Preparation of Ketones from Nitriles and Phosphoranes

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Supporting Information

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Experimental Section

General. All reagents were of commercial quality. All dry solvents were freshly distilled under nitrogen from the appropriate drying agent before use. ^1H and ^{13}C NMR spectra were recorded at 400 MHz using CDCl_3 as the internal standard. IR spectra were measured as thin films. All reactions were run under an N_2 atmosphere. TLC solvent mixtures are volume/volume. MTBE is methyl *t*-butyl ether, and PE is petroleum ether.

Current Data Parameters
NAME: B2P167B
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20011006
Time: 12.00
INSTRUM: spect
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 1
SWH: 5592.841 Hz
FIDRES: 0.110860 Hz
AQ: 2.120893 sec
RG: 48.3
DE: 89.400 usec
TE: 415.0 K
D1: 5.0000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 12.00 usec
PL1: 0.00 dB
SFO1: 400.1130007 MHz

F2 - Processing parameters
SI: 32768
SF: 400.1130007 MHz
WDW: no
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
RG: 327.68
SI: 32768
SF: 400.1130007 MHz
WDW: no
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00

PMCKM
170.05925 Hz/cm

AMX360 C-13 NMR GNP Probe Solvent CDCl3

Current Data Parameters
NAME B2P167Bc13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031006
Time 14.14

INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 423
DS 0

SMH 22623.701 Hz
FIDRES 0.345210 Hz
AQ 1.4463898 sec
RG 16384

DW 22.101 usec
DE 31.57 usec
TE 300.0 K
P1 8.00 usec
CNS12 150.0000000
CNS111 1.0000000

D20 0.006667 sec
S2 20 dB
HL1 3 dB
D1 6.00000000 sec

CPDPRG waitz16
P31 100.00 usec
D13 0.000040 sec
P2 16.0 usec

SF01 90.5648750 MHz
NUCLEUS 13C

F2 - Processing parameters
SI 32768

SF 90.5557639 MHz

WDW no

SSB 0

LB 0.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

F1P 225.528 ppm

F1 20422.88 Hz

F2P -24.304 ppm

F2 -2200.83 Hz
PPMCM 12.49159 ppm/cm
HZCM 1131.18506 Hz/cm

Current Data Parameters
 NAME B2P291P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040331
 Time 11.23
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 5
 DW 89.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300170 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.946 ppm
 F1 4780.07 Hz
 F2P -2.031 ppm
 F2 -812.77 Hz
 PPMCM 0.69888 ppm/cm
 HZCM 279.64203 Hz/cm

B4P23a2-c13

Current Data Parameters
NAME B4P23a2-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040923

Time 23.42
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG jvert
TD 65536
SOLVENT CDCl3
NS 792
DS 0
SWH 27173.912 Hz
FIDRES 0.414641 Hz
AQ 1.2059124 sec
RG 7298.2
DW 18.400 usec
DE 4.50 usec
TE 300.0 K
D1 6.00000000 sec
D11 0.03000000 sec
D13 0.00000300 sec
D20 0.00700000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
P2 21.00 usec
PL1 0.00 dB
SF01 100.6242995 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz

F2 - Processing Parameters
SI 32768
SF 100.6127290 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 250.042 ppm
F1 25157.42 Hz
F2P -20.042 ppm
F2 -2016.50 Hz
PPMCM 13.50421 ppm/cm
HZCM 1358.69580 Hz/cm