Metallated Nitriles: Halogen-Metal Exchange with α -Halonitriles

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Compound	Reference	¹ H NMR	¹³ C NMR
4a	1	S2	S3
4b		S4	S5
4ca		S6	S7
4cb		S8	S9
4d		S10	S11
5a		-	-
5b		S12	S13
5c		S14	S15
5d		S16	S17
5e		S18	S19
5f		S20	S21
5g		S22	S23
5h		S24	S25
References		S26

Current Data Parameters
 USER zhan
 NAME f1zjmd01
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030131
 Time 0.35
 INSTNM spect
 PROBD 5 mm QNP 1H
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 2048
 DS 8
 SMI 19230.770 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039860 sec
 RG 16384
 DW 26.000 usec
 DE 32.50 usec
 TE 300.0 K
 D12 0.0002000 sec
 DL6 23.00 dB
 D1 1.5000000 sec
 CPOPRG waltz16
 P31 110.00 usec
 D11 0.0300000 sec
 DL5 20.00 dB
 P1 6.20 usec
 SF01 75.4782456 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 65536
 SF 75.4677190 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 21.50 cm
 F1P 240.379 ppm
 F1 18140.87 Hz
 F2P 14.442 ppm
 F2 -1089.50 Hz
 PPM0K 11.85214 ppm/cm
 HZ0K 894.45435 Hz/cm

Current Data Parameters
 USER zhan
 NAME zh05_501
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030516
 Time 19.30

INSTRUM Spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 2

SMH 19230.770 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039860 sec

BG 8192
 DM 25.000 usec
 DE 32.50 usec

TE 300.0 K
 D12 0.00002000 sec
 DL6 23.00 dB

D1 1.50000000 sec
 CPDPRG waitz16
 P31 110.00 usec

D11 0.03000000 sec
 DL5 20.00 dB
 P1 6.20 usec

SFO1 75.4752455 MHz
 NUCLEUS 13C

F2 - Processing parameters
 SI 65536
 SF 75.4677190 MHz

WDW EM
 SSB 0
 LB 2.00 Hz

GB 0
 PC 1.00

1D NMR plot parameters
 CX 21.50 cm
 F1P 240.379 ppm

F1 181.40 87 Hz
 F2P -14.442 ppm
 F2 -1089.90 Hz

PPMCH 11.85214 ppm/cm
 HZCM 884.45435 Hz/cm

FFZY110.001
DATE 22-7-3

SF	300.133
SY	210.0
O1	4900.000
SI	8192
TD	8192
SM	6024.096
HZ/PT	1.471
PW	5.0
RD	2.500
AG	.680
RG	1
NS	8
TE	297
FW	7600
O2	5684.205
DP	4L P0
LB	0.0
GB	0.0
CX	25.00
CY	15.00
F1	10.001P
F2	-196P
HZ/CM	122.423
PPM/CM	.408
SR	3364.56

PPM

FFZY140.101
DATE 22-7-3

SF 75.475
SY 75.0
O1 6147.202
SI 16384
TD 16384
SW 17857.143
HZ/PT 2.180
PM 4.0
RD 3.000
AQ .459
RG 200
NS 214
TE 297
FW 22400
O2 4004.452
DP 20H BB
LB 0.0
GB 0.0
CX 25.00
CY 9.00
F1 220.014P
F2 .024P
HZ/CM 664.150
PPM/CM 8.800
SR -1399.02

120.806

77.400
76.990
76.560

46.235

39.504

32.344

27.172

21.860

FFZY109.001
DATE 22-7-3

SF 300.133
SY 210.0
O1 4900.000
S1 8192
TD 8192
SW 6024.096
HZ/PT 1.471
PM 5.0
RD 2.500
AQ .680
RG 1
NS 8
TE 297
FW 7600
O2 5684.205
DP 4L P0
LB 0.0
GB 0.0
CX 25.00
CY 0.0
F1 10.004P
F2 -193P
HZ/CM 122.423
PPM/CM .408
SR 3368.15

PPM

FFZY109.101
DATE 22-7-3

SF	75.469
SY	75.0
O1	61.47.202
SI	16384
TD	16384
SW	17857.143
HZ/PT	2.180
PW	4.0
RD	3.000
AG	.459
RG	200
NS	101
TE	297
FW	22400
O2	4004.452
DP	20H BB
LB	0.0
GB	0.0
CX	25.00
CY	12.50
F1	220.033P
F2	.024P
HZ/CM	664.150
PPM/CM	8.800
SR	-1388.12

119.200

77.432
77.001
76.573

45.979
45.113
42.028

32.145
27.177
26.396

Chloroform-d
 -7.25

BRIAN32.001
DATE 16-1-99
TIME 12:33

SOLVENT CDCl3
SF 300.133
SY 210.0
O1 4800.000
SI 16384
TD 16384
SM 4504.505
HZ/PT .550

PM 5.0
RD 2.500
AQ 1.819
RG 1
NS 8
TE 297

FW 5700
O2 5684.205
DP 4L P0

LB 0.0
GB 0.0
CX 25.00
CY 1.25
F1 10.001P
F2 -.198P
HZ/CM 122.444
PPM/CM 408
SR 3367.75

PPM

BRIAN32-101
DATE 10-1-99
TIME 13:21

SOLVENT CDCl3
SF 75.0
SY 75.0
01 6147.202
SI 16384
TD 16384
SW 17857.143
HZ/PT 2.180

PM 4.0
RD 3.000
AG .459
RG 200
NS 613
TE 297

FM 22400
02 4004.452
DP 20H BB

LB .200
GB 0.0
CX 25.00
CY 50
F1 220.004P
F2 -5.001P
HZ/CM 679.234
PPM/CM 9.000
SR -1396.84

117.559

77.434
77.000
77.000
77.000

38.734

31.708

24.950

21.685

¹ Walters, M. A.; Hoem, A. B.; McDonough, C. S. *J. Org. Chem.* **1996**, *61*, 55.