SUPPORTING INFORMATION

Oxygen Promoted Pd(II) Catalysis for the Coupling of Organoboron Compounds and Olefins

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Representative Experimental Procedure :

tert-Butyl acrylate **1** (64 mg, 0.5 mmol, 1 equiv.) was dissolved in DMF (2.5 mL, 0.2 M solution), and stirred at room temperature. To the clear solution, was added phenylboronic acid (74 mg, 0.6 mmol, 1.2 equiv.) followed by a single addition of Na₂CO₃ (106 mg, 1.0 mmol, 2 equiv.) and Pd(OAc)₂ (11 mg, 0.05 mmol, 0.1 equiv.). The reaction flask was fitted with an oxygen balloon, heated to 50 °C, and stirred for 3 h. The mixture was then diluted with ethyl acetate (20 mL), and washed with aqueous NaCl solution (3 X 10 mL). The organic layer was dried over anhydrous Na₂SO₄ and filtered. The filtrate was concentrated *in vacuo*, and subjected to flash chromatography (30 g of SiO₂). Elution with hexanes (100 mL), then 10:1 hexanes/EtOAc afforded *tert*-butyl *trans*-cinnamate (89 mg, 87%).

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021030
Time 11.02
INSTRUM spect
PROBHD 5 mm BBI X Y
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 3063.726 Hz
FIDRES 0.093497 Hz
AQ 5.3477874 sec
RG 362
DM 163.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.70 usec
PL1 0.00 dB
SF01 250.1315008 MHz

F2 - Processing parameters
SI 16384
SF 250.130072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CK 20.00 cm
F1P 10.000 ppm
f1 2901.30 Hz
F2P -0.500 ppm
f2 -125.07 Hz
PRGCM 0.52500 ppm/cm
HZCM 131.31825 Hz/cm

Current Data Parameters:

NAME	Carbon
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters:

Date_	Time
2002.03.11	9.17

INSTRUM spect

PROBHD 5 mm BBI X Y

PULPROG zgpg30

TD 32768

SOLVENT CDCl3

NS 1116

DS 4

SWH 13227.514 Hz

FIDRES 0.403677 Hz

AQ 1.2386804 sec

RG 5150.6

DW 37.800 usec

DE 6.00 usec

TE 300.0 K

D1 3.00000000 sec

D11 0.03000000 sec

D12 0.00000000 sec

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

NUC1	13C
P1	12.50 usec
PL1	0.00 dB
SFO1	62 9015035 MHz

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

CPDPRG2	NUC2	1H
PCPD2	130.00 usec	
PL2	3.00 dB	
PL12	30.00 dB	
PL13	32.00 dB	
SFO2	250.1310005 MHz	

F2 - Processing parameters:

SF	32768
SF	62 9592425 MHz
WDM	FM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

19 NMR file parameters:

EX	20.00 cm
F10 <td>2735.000 bpm</td>	2735.000 bpm
F11 <td>1762.401 Hz</td>	1762.401 Hz
F12 <td>5.000 bpm</td>	5.000 bpm
F13 <td>114.40 Hz</td>	114.40 Hz
PRPCH	11.000000 bpm/cm
Hz/CM	103 Hz/cm

Current Data Parameters

NAME	PROTON
EXNO	1
PRICNO	1

F2 - Acquisition Parameters

Date	Time
20021101	13.04

INSTRUM spect

PULPROG 5 mm BBI X Y

TD 32768

SOLVENT CDCl₃

NS 6

DS 4

SWH 3132.832 Hz

FIDRES 0.095606 Hz

AQ 5.2290226 sec

RG 181

DW 159.600 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

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

NUC1 ¹H

P1 6.50 usec

PL1 3.00 dB

SFO1 250.1315008 MHz

F2 - Processing parameters

SI	16384
SF	250.1300072 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	10.000 ppm
F1	2501.36 Hz
F2P	-0.500 ppm
F2	-125.07 Hz
PPMCM	0.52500 ppm/cm
HZCM	131.31825 Hz/cm

Table 2. From 6

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Current Data Parameters
NAME          carbon
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         2002101
Time          13.07
INSTRUM       spect
PROBHD        5 mm BBI X Y
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            320
DS            4
SWH           13227.514 Hz
FIDRES        0.403572 Hz
AQ            1.2386604 sec
RG            8192
DM            37.500 usec
DE            6.00 usec
TE            300.0 K
D1            3.00000000 sec
D11           0.02000000 sec
D12           0.00020000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            12.50 usec
PL1           0.00 dB
SI 01         62.9015035 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         120.00 usec
PL2           3.00 dB
PL12          30.00 dB
PL13          32.00 dB
SFO2          250.1310005 MHz

F2 - Processing parameters
S1            32768
SF            62.8952425 MHz
WON           LM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40

10 NMR plot parameters:
CX            20.00 cm
FID           2315.000 ppm
F1            132627.48 Hz
F2           -314.48 Hz
PRPCH         11.00000 ppm/cm
HZCM         6591.84706 Hz/cm
  
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Table 3. From 11

Current Data Parameters

NAME	PROTON
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20021122	9.19

INSTRUM spect

PROBHD 5 mm BBI X Y

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 8

DS 2

SWH 3053.726 Hz

FIDRES 0.093497 Hz

AQ 5.3477674 sec

RG 128

DH 163.200 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

***** CHANNEL f1 *****

NUC1 1H

P1 10.70 usec

PL1 0.00 dB

SFO1 250.1315008 MHz

F2 - Processing parameters

SI	SE
16384	250.130072 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

10 NMR plot parameters

CX	F1P	F1	F2P	F2	PPMCH	HZCM
20.00 cm	10.000 ppm	2501.30 Hz	-0.500 ppm	-125.07 Hz	0.52500 ppm/cm	131.31825 Hz/cm

Table 3. From 11

Current Data Parameters

NAME	VALUE	UNIT
EXPNO	1	
PROCNO	1	

F2 - Acquisition Parameters

NAME	VALUE	UNIT
Date_	20021123	
Time	11:14	
INSTRUM	spect	
PROBHD	5 mm BBI X Y	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	550	
DS	4	
SMH	13227.514	Hz
FIDRES	0.403672	Hz
AQ	1.2386804	sec
RG	6502	
DM	37.800	usec
DE	5.00	usec
TE	300.0	K
D1	3.00000000	sec
D12	0.03000000	sec
D12	0.0002000	sec

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

NAME	VALUE	UNIT
NUC1	13C	
P1	12.50	usec
PL1	0.00	dB
SFO1	62.5015035	MHz

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

NAME	VALUE	UNIT
CROPRG2	waltz16	
KUCC2	16	
FOF02	130.00	usec
PL2	3.00	dB
PL12	30.00	dB
PL13	32.00	dB
SFO2	250.1310005	MHz

F2 - Processing parameters

NAME	VALUE	UNIT
S1	32768	
SF	62.8952425	MHz
KDM	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

10 NMR plot parameters

NAME	VALUE	UNIT
CX	20.00	cm
F1P	215.000	ppm
F1	1352.40	Hz
F2P	-5.000	ppm
F2	-314.48	Hz
PRGCM	11.00000	ppm/cm
HZCM	691.84756	Hz/cm

Current Data Parameters

NAME	PROTON	EXPNO	PROCNO
NAME	proton	1	1
EXPNO	1		
PROCNO	1		

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DE	TE	DI
20021122	15.24	5 mm BBI X Y	5 mm BBI X Y	zgpg30	32768	CDCl3	6	4	3132.032 Hz	0.095006 Hz	5.2200226 sec	203.2	159.600 usec	300.0 K	1.00000000 sec

F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
16384	250.1300242 MHz	EM	0	0.30 Hz	0	1.00

1D NMR plot parameters

CX	F1P	F1	F2P	F2	PPMCM	HZCM
20.00 cm	10.000 ppm	2501.30 Hz	0.000 ppm	0.00 Hz	0.50000 ppm/cm	125.06501 Hz/cm

Current Data Parameters

NAME	PROTON
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	D1
20021107	14.16	SPECT	5 mm BBI X Y	zg30	32768	CDCl3	6	2	3063.726 Hz	0.693497 Hz	5.3477876 sec	203.2	163.200 usec	6.00 usec	300.0 K	1.00000000 sec

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

NUC1	HI
P1	10.70 usec
PL1	0.00 dB
SFO1	250.1315008 MHz

F2 - Processing parameters

SI	16384
SF	250.1300072 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

EX	20.00 cm
F1P	10.000 ppm
Z1	250.130 Hz
F2P	0.500 ppm
F2	125.07 Hz
PPMK	0.52500 ppm/cm
WCH	131.31073 Hz/cm

Current Data Parameters

NAME	Value
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20071107	20.39

INSTRUM spect

PROBHD 5 mm HPL X Y

PULPROG zgpg30

TD 32768

SOLVENT CDCl3

NS 466

DS 4

SWH 13277.514 Hz

FIDRES 0.403167 Hz

AQ 1.2346804 sec

RG 5160 6

DM 37.800 usec

DE 6.00 usec

TE 300.0 K

D1 3.00000000 sec

D11 0.03000000 sec

D12 0.0002000 sec

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

NUC1	PC1	PL1	SF01
13C	12.50 usec	0.00 dB	62.5015035 MHz

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

CPDPRG2	WALT16	NUC2	PC2	PL2	SF02
walt16	1H	130.00 usec	3.00 dB	30.00 dB	30.00 dB

F2 - Processing parameters

SF	SI	WDW	SSB	LB	GB	PC
62.5015035 MHz	32768	EM	0	1.00 Hz	0	1.40

1D F2 plot parameters

EX	EXP	F1	F2
20.00 usec	2715.000 dBm	132.768 MHz	1.000000 MHz

PROBHD 5 mm HPL X Y

PULPROG zgpg30

TD 32768

SOLVENT CDCl3

NS 466

DS 4

SWH 13277.514 Hz

FIDRES 0.403167 Hz

AQ 1.2346804 sec

RG 5160 6

DM 37.800 usec

DE 6.00 usec

TE 300.0 K

D1 3.00000000 sec

D11 0.03000000 sec

D12 0.0002000 sec

Current Data Parameters

NAME	proton
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20021123
Time	13.58
INSTRUM	spect
PROBHD	5 mm BBI X Y
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	6
DS	4
SWH	3132.832 Hz
FIDRES	0.095606 Hz
AQ	5.229226 sec
R6	362
DM	159.600 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	¹ H
P1	6.50 usec
PL1	3.00 dB
SFO1	250.1315008 MHz

F2 - Processing parameters

SI	16384
SF	250.130072 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	10.000 ppm
F1	2501.30 Hz
F2P	-0.500 ppm
F2	-125.07 Hz
PPMCM	0.52500 ppm/cm
HZCM	131.31825 Hz/cm

Current Data Parameters

NAME	VALUE
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20021101	15.02

INSTRUM spect

PROBHD 5 mm BRL X Y

PULPROG zgpg30

TD 32768

SOLVENT CDCl3

NS 909

DS 4

SWH 1327.514 Hz

FIDRES 0.405672 Hz

AQ 1.238600 sec

RG 5160.6

DM 37.800 usec

DE 6.00 usec

TE 300.0 K

D1 3.0000000 sec

D11 0.0300000 sec

D12 0.0002000 sec

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

NUC1	13C
P1	12.50 usec
PL1	0.00 dB
SFO1	62.5015035 MHz

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

CPDPRG2	zgpg30
NUC2 <td>1H</td>	1H
PCPD2	130.00 usec
PL2	3.00 dB
PL12	30.00 dB
PL13	32.00 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SF	32768
SR	6.2 8952625 MHz
WDM	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CX	20.00 cm
F1P	215.000 ppm
F1	135.2248 Hz
F2P	5.000 ppm
F2	314.48 Hz
NUC1CH	13.000000 ppm/c
NUC2CH	501.8460 Hz/cm