SUPPORTING INFORMATION

Room Temperature Zinc Chloride-Catalyzed Cycloisomerization of Alk-3-yn-1-ones: Synthesis of Substituted Furans

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¹H NMR spectrum for **3a** (CDCl₃)

Current Data Parameters

NAME Adam

EXPNO 1155

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060914

Time 10.04

INSTRUM spect

PROBHD 5 mm Multinu

PULPROG zg

TD 4096

SOLVENT CDCl3

NS 16

DS 2

SWH 2796.421 Hz

FIDRES 0.682720 Hz

AQ 0.7324148 sec

RG 362

DW 178.800 usec

DE 6.00 usec

TE 300.0 K

D1 5.00000000 sec

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

NUC1 1H

P1 10.00 usec

PL1 -3.00 dB

SFO1 200.1313509 MHz

F2 - Processing parameters

SI 32768

SF 200.1300031 MHz

WDW EM

SSB 0

LB 0.03 Hz

GB 0

PC 1.00

¹³C NMR spectrum for **3a** (CDCl₃)

Current Data Parameters

NAME Audrey

EXPNO 27

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060914

Time 8.59

INSTRUM spect

PROBHD 5 mm Multinu

PULPROG zgdc

TD 37686

SOLVENT CDCl3

NS 19000

DS 4

SWH 12562.814 Hz

FIDRES 0.333355 Hz

AQ 1.4999528 sec

RG 362

DW 39.800 usec

DE 6.00 usec

TE 300.0 K

DE 4.00000000 sec

d11 0.03000000 sec

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

NUC1 13C

P1 6.00 usec

PL1 1.00 dB

SFO1 50.3285046 MHz

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

CPDPRG2 waltz16

NUC2 1H

PCPD2 100.00 usec

PL2 -4.00 dB

PL12 16.72 dB

SFO2 200.1300000 MHz

F2 - Processing parameters

SI 32768

SF 50.3227247 MHz

WDW EM

SSB 0

LB 3.00 Hz

GB 0

PC 1.40

¹H NMR spectrum for **3b** (CDCl₃)

Current Data Parameters

NAME Adam

EXPNO 1134

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060912

Time 16.48

INSTRUM spect

PROBHD 5 mm Multinu

PULPROG zg

TD 4096

SOLVENT CDCl3

NS 16

DS 2

SWH 2796.421 Hz

FIDRES 0.682720 Hz

AQ 0.7324148 sec

RG 101.6

DW 178.800 usec

DE 6.00 usec

TE 300.0 K

D1 4.00000000 sec

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

NUC1 1H

P1 10.00 usec

PL1 -3.00 dB

SFO1 200.1313509 MHz

F2 - Processing parameters

SI 32768

SF 200.1300224 MHz

WDW EM

SSB 0

LB 0.03 Hz

GB 0

PC 1.00

S5

¹H NMR spectrum for **3c** (CDCl₃)

¹³C NMR spectrum for **3c** (CDCl₃)

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===== CHANNEL f1 =====
NUC1      1H
P1         10.00 usec
PL1        -3.00 dB
SFO1       200.1313509 MHz

F2 - Processing parameters
SI         32768
SF         200.1300088 MHz
WDW         EM
SSB         0
LB         0.03 Hz
GB         0
PC         1.00

Current Data Parameters
NAME       adam
EXPNO      1178
PROCNO     1

F2 - Acquisition Parameters
Date_      20060915
Time       20.40
INSTRUM    spect
PROBHD     5 mm Multinu
PULPROG    zg
TD          4096
SOLVENT    CDCl3
NS         16
DS         2
SWH         2796.421 Hz
FIDRES     0.682720 Hz
AQ          0.7324148 sec
RG          574.7
DE         178.800 usec
TE         6.00 usec
           300.0 K
D1         5.00000000 sec

```

¹³C NMR spectrum for **3d** (CDCl₃)

¹H NMR spectrum for **3e** (CDCl₃)

¹³C NMR spectrum for **3e** (CDCl₃)

Current Data Parameters

NAME Audrey

EXPNO 17

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060706

Time 8.47

INSTRUM spect

PROBHD 5 mm Multinu

PULPROG zgdc

TD 37686

SOLVENT CDCl₃

NS 9500

DS 4

SWH 12562.814 Hz

FIDRES 0.333355 Hz

AQ 1.4999528 sec

RG 90.5

DW 39.800 usec

DE 6.00 usec

TE 300.0 K

D1 4.0000000 sec

d11 0.03000000 sec

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

NUC1 ¹³C

P1 6.00 usec

PL1 1.00 dB

SFO1 50.3285046 MHz

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

CPDPRG2 waltz16

NUC2 ¹H

PCPD2 100.00 usec

PL2 -4.00 dB

PL12 16.72 dB

SFO2 200.1300000 MHz

F2 - Processing parameters

SI 32768

SF 50.3227232 MHz

WDW EM

SSB 0

LB 3.00 Hz

GB 0

PC 1.40

¹H NMR spectrum for **3f** (CDCl₃)

¹³C NMR spectrum for **3f** (CDCl₃)

Current Data Parameters

NAME Audrey

EXPNO 25

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060713

Time 9.10

INSTRUM spect

PROBHD 5 mm Multinu

PULPROG zgdc

TD 37686

SOLVENT CDCl3

NS 9500

DS 4

SWH 12562.814 Hz

FIDRES 0.333355 Hz

AQ 1.4999528 sec

RG 456.1

DW 39.800 usec

DE 6.00 usec

TE 300.0 K

D1 4.00000000 sec

d11 0.03000000 sec

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

NUC1 ¹³C

P1 6.00 usec

PL1 1.00 dB

SFO1 50.3285046 MHz

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

CPDPRG2 waltz16

NUC2 ¹H

PCPD2 100.00 usec

PL2 -4.00 dB

PL12 16.72 dB

SFO2 200.1300000 MHz

F2 - Processing parameters

SI 32768

SF 50.3226918 MHz

WDW EM

SSB 0

LB 3.00 Hz

GB 0

PC 1.40

¹H NMR spectrum for **3g** (CDCl₃)

Current Data Parameters
NAME Adam
EXPNO 1214
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060926
Time 10.54
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg
TD 4096
SOLVENT CDCl₃
NS 16
DS 2
SWH 2796.421 Hz
FIDRES 0.682720 Hz
AQ 0.7324148 sec
RG 128
DW 178.800 usec
DE 6.00 usec
TE 300.0 K
D1 5.0000000 sec

==== CHANNEL f1 =====
NUC1 ¹H
P1 10.00 usec
PL1 -3.00 dB
SFO1 200.1313509 MHz

F2 - Processing parameters
SI 32768
SF 200.1300085 MHz
WDW EM
SSB 0
LB 0.03 Hz
GB 0
PC 1.00

¹³C NMR spectrum for **3g** (CDCl₃)

Current Data Parameters
NAME Adam
EXPNO 1213
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060925
Time 19.07
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgdc
TD 37686
SOLVENT CDCl3
NS 751
DS 4
SWH 12562.814 Hz
FIDRES 0.333355 Hz
AQ 1.4999528 sec
RG 101.6
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 4.00000000 sec
d11 0.03000000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 6.00 usec
PL1 1.00 dB
SFO1 50.3285046 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.72 dB
SFO2 200.1300000 MHz

F2 - Processing parameters
SI 32768
SF 50.3227286 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

¹H NMR spectrum for **3h** (CDCl₃)

¹³C NMR spectrum for **3h** (CDCl₃)

Crystallography. X-ray data for compound **3d** were collected on a Siemens P4 diffractometer using a graphite monochromatic Cu K α radiation ($\lambda = 1.54178\text{\AA}$) and XSCANS (Bruker, version 2.31) software package. The data set was collected at 25°C and corrected for Lorentz and polarization effects. Data were corrected for absorption (XPREP, version 2006/1). Crystal stability was monitored by measuring three standard reflections every 97 reflections with no significant variations ($<\pm 3\%$). The X-SEED software platform, equipped with SHELX modules on a PC computer, was used for all structure solution (SHELXS-97) and refinement (SHELXL-97) calculations and molecular graphics. The structure was solved by direct methods, and refined by anisotropic full-matrix least-squares for all non-hydrogen atoms. The function, $\sum w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP + d + e \sin \theta]$ and $P = f[\max(f \text{ or } F_o^2)] + (1-f)F_c^2$. Crystal: transparent colorless block, $0.59 \times 0.38 \times 0.14$ mm, $\rho = 1.388$, $\mu = 3.274$, $F(000) = 728$, $T = 298$ K, $R1 = 0.0467$, $WR = 0.1214$, 2691 independent reflections [Cu K α ; $\theta \leq 62.48^\circ$] and 233 parameters. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were assigned ideal positions and refined using a riding model.

Table S1. Crystal data and structure refinement for **3d**.

Empirical formula	C ₂₀ H ₁₉ BrO	
Formula weight	355.27	
Temperature	298(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	$a = 7.7441(5)$ Å	$\alpha = 90^\circ$.
	$b = 6.2696(5)$ Å	$\beta = 92.327(7)^\circ$.
	$c = 35.046(3)$ Å	$\gamma = 90^\circ$.
Volume	1700.2(2) Å ³	
Z	4	
Density (calculated)	1.388 Mg/m ³	
Absorption coefficient	3.274 mm ⁻¹	
F(000)	728	
Crystal size	$0.59 \times 0.38 \times 0.14$ mm ³	
Theta range for data collection	5.05 to 62.48°.	
Index ranges	$h = -1 \rightarrow 8, k = -1 \rightarrow 7, l = -40 \rightarrow 40$	
Reflections collected	4084	
Independent reflections	2691 [R(int) = 0.0679]	
Completeness to $\theta = 62.48^\circ$	99.3%	
Absorption correction	Analytical	
Max. and min. transmission	0.6572 and 0.2483	
Data / restraints / parameters	2691 / 21 / 233	
Goodness-of-fit on F ²	1.040	
Final R indices [I > 2 σ (I)]	R1 = 0.0467, wR2 = 0.1214	
R indices (all data)	R1 = 0.0567, wR2 = 0.1307	
Largest diff. peak and hole	0.355 and -0.583 e ⁻ Å ⁻³	