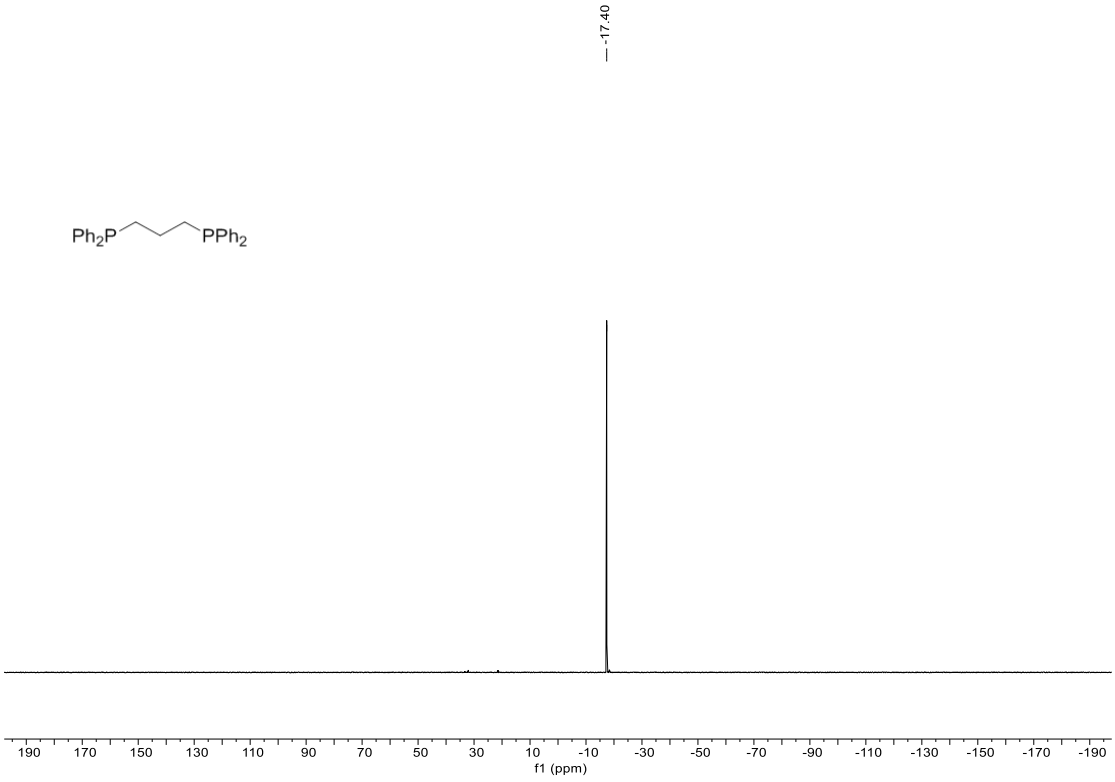
^{31}P NMR (162 MHz, $CDCl_3$) of **2bc**



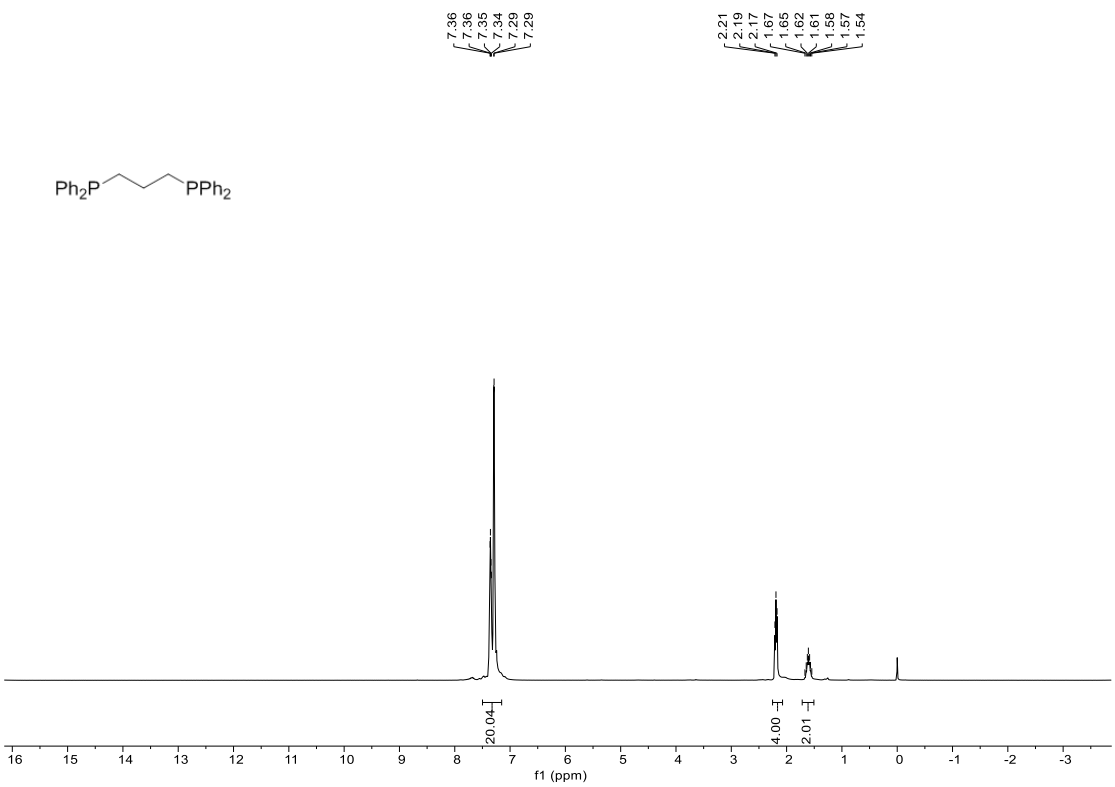
^{1}H NMR (400 MHz, $CDCl_3$) of **2bc**



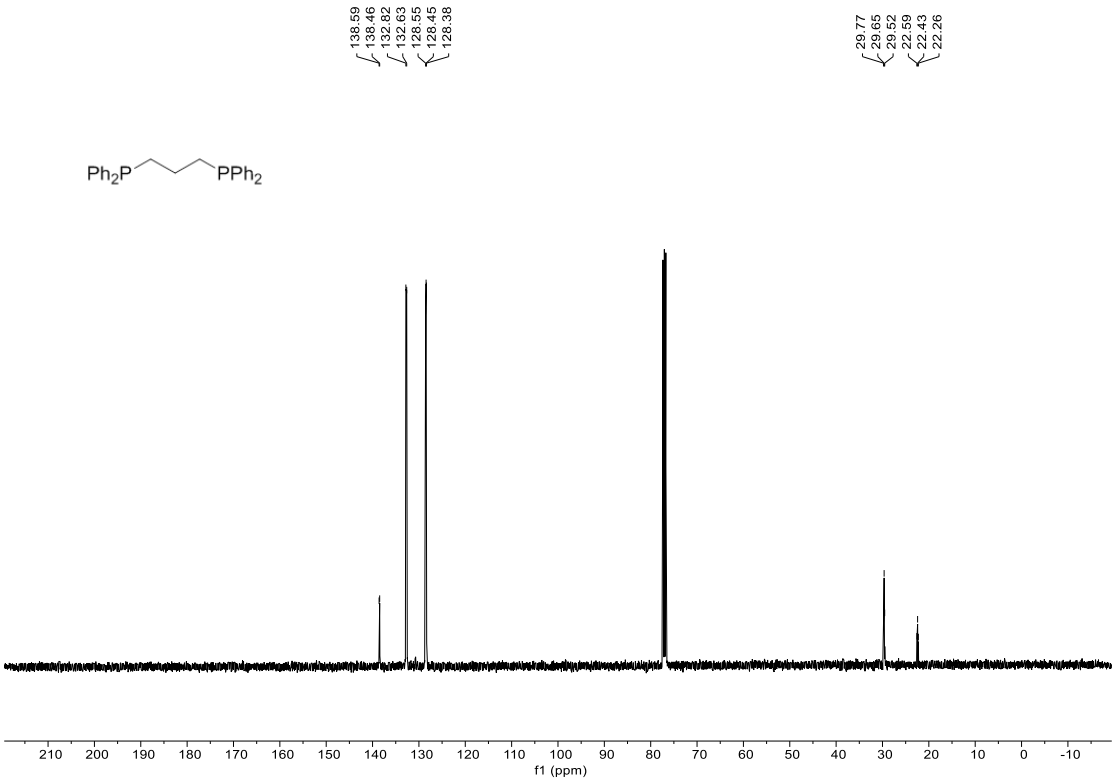
^{13}C NMR (101 MHz, $CDCl_3$) of **2bc**



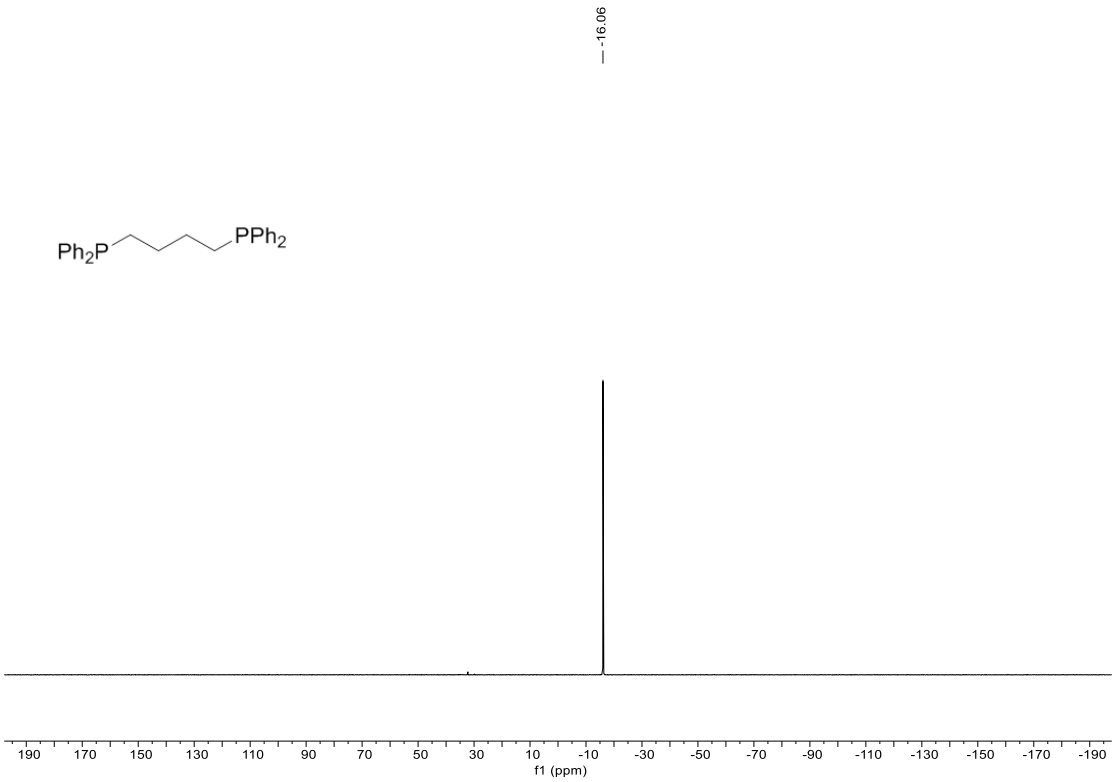
^{31}P NMR (162 MHz, $CDCl_3$) of **2bd**



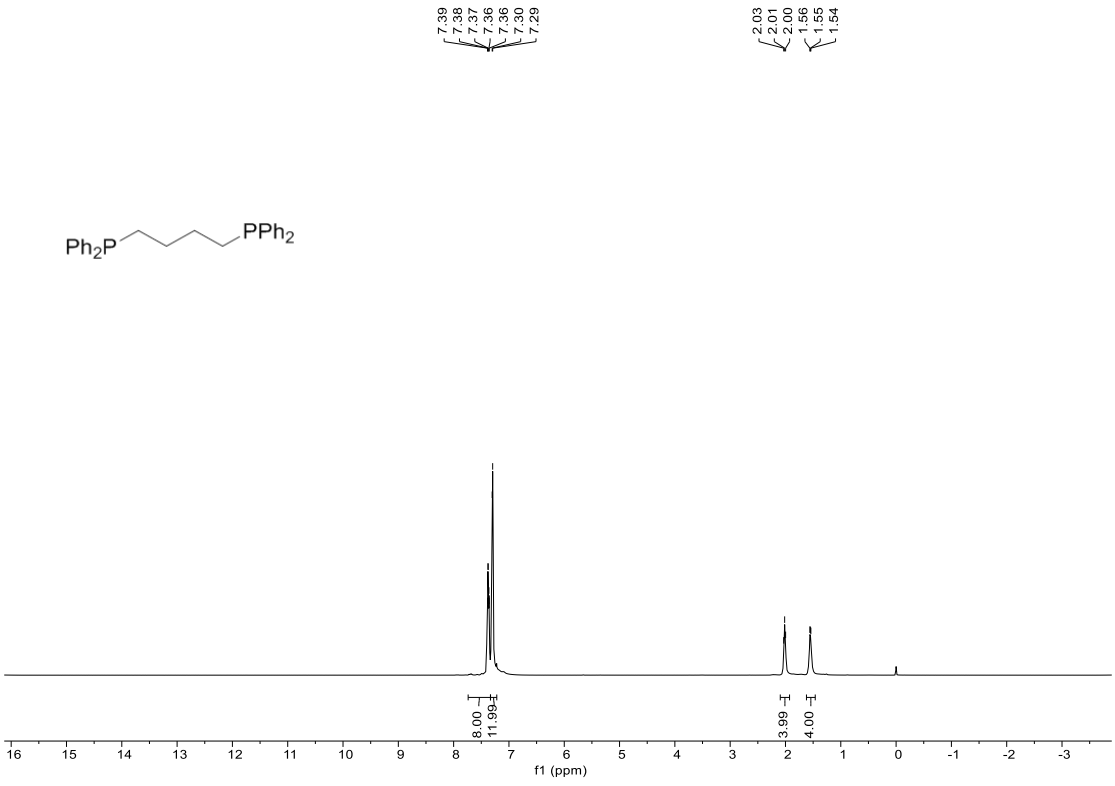
^{1}H NMR (400 MHz, $CDCl_3$) of **2bd**



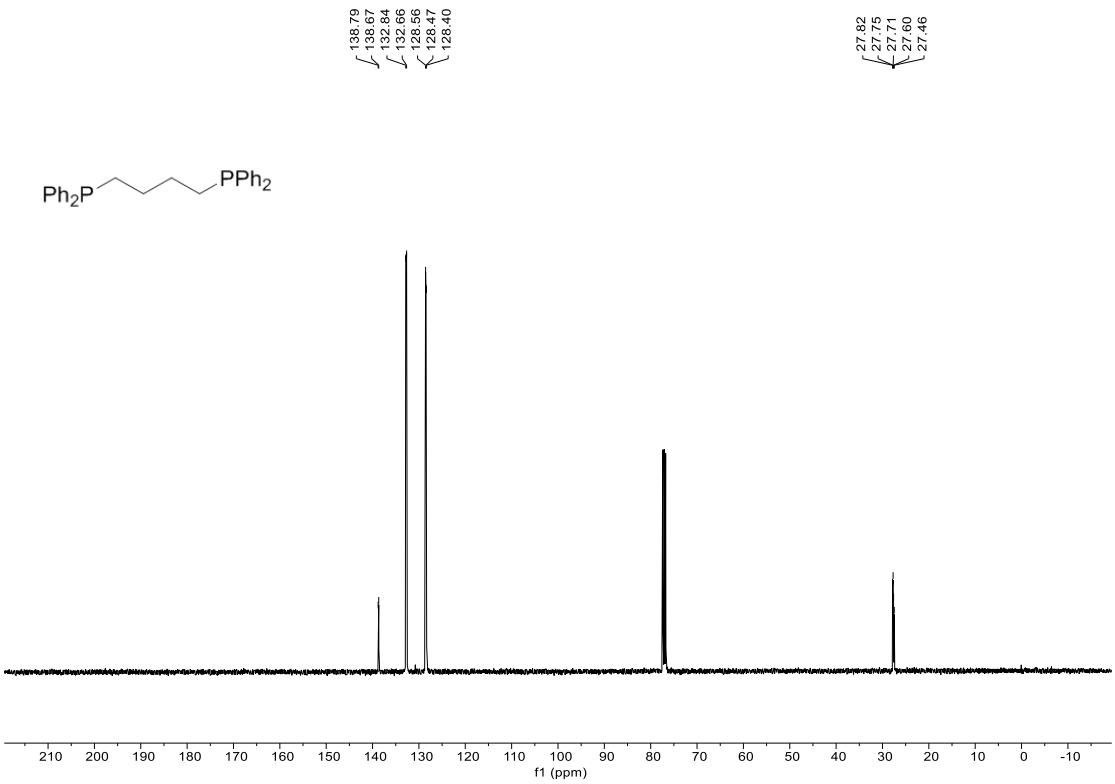
^{13}C NMR (101 MHz, $CDCl_3$) of **22bd**



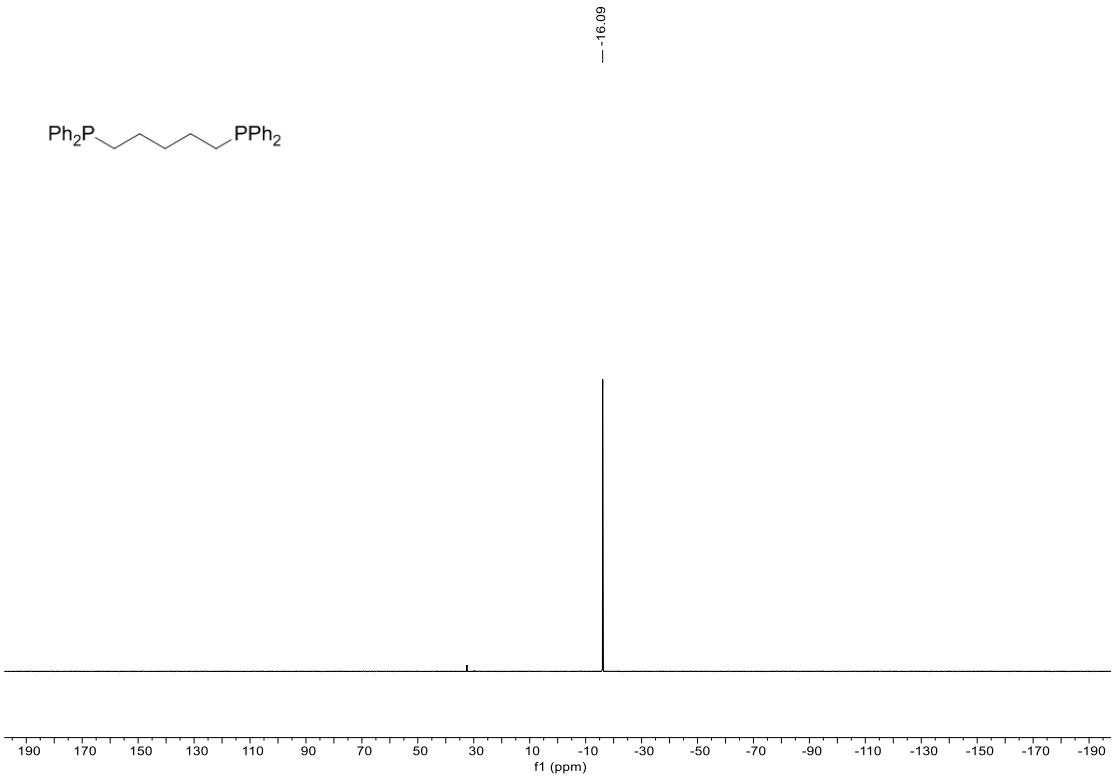
^{31}P NMR (162 MHz, $CDCl_3$) of **2be**



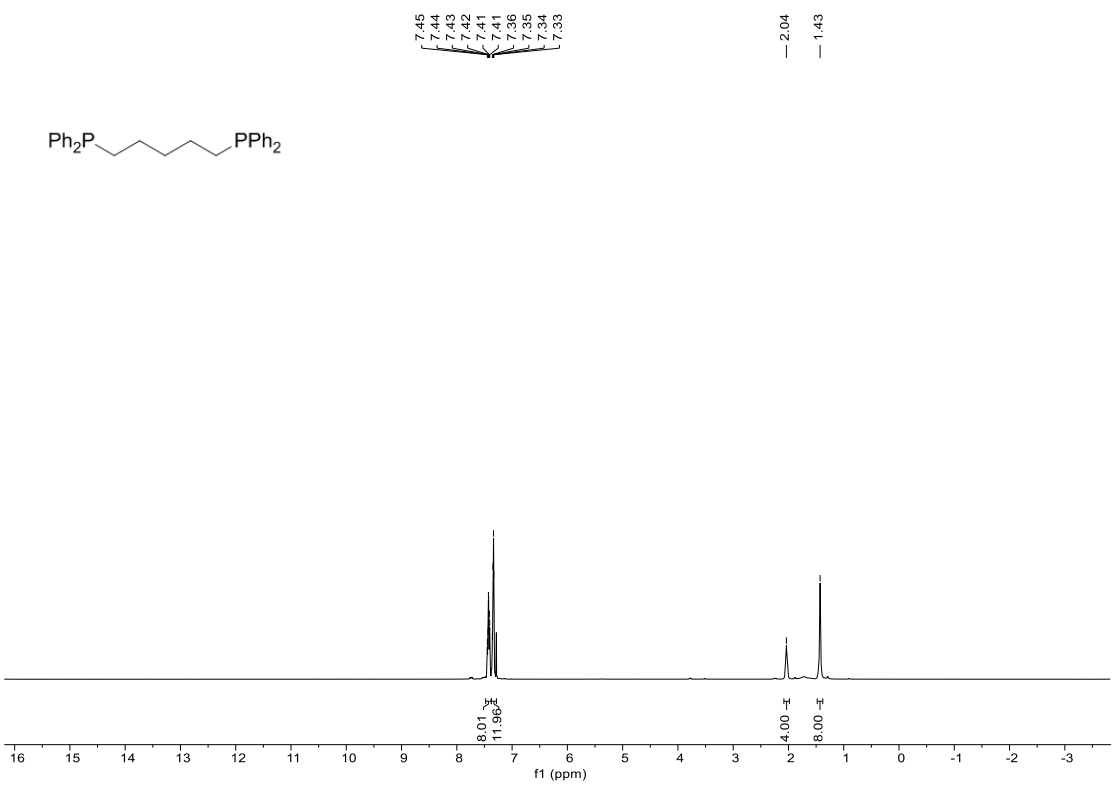
^{1}H NMR (400 MHz, $CDCl_3$) of **2be**



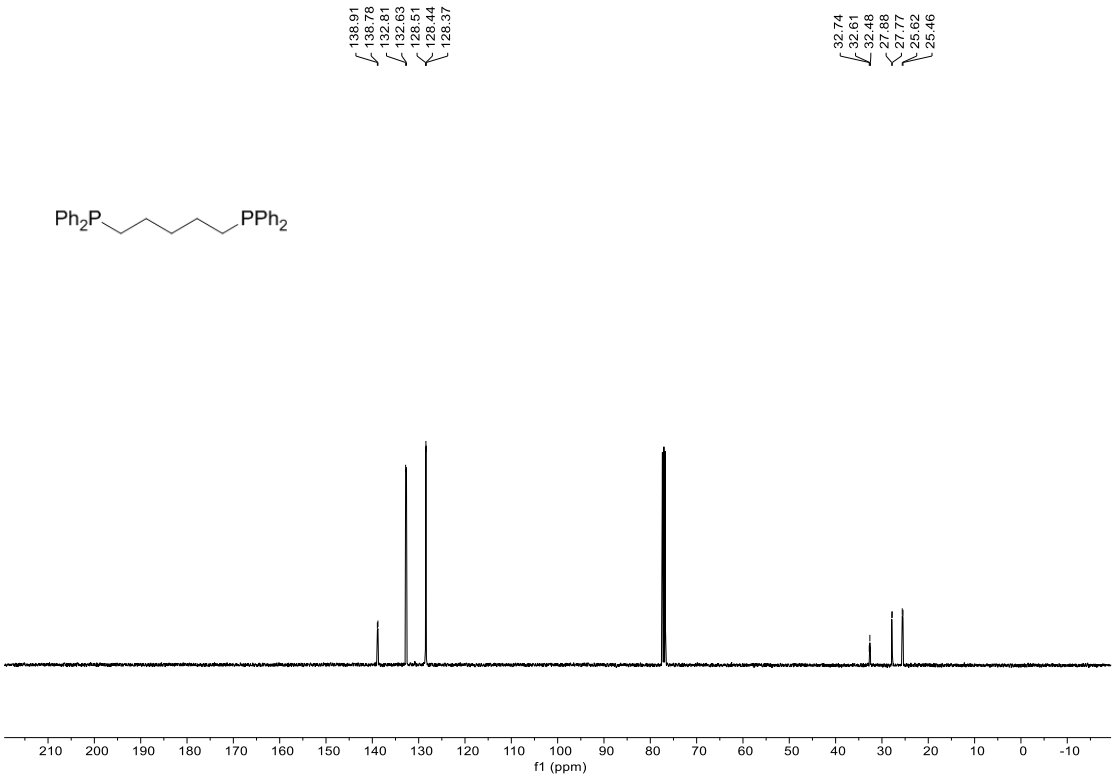
^{13}C NMR (101 MHz, $CDCl_3$) of **2be**



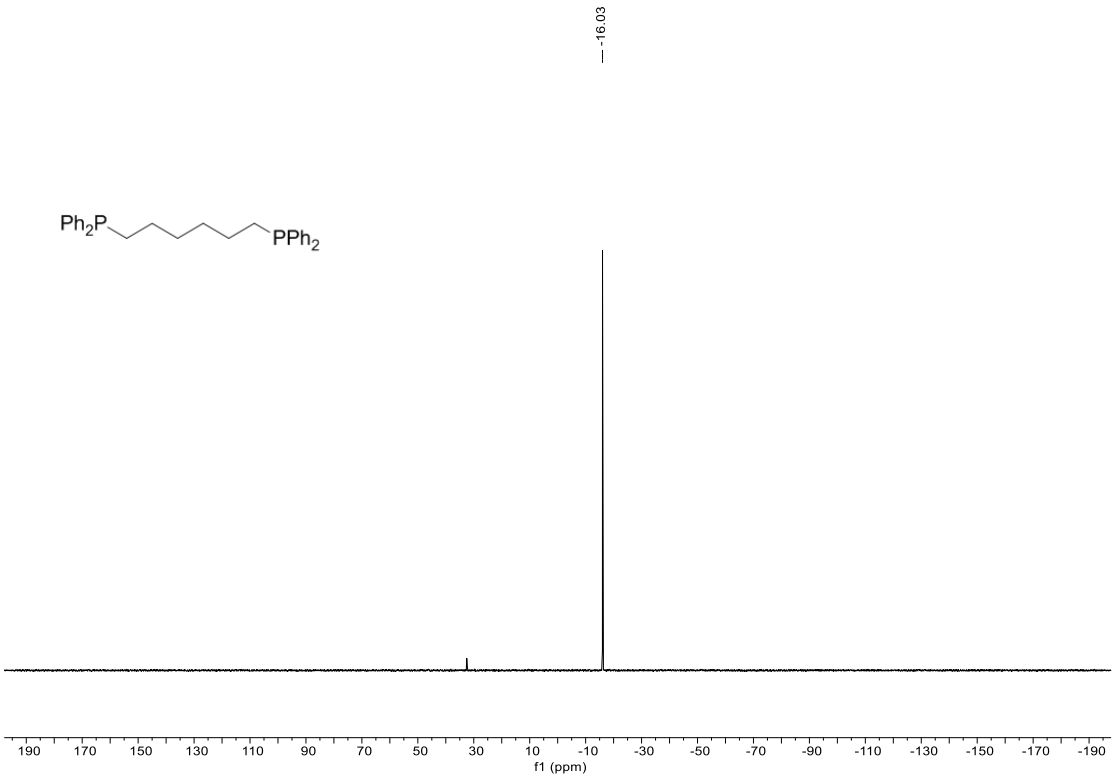
^{31}P NMR (162 MHz, $CDCl_3$) of **2bf**



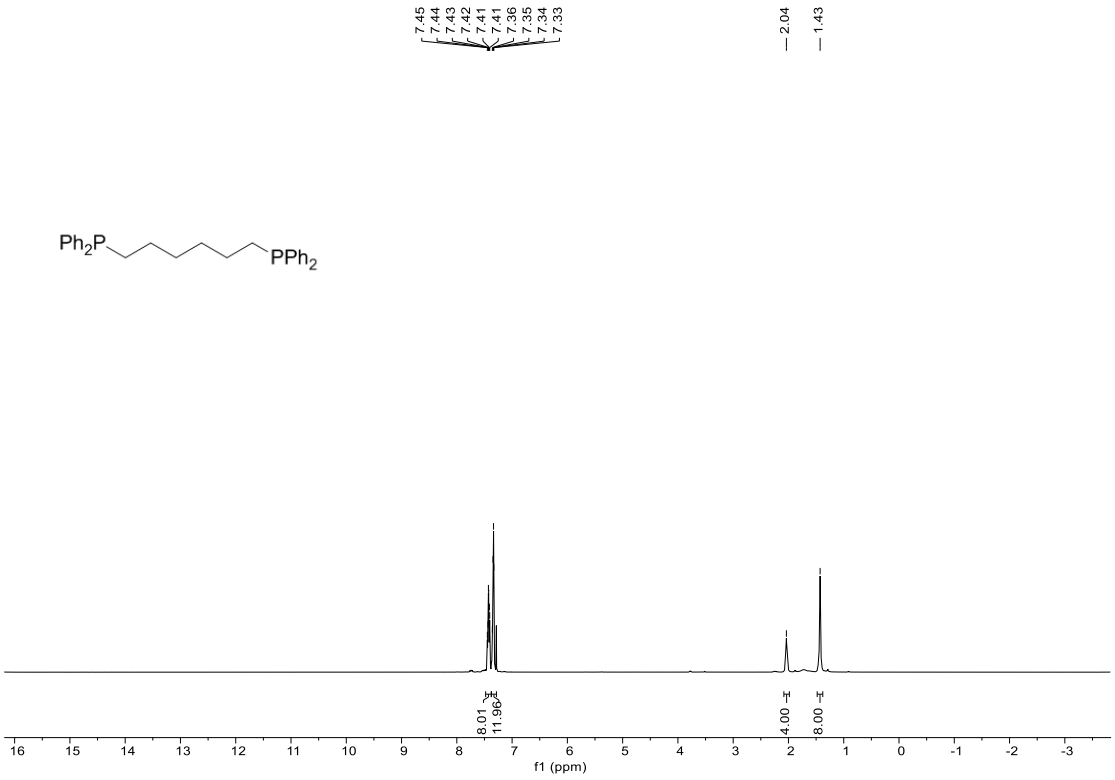
^{1}H NMR (400 MHz, $CDCl_3$) of **2bf**



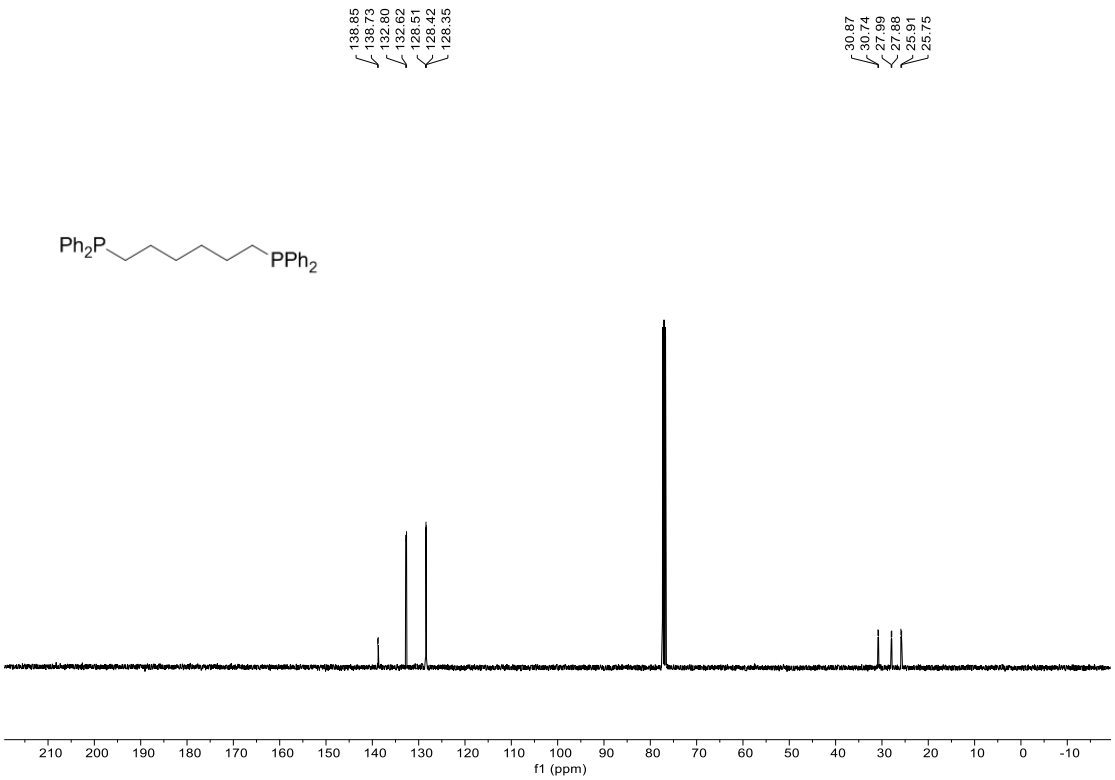
^{13}C NMR (101 MHz, $CDCl_3$) of **2bf**



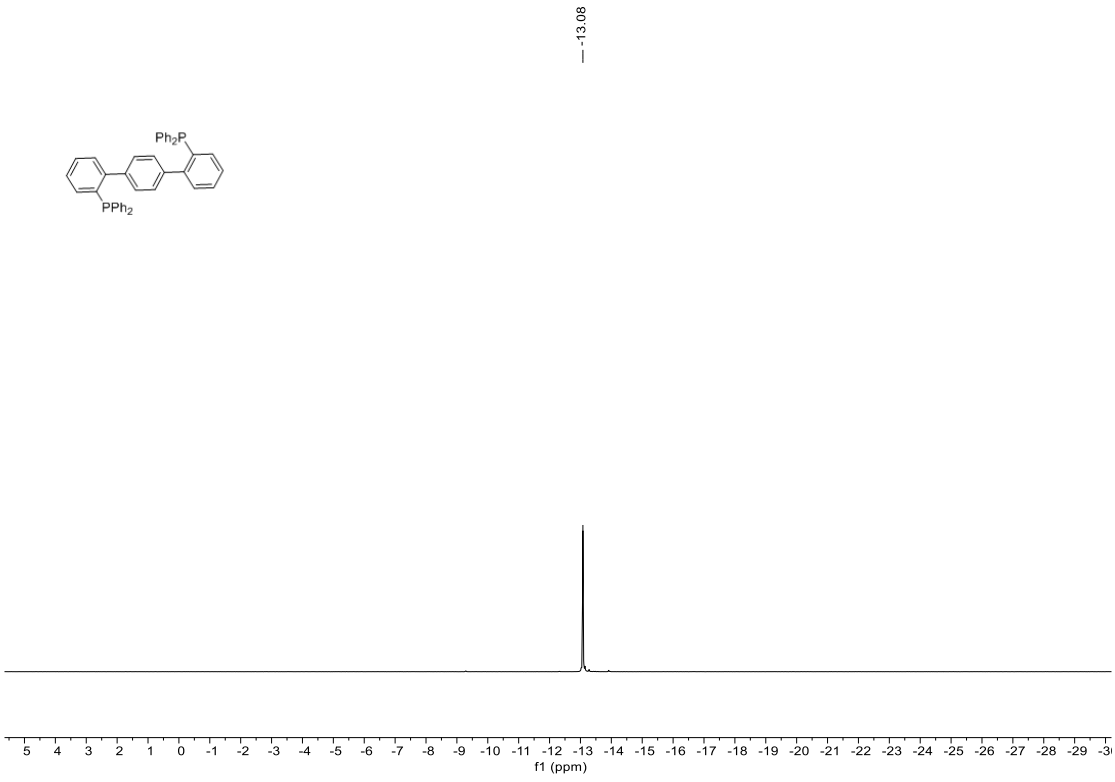
^{31}P NMR (162 MHz, $CDCl_3$) of **2bg**



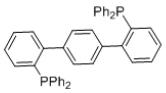
^{1}H NMR (400 MHz, $CDCl_3$) of **2bg**

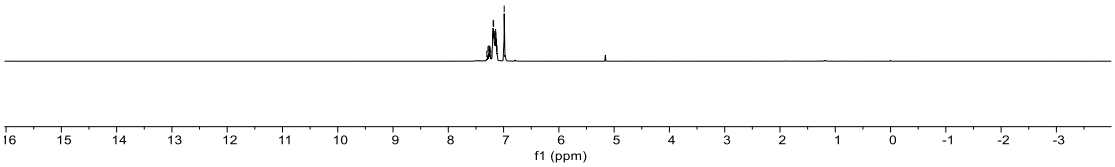


^{13}C NMR (101 MHz, $CDCl_3$) of **2bg**

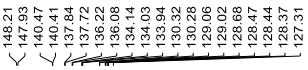


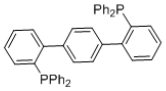
^{31}P NMR (162 MHz, $CDCl_3$) of **2bh**

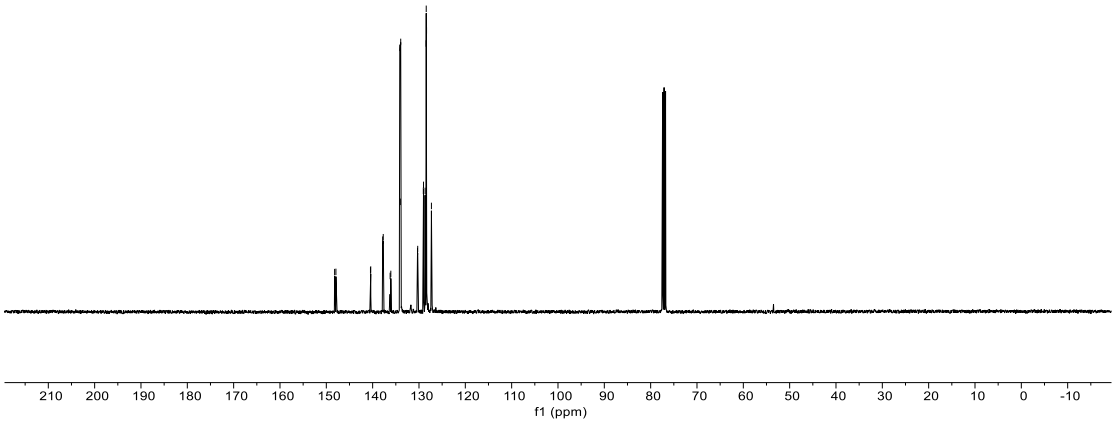




^{1}H NMR (400 MHz, $CDCl_3$) of **2bh**







^{13}C NMR (101 MHz, $CDCl_3$) of **2bh**

9. Symbolic Z-matrix of calculational molecules

1a:

0 1

O	0.00003400	-0.00006100	2.46054200
P	-0.00004300	-0.00002700	0.95822600
C	1.07515800	1.28563700	0.24194500
C	1.28608200	2.43902800	1.00888000
C	1.67186700	1.17288100	-1.02042900
C	2.07157800	3.47605800	0.50890200
H	0.84348400	2.50141600	1.99777600
C	2.45389700	2.21450100	-1.51886900
H	1.53994000	0.26812900	-1.60516900
C	2.65136500	3.36678800	-0.75638100
H	2.23537000	4.36713500	1.10709500
H	2.91631100	2.12283500	-2.49693400
H	3.26391200	4.17495500	-1.14447000
C	0.57584600	-1.57397800	0.24193800
C	0.17851700	-2.03533200	-1.01964800
C	1.47077400	-2.33231000	1.00812400
C	0.68984100	-3.23328800	-1.51813700
H	-0.54019400	-1.46950400	-1.60374300
C	1.97636700	-3.53095800	0.50813300
H	1.74712300	-1.97953800	1.99650000
C	1.59056600	-3.97936500	-0.75643900
H	0.37826200	-3.58865200	-2.49562100
H	2.66738300	-4.11750100	1.10574800
H	1.98438600	-4.91383700	-1.14454700
C	-1.65115300	0.28826500	0.24206700
C	-1.85214900	0.86297700	-1.01952100
C	-2.75529000	-0.10739000	1.00847200
C	-3.14531800	1.01946600	-1.51775500
H	-1.00276400	1.20218500	-1.60376900
C	-4.04620400	0.05437800	0.50871000
H	-2.58782800	-0.52308800	1.99683200
C	-4.24174800	0.61276800	-0.75581700
H	-3.29736400	1.46697100	-2.49523300
H	-4.89964500	-0.25055700	1.10648300
H	-5.24797900	0.73919400	-1.14373100

2a:

P	0.00012800	0.00028100	-1.27820200
C	0.23970300	-1.63183200	-0.44780200
C	-0.40691400	-2.74070600	-1.01501100
C	1.01828100	-1.81976900	0.70233700
C	-0.29414200	-4.00364300	-0.43689400
H	-1.00184700	-2.60980000	-1.91496500
C	1.14051700	-3.08671900	1.27415500
H	1.52751800	-0.97381000	1.15085100
C	0.48294300	-4.17983400	0.70932400
H	-0.80453900	-4.85094600	-0.88499500
H	1.74841300	-3.21853900	2.16451100
H	0.57907600	-5.16460900	1.15647500
C	1.29372900	1.02366800	-0.44753400
C	1.06674200	1.79342700	0.70148300
C	2.57783200	1.01659200	-1.01363600
C	2.10289900	2.53259200	1.27340700
H	0.07911400	1.81295900	1.14908900
C	3.61522800	1.74554900	-0.43539800
H	2.76229400	0.43480900	-1.91281000
C	3.37884900	2.50805600	0.70978600
H	1.91273800	3.12614400	2.16289200
H	4.60458700	1.72591100	-0.88261300
H	4.18366600	3.08355200	1.15704300
C	-1.53321700	0.60858600	-0.44770500
C	-2.08588600	0.02741900	0.70172900
C	-2.16995600	1.72336400	-1.01450100
C	-3.24443500	0.55475000	1.27335400
H	-1.60851200	-0.83727100	1.14964900
C	-3.32034200	2.25682000	-0.43659000
H	-1.75877900	2.17359000	-1.91407400
C	-3.86195800	1.67124300	0.70902900
H	-3.66308800	0.09354400	2.16310800
H	-3.79872700	3.12276500	-0.88437000
H	-4.76305600	2.08011700	1.15603400

-OTf:

S	0.92454600	-0.00000400	0.00002100
O	1.24145300	-0.23698900	1.42669700
O	1.24155200	-1.11708100	-0.91859600
O	1.24148100	1.35409200	-0.50813600
C	-0.93925200	-0.00004400	-0.00005700
F	-1.44271100	-1.17460300	0.44035900

F	-1.44276000	0.20591900	-1.23733600
F	-1.44265300	0.96870200	0.79700800

$Me(EtO)_2SiH$:

Si	0.21050000	0.92590100	-0.52054800
O	-0.91652200	-0.25381200	-0.18684500
C	-2.29929200	0.02870400	0.00834500
H	-2.43543400	0.65441100	0.90251500
H	-2.69743100	0.59160800	-0.84926700
C	0.21903000	2.20566500	0.84938800
H	0.96535700	2.98104100	0.64932900
H	-0.75605700	2.69658900	0.94005600
H	0.45166300	1.75425900	1.81946000
O	1.67872500	0.19204400	-0.68687600
C	2.30561400	-0.57910400	0.33971900
H	2.07176600	-0.16654300	1.33193800
C	-3.05151300	-1.28105900	0.16672200
H	-2.66451700	-1.83901700	1.02426100
H	-4.11925700	-1.09688500	0.32307200
H	-2.92986300	-1.89906600	-0.72710500
H	3.38670700	-0.47679300	0.19564700
C	1.89042100	-2.04140100	0.26498700
H	0.81307900	-2.13923500	0.41930000
H	2.13542800	-2.45275500	-0.71832800
H	2.41500800	-2.62706400	1.02791800
H	-0.06663700	1.55414800	-1.83632000

$Me(EtO)_2SiOH$:

Si	-0.22085200	-0.87564800	-0.11102600
O	0.82508500	0.41330100	-0.04834000
C	2.23816200	0.26495600	0.08476600
H	2.47518600	-0.24331300	1.03020300
H	2.62828600	-0.35841000	-0.73134200
C	0.04431800	-2.01814900	1.33341500
H	-0.68010500	-2.83681700	1.31036700
H	1.04660500	-2.45724200	1.31932200
H	-0.07545900	-1.48247300	2.28048200
O	-1.72978400	-0.21181700	-0.15669000
C	-2.11463900	0.94806200	0.58579500
H	-1.54351900	1.01776200	1.52164300
C	2.88126400	1.64008600	0.05339600
H	2.49595200	2.25888300	0.86894600
H	3.96796400	1.56052700	0.15911600

H	2.65878700	2.14282600	-0.89212500
H	-3.16835600	0.81592900	0.85490300
C	-1.92315500	2.21308700	-0.23657300
H	-0.86549400	2.34681000	-0.47518600
H	-2.48905200	2.14647000	-1.17061600
H	-2.27451300	3.08933200	0.31928000
O	-0.03084500	-1.78364500	-1.47956500
H	-0.35569400	-1.37217900	-2.28865900

$Me(EtO)_3Si$:

Si	0.11572500	-0.15615500	0.44089000
O	-1.11085500	0.82734300	-0.06738700
C	-1.08472400	2.24845500	0.07017500
H	-1.01381600	2.52279200	1.13296500
H	-0.19808800	2.64990200	-0.43596600
C	0.20773200	-0.18985900	2.30650600
H	1.06928300	-0.77221800	2.64829500
H	0.30402400	0.82097800	2.71548300
H	-0.69127200	-0.64016400	2.73944200
O	-0.14061400	-1.66763200	-0.16492900
C	-1.35262800	-2.40410000	0.00075900
H	-1.80191900	-2.19500900	0.98266300
C	-2.35306600	2.82250800	-0.53519200
H	-3.23471800	2.42477100	-0.02415300
H	-2.36190200	3.91375500	-0.44759400
H	-2.42129300	2.55679800	-1.59384800
H	-1.08346900	-3.46603900	-0.00972200
C	-2.34366500	-2.08965700	-1.11044800
H	-2.61227800	-1.03086200	-1.08926900
H	-1.89978500	-2.31313700	-2.08478600
H	-3.25199500	-2.69120000	-0.99509600
O	1.51454200	0.41661400	-0.22006200
C	2.74126300	-0.31397100	-0.23022700
H	3.06617200	-0.51809000	0.80062800
H	2.58894100	-1.27992000	-0.72721000
C	3.79311100	0.50357100	-0.95808700
H	3.94758500	1.46288600	-0.45564700
H	4.74675400	-0.03350600	-0.98519800
H	3.47489100	0.70214200	-1.98534000

IM1:

Si	-1.59552700	0.14199600	0.60778600

O	-0.04663800	-0.56399400	0.98981100
C	-2.14626200	1.07706000	2.10313700
H	-3.12095100	1.54422400	1.93729900
H	-2.22837700	0.40033900	2.95797800
H	-1.42247400	1.85784500	2.35434300
O	-1.44328500	1.00672500	-0.76777900
C	-1.26731600	2.42673800	-0.90898300
H	-0.84971900	2.84897700	0.00965800
C	2.04295100	-0.51097100	-0.59264700
H	-2.25477900	2.87167800	-1.07898700
C	-0.34138000	2.70232800	-2.07764200
H	0.64889700	2.28848500	-1.88089700
H	-0.73492200	2.25198100	-2.99335900
H	-0.24527600	3.78152800	-2.23362000
S	1.36271100	0.16427800	1.00700700
O	2.17630300	-0.38232200	2.07660400
O	1.19509300	1.60502800	0.83465800
F	2.15697300	-1.83626900	-0.50794500
F	3.23909300	0.03140100	-0.81090500
F	1.22440500	-0.20764200	-1.60378200
O	-2.53424300	-1.16117500	0.33652600
C	-2.55570700	-1.92934700	-0.87936500
H	-3.52644700	-2.43303200	-0.89816300
H	-2.50955200	-1.25080200	-1.73859200
C	-1.42502400	-2.94543200	-0.92611300
H	-1.45335000	-3.58914000	-0.04285000
H	-1.52683000	-3.57356400	-1.81733800
H	-0.44786100	-2.45867200	-0.96178500

IM2:

Si	-1.73405300	-0.87937300	-0.85053700
O	-0.00656800	-1.09131600	-0.75646100
C	-2.48882800	-1.98736600	0.43907300
H	-3.58173000	-1.95732800	0.39010500
H	-2.16636000	-3.02130500	0.28218800
H	-2.17885000	-1.68649800	1.44355900
O	-2.14944800	0.69511200	-0.72613900
C	-2.47847200	1.43189100	0.46676200
H	-2.25908800	0.83462300	1.35666800
C	1.97873600	0.55080200	-0.29515100
H	-3.55593900	1.62845900	0.43823400
C	-1.69231300	2.72840200	0.49768300
H	-0.62275000	2.52327900	0.56229200

H	-1.88407800	3.31466600	-0.40528900
H	-1.98651100	3.32311300	1.36850600
H	-1.95766600	-1.28519200	-2.24679300
S	0.90893700	-0.75192400	0.50139100
O	1.76253700	-1.88340800	0.81266700
O	0.11318400	-0.08899400	1.53269900
F	2.69064400	0.01142000	-1.27938000
F	2.79375800	1.04716500	0.63387700
F	1.21052600	1.52748900	-0.78300300

IM3:

Si	0.84750200	-1.28815800	-1.41766200
O	-0.44149900	-0.06112200	-1.19592200
P	-1.51684600	0.14576500	-0.09094500
H	-0.14395100	-2.39976400	-1.09040200
C	-3.11031000	-0.37034800	-0.76394500
C	-4.28766500	0.33507700	-0.48563300
C	-3.14896400	-1.52484300	-1.56101600
C	-5.50200700	-0.11897800	-0.99738900
H	-4.25295800	1.23738400	0.11509000
C	-4.36759400	-1.97157100	-2.06618600
H	-2.23008000	-2.06144600	-1.77520600
C	-5.54225100	-1.27068100	-1.78449800
H	-6.41417300	0.43008800	-0.78740800
H	-4.39950400	-2.86305800	-2.68410000
H	-6.48934700	-1.61967800	-2.18392900
C	-1.57346400	1.89258000	0.31239100
C	-2.17413600	2.32676500	1.50165800
C	-1.01327200	2.81331000	-0.58114800
C	-2.23216700	3.68974600	1.78393800
H	-2.57249400	1.60581100	2.20895800
C	-1.06812100	4.17241400	-0.28536800
H	-0.51344300	2.45976400	-1.47499300
C	-1.67988900	4.60971200	0.89057400
H	-2.69169400	4.03145500	2.70569300
H	-0.61602000	4.88685700	-0.96479700
H	-1.71414900	5.67028100	1.11931500
C	-1.20849600	-0.79527600	1.41438400
C	-0.08155000	-0.47557900	2.19070000
C	-2.06591200	-1.83550300	1.80029400
C	0.17349900	-1.20372700	3.34951300
H	0.59700900	0.30651200	1.86727400
C	-1.79678700	-2.55595600	2.96211900

H	-2.93238500	-2.08186700	1.19764900
C	-0.67940100	-2.23953100	3.73591200
H	1.04732800	-0.96430300	3.94655400
H	-2.45812700	-3.36277200	3.26091600
H	-0.47159900	-2.80330500	4.64020200
C	1.19081000	-1.63696100	-3.23062800
H	0.74833700	-0.85295400	-3.85337000
H	2.26706800	-1.62697300	-3.42107400
H	0.77630300	-2.60298300	-3.53165100
O	1.89664700	-1.63216800	-0.16174000
C	1.83651700	-2.79588100	0.64674300
H	0.79887800	-3.13749800	0.75973800
H	2.20161600	-2.50748400	1.63799000
C	2.70370700	-3.90051300	0.06120300
H	2.31044400	-4.22638900	-0.90748600
H	3.72235000	-3.53234800	-0.09117300
H	2.73848700	-4.76881800	0.72846300
S	2.47220800	1.32262400	-0.65095400
O	1.95849700	0.29666600	-1.66716100
O	1.56593600	1.51684500	0.49415400
O	2.97099200	2.50974300	-1.34093900
C	3.99477700	0.49968000	0.08575500
F	3.70541900	-0.12228500	1.23354900
F	4.90192600	1.45023200	0.34782400
F	4.52775600	-0.37617900	-0.77014100

IM3′:

Si	-1.94817300	0.16019800	-1.90681900
O	-0.30358000	-0.04929300	-1.44659800
P	0.56538200	0.01025900	-0.12279400
H	-2.22765000	1.59783700	-1.67520300
C	1.53134600	1.51795500	-0.19820200
C	2.83093900	1.55094700	0.32761300
C	0.95548400	2.67566000	-0.74631700
C	3.54786800	2.74513300	0.30941900
H	3.28202300	0.65224500	0.73411800
C	1.68165300	3.86332300	-0.75849000
H	-0.04431700	2.64561800	-1.16598000
C	2.97438800	3.89779000	-0.23009800
H	4.55573500	2.77364700	0.70904500
H	1.24291000	4.75883200	-1.18518900
H	3.53818500	4.82460800	-0.24517000
C	1.61618700	-1.43610500	-0.12231300

C	2.16818000	-1.90989700	1.07912500
C	1.93573800	-2.04759200	-1.34397500
C	3.04149100	-2.99435800	1.05080300
H	1.90847300	-1.44615400	2.02508700
C	2.80451000	-3.13577900	-1.35766600
H	1.49921700	-1.67953000	-2.26571100
C	3.35775100	-3.60540100	-0.16459000
H	3.46806100	-3.36680400	1.97584400
H	3.04854700	-3.61790300	-2.29807200
H	4.03454300	-4.45323300	-0.18109900
C	-0.46748800	0.00710400	1.34272900
C	-1.03696500	-1.20294000	1.77683500
C	-0.74329600	1.20409100	2.02197500
C	-1.87325400	-1.20815600	2.88816800
H	-0.82873500	-2.12677300	1.24865000
C	-1.59004000	1.18765400	3.12878200
H	-0.29327200	2.13497200	1.69540400
C	-2.15040800	-0.01512400	3.56185100
H	-2.30916200	-2.14085500	3.22972000
H	-1.80234700	2.11027700	3.65796900
H	-2.80181300	-0.02511000	4.42957200
C	-1.98307000	-0.39752600	-3.66835600
H	-1.25398600	0.14968500	-4.27300400
H	-1.75429800	-1.46569600	-3.73221700
H	-2.97644400	-0.23965300	-4.09881700
O	-2.87679300	-0.76297500	-0.92721300
C	-3.82428900	-0.27050700	0.04058900
H	-3.40402900	0.59750500	0.56357300
H	-3.94634700	-1.06885900	0.77564000
C	-5.14931900	0.07374100	-0.61503700
H	-5.03614600	0.89948000	-1.32539500
H	-5.54849400	-0.79195200	-1.14975700
H	-5.87842000	0.37922300	0.14176500

IM1-1:

P	-0.76824500	0.19560800	-0.42202100
C	-2.53062100	0.82493100	-0.51704800
C	-3.07072100	1.02707200	-1.79509700
C	-3.31300300	1.16166500	0.59752800
C	-4.37341800	1.49120300	-1.96210400
H	-2.45401100	0.83284900	-2.66774300
C	-4.60564800	1.65843500	0.43304200
H	-2.91268400	1.04250200	1.59539500

C	-5.14516400	1.81008300	-0.84426200
H	-4.77890600	1.62065800	-2.96109100
H	-5.19255300	1.92503200	1.30685900
H	-6.15562300	2.18794100	-0.96860900
C	-0.85888100	-0.23114200	1.43831800
C	-1.73309300	-1.26106800	1.82360000
C	-0.13687600	0.42482400	2.44043700
C	-1.87785000	-1.62901200	3.15849100
H	-2.30935500	-1.78542300	1.06599200
C	-0.27908300	0.06179000	3.78341700
H	0.54208400	1.22225900	2.17015400
C	-1.14662400	-0.96543900	4.14697900
H	-2.55803000	-2.43175700	3.42859700
H	0.29550800	0.58355000	4.54344400
H	-1.25378800	-1.24958400	5.18973000
C	-0.43798600	-1.56202600	-0.94653300
C	0.37992000	-2.40918200	-0.18817000
C	-0.88472200	-1.99505200	-2.20077800
C	0.74406500	-3.66353700	-0.67876400
H	0.74528800	-2.07559000	0.77456400
C	-0.55971900	-3.26551100	-2.67193400
H	-1.48705500	-1.33143800	-2.81384500
C	0.26516200	-4.09964000	-1.91423300
H	1.39712200	-4.30125400	-0.09035500
H	-0.93451900	-3.59851200	-3.63511200
H	0.53804400	-5.08137800	-2.28943100
H	-0.64074800	0.58064200	-1.81890500
O	0.55975500	1.19188700	-0.13833000
Si	2.14519900	0.92342800	-0.54048800
O	2.72469000	-0.24483800	0.46740600
C	3.67779500	-1.24222300	0.10625400
H	4.61738400	-0.77182200	-0.21367400
H	3.29601900	-1.83690000	-0.73408400
C	3.92335000	-2.13551300	1.30898100
H	4.65803700	-2.91068700	1.06798200
H	4.29719200	-1.54674500	2.15093200
H	2.99413500	-2.62108400	1.62068300
C	2.31824400	0.43435000	-2.33161100
H	1.91419300	1.21706500	-2.98072000
H	3.36735900	0.27905900	-2.60179600
H	1.76794600	-0.48754300	-2.54181900
O	2.95159000	2.32105000	-0.19481600
C	2.49634000	3.60635100	-0.62337300
H	2.57977800	3.68479600	-1.71709000

H	1.43826500	3.72987500	-0.36136600
C	3.34246600	4.67404500	0.04621600
H	3.02032300	5.67219600	-0.26794800
H	3.25109100	4.60345500	1.13368700
H	4.39651200	4.54849300	-0.21748600

IM2′:

P	-0.83269200	0.08281700	-0.03058100
C	0.00751800	0.41999700	1.51650700
C	0.68300100	1.64601800	1.64462300
C	-0.01749500	-0.48866900	2.58202000
C	1.34651100	1.94590500	2.82964700
H	0.68497700	2.35770300	0.82531000
C	0.64502700	-0.17548000	3.76814000
H	-0.54528800	-1.43016800	2.48569700
C	1.32883300	1.03417600	3.88993700
H	1.87057900	2.89021600	2.93152900
H	0.62708800	-0.87688000	4.59528300
H	1.84424200	1.27272000	4.81441500
C	-1.56730900	-1.55245700	-0.02126100
C	-0.74291600	-2.68977800	0.07269600
C	-2.96042800	-1.69143200	-0.11760600
C	-1.32258000	-3.95485600	0.06730000
H	0.33370200	-2.57739800	0.14525000
C	-3.52610700	-2.96503600	-0.11847800
H	-3.59456400	-0.81556200	-0.19311300
C	-2.71025000	-4.09292100	-0.02720800
H	-0.69197000	-4.83480900	0.13725200
H	-4.60250700	-3.07487500	-0.19369100
H	-3.15502300	-5.08260800	-0.03021100
C	-2.08230600	1.33215200	-0.30961300
C	-2.42356000	1.68620500	-1.62401600
C	-2.75425200	1.90408600	0.78150500
C	-3.43695200	2.61617400	-1.84022600
H	-1.89169600	1.24741800	-2.46085900
C	-3.77002900	2.82888800	0.55193600
H	-2.48032800	1.63603000	1.79652500
C	-4.10960000	3.18347500	-0.75535900
H	-3.69997800	2.90038500	-2.85339000
H	-4.29063500	3.27706600	1.39127200
H	-4.89845900	3.90780800	-0.92943500
O	0.17138000	0.22885600	-1.25079600
Si	1.68531600	-0.43762500	-1.70018600

C	1.39880500	-1.48663500	-3.18871900
H	0.68379400	-2.28277400	-2.96135600
H	1.00265100	-0.88911100	-4.01422200
C	3.46192300	-1.49719700	0.11893600
H	3.69180000	-2.54990700	-0.07436700
H	4.16510900	-0.88749800	-0.45942200
C	3.05591000	1.87587000	-1.18353000
H	2.33496800	2.68826000	-1.33296600
H	2.98801200	1.55322200	-0.13696000
C	4.46298600	2.33118500	-1.51541100
H	4.74407700	3.18027600	-0.88513500
H	5.18138500	1.52368200	-1.34835700
H	4.52815400	2.63865400	-2.56195500
C	3.56022300	-1.17922500	1.59841300
H	4.57096500	-1.38745800	1.96165500
H	3.33199900	-0.12690100	1.78761000
H	2.85511100	-1.78689400	2.17105100
O	2.11508600	-1.24896900	-0.33473100
O	2.69031300	0.79262300	-2.05749700
H	2.33183400	-1.94885100	-3.52330500

IM3′:

Si	-1.94817300	0.16019800	-1.90681900
O	-0.30358000	-0.04929300	-1.44659800
P	0.56538200	0.01025900	-0.12279400
H	-2.22765000	1.59783700	-1.67520300
C	1.53134600	1.51795500	-0.19820200
C	2.83093900	1.55094700	0.32761300
C	0.95548400	2.67566000	-0.74631700
C	3.54786800	2.74513300	0.30941900
H	3.28202300	0.65224500	0.73411800
C	1.68165300	3.86332300	-0.75849000
H	-0.04431700	2.64561800	-1.16598000
C	2.97438800	3.89779000	-0.23009800
H	4.55573500	2.77364700	0.70904500
H	1.24291000	4.75883200	-1.18518900
H	3.53818500	4.82460800	-0.24517000
C	1.61618700	-1.43610500	-0.12231300
C	2.16818000	-1.90989700	1.07912500
C	1.93573800	-2.04759200	-1.34397500
C	3.04149100	-2.99435800	1.05080300
H	1.90847300	-1.44615400	2.02508700
C	2.80451000	-3.13577900	-1.35766600

H	1.49921700	-1.67953000	-2.26571100
C	3.35775100	-3.60540100	-0.16459000
H	3.46806100	-3.36680400	1.97584400
H	3.04854700	-3.61790300	-2.29807200
H	4.03454300	-4.45323300	-0.18109900
C	-0.46748800	0.00710400	1.34272900
C	-1.03696500	-1.20294000	1.77683500
C	-0.74329600	1.20409100	2.02197500
C	-1.87325400	-1.20815600	2.88816800
H	-0.82873500	-2.12677300	1.24865000
C	-1.59004000	1.18765400	3.12878200
H	-0.29327200	2.13497200	1.69540400
C	-2.15040800	-0.01512400	3.56185100
H	-2.30916200	-2.14085500	3.22972000
H	-1.80234700	2.11027700	3.65796900
H	-2.80181300	-0.02511000	4.42957200
C	-1.98307000	-0.39752600	-3.66835600
H	-1.25398600	0.14968500	-4.27300400
H	-1.75429800	-1.46569600	-3.73221700
H	-2.97644400	-0.23965300	-4.09881700
O	-2.87679300	-0.76297500	-0.92721300
C	-3.82428900	-0.27050700	0.04058900
H	-3.40402900	0.59750500	0.56357300
H	-3.94634700	-1.06885900	0.77564000
C	-5.14931900	0.07374100	-0.61503700
H	-5.03614600	0.89948000	-1.32539500
H	-5.54849400	-0.79195200	-1.14975700
H	-5.87842000	0.37922300	0.14176500

IM4:

Si	1.08327500	-0.41038200	-1.87227600
O	-0.26316800	0.36825200	-1.36164200
P	-1.52228200	-0.17486600	-0.33375900
H	-1.38727900	-1.43802000	-1.05116200
C	-3.35578200	-0.30512400	-0.69728900
C	-4.27472200	0.74402800	-0.54317600
C	-3.82450800	-1.53455400	-1.18382000
C	-5.62439100	0.55233800	-0.83677500
H	-3.93925500	1.71225900	-0.19758200
C	-5.17624900	-1.73600100	-1.45385100
H	-3.11589400	-2.33866100	-1.36240200
C	-6.08145200	-0.68869500	-1.28025700
H	-6.32028100	1.37717800	-0.71738300

H	-5.51913600	-2.70117100	-1.81420300
H	-7.13414900	-0.83493000	-1.50271500
C	-1.59534900	1.57455100	0.39343200
C	-2.19276200	1.73225600	1.65365100
C	-1.16066800	2.72175400	-0.27938600
C	-2.34251200	2.99272400	2.22851100
H	-2.54567000	0.86019600	2.19555000
C	-1.31187700	3.98700500	0.29103500
H	-0.68698600	2.62383800	-1.24680500
C	-1.90074100	4.12736900	1.54627100
H	-2.80088400	3.08790000	3.20852300
H	-0.95794400	4.86245700	-0.24528200
H	-2.01104700	5.11119600	1.99248300
C	-1.00664400	-1.01769900	1.22751200
C	0.06629100	-0.50997900	1.96792200
C	-1.59586100	-2.22975700	1.60485400
C	0.54123700	-1.21022200	3.07698500
H	0.53360300	0.42229500	1.67409300
C	-1.13862900	-2.91233700	2.73104800
H	-2.41995600	-2.63480900	1.02495200
C	-0.06496700	-2.40503700	3.46668000
H	1.38642900	-0.81835300	3.63418500
H	-1.61547600	-3.84045400	3.03144100
H	0.29914500	-2.94262500	4.33695800
C	1.02917000	-0.85197600	-3.66786700
H	0.79468200	0.02790100	-4.27314000
H	1.98619300	-1.26036700	-4.00349400
H	0.24879900	-1.59930500	-3.84456300
O	1.55775700	-1.61278100	-0.87694500
C	1.15067400	-2.98152700	-0.80365600
H	1.35633600	-3.47150000	-1.76447900
H	0.07285800	-3.03439200	-0.61554500
C	1.91926900	-3.64556900	0.32225800
H	2.99559800	-3.55504400	0.15089200
H	1.67547500	-3.16943300	1.27393300
H	1.65974200	-4.70706400	0.38392900
S	2.98158800	1.46703500	-0.47431500
O	2.37467200	0.71018800	-1.74112000
O	1.94187700	1.81410400	0.48384100
O	3.92260100	2.45090400	-0.97607800
C	4.00025700	0.09816400	0.31667600
F	3.25369100	-0.59946900	1.16890000
F	4.99961600	0.67845900	0.98292700
F	4.49996500	-0.71220500	-0.61514700

IM4′:

Si	1.37830100	0.44716900	1.68597500
O	-0.20659600	0.24770200	1.75894900
P	-1.88599100	0.02250400	0.87355700
H	-2.28554700	0.08209800	2.21482300
C	-3.69228200	-0.12657300	0.33195600
C	-4.19843200	0.32566200	-0.89478600
C	-4.57105400	-0.76800500	1.21408300
C	-5.53758200	0.12833100	-1.23268700
H	-3.54726000	0.84746300	-1.58894900
C	-5.91063900	-0.96886200	0.88310300
H	-4.20494300	-1.11908400	2.17767600
C	-6.39679800	-0.52086800	-0.34556500
H	-5.91160500	0.48761000	-2.18695000
H	-6.57422600	-1.46835000	1.58276900
H	-7.43990600	-0.67061500	-0.60698000
C	-1.32864700	-1.57953800	0.20662200
C	-1.65971300	-1.93160500	-1.10771300
C	-0.57424500	-2.46219100	0.98906100
C	-1.19757500	-3.12939100	-1.64653700
H	-2.26578900	-1.27035800	-1.71489500
C	-0.14406600	-3.67448900	0.45593200
H	-0.30482000	-2.18465600	1.99920500
C	-0.44083800	-4.00270100	-0.86661300
H	-1.42878800	-3.37818900	-2.67722700
H	0.45207700	-4.34611300	1.06400700
H	-0.07628400	-4.93343400	-1.28894400
C	-1.51097400	1.51171000	-0.10665900
C	-0.61781200	1.44259700	-1.18029900
C	-2.17538400	2.71042200	0.17973000
C	-0.40316600	2.57334100	-1.96881600
H	-0.08218800	0.52585400	-1.39472700
C	-1.93076900	3.84352700	-0.59437400
H	-2.89069600	2.75766600	0.99516000
C	-1.04949200	3.77428900	-1.67556000
H	0.28307700	2.51196400	-2.80743000
H	-2.43770200	4.77466900	-0.36114900
H	-0.86918700	4.65325800	-2.28655800
C	2.14072700	0.59089800	3.37543700
H	1.88072800	-0.27390700	3.99218500
H	3.23026500	0.65074300	3.30504300
H	1.77522500	1.48650500	3.88742600

O	1.94371500	1.59734100	0.65105800
C	1.73266400	3.00190300	0.79177500
H	2.02378900	3.32417800	1.80184500
H	0.67005400	3.23044400	0.65761800
C	2.56864900	3.71930700	-0.25152600
H	3.62933000	3.49146000	-0.11479400
H	2.27458700	3.39400800	-1.25203100
H	2.42662100	4.80229000	-0.17896800
S	2.53345400	-1.40027300	-0.43237800
O	2.17276400	-0.95933600	1.03957000
O	1.52723000	-0.97385700	-1.39810400
O	2.99030900	-2.77923600	-0.38067900
C	4.06226400	-0.35398600	-0.76744300
F	3.73497500	0.77123500	-1.39448500
F	4.87775000	-1.06644500	-1.54840300
F	4.68985200	-0.06619600	0.37531100

IM5:

Si	-1.71006400	-0.71256200	-0.12041600
O	-1.32137800	-0.83067200	-1.70669300
C	-2.56425400	-2.16042300	0.63975800
H	-1.96388000	-3.06653800	0.51580700
H	-2.72049100	-1.99418600	1.70896900
H	-3.53677200	-2.32368200	0.16757300
O	-2.55419200	0.64677900	0.16561700
C	-2.20223800	1.96104000	-0.30547800
H	-3.13829700	2.44082300	-0.60559600
H	-1.56700400	1.88194900	-1.19425600
C	-1.51294300	2.75354100	0.79211200
H	-2.14729600	2.80439000	1.68112000
H	-0.56333300	2.29319900	1.07282100
H	-1.31309800	3.77428300	0.44977500
S	1.26146200	-0.93297900	0.31187200
O	-0.20279800	-0.53942300	0.76480300
O	1.21419200	-1.74886700	-0.90526400
O	2.04067300	-1.34487300	1.46164700
C	1.86755400	0.75191800	-0.20516800
F	1.05266400	1.24807300	-1.14262800
F	3.09589400	0.63510900	-0.69957200
F	1.87999300	1.57074800	0.84562800
H	-0.48996600	-1.29209800	-1.89941400

TS1:

Si	0.97717000	-0.58141800	-1.13279800
O	-0.15534500	0.66408800	-0.89090700
P	-1.43664100	-0.01061100	-0.11653300
H	-0.58466200	-1.34823800	-0.37351200
C	-2.80474500	-0.96621200	-0.90786600
C	-3.90982300	-0.32968300	-1.49121700
C	-2.73333700	-2.36731900	-0.93861400
C	-4.92070900	-1.08343300	-2.08730800
H	-3.97870800	0.75025500	-1.48391800
C	-3.75943800	-3.11898200	-1.50456500
H	-1.86356300	-2.86331500	-0.51905600
C	-4.85400200	-2.47614900	-2.08623000
H	-5.76334000	-0.57869900	-2.54919800
H	-3.69839800	-4.20274500	-1.50539100
H	-5.64702200	-3.05956500	-2.54381600
C	-2.31206000	1.63534500	0.04897800
C	-3.32721700	1.76549500	1.00862200
C	-2.02780200	2.72840900	-0.77963000
C	-4.04387700	2.95323100	1.13509300
H	-3.55730500	0.93420100	1.66824800
C	-2.74510300	3.91962700	-0.65387900
H	-1.23475600	2.64815600	-1.51252200
C	-3.75463200	4.03471300	0.30083200
H	-4.82320300	3.03696700	1.88663300
H	-2.50800800	4.75982800	-1.29958200
H	-4.30906200	4.96304600	0.39993700
C	-1.17319100	-0.34105200	1.65769700
C	-0.14457100	0.36674400	2.29274600
C	-1.90423700	-1.30632600	2.35780100
C	0.14982200	0.09663300	3.62849500
H	0.43779000	1.10058600	1.74450800
C	-1.61115400	-1.55832600	3.69814300
H	-2.69601000	-1.85856500	1.86139900
C	-0.58191400	-0.86123800	4.33284200
H	0.95461600	0.63717300	4.11652800
H	-2.18427300	-2.30153100	4.24403600
H	-0.35050400	-1.06471600	5.37378300
C	0.76138600	-1.59515400	-2.67742400
H	0.56049400	-0.92731000	-3.52082500
H	1.68784900	-2.13574700	-2.89193100
H	-0.05966700	-2.31041100	-2.59872200
O	1.75422900	-1.19303400	0.17389800
C	1.51865400	-2.33482000	0.98765400

H	0.45268900	-2.59098800	0.98356100
H	1.78192200	-2.04867600	2.01001500
C	2.36924200	-3.49998700	0.50843700
H	2.06784200	-3.81428300	-0.49615300
H	3.42067000	-3.20294400	0.47104300
H	2.26768100	-4.35674800	1.18259000
S	3.16385000	1.39954400	-0.74199300
O	2.28289600	0.45848700	-1.66201100
O	2.42689100	1.86004800	0.42964200
O	3.86868000	2.33032900	-1.60745000
C	4.46926000	0.18963000	-0.11190300
F	4.17487700	-0.22998000	1.11605500
F	5.63772600	0.83417000	-0.07876100
F	4.57544700	-0.86259100	-0.92909500

TS1′:

O	0.04231900	0.76288100	-0.48419300
P	-0.07577500	-0.92096600	0.12382500
C	1.58858200	-0.88546300	0.92857000
C	2.57635200	-1.82608600	0.61376600
C	1.77318800	-0.04212000	2.03368400
C	3.73775700	-1.90830900	1.38486000
H	2.44399400	-2.50108200	-0.22242900
C	2.93814400	-0.11639100	2.79172800
H	1.00083500	0.66495300	2.31580400
C	3.92298500	-1.05336600	2.47054100
H	4.49570400	-2.64302300	1.13353300
H	3.07207900	0.54678100	3.63994200
H	4.82596000	-1.12008400	3.06836900
C	0.08016100	-2.08040200	-1.25595400
C	-0.79677200	-3.16945600	-1.34057600
C	1.00984600	-1.83098900	-2.27490400
C	-0.73194000	-4.01925400	-2.44246500
H	-1.51814100	-3.35267300	-0.55038400
C	1.05955400	-2.68493100	-3.37621200
H	1.68507600	-0.98444400	-2.20391500
C	0.19328800	-3.77606500	-3.46037000
H	-1.40271900	-4.86945600	-2.50718300
H	1.77693600	-2.49646000	-4.16812100
H	0.23791700	-4.43783100	-4.31905500
C	-0.97141600	-1.59144200	1.58169700
C	-2.23612700	-1.09727500	1.92529100
C	-0.38733900	-2.61284900	2.35215200

C	-2.91529000	-1.62187100	3.02499000
H	-2.68499900	-0.29454300	1.35320400
C	-1.09047800	-3.15868900	3.42116400
H	0.60222700	-2.98335600	2.11287300
C	-2.35026300	-2.65947400	3.76432900
H	-3.88494000	-1.21986100	3.29964600
H	-0.64944500	-3.96599000	3.99633100
H	-2.88449900	-3.07608900	4.61193800
Si	-1.75381500	1.03955200	-1.10203700
O	-3.31232200	0.80365800	-0.55783500
C	-4.11343300	-0.34031800	-0.89255400
H	-4.34475300	-0.31640300	-1.96381700
H	-3.54435100	-1.25987900	-0.69491500
H	-1.50847600	-0.54731900	-0.36377300
C	-1.62173600	0.53467900	-2.88799800
H	-0.60834000	0.61503200	-3.28189400
H	-1.94196300	-0.50367400	-3.01314000
H	-2.28292500	1.16635300	-3.49014900
O	-1.54179000	2.62583300	-0.70182800
C	-2.58672600	3.61901000	-0.64862400
H	-3.40667700	3.34060600	-1.31768700
Si	1.38362500	1.87977600	-0.80841000
C	0.97088900	3.01209300	-2.21510900
H	0.56719100	2.48548600	-3.08198900
H	0.27051200	3.79540500	-1.92892300
H	1.91642600	3.47152900	-2.52414700
O	2.60065900	0.88538300	-1.25289800
O	1.75330600	2.64226800	0.58388300
C	0.87955400	3.45687100	1.38424200
H	0.00523800	2.86337300	1.67606600
H	0.51724700	4.29994600	0.78507300
C	3.97223500	0.96477200	-0.80686200
H	4.33475500	1.99129500	-0.93172400
H	4.00779300	0.71856200	0.25647000
C	-5.38467600	-0.30948500	-0.06684700
H	-5.93721600	0.61563900	-0.24946400
H	-6.02675600	-1.15507500	-0.32980100
H	-5.15777800	-0.36954800	1.00130500
C	4.80124600	-0.00138900	-1.62729300
H	5.84614200	0.03409400	-1.30521900
H	4.43732900	-1.02390400	-1.49846400
H	4.75838700	0.25468400	-2.68948400
C	1.64712500	3.94017200	2.59785300
H	2.51254400	4.53427100	2.29359200

H	1.00434200	4.56018500	3.22968600
H	2.00428300	3.09339700	3.19065900
H	-2.14121000	4.54512500	-1.02532000
C	-3.09078200	3.79092300	0.77213900
H	-3.54922400	2.86384100	1.12383600
H	-2.27018800	4.05887200	1.44386500
H	-3.83995300	4.58760000	0.81323500

TS1″:

Si	2.27804200	0.77721600	-0.18021400
O	1.36292800	0.52645400	1.09393100
P	-0.23178200	-0.00311400	0.08942600
H	0.82765100	0.15181100	-1.02537300
C	-1.36220200	-0.34348500	-1.34275900
C	-2.75270400	-0.39961900	-1.14561600
C	-0.83935700	-0.60324000	-2.61089800
C	-3.59457000	-0.71520100	-2.20804500
H	-3.17373400	-0.19785800	-0.16618700
C	-1.68404600	-0.91778200	-3.67716900
H	0.23579600	-0.56617200	-2.77752000
C	-3.06176200	-0.97393600	-3.47445700
H	-4.66728200	-0.75634000	-2.05031100
H	-1.26712300	-1.11572100	-4.65890700
H	-3.72203900	-1.21527400	-4.30085100
C	-1.05692500	1.45568100	0.78967400
C	-1.05959200	1.66731100	2.17692900
C	-1.67264100	2.38302000	-0.06393900
C	-1.70669800	2.78016400	2.70273300
H	-0.56539700	0.96597200	2.83691000
C	-2.28619800	3.51521100	0.47107300
H	-1.68230200	2.22143400	-1.13555300
C	-2.31316400	3.70852900	1.85175200
H	-1.73015600	2.92949700	3.77690100
H	-2.75168900	4.23699900	-0.19154300
H	-2.80475300	4.58214900	2.26692200
C	-0.27721700	-1.57789700	0.99178600
C	0.30686600	-1.70408300	2.26701800
C	-0.95422300	-2.67587900	0.43008900
C	0.17857200	-2.89411800	2.97465900
H	0.87448400	-0.88407200	2.68178700
C	-1.05735700	-3.86883500	1.14095400
H	-1.39481400	-2.60845200	-0.55467100
C	-0.50164100	-3.97783200	2.41511700

H	0.62263500	-2.97917000	3.96067700
H	-1.57396100	-4.71209700	0.69544500
H	-0.58906700	-4.90758600	2.96776300
C	2.41254700	2.43798500	-0.97410000
H	1.43796500	2.93335700	-0.94996000
H	3.11385400	3.05494000	-0.40001600
H	2.76942300	2.38387700	-2.00571000
O	3.41551800	-0.30813600	-0.51235300
C	4.53323500	-0.24996600	-1.43867000
H	4.27565700	0.39581600	-2.28505900
H	4.65453700	-1.26915900	-1.81008800
C	5.77823400	0.23703100	-0.72505100
H	5.65751700	1.26719200	-0.37510800
H	6.00369200	-0.40047300	0.13301600
H	6.63074300	0.21009400	-1.41004900

TS1‴:

P	-2.52297000	0.63013300	0.09238100
C	-4.34108100	0.53962100	0.58855800
C	-4.65924400	-0.20404300	1.73875600
C	-5.38065300	1.17403100	-0.09817600
C	-5.97478800	-0.32603100	2.17612900
H	-3.86634500	-0.68439200	2.30427400
C	-6.70383800	1.05556200	0.33989700
H	-5.17199500	1.76390400	-0.98242200
C	-7.00570400	0.30337000	1.47202100
H	-6.19802300	-0.90634400	3.06621200
H	-7.49658700	1.55340100	-0.20985900
H	-8.03289500	0.21210000	1.81023000
C	-2.66679100	1.76439300	-1.32746400
C	-3.14161400	1.25241300	-2.54306400
C	-2.31346800	3.11538400	-1.23169000
C	-3.22653100	2.08372300	-3.66052200
H	-3.48288600	0.22459800	-2.61146800
C	-2.40942800	3.94133100	-2.35108300
H	-1.97506800	3.52589100	-0.28644900
C	-2.85561600	3.42551600	-3.56891400
H	-3.59396200	1.68185100	-4.59929000
H	-2.14042700	4.98969900	-2.26928200
H	-2.92718700	4.07023200	-4.43876300
C	-1.99747400	1.35492800	1.69569100
C	-2.65899600	2.48713500	2.19307000

C	-0.97584800	0.76061200	2.44319300
C	-2.26031300	3.04994800	3.40422800
H	-3.48820700	2.91959200	1.64326200
C	-0.62154400	1.29570900	3.68130000
H	-0.47226600	-0.11596700	2.05711200
C	-1.24749400	2.44875700	4.15530500
H	-2.75650400	3.94190000	3.77278200
H	0.14851100	0.81031200	4.27299900
H	-0.95705500	2.87380000	5.11083100
O	-2.43884900	-0.94811200	-0.22974100
Si	-2.92000300	-2.25074600	-1.16101600
C	-1.78540800	-2.50358100	-2.60119500
H	-0.74316100	-2.53454800	-2.28334000
H	-2.02651200	-3.45225300	-3.08952800
C	-5.67694100	-2.21948200	-1.15864800
H	-5.77556600	-3.29641100	-0.97759100
H	-5.71744500	-1.70466200	-0.19553200
C	-2.96426400	-3.49539200	1.27773400
H	-2.34124500	-2.68163900	1.66790400
H	-4.00503100	-3.27639800	1.54775700
C	-2.53146000	-4.83018800	1.85348600
H	-2.63201500	-4.82469100	2.94341000
H	-3.14656600	-5.63989400	1.45234400
H	-1.48719600	-5.03762000	1.60191500
C	-6.77876500	-1.72048800	-2.07182900
H	-7.75700600	-1.89696900	-1.61441200
H	-6.66881700	-0.64649300	-2.24279900
H	-6.74587200	-2.23448700	-3.03642100
O	-4.40927900	-1.97127800	-1.79060900
O	-2.84187400	-3.54383300	-0.14886600
H	-1.90233800	-1.70682500	-3.33999100
H	-0.93714900	0.57034800	-0.23366700
Si	0.81266500	-0.05860000	-0.53683900
C	0.47189500	0.11883000	-2.36432600
H	0.79702800	-0.77880000	-2.89588500
H	-0.57034100	0.32185800	-2.60491100
H	1.07612500	0.95632200	-2.73101000
C	0.96115400	-2.48835600	0.86209000
H	2.00298000	-2.26643000	1.10860600
H	0.45734900	-2.77322200	1.79176900
C	0.87055400	-3.61591100	-0.15106100
H	1.35537200	-3.33069700	-1.09044300
H	1.36987000	-4.51132300	0.23419600
H	-0.17275200	-3.86548300	-0.35766000

C	1.01845700	2.64417600	-0.14932500
H	0.06456500	2.66046400	-0.68231300
H	1.79850600	2.95820900	-0.85183000
C	0.98030200	3.57158600	1.04963500
H	0.80928700	4.60127800	0.71931300
H	0.18538500	3.28853900	1.74144000
H	1.93425000	3.54347600	1.58420200
O	1.30730500	1.30728300	0.27967700
O	0.29221600	-1.31031400	0.40216300
O	2.49999200	-0.70025000	-0.76567300
P	3.87922100	-0.21664900	-0.20869000
C	4.02650600	-0.44918700	1.57540400
C	3.13464600	0.18959000	2.45781600
C	5.02481700	-1.29756200	2.08009600
C	3.25608100	-0.02329300	3.82776900
H	2.35520800	0.83249800	2.06671700
C	5.13199600	-1.50345500	3.45453100
H	5.71213900	-1.79506600	1.40603500
C	4.25035000	-0.86741300	4.32805200
H	2.57338500	0.47573900	4.50778900
H	5.90395600	-2.16072600	3.84037000
H	4.33753700	-1.02872000	5.39767500
C	5.10869100	-1.24032800	-1.02663800
C	6.40793600	-0.75778300	-1.23903800
C	4.76735900	-2.54767800	-1.40244700
C	7.36299900	-1.58624900	-1.82410000
H	6.66671500	0.25769000	-0.95741700
C	5.72824300	-3.36697400	-1.99005200
H	3.75741500	-2.90848200	-1.24365800
C	7.02344300	-2.88796400	-2.19829200
H	8.36809100	-1.21500200	-1.99361700
H	5.46663100	-4.37671700	-2.28828400
H	7.76894800	-3.52913500	-2.65723200
C	4.20423900	1.49664000	-0.64796700
C	4.56004900	2.45779000	0.30475000
C	4.08214400	1.85349400	-2.00085800
C	4.78205000	3.77552500	-0.09461500
H	4.65419900	2.18161700	1.34852100
C	4.30495300	3.17095100	-2.39081100
H	3.81075000	1.10547700	-2.73925700
C	4.65279900	4.13197600	-1.43724600
H	5.05514600	4.52230000	0.64334900
H	4.20926200	3.44869100	-3.43515800
H	4.82628200	5.15842200	-1.74341000

TS1-1:

Si	-1.75965800	1.46630500	0.01308200
O	-2.58464100	0.55171700	-1.13526600
C	-3.84988800	-0.07714000	-1.01778600
H	-4.37918900	0.27115100	-0.12449700
H	-4.45085800	0.21340800	-1.89016000
C	-3.67714300	-1.59140300	-0.99309100
H	-3.13707200	-1.92679700	-1.88330400
H	-3.09687800	-1.89872800	-0.11716600
H	-4.64857500	-2.09744300	-0.95837700
O	-0.53528900	0.53813000	1.02750500
P	0.62519700	0.05252000	0.07464500
H	-0.51053800	1.35080200	-1.00908100
C	1.83144900	1.30503800	-0.41872600
C	2.01624300	2.40236100	0.43271000
C	2.60843300	1.17432900	-1.57538100
C	2.96521500	3.37062400	0.11617900
H	1.41055200	2.49770700	1.32802800
C	3.56047700	2.14658000	-1.88140400
H	2.46159300	0.32806900	-2.23780200
C	3.73887600	3.24469900	-1.03978700
H	3.10120700	4.22461400	0.77216500
H	4.15935800	2.04675700	-2.78130300
H	4.47762700	4.00153600	-1.28376200
C	0.23019500	-1.10507200	-1.27557000
C	-0.15016600	-0.65577000	-2.54897800
C	0.27607200	-2.48364800	-1.01792100
C	-0.44872500	-1.57210300	-3.55219500
H	-0.23945300	0.40765500	-2.72931500
C	-0.05519000	-3.39612400	-2.01843900
H	0.56416600	-2.84623500	-0.03895200
C	-0.40989400	-2.94281000	-3.28803300
H	-0.73670700	-1.21392200	-4.53529100
H	-0.03046200	-4.45974700	-1.80410700
H	-0.66208800	-3.65426600	-4.06851300
C	1.58173800	-0.98079300	1.24747400
C	0.98384500	-1.44181400	2.42776800
C	2.90286600	-1.34764300	0.95552900
C	1.69864600	-2.26439800	3.29900600
H	-0.03332800	-1.14544100	2.65478600
C	3.61313300	-2.16956000	1.82708800
H	3.38003300	-0.98362500	0.05120300
C	3.01087400	-2.63050600	2.99970800

H	1.23029000	-2.61571000	4.21324200
H	4.63677900	-2.44647900	1.59486000
H	3.56590800	-3.26935800	3.67986900
C	-1.69724500	3.34630300	-0.13085700
H	-2.57312700	3.81935600	0.31997100
H	-0.80366700	3.72065300	0.38261800
H	-1.61190100	3.64381400	-1.18021800
O	-2.84659600	1.42695200	1.33365700
C	-3.01147100	0.36476700	2.24697200
H	-2.20217800	0.38045400	2.99243100
H	-2.95356200	-0.61493300	1.74720000
C	-4.35723200	0.50241300	2.94500900
H	-5.17619700	0.44311000	2.22114100
H	-4.49556300	-0.28856500	3.69070000
H	-4.42334200	1.47174600	3.44800700

TS2:

Si	1.53819800	0.46992000	1.85970500
O	0.01024500	0.25416700	2.14454500
P	-2.19936500	-0.00169400	0.54689800
H	-1.79619400	0.14955900	1.88296800
C	-4.00922400	-0.04311300	0.42478900
C	-4.67828200	0.32955000	-0.74965500
C	-4.74103500	-0.51631700	1.52279600
C	-6.06562700	0.22210700	-0.82303400
H	-4.11765500	0.71670900	-1.59388500
C	-6.12828100	-0.62055300	1.44404600
H	-4.22741500	-0.79996500	2.43697100
C	-6.79006200	-0.25333200	0.27138900
H	-6.58112400	0.51301600	-1.73266900
H	-6.69140900	-0.98371800	2.29756800
H	-7.87088600	-0.33303400	0.21201300
C	-1.55398000	-1.56788400	-0.06295300
C	-1.94847000	-2.03230200	-1.32612700
C	-0.64955000	-2.29878200	0.71677500
C	-1.41601700	-3.22057900	-1.81518500
H	-2.65733900	-1.46914900	-1.92520000
C	-0.12902100	-3.49128700	0.21791200
H	-0.32238900	-1.88686900	1.66409400
C	-0.50381900	-3.94611600	-1.04513000
H	-1.70529100	-3.57665500	-2.79861200
H	0.60259100	-4.03998300	0.80005000
H	-0.07554300	-4.86284400	-1.43746100

C	-1.62292000	1.37235700	-0.46846500
C	-0.51318400	1.19879100	-1.30151700
C	-2.27355200	2.61413400	-0.39481500
C	-0.06788500	2.26923700	-2.07566100
H	0.01622300	0.25529400	-1.33548200
C	-1.81396400	3.67752300	-1.16645300
H	-3.13439300	2.74642400	0.25298300
C	-0.71281300	3.50321600	-2.01027600
H	0.79820600	2.13118200	-2.71364400
H	-2.31310100	4.63957300	-1.11063700
H	-0.35651700	4.33453700	-2.61073200
C	2.66837200	0.70486900	3.33116000
H	2.54599400	-0.11812800	4.04124500
H	3.71602700	0.74113300	3.01993600
H	2.42950800	1.63389700	3.85894800
O	1.97020400	1.54696100	0.66040200
C	1.76922400	2.94668500	0.79355000
H	1.98189900	3.27353100	1.82272700
H	0.72042400	3.19144700	0.58265400
C	2.68891100	3.67000800	-0.17566900
H	3.73404000	3.43682600	0.04602400
H	2.48285500	3.35006900	-1.20009500
H	2.54662300	4.75404800	-0.11120400
S	2.65934800	-1.41328500	-0.31533400
O	2.26460000	-0.98778200	1.13138000
O	1.66945400	-1.02925300	-1.32042400
O	3.14434100	-2.78688900	-0.26722900
C	4.16920800	-0.34364400	-0.65786800
F	3.83358300	0.75582400	-1.32782000
F	5.01810200	-1.05828900	-1.40373400
F	4.77521300	-0.00451900	0.48382000