Room Temperature Cu(II)-Catalyzed Chemo- and Regioselective *Ortho*-Nitration of Arenes via C-H Functionalization

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Table of Contents

1. Mass spectra of reaction of mixture of **1a** S1
2. NMR (^1H and ^{13}C) Spectra **2a-v** S2-S45

NMR (^1H and ^{13}C) Spectra **2u-v** (Reproduced from *J. Org. Chem.* **2014**, 79, 8541. Copyright 2015 American Chemical Society)

Figure S1. Mass spectra of reaction mixture **1a** prior to work up. (Reproduced from *J. Org. Chem.* **2014**, 79, 8541. Copyright 2015 American Chemical Society)

SP-PH-PH-N-1H

exp4 PROTON

SAMPLE PREPARATION
 date Apr 4 2014 satmode n
 solvent cdcl3 wet n
 file exp
 ACQUISITION
 nu 6398.0 gain 0
 at 2.561 spin 0
 up 32768 hat 0.008
 fb 3600 pw20 16.200
 bs 4 alfa 10.000
 di 1.000
 ct 32 il n
 ct 32 in m
 TRANSMITTER
 tn N1 bs PROCESSING mn
 srfq 399.853 fn not used
 tof 363.1 fn DISPLAY
 pr 8.150 sp -65.9
 DECOUPLER
 dn C13 xfl wp 5010.5
 dof 0 xfp 3702.3
 ds mm xp 2894.9
 decwave g lp 124.5
 dpr 40
 def 17100 wc 268
 sc 0
 vs 52
 th 6
 ai cdc ph

SP-Pb-Pb-N-13C

exp5 CARBON

SAMPLE		PREPARATION	
date	Apr 4 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	n
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spin	not used
up	65536	het	0.008
fb	13800	pre90	9.500
hs	10	alfa	10.000
d1	1.000	FLAGS	
nt	10000	il	n
ct	640	in	n
TRANSMITTER		op	y
tn	cl3	hs	nn
sfrq	100.554	PROCESSING	
tof	1521.7	lb	0.50
typr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		wp	-247.9
dn	H1	wp	22435.8
dof	0	rf1	9246.5
dm	777	rfp	7764.9
decwave	w	rp	149.6
qprc	42	lp	-470.7
daf	10100	PLOT	
ws	268		
ac	0		
vs	531		
th	4		
al	cdc	ph

SP-3Me-3Me-N-1H

exp3 PROTON

SAMPLE		PREPARATION	
date	Apr 15 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	0
ACQUISITION		temp	25.0
av	6398.0	gain	32
at	2.561	spin	not used
up	32768	bat	0.008
eb	3600	pre90	16.300
bs	4	alpha	10.000
dl	1.000	FLAGS	
nt	32	il	n
ct	32	in	n
TRANSMITTER		dp	7
tn	H1	hs	mn
efrq	399.853	PROCESSING	
tofr	363.1	fn	not used
typr	58	DISPLAY	
pw	8.150	sp	-49.1
DECOUPLER		wp	4946.9
dn	C13	rf1	3702.3
dof	0	rfp	2894.9
dm	mm	rp	133.2
decwave	g	lp	-110.8
aper	40	PLOT	
daf	17100	wc	268
		ac	0
		vs	39
		th	7
		ai	cdc
		ph

SP-C-3ME-13C

Current Data Parameters
 NAME SP-C-3ME-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150421
 Time 10.43
 INSTRUM spect
 PULPROG zgpg30
 FIDRES 5 mm FAPBOC BS/PROG
 TD 32768
 SOLVENT CDCl3
 NS 507
 DS 2
 SWH 36057.691 Hz
 FWHM 1137.001 Hz
 AQ 0.4543823 sec
 RG 200.18
 DW 13.867 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 150.9279571 MHz
 ACQ1 150.9279571 MHz
 P1 10.50 usec
 PL1 95.00000000 W

===== CHANNEL f2 =====
 SF02 600.1724007 MHz
 ACQ2 600.1724007 MHz
 P2 10.50 usec
 PL2 95.00000000 W

===== CHANNEL f3 =====
 SF03 600.1724007 MHz
 ACQ3 600.1724007 MHz
 P3 10.50 usec
 PL3 95.00000000 W

F2 - Processing parameters
 SI 16384
 SF 150.9128316 MHz
 DS 2
 SWH 36057.691 Hz
 FWHM 1137.001 Hz
 AQ 0.4543823 sec
 RG 200.18
 DW 13.867 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.03000000 sec
 TD0 1

TP-SP-4Cl-Cl

8.959
8.943
8.266
8.263
7.730
7.727
7.715
7.711
7.687
7.673
7.573
7.559
7.260

10.720

-0.006

Current Data Parameters
NAME TP-SP-4Cl-Cl
EXPNO 1
PROCNO 1
Date_ 20150303
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO-200
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 14
DS 2
SWH 12018.250 Hz
FIDRES 0.170 Hz
AQ 1.3631488 sec
RG 47.16
DE 61.000000 sec
TE 298.4 K
T2 1.0000000 sec
T20 1
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 21.00000000 dB
F2 - Processing parameters
F2 120.150 MHz
WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

TP-SP-4Cl-Cl-13C

Current Data Parameters
NAME TP-SP-4Cl-Cl-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150202
Time 14.07
INSTRUM spect
PROBHD 5 mm PABBO-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 215
DS 2
SWH 36057.69 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 200.18
DM 13.867 usec
DE 6.50 usec
TE 298.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PL1 95.00000000 M

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
PCPD2 70.00 usec
PL2 21.00000000 M
PL12 0.61714000 M
PL13 0.30239999 M

F2 - Processing parameters
SI 32768
SF 150.9128220 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.40

/

3P-C-4F-13C

SP-4Me-4Me-N-13C

exp2 CARBON

SAMPLE		PRESATURATION	
date	May 7 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spin	not used
mp	65536	het	0.008
zb	13800	pw90	9.500
hs	10	alfa	10.000
dl	1.000	FLAGS	
nt	8000	il	n
ct	3600	in	n
TRANSMITTER		dp	y
tn	C13	hs	nn
sfreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
typr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		sp	-188.8
dn	H1	wp	21287.2
dof	0	rf1	9245.0
dm	yyy	rfp	7764.9
decwave	w	rp	65.5
dprc	42	lp	-387.3
dms	10100	PLOT	
vc		vc	268
sc		sc	0
vs		vs	1655
th		th	4
al		al	cdc ph

SP-4OMe-4OMe-N-1H

exp4 PROTON

SAMPLE		PREPARATION	
date	May 24 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/chem/da-	SPECIAL	25.0
ta/TP/SP/SP-01/SP--		temp	30
4OMe-4OMe-N-1H.fid		gain	not used
ACQUISITION		spin	not used
sw	6198.0	bat	0.008
at	2.561	pw90	16.300
np	32768	alfa	10.000
fb	3600	FLAGS	
bs	4	il	n
dl	1.000	in	n
nt	32	dp	y
ct	32	hs	nn
TRANSMITTER		PROCESSING	
tn	hl	fn	not used
strq	399.853	DISPLAY	-70.9
tof	363.1	sp	5017.1
tpwr	58	wp	3702.3
pw	8.150	rf1	2894.9
DECOUPLER		rfp	135.3
dn	cl3	tp	-111.4
dof	0	lp	PLOT
ds	nmn		
fs:ave	g	wc	268
	co	sc	0
	vs	147	
	th	al	cdc ph
			4

SP-4OMe-4OMe-N-11C

exp4 CARBON

SAMPLE		PREPARATION	
date	May 24 2014	setmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	25.0
ACQUISITION			
sw	25125.6	gain	30
at	1.304	spin	not used
mp	65536	het	0.008
zb	13800	pre90	9.500
hs	10	alpha	10.000
d1	1.000	FLAGS	
nt	9000	il	n
ct	1380	in	n
TRANSMITTER			
tn	cl3	hs	nn
sfreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
typr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER			
dn	h1	wp	-206.5
dof	0	rf1	21562.4
dm	yyy	rfp	9245.0
decwave	w	rp	7764.9
dprc	42	lp	63.8
daf	10100	PLOT	-340.5
wc			268
ec			0
vs			921
th			4
al			ph

SP-IPR

Sample Name:

SP-IPR

Data Collected on:

1170-MR-mercury400

Archive directory:

/export/home/champack/vmware/data

Sample directory:

File: SP-IPR

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 8 2014

Temp. 25.0 C / 298.1 K

Operator: chen

Relax. delay 1.000 sec

Pulse 45.0 degree

Acq. time 2.561 sec

Width 6398.0 Hz

32 repetitions

OBSERVE M1, 399.8509633 MHz

DATA PROCESSING

FT size 32768

Total time 2 min 12 sec

SP-IPR

Sample Name:
SP-IPR-13C
Data Collected on:
IITG-NMR-mercury400
Archive directory:
/home/chem/data/study
Sample directory:
SP-IPR-13C-01
FIDFile: SP-IPR-13C_CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 8 2014

Temp. 25.0 C / 298.1 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degree
Acq. time 1.304 sec
Width 25125.6 Hz
310 repetitions
OBSERVE C13, 100.5425863 MHz
DECOUPLE H1, 399.8529994 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 7 hr, 37 min

SP-4Et-4Et-1H

exp1 PROTON

SAMPLE PREPARATION
 date Apr 7 2014 satmode n
 solvent cdcl3 wet
 file /home/chem/da-
 ta/TP/SP/SP-01/SP-- temp 25.0
 4Et-4Et-1H.fid gain 18
 ACQUISITION spin not used
 sw 6398.0 hst 0.008
 at 2.561 pw90 16.300
 np 32768 alfa 10.000
 zb 3600
 bs 4 il n
 dl 1.000 in n
 nt 32 dp y
 ct 32 hs mn
 TRANSMITTER H1 fn not used
 tn
 sfrq 399.853 DISPLAY
 tof 363.1 sp -70.9
 tpr 58 wp 4995.3
 pw 8.150 rfl 3702.3
 DECOUPLER C13 rfp 2894.9
 dn 0 lp 134.6
 dof 0 lp -109.5
 dm mn
 decwave g wc 268
 dpr 40 sc 0
 daf 17100 vs 49
 ai cdc ph 2

SP-4Et-4Et-13C

exp9 CARBON

SAMPLE		PRESATURATION	
date	Apr 10 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spin	not used
np	65536	het	0.008
fb	13800	pw90	9.500
be	10	alfa	10.000
dl	1.000	FLAGS	
nt	8000	ll	n
ct	210	in	n
TRANSMITTER		qp	y
tn	Cl3	he	nm
sfrq	100.554	PROCESSING	
toF	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		sp	-109.9
dn	H1	wp	20598.6
dof	0	rfl	9251.9
dm	YYY	rfl	7764.9
decwave	w	rp	104.0
dpr	42	lp	-392.4
daf	10100	PLOT	
		vc	268
		sc	0
		vs	200
		th	5
		ai	cdc ph

SP-2-4-dim-N-IN

exp4 PROTON

SAMPLE		PREP	
date	May 5 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6398.0	gain	30
at	2.561	spin	not used
np	32768	het	0.008
fb	3600	pw90	16.300
hs	4	alpha	10.000
dl	1.000	FLAGS	
nt	32	il	n
ct	32	in	n
TRANSMITTER		dp	y
tn	h1	hs	nn
sfreq	399.853	PROCESSING	
tof	363.1	fn	not used
typer	58	DISPLAY	
pw	8.150	sp	-27.6
DECOUPLER		wp	4789.1
dn	cl3	xf1	3702.7
dof	0	rfp	2894.9
dm	nnn	rp	139.9
decwave	g	lp	-121.3
dpr	40	PLOT	
dmf	17100	vr	268
		zc	0
		vs	30
		th	2
		al	cdc ph

SP-2-4-dime-N-13C

exp5 CARBON

SAMPLE		PRESENTATION	
date	May 5 2014	satmode	n
solvent	cdcl3	wet	n
file			
ACQUISITION		SPECIAL	
sw	25125.6	temp	25.0
at	1.304	gain	30
sp	65536	not used	
fb	13800	bat	0.008
bs	10	yr90	9.500
dl	1.000	alfa	10.000
nt	6000	il	
ct	1470	in	n
tn	C13	dp	y
sfreq	100.554	hs	mn
tof	1521.7	lb	0.50
typr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		wp	-241.7
dn	H1	wp	20873.9
dof	0	xf1	9245.8
dm	YYY	xfp	7764.9
dacwave	w	xp	82.7
dprc	42	lp	-399.4
dmf	10100	PLOT	
		wc	268
		sc	0
		vs	444
		th	3
		ai	cdc ph

SP-3-4DMe-M-1H

exp2 PROTON

SAMPLE		PRESATURATION	
date	May 6 2014	satmode	n
solvent	cdcl3	wet	n
file			
ACQUISITION		SPECIAL	
sw	6198.0	temp	25.0
at	2.561	gain	18.0
np	32768	not used	
zb	3600	pw90	0.008
bs	4	pw90	16.300
dl	1.000	alpha	10.000
nt	32	flags	
ct	32		
TRANSMITTER		RECEIVER	
tn	H1	bn	nm
sfreq	399.853	PROCESSING	
tofr	363.1	fn	not used
typer	58	DISPLAY	
pw	8.150	sp	-27.6
DECOUPLER		wp	4920.7
dn	Cl3	rf1	3702.7
dof	0	rfp	2894.9
dm	nm	rp	135.3
decwave	g	lp	-108.4
dpr	40	PLOT	
daf	17100	vc	268
		sc	0
		vs	56
		th	6
		ai	cdc
		ph

SP-3-4DiMe-X-13C

exp3 CARBON

SAMPLE		PREPARATION	
date	May 8 2014	solvent	cdcl3
file	exp	temp	25.0
ACQUISITION			
sw	25125.6	gain	30
at	1.104	spin	not used
np	65536	bat	0.008
ps	13800	ps90	9.500
hs	10	alfa	10.000
d1	1.000	FLAOS	
nt	5000	il	n
ct	210	in	n
TRANSMITTER			
tn	cl3	hs	nm
afreq	100.624	PROCESSING	
tof	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER			
dn	h1	wp	-385.9
dof	0	rf1	21958.1
dm	yyy	rfp	9252.7
dmcwv	w	rp	7764.9
dprc	42	lp	96.1
daf	10100	PLOT	
wc	268		
sc	0		
vs	279		
th	4		
si	cdc	ph

SP-3-5D1Me-N-1H

exp3 PROTON

SAMPLE		PRESATURATION	
date	Apr 27 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/chem/ds-		
ta	SP-01/SP--	temp	25.0
3-5-dimEt-1H.fid	gain	18	
ACQUISITION	spin	not used	
sw	6388.0	bat	0.008
at	2.561	pre90	16.300
np	32768	alfa	10.000
fb	3600	FLAGS	
bs	4	il	n
dl	1.000	in	n
nt	32	dp	y
ct	32	hs	mn
TRANSMITTER		PROCESSING	
tn	hl	fn	not used
efrq	399.853	DISPLAY	
tofr	363.1	sp	-27.6
tpwr	58	wp	4951.5
pw	8.150	rf1	3702.7
DECOUPLER		rfp	2894.9
dn	cl3	rp	139.2
dof	0	lp	-124.7
dm	nmn	PLOT	
dacwave	g	wc	268
dprc	40	ec	0
daf	17100	vs	34
	th		6
	ai	cdc	ph

SP-3-5D1Me-M-13C

exp2 CARBON

SAMPLE		PREPARATION	
date	Apr 26 2014	setcode	n
solvent	cdcl3	wet	n
file	cdcl3	exp	SPECIAL
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spin	not used
up	65336	bat	0.008
fb	13800	pw90	9.500
hs	10	alfa	10.000
d1	1.000	FLAGS	
nt	2000	il	n
ct	190	in	n
TRANSMITTER		dp	y
tn	C13	hs	nm
sfreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
typr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		sp	-217.2
dn	H1	wp	21166.8
dof	0	rf1	9255.7
dm	yyy	rfp	7764.9
dwave	w	rp	105.6
dprc	42	lp	-390.1
dmf	10100	PLOT	
		wc	268
		sc	0
		vs	174
		th	4
		ai	cdc
		ph

SP-2Cl-Ph-N-13C

exp4 CARBON

SAMPLE		PREPARATION	
date	Apr 23 2014	setmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
ac	25125.6	gain	30
at	1.304	spin	not used
ap	65536	het	0.008
fb	13800	psf0	9.500
bs	10	alfa	10.000
dl	1.000	FLAGS	
nt	6000	il	n
ct	280	in	n
TRANSMITTER		dp	y
tn	Cl3	bs	nn
afreq	100.554	PROCESSING	
toif	1521.7	lb	0.50
tpwr	61	fn	not used
yw	4.750	DISPLAY	
DECOUPLER		wp	-168.1
dm	H1	wp	21389.9
dof	0	rfl	9258.8
dm	Y77	rfl	7764.9
decwave	w	rp	113.5
dpr	42	lp	-393.8
daf	10100	PLOT	
vc	268		
sc	0		
vs	154		
th			
ai	cdc	ph	8

exp4 PROTON

SAMPLE				PRESERVATION			
date	May 9 2014	solvent	cdcl3	stdmode	n	n	n
file		acq	exp	temp	SPECIAL		
sw	4398.0	gain	30				
at	2.561	spin	not used				
np	32768	bat	0.000				
eb	3600	pw90	16.300				
bs	4	slfs	10.000				
dl	1.000	FLAGS					
nt	32	il					
ct	32	in					
TRANSMITTER				dp	ny		
tn	hl	bs					
sfreq	399.853	fn	not used				
tof	363.1						
tpwr	58						
pw	8.150	wp	-40.5				
DECOUPLER				sp			
dn	cl3	rfl	5104.6				
doz	0	rfl	3702.3				
dm	mmn	rfl	2894.9				
ds	mmn	g	127.5				
decwave	g	lp	-103.6				
dpwr	40						
dmf	17100	vc	268				
		ac	0				
		vs	108				
		th	6				
		al	cdc				
		ph

SP-2Cl-4F-N-13C

exp\$ CARBON

SAMPLE		PRESATURATION	
date	May 9 2014	satmode	n
solvent	cdcl3	wt	n
file	exp	SPECIAL	n
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spn	not used
up	65536	bat	0.008
fb	13800	pw90	9.500
bs	10	alfa	10.000
d1	1.000	FLAGS	
nt	5000	il	n
ct	1000	in	n
TRANSMITTER		dp	y
tn	Cl3	hs	mn
sfrq	100.624	PROCESSING	
tof	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		sp	-603.7
dn	H1	wp	20942.9
dof	0	kfl	9246.5
dm	yyy	rff	7764.9
decwave	w	xy	54.2
dpr	42	lp	-316.6
dmf	10100	PLOT	
wc	268		
sc	0		
vs	395		
th	3		
ai	cdc	ph

SP-C-CLIPR-1H

SP-napthyl-1h-1

exp4 PROTON

SAMPLE		PREPARATION	
date	May 3 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/chem/da-	SPECIAL	25.0
ts/TP/SP/SP-01/SP--	napthyl-1h-1.fid	gain	18
ts/TP/SP/SP-01/SP--	napthyl-1h-1.fid	gain	18
ACQUISITION		spin	not used
sw	6398.0	hst	0.008
at	2.561	pw90	16.300
np	32768	alfa	10.000
fb	3600	FLAGS	
bs	4	il	n
dl	1.000	in	n
nt	32	dp	y
ct	32	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.853	DISPLAY	
tof	363.1	sp	-43.7
tpwr	58	wp	5246.0
pw	8.150	rfl	798.6
DECOUPLER		rfl	0
dn	Cl3	rp	134.6
dof	0	lp	-113.4
dm	mmn	plot	
decwave	g	wc	268
dqwr	40	sc	0
daf	17100	vs	291
	th	al	cdc ph
			5

SP-napthyl-13c

Sample Name:
SP-napthyl-13c
Data Collected on:
IITG-MMR-mercury400
Archive directory:
/home/chem/data/study
Sample directory:
AD_InAnSHI_1H-01
F1AF11: CARBON

Pulse Sequence: CARBON (zgpg3)
Solvent: cdcl3
Data collected on: May 3 2014

Temp. 282.4 C / 555.5 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degree
Acq. time 1.304 sec
Width 25125.6 Hz
280 repetitions

OSCILLATE C13, 100.5425878 MHz
DECOUPLE H1, 399.852994 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
F1F2 PROCESSING
1.5 sec bracketing 0.5 sec
F2 slice 85538
Total time 7 hr, 37 min

SP-2Cl-4-MO2-N-1E

exp6 PROTON

SAMPLE PREPARATION
 date Apr 22 2014 satmode n
 solvent cdcl3 wet n
 file /home/chem/da- SPECIAL 25.08
 ts/TP/SP/SP-01/SP-- temp 30
 2Cl-4-MO2-N-1E.fid gain not used
 ACQUISITION
 sw 6198.0 hat 0.008
 at 2.561 pw90 16.300
 rp 32768 alfa 10.000
 bs 3600 FLAGS
 4 l1 n
 1.000 in n
 32 dp Y
 nt 32 he nm
 ct 32 he nm
 TRANSMITTER M1 fn not used
 tn 399.853
 sfrq 363.1 sp 397.7
 tof 58 wp 5179.2
 pw 8.150 rf1 3702.3
 DECOUPLER Cl3 rfp 2894.9
 dn 144.6
 dof 0 lp -106.0
 dm non PLOT
 dscwave g wc 268
 dpr 40 sc 0
 *daf 17100 vs 54
 th 5
 ai cdr ph

SP-2Cl-4-NO2-H-13C

exp4 CARBON

SAMPLE		PREPARATION	
date	Apr 27 2014	anmode	n
solvent	cdcl3	wet	n
file	cdcl3	SPFICIAL	n
ACQUISITION			
sw	25125.6	gain	30
at	1.304	spin	not used
mp	65536	het	0.008
fb	13800	ps20	9.500
bs	10	alfa	10.000
dl	1.000	FLAGS	
nt	6000	il	n
ct	1340	in	n
TRANSMITTER			
tn	Cl3	hs	nn
afreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER			
dn	H1	wp	-264.7
dof	0	xf1	20684.5
ds	YYY	xfp	7764.9
dcurve	w	xfp	-148.0
dprz	42	lp	-445.2
daf	10100	PLOT	
vc	268		
sc	0		
vs	657		
th			
al	cdc	ph	6

SP-2F-48t-N-13C

exp4 CARBON

SAMPLE		PRESATURATION	
date	May 4 2014	antmode	n
solvent	cdcl3	wet	n
file			
ACQUISITION		SPECIAL	
sw	25125.6	temp	25.0
at	1.304	gain	30
up	65536	hst	not used
fb	13800	pw90	9.500
he	10	alpha	10.000
dl	1.000	FLAGS	
nt	6000	il	n
ct	90	in	n
TRANSMITTER		dp	y
tn	cl3	he	mn
afreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		wp	-116.0
dn	h1	wp	20736.6
dof	0	xf1	9258.0
dm	y77	rfp	7764.9
decwave	w	rp	117.1
qpr	42	lp	-396.1
daf	10100	PLOT	
		wc	268
		ac	0
		vs	156
		th	6
		ai	cdc
		ph

exp2 PROTON

SP-2-4-41m-Ph-N-13C

exp3 CARBON

SAMPLE		PREPARATION	
date	May 15 2014	satmode	n
solvent	dms	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	epim	not used
rp	65536	hst	0.008
fb	13800	ps90	9.500
hs	10	alfa	10.000
cl	1.000	FLAGS	
nt	10000	il	n
ct	1200	in	n
tn	CL3	hs	y
sfreq	100.554	PROCESSING	
tof	1521.7	lb	0.50
tpwr	41	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		wp	-138.8
dn	H1	wp	22698.0
do	0	rf1	8772.7
dm	Y77	rfp	7764.9
decwave	w	rp	84.7
qpr	42	lp	-383.5
qmf	10100	PLOT	
wc	263		
sc	c		
vs	276		
th	8		
ai	cdc	ph

SP-2-6dimethyl-N-1H

oxy2 PROTON

SAMPLE		PRESATURATION	
date	May 12 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/chem/da-		
ts/TP/SP-01/SP--	temp	SPECIAL	25.0
2-6dimethyl-N-1H-fi-	gain	18	
d	spin	not used	
ACQUISITION	het	0.008	
sv	6398.0	pr90	16.300
at	2.561	alfa	10.000
mp	32768		
fb	3600	il	FLAGS
ba	4	in	n
di	1.000	dp	y
nt	32	hs	mn
ct	32	PROCESSING	
TRANSMITTER	fn	not used	
tn	N1	DISPLAY	
afreq	399.853	wp	-79.9
tof	363.1	wp	4951.5
tpwr	58	rfl	3702.3
pw	8.150	rfl	2894.9
DECOUPLER	tp	134.5	
dm	CL3	lp	-109.0
dof	0	PLOT	
dm	min	wc	268
decwave	g	sc	0
dpr	40	vs	23
daf	17100	th	3
	ai	cdc	ph

SP-2-6dIme4Me-N-13C

exp2 CARBON

SAMPLE		PRESATURATION	
date	May 13 2014	setmode	n
solvent	cdcl3	wet	n
file	/home/chem/da-	SPECIAL	
ta/tp/SP/SP-01/SP--	temp	25.0	
2-6dIme4Me-N-13C.f-	gain	30	
	id	spin	not used
	hat	0.008	
ac	pw90	9.500	
at	1.304	alpha	10.000
tp	65536	FLAGS	
fb	13800	il	n
be	10	in	n
d1	1.000	dp	y
nt	2000	hs	nm
ct	50	PROCESSING	
tn	TRANSMITTER	lb	0.50
sfreq	100.554	fn	not used
tof	1521.7	wp	-187.3
tpwr	61	wp	20804.9
pw	4.750	rf1	9260.3
	DECOUPLER	rfp	7764.9
dn	H1	rp	104.6
dof	0	lp	-387.8
dm	YYY	PLOT	
decwave	w	wc	268
dpr	42	sc	0
dmf	10100	vs	88
	th	ah	cdc
	ph		6

SP-2-6-dime-4NO2-M-1H

exp4 PROTON

SAMPLE		PRESATURATION	
date	May 17 2014	satmode	n
solvent	cdcl3	wet	n
file			
ACQUISITION		SPECIAL	
sw	6398.0	gain	18
at	2.561	spin	not used
ap	32768	het	0.008
fb	3600	pw90	16.300
hs	4	alpha	10.000
dl	1.000	FLAGS	
nt	32	il	n
ct	32	in	n
TRANSMITTER		RECEIVER	
tn	H1	hs	mn
afreq	399.853	PROCESSING	
tof	363.1	fn	not used
typer	58	DISPLAY	
pw	8.150	sp	-31.9
DECOUPLER		wp	4898.8
dn	C13	xf1	3702.7
dof	0	xfp	2894.9
dm	mn	tp	136.3
decwave	g	lp	-118.5
dpr	40	FLOT	
def	17100	wc	268
		sc	0
		vs	65
		th	1
		ai	cdc
			ph

SP-2-6-dim-4NO2-M-13C

exp5 CARBON

SAMPLE		PRESATURATION	
date	May 18 2014	satmode	n
solvent	cdcl3	wet	n
file			
ACQUISITION		temp	25.0
sw	25125.6	gain	30
at	1.304	spin	not used
np	65536	het	0.008
fb	13800	pw90	9.500
bs	10	alife	10.000
dl	1.000	FLAGS	
nt	10000	fl	n
ct	210	in	n
TRANSMITTER		dp	y
tn	C13	hs	mn
sfrq	100.554	PROCESSING	
tof	1521.7	lb	0.50
tpwr	61	fn	not used
pw	4.750	DISPLAY	
DECOUPLER		sp	-263.2
dn	H1	wp	21183.6
dof	0	rf1	9250.4
dm	Y7Y	rfp	7764.9
decwave	w	rp	82.1
dpr	42	lp	-399.3
dpr	10100	PLOT	
wc	268		
sc	0		
vs	230		
th			
ai	cdc	ph	6

PULSE SEQUENCE	CROSSPOUSE EL 399.850602	DATA PROCESSING
Relax. delay 1.000 sec.	FT size 32768	Total time 1 minutes
Pulse 45.0 degrees		
Acq. time 2.561 sec		
Width 6398.0 Hz		
32 repetitions		

SP-487-NHAC1
 Solvent: cdcl3
 Temp: 25.0 C / 298.1 K
 Operator: chem
 File: SP-487-NHAC1
 Mercury-400 *H1Q-NMR*

SP-487_13C

Current Data Parameters
 NAME SP-487_13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140319
 Time 12.20
 INSTRUM spect
 PROBHD 5 mm FAPBBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 443
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 301.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9137348 MHz
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

<p>NAME: 2v</p>	<p>EXP: 01</p>	<p>DATE: 01/11/2019</p>	<p>TIME: 11:39:50</p>
<p>Relax. delay 1.000 sec</p>	<p>Solvent: cdcl3</p>	<p>FT size 12768</p>	<p>Temp. 25.0 C / 298.1 K</p>
<p>Pulse 45.0 degrees</p>	<p>Temp. 25.0 C / 298.1 K</p>	<p>Total time 1 minutes</p>	<p>Operator: chm</p>
<p>Acq. time 2.561 sec</p>	<p>Operator: chm</p>	<p>Mercury-400</p>	<p>11/11/2019</p>
<p>Width 6398.0 Hz</p>	<p>Mercury-400</p>	<p>11/11/2019</p>	<p>11/11/2019</p>
<p>132 repetitions</p>	<p>11/11/2019</p>	<p>11/11/2019</p>	<p>11/11/2019</p>

<p>EXPERIMENTAL</p> <p>Relax: delay: 1.000 sec</p> <p>Pulse: 45.0 degree</p> <p>Acq: time: 1.304 sec</p> <p>Width: 25125.6 Hz</p> <p>15470 repetitions</p>	<p>OBSERVE: 13C, 100.625893</p> <p>DECOUPLE: H1, 399.8529984</p> <p>Power: 42 dB</p> <p>continuously on</p> <p>WALTZ-16 modulated</p>	<p>DATA PROCESSING</p> <p>Line broadening: 0.5 Hz</p> <p>FT size: 65536</p> <p>Total time: 9.9 hours</p>	<p>SOLVENT: CDCl3</p> <p>Temp: 25.0 C / 298.1 K</p> <p>Operator: chem</p>
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