Supporting Information

Mono(boratabenzene) rare-earth metal dialkyl complexes: synthesis, structure and catalytic behaviors for styrene polymerization

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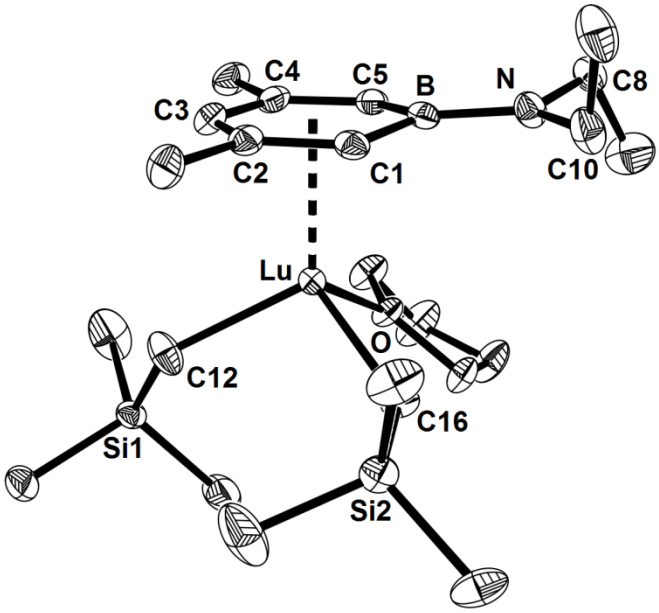


Fig. S1 Molecular structure of **2** with thermal ellipsoids set at 30% probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (◦): Lu–B 2.819(3), Lu–C1 2.663(3), Lu–C2 2.657(3), Lu–C3 2.655(3), Lu–C4 2.703(3), Lu–C5 2.712(3), Lu–C12 2.317(3), Lu–C16 2.323(3), Lu–O 2.248(2), B–N 1.436(4), B–N–C8 123.0(3), B–N–C10 122.0(3), C8–N–C10 114.7(3).

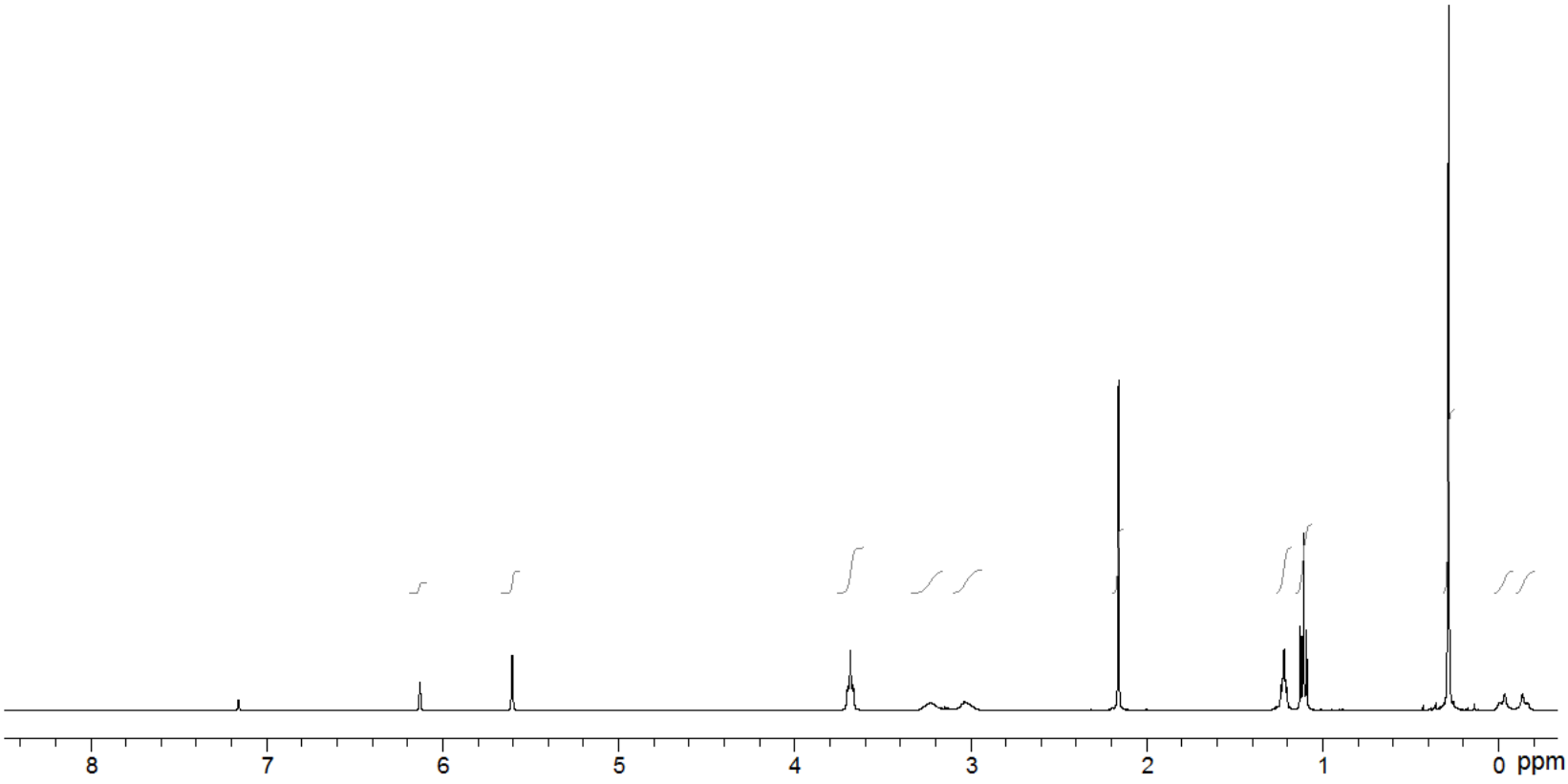


Fig. S2 ^{1}H NMR spectrum of **1** (400 MHz, C_6D_6, 25 ^{o}C).

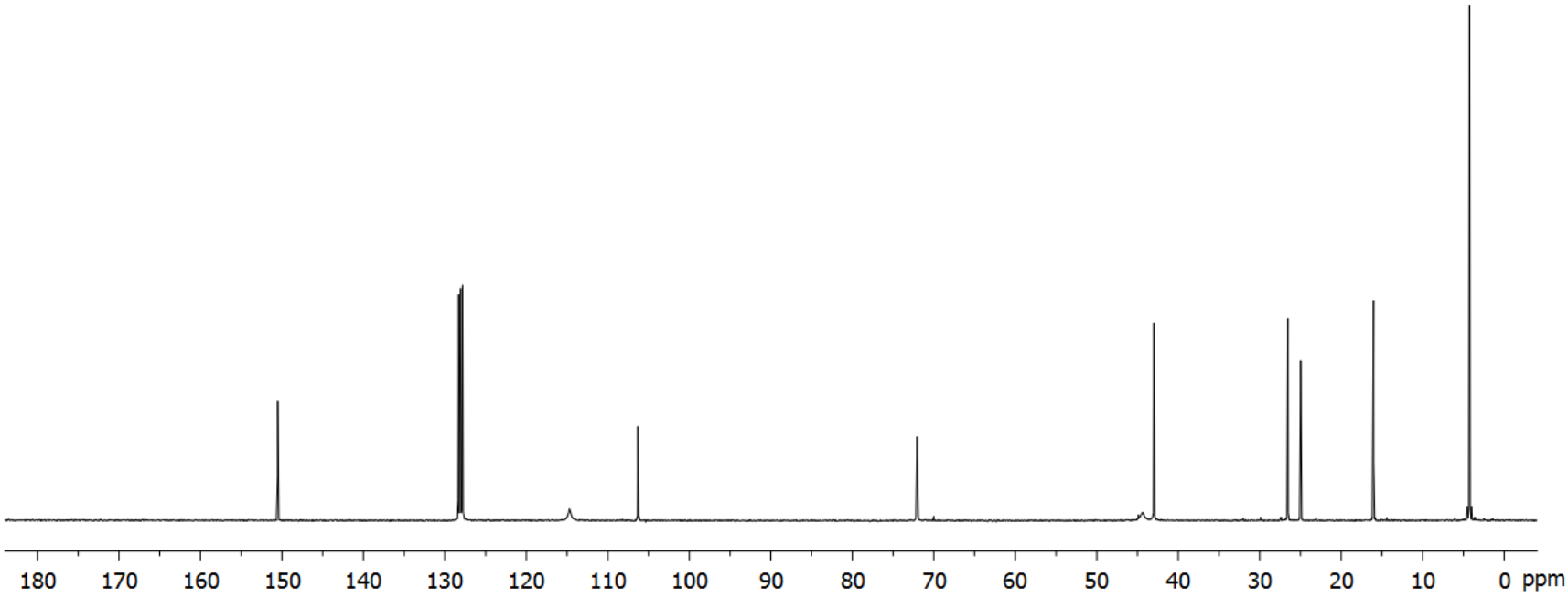
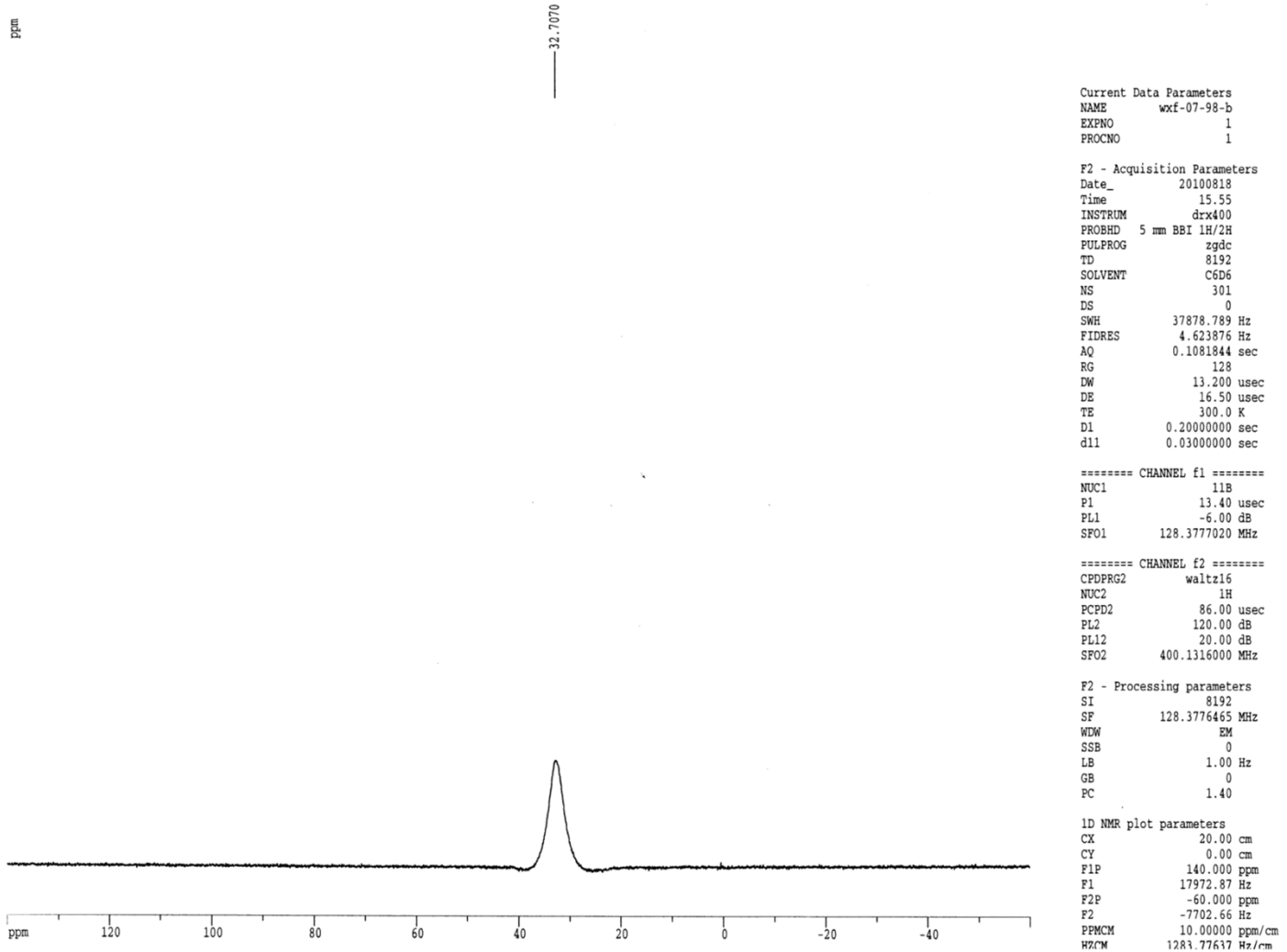


Fig. S3 ^{13}C NMR spectrum of **1** (100 MHz, C_6D_6, 25 ^{o}C).

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DE              16.50 usec
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P1                13.40 usec
PL1               -6.00 dB
SFO1        128.3777020 MHz

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NUC2                  1H
PCPD2              86.00 usec
PL2               120.00 dB
PL12               20.00 dB
SFO2        400.1316000 MHz

F2 - Processing parameters
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Fig. S4 ^{11}B NMR spectrum of **1** (128 MHz, C_6D_6, 25 ^{o}C).

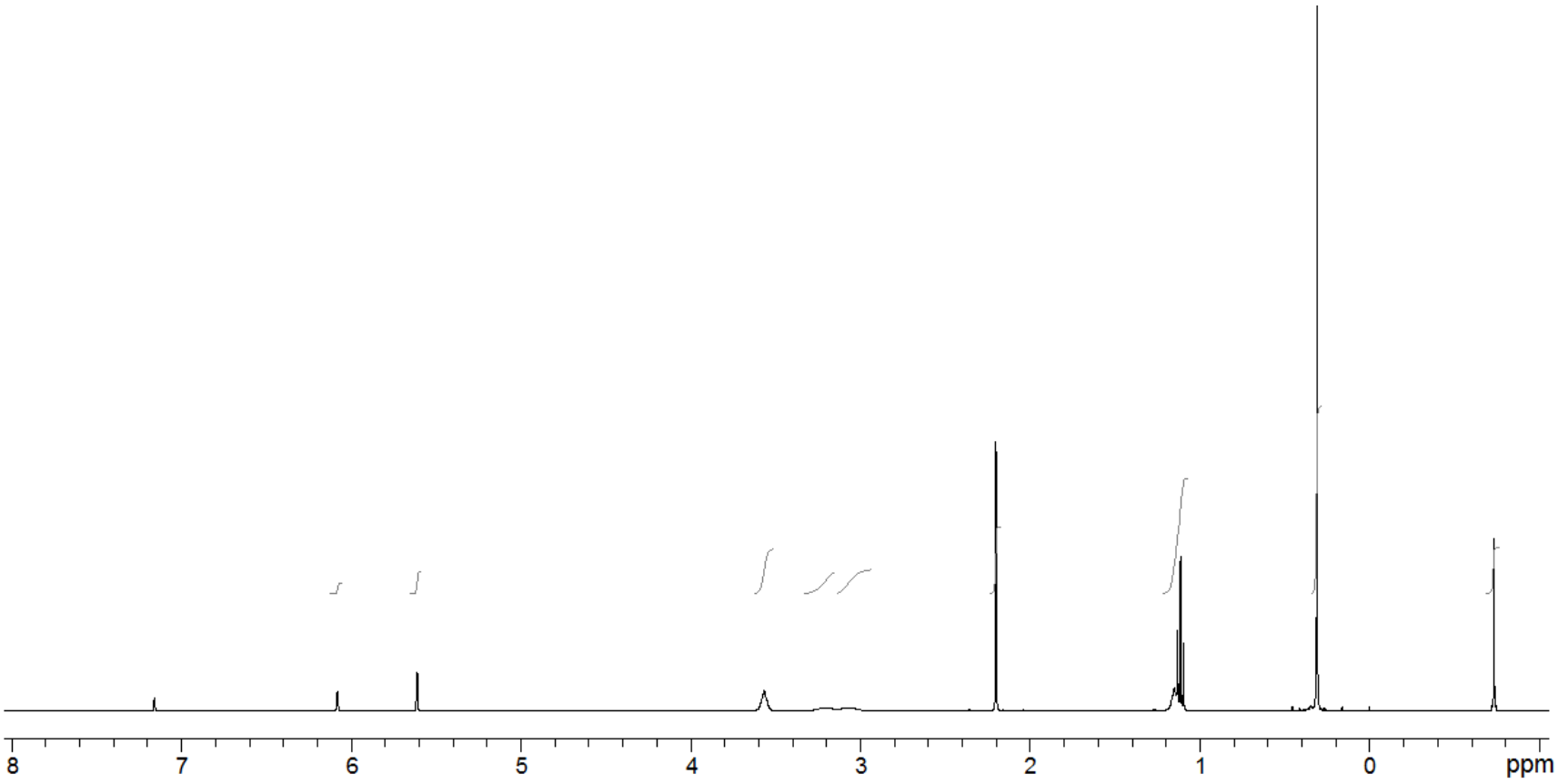


Fig. S5 ^{1}H NMR spectrum of **2** (400 MHz, C_6D_6, 25 ^{o}C).

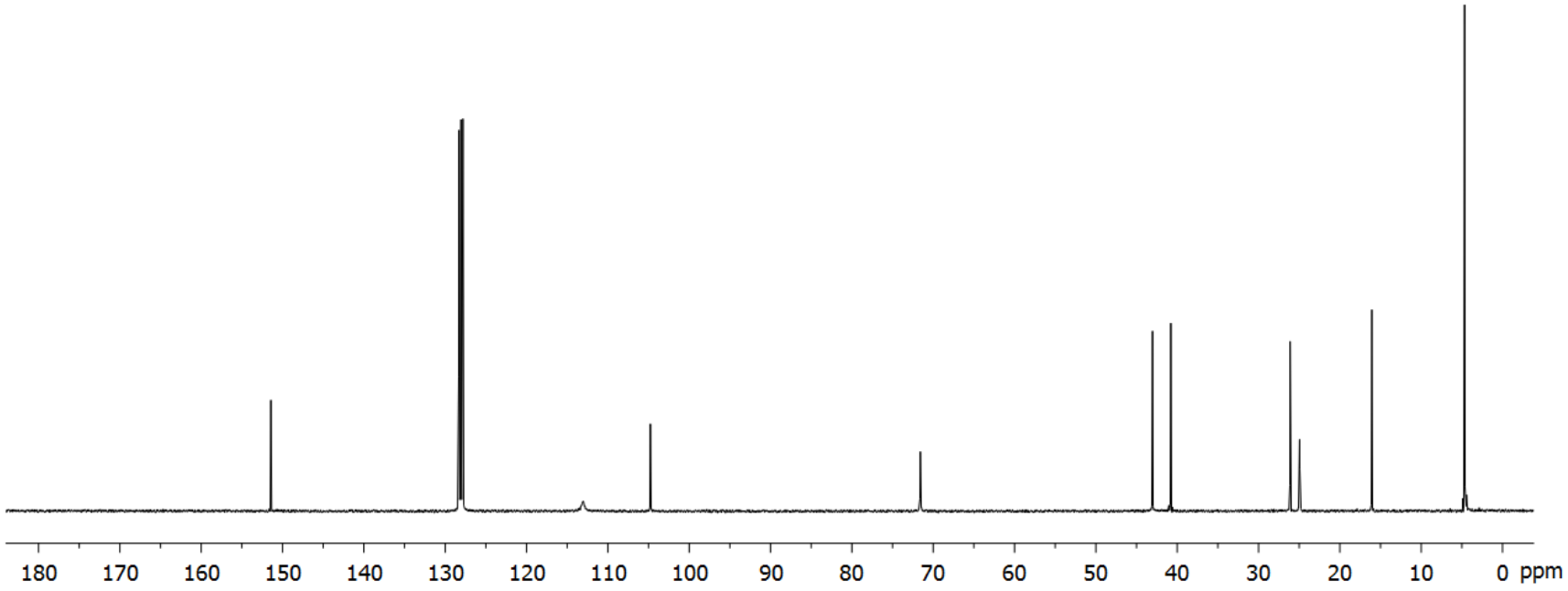
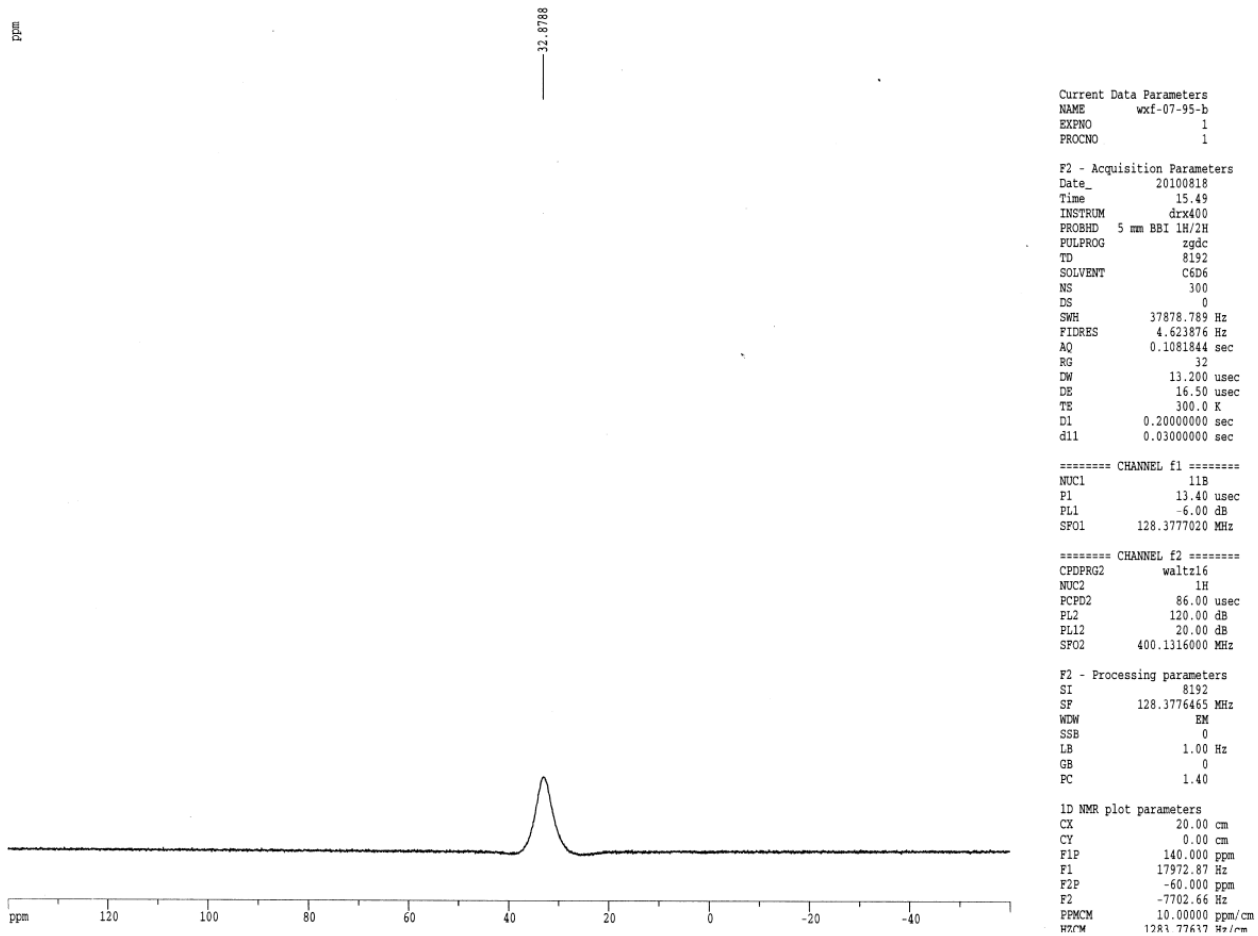


Fig. S6 ^{13}C NMR spectrum of **2** (100 MHz, C_6D_6, 25 ^{o}C).

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FIDRES         4.623876 Hz
AQ            0.1081844 sec
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DE               16.50 usec
TE                300.0 K
D1           0.20000000 sec
d11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                 11B
P1                13.40 usec
PL1               -6.00 dB
SFO1        128.3777020 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              86.00 usec
PL2               120.00 dB
PL12               20.00 dB
SFO2        400.1316000 MHz

F2 - Processing parameters
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WDW                   EM
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1D NMR plot parameters
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F1P             140.000 ppm
F1             17972.87 Hz
F2P             -60.000 ppm
F2             -7702.66 Hz
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Fig. S7 ^{11}B NMR spectrum of **2** (128 MHz, C_6D_6, 25 ^oC).

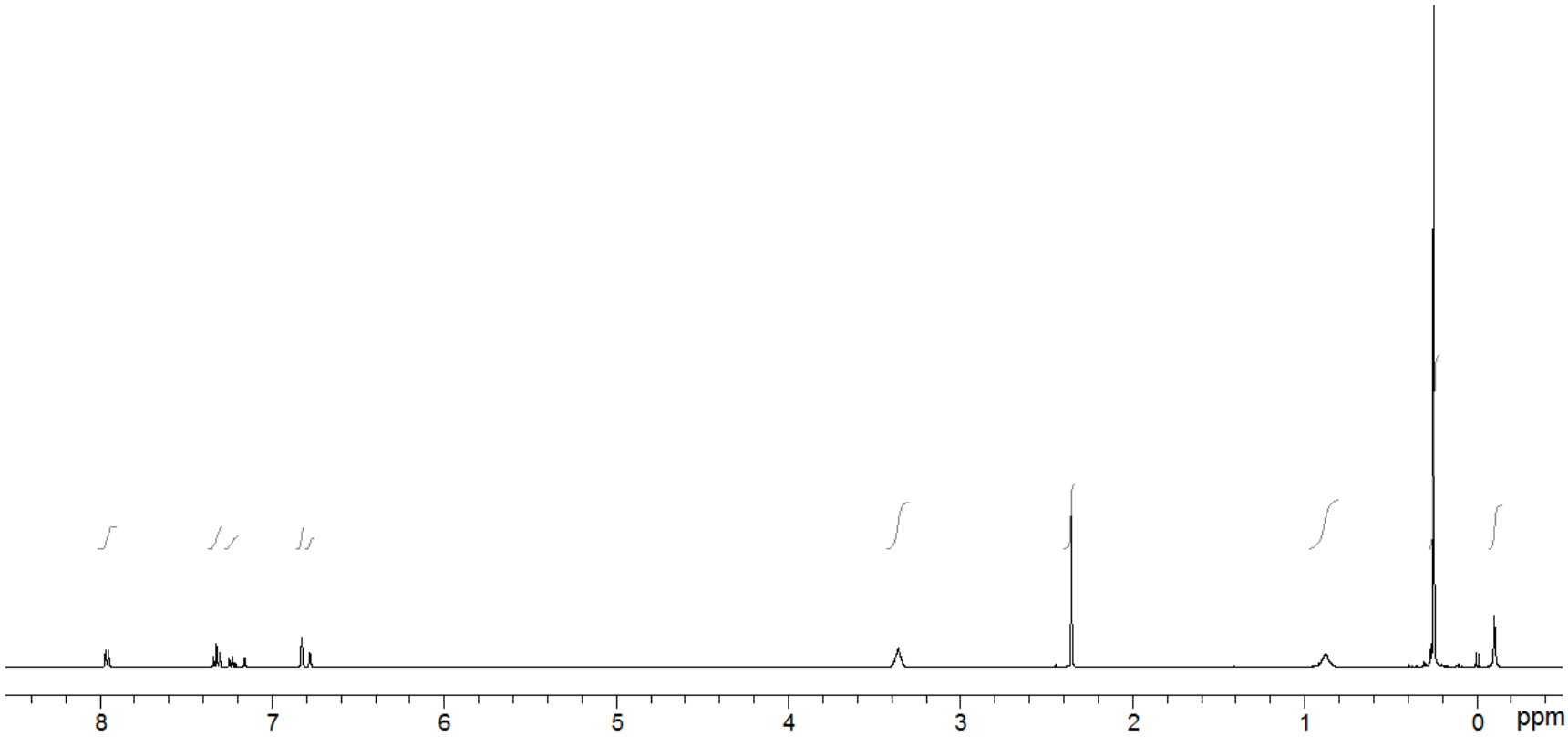


Fig. S8 ^{1}H NMR spectrum of **3** (400 MHz, C_6D_6, 25 ^{o}C).

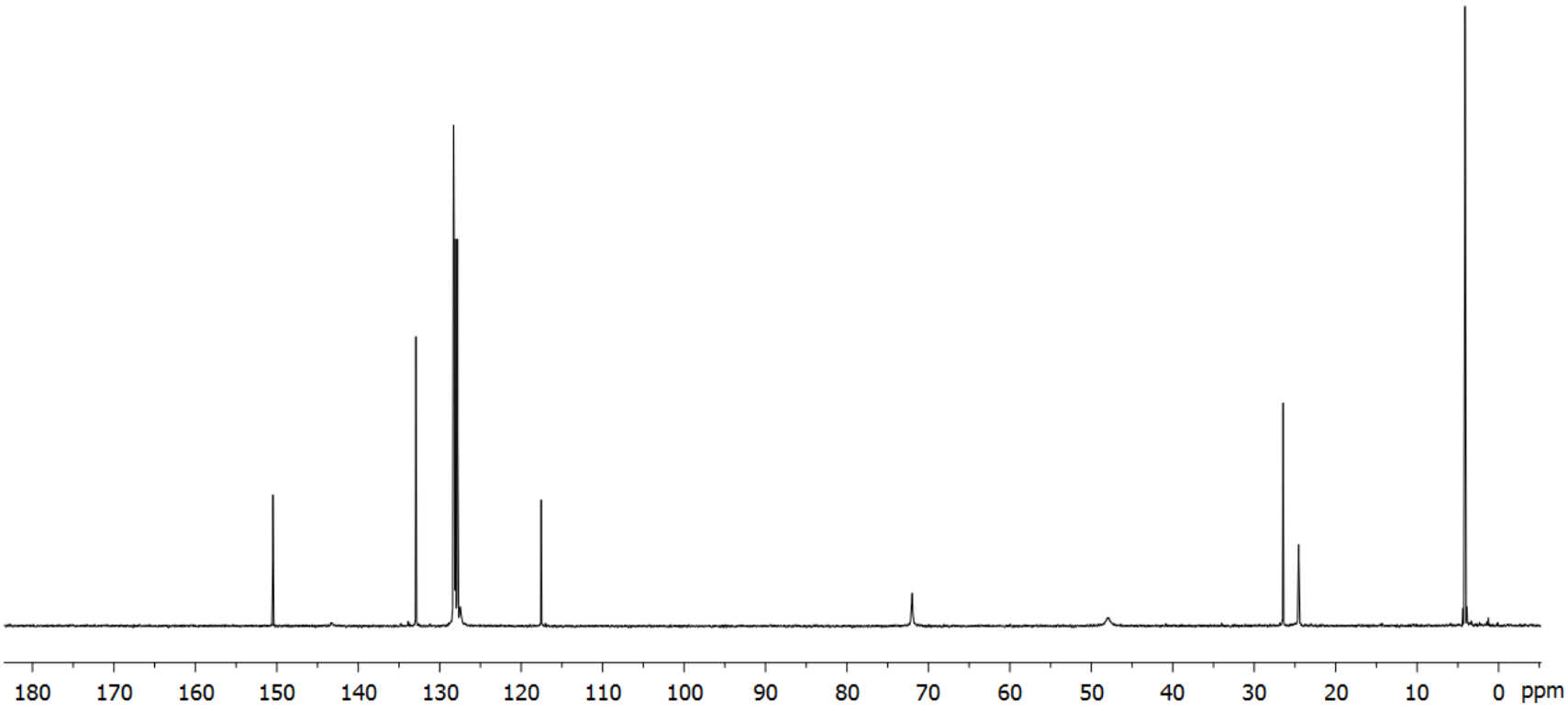
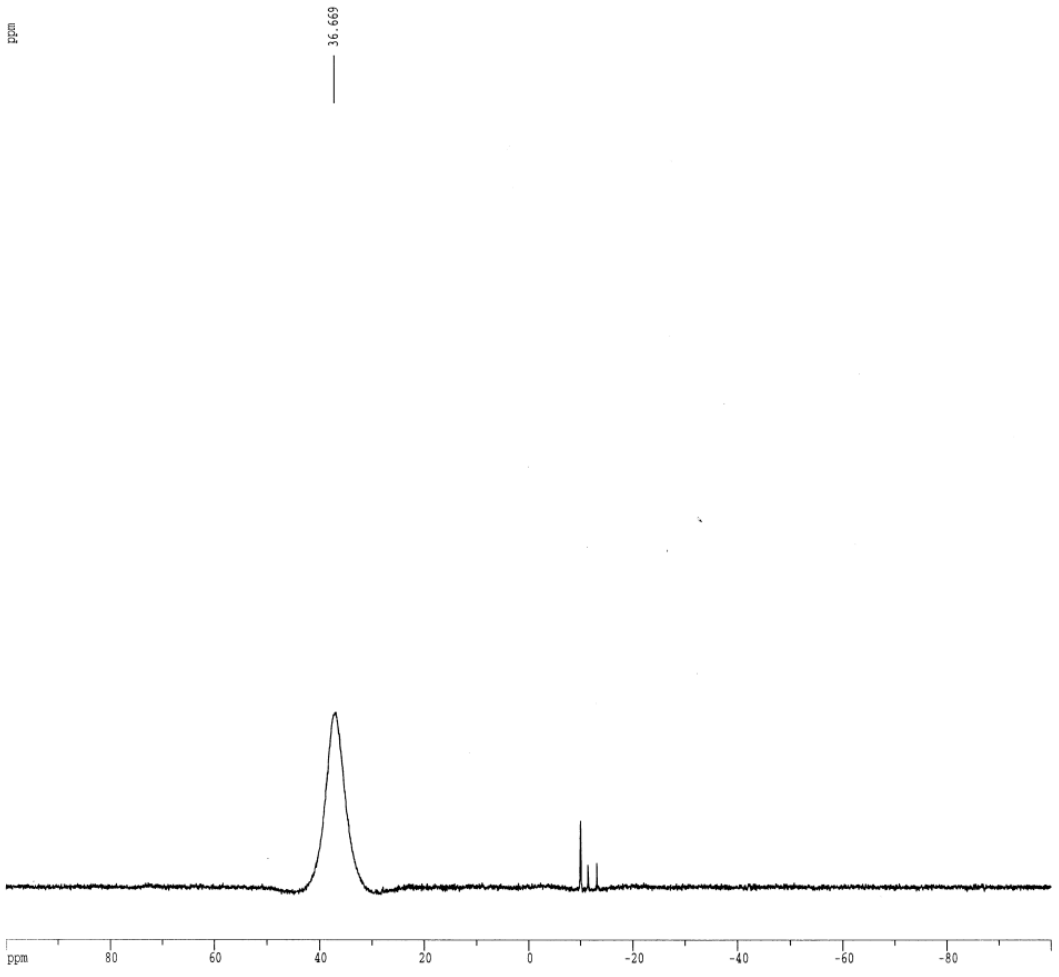


Fig. S9 ^{13}C NMR spectrum of **3** (100 MHz, C_6D_6, 25 °C).

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RG                   200
DW               12.975 usec
DE               18.54 usec
TE               300.0 K
D1           0.20000000 sec
d11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1               13.40 usec
PL1              -6.00 dB
SFO1        128.3792975 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            86.00 usec
PL2             120.00 dB
PL12             20.00 dB
SFO2        400.1315370 MHz

F2 - Processing parameters
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SF          128.3776464 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.00

1D NMR plot parameters
CX                20.00 cm
CY                 0.00 cm
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F1             12837.76 Hz
F2P            -100.000 ppm
F2            -12837.76 Hz
PPMCM          10.00000 ppm/cm
HZCM         1283.77637 Hz/cm
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Fig. S10 ^{11}B NMR spectrum of **3** (128 MHz, C_6D_6, 25 ^{o}C).

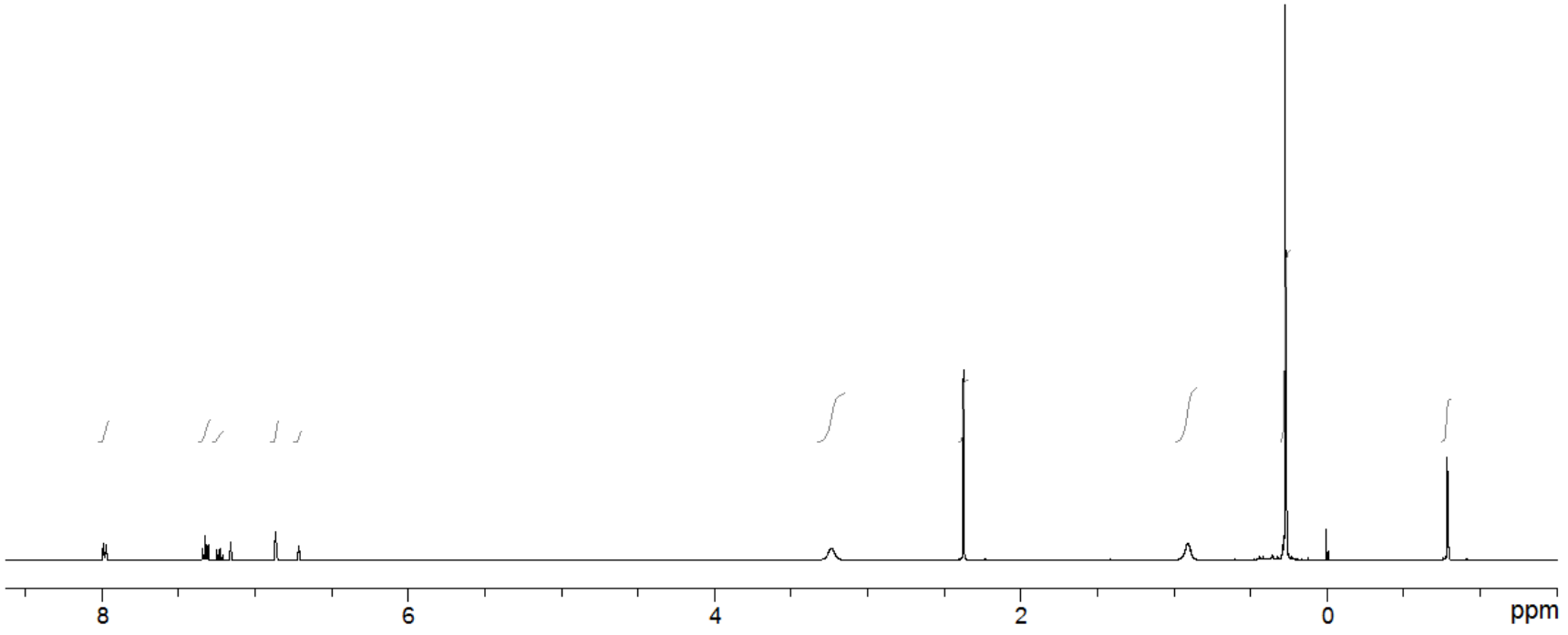


Fig S11 ^{1}H NMR spectrum of **4** (400 MHz, C_6D_6, 25 ^{o}C).

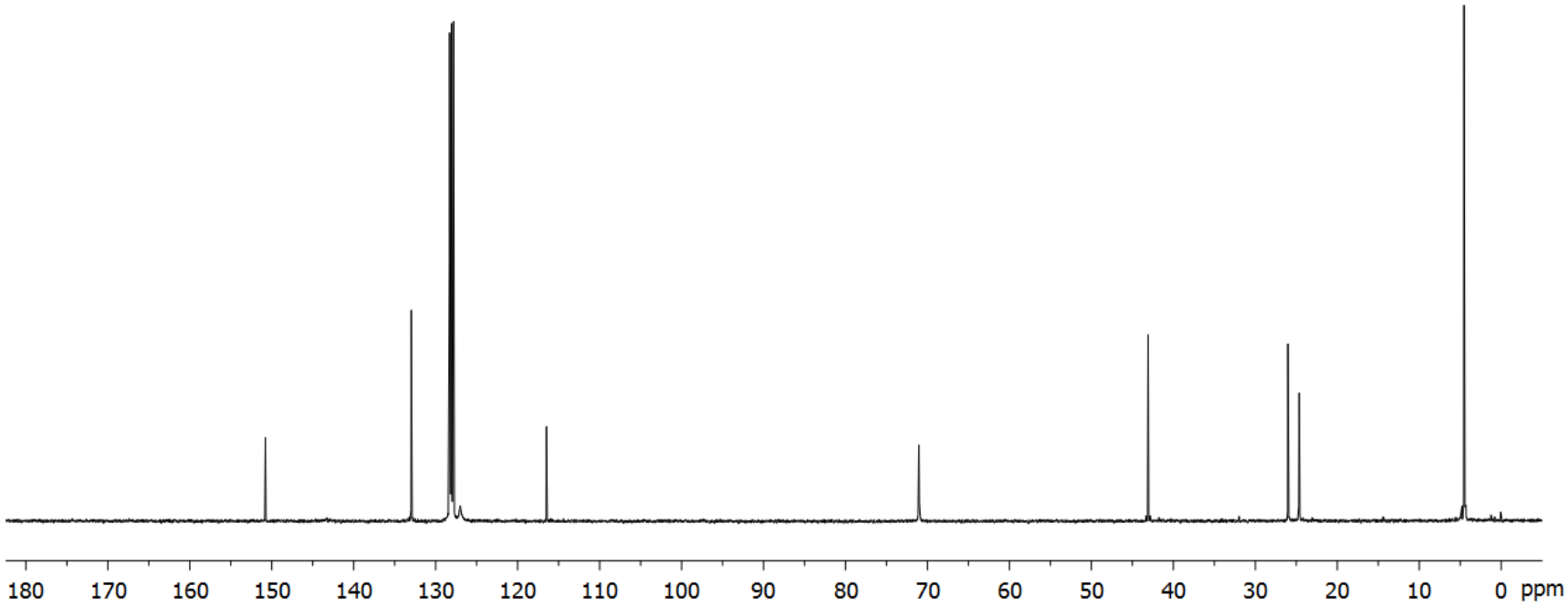
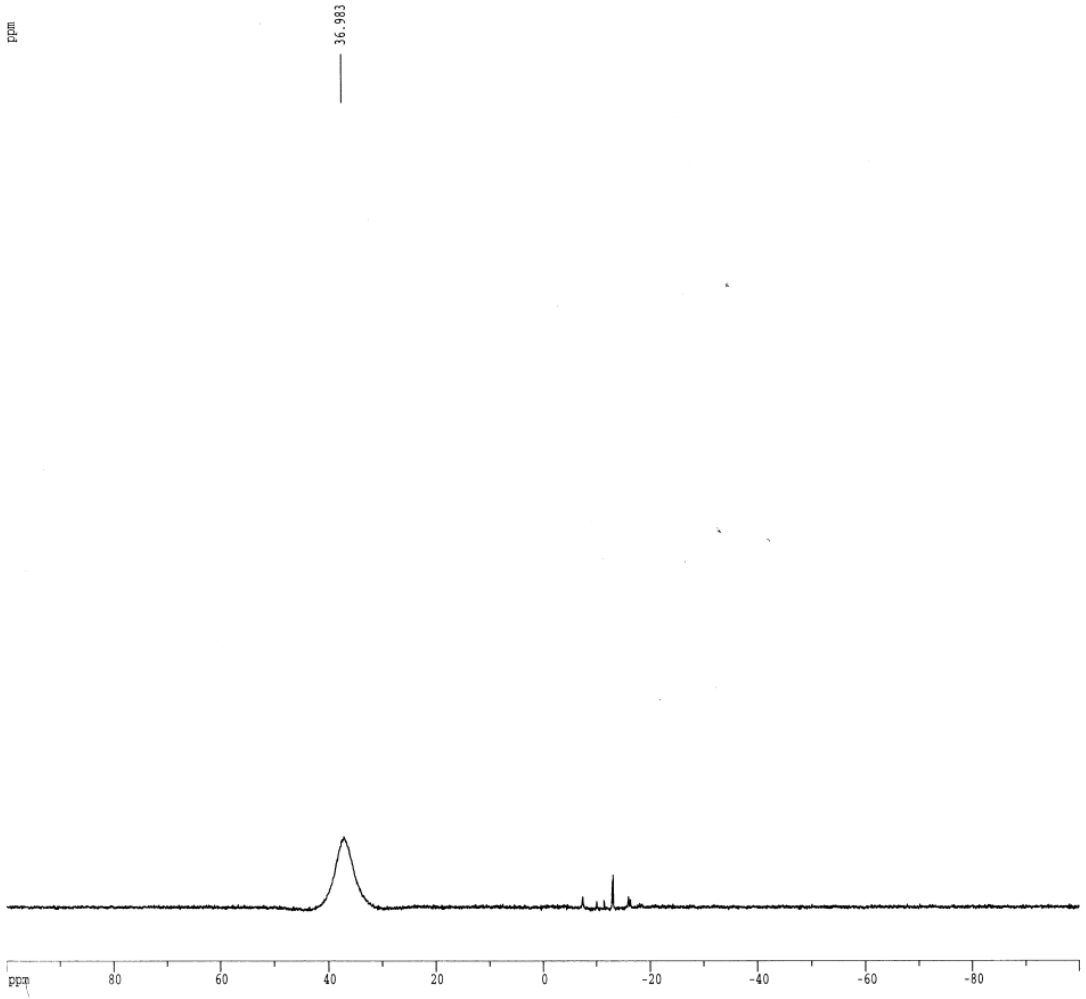


Fig. S12 ^{13}C NMR spectrum of **4** (100 MHz, C_6D_6, 25 °C).

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FIDRES         4.704058 Hz
AQ            0.1063412 sec
RG                   200
DW               12.975 usec
DE               18.54 usec
TE               300.0 K
D1           0.20000000 sec
d11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1               13.40 usec
PL1              -6.00 dB
SFO1        128.3792975 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            86.00 usec
PL2             120.00 dB
PL12             20.00 dB
SFO2        400.1315370 MHz

F2 - Processing parameters
SI                  8192
SF          128.3776464 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.00

1D NMR plot parameters
CX               20.00 cm
CY                0.00 cm
F1P             100.000 ppm
F1             12837.76 Hz
F2P            -100.000 ppm
F2            -12837.76 Hz
PPMCM          10.00000 ppm/cm
HZCM         1283.77637 Hz/cm
```

Fig. S13 ^{11}B NMR spectrum of **4** (128 MHz, C_6D_6, 25 ^{o}C).