

Supporting Information

Functionalized Dibenzo[*g,p*]chrysenes: Variable Photo- and Electronic Properties and Liquid Crystal Crystal Chemistry

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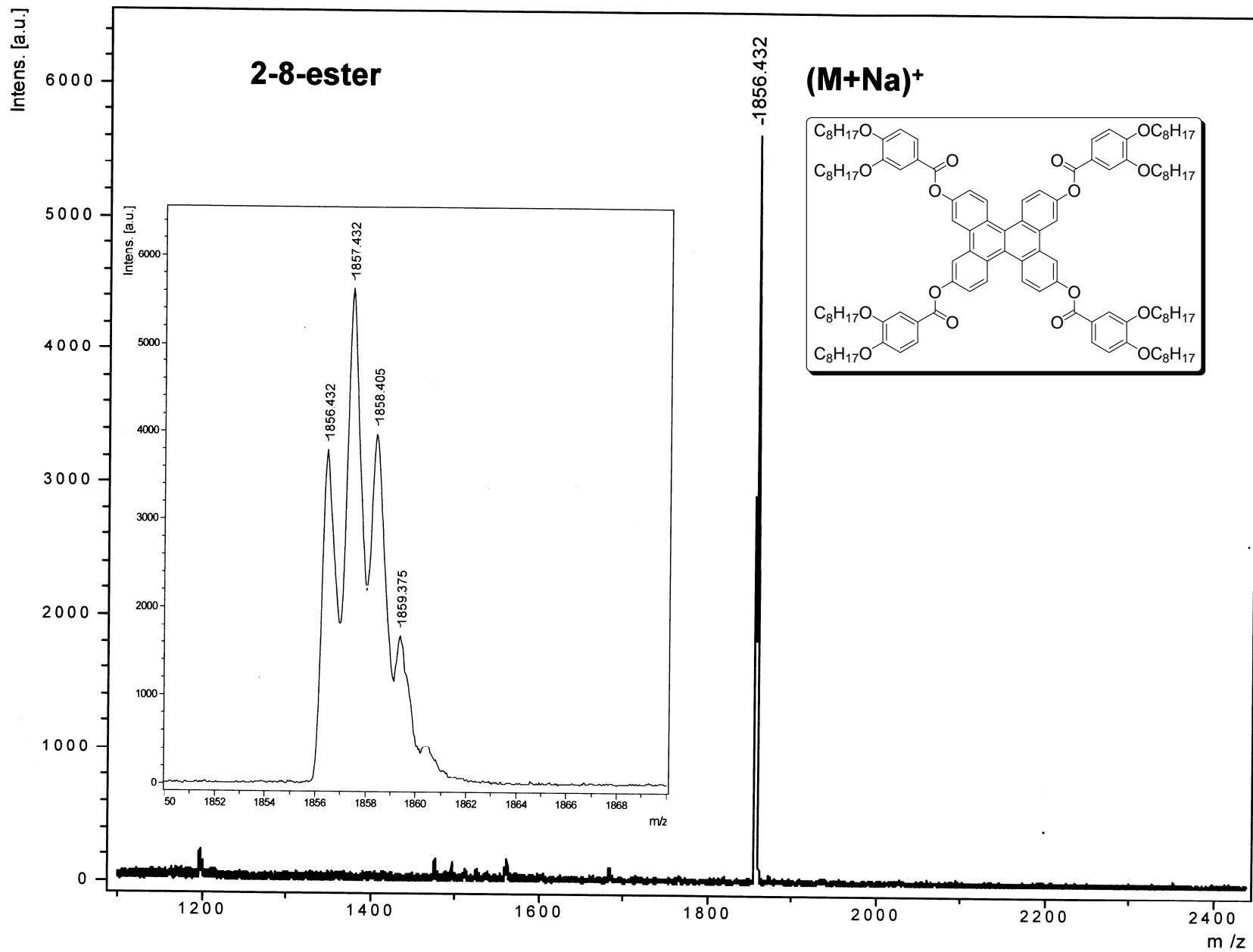
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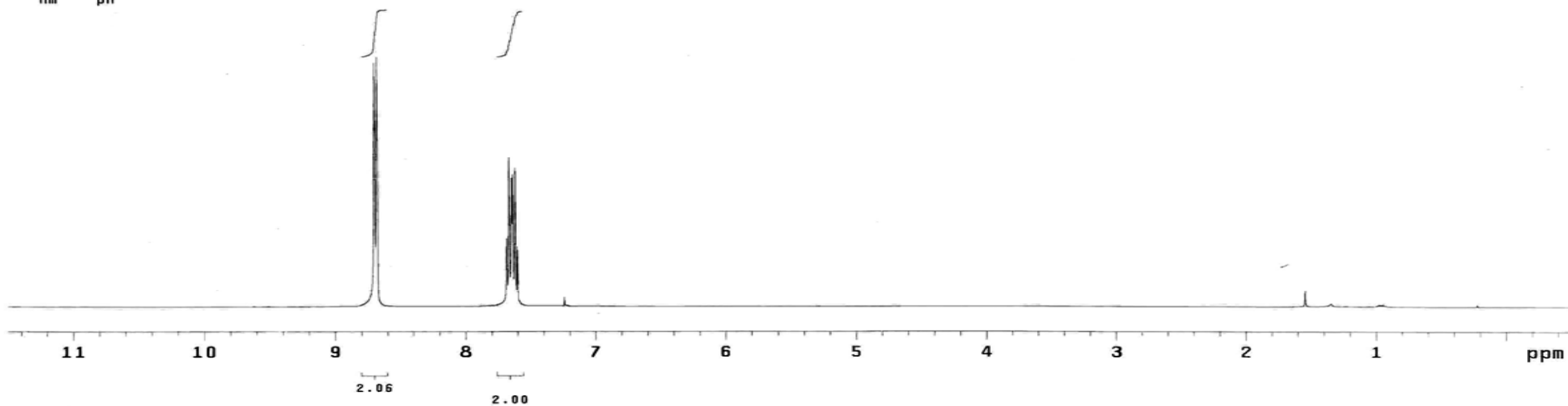
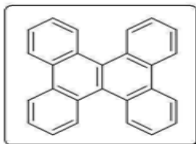


STANDARD 1H OBSERVE

exp1 std1h

SAMPLE DEC. & VT
date Feb 20 2006 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016 PROCESSING
sw 6009.6 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
d1 1.000 werr
tof 500.0 wexp
nt 100 wbs
ct 20 wnt
atlock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4805.3
vs 50
sc 0
wc 250
hzmm 5.23
is 65.85
rfl 3394.2
rfp 2899.3
th 10
ins 2.000
nm ph

8.702
8.697
8.686
8.683
7.687
7.684
7.670
7.667
7.650
7.647
7.641
7.638
7.620
7.617
7.604
7.600



13C OBSERVE

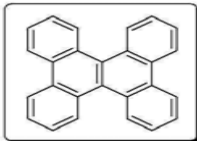
exp2 std13c

SAMPLE DEC. & VT
date Feb 20 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np PROCESSING
sw 25188.9 lb 3.00
fb 13800 wtfile
bs 4 proc
tpwr 58 fn not used
pw 6.5
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs
ct 160 wnt

alock n
gain not used

FLAGS
il n
in n
dp y

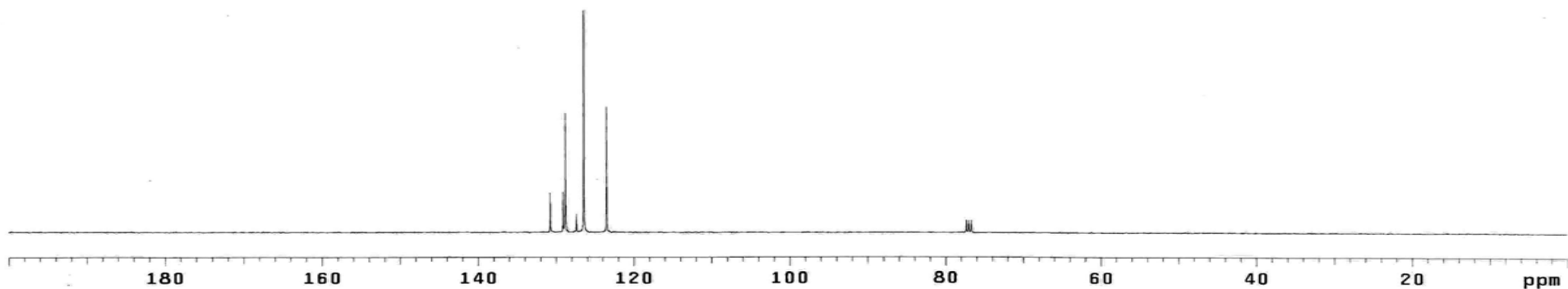
DISPLAY
sp -0.2
wp 20138.2
vs 45
sc 0
wc 250
hzmm 5.60
is 500.00
rfl 8854.5
rfp 7753.4
th 2
ins 100.000
nm ph



1

130.732
129.083
128.778
127.357
126.426
123.479

77.305
77.000
76.679

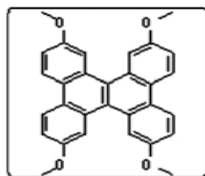


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red
expl std1h
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date May 14 2006
solvent CDC13
file
ACQUISITION exp
sfrq 400.447
tn H1
at 2.728
np 32768
sw 6006.0
fb 3400
bs 4
tpwr 59
pw 6.8
d1 1.000
tof 596.3
nt 100
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.6
vs 50
sc 0
wc 250
hzmm 3.17
is 37.68
rfl 408.2
rflp 0
th 3
ins 1.000
nm ph
DEC. & VT
dfrq 400.446
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
lb 0.10
wtfile
proc ft
fn 65536

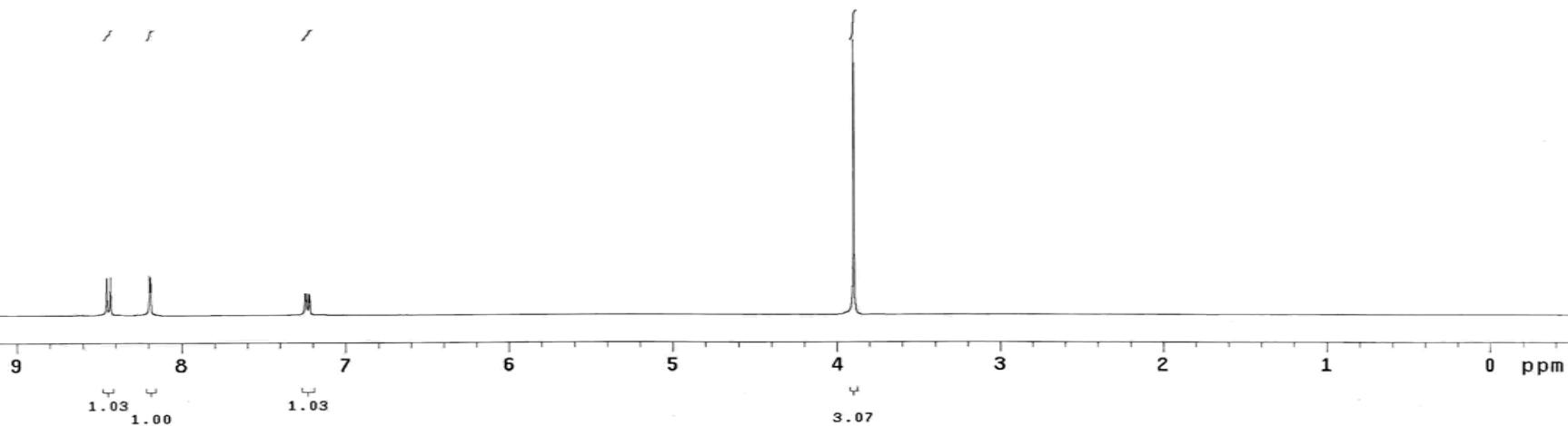
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8.454
8.432
8.194
8.188
7.248
7.242
7.226
7.220



2a

—3.897



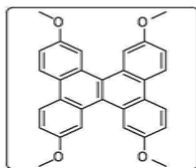
13C OBSERVE

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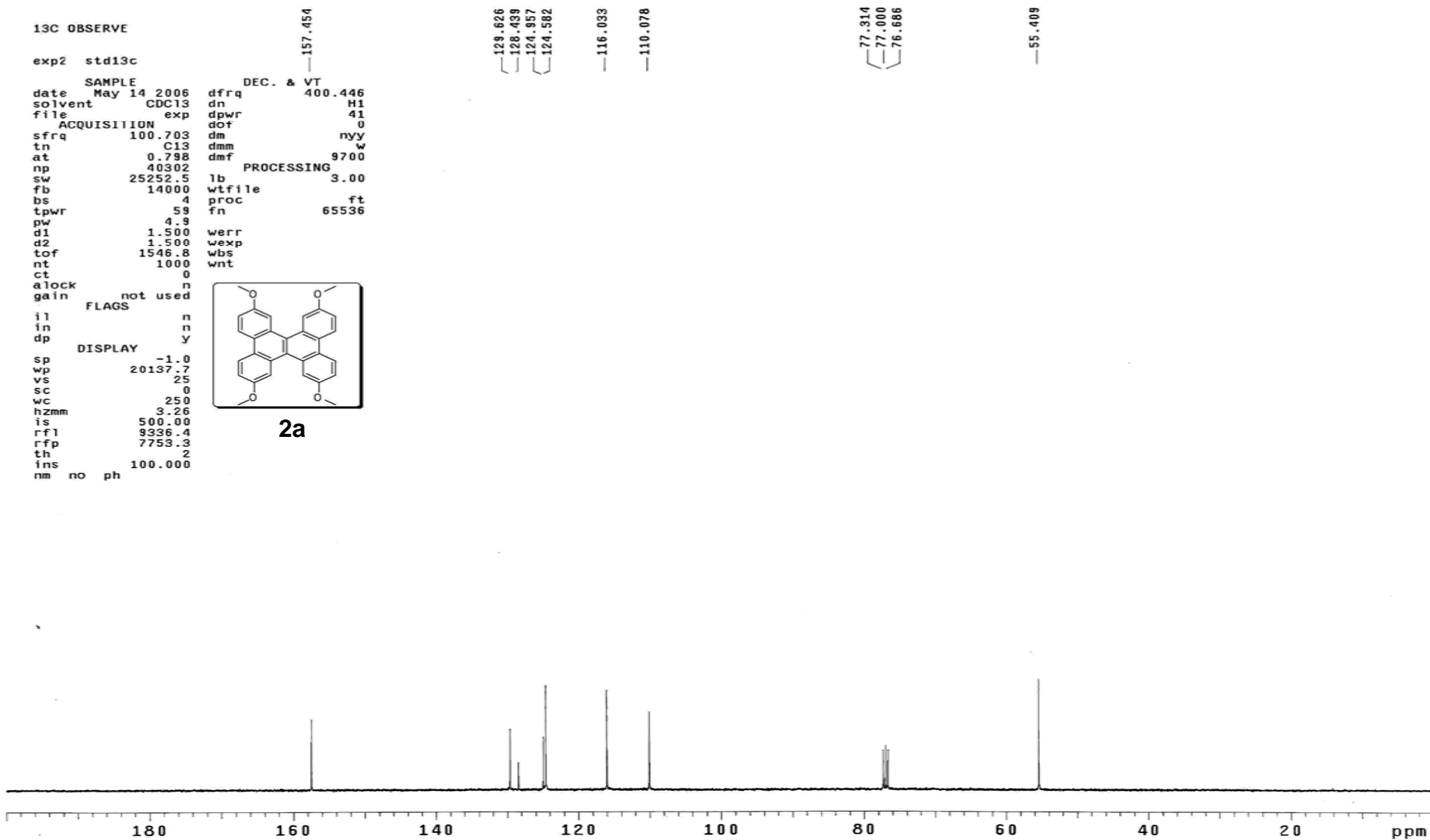
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SAMPLE
date May 14 2006 dfrq DEC. & VT 400.446
solvent CDC13 dn H1
file exp dpwr 41
ACQUISITION dof 0
sfrq 100.703 dm nyy
tn C13 dmm w
at 0.798 dmf 9700
np 40302
sw 25252.5 PROCESSING 3.00
fb 14000 wtfile
bs 4 proc ft
tpwr 59 fn 65536
pw 4.9
d1 1.500 werr
d2 1.500 wexp
tof 1546.8 wbs
nt 1000 wnt
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1.0
wp 20137.7
vs 25
sc 0
wc 250
hzmm 3.26
is 500.00
rf1 9336.4
rfp 7753.3
th 2
ins 100.000
nm no ph

```



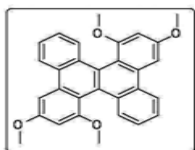
2a



```

exp1 std1h
SAMPLE
date Feb 9 2006 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION doT 0
sfrq 400.455 dm nnn
tn H1 dmm c
at 2.664 dmf 8000
np 32016 PROCESSING
sw 6009.6 lb 0.50
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0 werr
d1 1.000 wexp
tof 500.0 wbs wft aph
nt 100 wnt
ct 0
alock n
gain not used
FLAGS
f1 n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 1.53
is 39.76
rfl 496.0
rfp 0
th 5
ins 1.000
nm ph

```

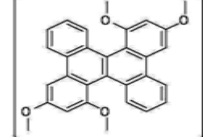


2b

8.464
8.445
7.799
7.796
7.779
7.776
7.713
7.707
7.480
7.476
7.460
7.456
7.451
7.446
7.430
7.427
7.238
6.765
6.760

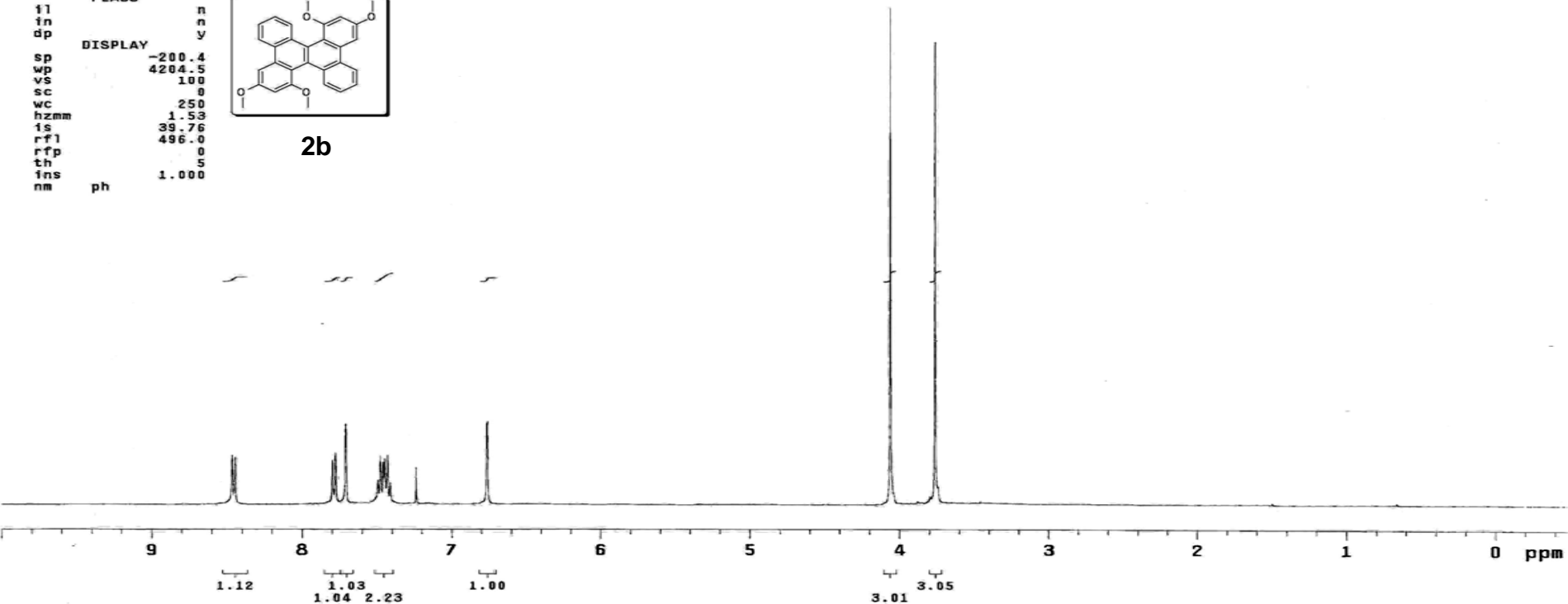
DEC. 8-VT

PROCESSING



2b

4.061
3.763

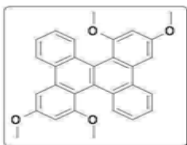


13C OBSERVE

exp2 std13c

```

SAMPLE
date Feb 9 2006 dfrq DEC. & VT 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmT 8000
np 32000
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 proc
tpwr 58 fn not used
pw 6.5
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs wft
CT 348 wnt
a1ock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 30
sc 0
wc 250
hzmm 17.72
is 500.00
rfl 8840.6
rfp 7753.4
th 4
ins 100.000
nm ph
  
```



2b

133.480
131.282
130.747
128.747
126.808
125.327
125.281
122.853
114.211

98.652
97.735

77.321
77.000
76.679

55.577
55.043

180

160

140

120

100

80

60

40

20

ppm


```

expl std1h
date Feb 14 2006
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 0
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 2.59
is 19.88
rf1 495.3
rfp 0
th 6
ins 2.000
nm ph

```

8.432
 8.412
 7.970
 7.950
 7.913
 7.508
 7.491
 7.469
 7.449
 7.240

DEC. & VT

dfrq 400.454

dn H1

dpwr 42

dof 0

dm nnn

dmm c

dmt 8000

PROCESSING

lb 0.50

wtfile

proc ft

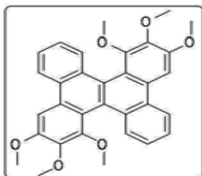
fn not used

werr

wexp

wbs wft aph

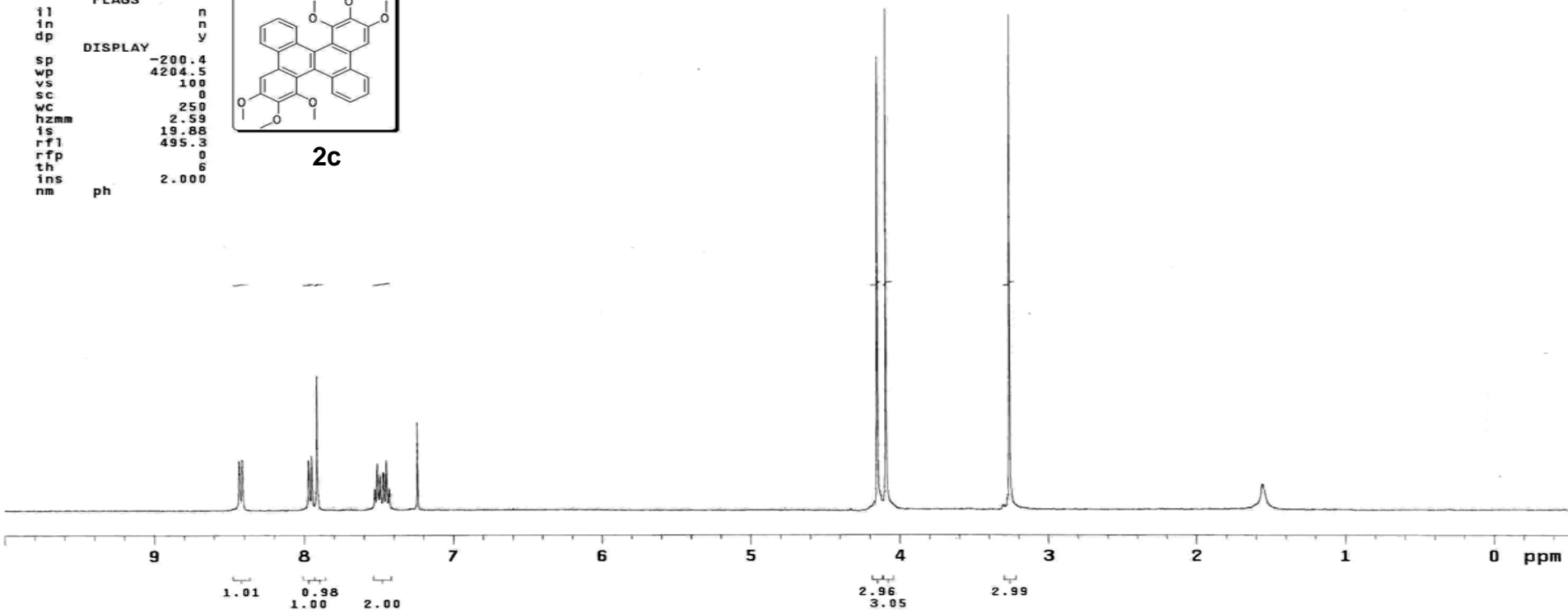
wnt



2c

4.148
 4.091

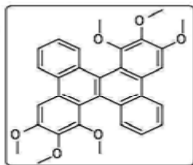
3.258



13C OBSERVE

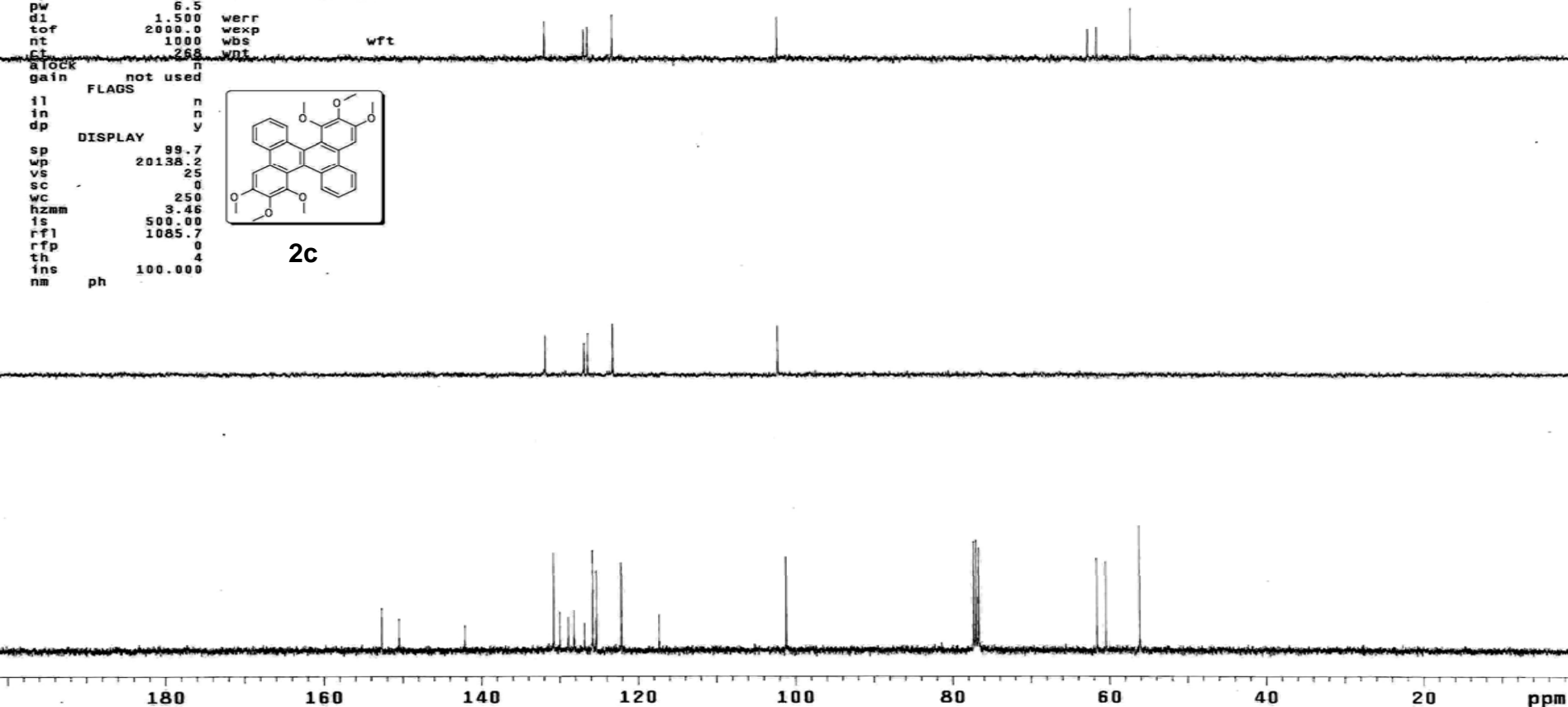
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solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dot 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 proc
tpwr 58 fn not used
pw 6.5
d1 1.500 verr
tof 2000.0 wexp
nt 1000 wbs
ct 268 wnt
a1ock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp 99.7
wp 20138.2
vs 25
sc 0
wc 250
hzmm 3.46
is 500.00
rfl 1085.7
rfp 0
th 4
ins 100.000
nm ph



2c

152.628
150.444
142.077
130.762
129.969
128.900
128.151
126.823
125.785
125.296
122.135
117.326
101.171
77.321
77.000
76.679
61.593
60.433
56.127

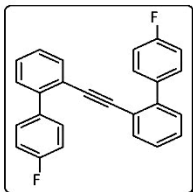


STANDARD 1H OBSERVE

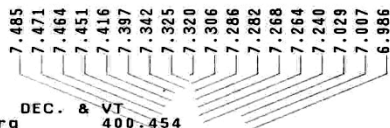
exp6 std1h

SAMPLE
date Mar 2 2006
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 4
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 1.74
is 101.28
rfl 3394.9
rfp 2899.3
th 9
ins 2.000
nm ph

DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm nnn
dmm c
dmf 8000
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt wft aph

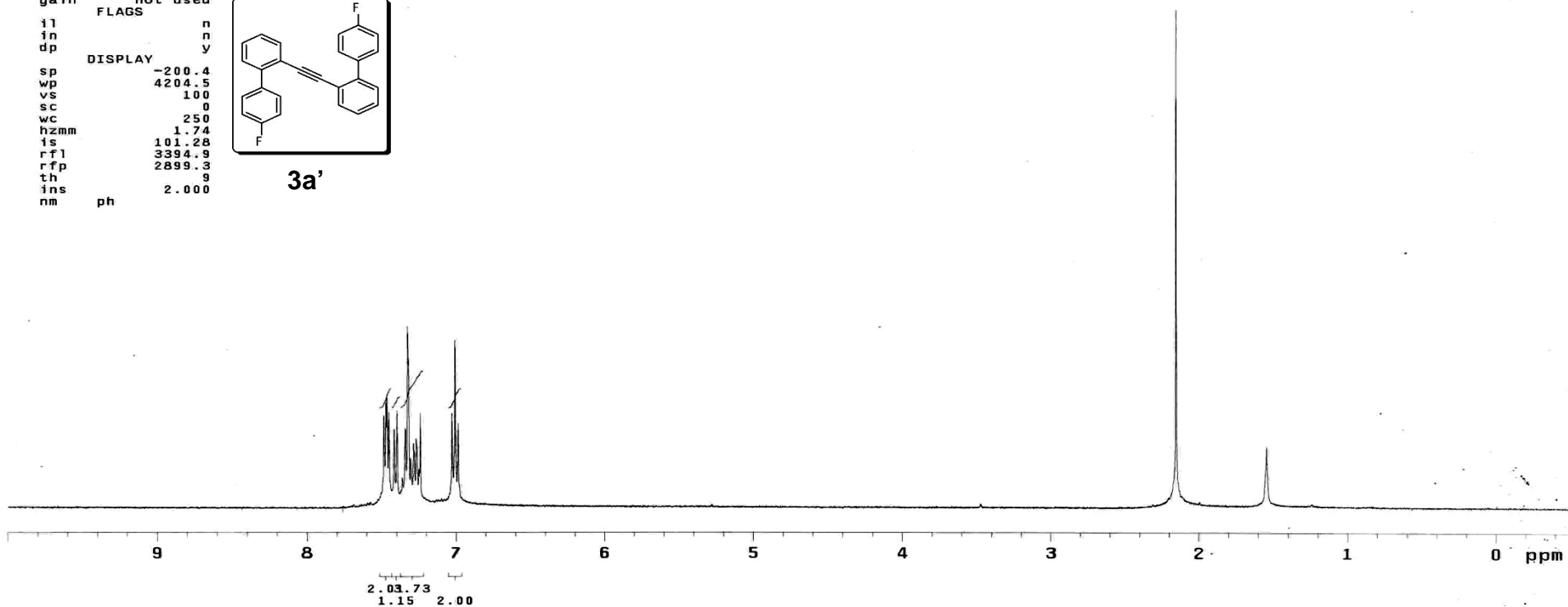


3a'



2.152

1.542



¹³C OBSERVE

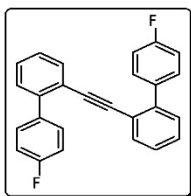
exp2 std13c

SAMPLE DEC. & VT
date Feb 20 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs wft

clock gain not used
FLAGS

il n
in n
dp y

DISPLAY
sp -0.2
wp 20138.2
vs 45
sc 0
wc 250
hzmm 80.56
is 500.00
rfl 8846.8
rfp 7753.4
th 6
ins 100.000
nm ph



3a'

163.515
161.072

142.413
136.290
132.961
130.885
130.793
129.342
128.548
127.083
121.509
114.852
114.638

91.780

77.305
77.000
76.679

180

160

140

120

100

80

60

40

20

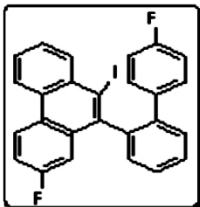
ppm

8.608
8.587
8.577
8.564
8.491
8.487
8.468
8.400
8.397
8.393
8.380
8.376
7.644
7.639
7.632
7.627
7.620
7.613
7.609
7.595
7.592
7.568
7.565
7.546
7.544
7.530
7.526
7.336

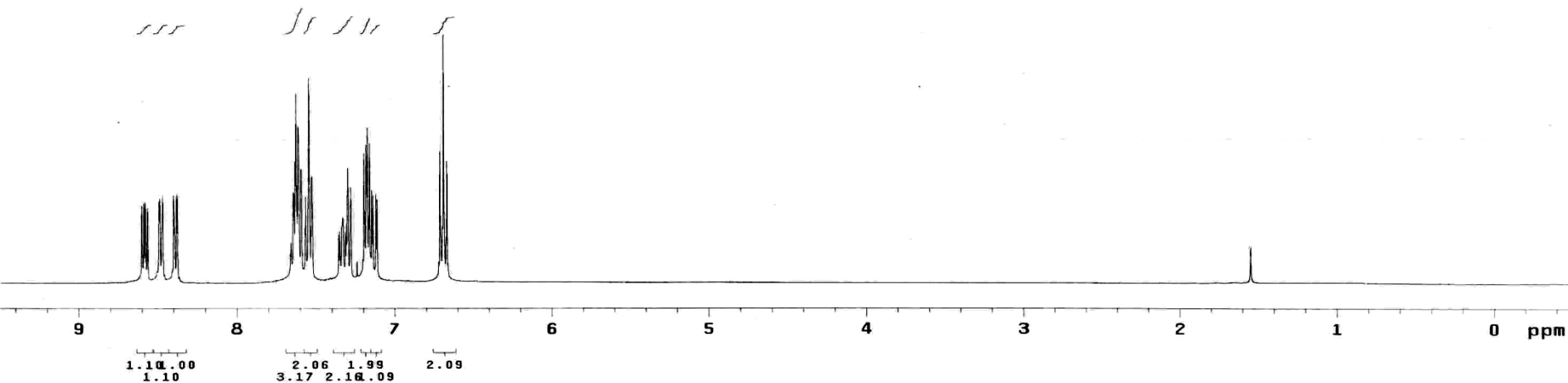
exp9 stdih

SAMPLE
date Feb 22 2006
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
d1 1.000
tof 500.0
nt 100
ct 4
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4004.2
vs 50
sc 0
wc 250
hzmm 3.91
is 77.24
rfl 3394.6
rfp 2899.3
th 11
ins 1.000
nm ph

DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm nnn
dmm c
dmf 8000
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs wft aph
wnt



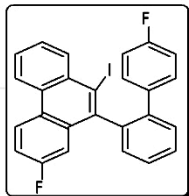
3a''



exp2 std13c

SAMPLE
date Feb 22 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 100.705
tn C13
at 0.635
np 32000
sw 25188.9
fb 13800
bs 4
tpwr 58
pw 6.5
d1 1.500
tof 2000.0
nt 1000
ct 108
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 100
sc 0
wc 250
hzmm 3.93
is 500.00
rfl 8849.9
th 7753.4
ins 7
nm ph 100.000

DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm YVY
dmm w
dmf 8000
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs wft
wnt



3a'

162.350
162.537
160.507
160.079
142.596
140.306
136.519
134.534
133.679
133.587
131.816
131.144
130.518
130.335
130.259
129.816
128.808
127.861
127.785
126.609
125.098
125.006
122.410
116.056
115.829
114.654
114.440
112.974
112.760
109.645

77.321
77.000
76.695

180

160

140

120

100

80

60

40

20

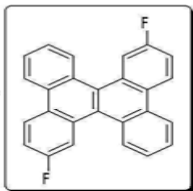
ppm

3.81
 3.73
 3.58
 3.40
 3.23
 3.20
 3.03
 2.95
 2.85
 2.75
 2.66
 2.50
 2.45
 2.22
 2.16
 2.08
 2.05
 1.98
 1.94
 1.80
 1.62
 1.56
 1.50
 1.42
 1.37
 1.33
 1.26
 1.10
 1.00
 0.94
 0.80
 0.62
 0.56
 0.50
 0.42
 0.37
 0.33
 0.26
 0.10
 0.00

exp1 stdin
 SAMPLE
 date Feb 23 2006
 solvent CDCl3
 file exp
 ACQUISITION
 sfrq 400.455
 tn H1
 at 2.664
 np 32016
 sw 6009.6
 fb 3400
 bs 4
 tpwr 58
 pw 6.0
 dl 1.000
 tof 500.0
 nt 100
 ct 16
 alock n
 gain not used
 FLAGS
 il n
 in n
 dp y
 DISPLAY
 sp -200.4
 wp 4204.5
 vs 45
 sc 0
 wc 250
 hzmm 16.82
 ls 32.15
 rfl 3394.9
 rfp 2899.3
 th 5
 ins 1.000
 nm ph

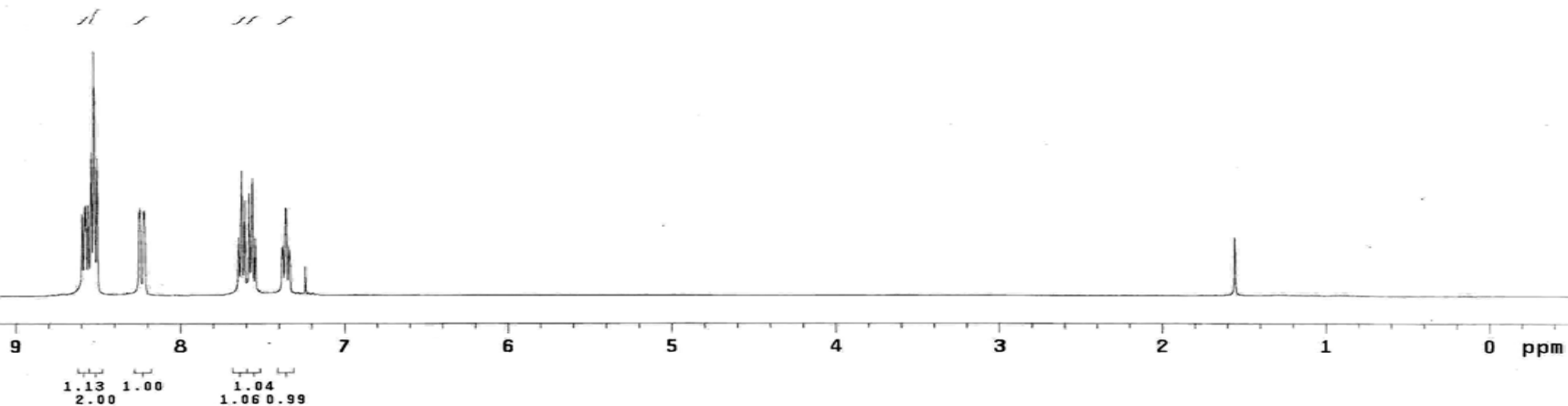
DEC. & VT
 dfrq 400.454
 dn H1
 dpwr 42
 dof 0
 dm nnn
 dmm c
 dmf 8000
 PROCESSING
 lb 0.10
 wtfile
 proc ft
 fn not used
 werr
 wexp
 wbs wft aph
 wnt

7.861
 7.848
 7.845
 7.827
 7.810
 7.807
 7.784
 7.780
 7.762
 7.750
 7.742
 7.733
 7.729
 7.716
 7.706
 7.693
 7.680
 7.660
 7.656
 7.654
 7.641
 7.637



3a

1.556



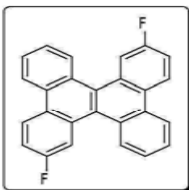
¹³C OBSERVE

exp2 std13c

SAMPLE DEC. & VT
date Feb 23 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 2.000 werr
tof 2000.0 wexp
nt 10000 wbs wft
CT 86 WDT

alock n
gain not used
FLAGS
il n
in n
dp y

DISPLAY
sp -0.2
wp 20138.2
vs 45
sc 0
wc 250
hzmm 2.00
is 500.00
rfl 8842.2
rfp 7753.4
th 5
ins 100.000
nm no ph



3a

162.583
160.155

130.411
130.320
128.472
128.167
127.632
127.388
126.976
126.548
125.815
125.724
123.418
115.280
115.051
113.966
113.737

77.321
77.000
76.695

180

160

140

120

100

80

60

40

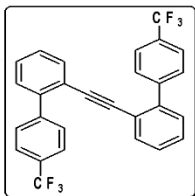
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ppm

n
exp3 std1h

SAMPLE
date Feb 24 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 16
alock n
gain not used
FLAGS n
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzm 2.28
is 215.67
rfl 3394.9
rfp 2899.3
th 3
ins 2.000
nm ph

DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm nnn
dmm c
dmf 8000
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt wft aph



3b'

7.566
7.413
7.394
7.376
7.362
7.358
7.335
7.318
7.313
7.240

1.540

9

8

7

6

5

4

3

2

1

0

ppm

0.92
1.08

13C OBSERVE

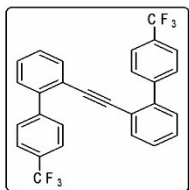
exp4 std13c

SAMPLE DEC. & VT
date Feb 24 2006 dfrq 400.454
solvent CDCl3 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm yyw
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 wproc ft
tpwr 58 fn not used
pw 6.5
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs wft
Gt 728 wot

LOCK gain not used

FLAGS
il n
in n
dp y

DISPLAY
sp -0.2
wp 20138.2
vs 50
sc 0
wc 250
hzmm 28.05
is 500.00
rfl 8837.6
rfp 7753.4
th 3
ins 100.000
nm ph



3b'

143.955
142.138
133.022
129.633
129.510
129.404
128.778
127.816
124.853
124.808
121.464
91.689
77.321
77.000
76.695

180

160

140

120

100

80

60

40

20

ppm

8.707
8.685
8.697
8.681
8.773
8.742
8.734
8.718
8.702
8.687
8.678
8.660
8.647
8.636
8.619
8.612
8.604
8.599
8.595
8.579
8.567
8.555
8.540
8.538
8.521
8.517
8.503
8.498
8.488

exp4 std1h

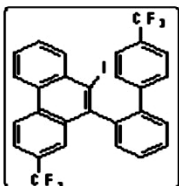
SAMPLE
date Mar 1 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
d1 1.000
tof 500.0
nt 100
ct 56
alock n
gain not used

DEC. & VT
dfrq 400.454
dn H1
dpwr 42
dof 0
dm nnn
dmm c
dmf 8000

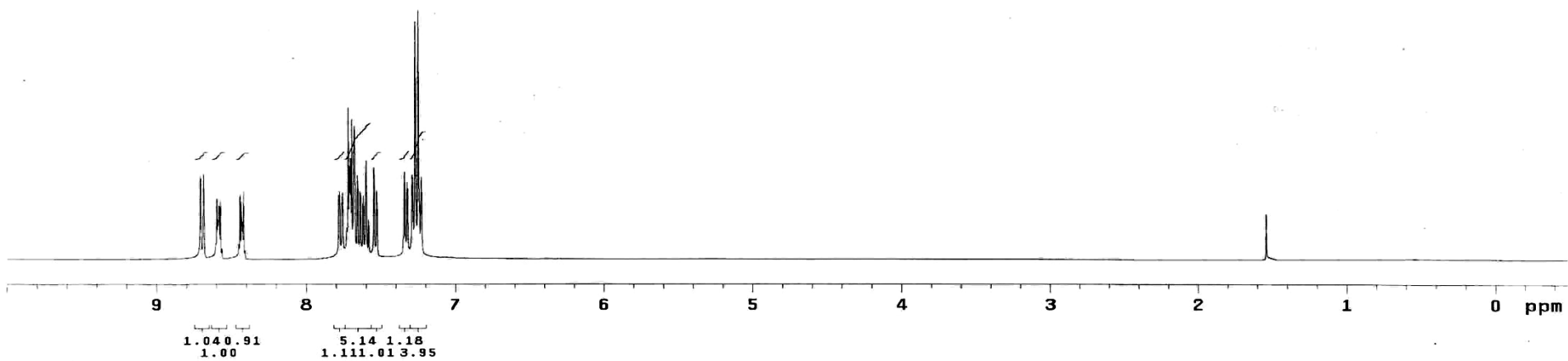
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt wft aph

FLAGS
f1 n
f2 n
dp y

DISPLAY
sp -200.4
wp 4204.5
vs 50
sc 0
wc 250
hzmm 2.73
is 125.00
rf1 495.3
rfp 0
th 8
ins 1.000
nm ph



3b''



13C OBSERVE

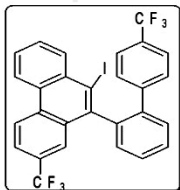
exp2 std13c

SAMPLE DEC. & VT
date Mar 3 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb wtfile 1.00
fb 13800 proc ft
bs 4 fn not used
tpwr 58
pw 6.5
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs
ct 508 wnt

alock n
gain not used

il n
in n
dp y

DISPLAY
sp -0.2
wp 20138.2
vs 45
sc 0
wc 250
hzmm 11.86
is 500.00
rfl 8848.3
rfp 7753.4
th 1
ins 100.000
nm ph



3b''

129.510
129.434
129.220
129.159
129.022
128.930
128.747
128.610
128.518
128.426
128.289
128.136
128.029
127.800
125.540
125.495
125.449
125.327

77.321
77.000
76.679

180

160

140

120

100

80

60

40

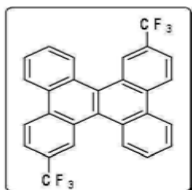
20

ppm

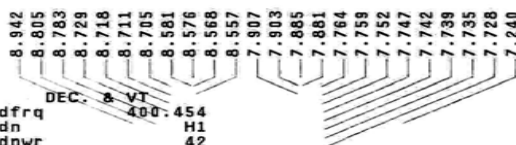
exp1 std1h

SAMPLE
date Mar 6 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 24
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4805.3
vs 50
sc 0
wc 250
hzmm 3.37
is 113.40
rfl 3394.6
rpf 2899.3
th 11
ins 1.000
nm ph

DEC. & VI
400.454
H1
42
0
nnn
c
8000
PROCESSING
lb 0.10
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt wft aph



3c



1.530

11 10 9 8 7 6 5 4 3 2 1 ppm

1.02.09
1.02.09

0.99
2.05

¹³C OBSERVE

exp2 std13c

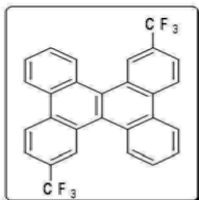
SAMPLE		DEC. & VT	
date	Mar 6 2006	dfrq	400.454
solvent	CDC13	dn	H1
file	exp	dpwr	42
ACQUISITION		dof	0
sfrq	100.705	dm	yyy
tn	C13	dmm	w
at	0.635	dmf	8000
np	32000	PROCESSING	
sw	25188.9	lb	3.00
fb	13800	wtfile	
bs	4	proc	ft
tpwr	58	fn	not used
pw	6.5		
dl	1.500	werr	
tor	2000.0	wexp	
nt	1000	wbs	
ct	368	wnt	wft
alock	n		
gain	not used		

FLAGS

il	n
in	n
dp	y

DISPLAY

sp	-0.2
wp	20138.2
vs	30
sc	0
wc	250
hzmm	6.19
is	500.00
rfl	8839.1
rfp	7753.4
th	3
ins	100.000
nm	ph



3c

133.206
130.014
129.495
129.373
129.220
128.701
128.487
128.136
127.709
127.327
126.090
125.769
124.533
124.120
123.021

77.321
77.000
76.695

180 160 140 120 100 80 60 40 20 ppm

exp1 stdih

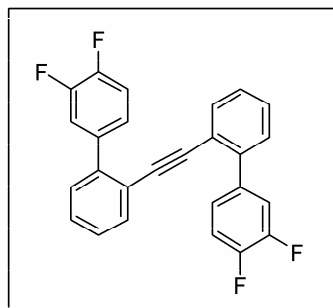
SAMPLE
date Jul 28 2006
solvent CDCl3
file exp
ACQUISITION
sfrq 400.447
tn H1
at 2.728
np 32768
sw 6006.0
fb 3400
bs 4
tpwr 59
pw 6.8
dl 1.000
tof 596.3
nt 100
ct 24
alock n
gain not used

FLAGS
il n
in n
dp y

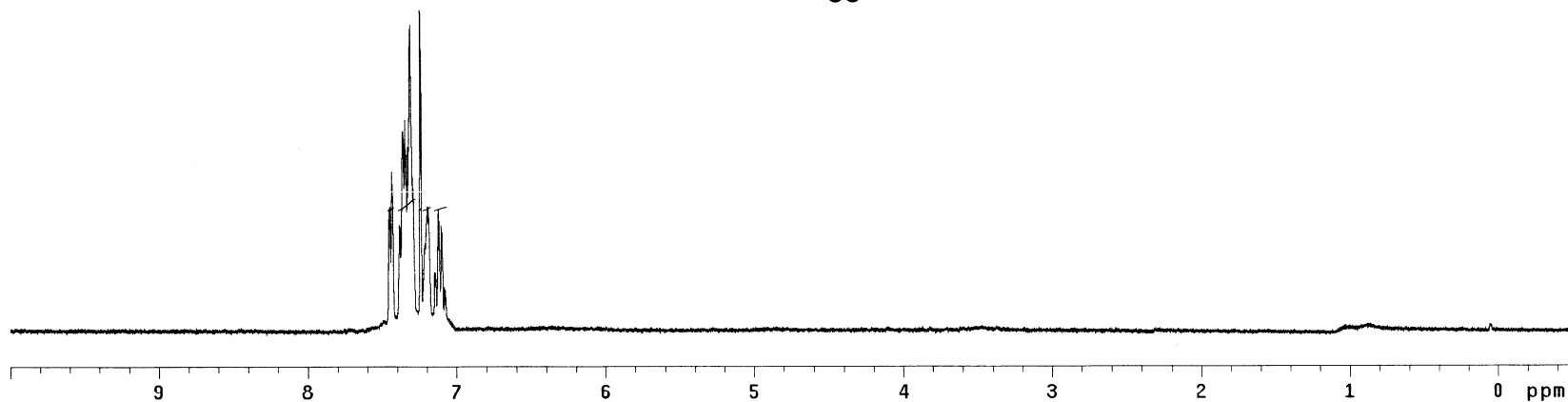
DISPLAY
sp -200.4
wp 4204.6
vs 100
sc 0
wc 250
hzmm 16.82
is 49.71
rfl 406.9
rfp 0
th 10
ins 100.000
nm ph

7.380
7.361
7.357
7.350
7.345
7.340
7.332
7.327
7.320
7.316
7.311
7.297
7.291
7.245
7.241
7.235
7.215
7.210
7.204
7.199
7.194
7.189
7.148

DEC. & VT
400.446
111
20
0
nnn
c
200
PROCESSING
lb 0.10
wtfile
proc ft
fn 65536
werr
wexp
wbs
wnt



3c'



11.1019354
4913165

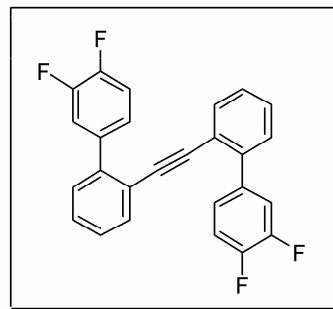
exp3 std13c

SAMPLE DEC. & VT
date Jul 29 2006 dfrq 400.447
solvent cd2cl2 dn H1
file exp dpwr 41
ACQUISITION dof 0
sfrq 100.703 dm nyy
tn C13 dmm w
at 0.798 dmf 9700
np 40302 PROCESSING
sw 25252.5 lb 1.00
fb 14000 wtfile
bs 4 proc ft
tpwr 59 fn 65536
pw 4.3
d1 0.500 werr
d2 1.500 wexp
tof 1546.8 wbs
nt 10000 wnt
ct 788
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.4
wp 20137.7
vs 150
sc 0
wc 250
hzmm 80.55
is 500.00
rfl 6948.9
rfp 5417.2
th 4
ins 100.000
nm ph

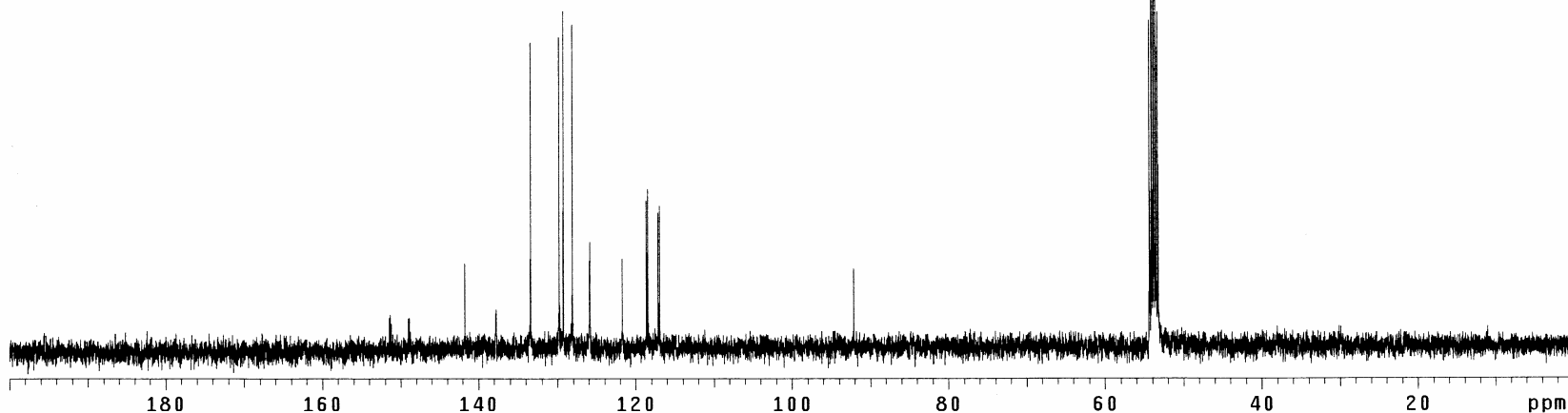
151.482
151.329
149.017
148.887
141.700
137.713
133.373
129.753
129.241
128.070
125.850
125.812
121.679
118.610
116.434
117.133
116.957

92.129

54.320
54.053
53.777
53.509
53.241



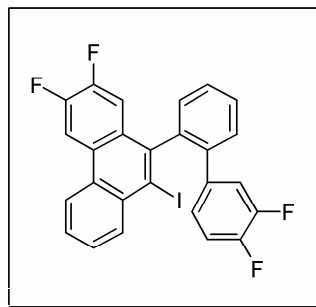
3c'



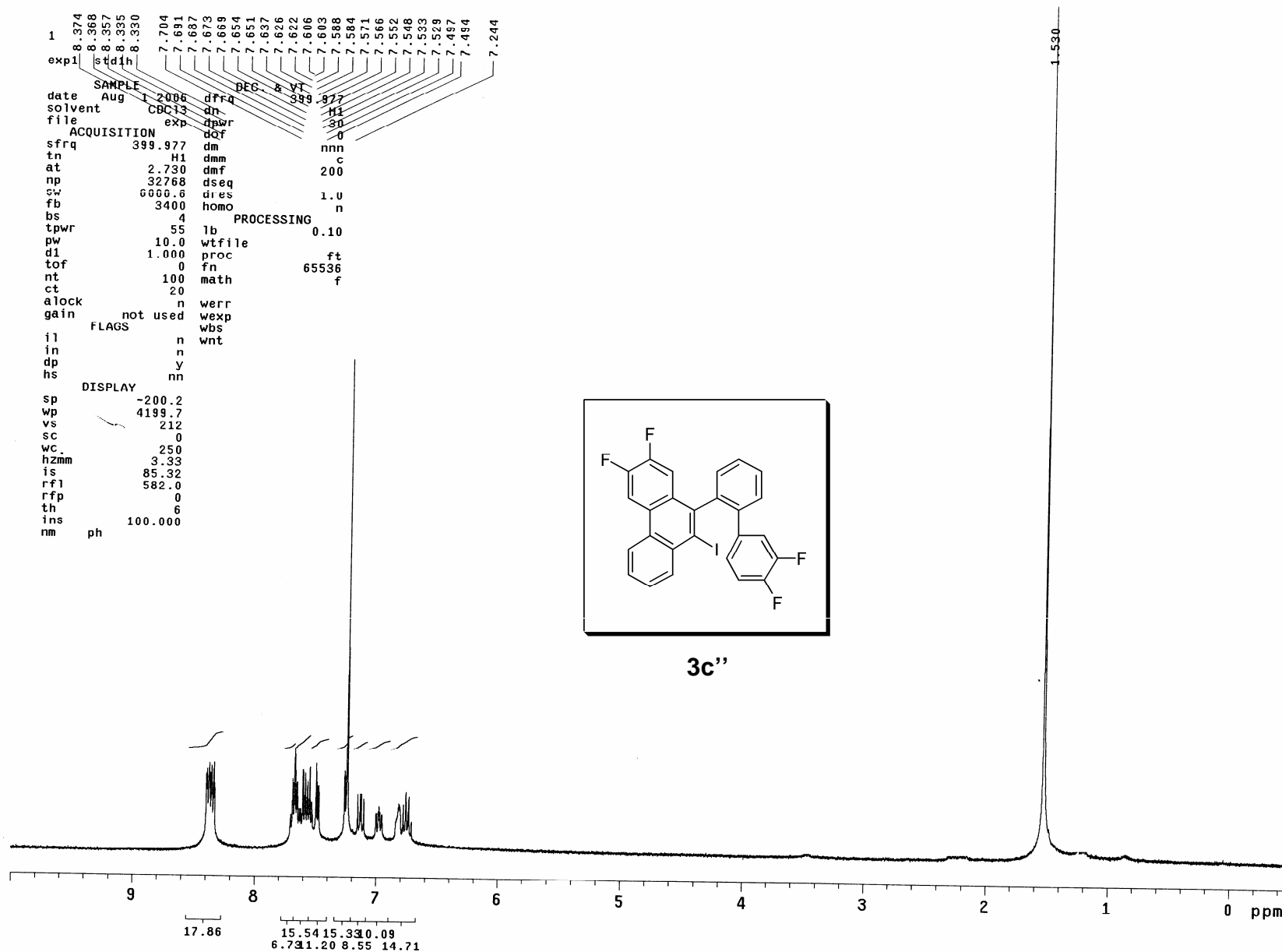
1
 exp1 8.374
 8.368
 8.357
 8.335
 8.330
 7.704
 7.691
 7.687
 7.673
 7.669
 7.654
 7.651
 7.637
 7.626
 7.622
 7.606
 7.603
 7.588
 7.584
 7.571
 7.566
 7.552
 7.548
 7.533
 7.529
 7.497
 7.494
 7.244

SAMPLE
 date Aug 1 2006
 solvent CDCl3
 file exp dqr
 ACQUISITION
 sfrq 399.977
 tn H1
 at 2.730
 np 32768
 sw 6000.6
 fb 3400
 bs 4
 tpwr 55
 pw 10.0
 d1 1.000
 tof 0
 nt 100
 ct 20
 alock not used
 gain not used
 FLAGS
 il n
 in n
 dp y
 hs nn
 DISPLAY
 sp -200.2
 wp 4199.7
 vs 212
 sc 0
 wc 250
 hzmm 3.33
 is 85.32
 rfl 582.0
 rfp 0
 th 6
 ins 100.000
 nm ph

DEC. & VT
 399.977
 H1
 30
 0
 nnn
 c
 dmm
 dmf
 dseq
 dres
 homo
 lb
 wtfile
 proc
 fn
 math
 werr
 wexp
 wbs
 wnt
 0.10
 ft
 65536
 f



3c''



ent Data Parameters
P59-P
NO 2
CNO 1

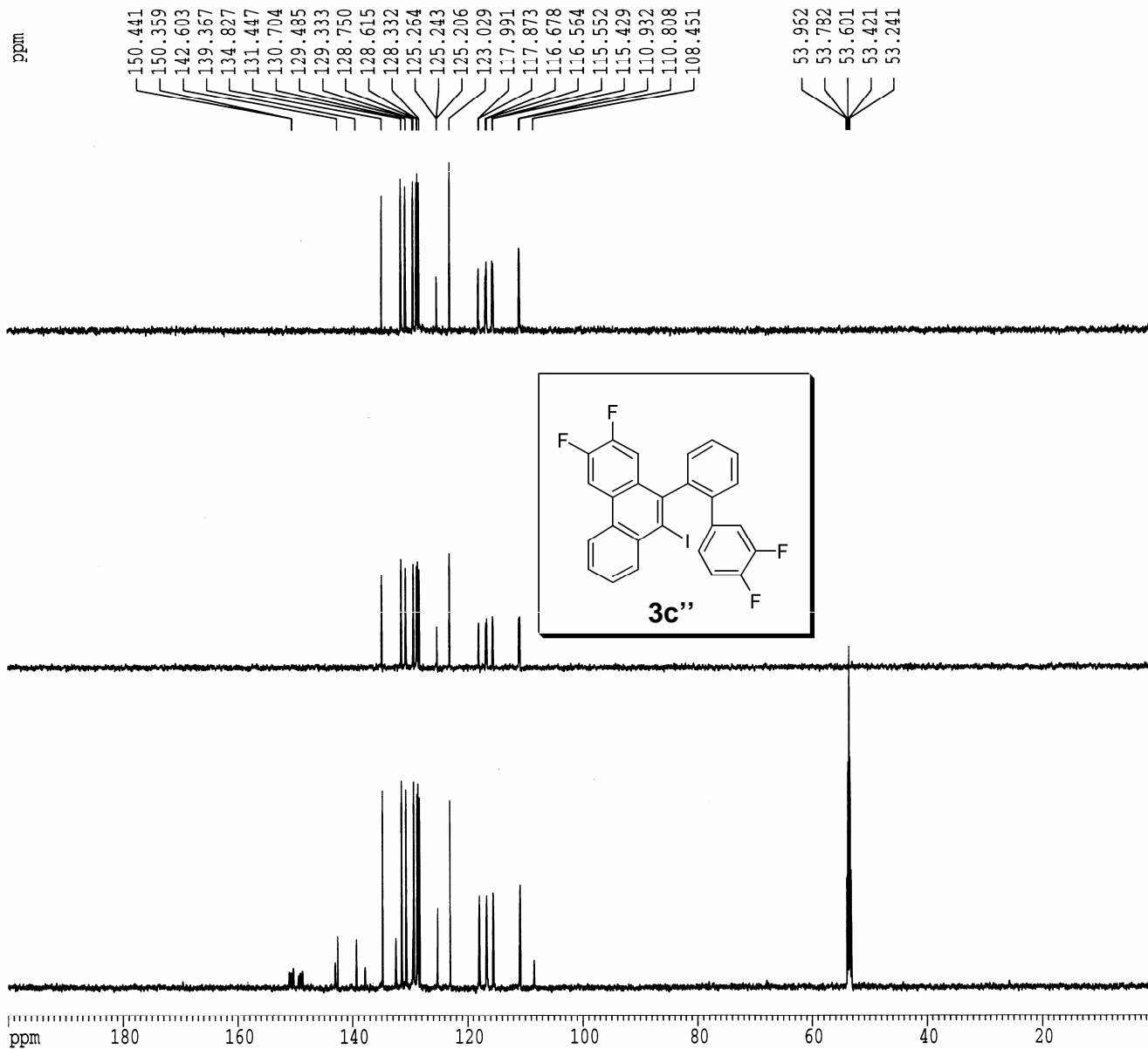
Acquisition Parameters
20061119
16.38
SRUM spect
BHD 5 mm QNP 1H/1
PROG zgpg
32768
VENT Acetone
1410
0
45045.047 Hz
1.374666 Hz
0.3637748 sec
4096
11.100 usec
6.50 usec
302.4 K
3.00000000 sec
0.03000000 sec
TA 2.90000010 sec
EST 0.00000000 sec
RK 0.01500000 sec

==== CHANNEL f1 =====
13C
8.00 usec
0.00 dB
150.7560381 MHz

==== CHANNEL f2 =====
PRG2 waltz16
1H
92.00 usec
120.00 dB
12.00 dB
14.00 dB
599.4829974 MHz

Processing parameters
65536
150.7393373 MHz
EM
0
3.00 Hz
0
0.50

NMR plot parameters
20.00 cm
6.00 cm
200.000 ppm
30147.87 Hz
0.000 ppm
0.00 Hz
10.00000 ppm/cm
1507.39331 Hz/cm



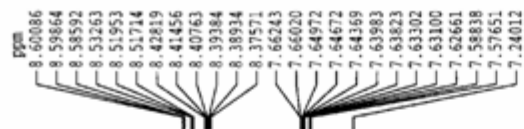
Current Data Parameters
 E DIF-160-P
 NO 1
 CNO 1

- Acquisition Parameters
 e. 20061109
 e 2.00
 TRUM spect
 BHD 5 mm QNP 1H/1
 PROG zg
 32768
 VENT CDC13
 16
 0
 7861.635 Hz
 RES 0.239918 Hz
 2.0840948 sec
 512
 63.600 usec
 6.50 usec
 308.0 K
 1.50000000 sec
 EST 0.00000000 sec
 RK 0.01500000 sec

===== CHANNEL f1 =====
 1 1H
 10.00 usec
 3.00 dB
 1 599.4829974 MHz

- Processing parameters
 32768
 599.4800276 MHz
 no
 0
 0.00 Hz
 0
 1.00

QMR plot parameters
 20.00 cm
 10.00 cm
 10.000 ppm
 5994.80 Hz
 -0.500 ppm
 -299.74 Hz
 CM 0.52500 ppm/cm
 M 314.72702 Hz/cm



3c



ent Data Parameters
 027-160-9
 2
 1

Acquisition Parameters
 20061109
 2.01
 spect
 5 mm QNP 1H/1
 32768
 32768
 Acetone
 3072
 0

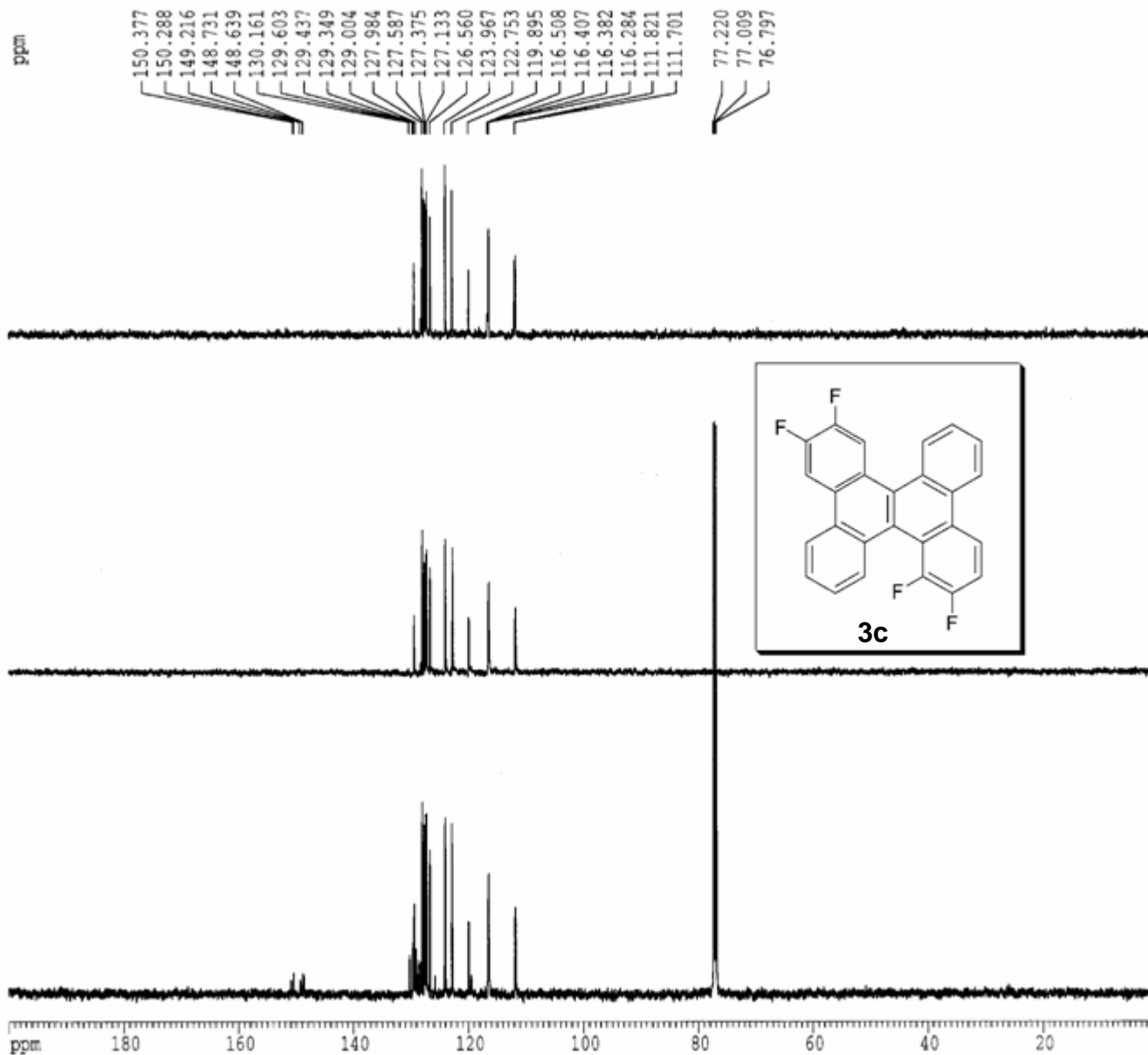
45045.047 Hz
 1.374466 Hz
 0.1637748 sec
 4096
 11.100 usec
 6.50 usec
 308.0 K
 3.0000000 sec
 0.0300000 sec
 2.9000000 sec
 0.0000000 sec
 0.0150000 sec

===== CHANNEL f1 =====
 13C
 4.50 usec
 0.00 dB
 150.7560381 MHz

===== CHANNEL f2 =====
 1H
 92.00 usec
 120.00 dB
 11.30 dB
 14.00 dB
 599.6829974 MHz

Processing parameters
 65536
 150.7393594 MHz
 0
 3.00 Hz
 0
 0.50

QNP plot parameters
 20.00 cm
 10.00 cm
 200.000 ppm
 30147.87 Hz
 0.000 ppm
 0.00 Hz
 10.00000 ppm/cm
 1507.39368 Hz/cm



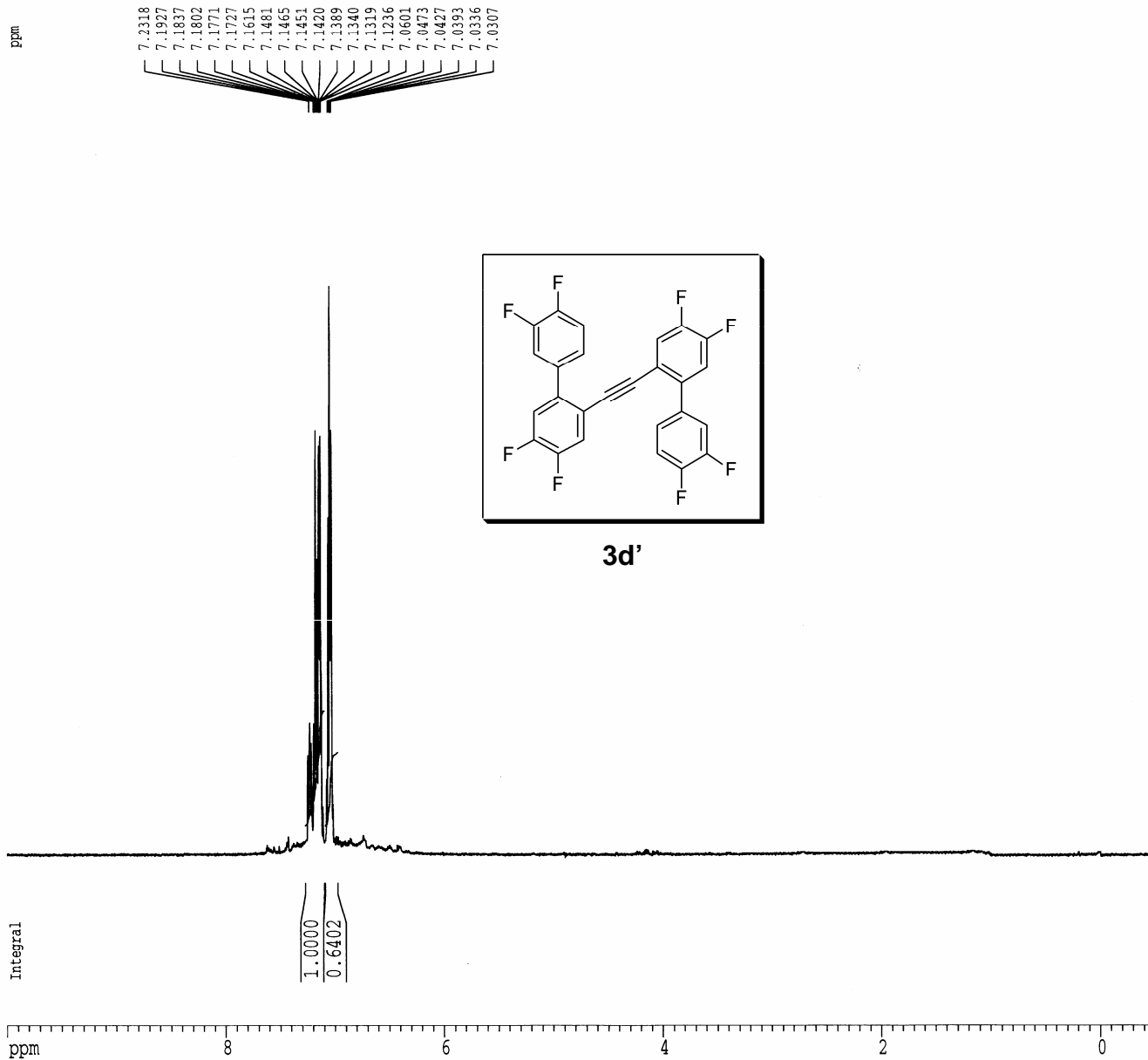
Current Data Parameters
Pulse Program: DIF-147-P
NO: 1
CNO: 1

Acquisition Parameters
Date_: 20061012
Time: 15.51
Pulse Program: spect
BHD: 5 mm QNP 1H/1
PROG: zg
32768
VENT: CDC13
16
0
8389.262 Hz
RES: 0.256020 Hz
1.9530228 sec
128
59.600 usec
6.50 usec
310.5 K
EST: 1.50000000 sec
RK: 0.00000000 sec
0.01500000 sec

==== CHANNEL f1 =====
1 1H
9.30 usec
3.00 dB
1 599.4829974 MHz

Processing parameters
32768
599.4800673 MHz
no
0
0.00 Hz
0
1.00

NMR plot parameters
20.00 cm
10.00 cm
10.000 ppm
5994.80 Hz
-0.500 ppm
-299.74 Hz
CM 0.52500 ppm/cm
M 314.72702 Hz/cm



rent Data Parameters
E DIF-147-P
NO 2
CNO 1

- Acquisition Parameters

20061012
15.56
spect
BHD 5 mm QNP 1H/1
PROG zgpg
32768
VENT CDC13
1024
0
45045.047 Hz
1.374666 Hz
0.3637748 sec
1024
11.100 usec
6.50 usec
308.9 K
3.00000000 sec
0.03000000 sec
TA 2.90000010 sec
EST 0.00000000 sec
RK 0.01500000 sec

==== CHANNEL f1 =====

1 13C
4.70 usec
0.00 dB
1 150.7559473 MHz

==== CHANNEL f2 =====

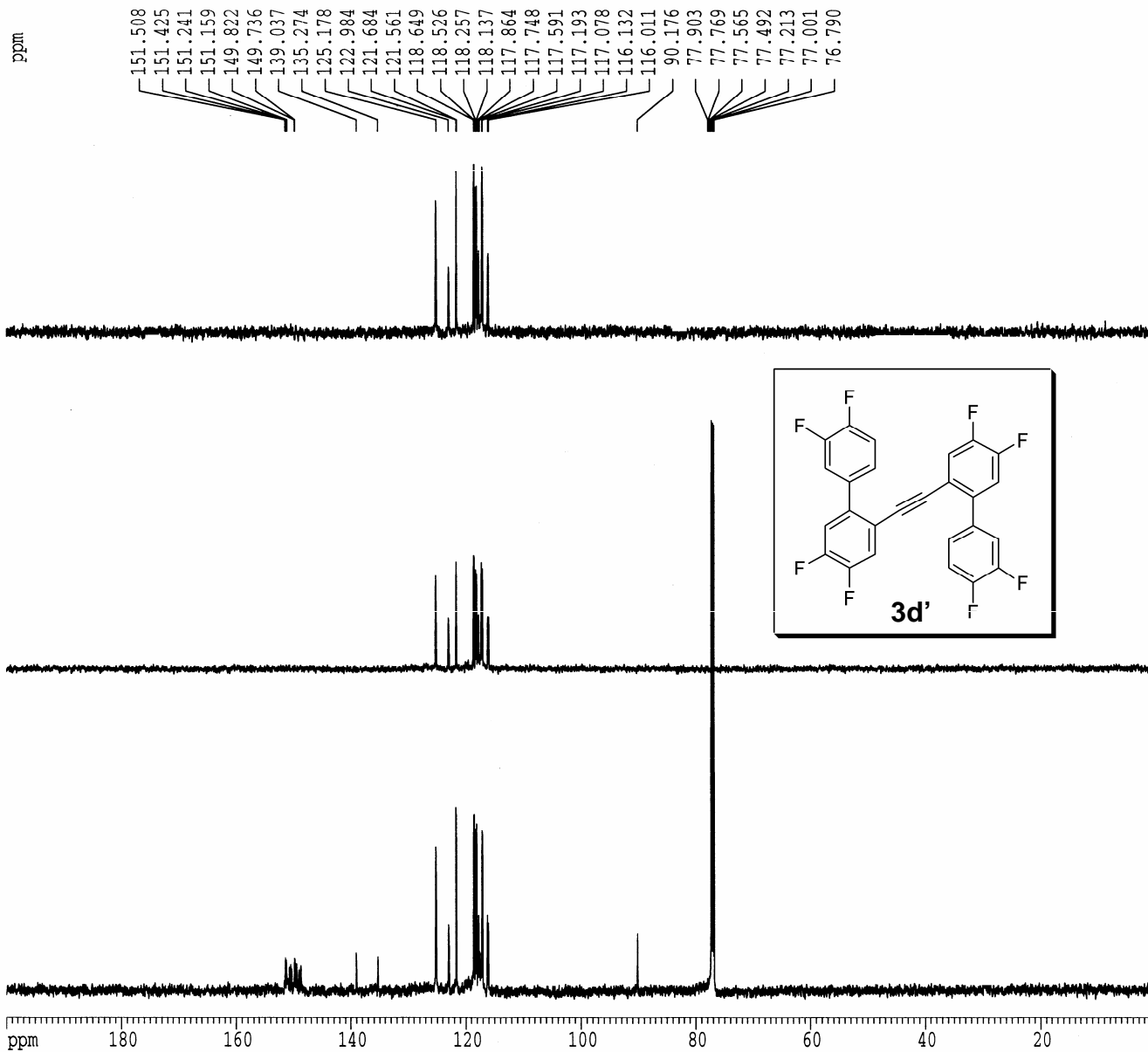
PRG2 waltz16
2 1H
D2 92.00 usec
120.00 dB
2 11.30 dB
3 14.00 dB
2 599.4829974 MHz

- Processing parameters

65536
150.7393524 MHz
EM
0
3.00 Hz
0
0.50

NMR plot parameters

20.00 cm
10.00 cm
200.000 ppm
30147.87 Hz
0.000 ppm
0.00 Hz
10.00000 ppm/cm
M 1507.39355 Hz/cm



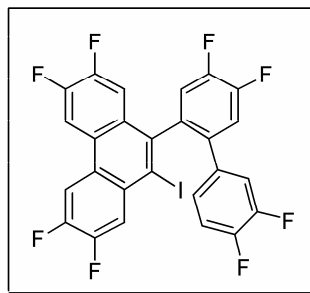
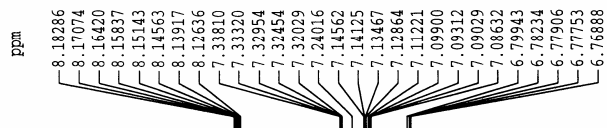
Current Data Parameters
E DIF-163-P
NO 1
CNO 1

Acquisition Parameters
e 20061024
e 15.51
TRUM spect
BHD 5 mm QNP 1H/1
PROG zg
32768
VENT CDC13
16
0
12019.230 Hz
RES 0.366798 Hz
1.3631988 sec
128
41.600 usec
6.50 usec
302.0 K
1.5000000 sec
EST 0.0000000 sec
RK 0.0150000 sec

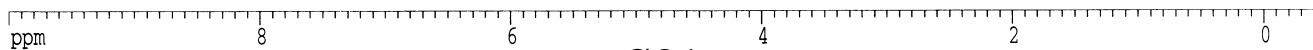
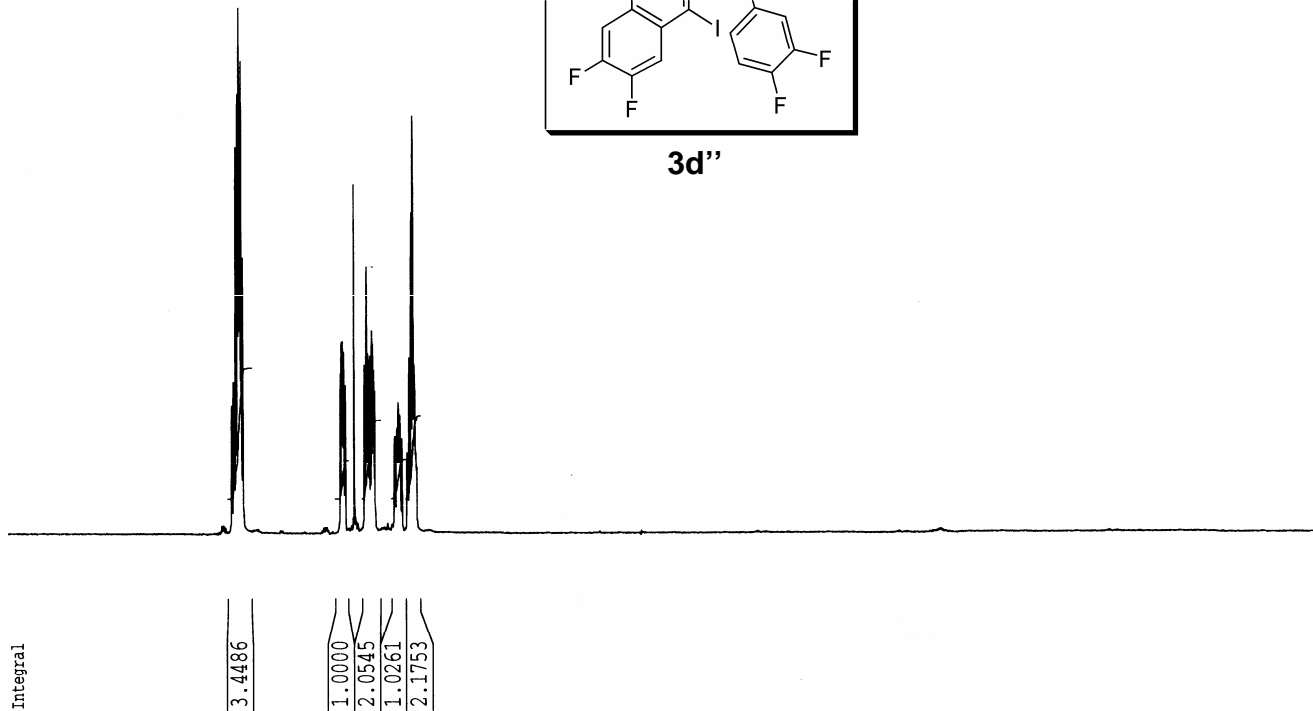
===== CHANNEL f1 =====
1 1H
10.30 usec
2.00 dB
1 599.4829974 MHz

Processing parameters
32768
599.4800279 MHz
no
0
0.00 Hz
0
1.00

NMR plot parameters
20.00 cm
10.00 cm
10.000 ppm
5994.80 Hz
-0.500 ppm
-299.74 Hz
CM 0.52500 ppm/cm
M 314.72702 Hz/cm



3d''



ent Data Parameters
DIF-163-P
0 2
NO 1

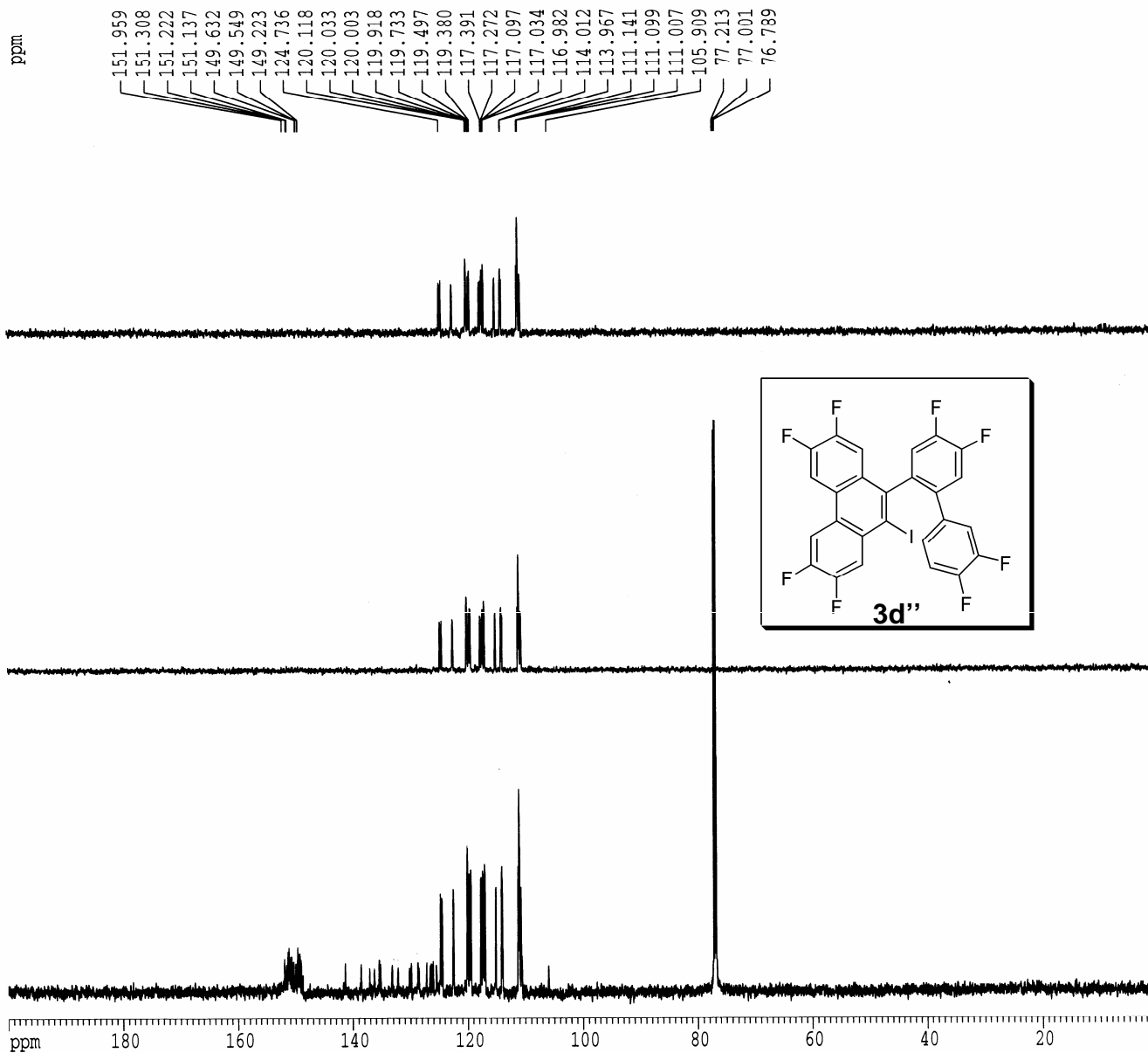
Acquisition Parameters
20061024
15.59
spt
HD 5 mm QNP 1H/1
PROG zgpg
32768
ENT CDC13
500
0
45045.047 Hz
1.374666 Hz
0.3637748 sec
512
11.100 usec
6.50 usec
302.1 K
3.00000000 sec
0.03000000 sec
2.90000010 sec
0.00000000 sec
0.01500000 sec

==== CHANNEL f1 =====
13C
4.70 usec
0.00 dB
150.7559473 MHz

==== CHANNEL f2 =====
PRG2 waltz16
1H
92.00 usec
120.00 dB
11.30 dB
14.00 dB
599.4829974 MHz

Processing parameters
65536
150.7393682 MHz
EM
0
3.00 Hz
0
0.50

2D plot parameters
20.00 cm
10.00 cm
200.000 ppm
30147.87 Hz
0.000 ppm
0.00 Hz
10.00000 ppm/cm
1507.39368 Hz/cm



S32

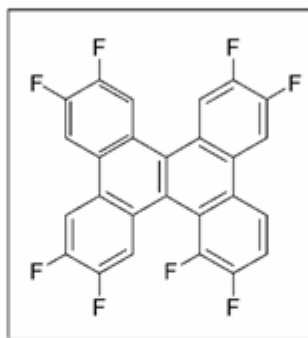
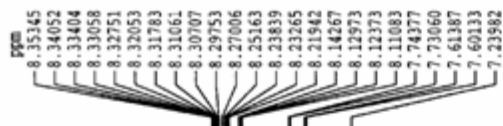
Experiment Data Parameters
 E DIF-162-P
 VO 1
 CNO 1

Acquisition Parameters
 Date_ 20061108
 Time 17.29
 INSTRUM spect
 PWD 5 mm QNP 1H/1
 PROG zg
 FID 32768
 VSWT CDC13
 SFO 16
 O 0
 F1 7861.635 Hz
 RES 0.239918 Hz
 AQ 2.0840948 sec
 SI 512
 SF 63.600 usec
 EX 6.50 usec
 K 307.7 K
 1.50000000 sec
 FST 0.00000000 sec
 RK 0.01500000 sec

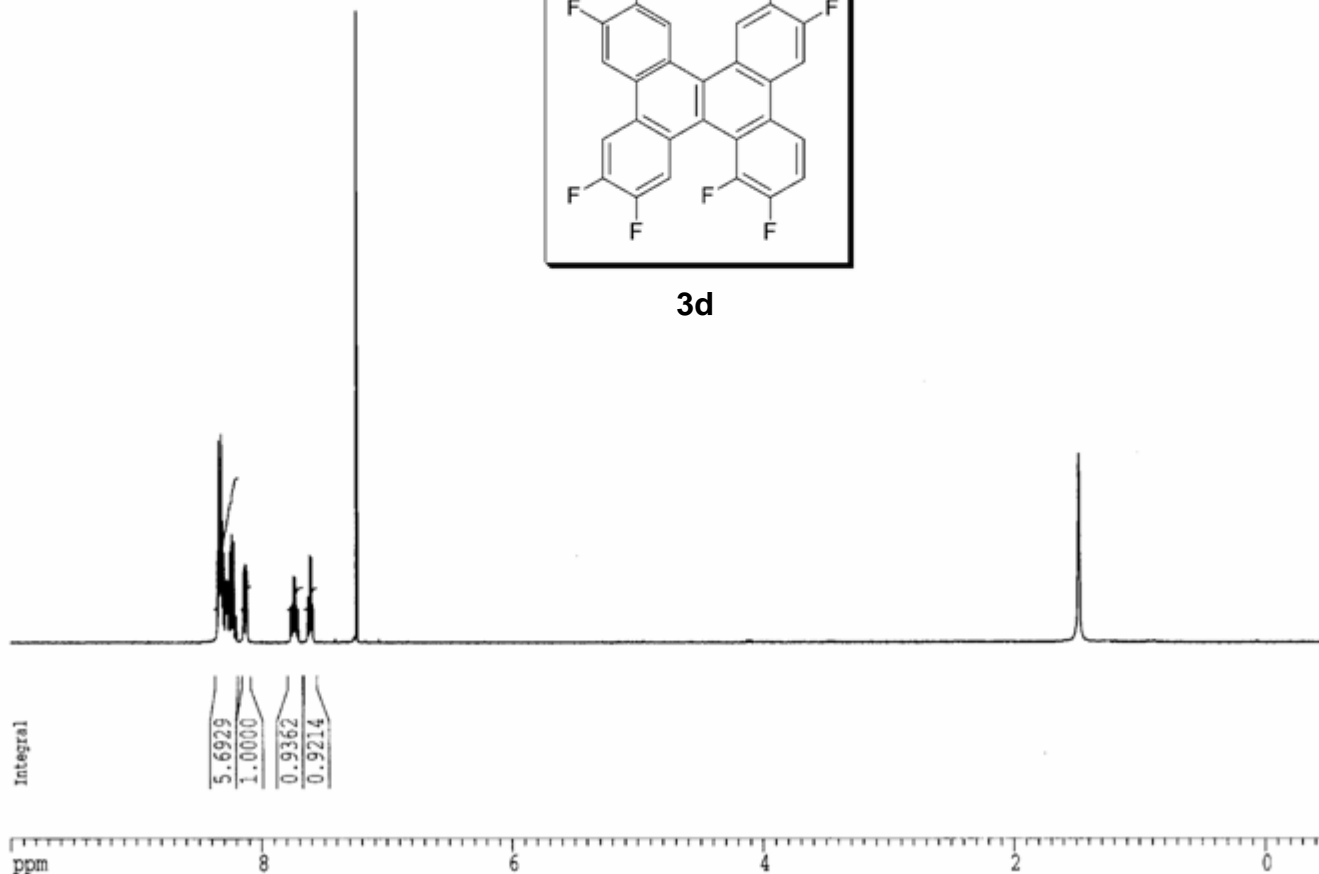
===== CHANNEL f1 =====
 L 1H
 T1 10.00 usec
 P 3.00 dB
 FREQ 599.4829974 MHz

Processing parameters
 32768
 599.4800273 MHz
 no
 0
 0.00 Hz
 0
 1.00

===== 1H NMR plot parameters =====
 20.00 cm
 10.00 cm
 10.000 ppm
 5994.80 Hz
 -0.500 ppm
 -299.74 Hz
 0.52500 ppm/cm
 314.72702 Hz/cm



3d



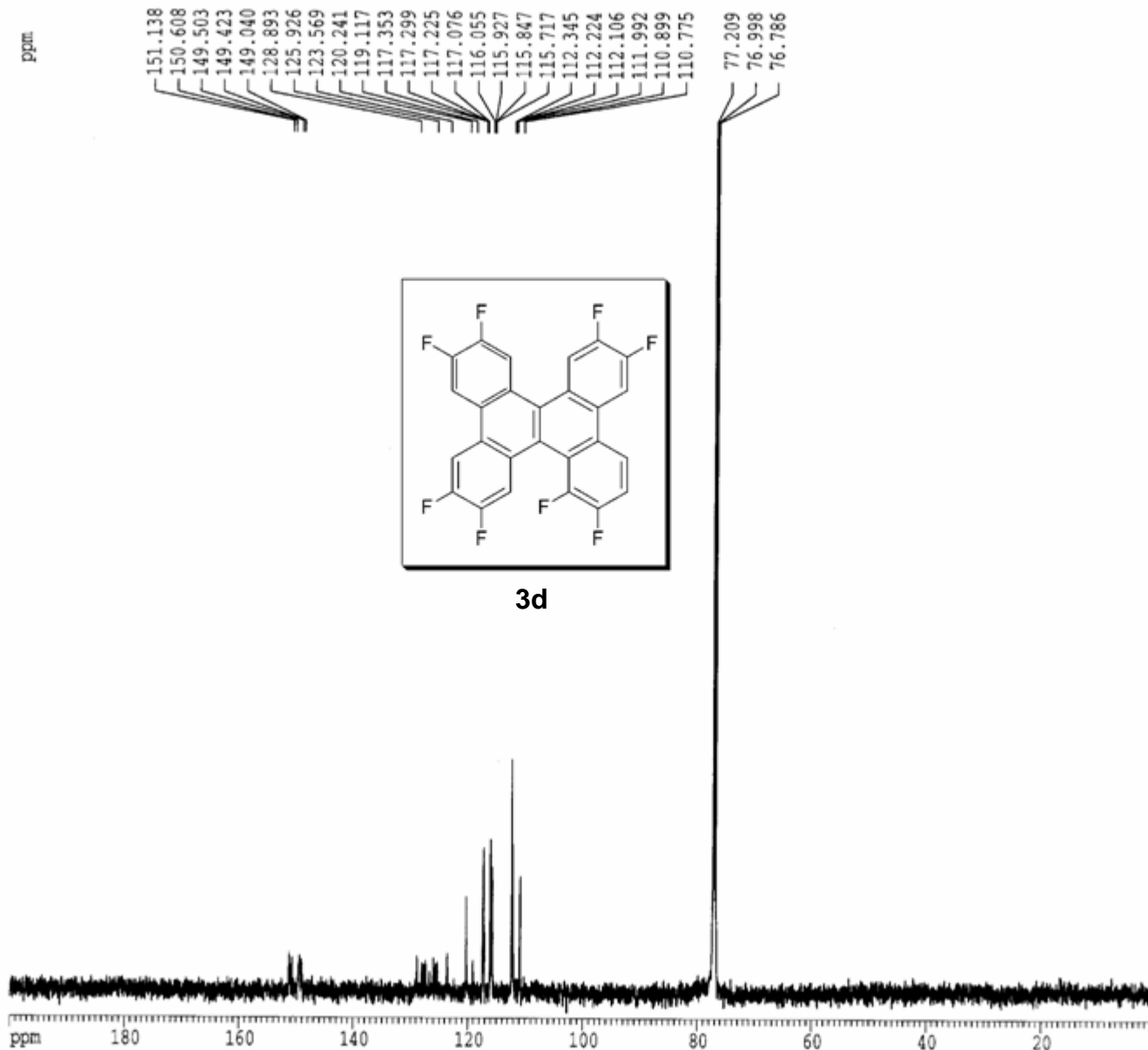
Current Data Parameters
 NS 121P-182-P
 PWD 2
 DCHO 1

Acquisition Parameters
 Date_ 20061108
 Time 17.33
 STRUM spect
 NMRD 5 mm QNP 1H/1
 PPG 32768
 FREQ 400
 ACQNT Acetone
 2011
 0
 45045.047 Hz
 1.374666 Hz
 0.3637768 sec
 4096
 11.100 usec
 6.50 usec
 309.0 K
 3.00000000 sec
 0.03000000 sec
 2.90000010 sec
 0.00000000 sec
 0.01500000 sec

===== CHANNEL f1 =====
 F1 13C
 4.50 usec
 0.00 dB
 150.7560381 MHz
 ===== CHANNEL f2 =====
 F2 1H
 92.00 usec
 120.00 dB
 11.30 dB
 14.00 dB
 599.4829974 MHz

Processing parameters
 65536
 150.7393566 MHz
 0
 3.00 Hz
 0
 0.50

===== plot parameters =====
 20.00 cm
 30.00 cm
 230.000 ppm
 30147.87 Hz
 0.000 ppm
 0.00 Hz
 10.00000 ppm/cm
 1507.39355 Hz/cm



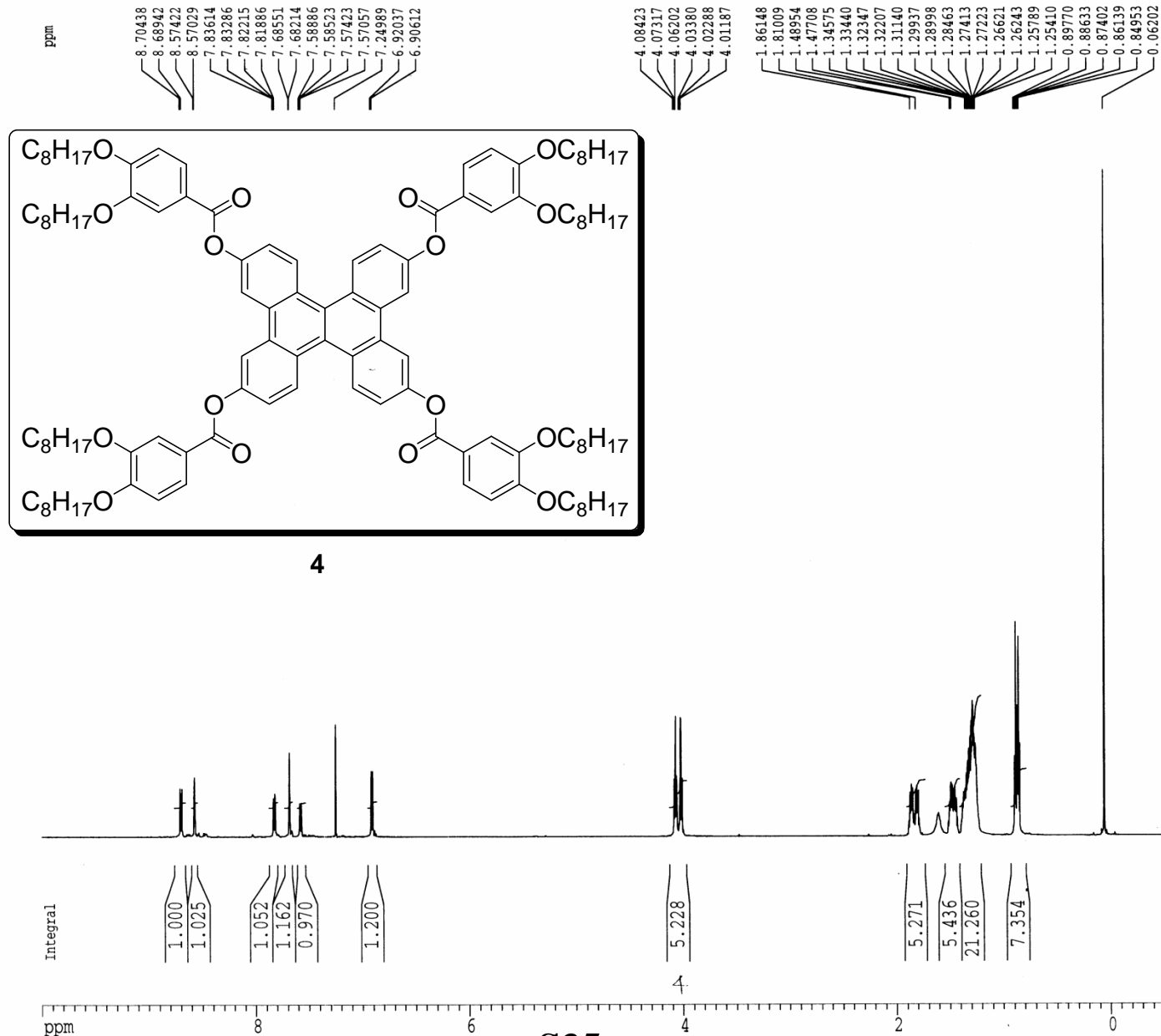
Current Data Parameters
 NAME ester-2-OC8H17
 XPNO 1
 PROCNO 1

2 - Acquisition Parameters
 Date_ 20060927
 Time 13.58
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg
 D 32768
 SOLVENT CDCl3
 S 16
 S 0
 WH 12019.230 Hz
 IDRES 0.366798 Hz
 Q 1.3631988 sec
 G 128
 W 41.600 usec
 E 6.50 usec
 E 0.0 K
 I 1.50000000 sec
 CREST 0.00000000 sec
 CWPR 0.01500000 sec

===== CHANNEL f1 =====
 UC1 1H
 I 9.80 usec
 L1 3.00 dB
 FO1 599.5035970 MHz

2 - Processing parameters
 I 32768
 F 599.5000213 MHz
 DW no
 SB 0
 B 0.00 Hz
 B 0
 C 1.00

D NMR plot parameters
 X 20.00 cm
 Y 12.00 cm
 I 10.000 ppm
 I 5995.00 Hz
 I 2P -0.500 ppm
 I 2 -299.75 Hz
 PMCM 0.52500 ppm/cm
 ZCM 314.73749 Hz/cm



Current Data Parameters
 ME ester-2-OC8H17
 PNO 2
 DCNO 1

- Acquisition Parameters

ce_ 20060927
 ne 14.03
 STRUM spect
 DBHD 5 mm QNP 1H/1
 LPROG zgpg
 32768
 LVENT CDCl3
 758
 0
 H 45045.047 Hz
 DRES 1.374666 Hz
 0.3637748 sec
 2048
 11.100 usec
 6.50 usec
 0.0 K
 3.00000000 sec
 0.03000000 sec
 2.90000010 sec
 0.00000000 sec
 WRK 0.01500000 sec

==== CHANNEL f1 =====

C1 13C
 4.70 usec
 1 0.00 dB
 D1 150.7609769 MHz

==== CHANNEL f2 =====

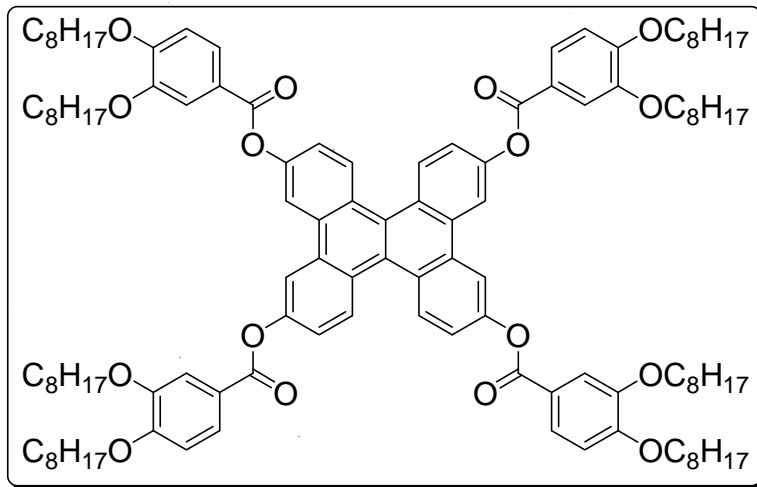
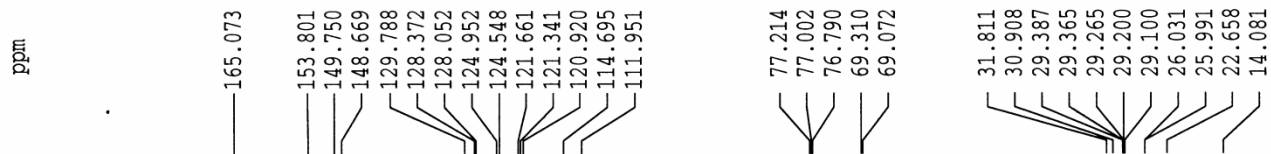
DPRG2 waltz16
 C2 1H
 PD2 92.00 usec
 2 120.00 dB
 12 11.30 dB
 13 14.00 dB
 02 599.5029975 MHz

- Processing parameters

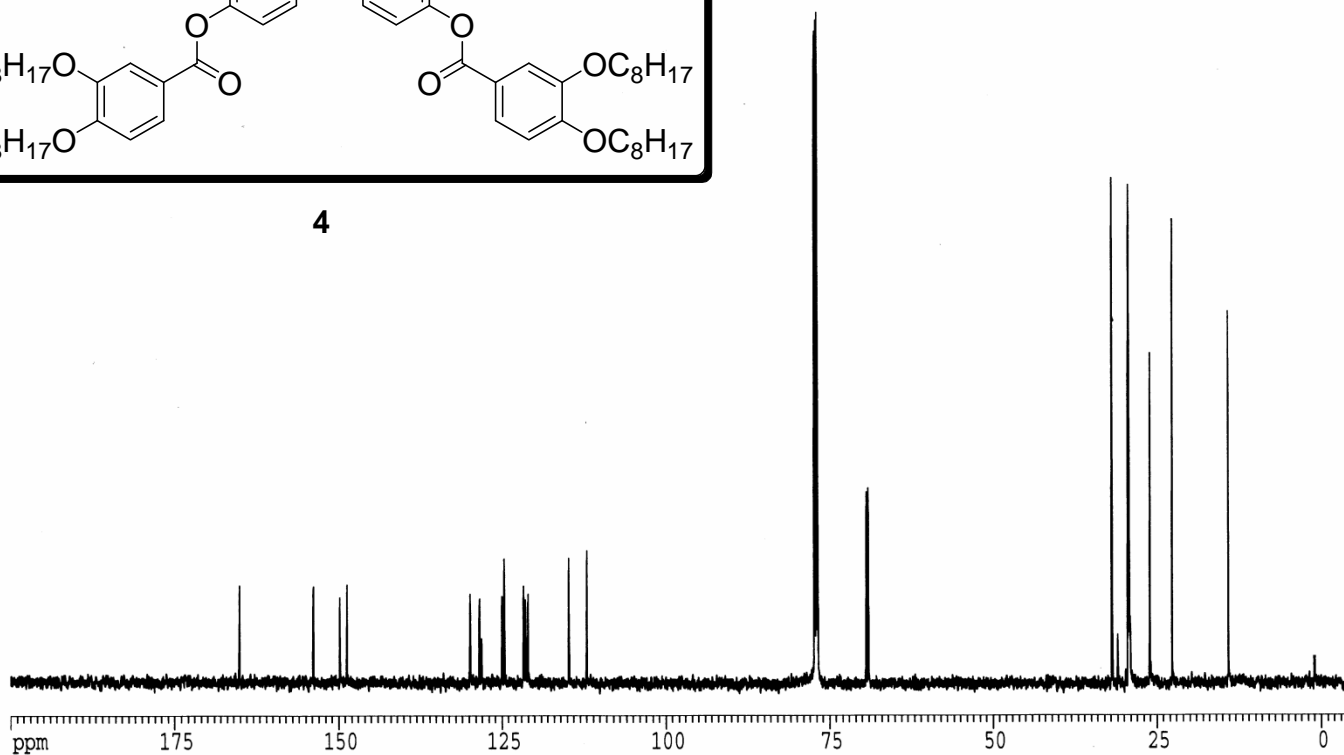
65536
 150.7443988 MHz
 W EM
 B 0
 3.00 Hz
 0
 0.50

NMR plot parameters

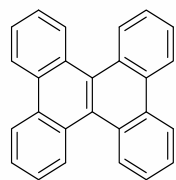
20.00 cm
 10.00 cm
 P 200.000 ppm
 30148.88 Hz
 P -5.000 ppm
 -753.72 Hz
 MCM 10.25000 ppm/cm
 CM 1545.13025 Hz/cm



4

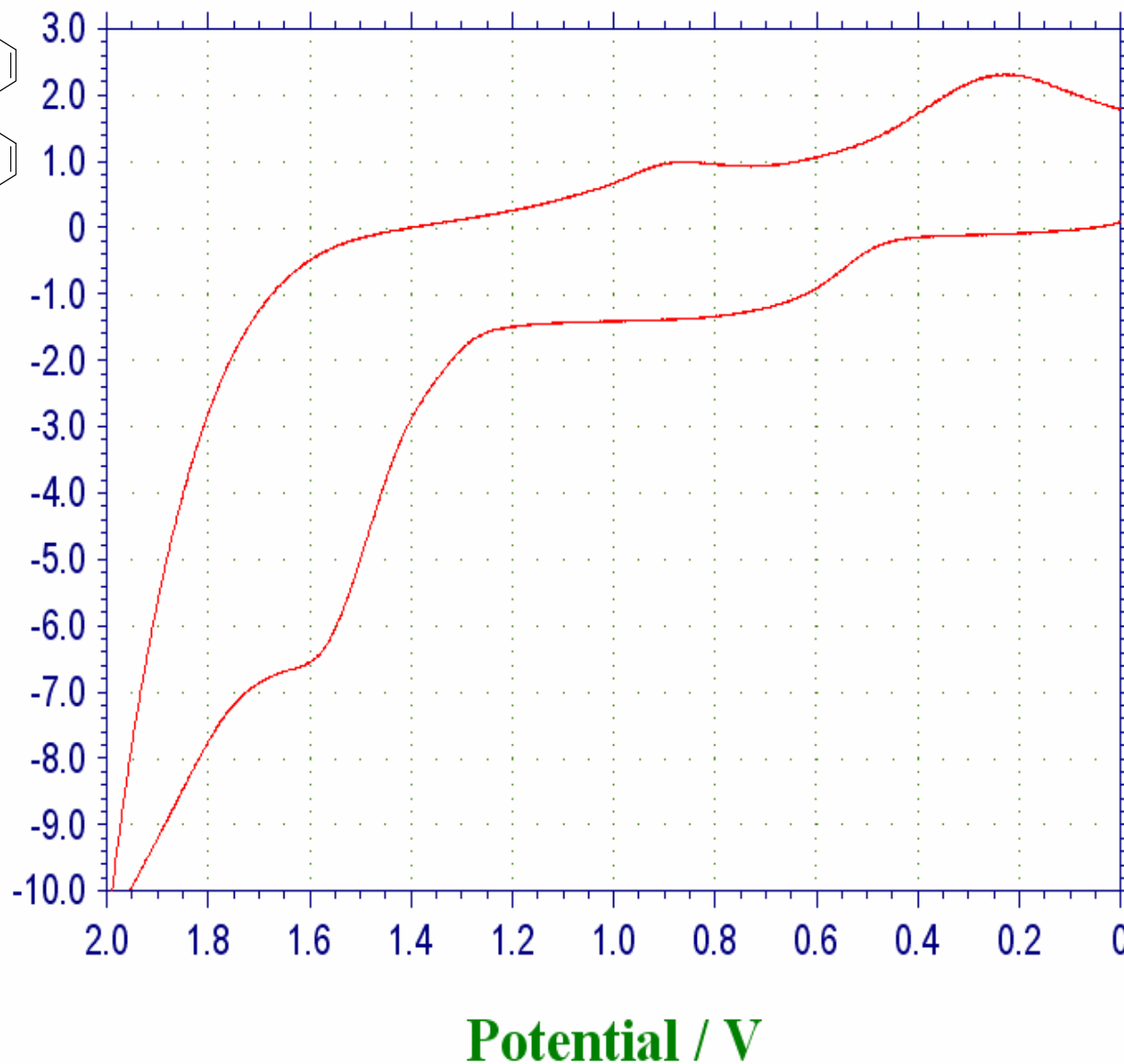


S36



1

Current / 1e-6A



Apr. 15, 2006 16:43:05

Tech: CV

File: All-H-ref.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = 0

Init P/N = P

Scan Rate (V/s) = 0.1

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-6

Segment 1:

Segment 2:

Figure S1. Cyclic voltammetry of **1**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

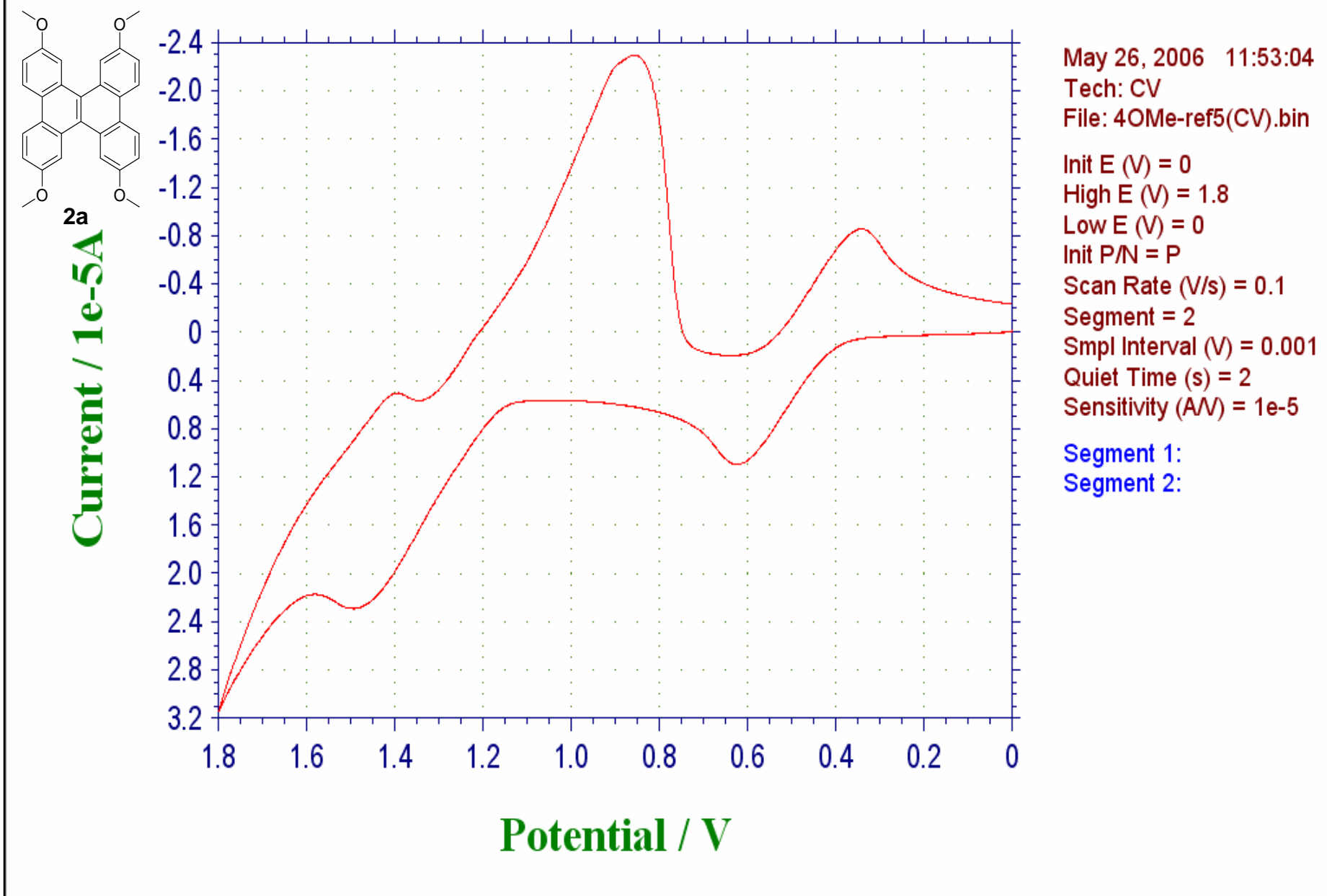
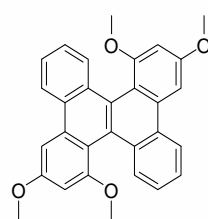
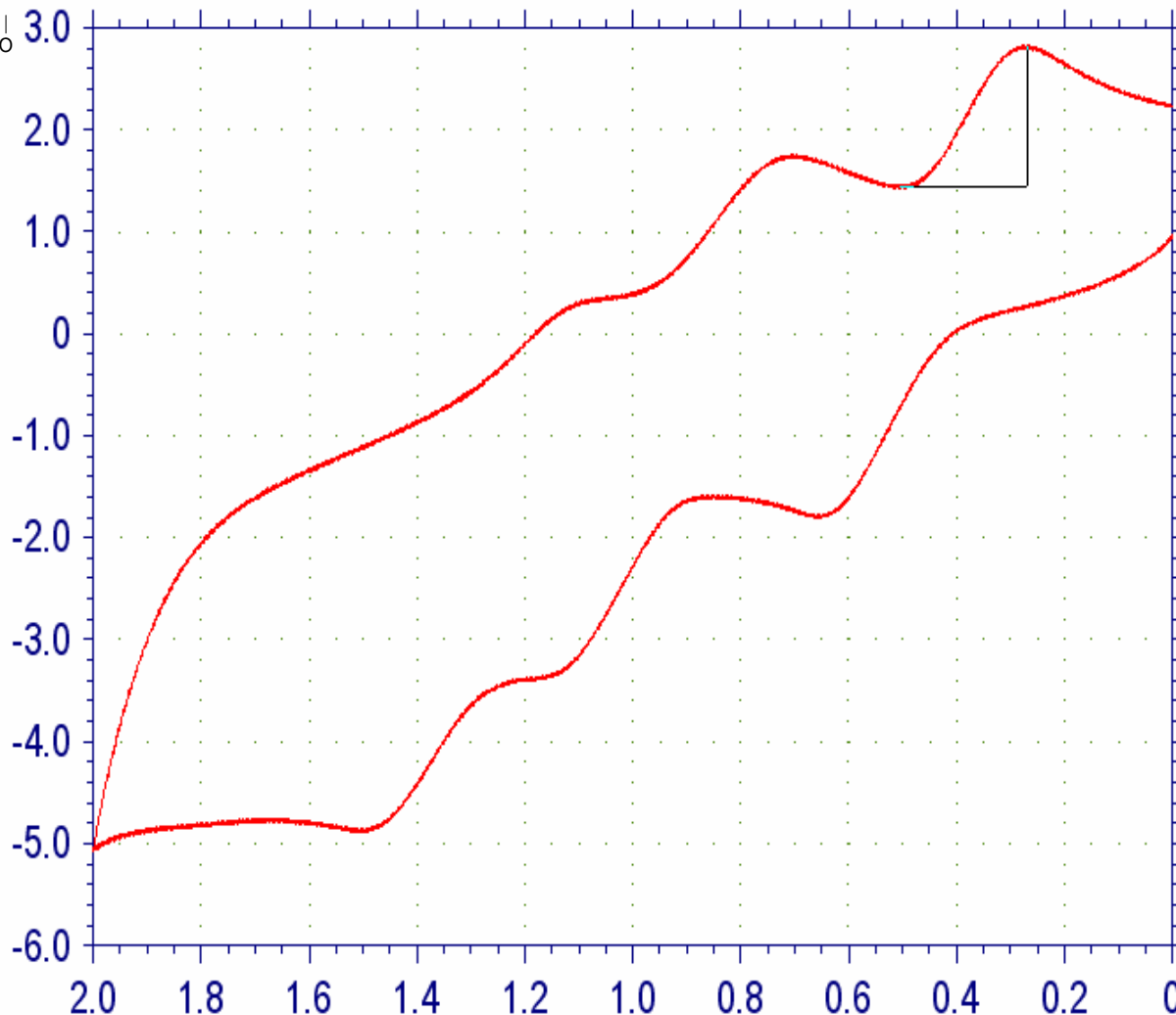


Figure S2. Cyclic voltammetry of **2a**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)



2b

Current / 1e-6A



Potential / V

Apr. 15, 2006 17:59:56

Tech: CV

File: 2OMe-ref-2.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = 0

Init P/N = P

Scan Rate (V/s) = 0.1

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 2e-6

Segment 1:

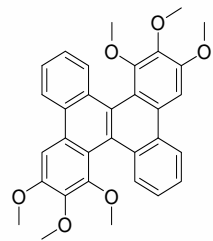
Segment 2:

Ep = 0.269V

ip = 1.384e-6A

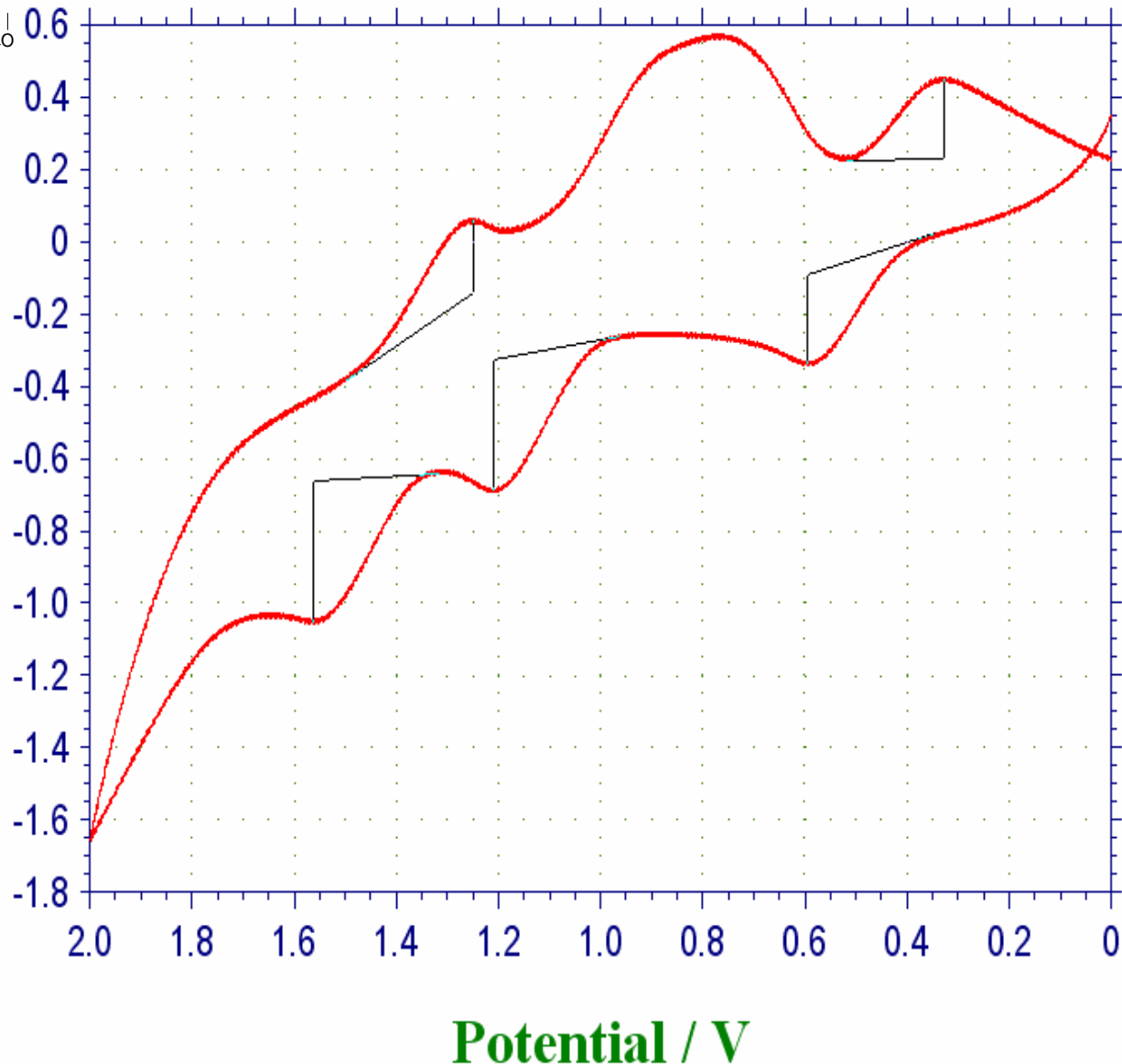
Ah = 1.584e-6C

Figure S3. Cyclic voltammetry of **2b**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)



2c

Current / 1e-5A



Apr. 15, 2006 18:35:16

Tech: CV

File: 3OMe-ref-3.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = 0

Init P/N = P

Scan Rate (V/s) = 0.1

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 2e-6

Segment 1:

Ep = 0.596V

ip = -2.507e-6A

Ah = -2.833e-6C

Ep = 1.209V

ip = -3.657e-6A

Ah = -4.029e-6C

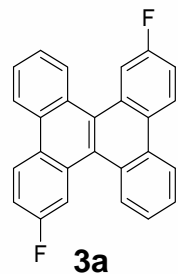
Ep = 1.564V

ip = -3.943e-6A

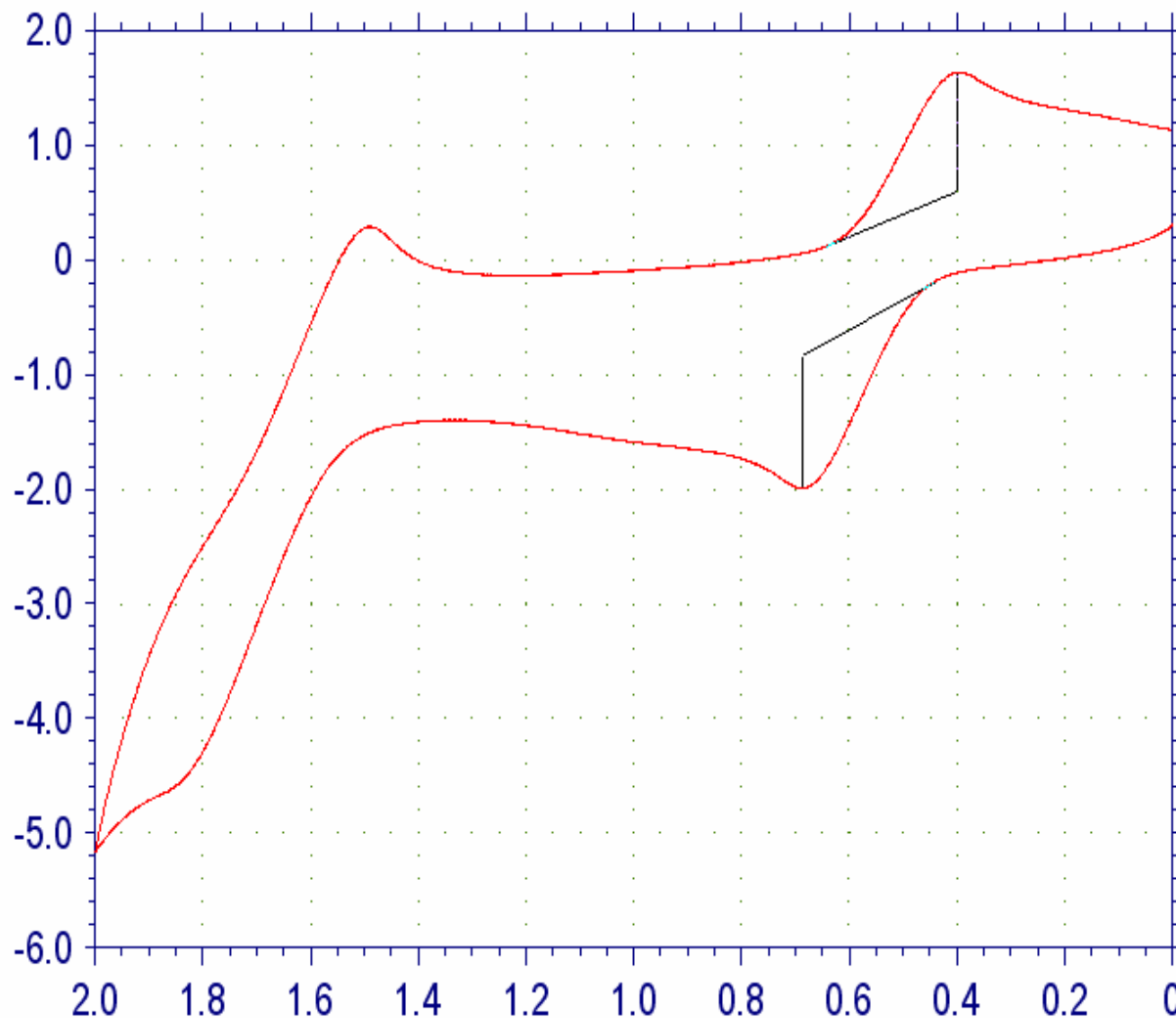
Ah = -4.571e-6C

Segment 2:

Figure S4. Cyclic voltammetry of **2c**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)



Current / 1e-6A



Potential / V

Apr. 15, 2006 17:12:47

Tech: CV

File: 2F-ref-2.bin

Init E (V) = 0

High E (V) = 2

Low E (V) = 0

Init P/N = P

Scan Rate (V/s) = 0.1

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-6

Segment 1:

Ep = 0.687V

ip = -1.160e-6A

Ah = -1.414e-6C

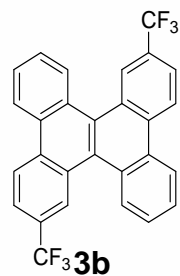
Segment 2:

Ep = 0.398V

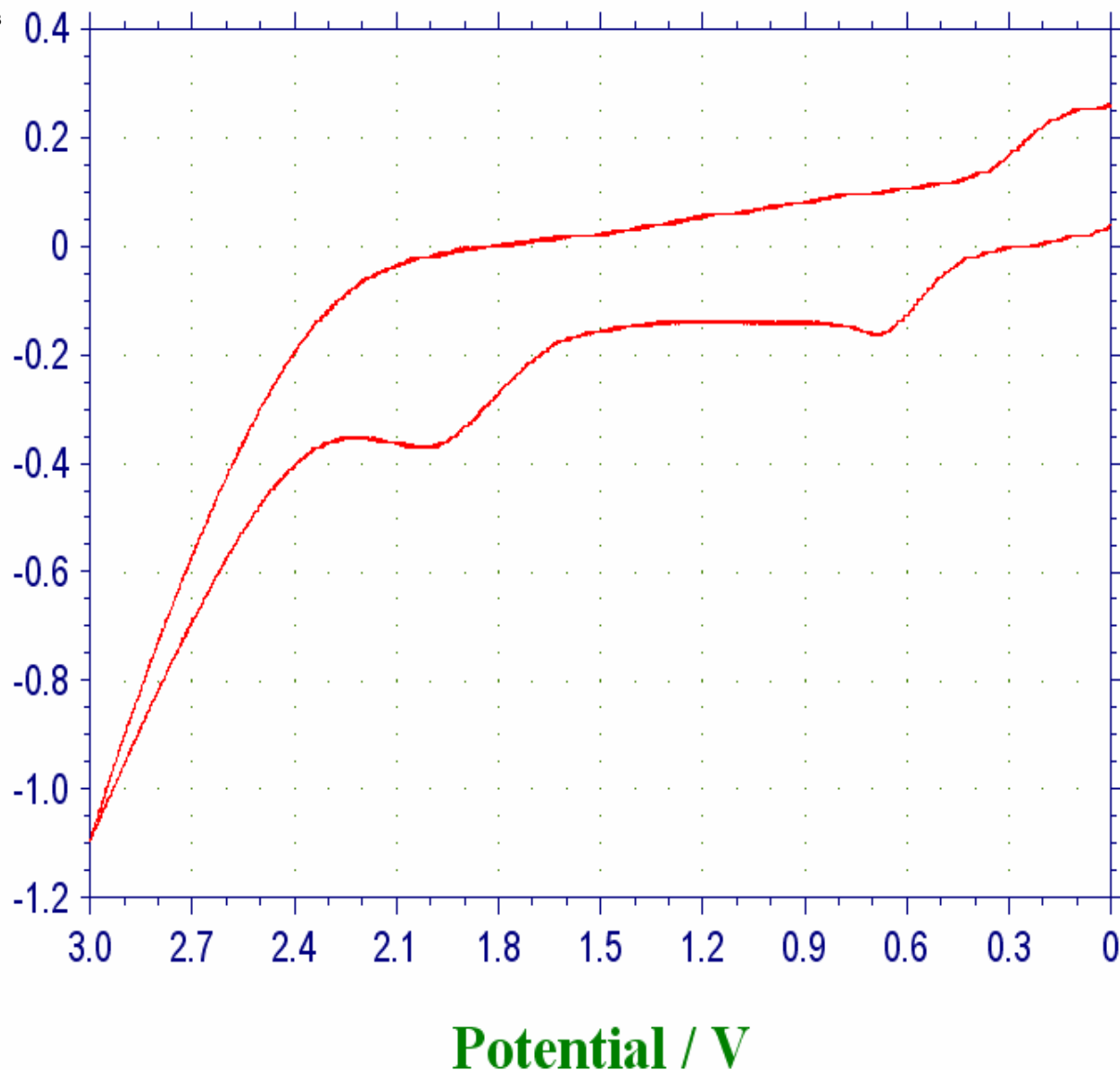
ip = 1.046e-6A

Ah = 1.205e-6C

Figure S5. Cyclic voltammetry of **3a**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)



Current / 1e-5A



Apr. 15, 2006 17:41:16

Tech: CV

File: CF3-ref-4.bin

Init E (V) = 0

High E (V) = 3

Low E (V) = 0

Init P/N = P

Scan Rate (V/s) = 0.1

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 2e-5

Segment 1:

Segment 2:

Figure S6. Cyclic voltammetry of **3b**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

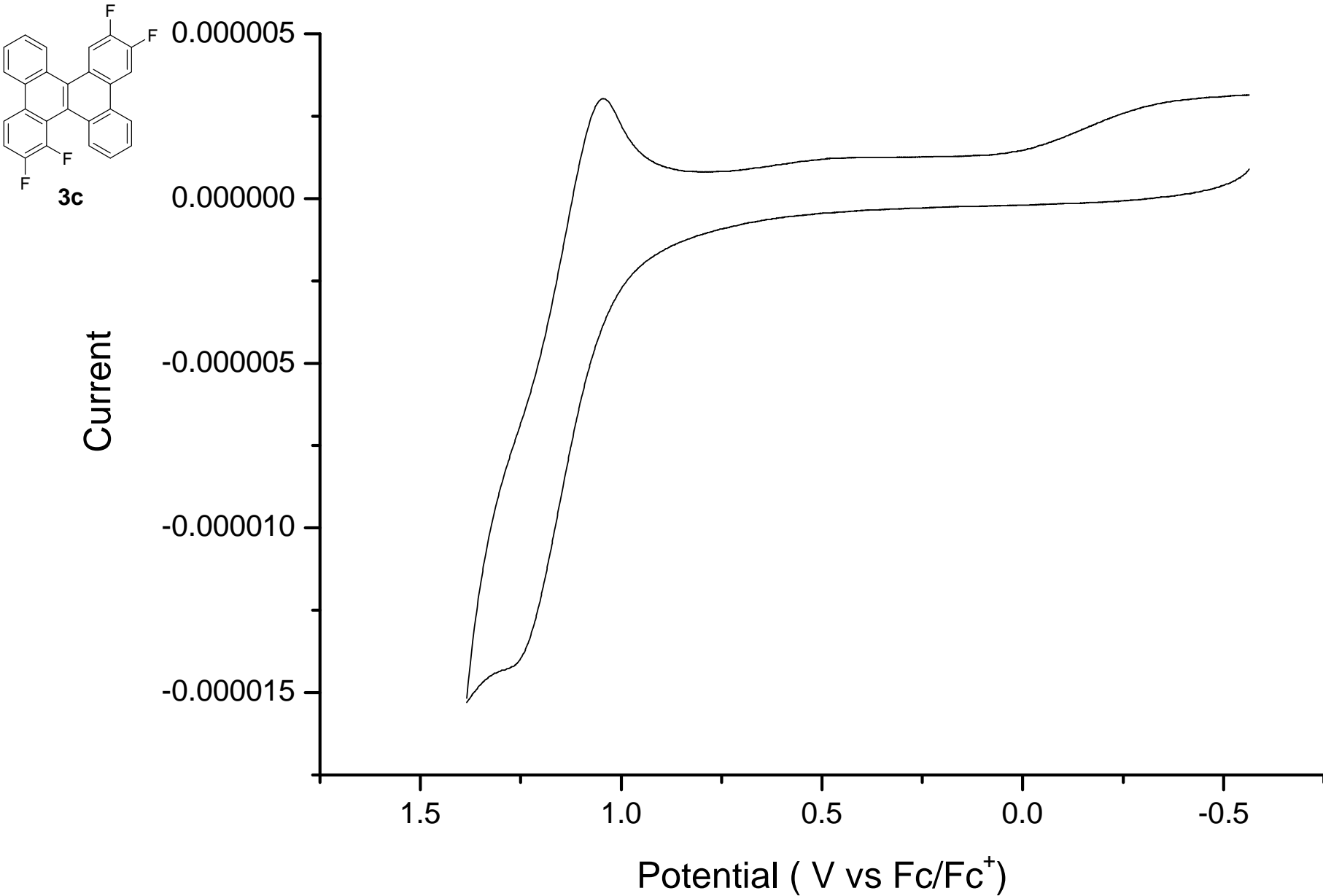


Figure S7. Cyclic voltammetry of **3c**: (Sample concentration was $1 \times 10^{-3} \text{ M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as eference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

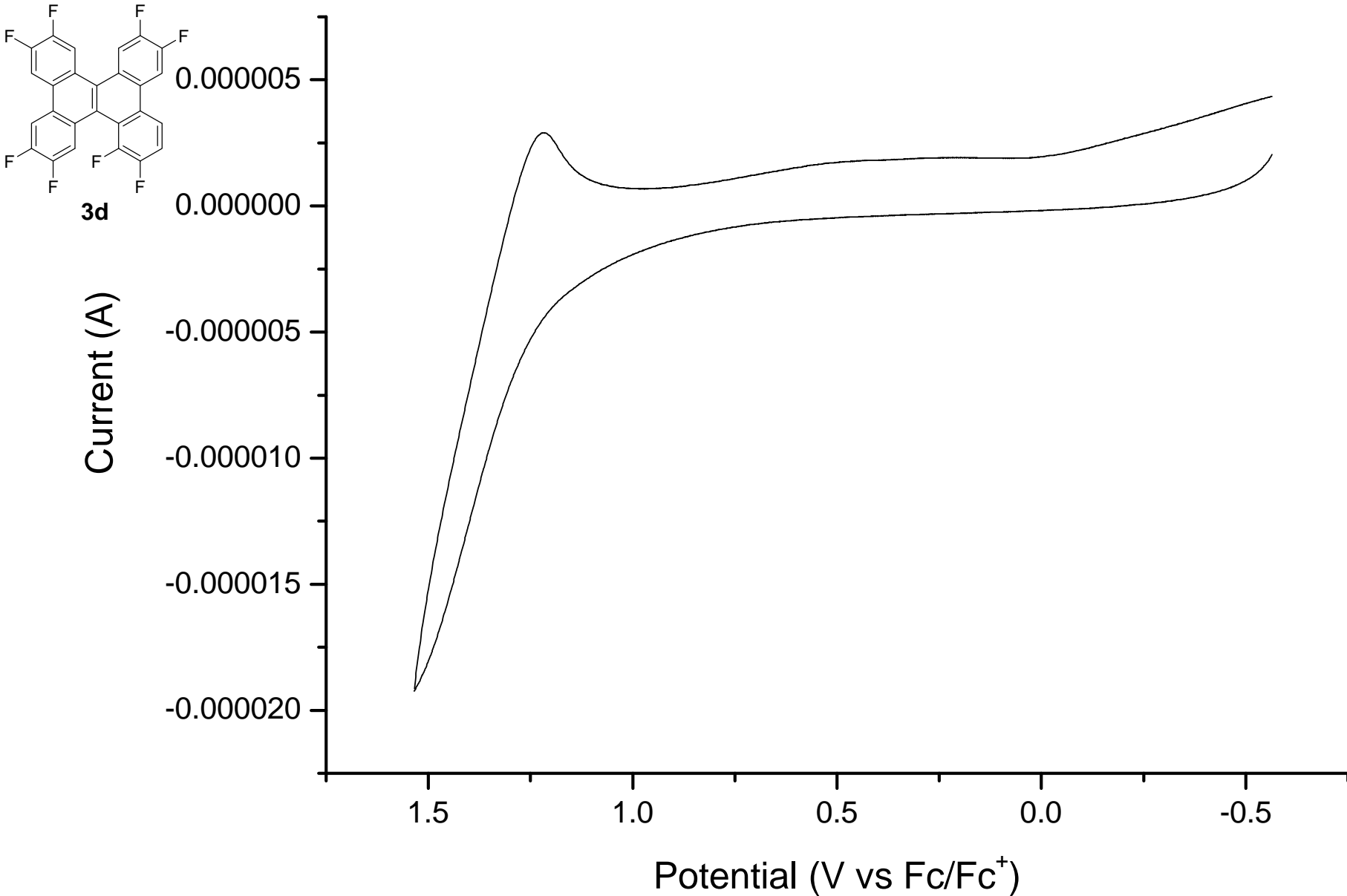


Figure S8. Cyclic voltammetry of **3d**: (Sample concentration was $1 \times 10^{-3} \text{ M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

TG/DTA		<Sample>	<Comment>	<Temp. program [C]	[C/min]	[min]
<Name>	080602A	1		1*	25.0- 900.0	5.00 0.00
<Date>	86/08/01 10:54			<Gas>		
		3.485 mg		N2	100.0 ml/min	
		(3.485 mg)		no	0.0 ml/min	
		<Reference>				
		Pt				
		0.000 mg	<Sampling>			
			0.5 sec			

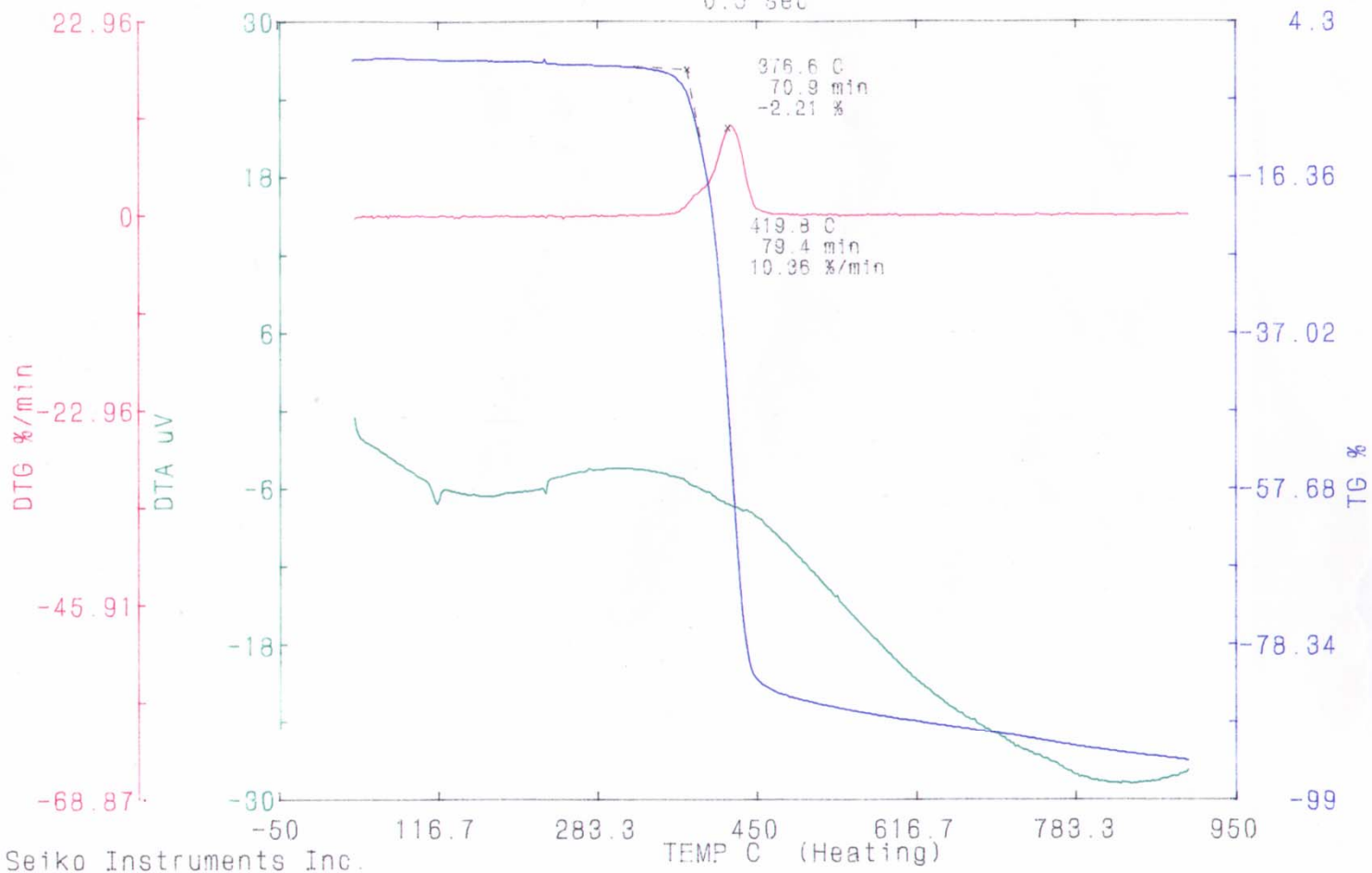


Figure S8. The TGA measurement of **4**