

Supporting Information for:

Palladium and platinum complexes of tellurium-containing imidodiphosphate ligands: nucleophilic attack of

Li[(PⁱPr₂)(TePⁱPr₂)N] on coordinated 1,5-cyclooctadiene

Stuart D. Robertson, Jamie S. Ritch and Tristram Chivers*

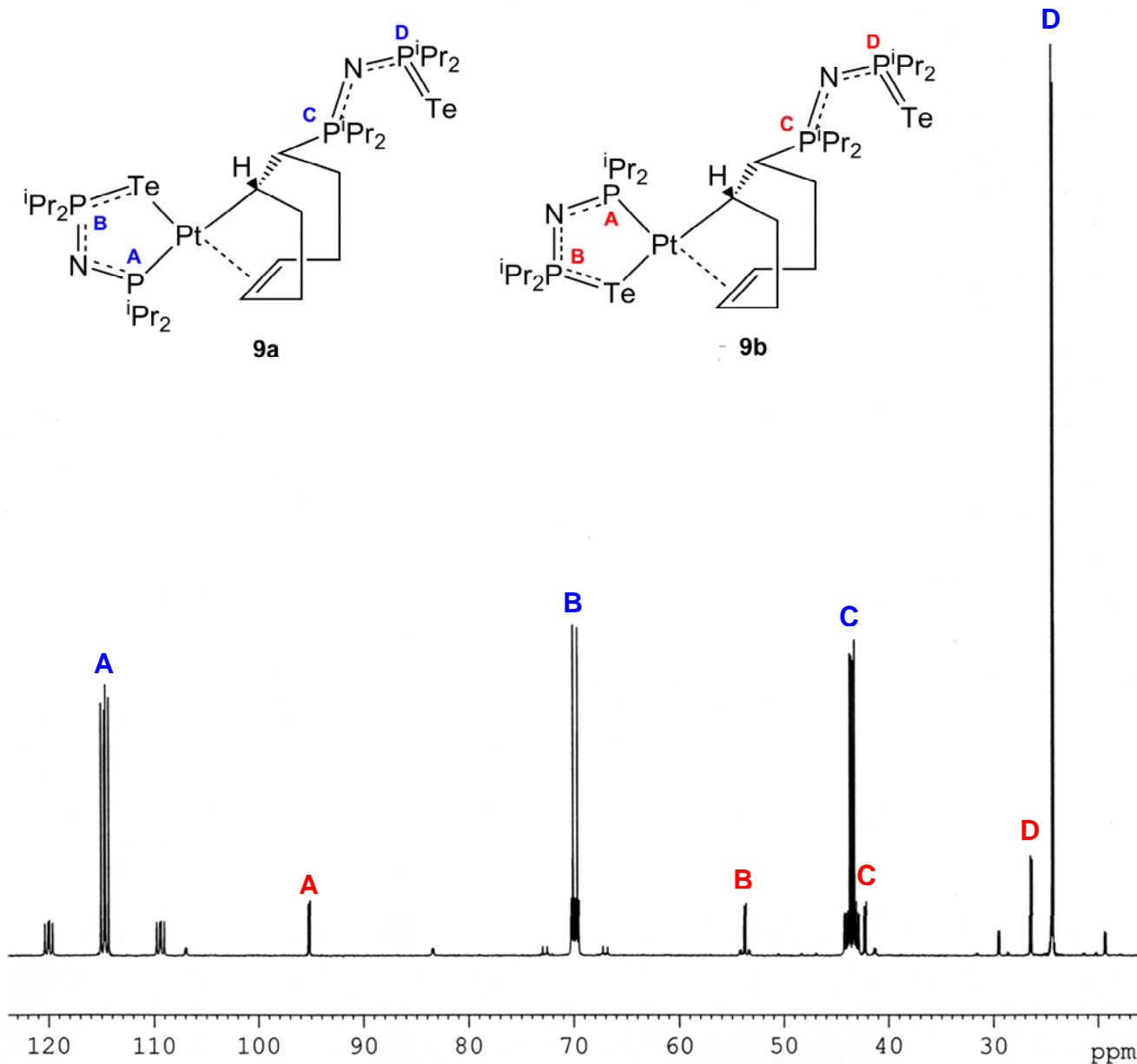
Department of Chemistry, University of Calgary, 2500 University Drive NW, Calgary, Alberta, Canada, T2N 1N4.

E-mail: chivers@ucalgary.ca; Fax: +1 403 289 9488; Tel: +1 403 220 5741

Contents:

Multinuclear NMR Spectra of Complexes **8** and **9**

³¹P NMR Spectrum (*d*₈-THF) of 9



Current Data Parameters
 NAME 90401jrl
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090401
 Time_ 13.01
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc30
 TD 32768
 SOLVENT D2O
 NS 326
 DS 0
 SWH 48661.801 Hz
 FIDRES 1.485040 Hz
 AQ 0.3367412 sec
 RG 4597.6
 DW 10.275 usec
 DE 14.68 usec
 TE 296.8 K
 D1 1.0000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

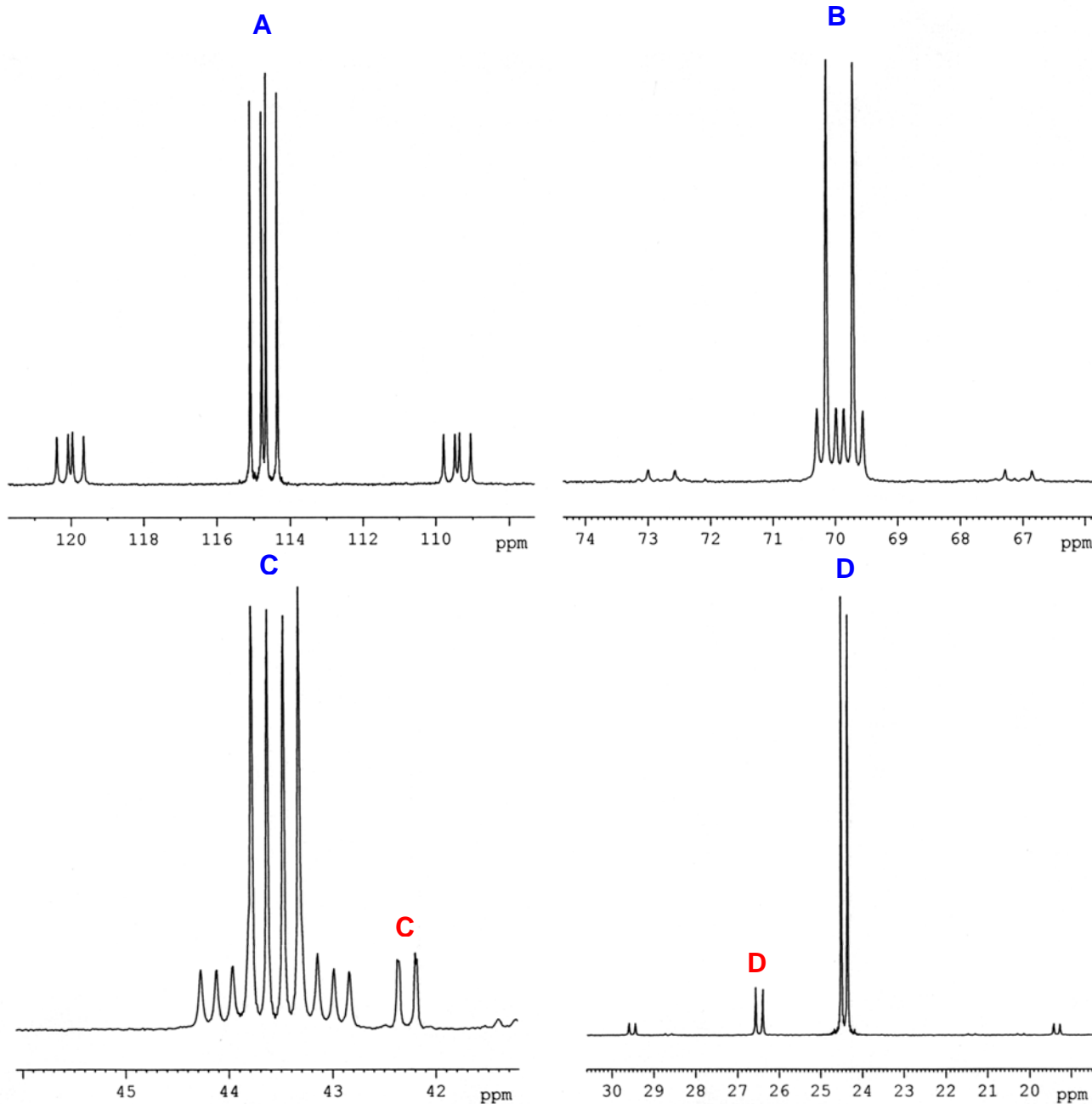
===== CHANNEL f1 =====
 NUC1 31P
 P1 6.60 usec
 PL1 -2.00 dB
 SFO1 161.7102994 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SFO2 399.4572000 MHz

F2 - Processing parameters
 SI 32768
 SF 161.7022045 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.97 cm
 F1P 130.000 ppm
 F1 21021.29 Hz
 F2P 10.000 ppm
 F2 1617.02 Hz
 PPMCM 6.00000 ppm/cm
 HZCM 970.21320 Hz/cm

Selected Expansions of the ^{31}P NMR Spectrum (d_8 -THF) of **9**



Current Data Parameters

NAME 90401jrl
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20090401
Time_ 13.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 32768
SOLVENT D2O
NS 326
DS 0
SWH 48661.801 Hz
FIDRES 1.485040 Hz
AQ 0.3367412 sec
RG 4597.6
DW 10.275 usec
DE 14.68 usec
TE 296.8 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====

NUC1 31P
P1 6.60 usec
PL1 -2.00 dB
SFO1 161.7102994 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 399.4572000 MHz

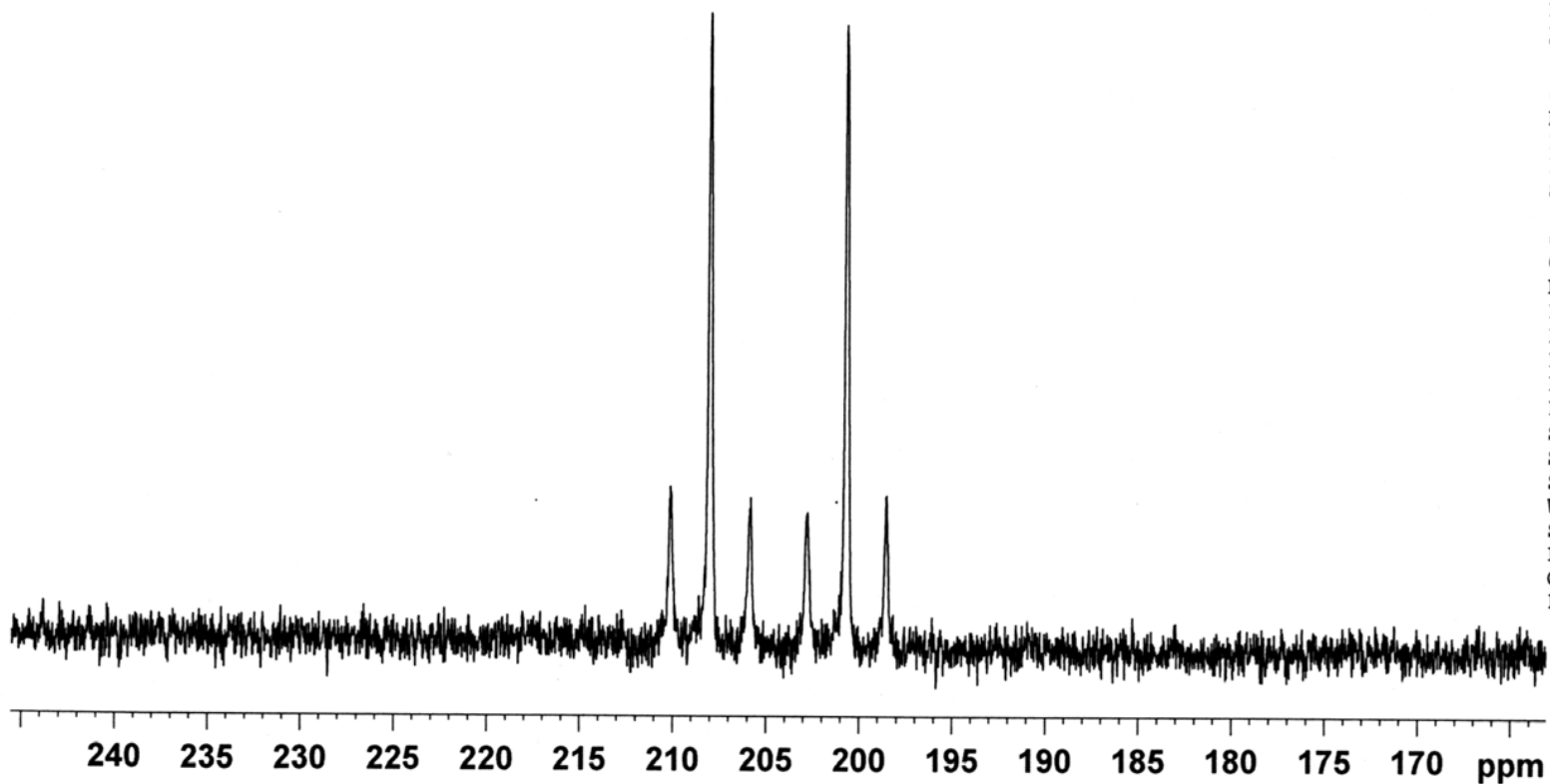
F2 - Processing parameters

SI 32768
SF 161.7022045 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 130.000 ppm
F1 21021.29 Hz
F2P 10.000 ppm
F2 1617.02 Hz
PPMCM 6.00000 ppm/cm
HZCM 970.21320 Hz/cm

¹²⁵Te NMR Spectrum (*d*₈-THF) of 9 (first window)

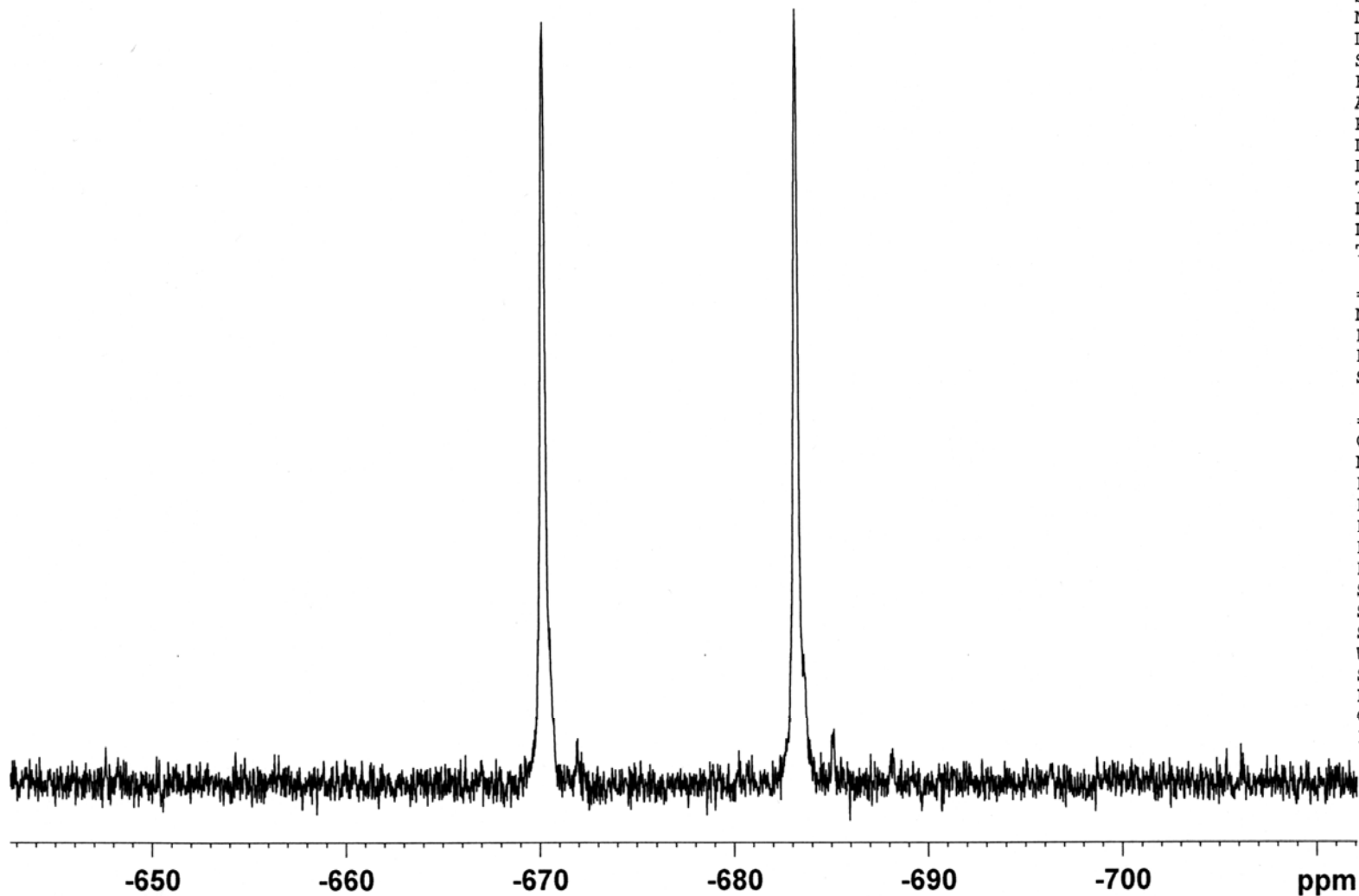


```
NAME          90313jrl
EXPNO         2
PROCNO       1
Date_        20090313
Time         20.14
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zgdc30
TD          32768
SOLVENT      THF
NS          36053
DS           4
SWH         75187.969 Hz
FIDRES      2.294555 Hz
AQ          0.2179572 sec
RG          32768
DW          6.650 usec
DE          50.00 usec
TE          298.5 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0         1
```

```
===== CHANNEL f1 =====
NUC1          125Te
P1            5.50 usec
PL1           3.00 dB
SFO1          126.2748044 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           0.00 dB
PL12          15.00 dB
PL2W          15.07131863 W
PL12W         0.47659695 W
SFO2          400.1816007 MHz
SI            32768
SF            126.2557224 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

¹²⁵Te NMR Spectrum (*d*₈-THF) of 9 (second window)

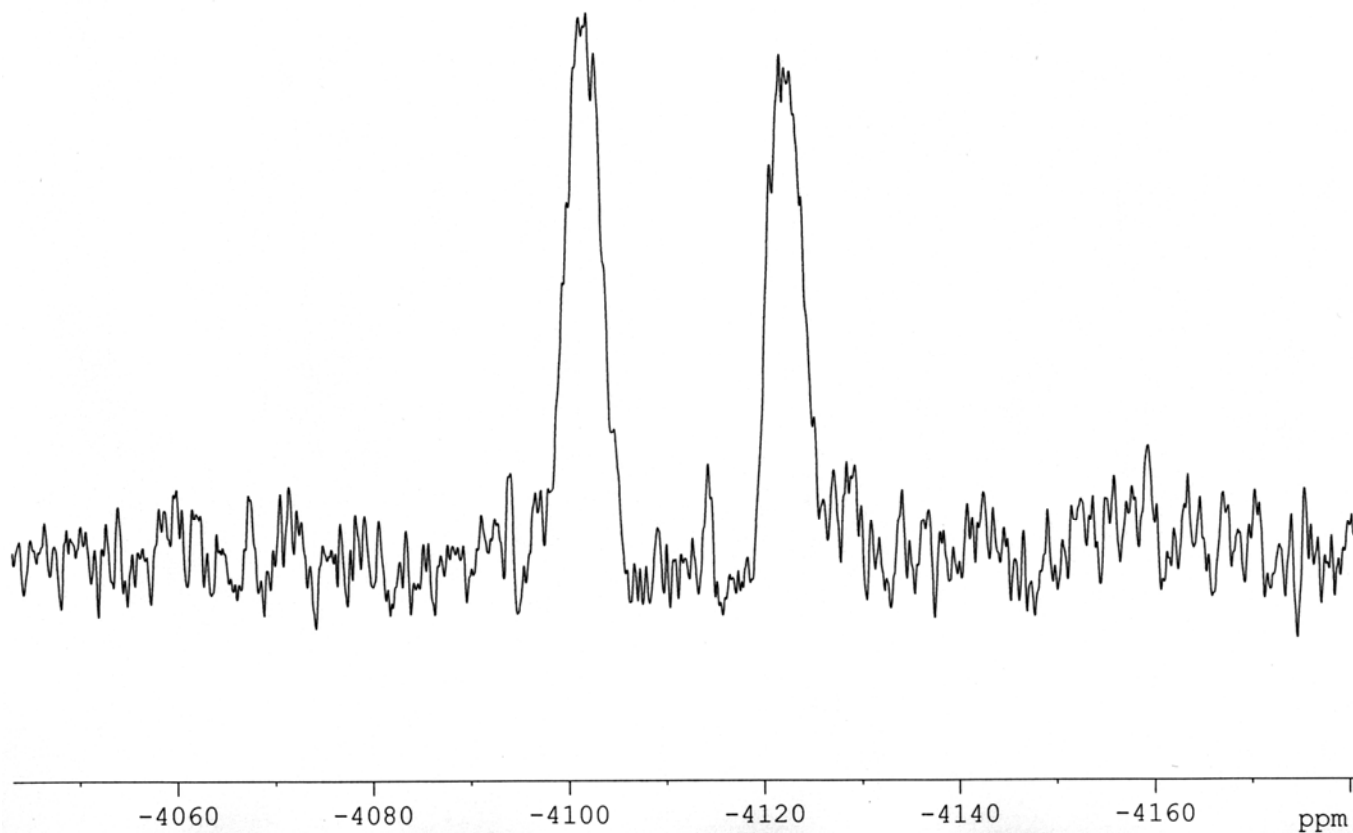


NAME 90316jr2
EXPNO 3
PROCNO 1
Date_ 20090316
Time_ 19.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 32768
SOLVENT THF
NS 36414
DS 4
SWH 75187.969 Hz
FIDRES 2.294555 Hz
AQ 0.2179572 sec
RG 32768
DW 6.650 usec
DE 50.00 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 125Te
P1 5.50 usec
PL1 3.00 dB
SFO1 126.2003134 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 15.07131863 W
PL12W 0.47659695 W
SFO2 400.1816007 MHz
SI 32768
SF 126.2557224 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{195}Pt NMR Spectrum (d_8 -THF) of 9



Current Data Parameters
NAME 81003jrl
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date 20081005
Time 4.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT THF
NS 17000
DS 2
SWH 70422.539 Hz
FIDRES 2.149125 Hz
AQ 0.2327028 sec
RG 32768
DW 7.100 usec
DE 50.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 195Pt
P1 9.30 usec
PL1 -2.00 dB
SFO1 85.4920237 MHz

F2 - Processing parameters
SI 32768
SF 85.8710429 MHz
WDW EM
SSB 0
LB 30.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P -599.724 ppm
F1 -51498.96 Hz
F2P -1800.275 ppm
F2 -154591.52 Hz
PPMCM 60.02755 ppm/
HZCM 5154.62793 Hz/c

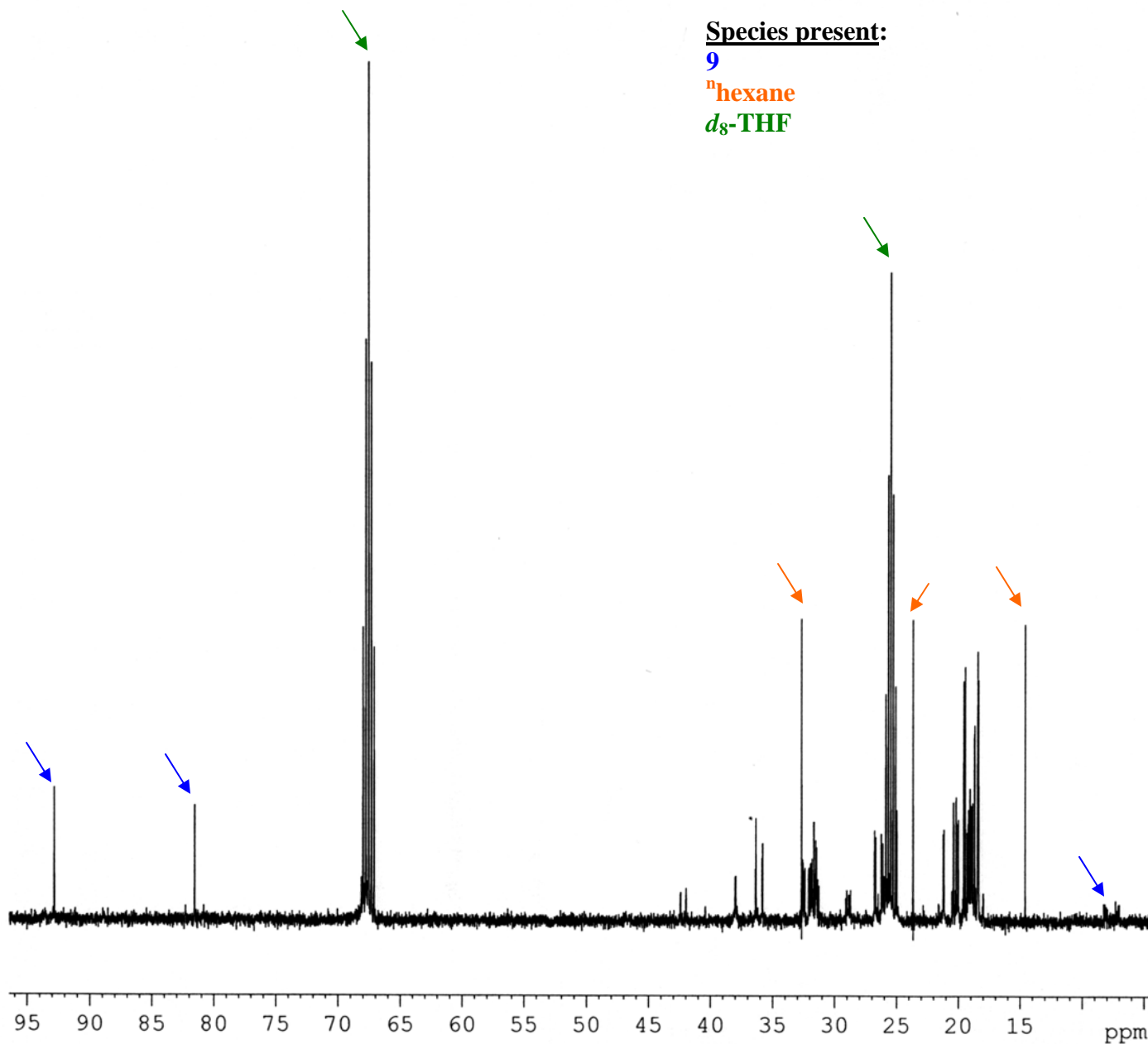
¹³C NMR Spectrum (*d*₈-THF) of 9

Species present:

9

ⁿhexane

*d*₈-THF



Current Data Parameters
NAME 90401jr1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090401
Time_ 13.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 32768
SOLVENT CDC13
NS 2150
DS 2
SWH 27662.518 Hz
FIDRES 0.844193 Hz
AQ 0.5923316 sec
RG 32768
DW 18.075 usec
DE 50.00 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
SFO1 100.4530843 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 17.80 dB
SFO2 399.4572000 MHz

F2 - Processing parameters
SI 32768
SF 100.4429251 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P 100.000 ppm
F1 10044.29 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 5.00000 ppm/cm
HZCM 502.21463 Hz/cm

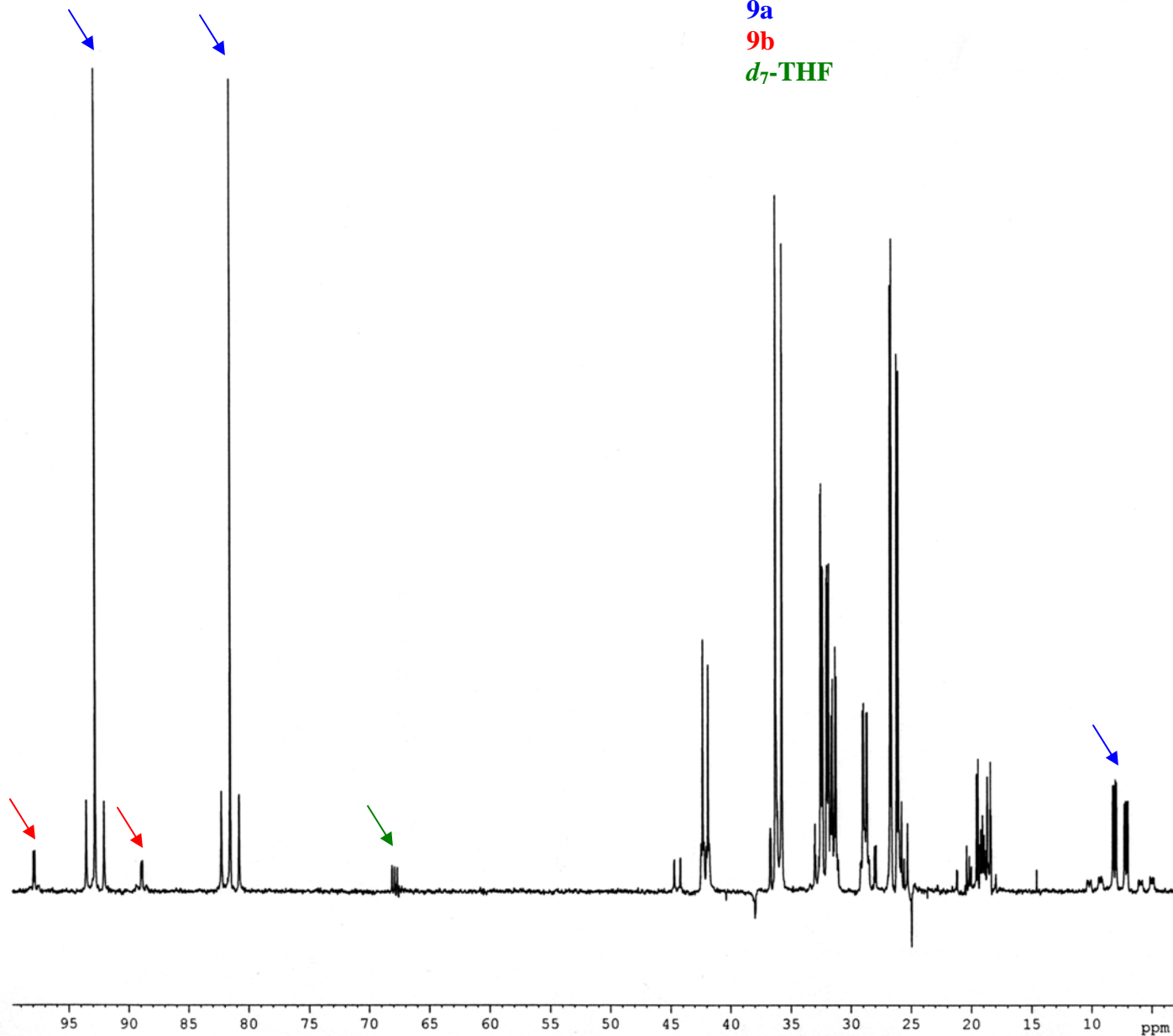
DEPT-90 NMR Spectrum (d_8 -THF) of 9

Species present:

9a

9b

d_7 -THF



Current Data Parameters
NAME 90401jr1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090401
Time_ 15.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept90
TD 32768
SOLVENT CDCl3
NS 37411
DS 0
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 32768
DW 19.900 usec
DE 29.00 usec
TE 296.9 K
CNST2 145.0000000
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000993 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

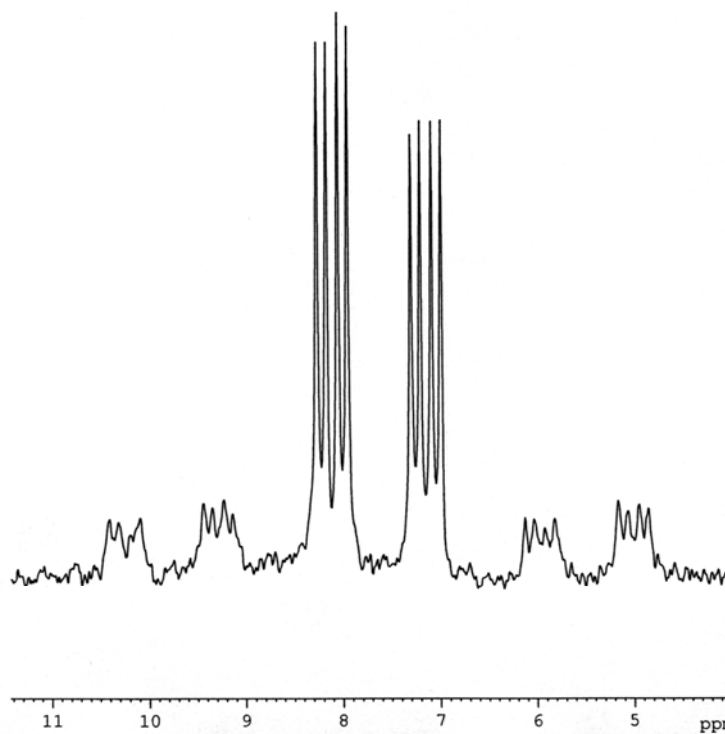
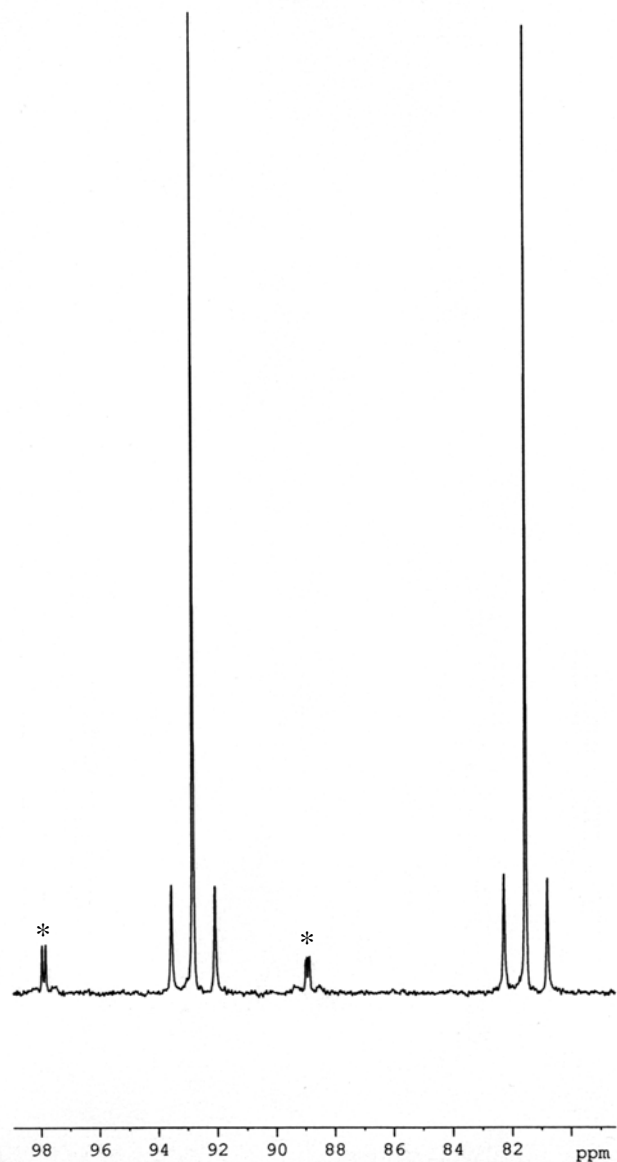
==== CHANNEL f1 =====
NUC1 13C
P1 7.80 usec
p2 15.60 usec
PL1 -2.00 dB
SFO1 100.4546033 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.50 usec
p4 19.00 usec
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.00 dB
SFO2 399.4572000 MHz

F2 - Processing parameters
SI 32768
SF 100.4429261 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 15.822 ppm
F1 1589.17 Hz
F2P 1.877 ppm
F2 188.53 Hz
PPMCM 0.69723 ppm/c
HZCM 70.03214 Hz/cm

Selected Expansions of the DEPT-90 NMR Spectrum (d_8 -THF) of 9a (asterisks denote 9b)



```
Current Data Parameters
NAME          90401jr1
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20090401
Time_         15.10
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       dept90
TD            32768
SOLVENT       CDC13
NS            37411
DS            0
SWH           25125.629 Hz
FIDRES        0.766773 Hz
AQ            0.6521332 sec
RG            32768
DW            19.900 usec
DE            29.00 usec
TE            296.9 K
CNST2         145.0000000
D1            1.00000000 sec
d2            0.00344828 sec
d12           0.00002000 sec
DELTA         0.00000993 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

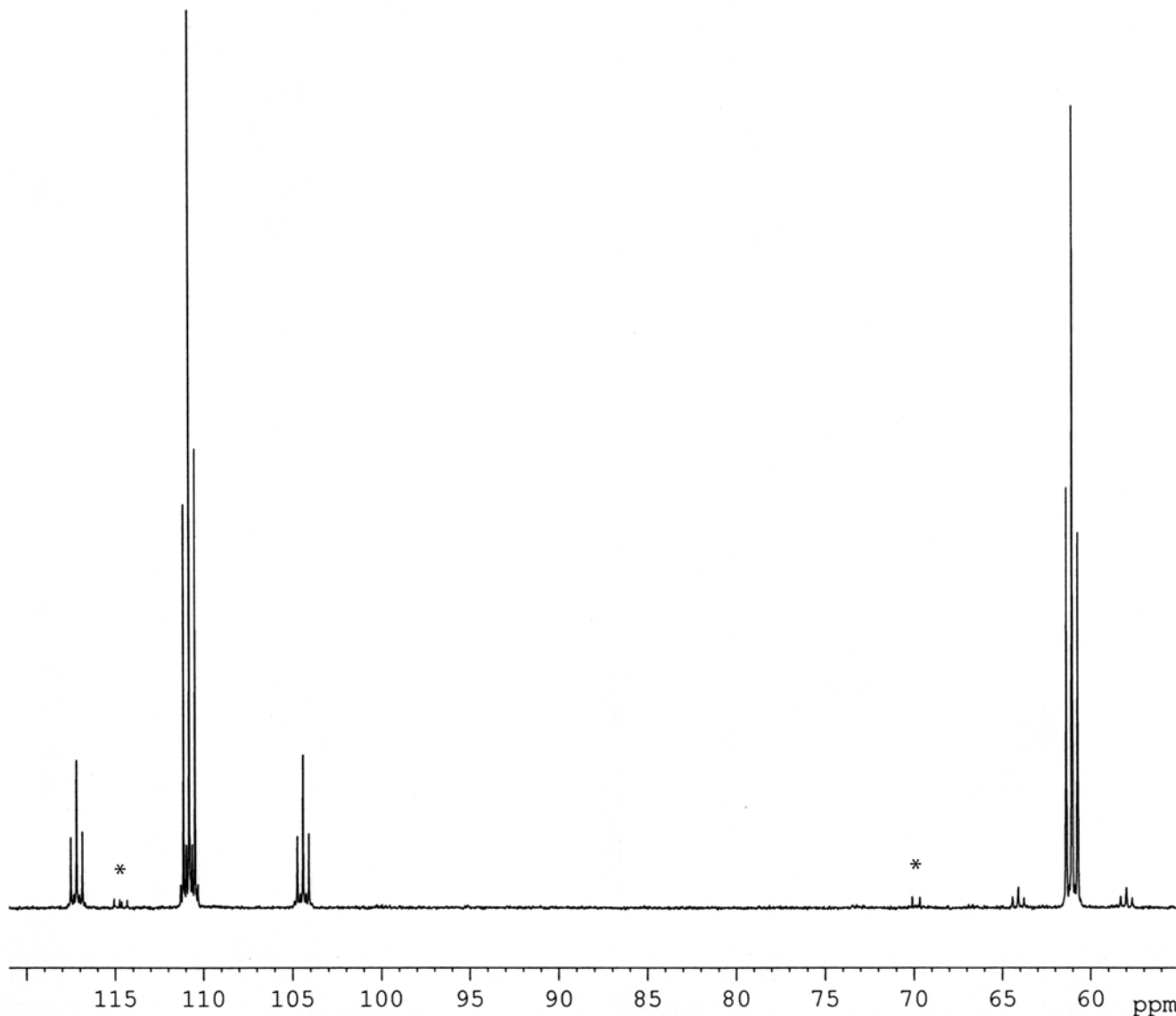
===== CHANNEL f1 =====
NUC1          13C
P1            7.80 usec
p2            15.60 usec
PL1           -2.00 dB
SFO1          100.4546033 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            9.50 usec
p4            19.00 usec
PCPD2         80.00 usec
PL2           -2.00 dB
PL12          18.00 dB
SFO2          399.4572000 MHz

F2 - Processing parameters
SI            32768
SF            100.4429261 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40

1D NMR plot parameters
CX            20.00 cm
F1P           15.822 ppm
F1            1589.17 Hz
F2P           1.877 ppm
F2            188.53 Hz
PPMCM         0.69723 ppm/c
HZCM          70.03214 Hz/cm
```

³¹P NMR Spectrum (*d*₈-THF) of *trans*-8 (asterisks denote 9a as a minor impurity)



Current Data Parameters
NAME 81003jr1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20081003
Time 10.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 32768
SOLVENT D2O
NS 1007
DS 0
SWH 48661.801 Hz
FIDRES 1.485040 Hz
AQ 0.3367412 sec
RG 8192
DW 10.275 usec
DE 14.68 usec
TE 298.0 K
D1 1.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

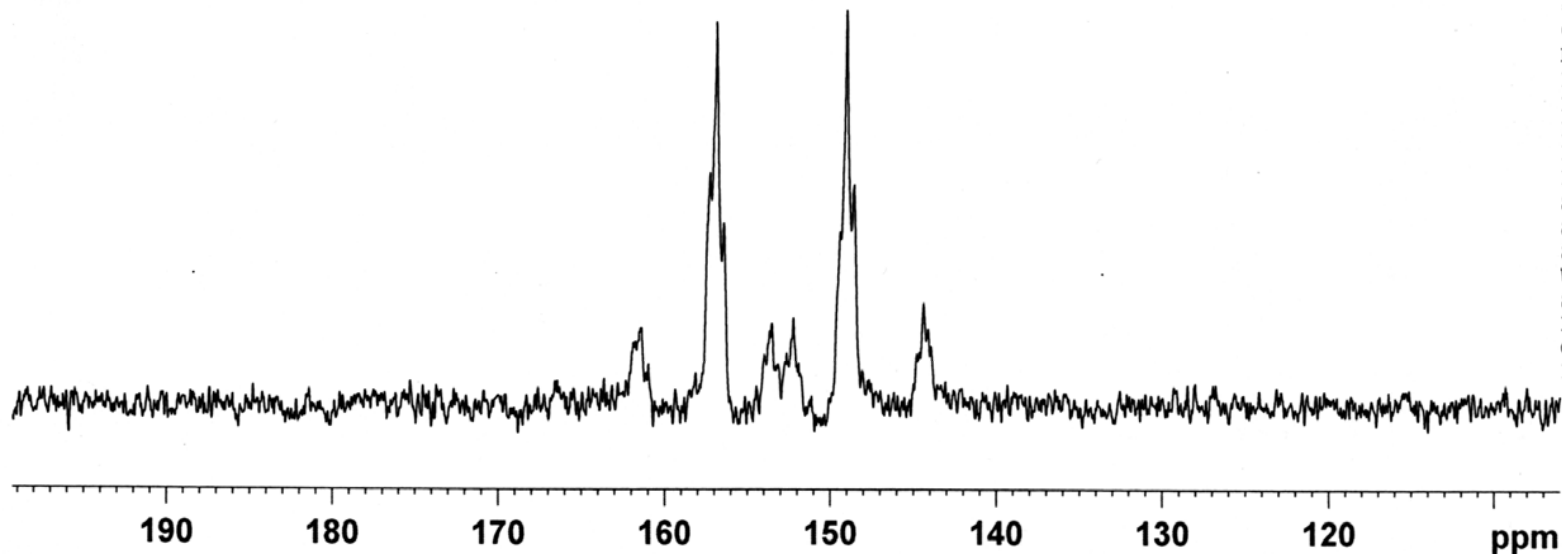
===== CHANNEL f1 =====
NUC1 31P
P1 6.60 usec
PL1 -2.00 dB
SFO1 161.7102994 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 18.00 dB
SFO2 399.4572000 MHz

F2 - Processing parameters
SI 32768
SF 161.7022045 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.99 cm
F1P 130.000 ppm
F1 21021.29 Hz
F2P 20.000 ppm
F2 3234.04 Hz
PPMCM 5.50000 ppm/cm
HZCM 889.36212 Hz/cm

¹²⁵Te NMR Spectrum (*d*₈-THF) of *trans*-8



NAME 81216jr1
EXPNO 3
PROCNO 1
Date_ 20081216
Time 19.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 32768
SOLVENT THF
NS 35000
DS 4
SWH 75187.969 Hz
FIDRES 2.294555 Hz
AQ 0.2179572 sec
RG 32768
DW 6.650 usec
DE 50.00 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 125Te
P1 5.50 usec
PL1 3.00 dB
SFO1 126.2748044 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 15.07131863 W
PL12W 0.47659695 W
SFO2 400.1816007 MHz
SI 32768
SF 126.2557224 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 1.40

¹⁹⁵Pt NMR Spectrum (*d*₈-THF) of *trans*-8

