Supporting Information

Chiral Wide Bite Angle Diphosphine Ligands: Synthesis, Coordination Chemistry and Application in Pd-catalyzed Allylic Alkylation

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1- Compound 11F

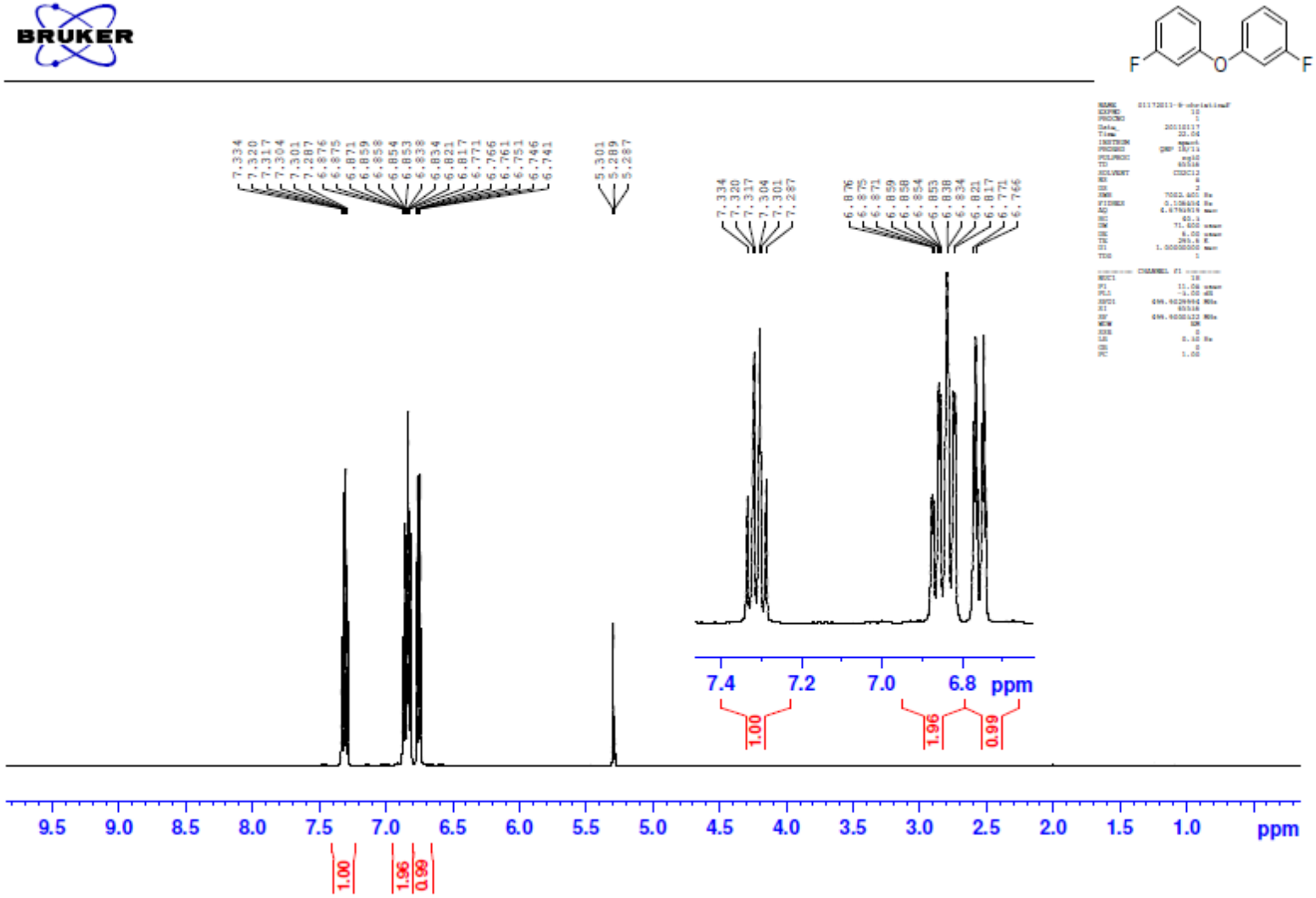


Figure S1 **^{1}H NMR spectrum of compound 11F** (500 MHz, CD_2Cl_2, 296 K)

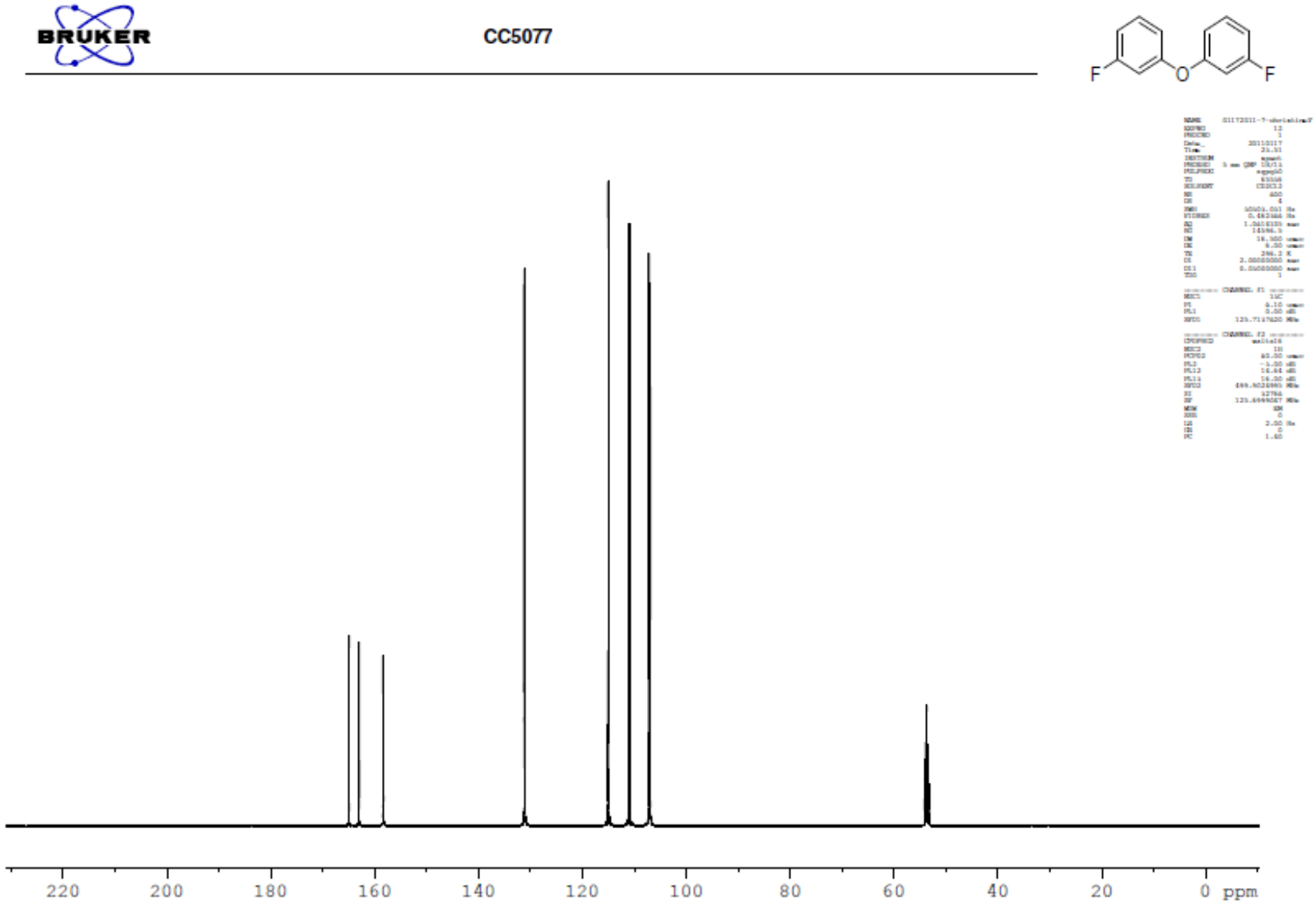


Figure S2 $^{13}C\{^{1}H\}$ **NMR spectrum of compound 11F** (126 MHz, CD_2Cl_2, 295 K)

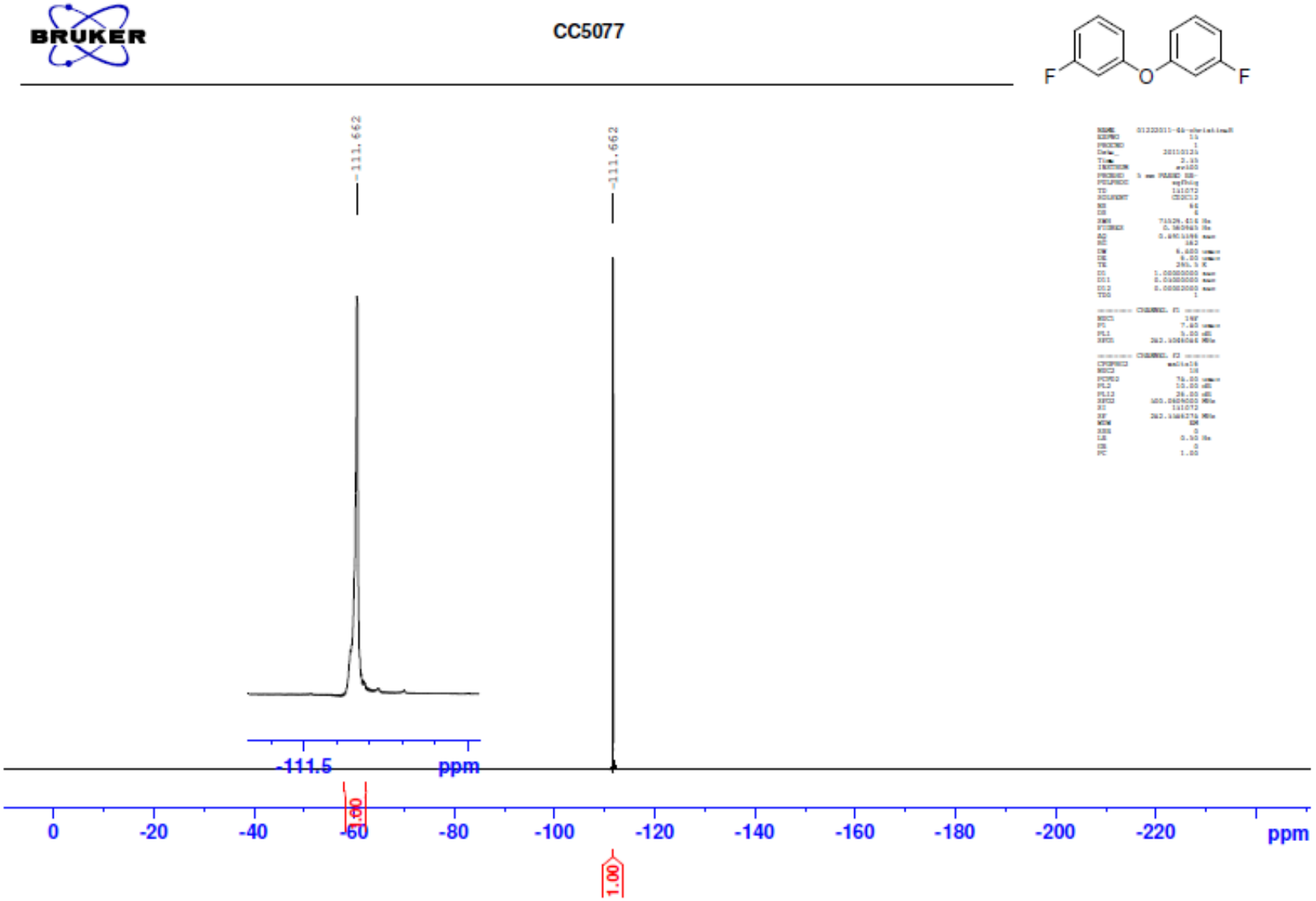


Figure S3 $^{19}F\{^{1}H\}$ **NMR spectrum of compound 11F** (282 MHz, CD_2Cl_2, 295 K)

2- Compound 11OMe

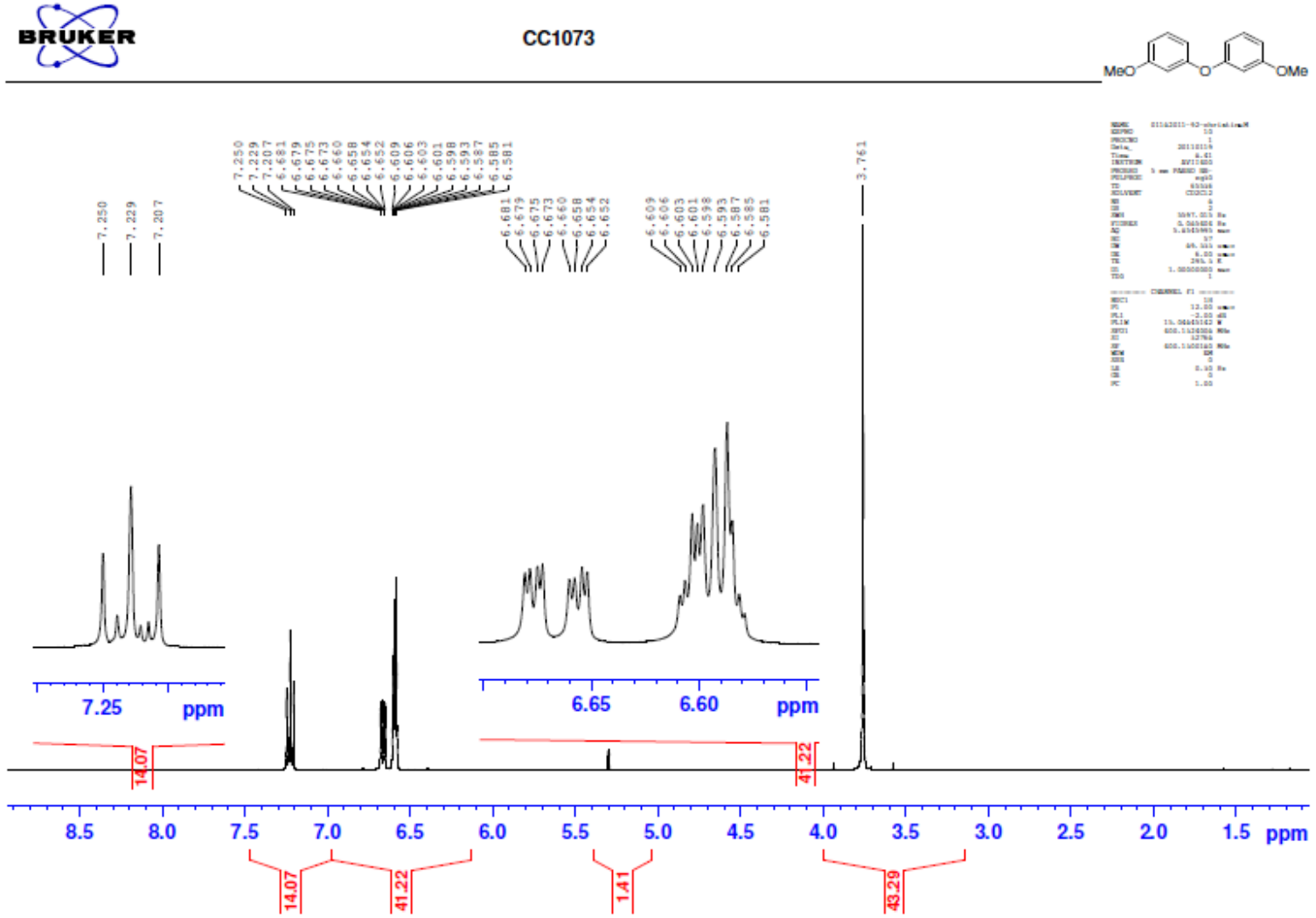


Figure S4 **^{1}H NMR spectrum of compound 11OMe** (400 MHz, CD_2Cl_2, 295 K)

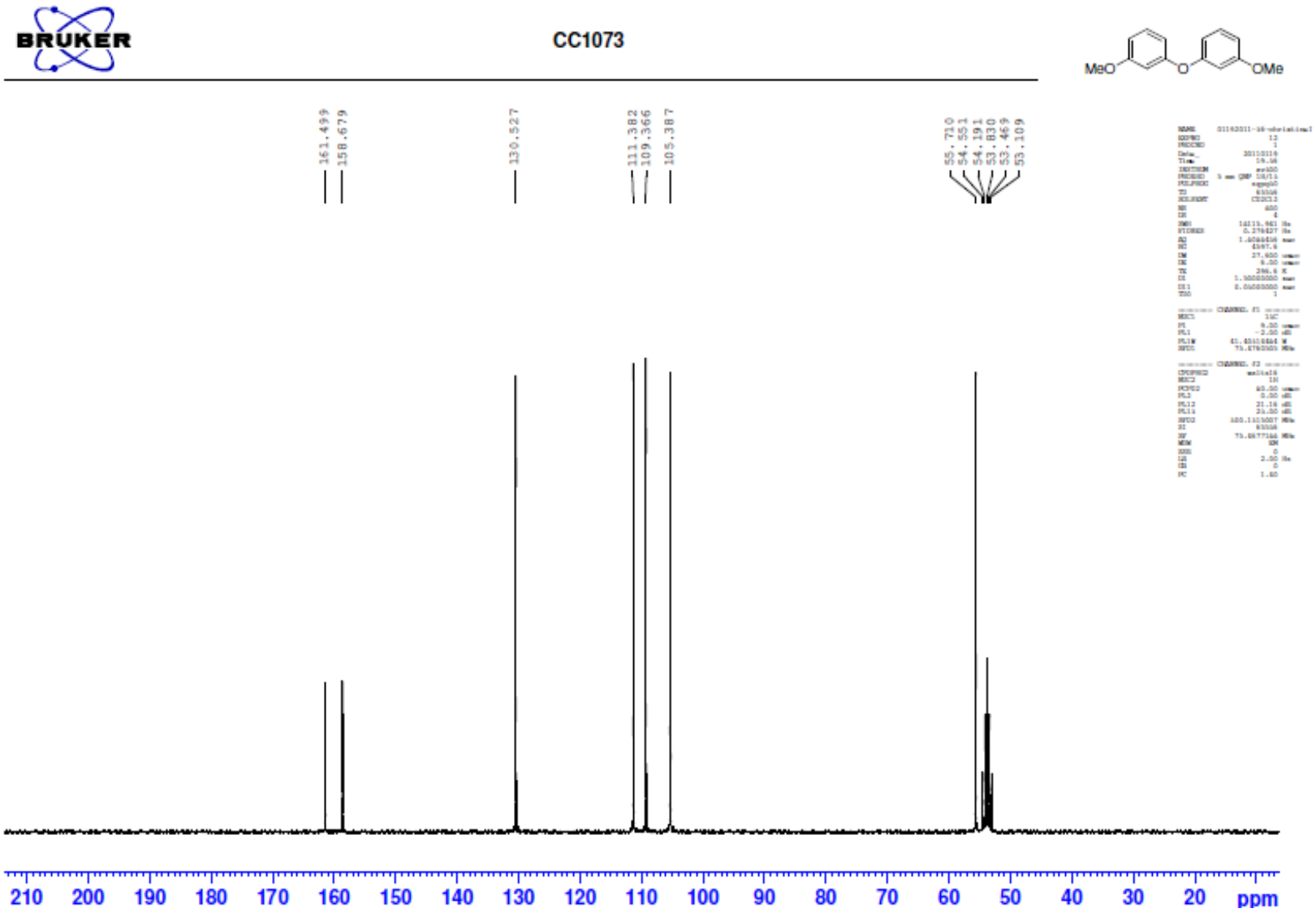


Figure S5 $^{13}C\{^{1}H\}$ **NMR spectrum of compound 11OMe** (75 MHz, CD_2Cl_2, 295 K)

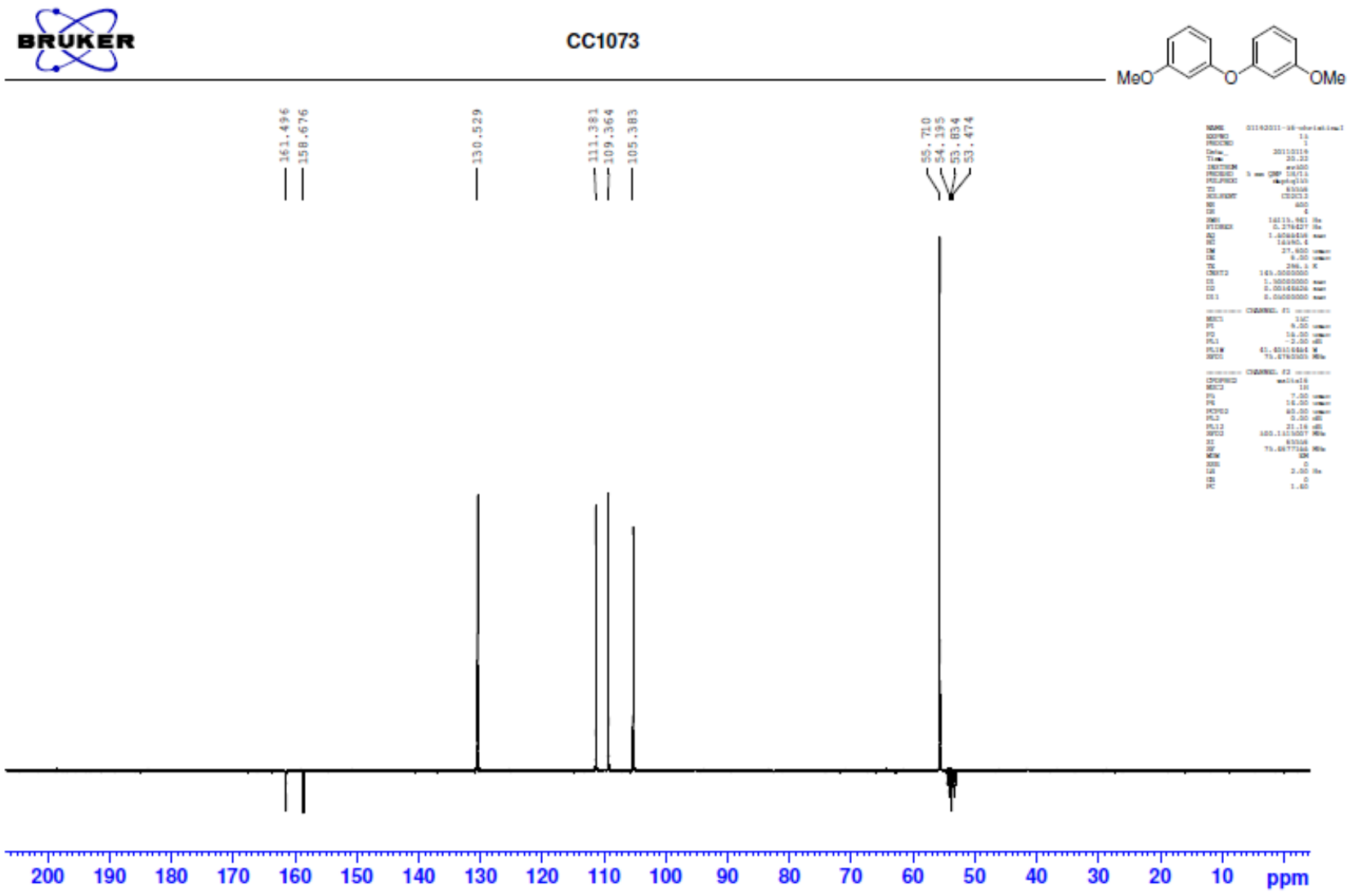


Figure S6 **^{13}C APT NMR spectrum of compound 11OMe** (75 MHz, CD_2Cl_2, 295 K)

3- Compound 12

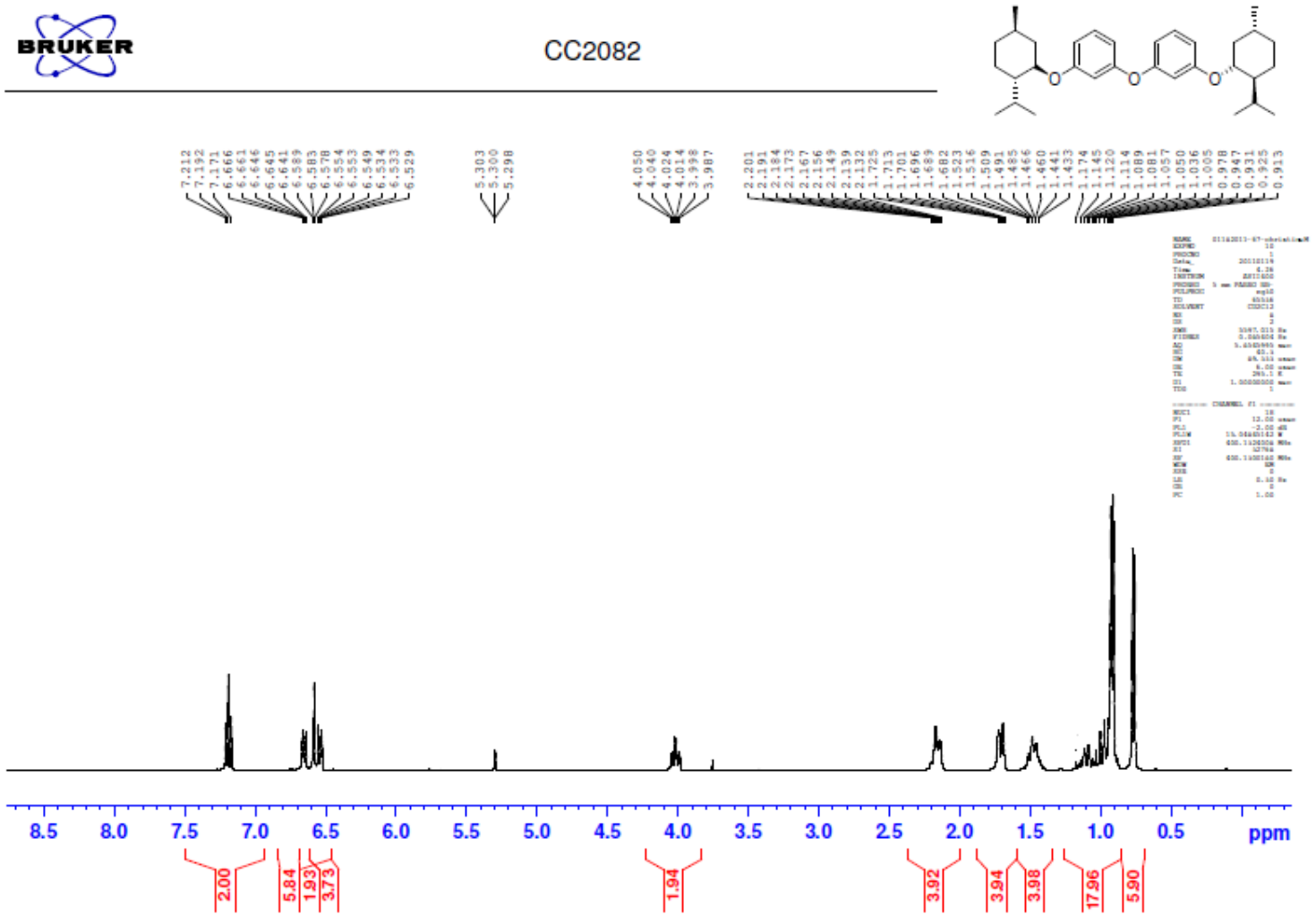


Figure S7 **^{1}H NMR spectrum of compound 12** (400 MHz, CD_2Cl_2, 295 K)

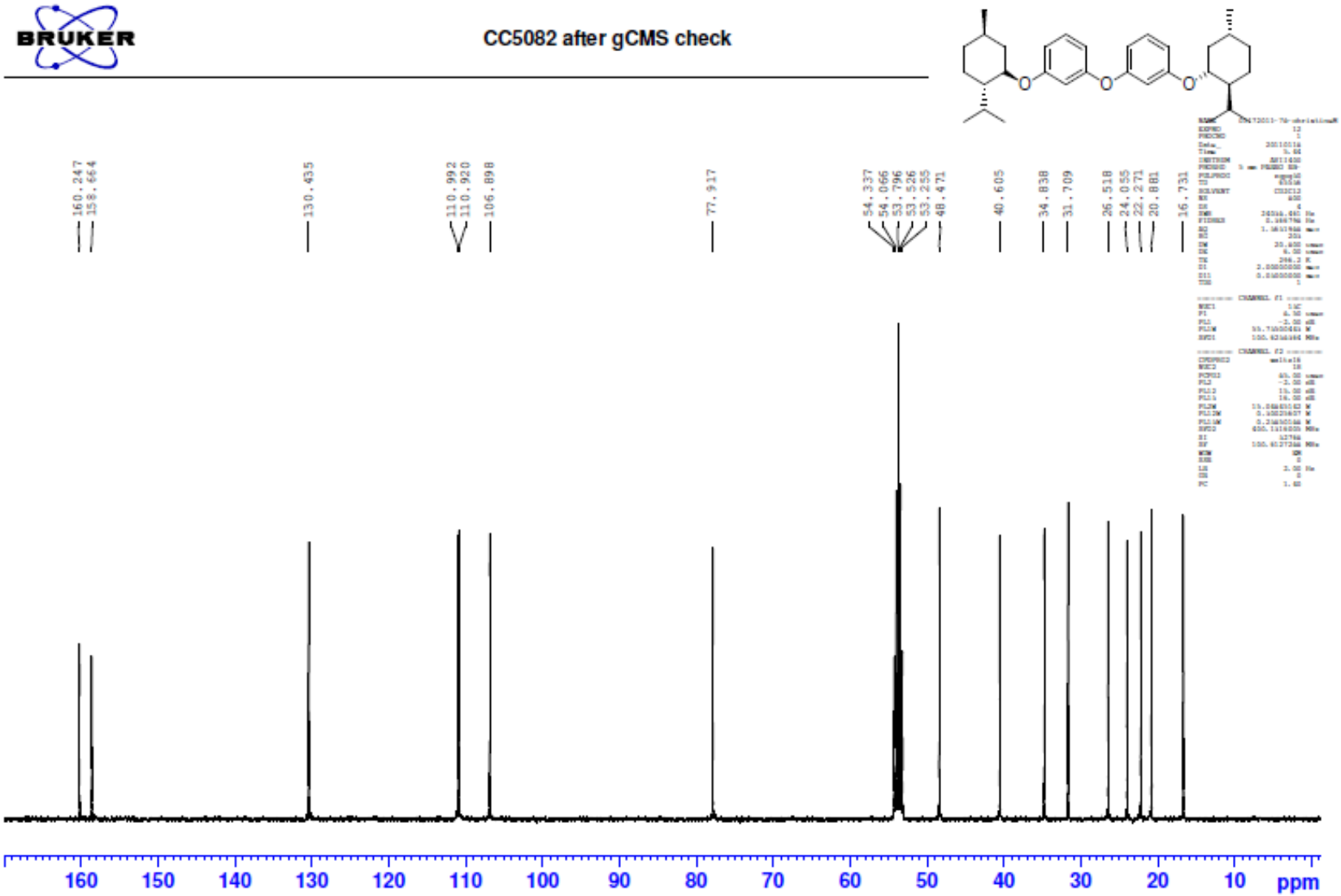


Figure S8 **$^{13}C\{^{1}H\}$ NMR spectrum of compound 12** (101 MHz, CD_2Cl_2, 295 K)

4- Compound 13

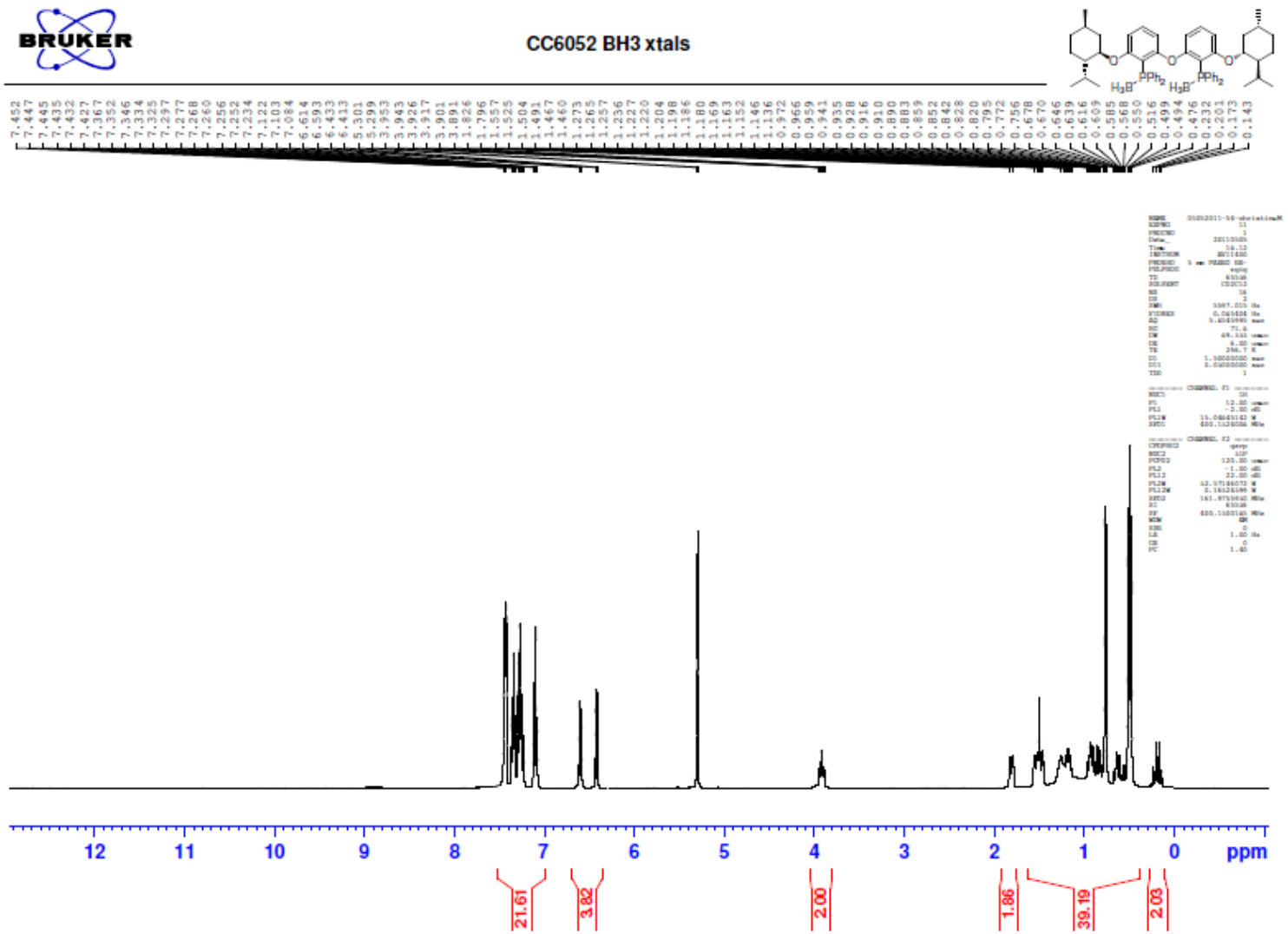


Figure S9 **^{1}H NMR spectrum of compound 13** (400 MHz, CD_2Cl_2, 296 K)

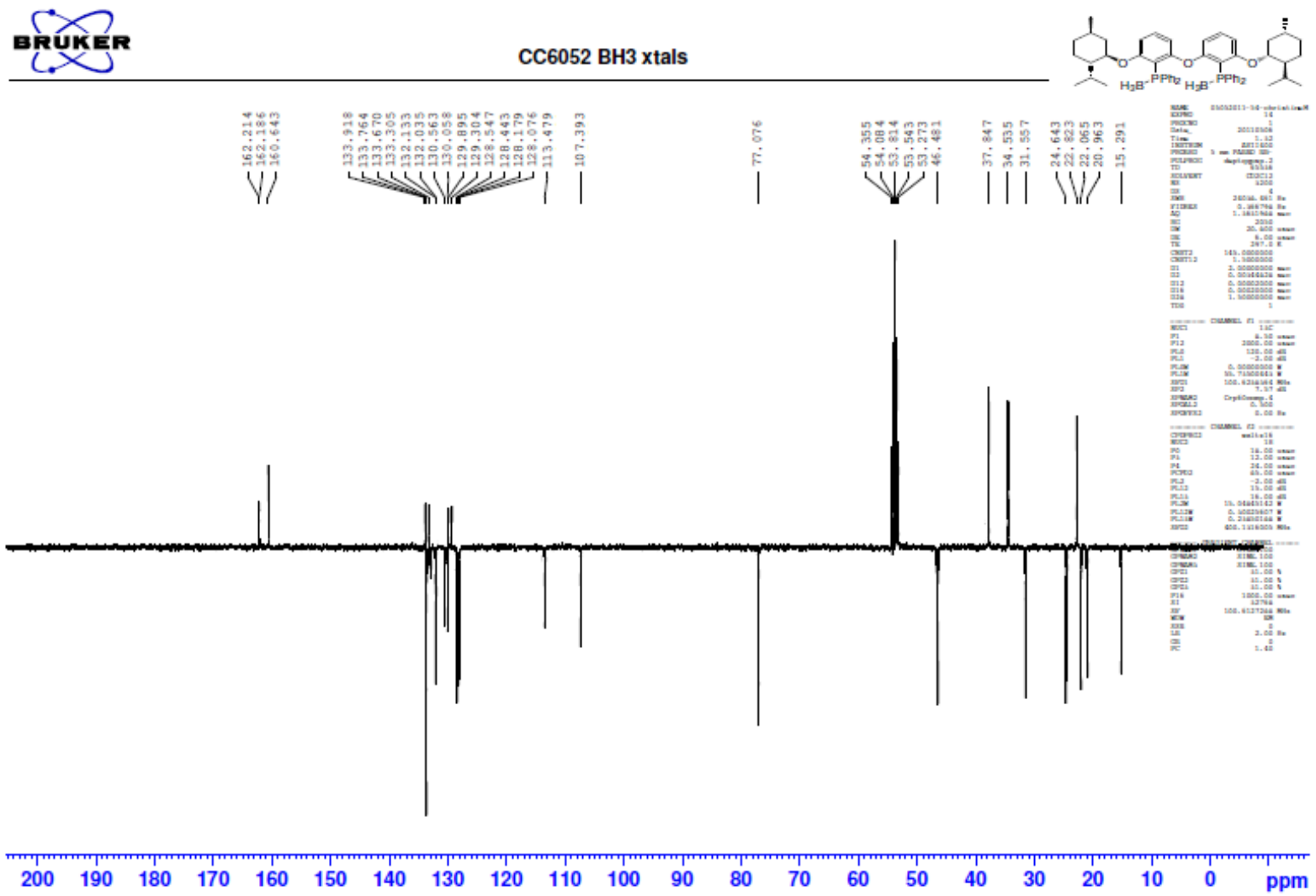


Figure S10 **^{13}C APT NMR spectrum of compound 13** (101 MHz, CD_2Cl_2, 296 K)

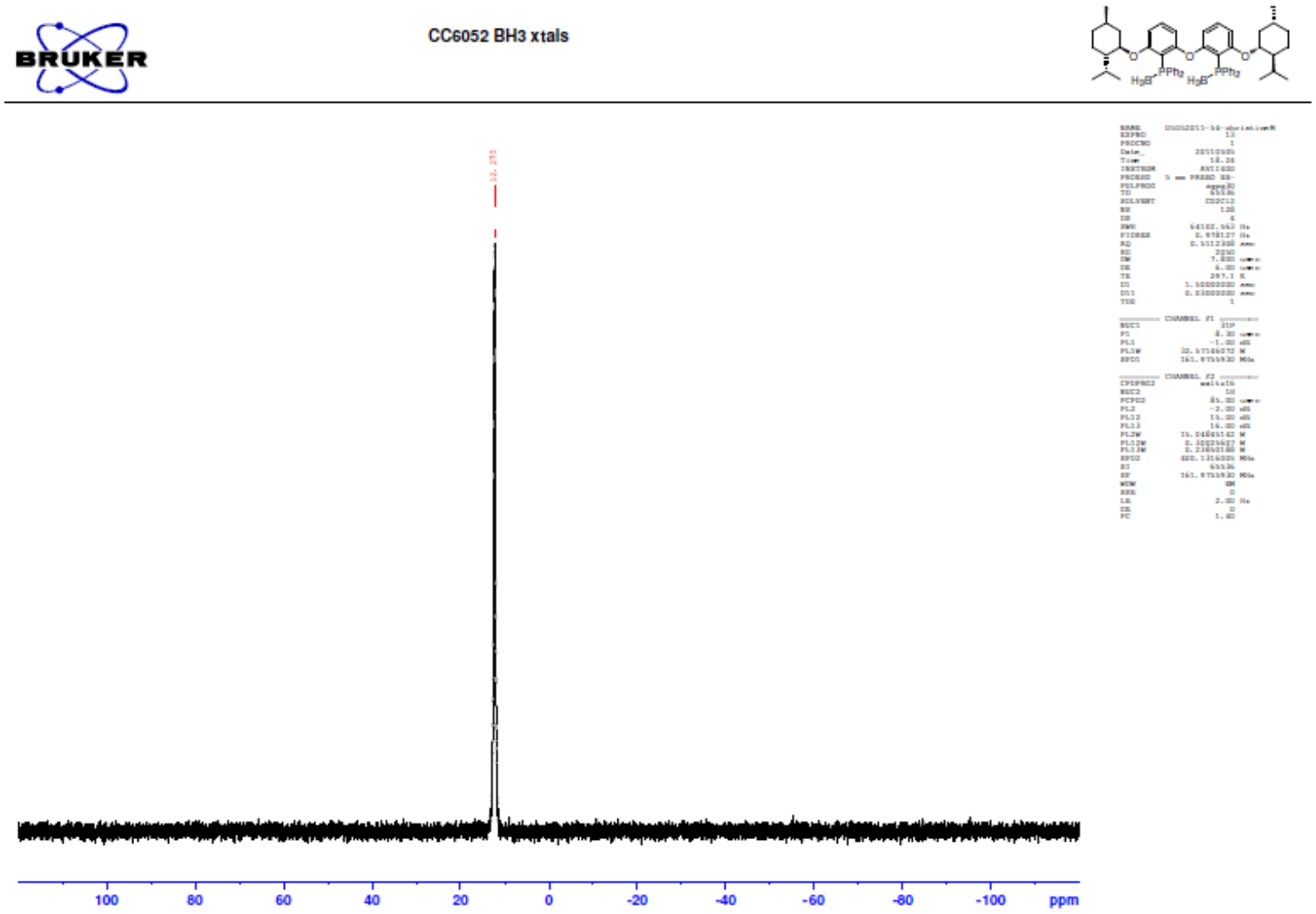


Figure S11 $^{31}P\{^{1}H\}$ **NMR spectrum of compound 13** (161 MHz, CD_2Cl_2, 296 K)

5- Compound 14

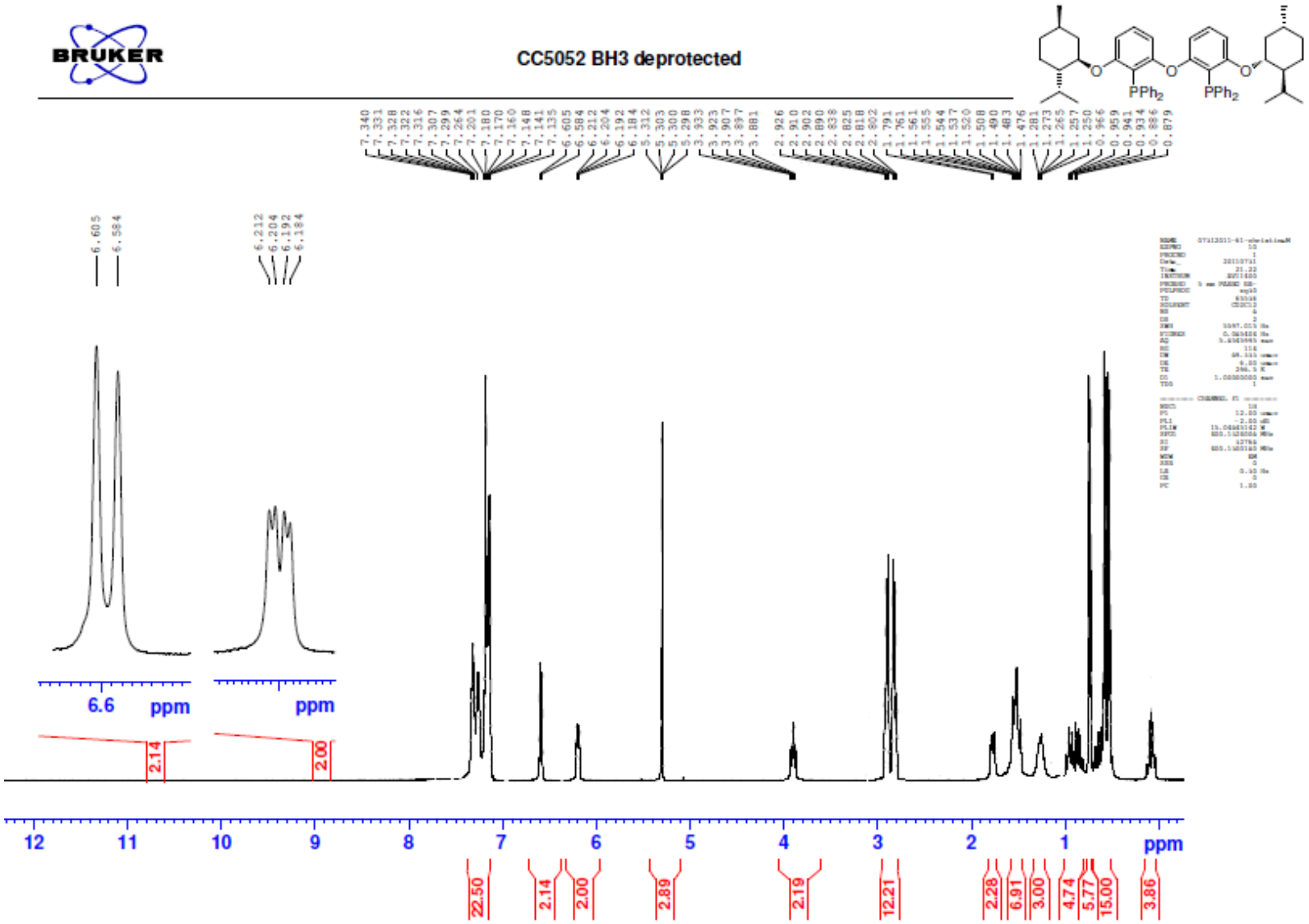


Figure S12 **^{1}H NMR spectrum of compound 14** (400 MHz, CD_2Cl_2, 296 K)

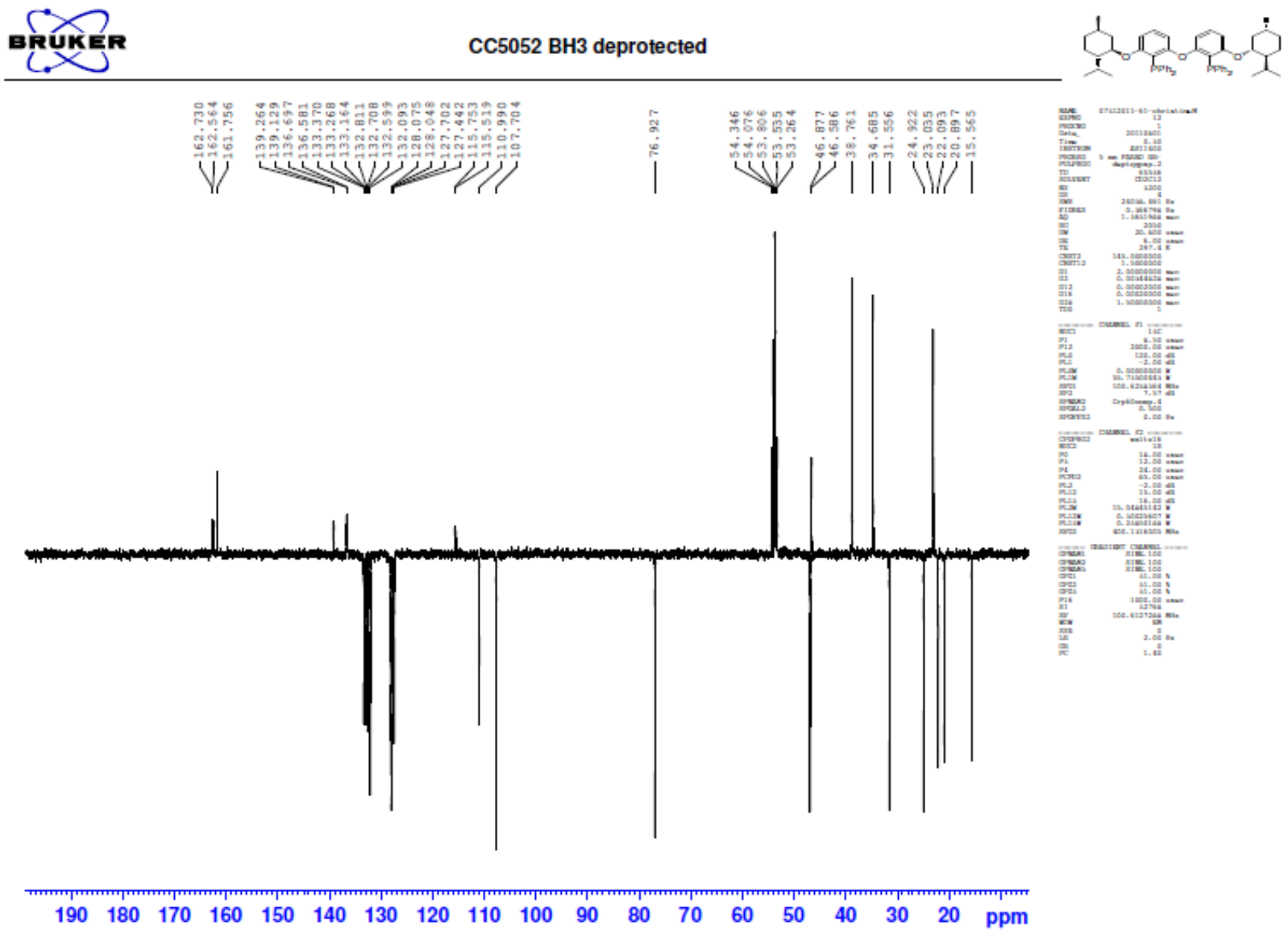


Figure S13 **^{13}C APT NMR spectrum of compound 14** (101 MHz, CD_2Cl_2, 296 K)

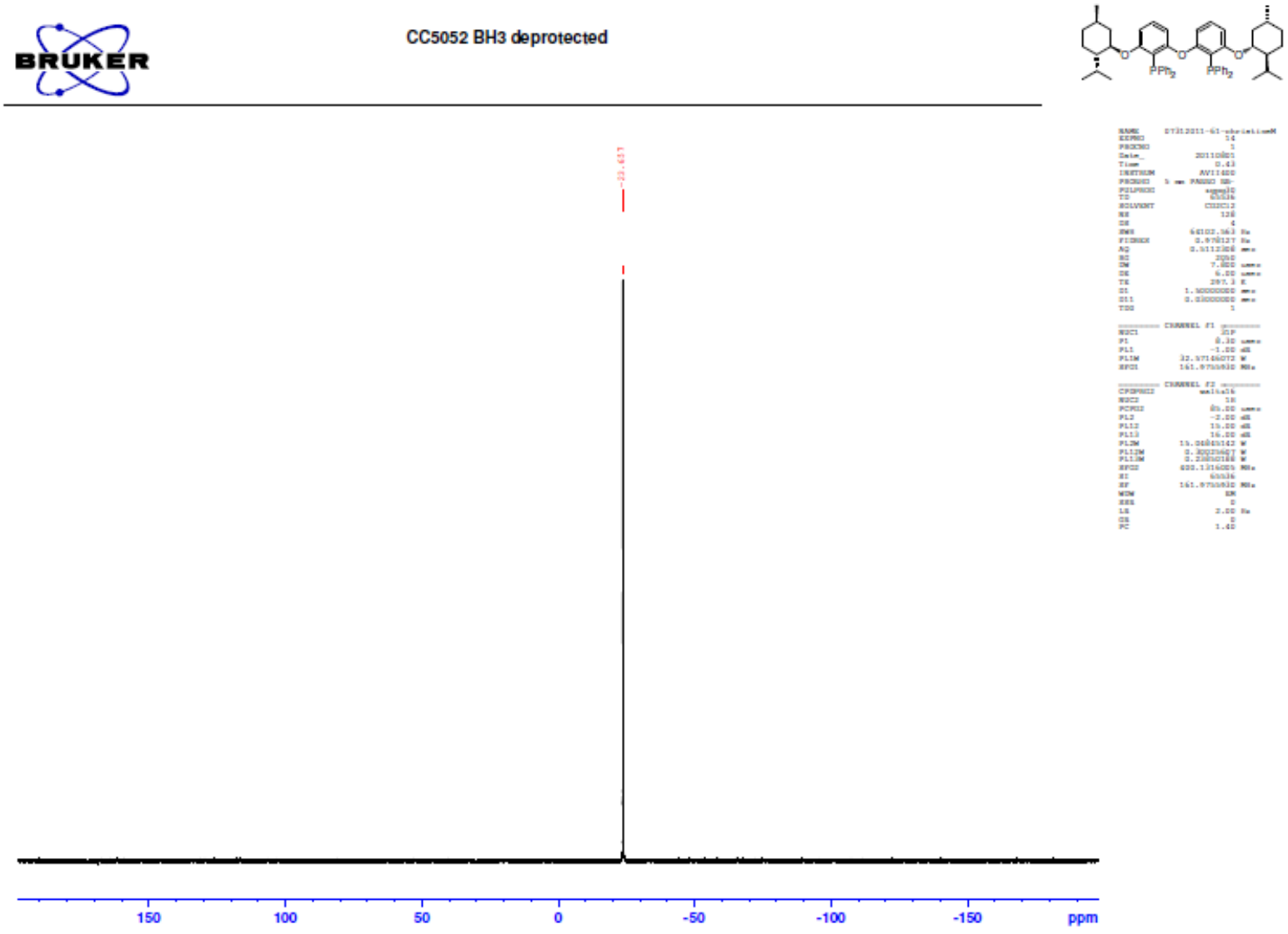


Figure S14 **$^{31}P\{^{1}H\}$ NMR spectrum of compound 14** (161 MHz, CD_2Cl_2, 296 K)

6- Compound 15

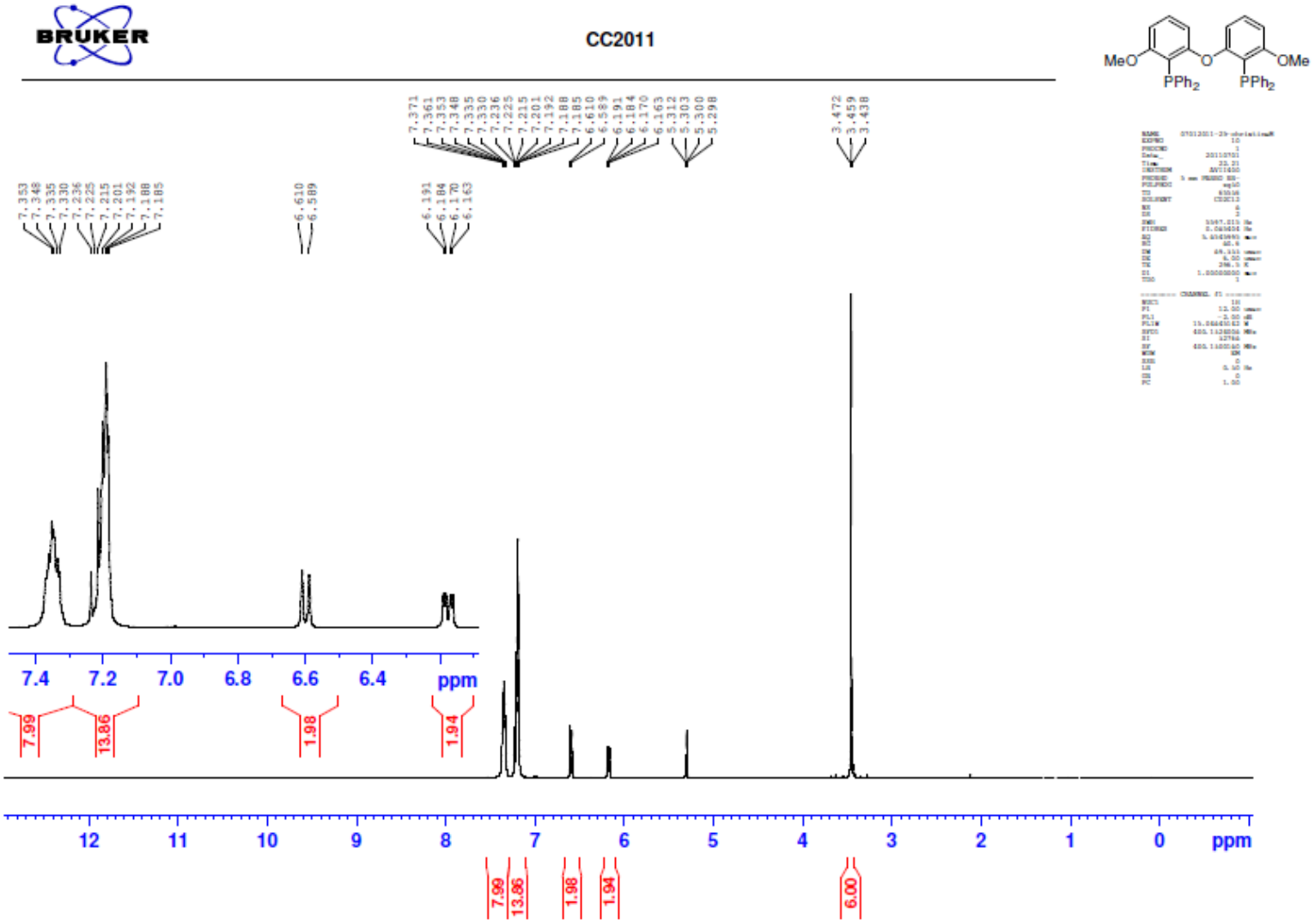


Figure S15 **^{1}H NMR spectrum of compound 15** (400 MHz, CD_2Cl_2, 296 K)

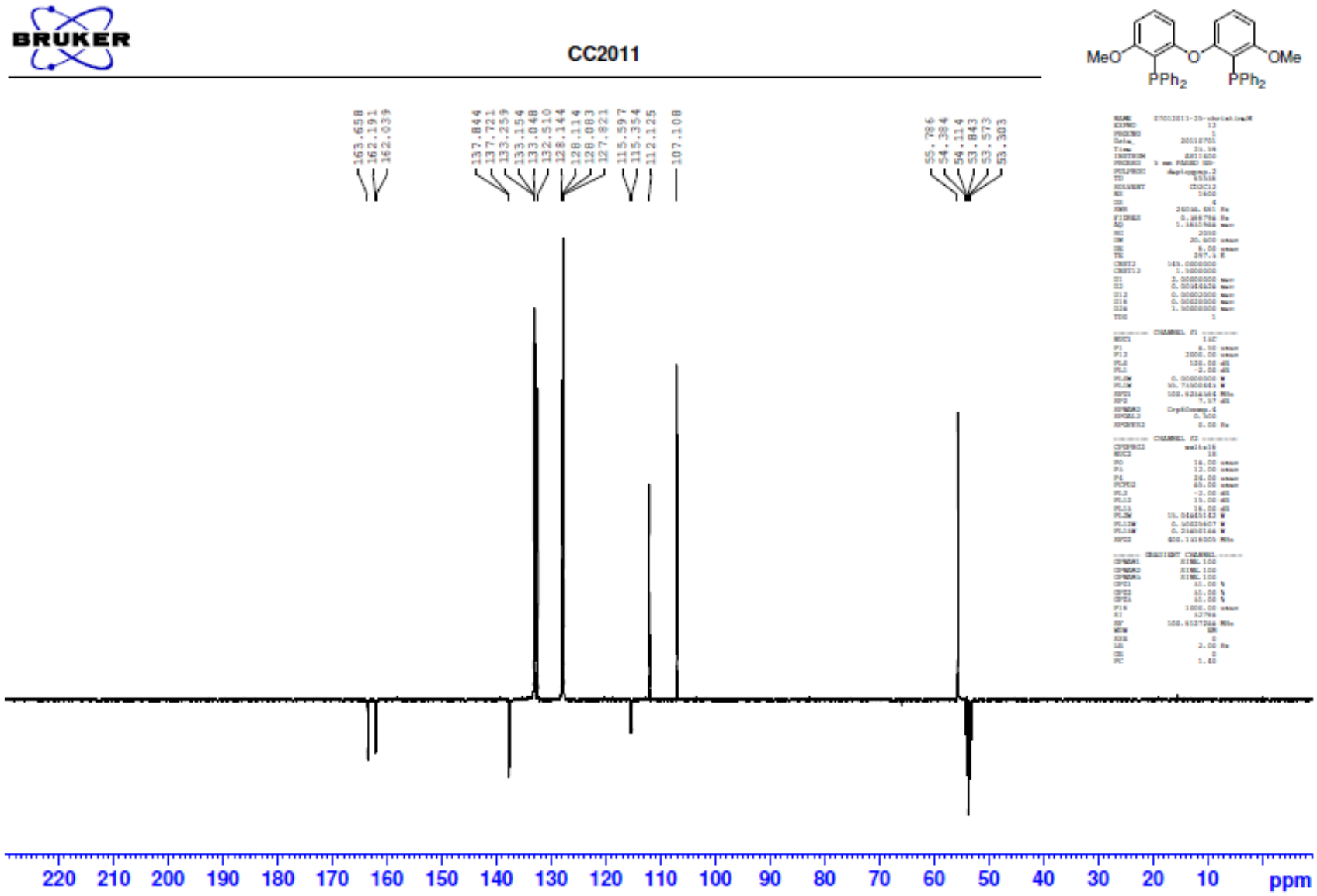


Figure S16 **^{13}C APT NMR spectrum of compound 15** (101 MHz, CD_2Cl_2, 296 K)

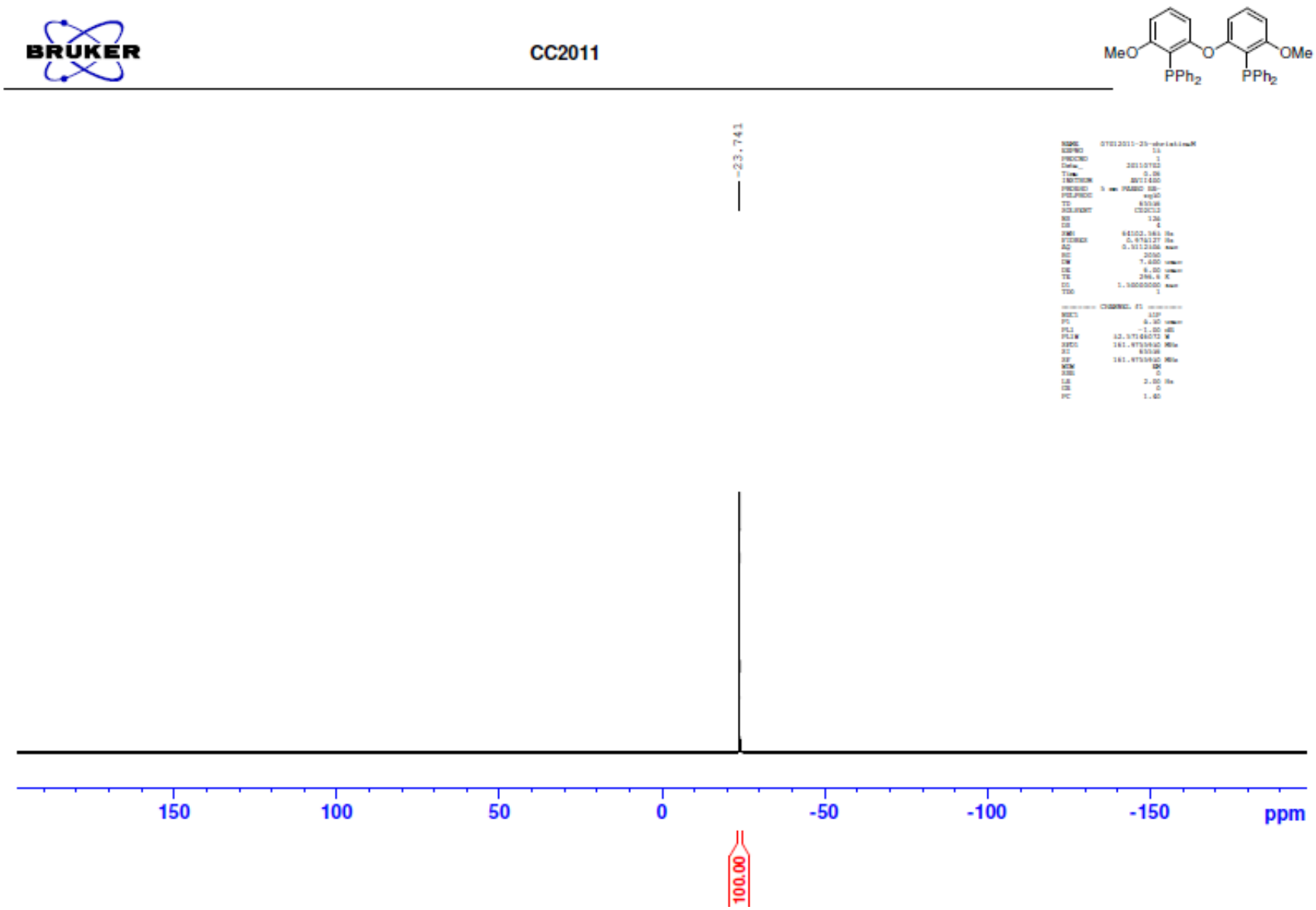


Figure S17 $^{31}P\{^{1}H\}$ **NMR spectrum of compound 15** (161 MHz, CD_2Cl_2, 296 K)

7- Compound 17a

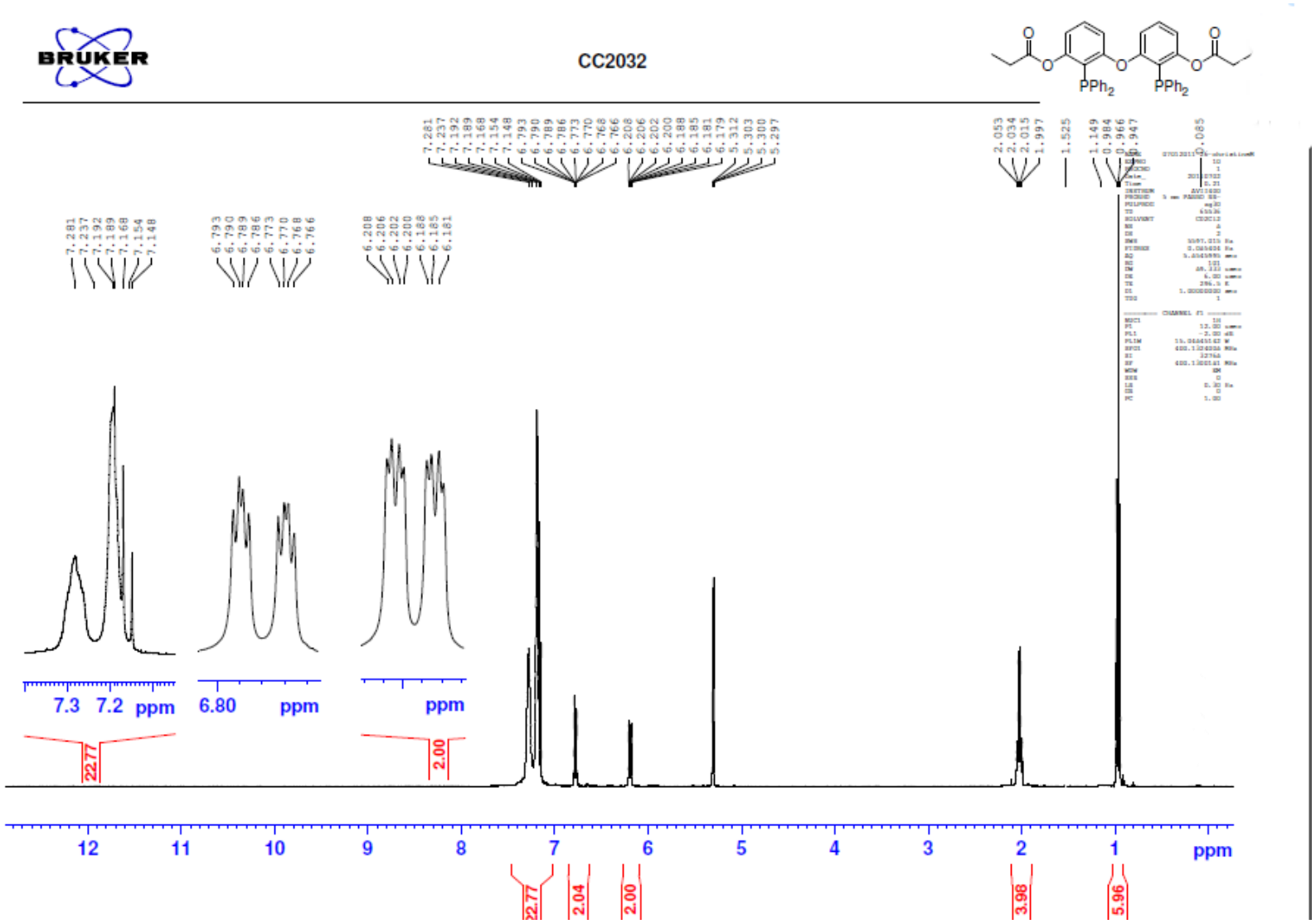


Figure S18 **^{1}H NMR spectrum of compound 17a** (400 MHz, CD_2Cl_2, 297 K)

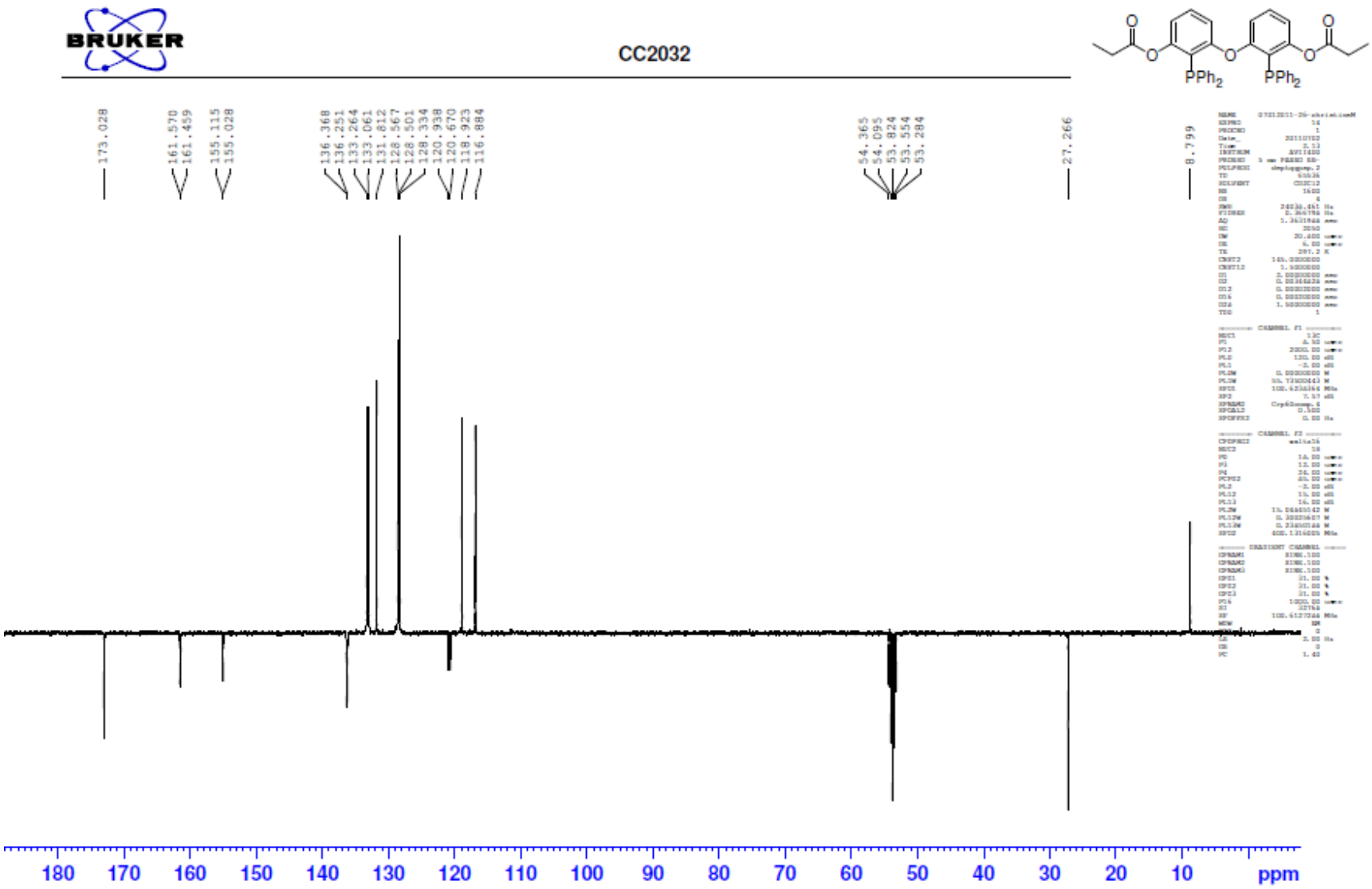


Figure S19 **^{13}C APT NMR spectrum of compound 17a** (101 MHz, CD_2Cl_2, 297 K)

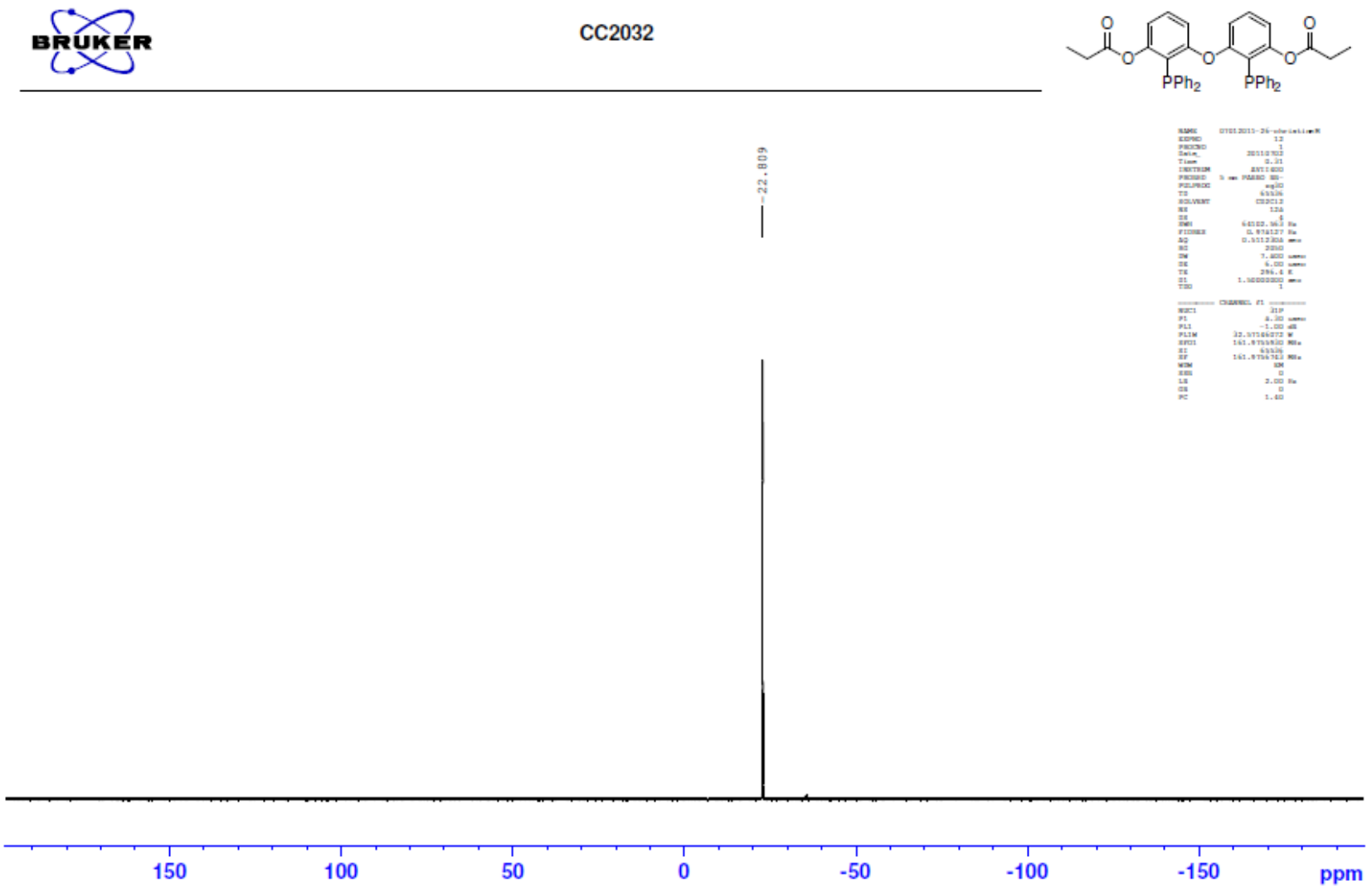


Figure S20 **$^{31}P\{^{1}H\}$ NMR spectrum of compound 17a** (161 MHz, CD_2Cl_2, 297 K)

8- Compound 17a

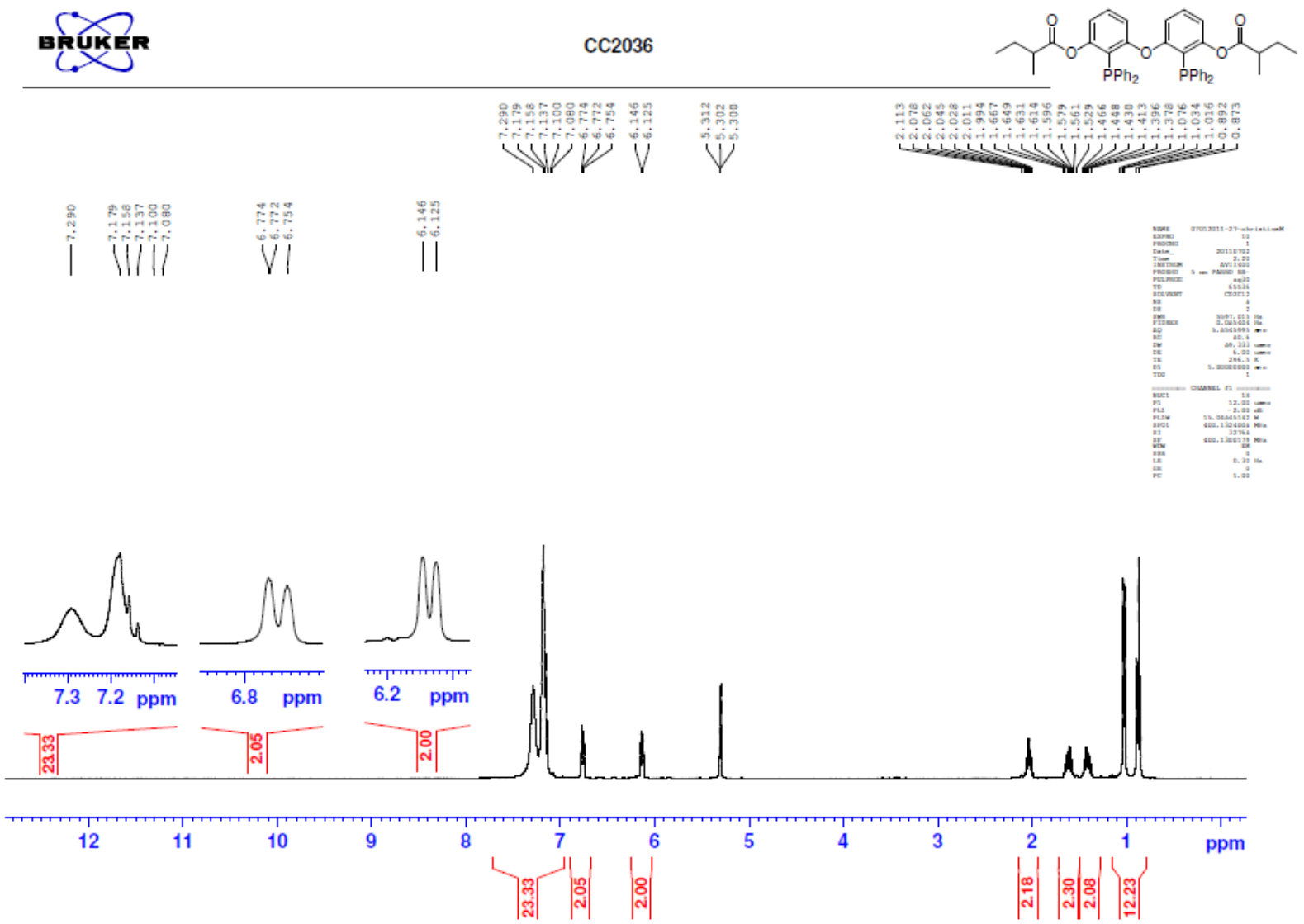


Figure S21 **^{1}H NMR spectrum of compound 17b** (400 MHz, CD_2Cl_2, 297 K)

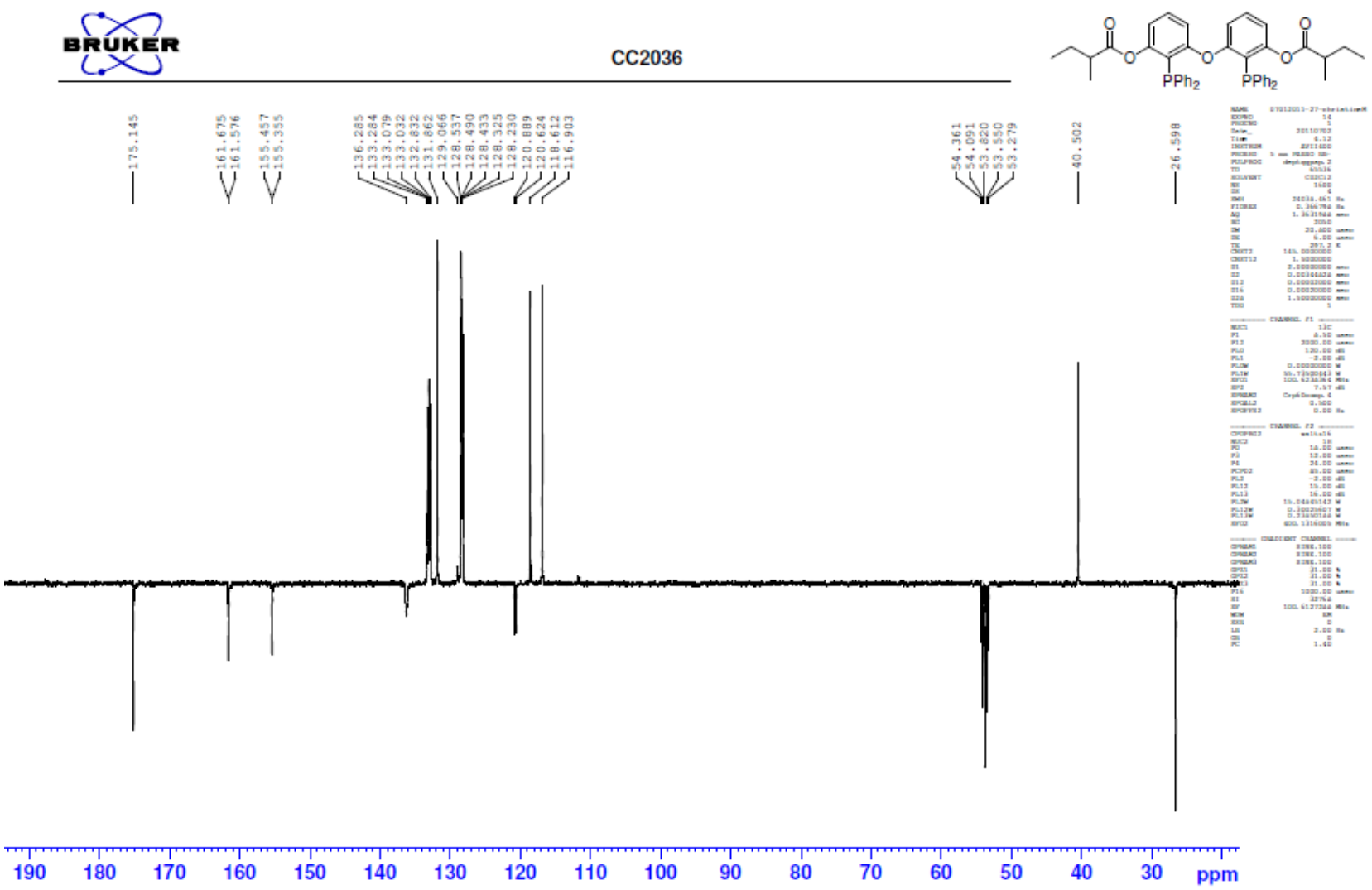


Figure S22 **^{13}C APT NMR spectrum of compound 17b** (101 MHz, CD_2Cl_2, 297 K)

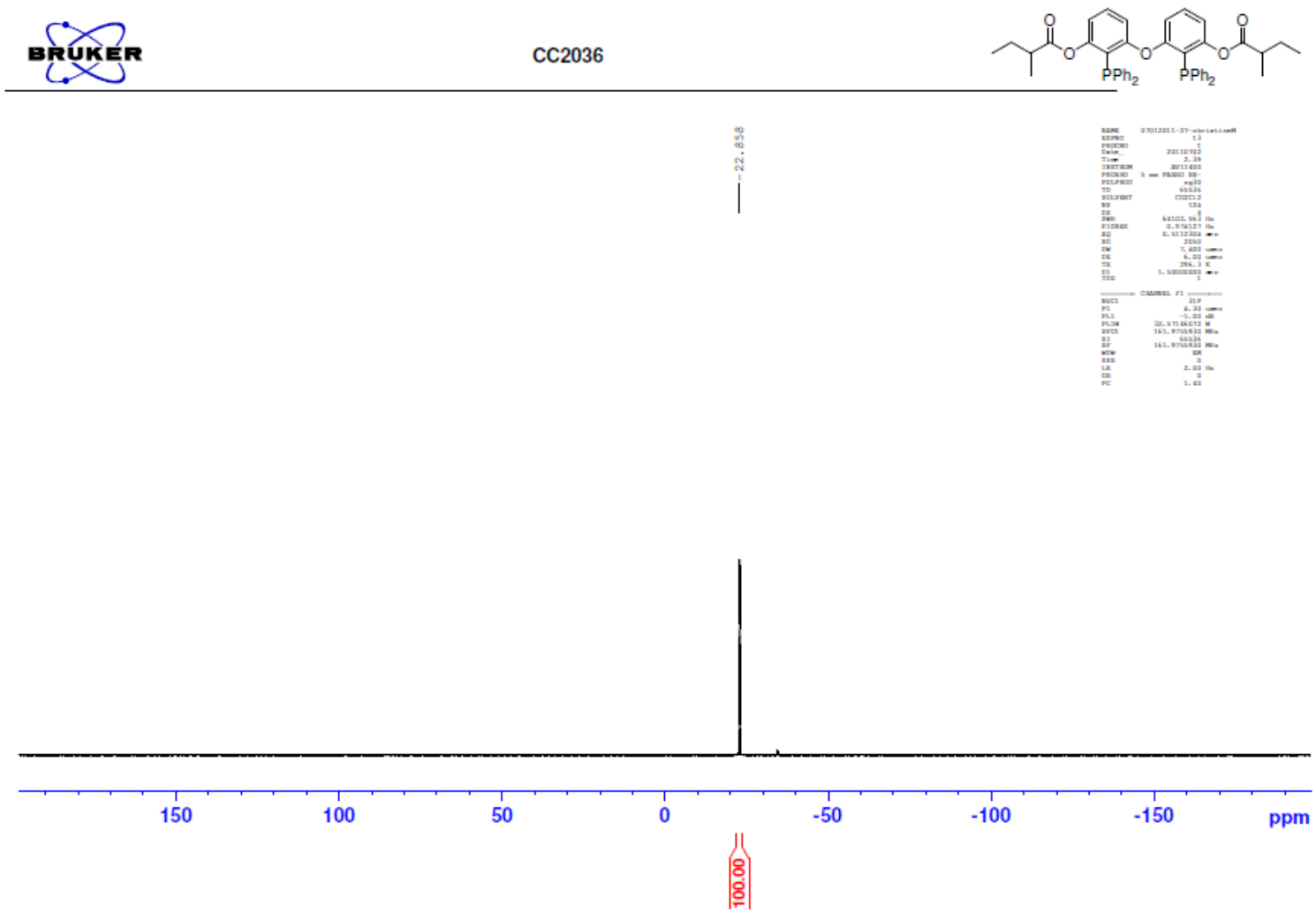


Figure S23 $^{31}P\{^{1}H\}$ **NMR spectrum of compound 17b** (161 MHz, CD_2Cl_2, 297 K)

9- Compound 17c

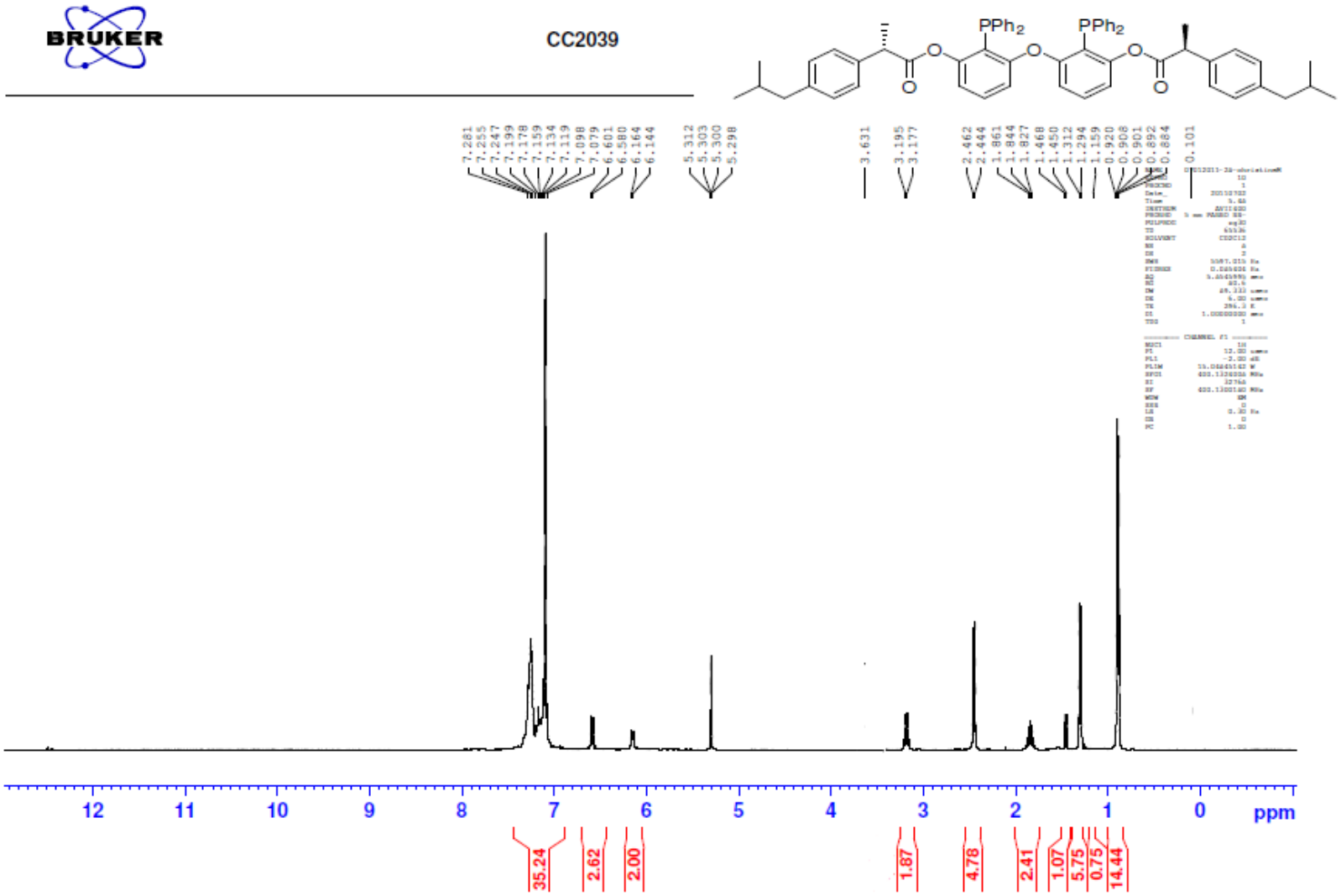
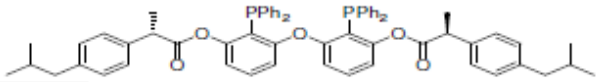


Figure S24 **^{1}H NMR spectrum of compound 17c** (400 MHz, CD_2Cl_2, 297 K)



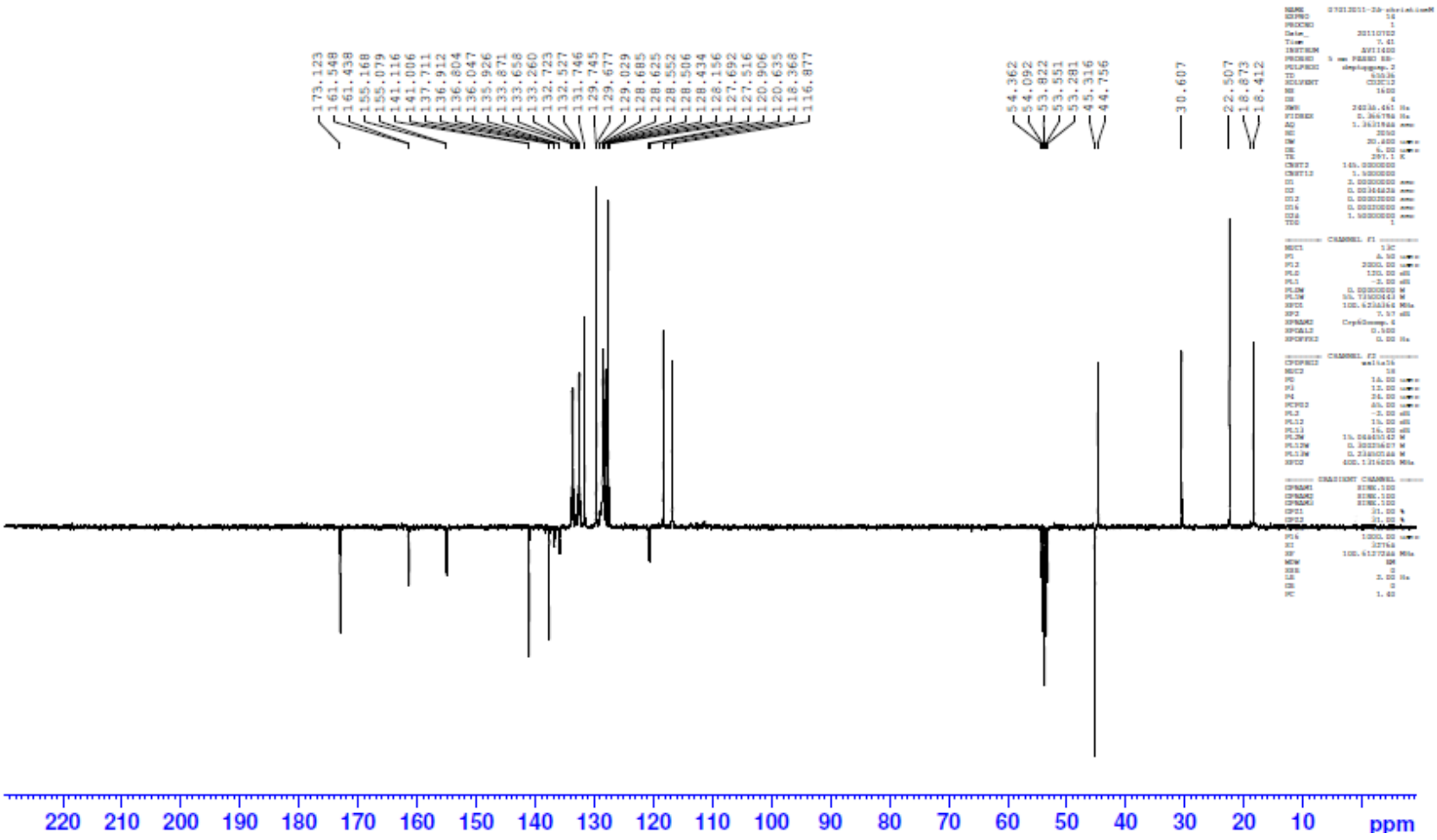


Figure S25 **^{13}C APT NMR spectrum of compound 17c** (101 MHz, CD_2Cl_2, 297 K)

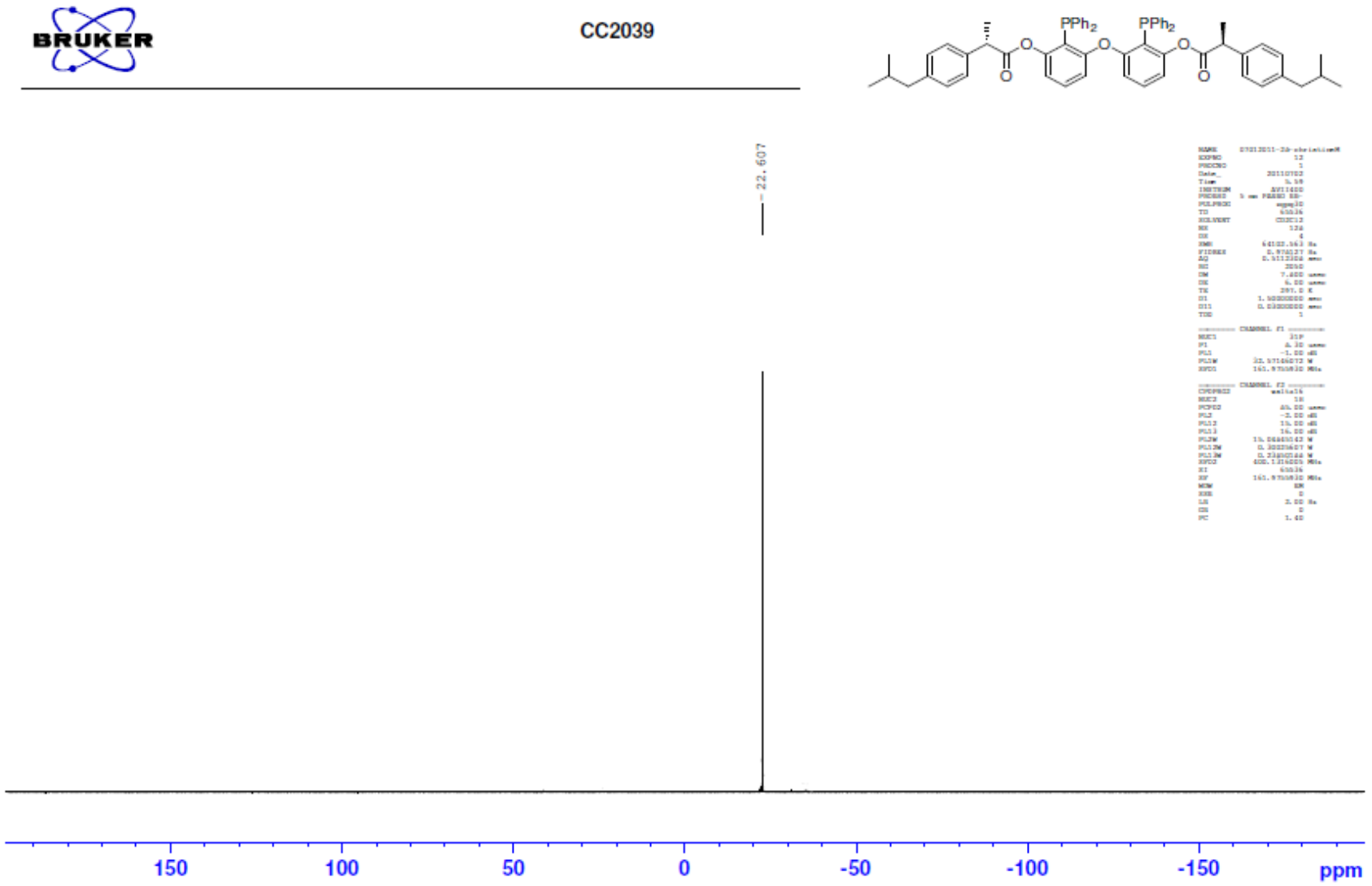


Figure S26 **$^{31}P\{^{1}H\}$ NMR spectrum of compound 17c** (161 MHz, CD_2Cl_2, 297 K)

10- Compound 17d

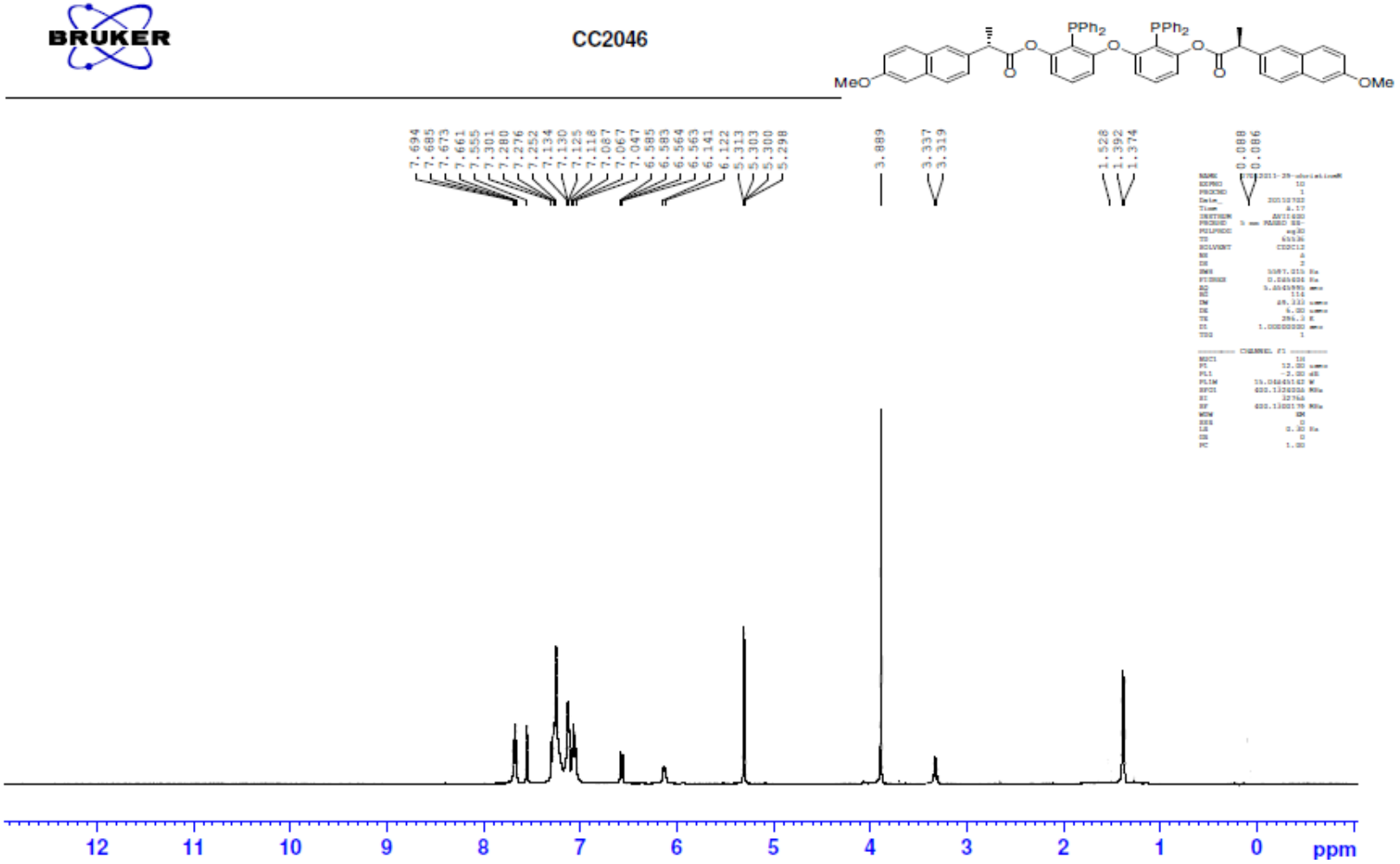


Figure S27 **^{1}H NMR spectrum of compound 17c** (400 MHz, CD_2Cl_2, 297 K)

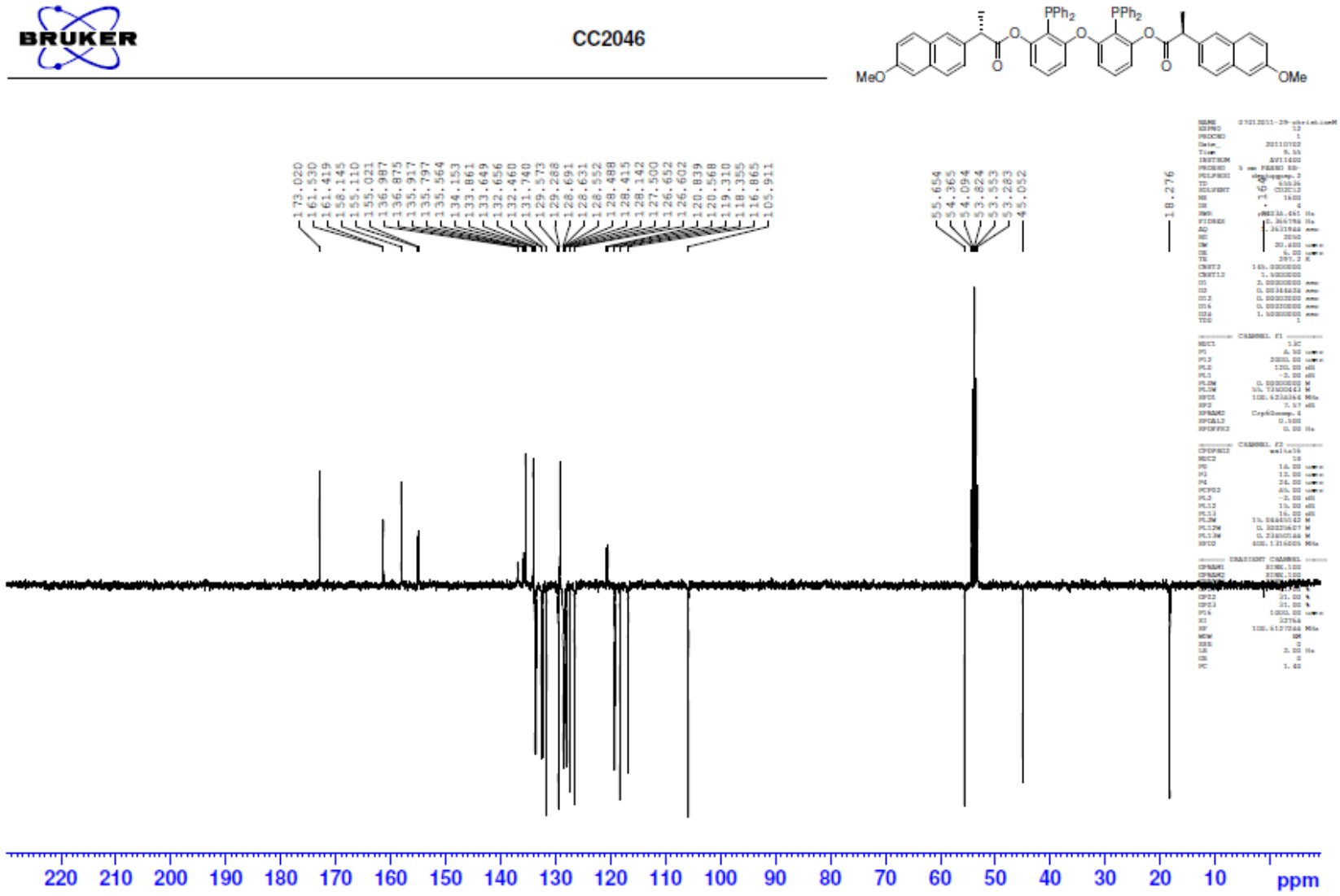


Figure S28 **^{13}C APT NMR spectrum of compound 17c** (101 MHz, CD_2Cl_2, 297 K)

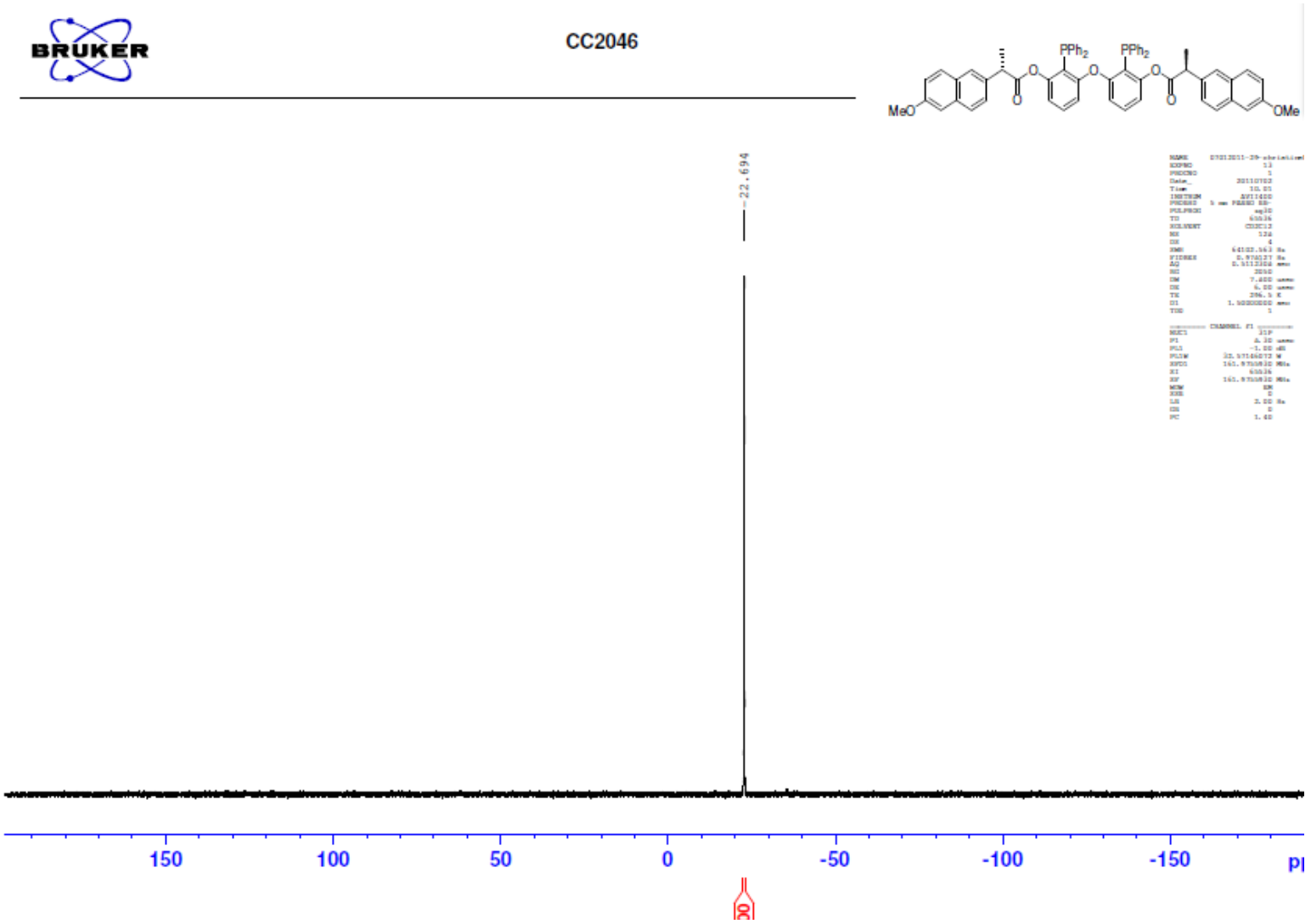


Figure S29 $^{31}P\{^{1}H\}$ **NMR spectrum of compound 17c** (161 MHz, CD_2Cl_2, 297 K)

11- Platinum Complexes

[$PtCl_2$(**15**)]

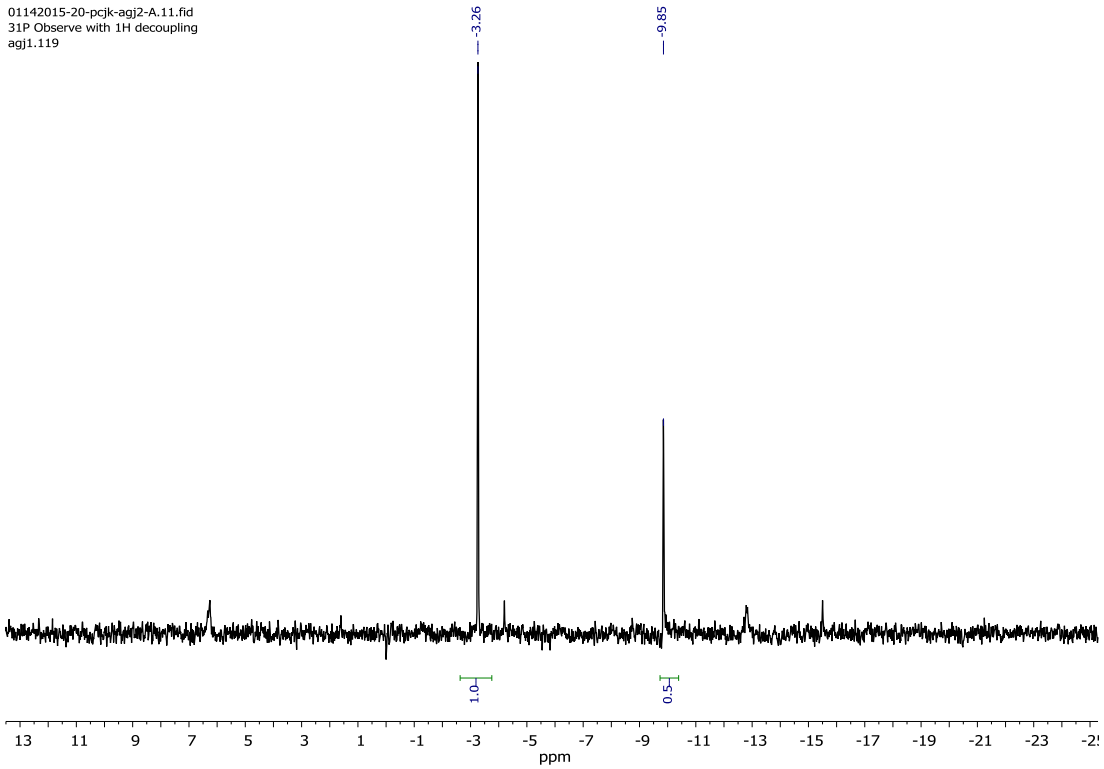


Figure S30: $^{31}P\{^1H\}$ NMR of $PtCl_2$(15) (202 MHz, $CDCl_3$)

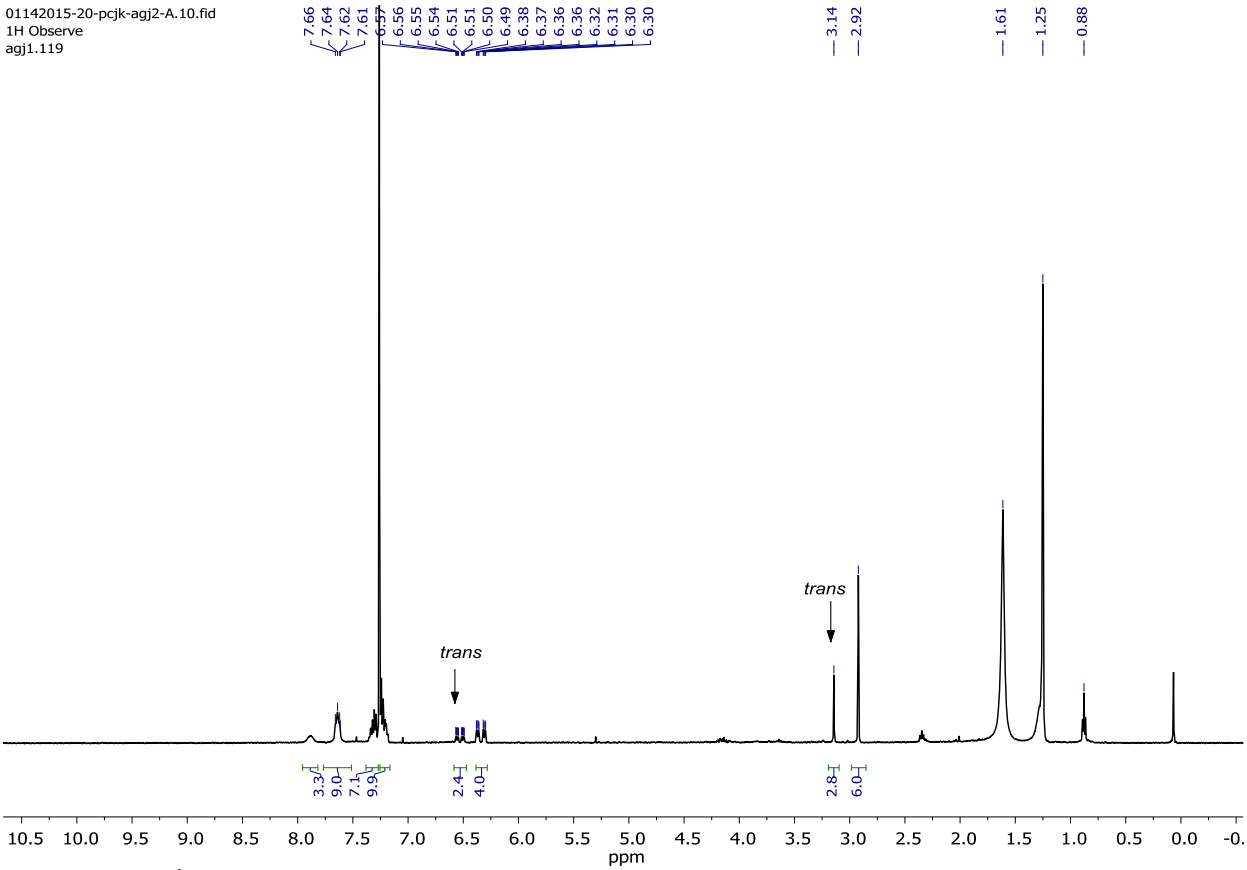


Figure S31: ^{1}H NMR of $PtCl_2$(15) (500 MHz, $CDCl_3$) (major product *cis*-isomer, minor product *trans*-isomer)

[$PtCl_2$(**17a**)]

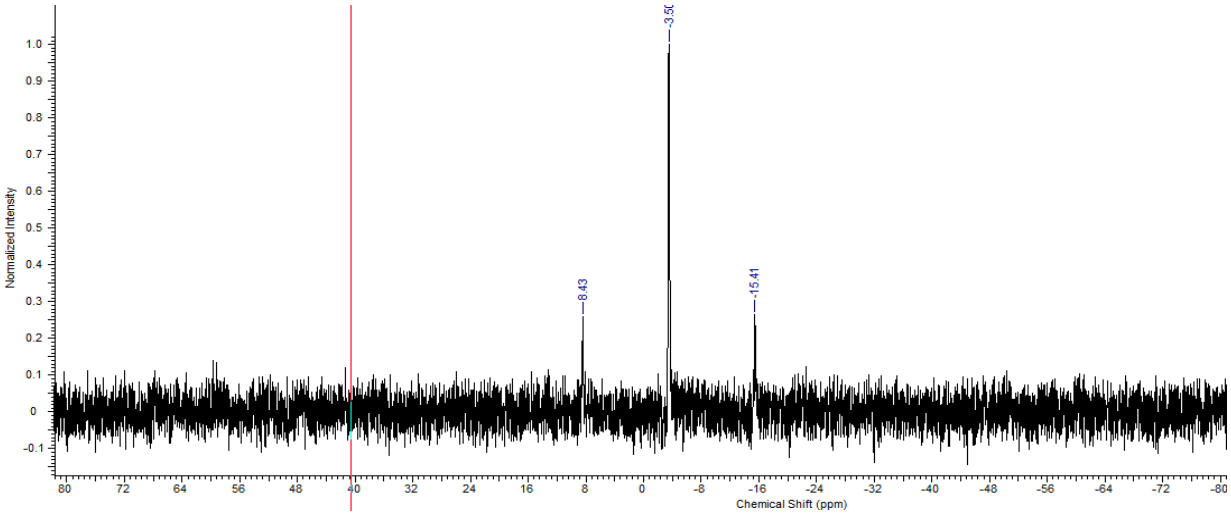


Figure S32: $^{31}P\{^{1}H\}$ NMR of $PtCl_2$(17a) (162 MHz, $CDCl_3$)

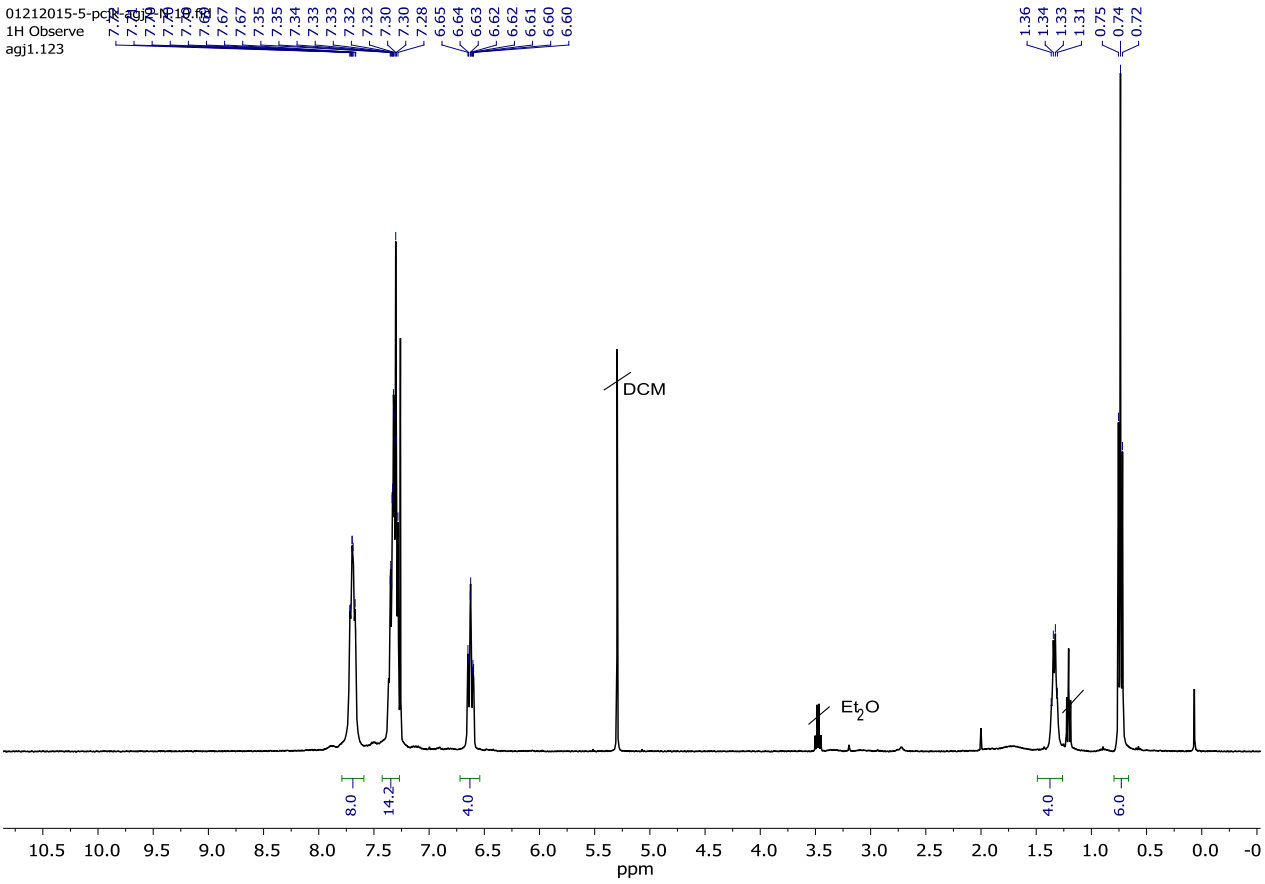


Figure S33: ^{1}H NMR of $PtCl_2$(17a) (400 MHz, $CDCl_3$)

[$PtCl_2$(**17b**)]

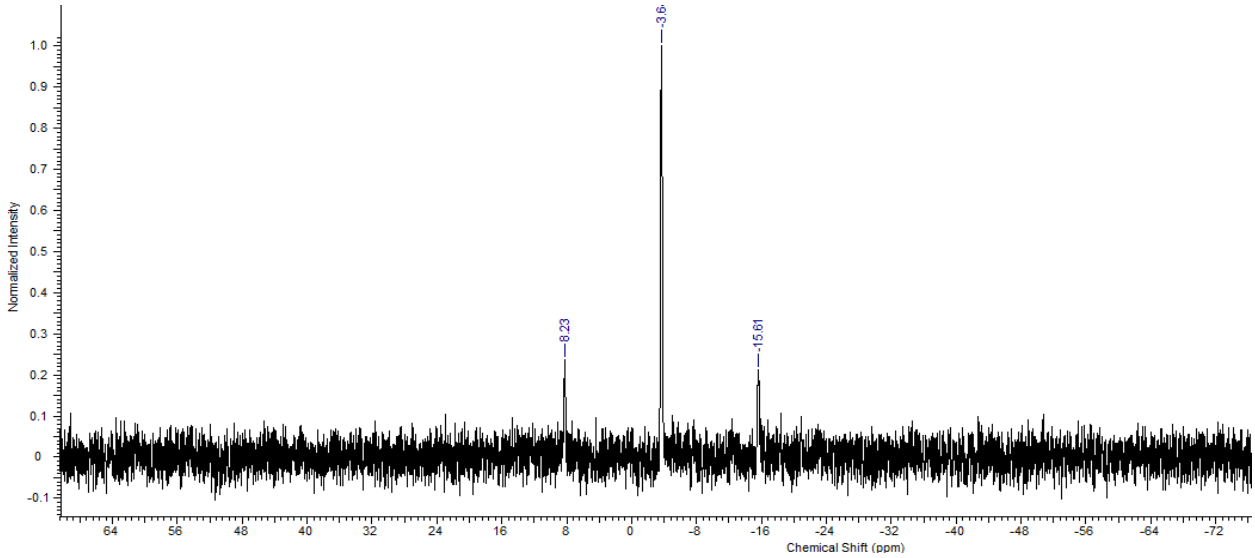


Figure S34: $^{31}P\{^1H\}$ NMR of $PtCl_2$(17b) (162 MHz, $CDCl_3$)

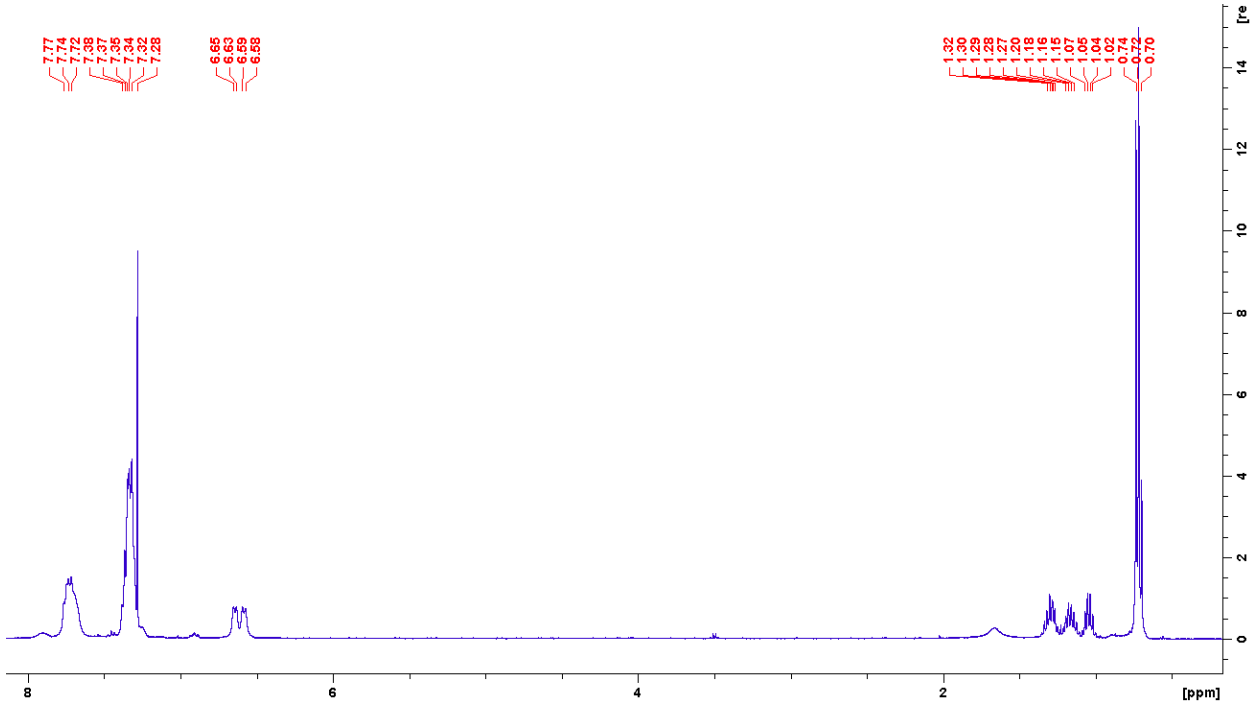


Figure S35: ^1H NMR of $PtCl_2$(17b) (400 MHz, $CDCl_3$)

[$PtCl_2$(**17c**)]

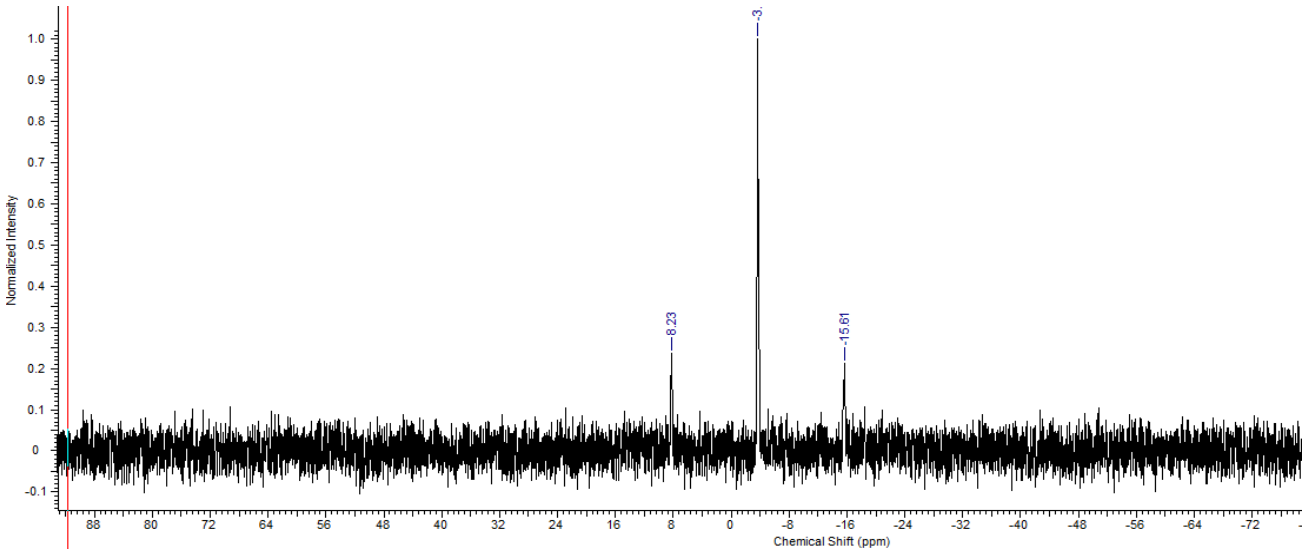


Figure S36: $^{31}P\{^1H\}$ NMR of $PtCl_2$(17c) (162 MHz, $CDCl_3$)

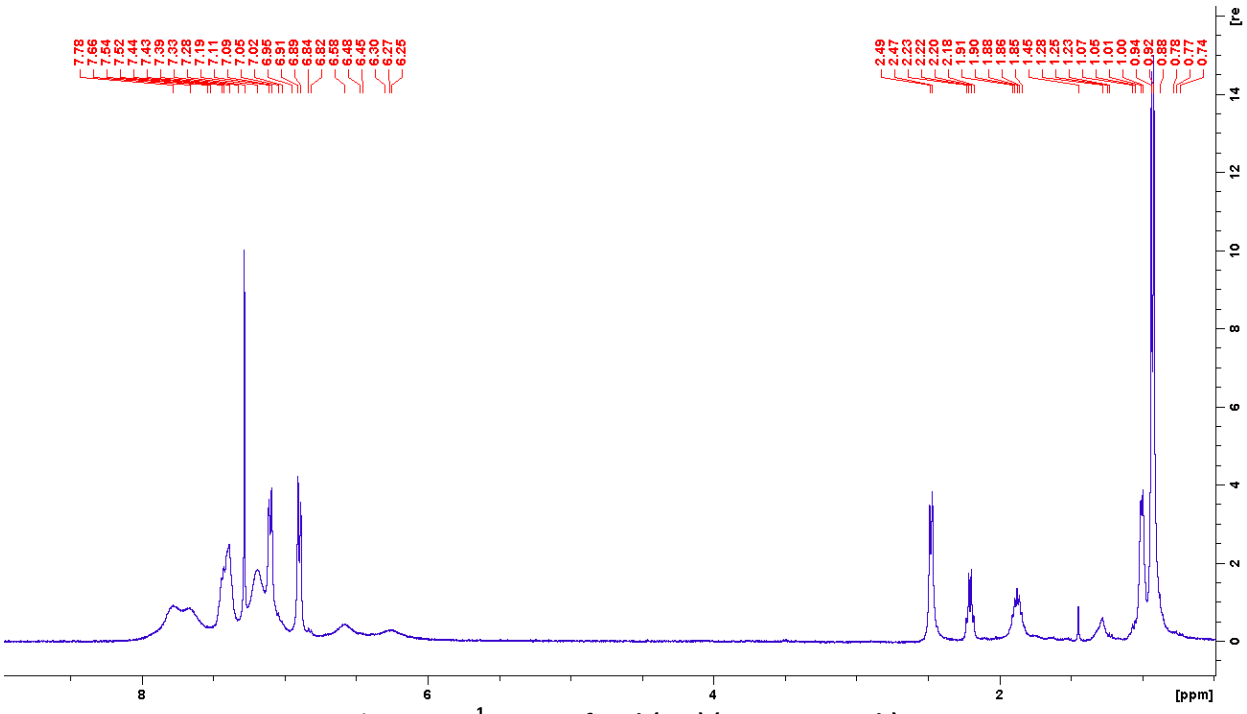


Figure S37: ^1H NMR of $PtCl_2$(17c) (400 MHz, $CDCl_3$)

12- Phosphine selenide compounds

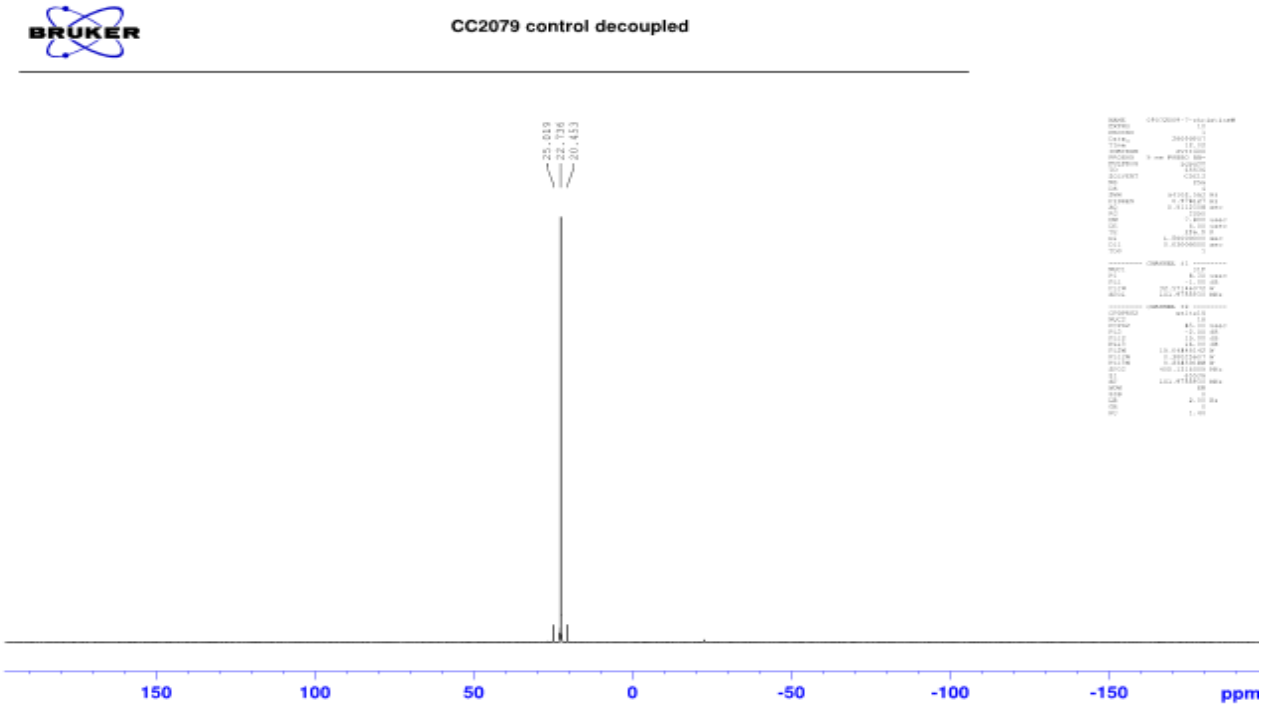


Figure S38 $^{31}P\{^{1}H\}$ **NMR spectrum of diselenide of 15** (161 MHz, CD_2Cl_2, 297 K)

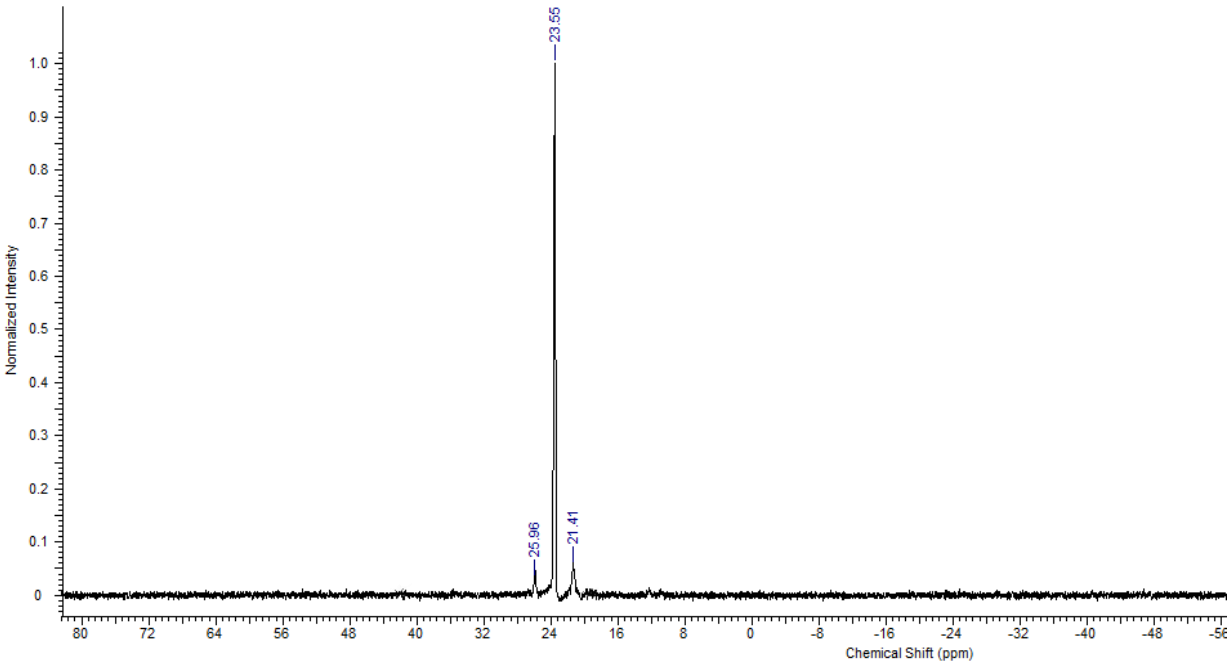


Figure S39 **$^{31}P\{^{1}H\}$ NMR spectrum of diselenide of 17a** (161 MHz, CD_2Cl_2, 297 K)

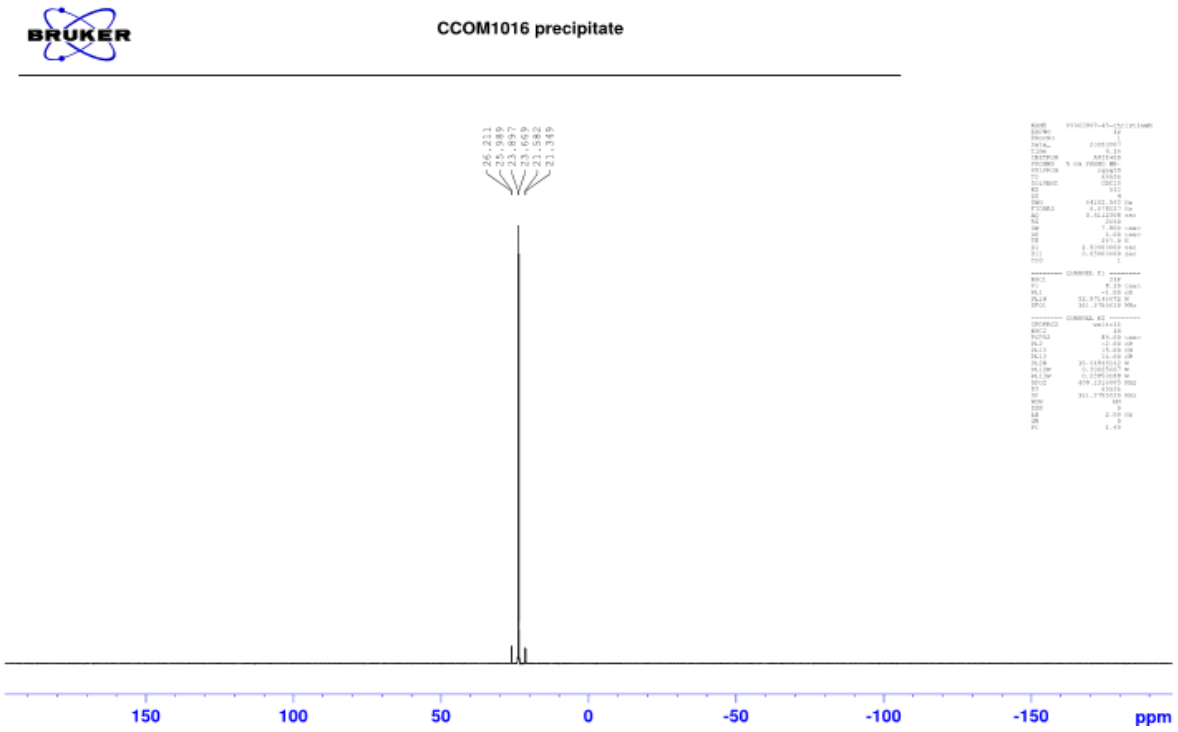


Figure S40 **$^{31}P\{^{1}H\}$ NMR spectrum of diselenide of 17b** (161 MHz, CD_2Cl_2, 297 K)

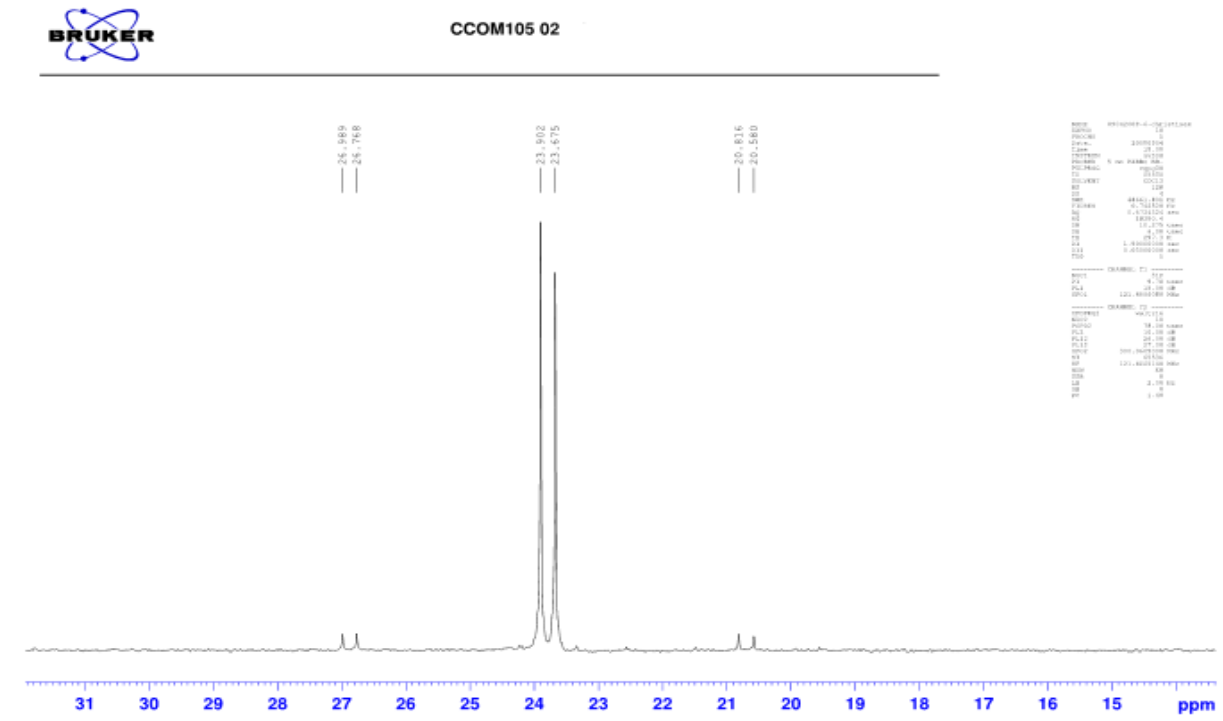


Figure S41 **$^{31}P\{^{1}H\}$ NMR spectrum of diselenide of 17c** (161 MHz, CD_2Cl_2, 297 K)

13- Nickel complexes

[Ni(**15**)$(CO)_2$]

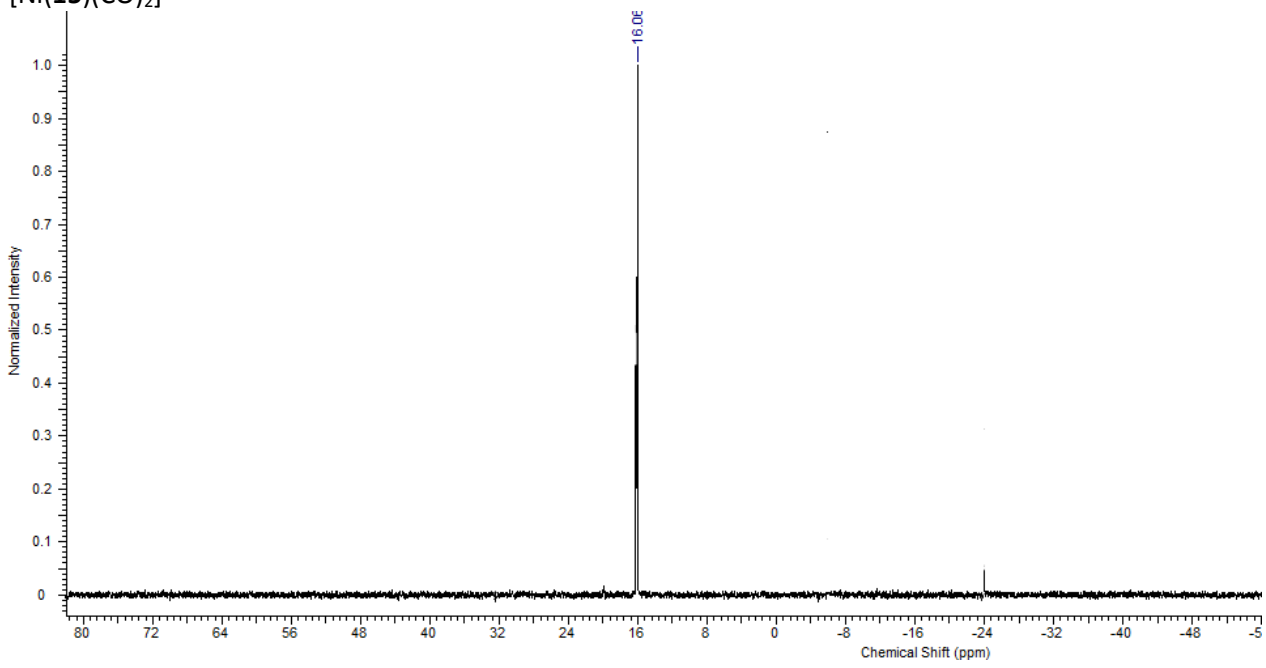


Figure S42 **$^{31}P\{^{1}H\}$ NMR spectrum of [Ni(15)$(CO)_2$]** (161 MHz, CD_2Cl_2, 297 K)

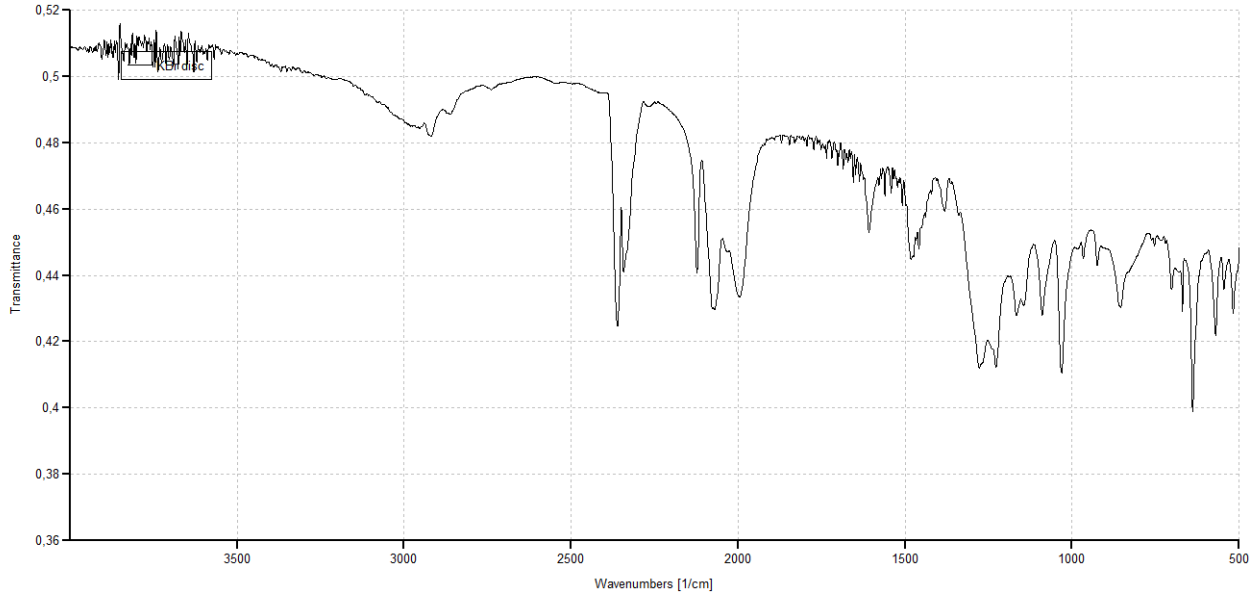


Figure S43 **IR spectrum of [Ni(15)(CO)$_2$]** (KBr)

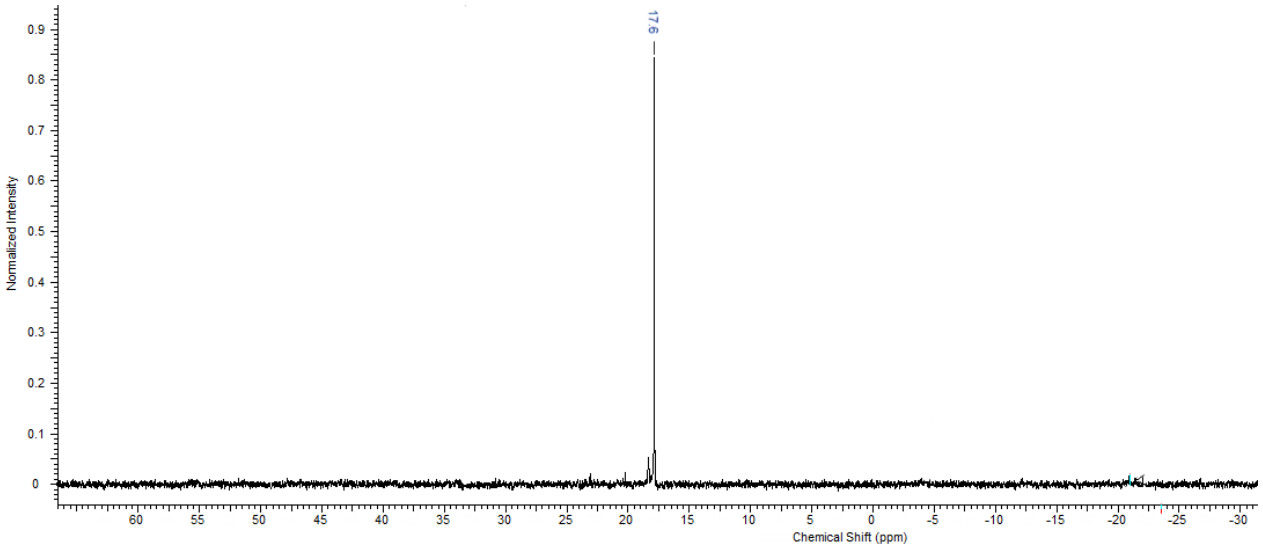


Figure S44 **$^{31}P\{^1H\}$ NMR spectrum of [Ni(17a)(CO)$_2$]** (161 MHz, CD_2Cl_2, 297 K)

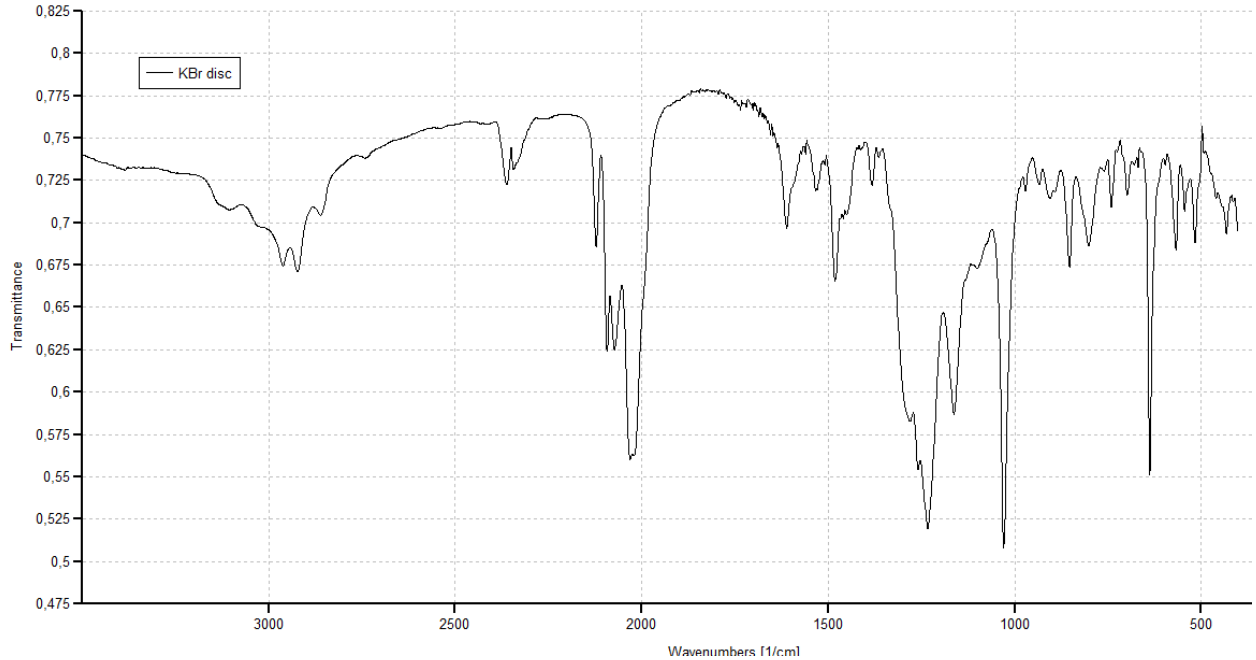


Figure S45 **IR spectrum of [Ni(17a)(CO)$_2$]** (KBr)

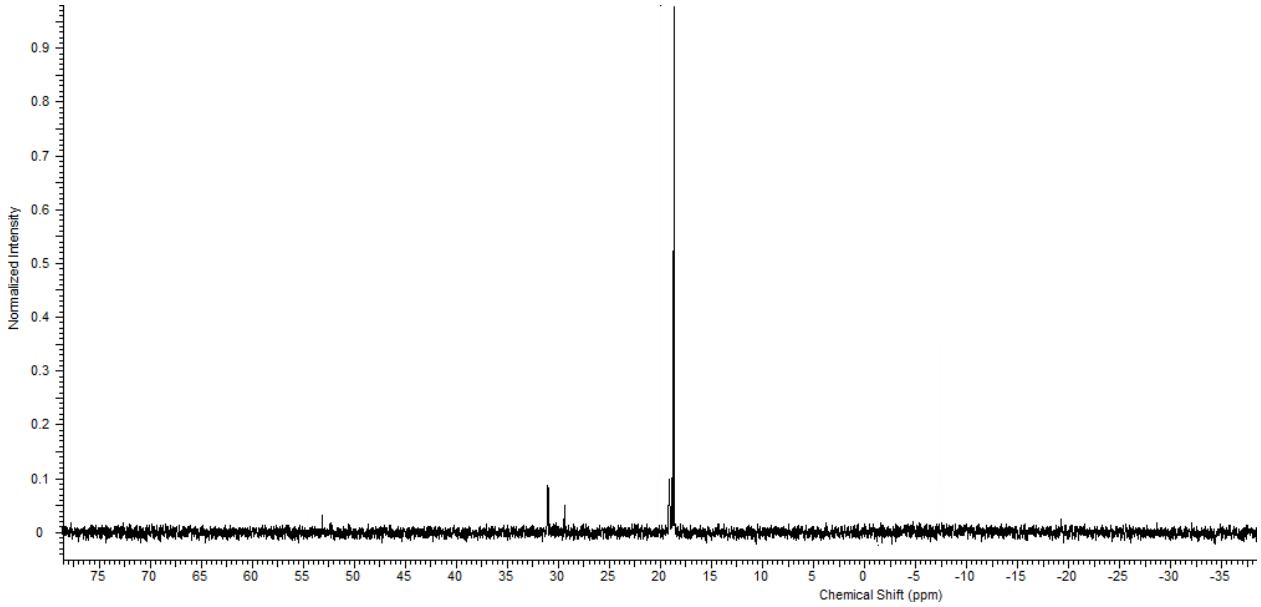


Figure S46 **$^{31}P\{^1H\}$ NMR spectrum of [Ni(17b)(CO)$_2$]** (161 MHz, CD_2Cl_2, 297 K)

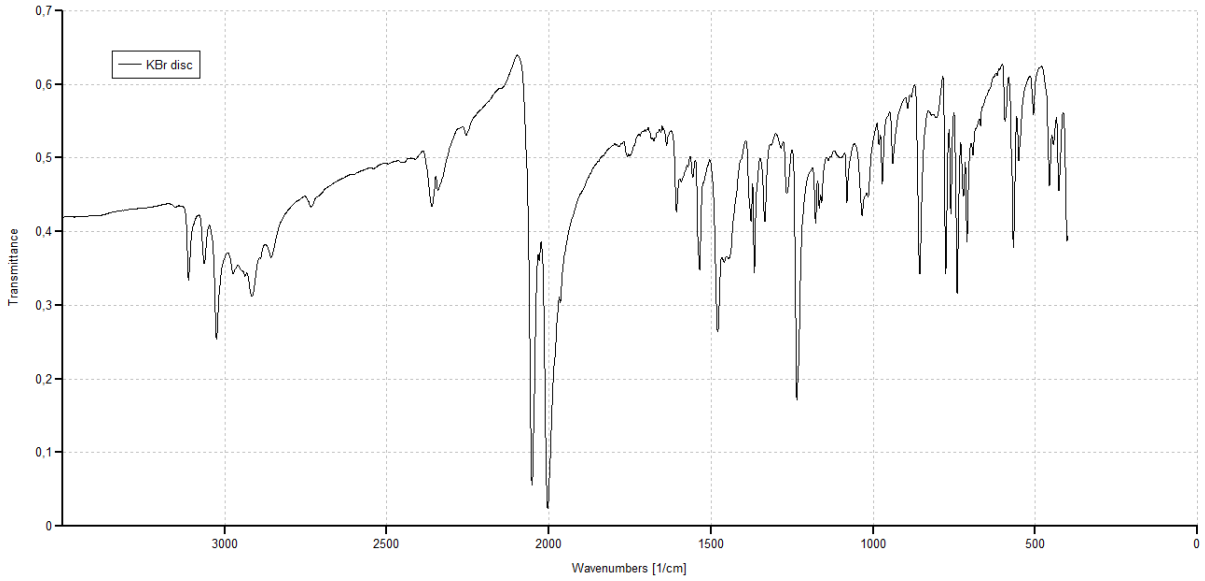


Figure S47 **IR spectrum of [Ni(17b)(CO)$_2$]** (KBr)

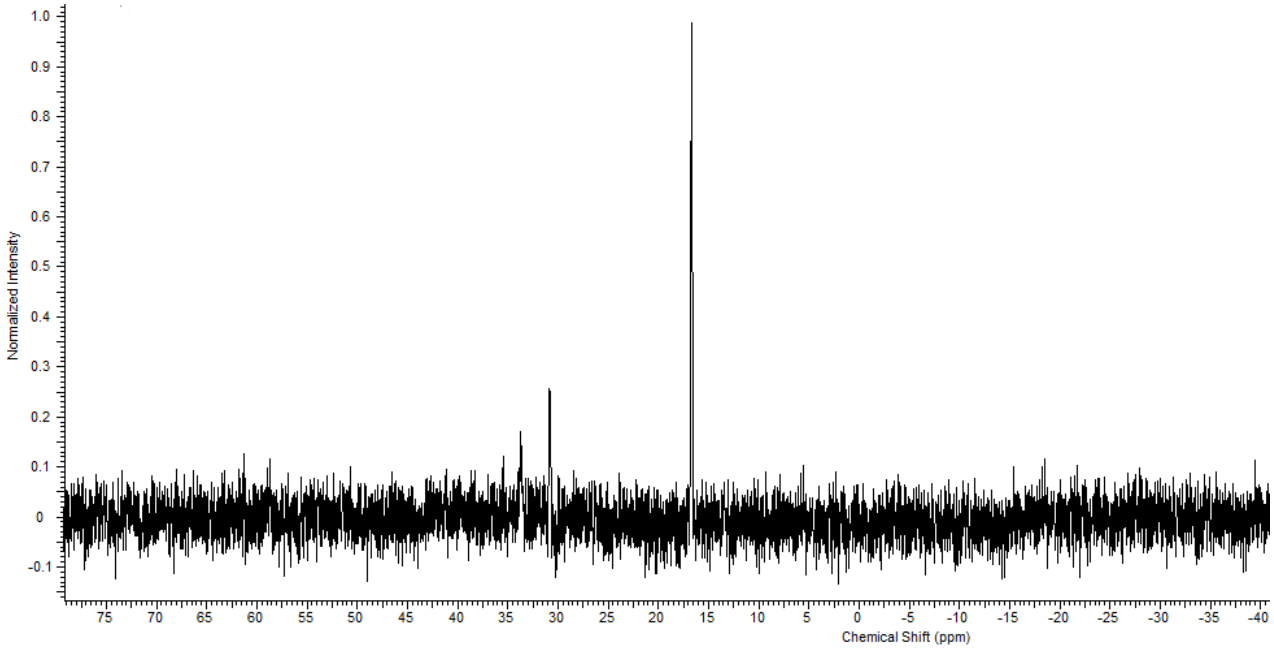


Figure S48 **^{31}P{^{1}H} NMR spectrum of [Ni(17c)(CO)$_2$]** (161 MHz, CD_2Cl_2, 297 K)

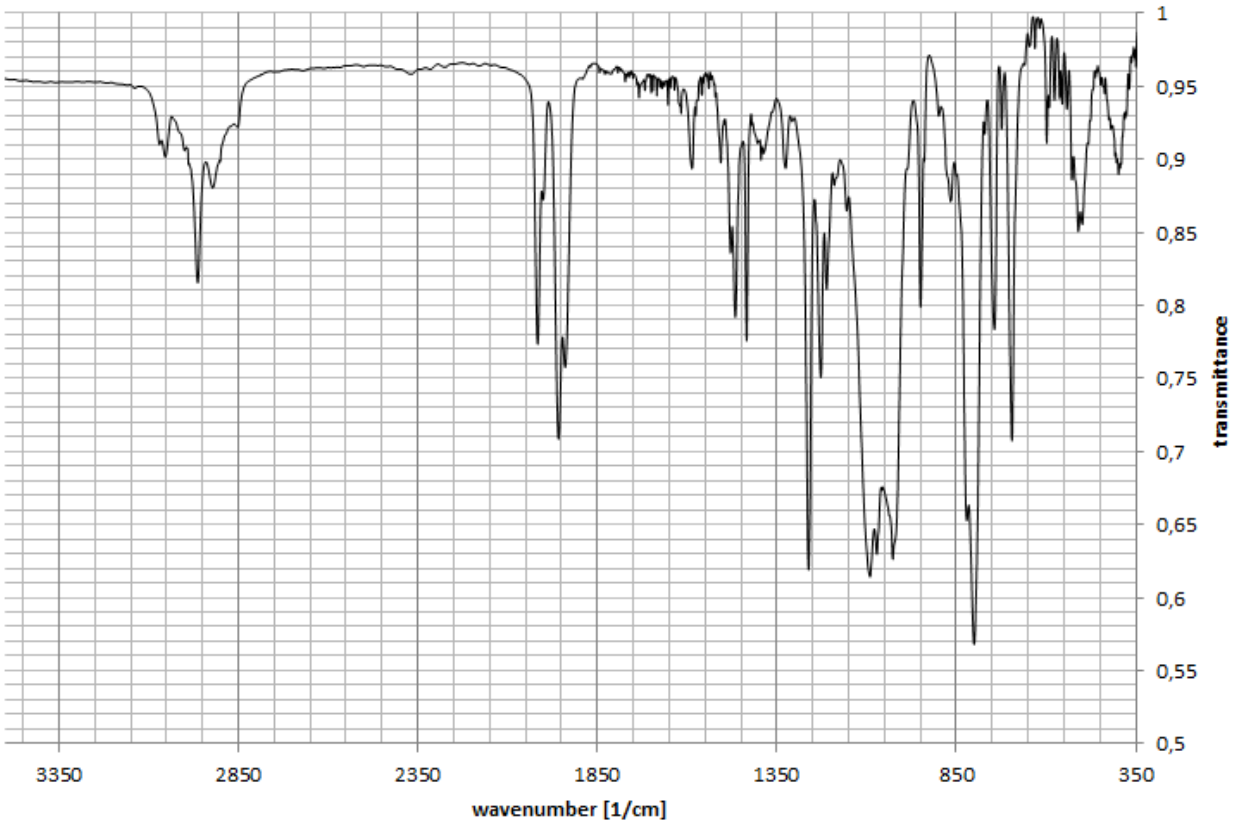


Figure S49 **IR spectrum of [Ni(17c)(CO)$_2$]** (KBr)

14- Palladium complexes

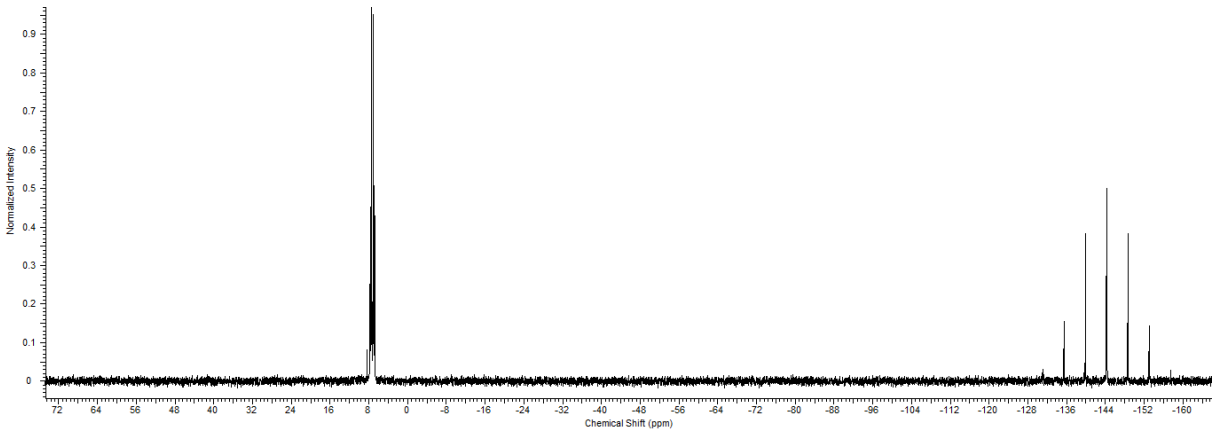


Figure S50 **^{31}P{^{1}H} NMR spectrum of [Pd(η^3-allyl)(14)]$^+$** (161 MHz, CD_2Cl_2, 297 K)

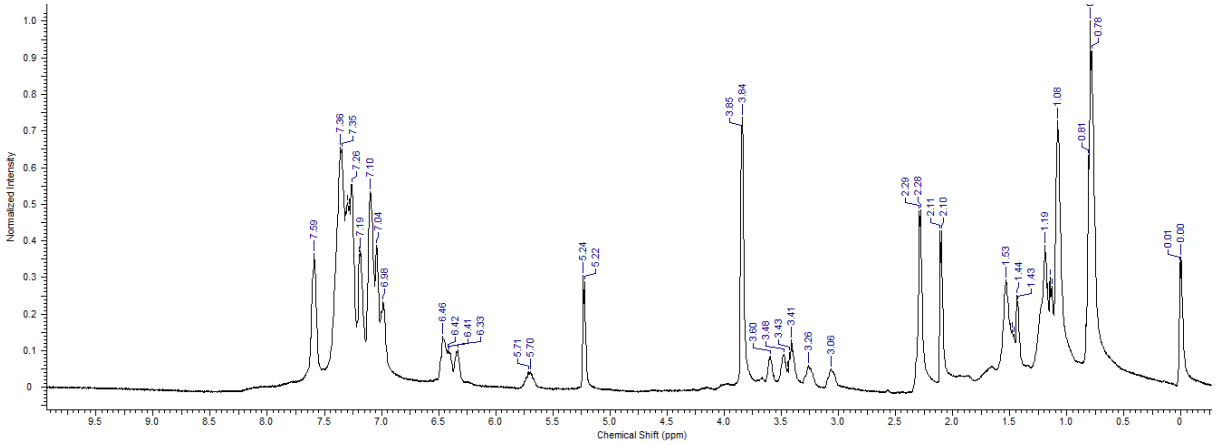


Figure S51 **^{1}H NMR spectrum of [Pd(η^3-allyl)(14)]$^+$** (400 MHz, CD_2Cl_2, 297 K)

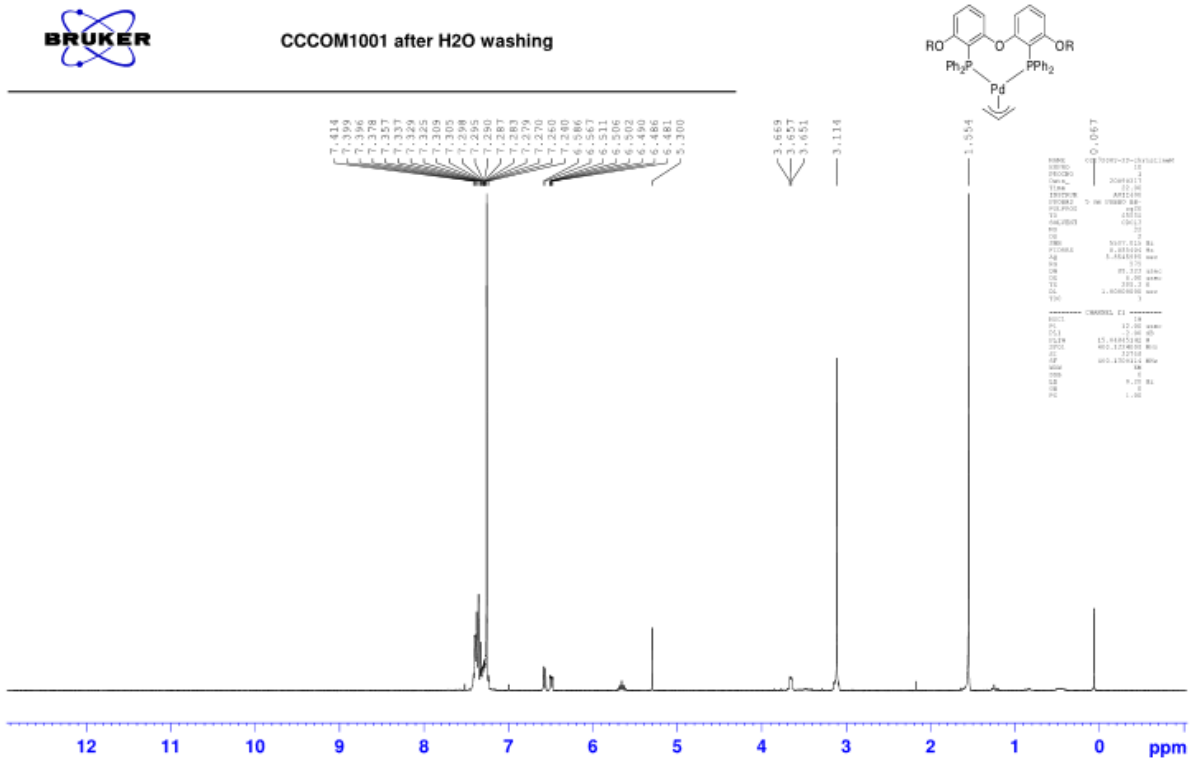


Figure S52 **^{1}H NMR spectrum of [Pd(η^3-allyl)(15)]$^+$** (500 MHz, CD_2Cl_2, 297 K)

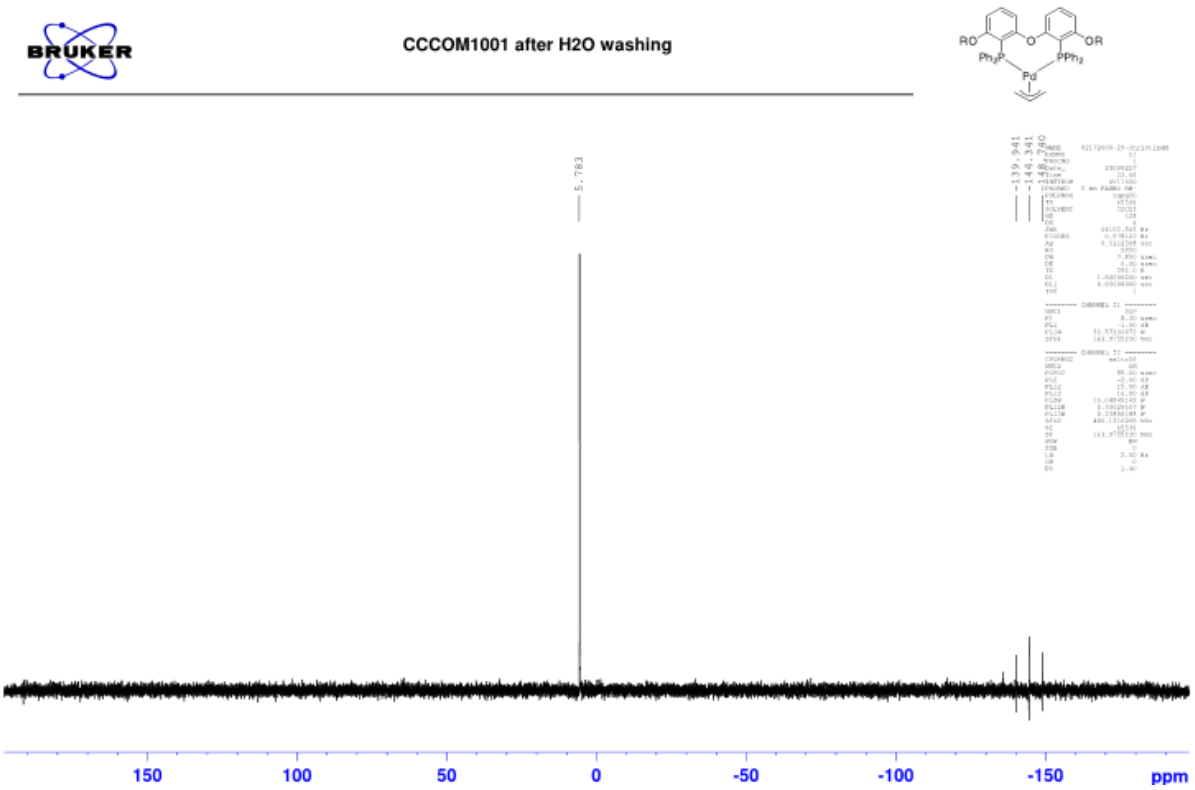


Figure S53 $^{31}P\{^{1}H\}$ NMR spectrum of **[Pd(η^3-allyl)(15)]$^+$** (202 MHz, CD_2Cl_2, 297 K)

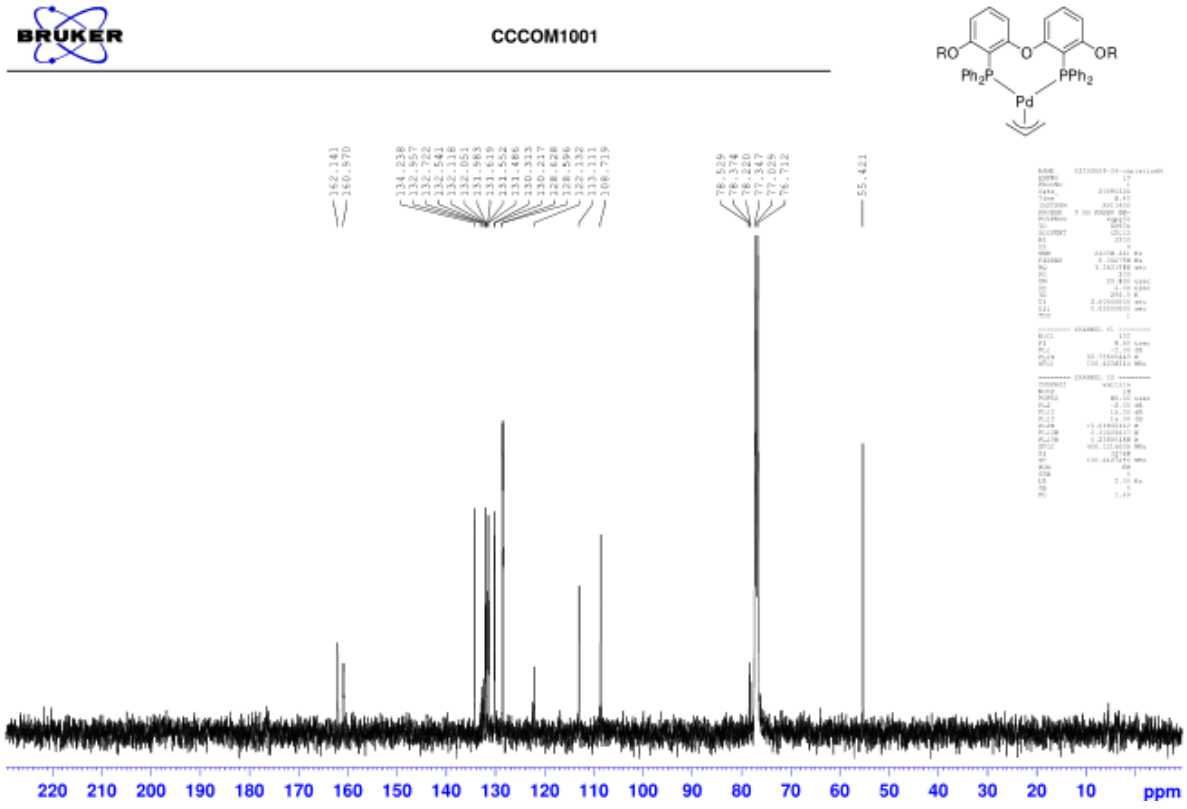


Figure S54 $^{13}C\{^{1}H\}$ NMR spectrum of **[Pd(η^3-allyl)(15)]$^+$** (100 MHz, CD_2Cl_2, 297 K)

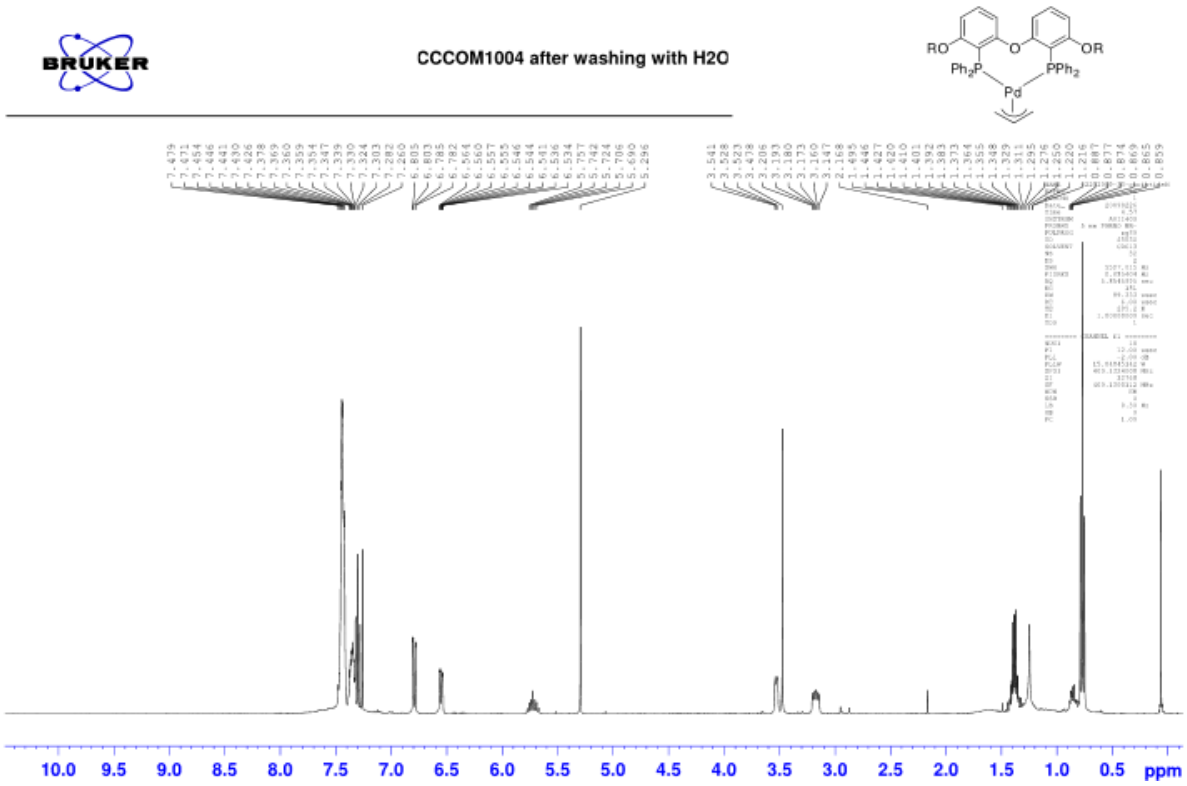


Figure S55 **^{1}H NMR spectrum of [Pd(η^3-allyl)(17a)]$^{+}$** (400 MHz, CD_2Cl_2, 297 K)

Figure S56 **^{31}P{^{1}H} NMR spectrum of [Pd(η^3-allyl)(17a)]$^{+}$** (161 MHz, CD_2Cl_2, 297 K)

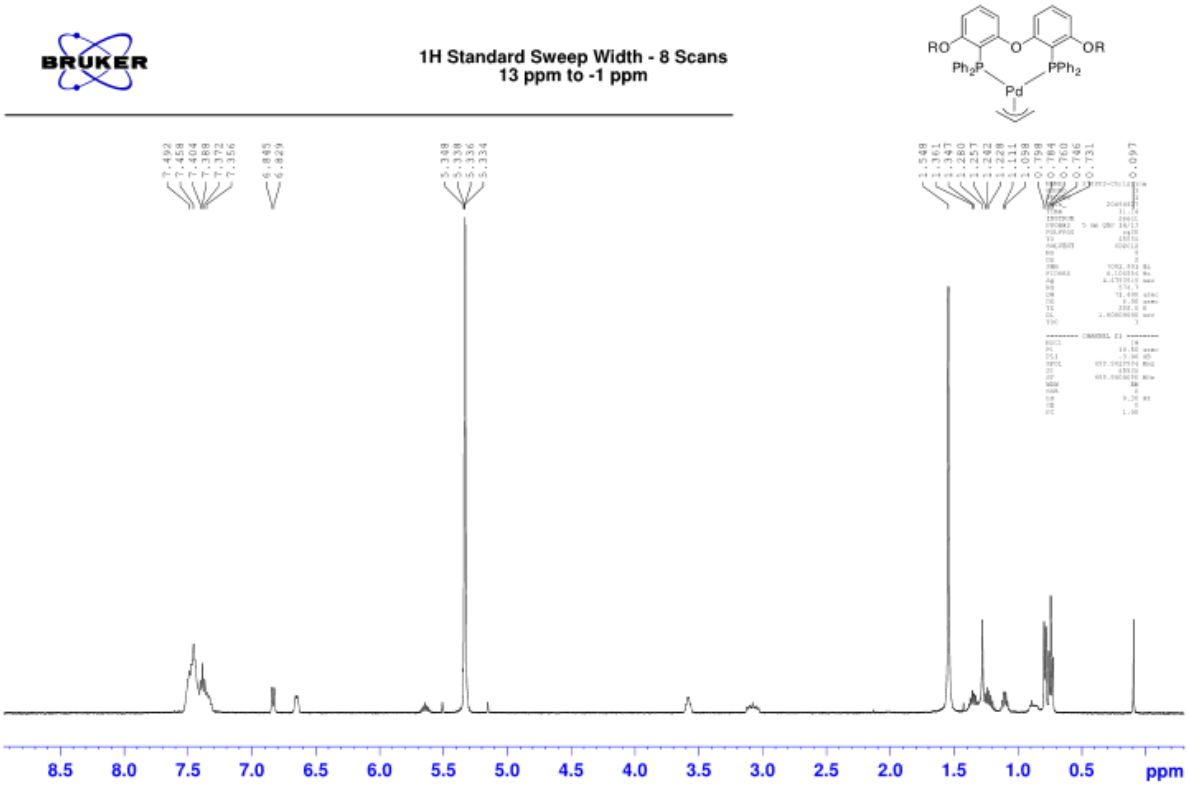


Figure S57 **^{1}H NMR spectrum of [Pd(η^3-allyl)(17b)]$^{+}$** (400 MHz, CD_2Cl_2, 297 K)

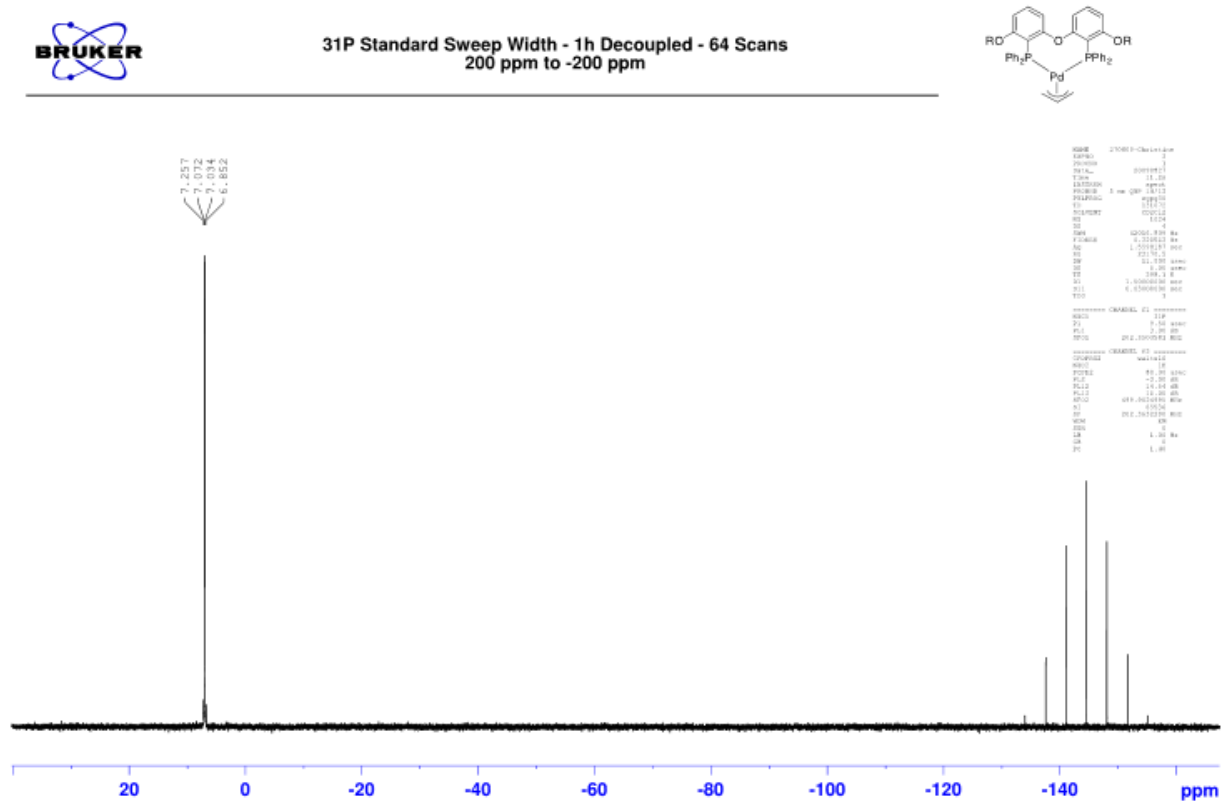


Figure S58 **^{31}P{^{1}H} NMR spectrum of [Pd(η^3-allyl)(17b)]$^{+}$** (161 MHz, CD_2Cl_2, 297 K)

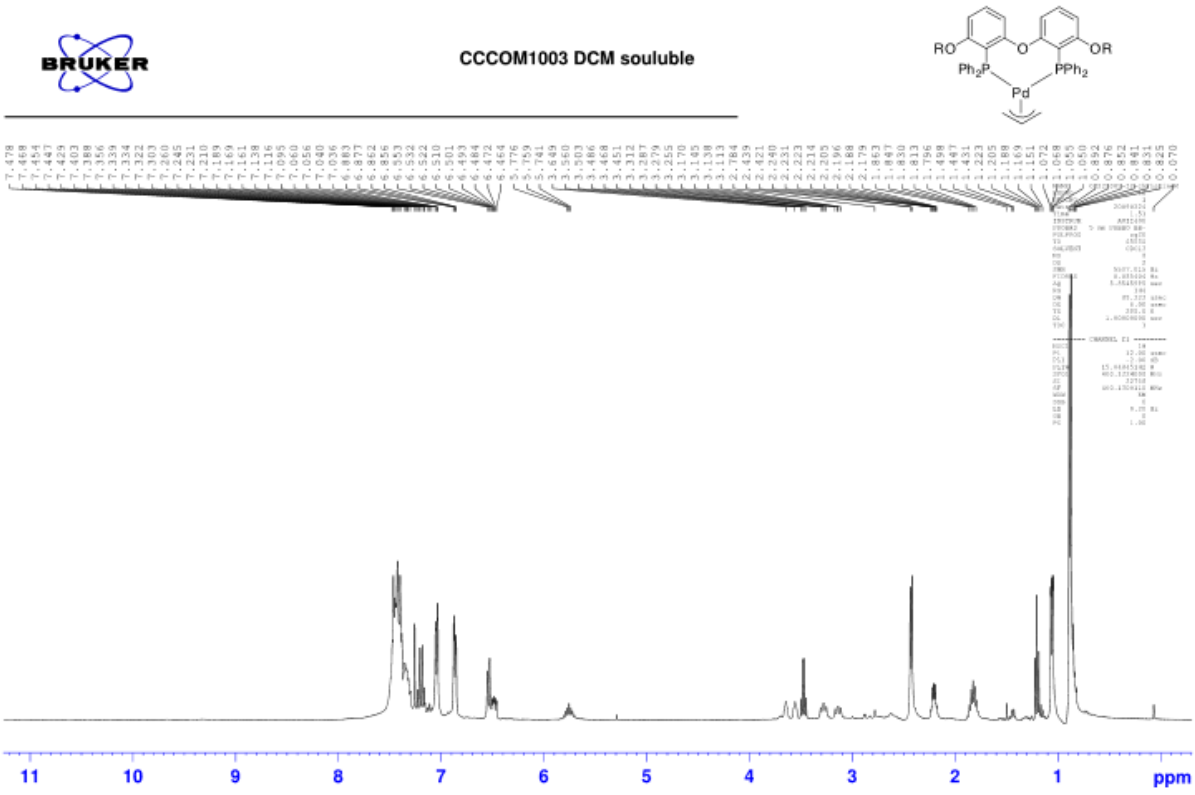


Figure S59 **^{1}H NMR spectrum of [Pd(η^3-allyl)(17c)]$^{+}$** (400 MHz, CD_2Cl_2, 297 K)

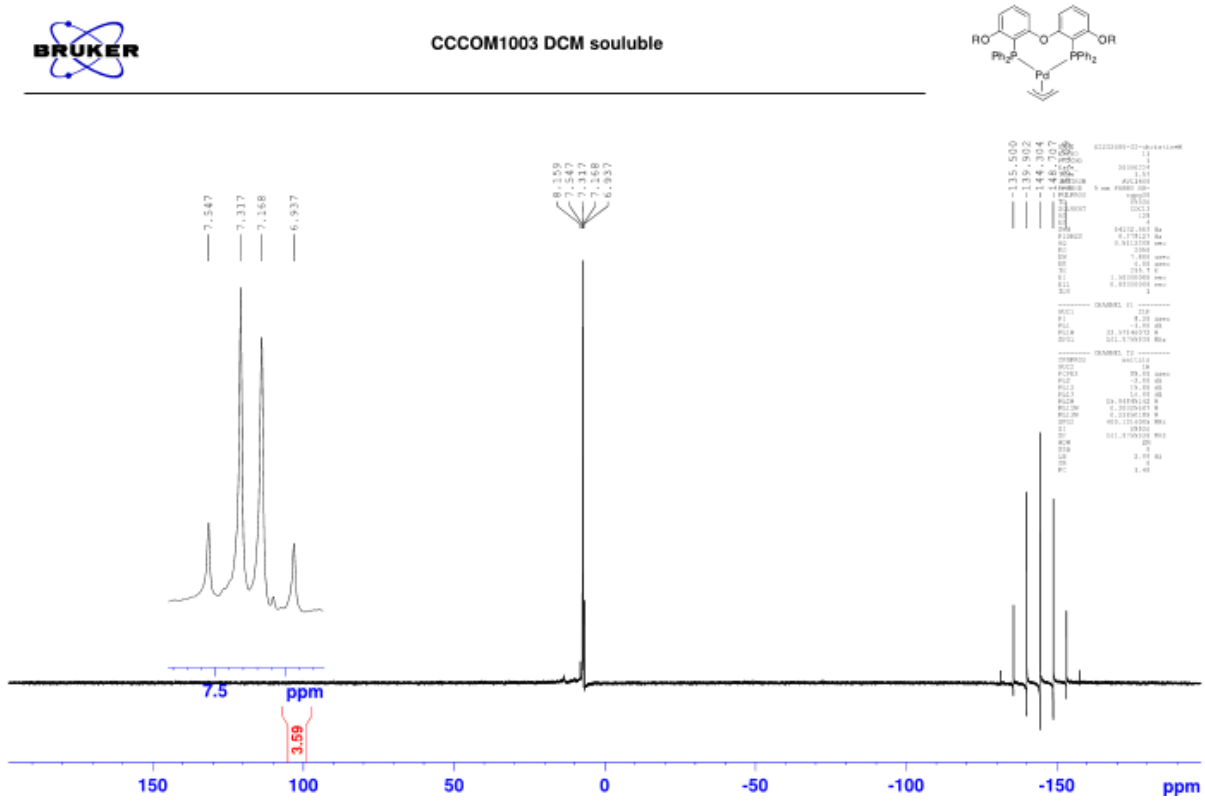


Figure S60 **^{31}P{^{1}H} NMR spectrum of [Pd(η^3-allyl)(17c)]$^{+}$** (161 MHz, CD_2Cl_2, 297 K)

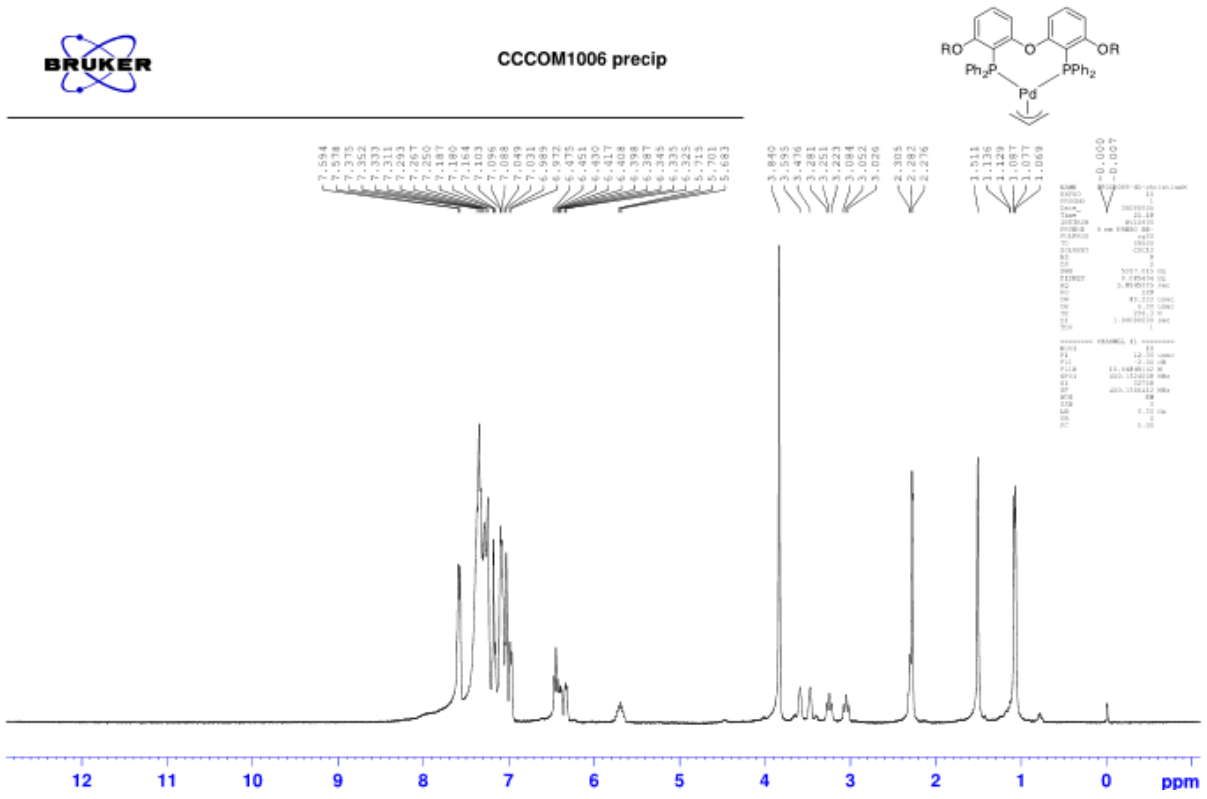


Figure S61 **^{1}H NMR spectrum of [Pd(η^3-allyl)(17d)]$^{+}$** (400 MHz, CD_2Cl_2, 297 K)

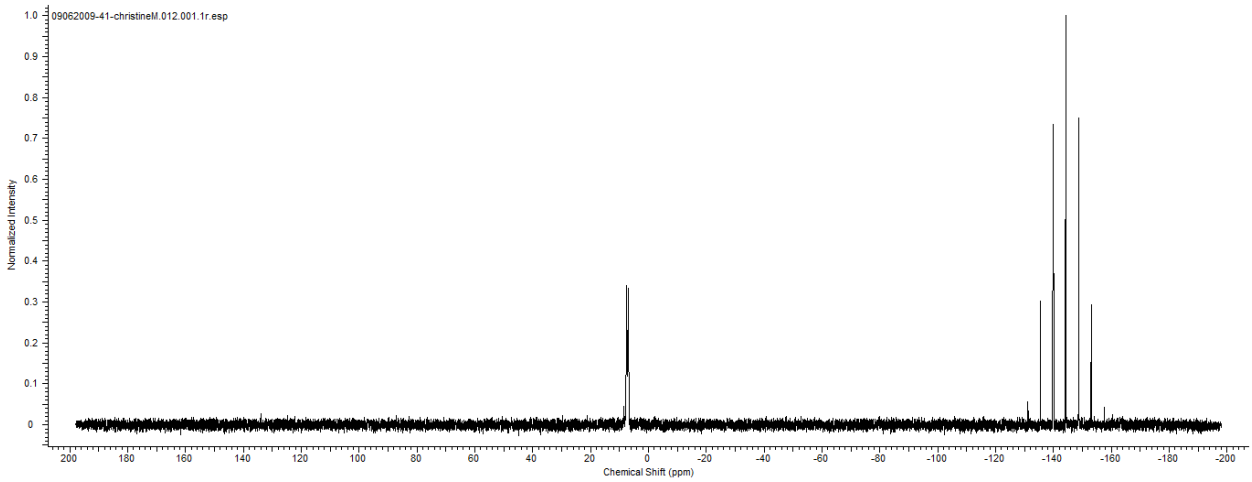


Figure S62 **^{31}P{^{1}H} NMR spectrum of [Pd(η^3-allyl)(17d)]$^{+}$** (161 MHz, CD_2Cl_2, 297 K)