1,1,1-Tris(hydroxymethyl)ethane as a New, Efficient, and Versatile Tripod-Ligand for Copper-Catalyzed Cross-Coupling Reactions of Aryl Iodides with Amides, Thiols, and Phenols

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Typical Procedure (Table 1, entry 10): Cs₂CO₃ (661 mg, 2.03 mmol), CuI (19 mg, 0.1 mmol, 10 mol%), and 1,1,1-tris(hydroxymethyl)ethane (12 mg, 0.1 mmol, 10 mol%) were added to a screw-capped test tube with a septum. The tube was evacuated with heating and back-filled with nitrogen three times. Dioxane (1.8 mL), DMF (0.2 mL), iodobenzene (0.112 mL, 1.0 mmol), and 2-pyrrolidone (0.094 mL, 1.2 mmol) were added by syringe at room temperature. After the septum of tube was exchanged with a Teflon screw-cap, the reaction mixture was heated at 110 °C for 24 h, and then allowed to cool to room temperature. The reaction mixture was directly passed through celite. After rinsed with further 50 mL of ethyl acetate, the combined filtrate was evaporated by vacuum to yield the crude product. The residue was purified by column chromatography on silica gel using hexane/ethyl acetate (1:1) as eluent to give a white solid of 1-phenylpyrrolidin-2-one (158.1 mg, 98 %).

1-Phenylpyrrolidin-2-one (Table 2, entry 1)

White solid; ¹H NMR(400 MHz, CDCl₃) δ 7.61(2H, d, J=7.6 Hz), 7.37(2H, t, J=7.2 Hz), 7.15(1H, t, J=7.2 Hz), 3.87(2H, t, J=6.8 Hz), 2.62(2H, t, J=8.0 Hz), 2.15-2.20(2H, m)

¹³C NMR(100 MHz, CDCl₃) δ 17.6, 32.5, 48.4, 119.6, 124.1, 128.5, 139.1, 173.9.

Reference: Cristau, H. -J.; Cellier, P. P.; Spindler J. -F.; Taillefer, M. *Chem. Eur. J.* **2004**, *10*, 5607

1-(4-Methoxyphenyl)pyrrolidin-2-one (Table 2, entry 3)

White solid; ^1H NMR (400 MHz, CDCl_3) δ 7.49(2H, d, $J=8.8$ Hz), 6.89(2H, d, $J=9.2$ Hz), 3.81(2H, t, $J=6.4$ Hz), 3.79(3H, s), 2.58(2H, t, $J=8.0$ Hz), 2.09-2.17(2H, m).

^{13}C NMR (100 MHz, CDCl_3) δ 17.8, 32.3, 49.0, 55.3, 113.9, 121.7, 132.5, 156.4, 173.8.

Reference: Easton, C. J.; Pitt, M. J.; Ward, C. M. *Tetrahedron* **1995**, 51, 12781.

1-(2-Methoxyphenyl)-2-pyrrolidinone (Table 2, entry 5)

Brown oil; ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.29(2H, m), 6.95-6.99(2H, m), 3.83(3H, s), 3.75(2H, t, $J=6.8$ Hz), 2.55(2H, t, $J=8.0$ Hz), 2.14-2.21(2H, m).

^{13}C NMR (100 MHz, CDCl_3) δ 18.74, 31.01, 49.76, 55.43, 111.89, 120.67, 127.07, 128.42, 128.45, 154.66, 174.98.

Reference: Duplantier, A. J.; Andresen, C. J.; Cheng, J. A.; Cohan, V. L.; Decker, C.; DiCapua, F. M.; Kraus, K. G.; Johnson, K. L.; Turner, C. R.; UmLand, J. P.; Watson, J. W.; Wester, R. T.; William, A. S.; William, J. A. *J. Med. Chem.* **1998**, 41, 2268.

1-(4-Acetylphenyl)pyrrolidin-2-one (Table 2, entry 7)

White solid; ^1H NMR (400 MHz, CDCl_3) δ 7.98(2H, d, $J=9.2$ Hz), 7.75(2H, d, $J=9.2$ Hz), 3.91(2H, t, $J=7.2$ Hz), 2.65(2H, t, $J=8.4$ Hz), 2.59(3H, s), 2.17-2.24(2H, m).

^{13}C NMR (100 MHz, CDCl_3) δ 17.3, 25.9, 47.9, 118.1, 128.8, 131.9, 143.1, 174.3, 196.4.

EI-MS m/z (rel.int %): 203(M^+ , 43), 188(100), 148(34), 105(15), 77(12).

HRMS Calcd. for $\text{C}_{12}\text{H}_{13}\text{NO}_2$: 203.0954; Found : 203.0946.

3-Phenyloxazolidin-2-one (Table 2, entry 10)

White solid; ^1H NMR (400 MHz, CDCl_3) δ 7.55 (2H, d, $J=7.6$ Hz), 7.39 (2H, t, $J=7.6$ Hz), 7.15 (1H, t, $J=7.6$ Hz), 4.49 (2H, t, $J=8.4$ Hz), 4.07 (2H, t, $J=8.4$ Hz).

^{13}C NMR (100 MHz, CDCl_3) δ 45.0, 61.2, 118.0, 123.9, 128.9, 138.1, 155.2.

Reference: Cristau, H. -J.; Cellier, P. P.; Spindler J. -F.; Taillefer, M. *Chem. Eur. J.* **2004**, *10*, 5607.

Diphenyl sulfide (Table 3, entry 1)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.21-7.36 (10H, m)

^{13}C NMR (100 MHz, CDCl_3) δ 127.0, 129.1, 131.0, 135.8.

Reference: Bates, C. G.; Gujadhur, R. K.; Venkataraman, D. *Org. Lett.* **2002**, *4*, 2803.

1-Methoxy-4-(phenylthio)benzene (Table 3, entry 2 and 5)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.40 (2H, d, $J=8.4$ Hz), 7.09-7.23 (5H, m), 6.88 (2H, d, $J=8.4$ Hz), 3.78 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 55.2, 114.9, 124.2, 125.7, 128.1, 128.8, 135.2, 138.5, 159.7.

Reference: Bates, C. G.; Gujadhur, R. K.; Venkataraman, D. *Org. Lett.* **2002**, *4*, 2803.

1-Methoxy-2-(phenylthio)benzene (Table 3, entry 3 and 7)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.19-7.35 (6H, m), 7.07 (1H, dd, $J=7.6$ Hz), 6.82-6.88 (2H, m), 3.82 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 55.7, 110.8, 121.1, 123.9, 126.9, 128.3, 129.0, 131.3, 131.6, 134.5, 157.3.

Reference: Bates, C. G.; Gujadhur, R. K.; Venkataraman, D. *Org. Lett.* **2002**, *4*, 2803.

4-Phenylsulfanylacetophenone (Table 3, entry 4)

White solid; ^1H NMR (400 MHz, CDCl_3) δ 7.80 (2H, d, $J=8.4$ Hz), 7.47-7.50 (2H, m), 7.37-7.39 (3H, m), 7.20 (2H, d, $J=8.4$ Hz), 2.53 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 26.3, 127.4, 128.6, 128.8, 129.5, 131.9, 133.6, 134.4, 144.7, 196.9.

Reference: Itoh, T.; Mase, T. *Org. Lett.* **2004**, 6, 4587.

4-Chlorodiphenyl sulfide (Table 3, entry 6)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.25-7.38 (9H, m).

^{13}C NMR (100 MHz, CDCl_3) δ 127.39, 129.28, 129.29, 131.28, 131.98, 132.95, 134.62, 135.08.

Reference: Ishiyama, T.; Mori, M.; Suzuki, A.; Miyaura, N. *J. Organometallic Chem.* **1996**, 525, 225

(n-Dodecylthio)benzene (Table 3, entry 8)

White solid; ^1H NMR (400 MHz, CDCl_3) δ 7.11-7.31 (5H, m), 2.89 (2H, t), 1.12-1.67 (20H, m), 0.88 (3H, t).

^{13}C NMR (100 MHz, CDCl_3) δ 14.07, 22.66, 28.82, 29.11, 29.14, 29.32, 29.48, 29.55, 29.62, 31.89, 33.52, 125.52, 128.73, 137.08.

Reference: Pastor, S. D.; Hessel, E. T. *J. Org. Chem.* **1985**, 50, 4812.

Diphenyl ether (Table 4, entry 1)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.35 (4H, m), 7.09-7.11 (2H, m), 7.01-7.02 (4H, m).

^{13}C NMR (100 MHz, CDCl_3) δ 118.8, 123.1, 129.6, 157.1.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

1-Methoxy-4-phenoxybenzene (Table 4, entry 2)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.25-7.32 (2H, m), 6.86-7.06 (7 H, m), 3.80 (3 H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 55.6, 114.8, 117.5, 120.8, 122.4, 129.6, 150.1, 155.9, 158.5.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

Phenyl *m*-tolyl ether (Table 4, entry 3)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.34 (2H, m), 7.19-7.22 (1H, m), 7.08-7.10 (1H, m), 6.99-7.01 (2H, m), 6.91-6.92 (1H, m), 6.80-6.83 (2H, m), 2.32 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 21.4, 115.8, 118.7, 119.5, 123.0, 124.0, 129.4, 129.6, 139.8, 157.1, 157.3.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

2-Methylphenyl phenyl ether (Table 4, entry 4)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.23-7.31 (3H, m), 7.01-7.17 (3H, m), 6.88-6.91 (3H, m), 2.24 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 16.1, 117.3, 119.8, 122.3, 123.9, 127.1, 129.6, 130.0, 131.4, 154.5, 157.9.

Reference: Cristau, H. J.; Cellier, P. P.; Hamada, S.; Spindler, J. F.; Tailleiter, M. *Org. Lett.* **2004**, 6, 913

3,5-Dimethylphenyl phenyl ether (Table 4, entry 5)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.34 (2H, m), 7.08-7.10 (1 H, m), 6.99-7.01 (2H, m), 6.75 (1 H, s), 6.63 (1 H, s), 2.28 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 21.3, 116.5, 118.8, 122.9, 124.9, 129.6, 139.5, 157.1, 157.4.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

Phenyl 4-methylphenyl ether (Table 4, entry 6)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.28-7.31 (2H, m), 7.12-7.13 (2H, m), 7.04-7.06 (1H, m), 6.96-6.98 (2H, m), 6.90-6.91 (2H, m), 2.32 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 20.7, 118.3, 119.1, 122.8, 129.6, 130.2, 132.8, 154.6, 157.7.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

1-Methoxy-4-*m*-tolyloxybenzene (Table 4, entry 7)

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.16 (2H, t, $J=7.8$ Hz), 6.96-6.97 (2H, m), 6.84-6.88 (3H, m), 6.73-6.75 (2H, m), 3.79 (3H, s), 2.30 (3H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 21.4, 55.6, 114.5, 114.7, 118.2, 120.8, 123.2, 129.3, 139.7, 150.1, 155.7, 158.4.

Reference: Ma, D.; Cai, Q. *Org. Lett.* **2003**, 5, 3799.

3',5'-Dimethyl-4-methoxydiphenyl ether (Table 4, entry 8)

Colorless solid; ^1H NMR (400 MHz, CDCl_3) δ 6.97 (2H, d, $J=9.0$ Hz), 6.88 (2H, d, $J=9.6$ Hz), 6.68 (1H, s), 6.55 (2H, s), 3.80 (3H, s), 2.26 (6H, s).

^{13}C NMR (100 MHz, CDCl_3) δ 21.3, 55.6, 114.7, 115.2, 120.8, 124.1, 139.4, 150.2, 155.7, 158.4.

Reference: Cristau, H. J.; Cellier, P. P.; Hamada, S.; Spindler, J. F.; Tailleter, M. *Org. Lett.* **2004**, 6, 913.

STANDARD 1H OBSERVE

exp1 std1h

SAMPLE

date Mar 24 2006

solvent CDC13

file exp

ACQUISITION

sfrq 400.444

tn H1

at 2.728

np 32768

sw 6006.0

fb not used

bs 4

tpwr 57

pw 6.0

d1 0

tof 500.0

nt 128

ct 52

alock n

gain 6

il FLAGS

in n

dp y

DISPLAY

sp -200.3

wp 4004.2

vs 45

sc 0

wc 250

hzmm 16.02

is 1276.91

rfl 496.5

rfp 0

th 2

ins 100.000

nm ph

DEC. & VT

dfrq 400.448

dn H1

dpwr 30

dof 0

dm nnn

dmm c

dmt 200

PROCESSING

lb 0.10

wtfile

proc ft

fn 65536

werr

wexp

wbs

wnt

n

6

n

n

y

-200.3

4004.2

45

0

250

16.02

1276.91

496.5

0

2

100.000

ph

7.510
7.490
7.268
7.249
7.229
7.043
7.025
7.006

3.714
3.697
3.679

2.480
2.459
2.439
2.033
2.014
1.985
1.976
1.957

1-Phenylpyrrolidin-2-one
Table 2, entry 1

13C OBSERVE

exp5 std13c

SAMPLE DEC. & VT
 date Mar 24 2006 dfrq 400.443
 solvent CDC13 dn H1
 file exp dpwr 39
 ACQUISITION dof 0
 sfrq 100.703 dm YYY
 tn C13 dmm w
 at 1.000 dmf 10600
 np 56022 PROCESSING
 sw 28011.2 lb 1.00
 fb 15400 wtfile
 bs 8 proc ft
 tpwr 57 fn 65536
 pw 6.7
 d1 2.000 werr
 tof 2056.1 wexp
 nt 10000 wbs
 ct 80 wnt
 alock n
 gain 36

FLAGS
 il n
 in n
 dp y

DISPLAY
 sp -0.4
 wp 20137.9
 vs 96
 sc 0
 wc 250
 hzmm 80.55
 is 500.00
 rfl 10219.9
 rfp 7753.2
 th 4
 ins 100.000
 nm no ph

STANDARD 1H OBSERVE

exp1 std1h

SAMPLE DEC. & VT
 date Mar 13 2006 dfrq 400.443
 solvent CDC13 dn H1
 file exp dpwr 30
 ACQUISITION dof 0
 sfrq 400.444 dm nnn
 tn H1 dmm c
 at 2.728 dmf 200
 np 32768
 sw 6006.0 lb 0.10
 fb not used wtfile ft
 bs 4 proc
 tpwr 57 fn 65536
 pw 6.0
 d1 0 werr
 tof 500.0 wexp
 nt 128 wbs
 ct 104 wnt
 alock n
 gain 6
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -200.3
 wp 4004.2
 vs 83
 sc 0
 wc 250
 hzmm 16.02
 is 1410.08
 rfl 459.3
 rfp 0
 th 2
 ins 2.000
 nm ph

```

13C OBSERVE
exp1 std13c
SAMPLE
date Mar 21 2006 dfrq DEC. & VT 400.443
solvent CDC13 dn H1
file exp dpwr 39
ACQUISITION dof 0
sfrq 100.703 dm yyy
tn C13 dmm w
at 1.000 dmf 10600
np 56022 PROCESSING
sw 28011.2 lb 1.00
fb 15400 wtfile
bs 8 proc ft
tpwr 57 fn 65536
pw 6.7
d1 2.000 werr
tof 2056.1 wexp
nt 10000 wbs
ct 256 wnt
alock n
gain 36
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 20137.9
vs 88
sc 0
wc 250
hzmm 80.55
is 500.00
rf1 10202.8
rfp 7753.2
th 5
ins 100.000
nm no ph

```

1-(4-Methoxyphenyl)pyrrolidin-2-one
Table 2, entry 3

13C OBSERVE

exp1 std13c

SAMPLE		DEC. & VT	
date	Mar 25 2006	dfrq	400.443
solvent	CDC13	dn	H1
file	exp	dpwr	39
ACQUISITION		dof	0
sfrq	100.703	dm	VYV
tn	C13	dmm	w
at	1.000	dmf	10600
np	56022	PROCESSING	
sw	28011.2	lb	1.00
fb	15400	wtfile	
bs	8	proc	ft
tpwr	57	fn	65536
pw	6.7		
d1	2.000	werr	
tof	2056.1	wexp	
nt	5000	wbs	
ct	776	wnt	
alock	n		
gain	36		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	20137.9		
vs	53		
sc	0		
wc	250		
hzmm	80.55		
is	500.00		
rfl	10203.6		
rfp	7753.2		
th	2		
ins	100.000		
nm	no	ph

STANDARD 1H NMR

exp1 std1h

SAMPLE

date May 25 2006 dfrq 400.443

solvent CDCl3 dn H1

file exp dpwr 30

ACQUISITION

sfrq 400.444 dm 0

tn H1 dmm nnn

at 2.728 dmf 200

np 32768

sw 6006.0 lb 0.10

fb not used wtfile

bs 4 proc ft

tpwr 57 fn 65536

pw 6.0

dl 0 werr

tof 500.0 wexp

nt 128 wbs

ct 96 wnt

alock n

gain 20

FLAGS

il n

in n

dp Y

DISPLAY

sp -200.3

wp 4004.2

vs 64

sc 0

wc 250

h2mm 16.02

is 10883.02

rfl 469.1

rfp 0

th 4

ins 100.000

nm ph

4.511
4.492
4.471
4.092
4.070
4.052

1.575

-0.001

13C OBSERVE

exp1 std13c

SAMPLE DEC. & VT
date Mar 25 2006 dfrq 400.443
solvent CDC13 dn H1
file exp dpwr 39
ACQUISITION dof 0
sfrq 100.703 dm yyy
tn C13 dmm w
at 1.000 dmf 10600
np 56022 PROCESSING
sw 28011.2 lb 1.00
fb 15400 wtfile
bs 8 proc ft
tpwr 57 fn 65536
pw 6.7
d1 2.000 werr
tof 2056.1 wexp
nt 10000 wbs
ct 72 wnt
alock n
gain 36
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 22152.0
vs 67
sc 0
wc 250
hzmm 88.61
is 500.00
rfl 10205.3
rfp 7753.2
th 3
ins 100.000
nm no ph

3-Phenyloxazo-2-one
Table 2, entry 10

STANDARD 1H NMR

exp1 std1h

SAMPLE

date May 25 2006

solvent CDC13

file exp

ACQUISITION

sfrq 400.444

tn H1

at 2.728

np 32768

sw 6006.0

fb not used

bs 4

tpwr 57

pw 6.0

d1 0

tof 500.0

nt 128

ct 40

alock n

gain 20

FLAGS

il n

in n

dp y

DISPLAY

sp -200.3

wp 4004.2

vs 62

sc 0

wc 250

hzmm 16.02

is 1356.85

rfl 474.4

rfp 0

th 3

ins 100.000

nm ph

DEC. & VT

400.443

H1

30

0

nnn

c

200

PROCESSING

0.10

ft

65536

7.188

7.185

7.151

7.146

7.136

7.134

7.131

7.106

7.299

7.296

7.293

7.289

7.278

7.275

7.254

7.250

7.247

7.242

7.239

7.234

7.229

7.222

7.218

7.215

7.212

Diphenyl sulfide
Table 3, entry 1

13C OBSERVE

exp1 std13c

SAMPLE DEC. & VT
date May 25 2006 dfrq 400.443
solvent CDC13 dn H1
file exp dpwr 39
ACQUISITION dof 0
sfrq 100.703 dm yyy
tn C13 dmm w
at 1.000 dmf 10600
np 56022 PROCESSING
sw 28011.2 lb 1.00
fb 15400 wtfile
bs 8 proc ft
tpwr 57 fn 65536
pw 6.7
d1 2.000 werr
tof 2056.1 wexp
nt 10000 wbs
ct 176 wnt
alock n
gain 36
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 20137.9
vs 39
sc 0
wc 250
hzmm 80.55
is 500.00
rfl 10189.9
rfp 7753.2
th 2
ins 100.000
nm no ph

135.801
131.038
129.171
127.023

77.323
77.000
76.686

Diphenyl sulfide
Table 3, entry 1

13C OBSERVE

exptl std13c

SAMPLE DEC. & VT
date Apr 1 2006 dfrq 400.443
solvent CDC13 dn H1
file exp dpwr 39
ACQUISITION dof 0
sfrq 100.703 dm yyy
tn C13 dmm w
at 1.000 dmf 10600
np 56022 PROCESSING
sw 28011.2 lb 1.00
fb 15400 wtfile
bs 8 proc ft
tpwr 57 fn 65536
pw 6.7
d1 2.000 werr
tof 2056.1 wexp
nt 10000 wbs
ct 104 wnt
alock n
gain 36
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 22152.0
vs 97
sc 0
wc 250
hzmm 88.61
is 500.00
rfl 10207.9
rfp 7753.2
th 4
ins 100.000
nm no ph

159.734
138.518
135.241
128.831
128.109
125.656
124.204
114.899
77.314
77.000
76.677
55.206

1-Methoxy-4-(phenylthio)benzene
Table 3, entry 2 and 5

200 180 160 140 120 100 80 60 40 20 ppm

13C OBSERVE

exp1 std13c

SAMPLE		DEC. & VT	
date	Apr 10 2006	dfrq	400.443
solvent	CDC13	dn	H1
file	exp	dpwr	39
ACQUISITION		dof	0
sfrq	100.703	dm	YYY
tn	C13	dmm	w
at	1.000	dmf	10600
np	56022	PROCESSING	
sw	28011.2	lb	1.00
fb	15400	wtfile	
bs	8	proc	ft
tpwr	57	fn	65536
pw	6.7	werr	
d1	2.000	wexp	
tof	2056.1	wbs	
nt	10000	wnt	
ct	168		
alock	n		
gain	36		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	20137.9		
vs	76		
sc	0		
wc	250		
hzmm	2.43		
is	500.00		
rfl	10208.7		
rfp	7753.2		
th	5		
ins	100.000		
nm	no ph

13C OBSERVE

exp1 std13c

SAMPLE		DEC. & VT	
date	Apr 8 2006	dfreq	400.443
solvent	CDCl3	dn	H1
file	exp	dpwr	39
ACQUISITION		dof	0
sfrq	100.703	dm	VYV
tn	C13	dmm	w
at	1.000	dmf	10600
np	56022	PROCESSING	
sw	28011.2	lb	1.00
fb	15400	wtfile	
bs	8	proc	ft
tpwr	57	fn	65536
pw	6.7		
d1	2.000	werr	
tof	2056.1	wexp	
nt	10000	wbs	
ct	112	wnt	
alock	n		
gain	36		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	22152.0		
vs	99		
sc	0		
wc	250		
hzmm	3.03		
is	500.00		
rfl	10204.5		
rfp	7753.2		
th	4		
ins	100.000		
nm	no ph

STANDARD 1H OBSERVE

exp1 std1h

SAMPLE
 date May 20 2006 dfrq 400.443
 solvent CDC13 dn H1
 file exp dpwr 30
 ACQUISITION
 sfrq 400.444 dof 0
 tn H1 dmm nnn
 at 2.728 dmf 200
 np 32768
 sw 6006.0 lb 0.10
 fb not used wtfile
 bs 4 proc ft
 tpwr 57 fn 65536
 pw 6.0
 d1 0 werr
 tof 500.0 wexp
 nt 128 wbs
 ct 28 wnt
 alock n
 gain 20
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -200.3
 wp 4004.2
 vs 75
 sc 0
 wc 250
 hzmm 0.55
 is 500.00
 rfl 470.0
 rfp 0
 th 20
 ins 100.000
 nm ph

7.337
 7.333
 7.317
 7.257
 7.253

PROCESSING

4-Chlorodiphenyl sulfide
 Table 3, entry 6

¹³C OBSERVE

exp1 std13c

SAMPLE		DEC. & VT	
date	Apr 20 2006	dfrq	400.443
solvent	CDC13	dn	H1
file	exp	dpwr	39
ACQUISITION		dof	0
sfrq	100.703	dm	YY
tn	C13	dmm	w
at	1.000	dmf	10600
np	56022	PROCESSING	
sw	28011.2	lb	1.00
fb	15400	wtfile	
bs	8	proc	ft
tpwr	57	fn	65536
pw	6.7		
d1	2.000	werr	
tof	2056.1	wexp	
nt	10000	wbs	
ct	120	wnt	
alock	n		
gain	36		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	20137.9		
vs	64		
sc	0		
wc	250		
hzmm	80.55		
is	500.00		
rfl	10195.9		
rfp	7753.2		
th	2		
ins	100.000		
nm	no	ph

4-Chlorodiphenyl sulfide
Table 3, entry 6

STANDARD 1H NMR OBSERVED

7.17	7.14	7.10	7.06	7.04	7.03	7.02	7.01	7.00	6.99	6.98	6.97	6.96	6.95	6.94	6.93	6.92	6.91	6.90	6.89	6.88	6.87	6.86	6.85	6.84	6.83	6.82	6.81	6.80	6.79	6.78	6.77	6.76	6.75	6.74	6.73	6.72	6.71	6.70	6.69	6.68	6.67	6.66	6.65	6.64	6.63	6.62	6.61	6.60	6.59	6.58	6.57	6.56	6.55	6.54	6.53	6.52	6.51	6.50	6.49	6.48	6.47	6.46	6.45	6.44	6.43	6.42	6.41	6.40	6.39	6.38	6.37	6.36	6.35	6.34	6.33	6.32	6.31	6.30	6.29	6.28	6.27	6.26	6.25	6.24	6.23	6.22	6.21	6.20	6.19	6.18	6.17	6.16	6.15	6.14	6.13	6.12	6.11	6.10	6.09	6.08	6.07	6.06	6.05	6.04	6.03	6.02	6.01	6.00	5.99	5.98	5.97	5.96	5.95	5.94	5.93	5.92	5.91	5.90	5.89	5.88	5.87	5.86	5.85	5.84	5.83	5.82	5.81	5.80	5.79	5.78	5.77	5.76	5.75	5.74	5.73	5.72	5.71	5.70	5.69	5.68	5.67	5.66	5.65	5.64	5.63	5.62	5.61	5.60	5.59	5.58	5.57	5.56	5.55	5.54	5.53	5.52	5.51	5.50	5.49	5.48	5.47	5.46	5.45	5.44	5.43	5.42	5.41	5.40	5.39	5.38	5.37	5.36	5.35	5.34	5.33	5.32	5.31	5.30	5.29	5.28	5.27	5.26	5.25	5.24	5.23	5.22	5.21	5.20	5.19	5.18	5.17	5.16	5.15	5.14	5.13	5.12	5.11	5.10	5.09	5.08	5.07	5.06	5.05	5.04	5.03	5.02	5.01	5.00	4.99	4.98	4.97	4.96	4.95	4.94	4.93	4.92	4.91	4.90	4.89	4.88	4.87	4.86	4.85	4.84	4.83	4.82	4.81	4.80	4.79	4.78	4.77	4.76	4.75	4.74	4.73	4.72	4.71	4.70	4.69	4.68	4.67	4.66	4.65	4.64	4.63	4.62	4.61	4.60	4.59	4.58	4.57	4.56	4.55	4.54	4.53	4.52	4.51	4.50	4.49	4.48	4.47	4.46	4.45	4.44	4.43	4.42	4.41	4.40	4.39	4.38	4.37	4.36	4.35	4.34	4.33	4.32	4.31	4.30	4.29	4.28	4.27	4.26	4.25	4.24	4.23	4.22	4.21	4.20	4.19	4.18	4.17	4.16	4.15	4.14	4.13	4.12	4.11	4.10	4.09	4.08	4.07	4.06	4.05	4.04	4.03	4.02	4.01	4.00	3.99	3.98	3.97	3.96	3.95	3.94	3.93	3.92	3.91	3.90	3.89	3.88	3.87	3.86	3.85	3.84	3.83	3.82	3.81	3.80	3.79	3.78	3.77	3.76	3.75	3.74	3.73	3.72	3.71	3.70	3.69	3.68	3.67	3.66	3.65	3.64	3.63	3.62	3.61	3.60	3.59	3.58	3.57	3.56	3.55	3.54	3.53	3.52	3.51	3.50	3.49	3.48	3.47	3.46	3.45	3.44	3.43	3.42	3.41	3.40	3.39	3.38	3.37	3.36	3.35	3.34	3.33	3.32	3.31	3.30	3.29	3.28	3.27	3.26	3.25	3.24	3.23	3.22	3.21	3.20	3.19	3.18	3.17	3.16	3.15	3.14	3.13	3.12	3.11	3.10	3.09	3.08	3.07	3.06	3.05	3.04	3.03	3.02	3.01	3.00	2.99	2.98	2.97	2.96	2.95	2.94	2.93	2.92	2.91	2.90	2.89	2.88	2.87	2.86	2.85	2.84	2.83	2.82	2.81	2.80	2.79	2.78	2.77	2.76	2.75	2.74	2.73	2.72	2.71	2.70	2.69	2.68	2.67	2.66	2.65	2.64	2.63	2.62	2.61	2.60	2.59	2.58	2.57	2.56	2.55	2.54	2.53	2.52	2.51	2.50	2.49	2.48	2.47	2.46	2.45	2.44	2.43	2.42	2.41	2.40	2.39	2.38	2.37	2.36	2.35	2.34	2.33	2.32	2.31	2.30	2.29	2.28	2.27	2.26	2.25	2.24	2.23	2.22	2.21	2.20	2.19	2.18	2.17	2.16	2.15	2.14	2.13	2.12	2.11	2.10	2.09	2.08	2.07	2.06	2.05	2.04	2.03	2.02	2.01	2.00	1.99	1.98	1.97	1.96	1.95	1.94	1.93	1.92	1.91	1.90	1.89	1.88	1.87	1.86	1.85	1.84	1.83	1.82	1.81	1.80	1.79	1.78	1.77	1.76	1.75	1.74	1.73	1.72	1.71	1.70	1.69	1.68	1.67	1.66	1.65	1.64	1.63	1.62	1.61	1.60	1.59	1.58	1.57	1.56	1.55	1.54	1.53	1.52	1.51	1.50	1.49	1.48	1.47	1.46	1.45	1.44	1.43	1.42	1.41	1.40	1.39	1.38	1.37	1.36	1.35	1.34	1.33	1.32	1.31	1.30	1.29	1.28	1.27	1.26	1.25	1.24	1.23	1.22	1.21	1.20	1.19	1.18	1.17	1.16	1.15	1.14	1.13	1.12	1.11	1.10	1.09	1.08	1.07	1.06	1.05	1.04	1.03	1.02	1.01	1.00	0.99	0.98	0.97	0.96	0.95	0.94	0.93	0.92	0.91	0.90	0.89	0.88	0.87	0.86	0.85	0.84	0.83	0.82	0.81	0.80	0.79	0.78	0.77	0.76	0.75	0.74	0.73	0.72	0.71	0.70	0.69	0.68	0.67	0.66	0.65	0.64	0.63	0.62	0.61	0.60	0.59	0.58	0.57	0.56	0.55	0.54	0.53	0.52	0.51	0.50	0.49	0.48	0.47	0.46	0.45	0.44	0.43	0.42	0.41	0.40	0.39	0.38	0.37	0.36	0.35	0.34	0.33	0.32	0.31	0.30	0.29	0.28	0.27	0.26	0.25	0.24	0.23	0.22	0.21	0.20	0.19	0.18	0.17	0.16	0.15	0.14	0.13	0.12	0.11	0.10	0.09	0.08	0.07	0.06	0.05	0.04	0.03	0.02	0.01	0.00
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exp1 std1h

SAMPLE

date May 14 2006 dffg 400.443

solvent CDC13 dn H1

file exp dpwr 30

ACQUISITION

sfrq 400.444 dof 0

tn H1 dm nnn

at 2.728 dmm C

np 32768 dmf 200

sw 6006.0 lb 0.10

fb not used wtfile

bs 4 proc ft

tpwr 57 fn 65536

pw 6.0

d1 0 werr

tof 500.0 wexp

nt 128 wbs

ct 48 wnt

alock n

gain 0

FLAGS

il n

in n

dp y

DISPLAY

sp -200.3

wp 3804.1

vs 108

sc 0

wc 250

hzmm 15.22

is 6299.66

rfl 487.2

rfl 0

th 2

ins 100.000

nm ph

(n-Dodecylthio)benzene

Table 3, entry 8

13C OBSERVE

exp1 std13c

SAMPLE		DEC. & VT	
date	May 14 2006	dfrq	400.443
solvent	CDC13	dn	H1
file	exp	dpwr	39
ACQUISITION		dof	0
sfrq	100.703	dm	yyy
tn	C13	dmm	w
at	1.000	dmf	10600
np	56022	PROCESSING	
sw	28011.2	lb	1.00
fb	15400	wtfile	
bs	8	proc	ft
tpwr	57	fn	65536
pw	6.7		
d1	2.000	werr	
tof	2056.1	wexp	
nt	10000	wbs	
ct	72	wnt	
alock	n		
gain	36		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-0.4		
wp	22152.0		
vs	108		
sc	0		
wc	250		
hzmm	88.61		
is	500.00		
rfl	10197.6		
rfp	7753.2		
th	4		
ins	100.000		
nm	no ph

mH

exp15 s2pu1

SAMPLE DEC. & VT
date Sep 21 2006 dfrq 599.938
solvent CDCl3 dn H1
file exp dpwr 30
ACQUISITION dof 0
sfrq 599.939 dm nnn
tn H1 dmm c
at 2.000 dmf 200
np 32000 dseq
sw 8000.0 dres 1.0
fb not used homo n
bs 8 temp 18.0
tpwr 59 DEC2
pw 5.5 dfrq2 0
d1 1.000 dn2
tof 500.0 dpwr2 1
nt 32 dof2 0
ct 32 dm2 n
alock n dmm2 c
gain 30 dmf2 200
FLAGS
il n dseq2 1.0
in n homo2 n
dp y PROCESSING
hs nn wfile
DISPLAY
sp -300.3 ft
wp 6898.9 fn not used
vs 65 math f
sc 0 werr
wc 250 wexp
hzmm 27.60 wbs
is 4262.39 wnt wft
rfl 503.4
rfp 0
th 44
ins 10.000
nm cdc ph

Diphenyl ether
Table 4, entry 1

mH-0921

exp16 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	37
ACQUISITION		dof	0
sfrq	150.870	dm	nyy
tn	C13	dmm	w
at	1.000	dmf	10101
np	79974	dseq	
sw	40000.0	dres	1.0
fb	not used	homo	n
bs	16	temp	18.0
tpwr	56	DEC2	
pw	6.0	dfrq2	0
d1	0.500	dn2	
d2	1.500	dpwr2	1
tof	2500.0	dof2	0
nt	20000	dm2	n
ct	112	dmm2	c
alock	n	dmf2	10000
gain	58	dseq2	
FLAGS		dres2	1.0
il	n	homo2	n
in	n	PROCESSING	
dp	y	lb	3.00
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-1508.6	fn	not used
wp	34696.0	math	f
vs	47		
sc	0	werr	
wc	250	wexp	
hzmm	138.79	wbs	
is	500.00	wnt	
rfl	4050.1		
rfp	0		
th	3		
ins	100.000		
nm	cdc ph

Diphenyl ether
Table 4, entry 1

13C OBSERVE

exp4 std13c

SAMPLE DEC. & VT
 date Sep 8 2006 dfrq 400.443
 solvent CDC13 dn H1
 file exp dpwr 39
 ACQUISITION dof 0
 sfrq 100.703 dm yyy
 tn C13 dmm w
 at 1.000 dmf 10600
 np 56022
 sw 28011.2 lb 1.00
 fb 15400 wtfile
 bs 8 proc ft
 tpwr 57 fn 65536
 pw 6.7
 d1 2.000 werr
 tof 2056.1 wexp
 nt 10000 wbs
 ct 80 wnt
 alock n
 gain 36
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -0.4
 wp 22152.0
 vs 78
 sc 0
 wc 250
 hzmm 88.61
 is 500.00
 rfl 10195.1
 rfp 7753.2
 th 5
 ins 100.000
 nm no ph

158.486
 155.863
 150.090

129.570
 122.387
 120.783
 117.548
 114.814

77.314
 76.992
 76.677

55.597

1-Methoxy-4-phenoxybenzene
 Table 4, entry 2

5H-0921

exp15 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION			
sfrq	599.939	dm	nmn
tn	H1	dmm	c
at	2.000	dmf	200
np	32000	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	8	temp	18.0
tpwr	59	DEC2	
pw	5.5	dfrq2	0
d1	1.000	dn2	
tof	500.0	dpwr2	1
nt	32	dof2	0
ct	32	dm2	n
alock	n	dmm2	c
gain	30	dmf2	200
FLAGS			
il	n	dseq2	
in	n	dres2	1.0
dp	y	homo2	n
hs	nn	PROCESSING	
		wtfile	ft
sp	DISPLAY -300.3	proc	not used
wp	6299.3	fn	f
vs	110	math	
sc	0	werr	
wc	250	wexp	
hzmm	25.20	wbs	
is	8443.59	wnt	wft
rfl	502.0		
rfp	0		
th	24		
ins	10.000		
nm	cdc ph		

7.330
7.256
7.011

1.730.90.83
0.84.62.54

2.328

Phenyl *m*-tolyl ether
Table 4, entry 3

0.000

2.54

5C-0921

exp16 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	37
ACQUISITION		dof	0
sfrq	150.870	dm	nyy
tn	C13	dmm	w
at	1.000	dmf	10101
np	79974	dseq	
sw	40000.0	dres	1.0
fb	not used	homo	n
bs	16	temp	18.0
tpwr	56	DEC2	
pw	6.0	dfrq2	0
d1	0.500	dn2	
d2	1.500	dpwr2	1
tof	2500.0	dof2	0
nt	20000	dm2	n
ct	32	dmm2	c
alock	n	dmf2	10000
gain	58	dseq2	
FLAGS		dres2	1.0
il	n	homo2	n
in	n	PROCESSING	
dp	y	lb	3.00
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-1508.6	fn	not used
wp	34696.0	math	f
vs	64		
sc	0	werr	
wc	250	wexp	
hzmm	138.79	wbs	
ls	500.00	wnt	
rfl	15665.9		
rfp	11615.7		
th	7		
ins	100.000		
nm	cdc ph

Phenyl *m*-tolyl ether
Table 4, entry 3

13C OBSERVE

exp1 std13c

SAMPLE DEC. & VT
date Sep 22 2006 dfrq 400.443
solvent CDC13 dn H1
file exp dpwr 39
ACQUISITION dof 0
sfrq 100.703 dm yyy
tn C13 dmm w
at 1.000 dmf 10600
np 56022 PROCESSING
sw 28011.2 lb 3.00
fb 15400 wtfile
bs 8 proc ft
tpwr 57 fn 65536
pw 6.7
d1 2.000 werr
tof 2056.1 wexp
nt 10000 wbs
ct 288 wnt
alock n
gain 36
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 22152.0
vs 66
sc 0
wc 250
hzmm 88.61
is 500.00
rfl 10190.8
rfp 7753.2
th 4
ins 100.000
nm no ph

2-Methylphenyl phenyl ether
Table 4, entry 4

3C-0921

exp15 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION			
sfrq	599.939	dm	nnn
tn	H1	dmm	c
at	2.000	dmf	200
np	32000	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	8	temp	18.0
tpwr	59	DEC2	
pw	5.5	dfrq2	0
d1	1.000	dn2	
tof	500.0	dpwr2	1
nt	32	dof2	0
ct	32	dm2	n
alock	n	dmm2	c
gain	30	dmf2	200
il	n	dseq2	
in	n	dres2	1.0
dp	y	homo2	n
hs	nn	PROCESSING	
DISPLAY		wtfile	ft
sp	-300.3	proc	not used
wp	6299.3	fn	f
vs	140	math	
sc	0	werr	
wc	250	wexp	
hzmm	25.20	wbs	
is	5937.39	wnt	wft
rfl	501.5		
rfp	0		
th	14		
ins	10.000		
nm	cdc ph

3, 5-Dimethylphenyl phenyl ether
Table 4, entry 5

3C-0921

exp16 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	37
ACQUISITION		dof	0
sfrq	150.870	dm	nyy
tn	C13	dmm	w
at	1.000	dmd	10101
np	79974	dseq	
sw	40000.0	dres	1.0
fb	not used	homo	n
bs	16	temp	18.0
tpwr	56	DEC2	
pw	6.0	dfrq2	0
d1	0.500	dn2	
d2	1.500	dpwr2	1
tof	2500.0	dof2	0
nt	20000	dm2	n
ct	32	dmm2	c
alock	n	dmd2	10000
gain	58	dseq2	
FLAGS		dres2	1.0
il	n	homo2	n
in	n	PROCESSING	
dp	y	lb	3.00
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-1508.6	fn	not used
wp	34696.0	math	f
vs	82		
sc	0	werr	
wc	250	wexp	
hzmm	138.79	wbs	
is	500.00	wnt	
rfl	15672.0		
rfp	11615.7		
th	7		
ins	100.000		
nm	cdc ph

3, 5-Dimethylphenyl phenyl ether
Table 4, entry 5

1-0922

exp20 s2pu1

SAMPLE		DEC. & VT	
date	Sep 22 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION			
sfrq	599.939	dm	nnn
tn	H1	dmm	c
at	2.000	dmf	200
np	32000	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	8	temp	20.0
tpwr	59	DEC2	
pw	5.5	dfrq2	0
d1	1.000	dn2	
tof	500.0	dpwr2	1
nt	32	dof2	0
ct	32	dm2	n
alock	n	dmm2	c
gain	30	dmf2	200
FLAGS			
il	n	dseq2	
in	n	dres2	1.0
dp	y	homo2	n
hs	nn	PROCESSING	
DISPLAY			
sp	-300.3	proc	ft
wp	6299.3	fn	not used
vs	112	math	f
sc	0	werr	
wc	250	wexp	
hzmm	25.20	wbs	
is	914.51	wnt	wft
rfl	529.3		
rfp	0		
th	27		
ins	10.000		
nm	cdc ph

1-0922

exp21 s2pu1

SAMPLE		DEC. & VT	
date	Sep 22 2006	dfrq	599.938
solvent	CDCl3	dn	H1
file	exp	dpwr	37
ACQUISITION			
sfrq	150.870	dof	nyy
tn	C13	dmm	w
at	1.000	dmf	10101
np	79974	dseq	
sw	40000.0	dres	1.0
fb	not used	homo	n
bs	16	temp	20.0
tpwr	56	DEC2	
pw	6.0	dfrq2	0
d1	0.500	dn2	
d2	1.500	dpwr2	1
tof	2500.0	dof2	0
nt	20000	dm2	n
ct	0	dmm2	c
alock	n	dmf2	10000
gain	58	dseq2	
il	n	dres2	1.0
in	n	homo2	n
dp	y	PROCESSING	
hs	nn	lb	3.00
sp	DISPLAY	wtfile	
wp	-1508.6	proc	ft
vs	34696.0	fn	not used
sc	76	math	f
wc	0	werr	
hzmm	250	wexp	
is	138.79	wbs	
rf1	500.00	wnt	
rfp	15662.8		
th	11615.7		
ins	6		
nm	100.000		
cdc	ph

Phenyl 4-methylphenyl ether
Table 4, entry 6

6-0921

exp15 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	599.939	dm	nnn
tn	H1	dmm	c
at	2.000	dmf	200
np	32000	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	8	temp	18.0
tpwr	59	DEC2	
pw	5.5	dfrq2	0
d1	1.000	dn2	
tof	500.0	dpwr2	1
nt	32	dof2	0
ct	32	dm2	n
alock	n	dmm2	c
gain	30	dmf2	200
FLAGS		dseq2	
il	n	dres2	1.0
in	n	homo2	n
dp	y	PROCESSING	
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-300.3	fn	not used
wp	6299.3	math	f
vs	120		
sc	0	werr	
wc	250	wexp	
hzmm	25.20	wbs	
is	1918.84	wnt	wft
rf1	512.7		
rfp	0		
th	25		
ins	10.000		
nm	cdc ph

6-0921

exp16 s2pu1

SAMPLE DEC. 2 2006
 date Sep 21 2006 dfrq 599.938
 solvent CDC13 dn H1
 file exp dpwr 37
 ACQUISITION dof 0
 sfrq 150.870 dm nyv
 tn C13 dmm w
 at 1.000 dmf 10101
 np 79974 dseq
 sw 40000.0 dres 1.0
 fb not used homo n
 bs 16 temp 18.0
 tpwr 56 DEC2
 pw 6.0 dfrq2 0
 d1 0.500 dn2
 d2 1.500 dpwr2 1
 tof 2500.0 dof2 0
 nt 20000 dm2 n
 ct 48 dmm2 c
 alock n dmf2 10000
 gain 58 dseq2
 FLAGS dres2 1.0
 il n homo2
 in n PROCESSING
 dp y lb 3.00
 hs nn wtfle
 DISPLAY proc
 sp -1508.6 fn not used
 wp 34696.0 math f
 vs 66
 sc 0 werr
 wc 250 wexp
 hzmm 138.79 wbs
 is 500.00 wnt
 rfl 15660.4
 rfp 11615.7
 th 8
 ins 100.000
 nm cdc ph

4-0921

exp15 s2pul

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	599.939	dm	nnn
tn	H1	dmm	c
at	2.000	dmf	200
np	32000	dseq	
sw	8000.0	dres	1.0
fb	not used	homo	n
bs	8	temp	18.0
tpwr	59	DEC2	
pw	5.5	dfrq2	0
d1	1.000	dn2	
tof	500.0	dpwr2	1
nt	32	dof2	0
ct	32	dm2	n
alock	n	dmm2	c
gain	30	dmf2	200
FLAGS		dseq2	
il	n	dres2	1.0
in	n	homo2	n
dp	y	PROCESSING	
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-300.3	fn	not used
wp	6299.3	math	f
vs	102		
sc	0	werr	
wc	250	wexp	
hzmm	25.20	wbs	
is	3134.39	wnt	wft
rfl	503.9		
rfp	0		
th	16		
ins	10.000		
nm	cdc ph

3',5'-Dimethyl-4-methoxydiphenyl ether
Table 4, entry 8

4-0921

exp16 s2pu1

SAMPLE		DEC. & VT	
date	Sep 21 2006	dfrq	599.938
solvent	CDC13	dn	H1
file	exp	dpwr	37
ACQUISITION			
sfrq	150.870	dof	0
tn	C13	dm	nyy
at	1.000	dmm	w
np	79974	dmf	10101
sw	40000.0	dseq	
fb	not used	dres	1.0
bs	16	homo	n
tpwr	56	temp	18.0
		DEC2	
pw	6.0	dfrq2	0
d1	0.500	dn2	
d2	1.500	dpwr2	1
tof	2500.0	dof2	0
nt	20000	dm2	n
ct	160	dmm2	c
alock		dmf2	10000
gain	58	dseq2	
FLAGS			
il	n	dres2	1.0
in	n	homo2	n
dp	y	PROCESSING	
hs	nn	lb	3.00
		wtfile	
DISPLAY			
sp	-1508.6	proc	ft
wp	34696.0	fn	not used
vs	88	math	f
sc	0	werr	
wc	250	wexp	
hzmm	138.79	wbs	
is	500.00	wnt	
rfl	15663.5		
rfp	11615.7		
th	10		
ins	100.000		
nm	cdc ph

3',5'-Dimethyl-4-methoxydiphenyl ether
Table 4, entry 8