Base-Free Mizoroki-Heck Reaction Catalysed by Rhodium Complexes

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Supporting information

General Procedures

¹H NMR and ¹³C NMR spectra were recorded on a Avance 300 or Avance 400 instruments; chemical shifts (δ) are reported in ppm relative to Me₄Si; coupling constants (*J*) are reported in Hz and refer to apparent peak multiplicities. ²H NMR spectra were recorded on a Bruker Avance 400 instrument at 61.4 MHz using benzene-*d*₆ as an internal reference. Mass spectra were determined on a Ribermag instrument. High resolution mass spectra were performed on a Varian MAT311 at the Université Pierre et Marie Curie (Paris). Thin layer chromatography was carried out on silica-gel plates (Merck F254), spots were detected with UV light and revealed with KMnO₄ solution. GC analyses were performed on a Hewlett-Packard instrument equipped with a J&W Scientific DB-1701 capillary column (15 m, Ø = 0.25 µm), using an ionization flame detector.

Potassium organotrifluoroborates¹ were prepared according to published procedures. Dioxane and acetone were distilled from CaH₂. Activated alkenes were freshly distilled before use.

Typical procedure for rhodium-catalyzed alkenylation of potassium aryltrifluoroborates: preparation of (butyl 3-(4-methoxyphenyl)acrylate (entry 3): To a mixture of potassium trifluoro(4-methoxyphenyl)borate (1 mmol, 214 mg), chlorobis(ethylene)rhodium(I) dimer (15 µmol, 5.8 mg) and triphenylphosphane (60 µmol, 15.7 mg) in degassed dioxane (2 mL) and degassed acetone (0.5 mL) was added butyl acrylate (2 mmol, 288 µl), under an argon atmosphere. The flask was placed in a preheated oil bath at 80°C. The mixture was stirred until completion of the reaction (followed by GC analysis). After concentration under reduced pressure, the crude mixture was purified by silica gel chromatography eluting with cyclohexane/ethyl acetate (95:5) to afford 217 mg of analytically pure alkene **3d** as a colorless oil (yield 92%).

1-(3-Bromophenyl)-hex-1-en-3-one 3m (entry 12):

Reaction of potassium 3-bromophenyltrifluoroborate (1 mmol, 263 mg) and hex-1-en-3-one (3 mmol, 294 mg) afforded 213 mg of enone **3m** as a pale yellow oil (yield 84%). GC (50 kPa, 70°C during 1 min then 20°C/min up to 210°C): *t*_R 10.00 min. R_f (petroleum ether / ethyl acetate 20/1): 0.24. ¹H NMR (CDCl₃, 300 MHz) δ = 7.69 (t app, *J* = 1.8 Hz, 1H), 7.46 (d, *J* = 16.4 Hz, 1H), 7.44-7.52 (m, 2H), 7.25 (t, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 16.2 Hz, 1H), 2.64 (t, *J* = 7.4 Hz, 2H), 1.72 (sext. app., *J* = 7.3 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H). ¹³C NMR (CDCl₃, 75 MHz) δ = 200.0, 140.4, 136.8, 133.1, 130.8, 130.4, 127.3, 126.8, 123.8, 43.1, 17.7, 13.8. MS (70 eV): *m/z* (%) = 254 (8), 252 (8) [M]⁺, 211 (85), 209 (100) [M-C₃H₇]⁺, 183 (26), 181 (29) [M-COC₃H₇]⁺, 173 (65) [M-Br]⁺, 102 (63) [C₆H₄CHCH]⁺. HRMS for C₁₂H₁₄BrO calculated 253.0223 and 255.0202; found 253.0224 and 255.0203 [M+H]⁺.

1-(2-Methylphenyl)-hex-1-en-3-one 3n (entry 13):

¹ a) Darses, S.; Genet, J.-P. *Eur. J. Org. Chem.* **2003**, 4313. (b) Darses, S.; Michaud, G.; Genet, J.-P. *Eur. J. Org. Chem.* **1999**, 1875.

Reaction of potassium 3-methylphenyltrifluoroborate (1 mmol, 198 mg) and hex-1-en-3-one (2 mmol, 48 mg) afforded 162 mg of enone **3n** as a pale yellow oil (yield 86%). GC (50 kPa, 70°C during 1 min then 20°C/min up to 210°C): t_R 8.20 min. Rf (petroleum ether / ethyl acetate 4/1): 0.78. 1H NMR ($CDCl_3$, 300 MHz) δ = 7.86 (d, J = 16.0 Hz, 1H), 7.56-7.59 (m, 1H), 7.11-7.31 (m, 3H), 6.67 (d, J = 16.0 Hz, 1H), 2.65 (t, J = 7.3 Hz, 2H), 2.45 (s, 3H), 1.73 (sext. app., J = 7.4 Hz, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ = 200.4, 139.8, 137.9, 133.6, 130.8, 130.1, 127.2, 126.4, 126.3, 43.1, 19.8, 17.8, 13.9. MS (70 eV): m/z (%) = 188 (9) $[M]^+$, 173 (33) $[M-CH_3]^+$, 145 (100) $[M-C_3H_7]^+$, 117 (32) $[M-COC_3H_7]^+$, 115 (51), 91 (23) $[CH_3C_6H_4]^+$. HRMS for $C_{13}H_{17}O$ calculated 189.1274; found 189.1273 $[M+H]^+$.

All other products were identified by comparison of spectroscopic data with authentic sample or with those reported in the literature: **1b** [83160-20-7], **3a** [52392-64-0], **3b** [125950-99-4], **3c** [114833-06-6], **3d** [346586-17-2], **3e** [220466-27-3], **3f** [352-03-4], **3g** [24393-48-4], **3h** [527759-23-5], **3i** [202476-39-9], **3j** [202476-40-2], **3k** [99564-46-2], **3l** [99564-62-2], **3o** [103-36-6], **5a** [116144-99-1], **5b** [87482-94-8].

7.481
7.427
7.375
7.347
7.280
7.251
7.189
6.291
6.238

1.458

Current Data Parameters
 NAME gl3fv55
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060314
 Time_ 0.06
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 362
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300274 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

28.164
26.887

80.661
77.465
77.041
76.617

142.051
135.795
133.150
129.078
120.783

166.003

Current Data Parameters
NAME gl6fv55
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060317
Time_ 1.40
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 18390.4
DW 27.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.03000000 sec
d12 0.0002000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME g01fv46
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060301
Time 21.47
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 14596.5
DW 27.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME g28rm487
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060301
 Time 4.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 362
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.1000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300282 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME g28rm487
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060301
 Time_ 4.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 800
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088436 sec
 RG 16384
 DW 27.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.70 usec
 PL1 -1.00 dB
 SFO1 75.4756731 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 22.50 dB
 PL13 22.50 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4676462 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME g11rm
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051011
Time 14.52
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 362
DM 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 0.00 dB
SF01 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.50 cm
CY 13.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.44444 ppm/cm
HZCM 133.39111 Hz/cm

Current Data Parameters
NAME g11fv2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051012
Time_ 0.50
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 11585.2
DW 27.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4678187 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME g27fv45
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date 20060228
 Time 4.44
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 143.7
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300276 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME g27fv45
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060228
 Time_ 4.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 400
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088436 sec
 RG 16384
 DW 27.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.70 usec
 PL1 -1.00 dB
 SFO1 75.4756731 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 22.50 dB
 PL13 22.50 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME g27fv47
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060228
 Time_ 8.28
 INSTRUM spect
 PROBD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 71.8
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300374 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

```

Current Data Parameters
NAME      g27fv47
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20060228
Time      8.26
INSTRUM   spect
PROBHD    5 mm QNP 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         400
DS         0
SWH        18115.941 Hz
FIDRES     0.276427 Hz
AQ         1.8088436 sec
RG         13004
DW         27.600 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         7.70 usec
PL1        -1.00 dB
SFO1       75.4756731 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.00 dB
PL12       22.50 dB
PL13       22.50 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677490 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```

Current Data Parameters
 NAME g27fv48
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060228
 Time 0.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542380 sec
 RG 812.7
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300275 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME g01fv48
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060301
Time_ 23.41
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 18390.4
DW 27.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME g04ab16
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070505
Time_ 3.20
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 18390.4
DE 27.600 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

8.311
8.253
8.236
8.178
8.109
8.082
7.806
7.793
7.779
7.767
7.761
7.647
7.623
7.500
7.482
7.477
7.472
7.456
7.449
7.429
7.425
7.415
7.406
7.402
7.389
7.363
7.181
6.348
6.290
6.285
6.228
5.188
4.157
4.134
4.110
4.084
4.060
1.328
1.305
1.281

Current Data Parameters
 NAME g04ab18
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20070505
 Time 1.22
 INSTRUM spect
 PROHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542380 sec
 RG 90.5
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300300 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

```

Current Data Parameters
NAME      g04abi8
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20070505
Time      1.20
INSTRUM   spect
PROBHD    5 mm QNP 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         800
DS         0
SWH        18115.941 Hz
FIDRES     0.276427 Hz
AQ         1.8088436 sec
RG         18390.4
DE         27.600 usec
TE         -300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         7.70 usec
PL1        -1.00 dB
SFO1       75.4756731 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         0.00 dB
PL12        22.50 dB
PL13        22.50 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI          32768
SF          75.4677490 MHz
WDW         EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40

```

Current Data Parameters
NAME g09nm
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070509
Time 10:59
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 32
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 362
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 0.1000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 7.10 usec
PL1 0.00 dB
SF01 300.1318008 MHz

F2 - Processing parameters

SI 32768
SF 300.1300051 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

ID NMR plot parameters

CX 22.50 cm
CY 0.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.44444 ppm/cm
HZCM 133.39111 Hz/cm

```

Current Data Parameters
NAME      g07rm770
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20070507
Time      22:38
INSTRUM   spect
PROBHD    5 mm QNP 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2000
DS         0
SWH        18115.941 Hz
FIDRES     0.276427 Hz
AQ         1.8088436 sec
RG         18390.4
DW         27.600 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.0002000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         7.70 usec
PL1        -1.00 dB
SFO1       75.4756731 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0.00 dB
PL12       22.50 dB
PL13       22.50 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677490 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40

```

Current Data Parameters
NAME g24cm
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061124
Time 10.39
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 362
CW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 0.00 dB
SF01 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.50 cm
CY 0.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPHMM 0.44444 ppm/cm
HZCM 133.39111 Hz/cm

Current Data Parameters
 NAME g24m278
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061125
 Time 0.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 400
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088436 sec
 RG 14596.5
 DW 27.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.70 usec
 PL1 -1.00 dB
 SFO1 75.4756731 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 22.50 dB
 PL13 22.50 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME g01rm
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061201
 Time 9:58
 INSTRUM spect
 PROBHD 5 mm QNP 1H/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 143.7
 DW 81.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.10 usec
 PL1 0.00 dB
 SF01 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300061 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 CY 13.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPVCM 0.44444 ppm/cm
 HZCM 133.39111 Hz/cm

Current Data Parameters
NAME g30rm759
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061130
Time 23.13
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zgpg30
TD 65336
SOLVENT CDCl3
NS 800
DS 0
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8088436 sec
RG 14596.5
DM 27.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -1.00 dB
SFO1 75.4756731 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 22.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

7.786
7.733
7.488
7.482
7.457
7.201
7.182
7.174
7.169
7.158
7.152
7.131
7.111
7.087
6.598
6.544

2.570
2.546
2.522
2.343

1.668
1.644
1.619
1.594
1.570

0.921
0.897
0.872

Current Data Parameters
NAME g04rm756
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20070505
Time 2.23
INSTRUM spect
PROBHD 5 mm QNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 71.8
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.10 usec
PL1 0.00 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300334 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME g04m756
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070505
 Time_ 2.20
 INSTRUM spect
 PROBD 5 mm QNP 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 800
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088436 sec
 RG 18390.4
 DW 27.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 7.70 usec
 PL1 -1.00 dB
 SFO1 75.4756731 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 22.50 dB
 PL13 22.50 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 WDW 0
 SSB 3.00 Hz
 LB 0
 GB 0
 PC 1.40

```
Current Data Parameters
NAME          g21eg
EXPNO         4
PROCNO        1
```

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	SOLVENT	NS	DS	SWH	FIDRES	RG	LOW	DE	TE	D1		
20060321	11:27	spect	5 mm QNP 1H/	zg30	32768	CDCl3	16	0	6172.839 Hz	0.188380	2.6542560 sec	362	81.000 usec	6.50 usec	300.0 K	0.10000000 sec