

Supporting Information

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

Rupsha Chaudhuri,[†] Ming-Yu Hsu,[†] Chia-Wen Li,[†] Cheng-I Wang,[†] Chun-Jung Chen,[‡]
Chung K. Lai,[‡] Li-Yin Chen,[§] Su-Hao Liu,[§] Chung-Chih Wu,[§] and Rai-Shung Liu^{†*}

[†]Department of Chemistry, National Taing-Hua University, Hsinchu,

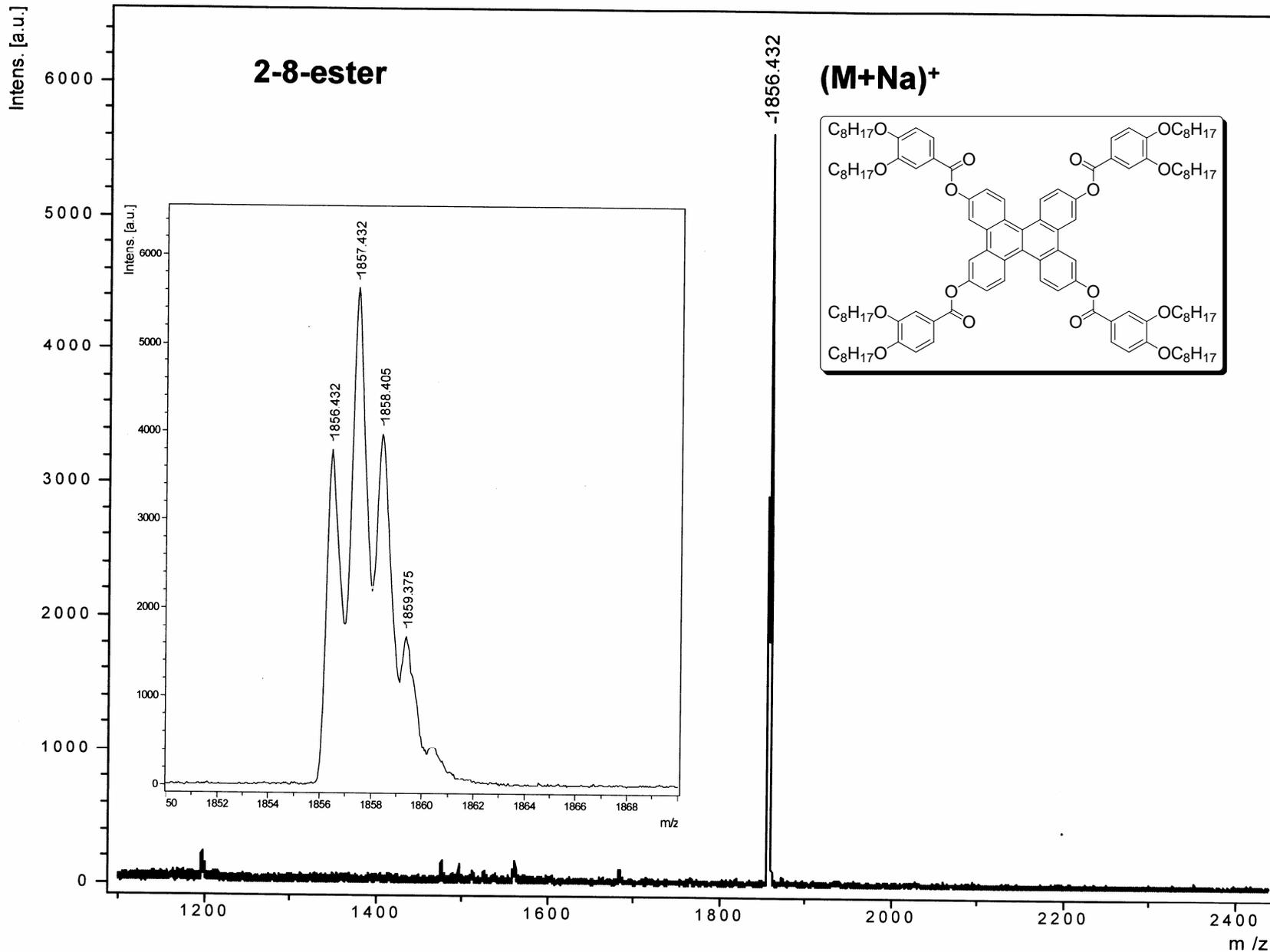
[‡]Department of Chemistry, National Central University, Chungli,

[§]Department of Electric Engineering and Graduate Institute of Photonics and Optoelectronics, National Taiwan University, Taipei, Taiwan, ROC.

rsliu@mx.nthu.edu.tw

Contents:

(1) MALDI-TOF (M+Na) ⁺ for compound 4-----	S2
(2) NMR Spectra for key compounds-----	S3
(3) Cyclic Voltammograms for key compound-----	S36
(4) The TGA measurement for 4-----	S45

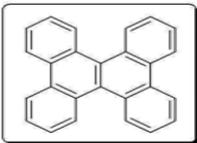


STANDARD 1H OBSERVE

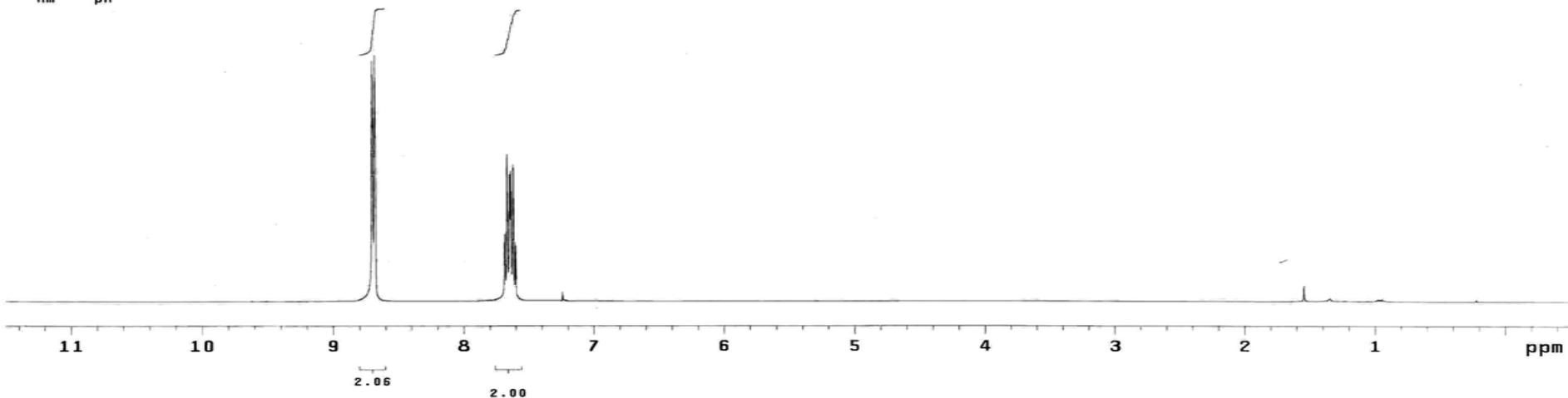
exp1 std1h

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
 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 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



1

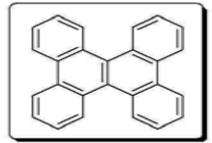


13C OBSERVE

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 1380.0 wtfile
bs 4 proc
tpwr 58 ft
pw 6.5 fn not used
d1 1.500 werr
tof 2000.0 wexp
nt 1000 wbs
ct 160 wnt

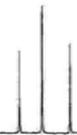
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -0.2
wp 20138.2
vs 45
sc 0
wc 250
hzmm 5.60
is 500.00
rfl 8854.5
rfp 7753.4
th 2
ins 100.000
nm ph



1

130.732
129.083
128.778
127.357
126.426
123.479

77.305
77.000
76.679

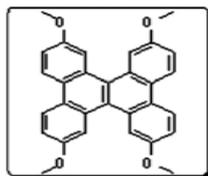


180 160 140 120 100 80 60 40 20 ppm

```

red
expl std1h
SAMPLE DEC. & VT
date May 14 2006 dfrq 400.446
solvent CDC13 dn H1
file exp dpwr 30
ACQUISITION exp dof 0
sfrq 400.447 dm nnn
tn H1 dmm c
at 2.728 dmf 200
np 32768 PROCESSING
sw 6006.0 lb 0.10
fb 3400 wtfile
bs 4 proc
tpwr 59 fn 65536
pw 6.8
d1 1.000 werr
tof 596.3 wexp
nt 100 wbs
ct 0 wnt
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
th 3
ins 1.000
nm ph

```



2a

8.454
8.432
8.194
8.188
7.248
7.242
7.226
7.220

3.897

9 8 7 6 5 4 3 2 1 0 ppm

1.03
1.00

1.03

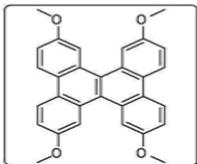
3.07

13C OBSERVE

exp2 std13c

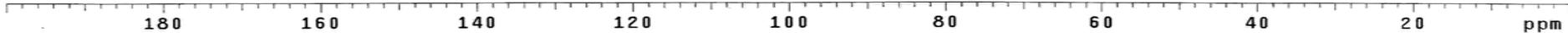
```

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 lb 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

129.626
128.439
124.957
124.582
116.033
110.078
77.314
77.000
76.686
55.409

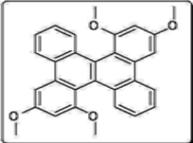


```

expt stdih
SAMPLE
date Feb 9 2006 dfrq 400.454
solvent COCl3 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 Ib 0.50
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 wft aph
ct 0 wnt
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 1.53
is 39.76
rfl 496.0
rfp 0
th 5
ins 1.000
nm ph

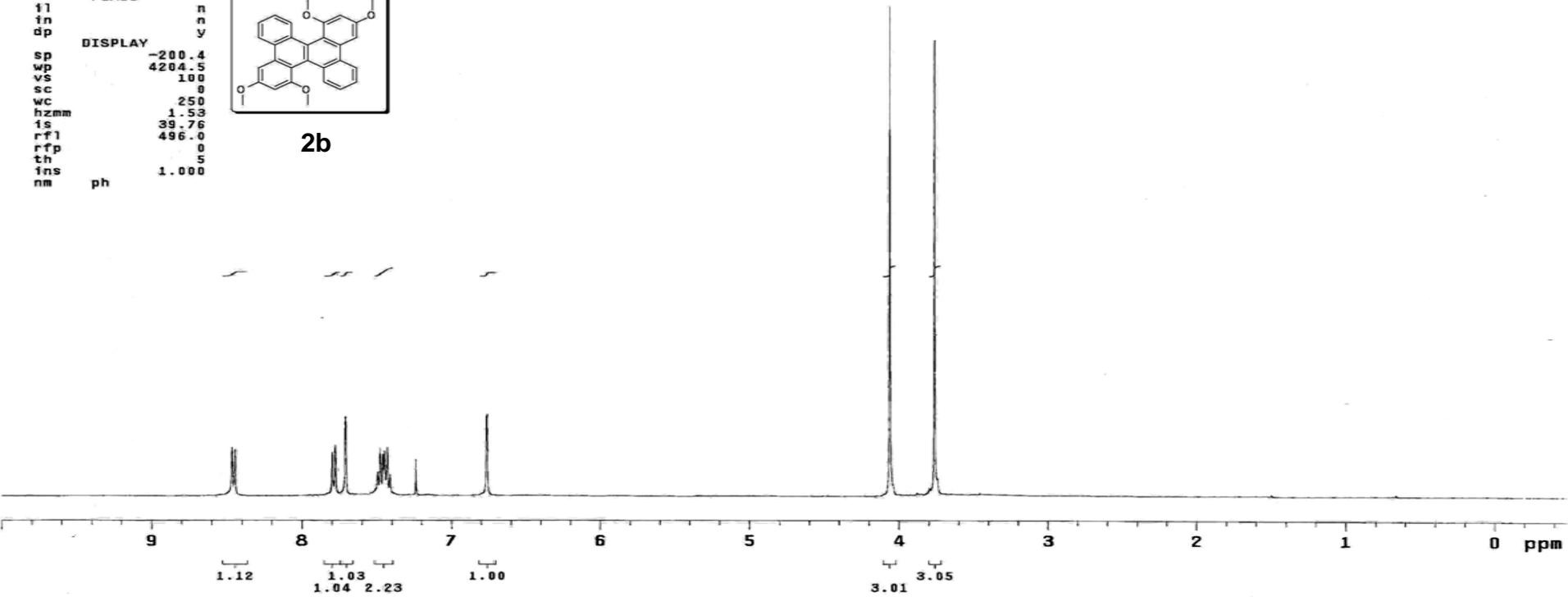
```

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



2b

4.061
3.763

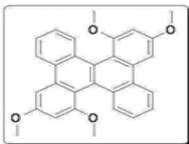


13C OBSERVE

exp2 std13c

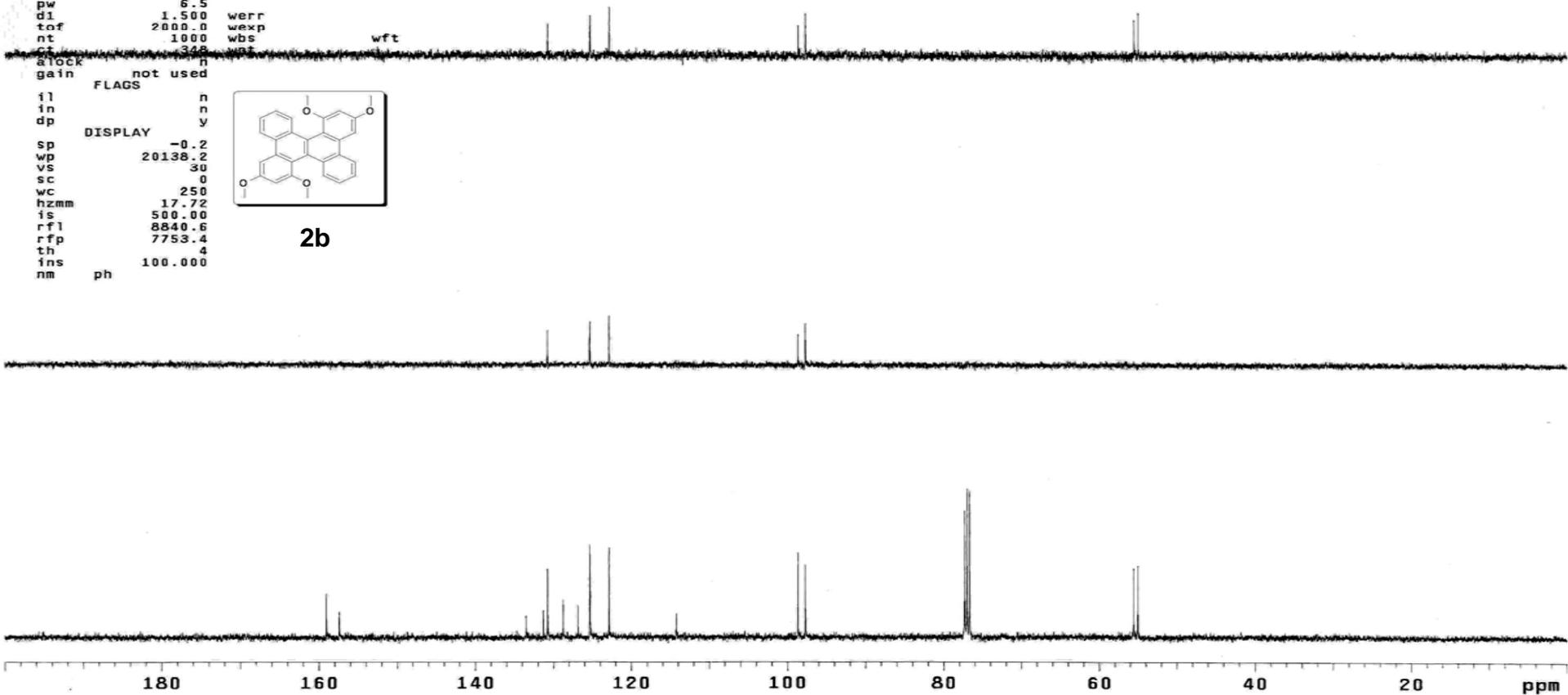
SAMPLE
date Feb 9 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm w
at 0.635 dmf 8000
np 32000
sw 25188.9 lb 1.00
fb 13800 wfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
dl 1.500 werr
tof 2000.0 wexp
nt 1000 wbs
ct 348 wft

LOCK not used
gain
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
ins 100.000
nm ph



2b

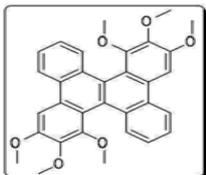
133.480
131.282
130.747
128.747
126.808
125.327
125.281
122.853
114.211
98.652
97.735
77.321
77.000
76.679
55.577
55.043



```

expl stdih
SAMPLE
date Feb 14 2006 dfrq DEC. & VT 400.454
solvent CDC13 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 0.50
fb 3400 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.0
dl 1.000 werr
tof 500.0 wexp
nt 100 wbs wft aph
ct 0 wnt
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

```

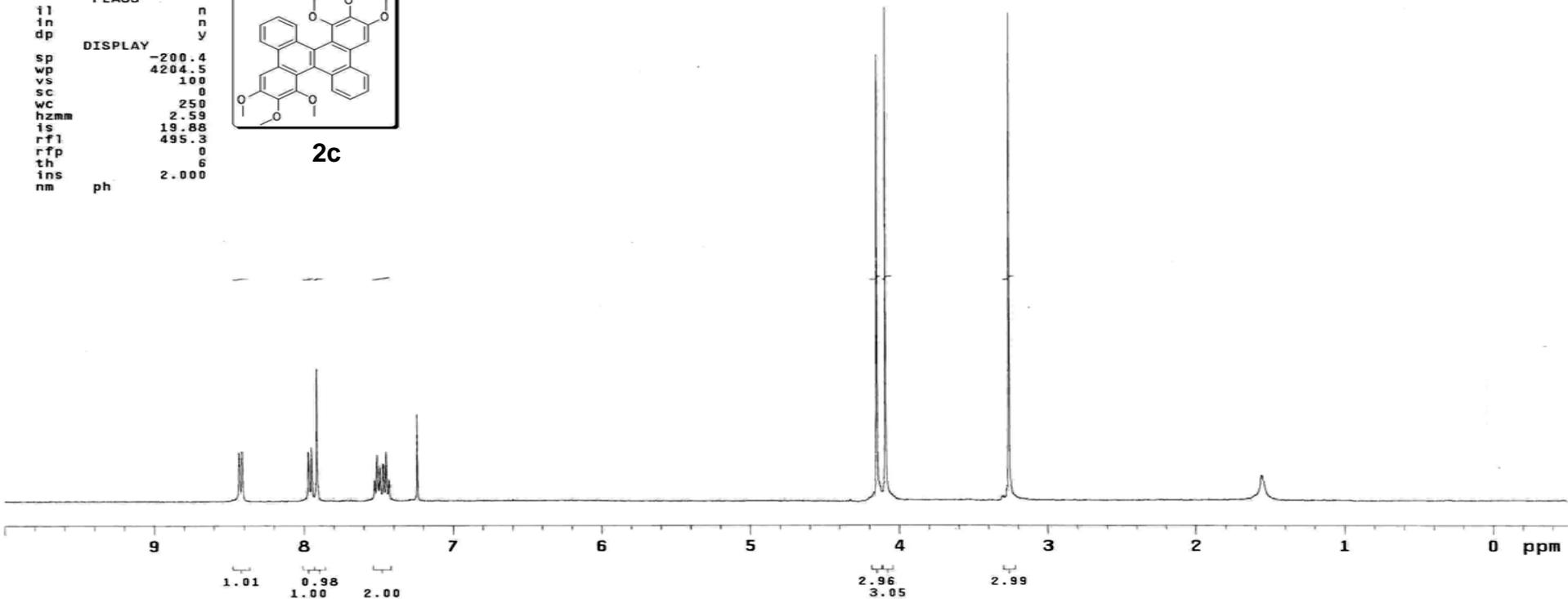


2c

8.432
8.412
7.970
7.950
7.913
7.508
7.491
7.469
7.449
7.240

4.148
4.091

3.258



13C OBSERVE

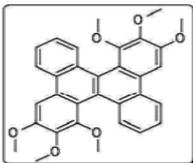
exp6 std13c

SAMPLE DEC. & VT
date Feb 15 2006 dfrq 400.454
solvent CDC13 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 ft
tpwr 58 fn not used
pw 6.5
d1 1.500 verr
tof 2000.0 wexp
nt 1000 wbs wft
ct 268 wnt

LOCK gain not used

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

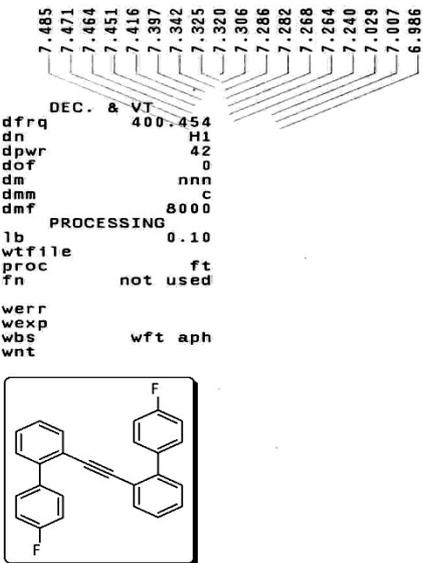
180 160 140 120 100 80 60 40 20 ppm

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



2.152

1.542

13C OBSERVE

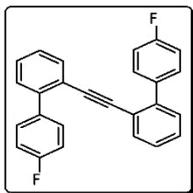
exp2 std13c

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 PROCESSING 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

lock 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 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
127.063

121.509

114.852
114.638

91.780

77.305
77.000
76.679

180

160

140

120

100

80

60

40

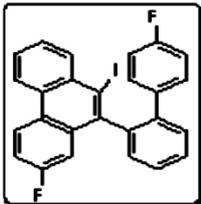
20

ppm

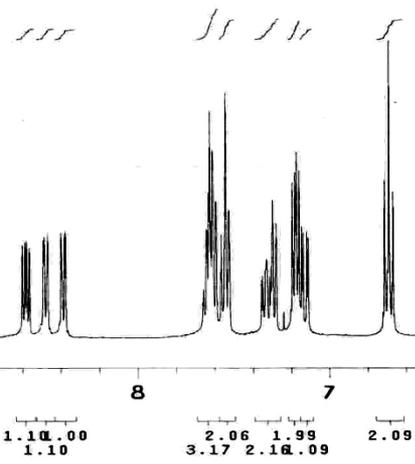
8.609
8.587
8.577
8.564
8.491
8.487
8.468
8.400
8.397
8.393
8.380
8.376
7.644
7.639
7.632
7.627
7.620
7.613
7.609
7.595
7.592
7.568
7.565
7.546
7.544
7.530
7.526
7.336

SAMPLE
date Feb 22 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 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''



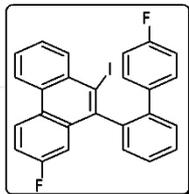
exp2 std13c

SAMPLE
date Feb 22 2006
solvent CDC13
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
hznm 3.93
is 500.00
rfl 8849.9
rfp 7753.4
th 7
ins
nm ph 100.000

DEC. & VT
162.950
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
125.096
125.006
122.410
116.056
115.829
114.654
114.440
112.974
112.760
109.645

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''

77.321
77.000
76.695

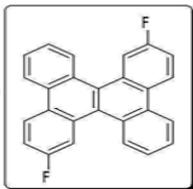
180 160 140 120 100 80 60 40 20 ppm

```

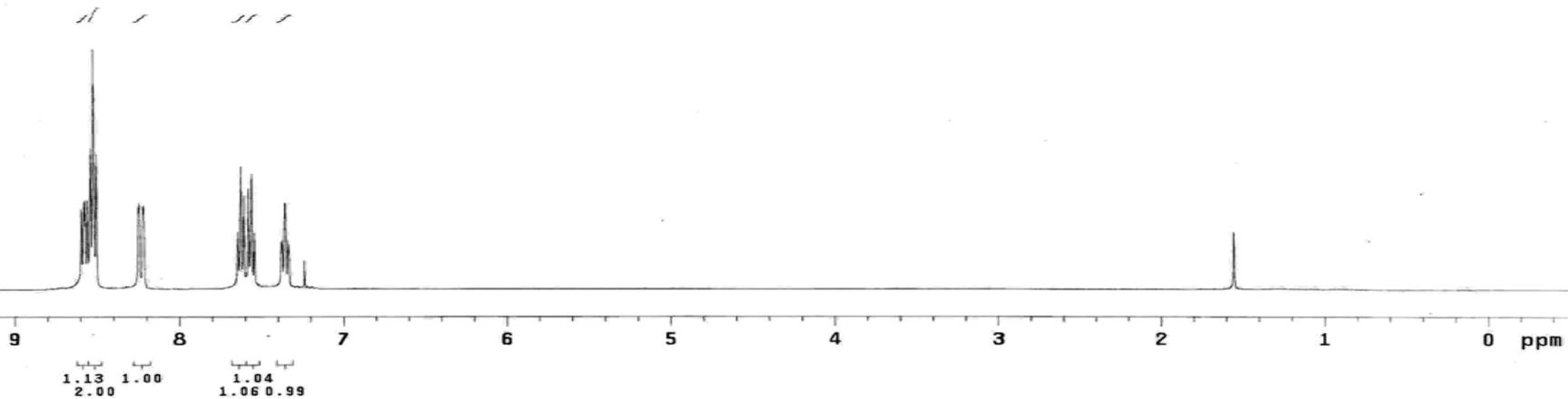
8.981
8.973
8.958
8.940
8.923
8.920
8.903
8.890
8.845
8.822
8.716
7.648
7.645
7.627
7.610
7.607
7.584
7.580
7.562
7.560
7.542
7.383
7.379
7.376
7.373
7.363
7.360
7.356
7.354
7.341
7.337

```

exp1 st01h
 SAMPLE
 date Feb 23 2006 dfrq DEC. & VT 400.454
 solvent CDC13 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
 dl 1.000 werr
 tot 500.0 wexp
 nt 100 wbs wft aph
 ct 16 wnt
 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
 is 32.15
 rfl 3394.9
 rfp 2899.3
 th 5
 ins 1.000
 nm ph



3a



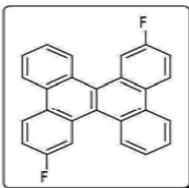
—1.556

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 wfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
dl 2.000 werr
tof 2000.0 wexp
nt 10000 wbs
ct 86 wdt

alock n
gain not used
FLAGS
ll 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

20

ppm

```

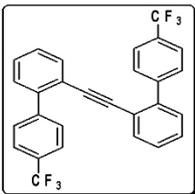
n
exp3 std1h
SAMPLE
date Feb 24 2006
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4204.5
vs 100
sc 0
wc 250
hzmm 2.28
is 215.67
rfl 3394.9
rfp 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

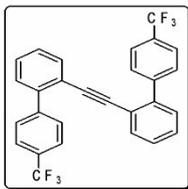
0.92
1.08

13C OBSERVE

exp4 std13c

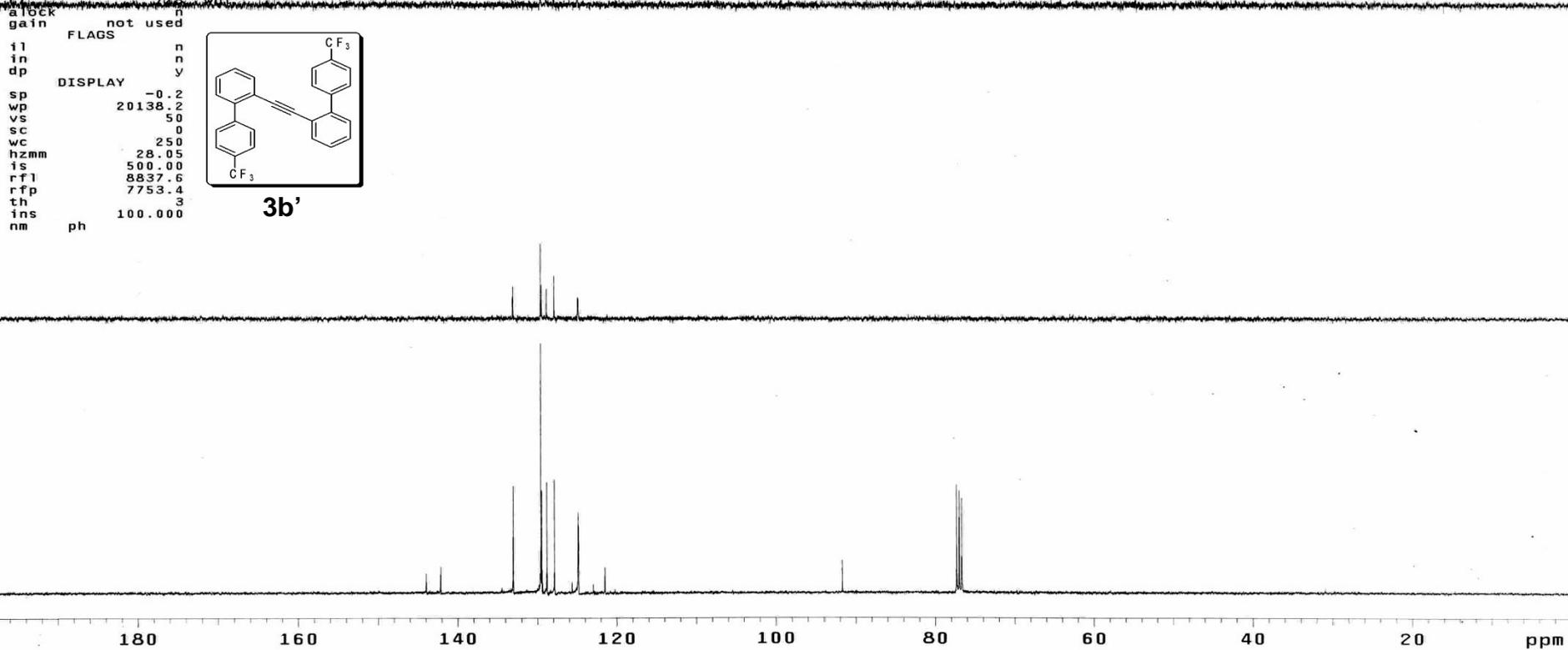
SAMPLE DEC. & VT
date Feb 24 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION dof 0
sfrq 100.705 dm yyy
tn C13 dmm yw
at 0.635 dmf 8000
np 32000 PROCESSING
sw 25188.9 lb 1.00
fb 13800 wtfile
bs 4 proc ft
tpwr 58 fn not used
pw 6.5
d1 1.500 verr
tof 2000.0 wexp
nt 1000 wbs
G 728 wgt

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
ins 100.000
nm ph



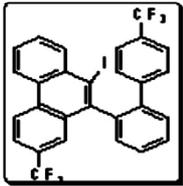
3b'

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

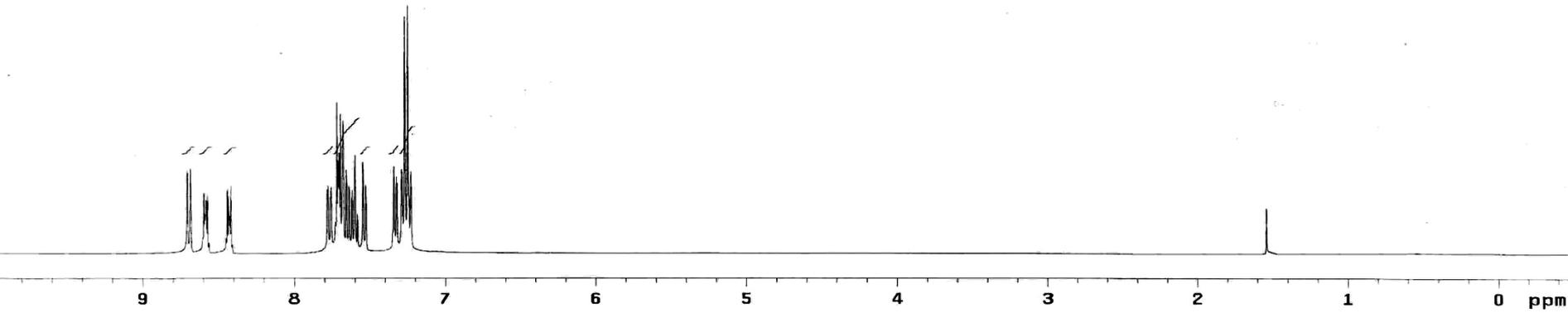


8.707
8.685
8.497
8.481
8.473
8.442
8.434
8.418
8.382
8.378
8.360
8.356
7.719
7.712
7.709
7.704
7.702
7.695
7.679
7.659
7.657
7.655
7.640
7.638
7.636
7.621
7.617
7.603
7.598
7.548

exp4 std1h
SAMPLE 1 2006 DEC. & VT 400.454
date Mar 1 2006 dfrq 400.454
solvent CDC13 dn H1
file exp dpwr 42
ACQUISITION exp 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 wft aph
ct 56 wnt
alock n
gain not used
FLAGS
i) n
in 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''



1.040.91
1.00
5.14 1.18
1.111.01 3.95

13C OBSERVE

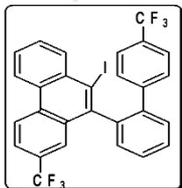
exp2 std13c

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 PROCESSING
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
FLAGS
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

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



3b''

180 160 140 120 100 80 60 40 20 ppm

```

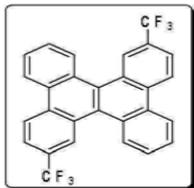
exp1 std1h
SAMPLE
date Mar 6 2006
solvent CDC13
file exp
ACQUISITION
sfrq 400.455
tn H1
at 2.664
np 32016
sw 6009.6
fb 3400
bs 4
tpwr 58
pw 6.0
dl 1.000
tof 500.0
nt 100
ct 24
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -200.4
wp 4805.3
vs 50
sc 0
wc 250
hzmm 3.37
is 113.40
rf1 3394.6
rfp 2899.3
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
wft aph
wnt

```



3c

////// //

8.942
8.805
8.783
8.729
8.718
8.711
8.705
8.581
8.576
8.568
8.557
7.907
7.903
7.885
7.881
7.764
7.759
7.752
7.747
7.742
7.739
7.735
7.728
7.240

1.530

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

1.02 0.9
1.02 0.9
0.99
2.05

¹³C OBSERVE

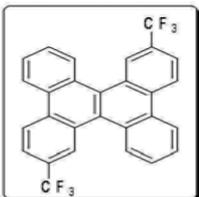
exp2 std13c

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
rpf	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

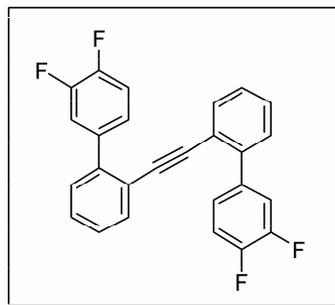
77.321
77.000
76.695

180 160 140 120 100 80 60 40 20 ppm

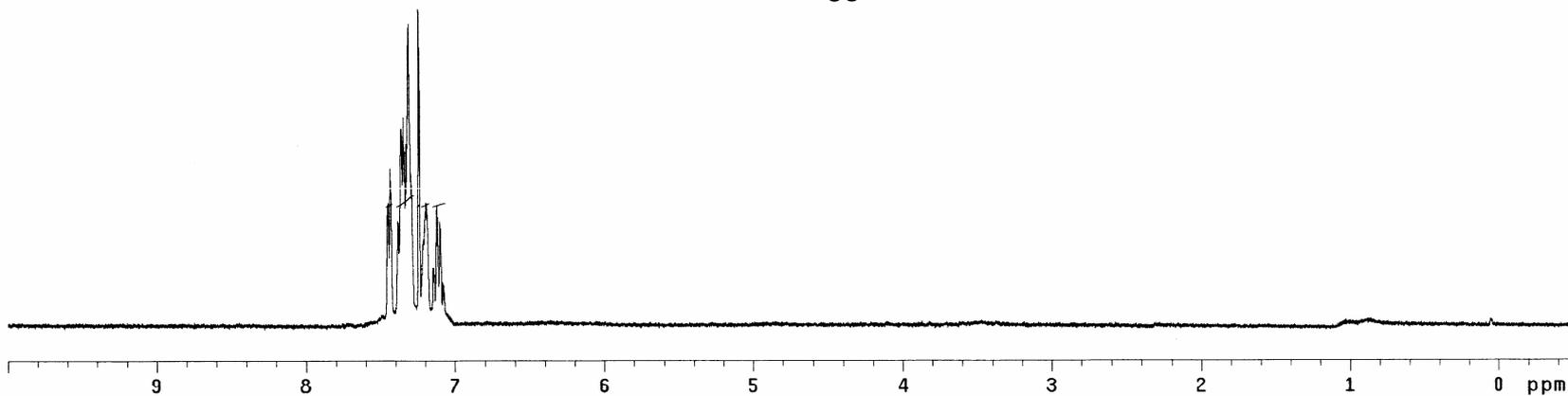
```

exp1 stdih
SAMPLE
date Jul 28 2006 dfrq DEC 400.446
solvent CDC13 dn H1
file exp dpwr 30
ACQUISITION dof 9
sfrq 400.447 dm nnn
tn H1 dmm c
at 2.728 dmf 200
np 32768 PROCESSING
sw 6006.0 lb 0.10
fb 3400 wtfile
bs 4 proc ft
tpwr 59 fn 65536
pw 6.8
dl 1.000 werr
tof 596.3 wexp
nt 100 wbs
ct 24 wnt
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

```



3c'



11.0018354
4913165

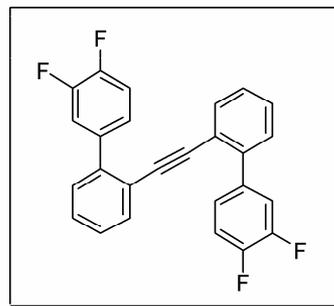
exp3 std13c

SAMPLE DEC. & VT
date Jul 29 2006 dfrq 400.447
solvent cd2c12 dn H1
file exp dpwr 41
ACQUISITION dof 0
sfrq 100.703 dm nyq
tn C13 dmm w
at 0.798 dmf 9700
np 40302 PROCESSING
sw 25252.5 lb 1.00
fb 14000 wtf file
bs 4 PROC
tpwr 59 fn 65536
pw 4.9
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

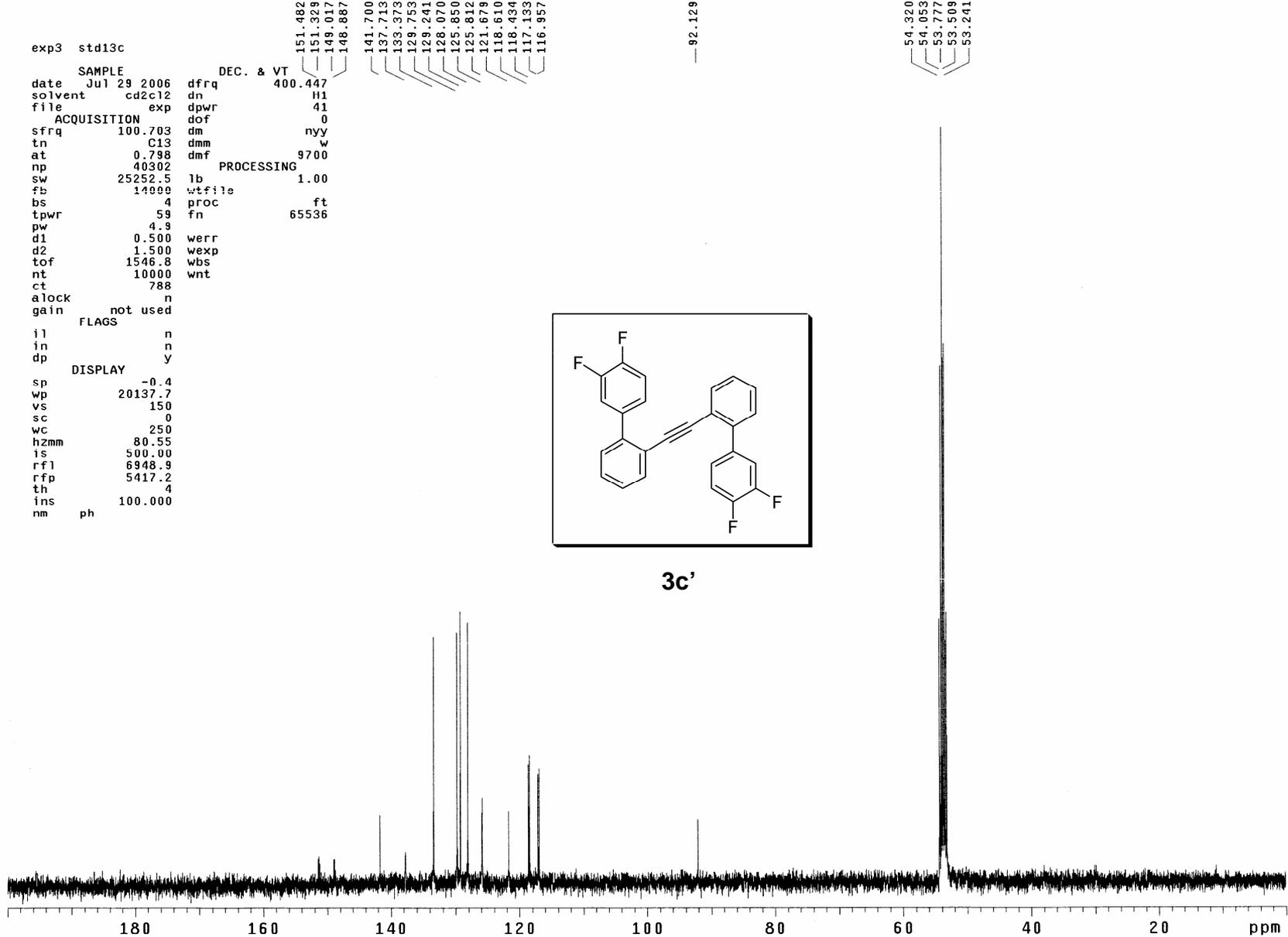
151.482
151.329
149.017
148.887
141.700
137.713
138.973
129.753
129.241
128.070
125.850
125.812
121.679
118.610
118.434
117.133
116.957

92.129

54.320
54.053
53.777
53.509
53.241



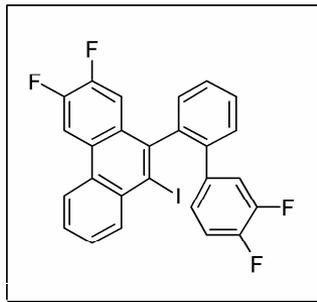
3c'



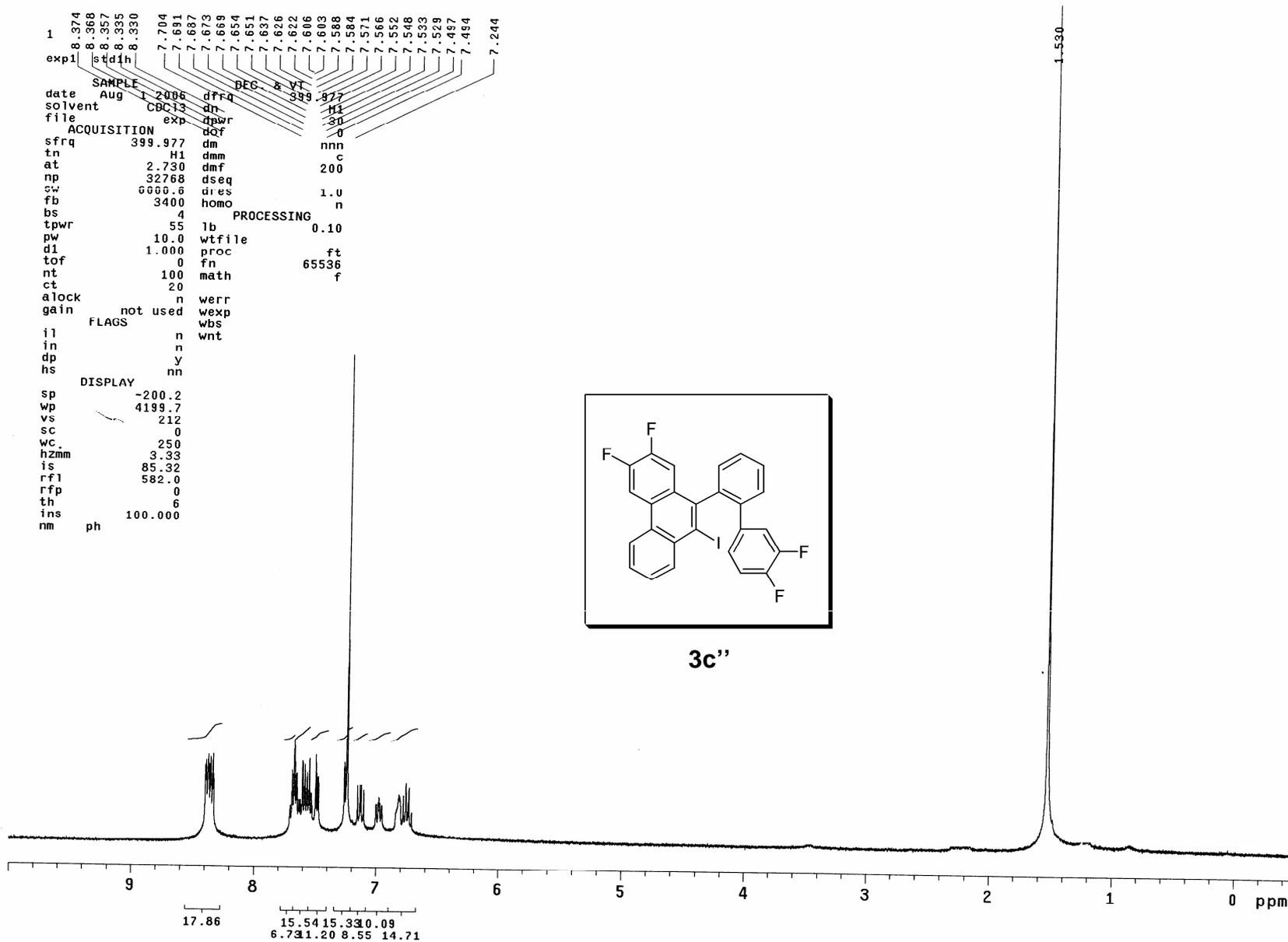
```

1
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
7.487
7.484
7.244
exp1
SAMPL
date Aug 1 2006 dff4
solvent CDCl3 dn H1
file exp dswr 30
ACQUISITION
sfrq 399.977 dm nnn 0
tn H1 dmm c
at 2.730 dmf 200
np 32768 dseq
sw 6666.6 dres 1.0
fb 3400 homo n
bs 4
tpwr 55 lb 0.10
pw 10.0 wtfile
d1 1.000 proc ft
tof 0 fn 65536
nt 100 math f
ct 20
alock not used werr
gain not used wexp
wbs
wnt
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

```



3c''



ent Data Parameters
 P59-P
 NO 2
 NO 1

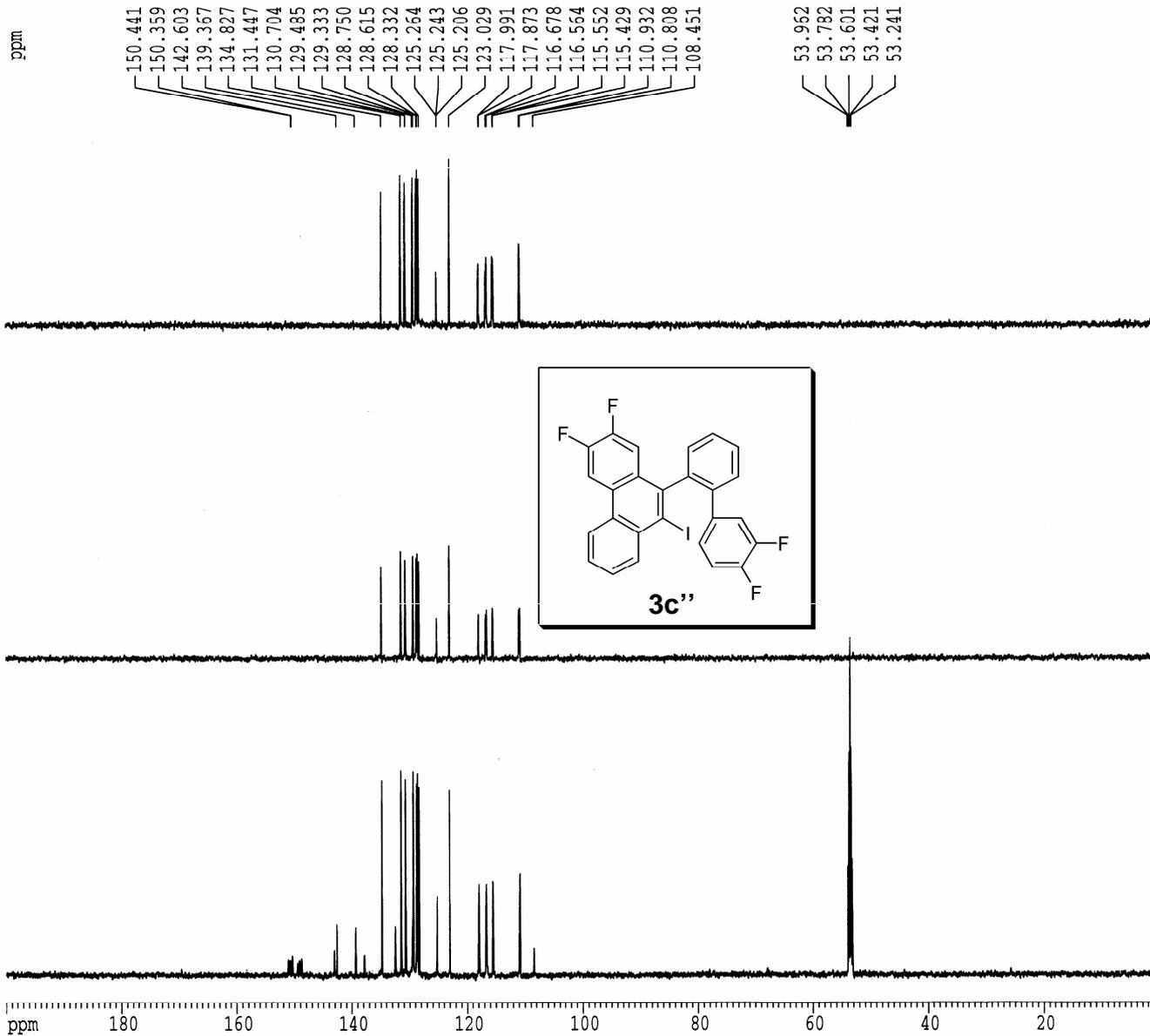
Acquisition Parameters
 20061119
 16.38
 spect
 5 mm QNP 1H/1
 299g
 12768
 Acetone
 1410
 0
 45045.047 Hz
 1.374666 Hz
 0.3637748 sec
 4096
 11.100 usec
 6.50 usec
 302.4 K
 3.0000000 sec
 0.0300000 sec
 2.9000010 sec
 0.0000000 sec
 0.0150000 sec

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

==== CHANNEL f2 =====
 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

MNR 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 :
CNO :

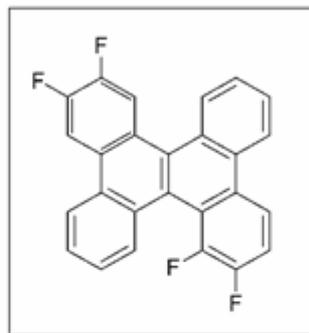
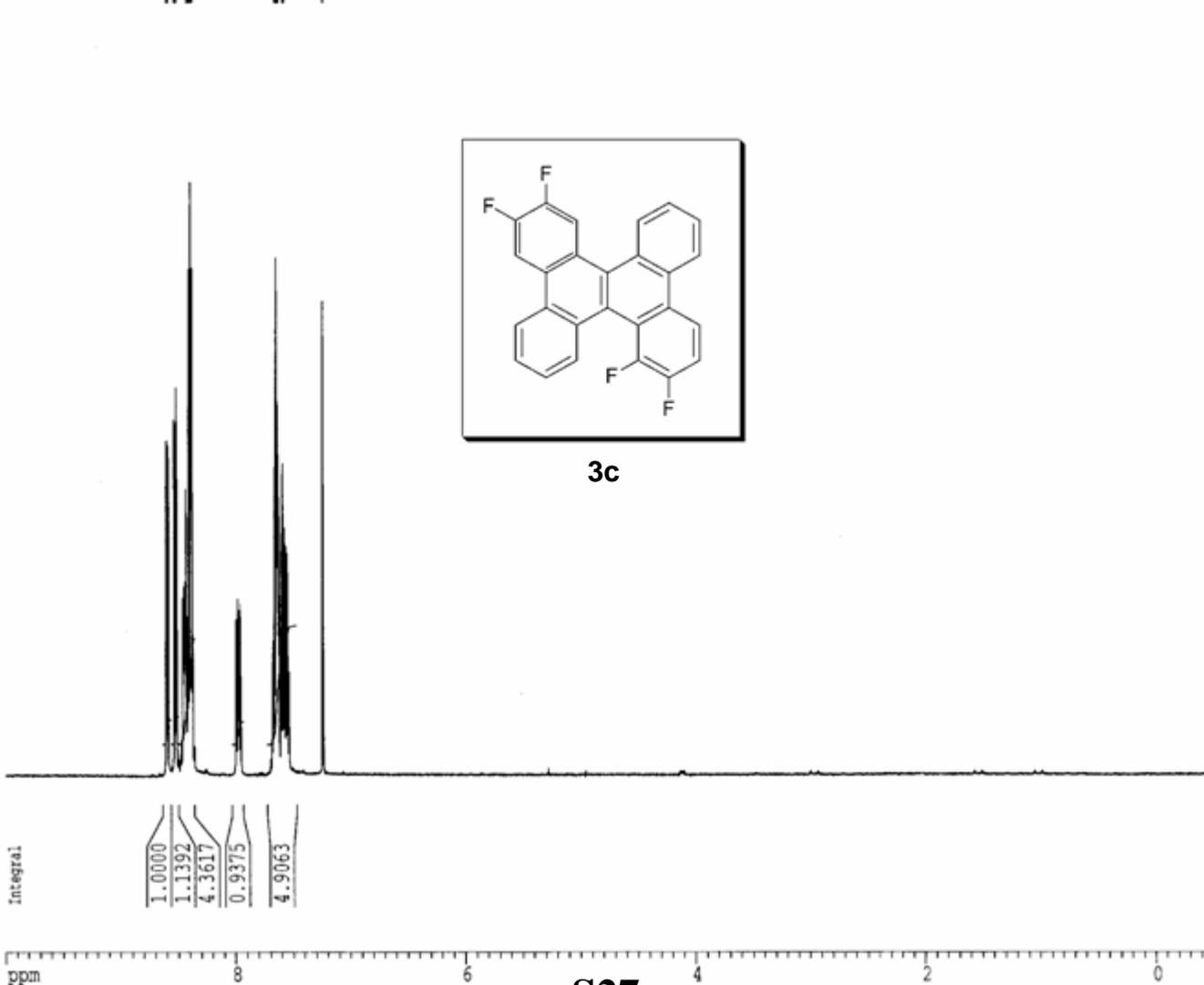
Acquisition Parameters
Date_ 20061109
Time_ 2.00
TRIM spect
PULPROG 5 mm QNP 1H/1
PROG zg
AQ 32768
RG 16
SD 0
FIDRES 7861.635 Hz
RES 0.239918 Hz
AQ 2.0840948 sec
SFO 512
PC 63.600 usec
PR 6.50 usec
K 308.0 K
SOLVENT 1.50000000 sec
EST 0.00000000 sec
RK 0.01500000 sec

==== CHANNEL f1 =====
1 1H
P1 10.00 usec
PL 3.00 dB
F1 599.4829974 MHz

Processing parameters
32768
599.4800276 MHz
no
0
0.00 Hz
0
1.00

===== F2 =====
F2 13C
P2 10.00 cm
PL 10.00 ppm
SFO 5994.80 Hz
PC 0.500 ppm
PR -299.74 Hz
SOLVENT 0.52500 ppm/cm
M 314.72702 Hz/cm

8.60086
8.59864
8.58592
8.53263
8.51953
8.51714
8.42819
8.41456
8.40763
8.39384
8.38934
8.37571
7.66243
7.66020
7.64972
7.64672
7.64369
7.63983
7.63823
7.63302
7.63100
7.62661
7.58838
7.57651
7.24012



3c

ent Data Parameters
E 02P-160-P
NO 2
NO 1

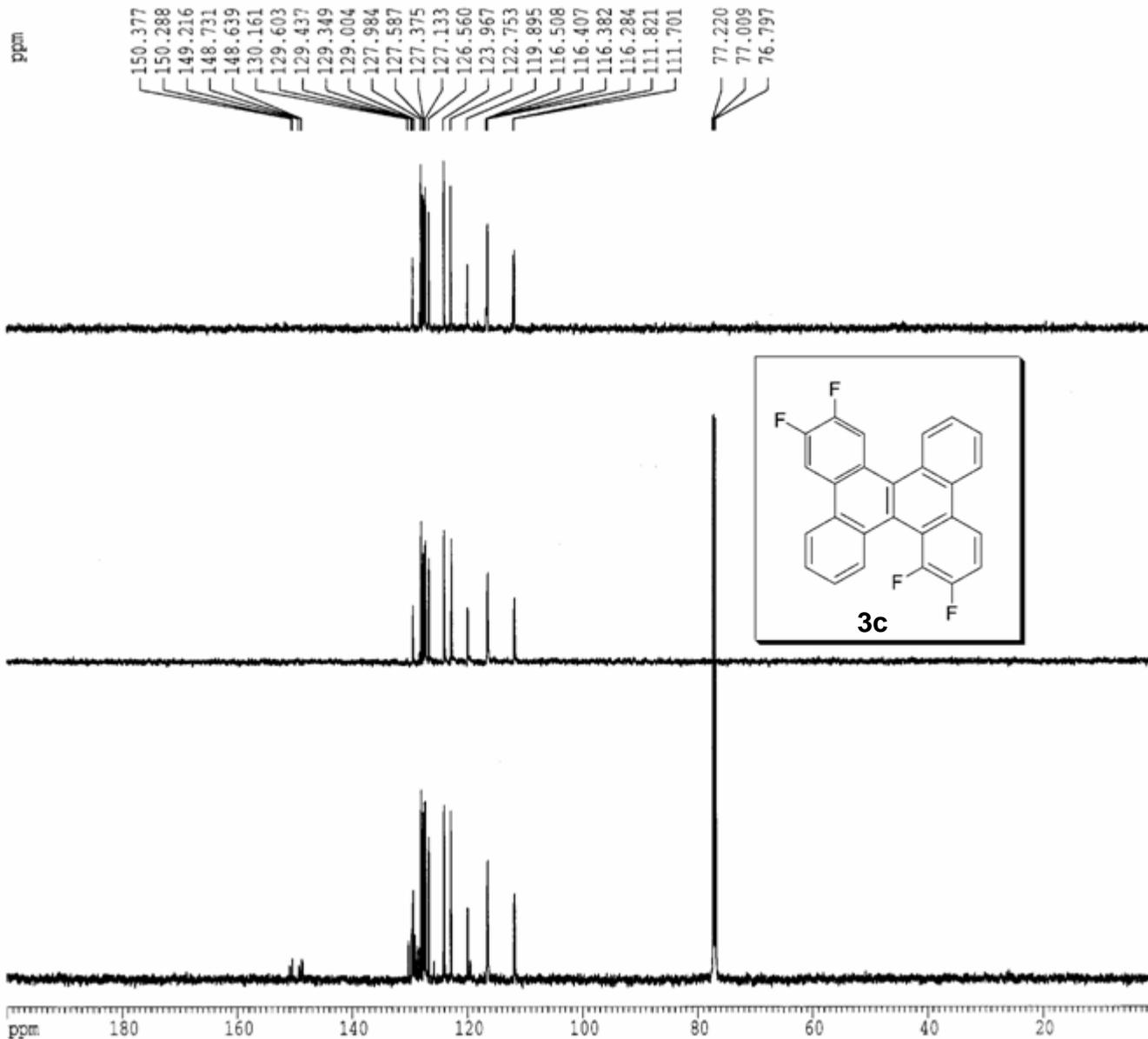
Acquisition Parameters
Date_ 20061109
Time 2.01
PROB spect
PULPROG zgpg
PROG 5 mm QNP 1H/1
PROC 32768
F2 101.6261200
F1 45045.047 Hz
AQ 1.374666 Hz
RG 0.1637748 sec
SFO 4096
AQ 11.100 usec
RG 6.50 usec
K 308.0 K
SFO 3.0000000 sec
RG 0.0300000 sec
SFO 2.9000000 sec
RG 0.0000000 sec
SFO 0.0150000 sec

==== CHANNEL f1 =====
NUC1 13C
PULPROG zgpg
RG 4.50 usec
SFO 101.6261200 MHz

==== CHANNEL f2 =====
PROB2 mlti16
PULPROG 1H
RG 92.00 usec
SFO 120.00 dB
RG 11.30 dB
SFO 14.00 dB
SFO 599.6829974 MHz

Processing parameters
SFO 65036
F2 150.7191594 MHz
SFO 0
RG 3.00 Hz
SFO 0
RG 0.50

===== plot parameters =====
SFO 20.00 cm
RG 10.00 cm
SFO 200.000 ppm
RG 30147.87 Hz
SFO 0.000 ppm
RG 0.00 Hz
SFO 10.00000 ppm/cm
RG 1507.39368 Hz/cm



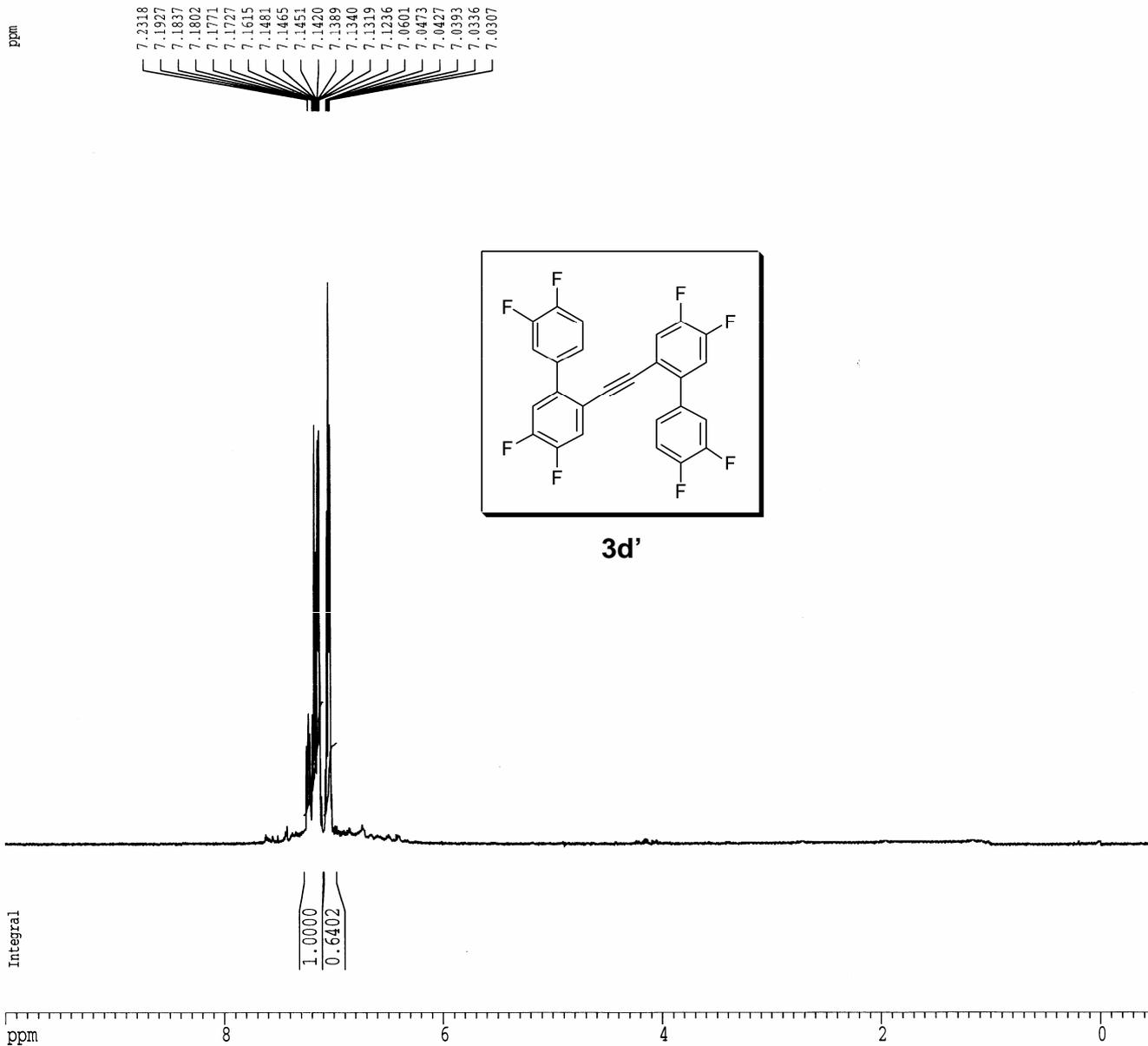
Current Data Parameters
NAME DIF-147-P
PULPROG zgpg30
SOLVENT CDCl3
NS 1
DS 1

Acquisition Parameters
Date_ 20061012
Time 15.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PROG zgpg30
PULPROG zgpg30
SOLVENT CDCl3
NS 1
DS 1
AQ 8389.262 Hz
RES 0.256020 Hz
AQ 1.9530228 sec
SFO 128
AQ 59.600 usec
SFO 6.50 usec
SFO 310.5 K
EST 1.50000000 sec
PRK 0.00000000 sec
PRK 0.01500000 sec

==== CHANNEL f1 =====
P1 1H
P1 9.30 usec
P1 3.00 dB
F1 599.4829974 MHz

Processing parameters
SFO 32768
F1 599.4800673 MHz
AQ 0.00 Hz
SFO 0
P1 1.00

NMR plot parameters
SFO 20.00 cm
AQ 10.00 cm
SFO 10.000 ppm
F1 5994.80 Hz
SFO -0.500 ppm
F1 -299.74 Hz
SFO 0.52500 ppm/cm
F1 314.72702 Hz/cm



Experiment Data Parameters
NAME DIF-147-P
PULPROG zgpg
TD 32768
SFO 500.136
AQ 1.024
RG 0
WDW EM
SSB 0
LB 45045.047 Hz
GB 1.374666 Hz
PC 0.3637748 sec
TC 1.024 sec
DC 11.100 usec
AS 6.50 usec
SC 308.9 K
EC 3.00000000 sec
FC 0.03000000 sec
TA 2.90000010 sec
EST 0.00000000 sec
RK 0.01500000 sec

Acquisition Parameters

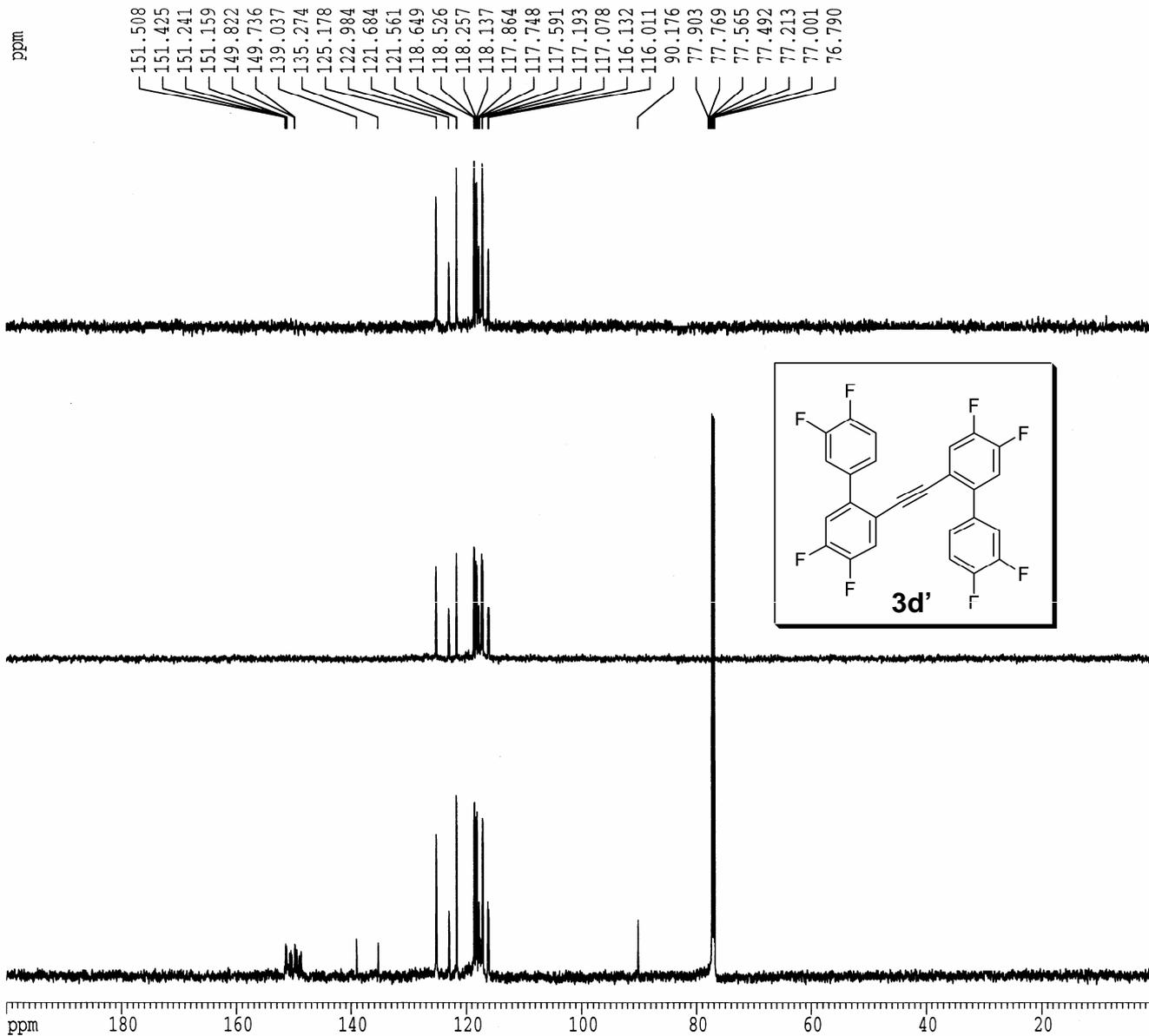
===== CHANNEL f1 =====
1 13C
4.70 usec
0.00 dB
1 150.7559473 MHz
===== CHANNEL f2 =====
PRG2 waltz16
2 1H
D2 92.00 usec
120.00 dB
2 11.30 dB
3 14.00 dB
2 599.4829974 MHz

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

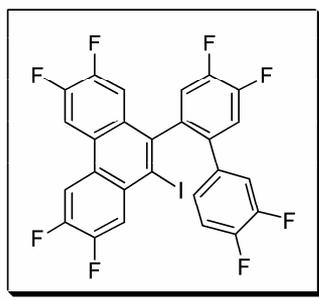
Acquisition Parameters
e_ 20061024
e 15.51
TRUM spect
BHD 5 mm QNP 1H/1
PROG zg
32768
VENT CDC13
16
0
12019.230 Hz
RES 0.366798 Hz
1.3631988 sec
128
41.600 usec
6.50 usec
302.0 K
1.5000000 sec
EST 0.0000000 sec
RK 0.0150000 sec

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

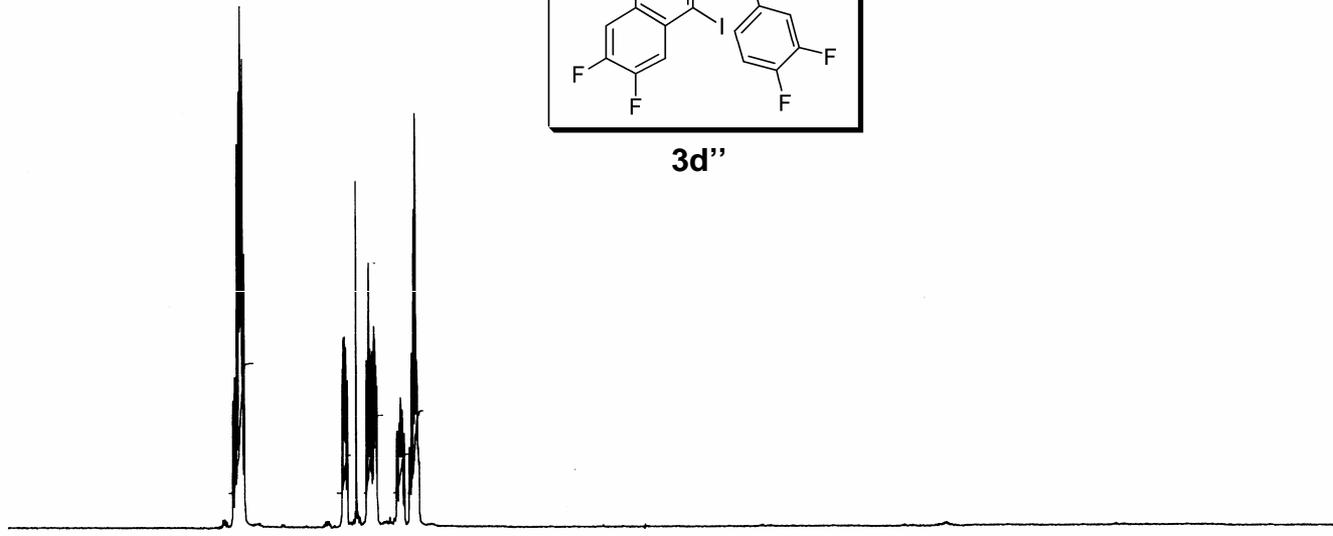
Processing parameters
32768
599.4800279 MHz
no
0
0.00 Hz
0
1.00

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

ppm
8.18286
8.17074
8.16420
8.15837
8.15143
8.14563
8.13917
8.12636
7.33810
7.33320
7.32954
7.32454
7.32029
7.24016
7.14562
7.14125
7.13467
7.12864
7.11221
7.09900
7.09312
7.09029
7.08632
6.79943
6.78234
6.77906
6.77753
6.76888



3d''



Integral
3.4486
1.0000
2.0545
1.0261
2.1753

ppm
8
6
4
2
0

ent Data Parameters
DIF-163-P
0
NO 1

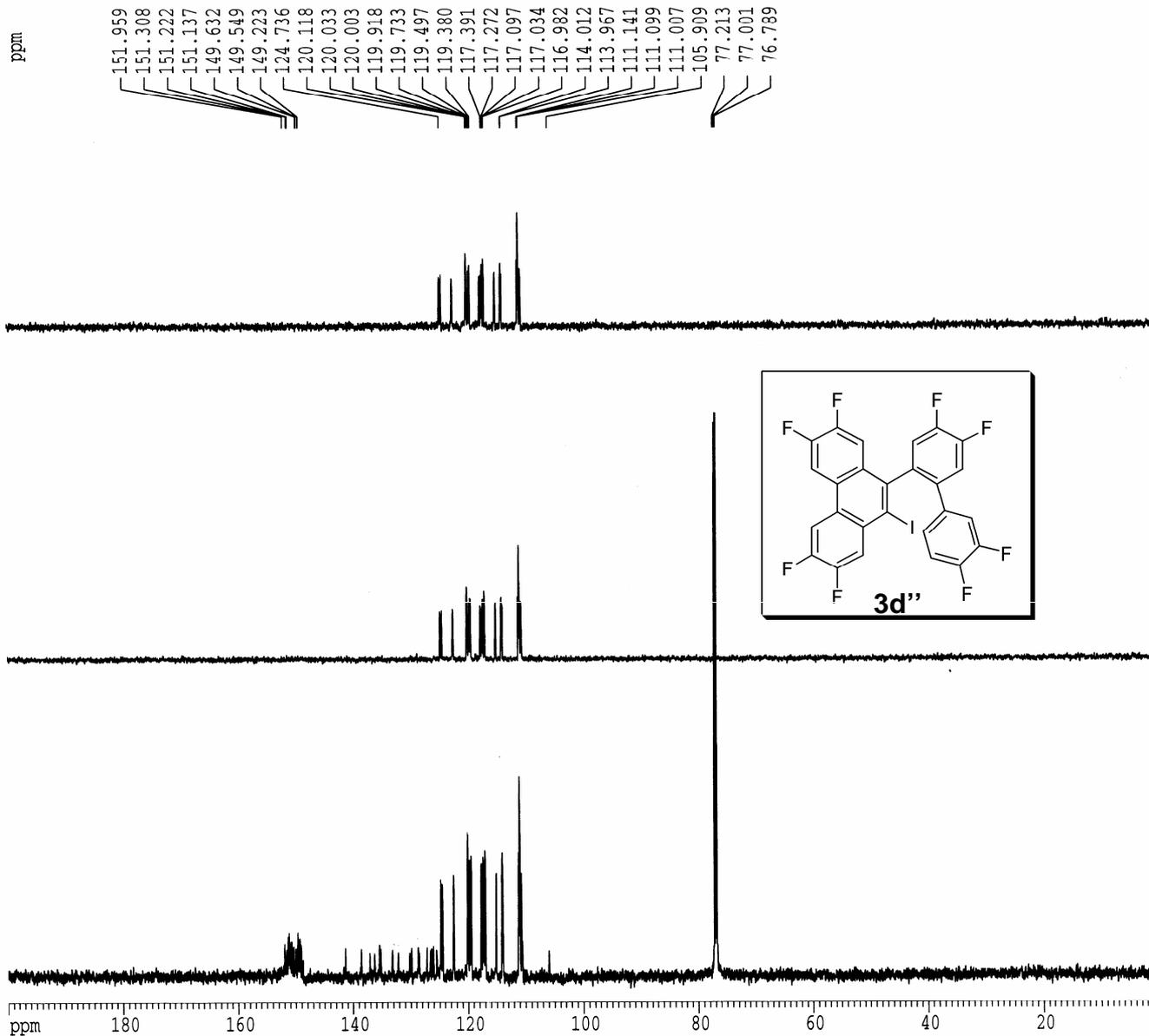
Acquisition Parameters
20061024
15.59
SPRM spect
HD 5 mm QNP 1H/1
PROG zgpg
32768
EMT CDC13
500
0
45045.047 Hz
1.374666 Hz
0.3637748 sec
512
11.100 usec
6.50 usec
302.1 K
3.00000000 sec
0.03000000 sec
2.90000010 sec
0.00000000 sec
0.01500000 sec

==== 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

MR 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



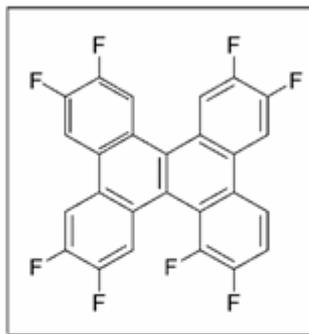
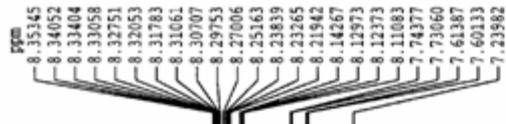
Experiment Data Parameters
E DIF-162-P
NO 1
CNO 1

Acquisition Parameters
Date_ 20061108
Time 17.29
Pulse PROGRAM spect
Pulse PROG 2g
SFO 32768
WDW CDCL3
SSB 16
GB 0
AQ 7861.635 Hz
RES 0.239918 Hz
AQ 2.0840948 sec
SFO 512
AQ 63.600 usec
SFO 6.50 usec
SFO 307.7 K
SFO 1.5000000 sec
SFO 0.0000000 sec
SFO 0.0150000 sec

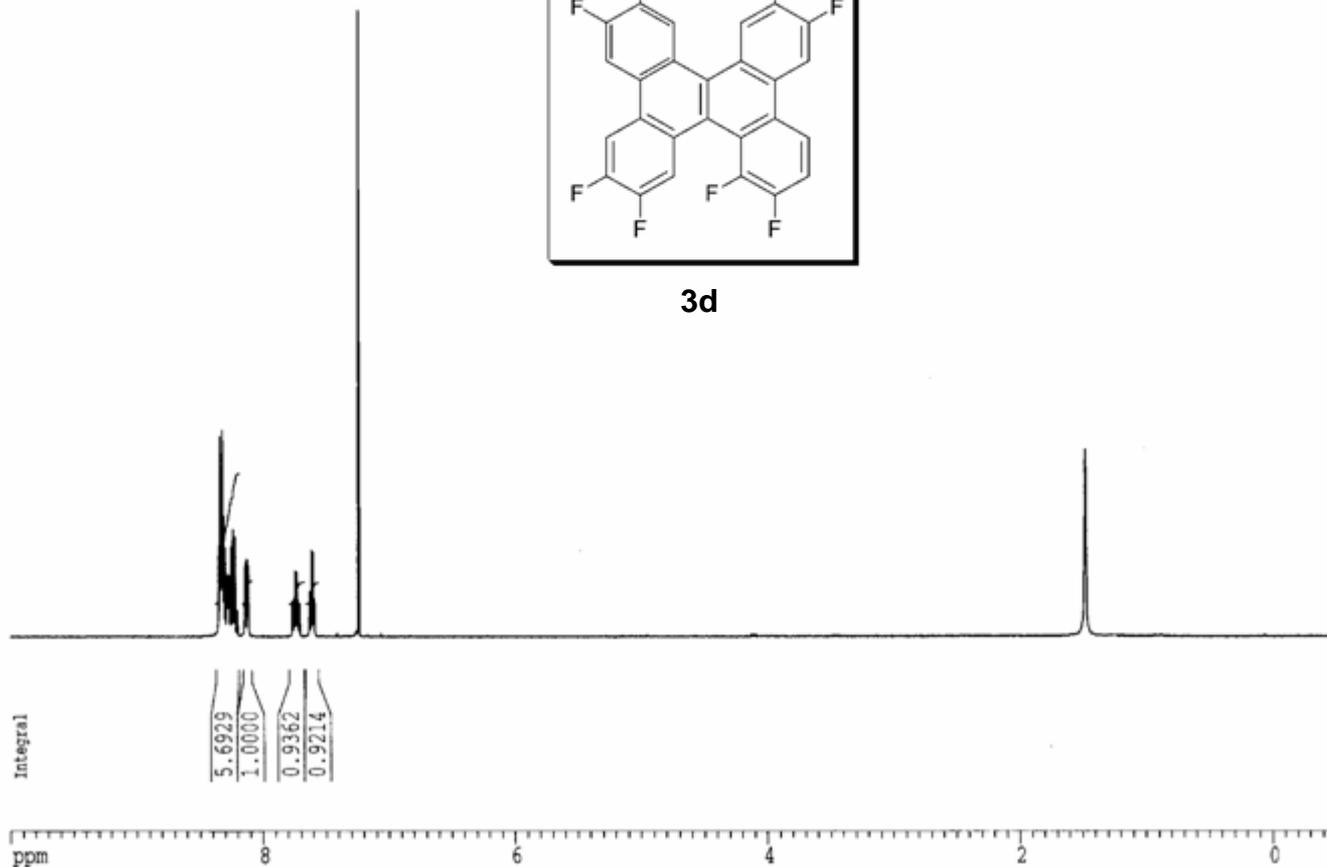
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 3.00 dB
FREQ1 599.4829974 MHz

Processing parameters
SFO 32768
FREQ1 599.4800273 MHz
NUC1 no
AQ 0
RES 0.00 Hz
SFO 0
GB 1.00

===== F2 plot parameters =====
SFO 20.00 cm
P1 10.00 cm
PL1 10.000 ppm
FREQ1 5994.80 Hz
SFO -0.500 ppm
P1 -299.74 Hz
SFO 0.52500 ppm/cm
P1 314.72702 Hz/cm



3d



```

Current Data Parameters
NAME      DIP-182-P
PNO      2
DINO      1

- Acquisition Parameters
Date_     20061108
Time      17.33
STRM      spect
NAME      5 mm QNP 1H/1
PROG      zgpg
PROC      32768
EVENT     Acetone
         2011
         0
FID       45045.047 Hz
AQ        1.374666 Hz
RG        0.5637768 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

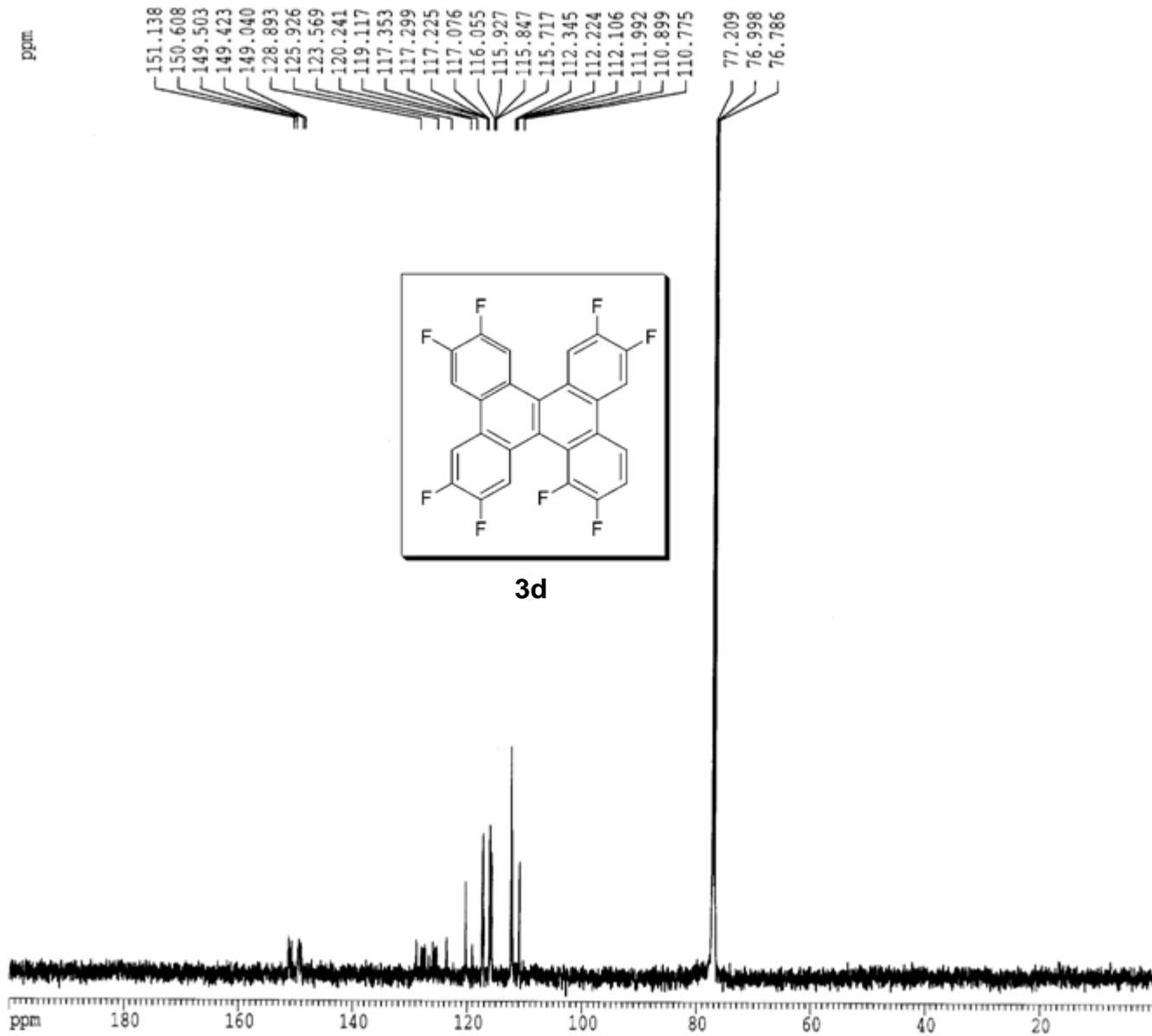
===== CHANNEL f1 =====
NUC1      13C
P1        4.50 usec
PL1       0.00 dB
RF1       150.7560381 MHz

===== CHANNEL f2 =====
PRG2      waltz16
NUC2      1H
PC2       92.00 usec
PL2       120.00 dB
PL3       11.30 dB
PL4       14.00 dB
RF2       599.4829974 MHz

- Processing parameters
SI         65536
SF         150.7393566 MHz
AQ         0
RG         3.00 Hz
WDW        0
SSB        0.50

===== F2 plot parameters =====
X1         20.00 cm
X2         10.00 cm
Y1         290.000 ppm
Y2         30147.87 Hz
          0.000 ppm
          0.00 Hz
          10.00000 ppm/cm
          1507.39355 Hz/cm

```



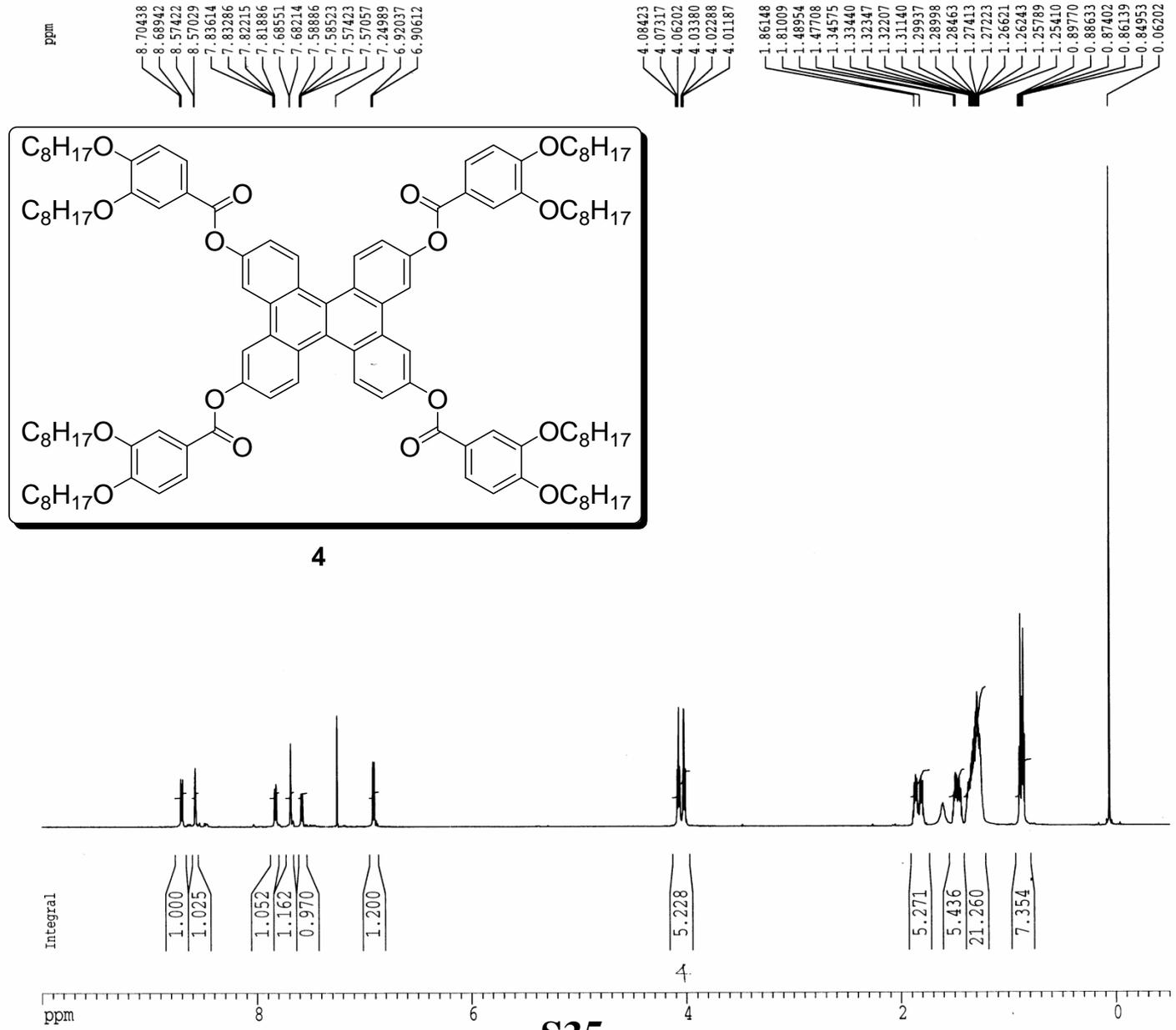
Current Data Parameters
 NAME ester-2-OC8H17
 XPNO 1
 PROCNO 1

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
 VIDRES 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
 CNRK 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
 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
 Name ester-2-OC8H17
 PNO 2
 DCNO 1

Acquisition Parameters
 Date_ 20060927
 Time 14.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 P1PROG zgpg
 F2 32768
 SOLVENT CDCl3
 T1 758
 T2 0
 FIDRES 45045.047 Hz
 AQRES 1.374666 Hz
 SFO 0.3637748 sec
 AQ 2048
 F1 11.100 usec
 F2 6.50 usec
 K 0.0 K
 SFO 3.0000000 sec
 SFT 0.0300000 sec
 SFA 2.9000010 sec
 SFB 0.0000000 sec
 SFC 0.0150000 sec

==== CHANNEL f1 =====
 C1 13C
 P1 4.70 usec
 PL 0.00 dB
 D1 150.7609769 MHz
 ===== CHANNEL f2 =====
 DPRG2 waltz16
 C2 1H
 PD2 92.00 usec
 P2 120.00 dB
 P12 11.30 dB
 P13 14.00 dB
 P02 599.5029975 MHz

Processing parameters
 SFO 65536
 F0 150.7443988 MHz
 W EM
 B 0
 SFO 3.00 Hz
 K 0
 SFO 0.50

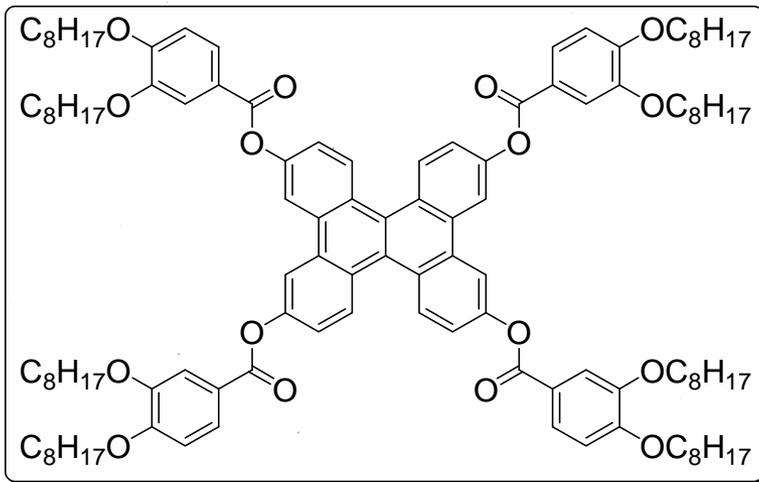
NMR plot parameters
 X 20.00 cm
 Y 10.00 cm
 P 200.000 ppm
 F 30148.88 Hz
 P -5.000 ppm
 F -753.72 Hz
 CM 10.25000 ppm/cm
 CM 1545.13025 Hz/cm

ppm

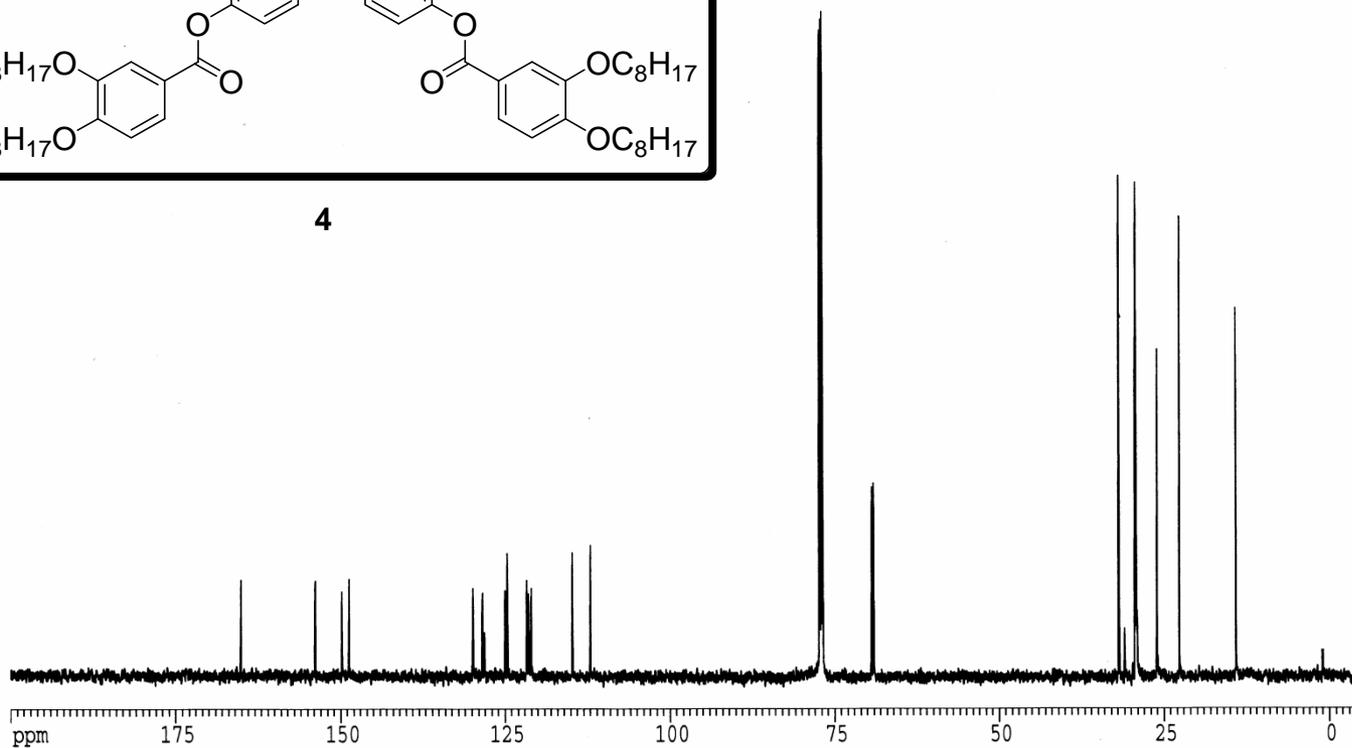
165.073
 153.801
 149.750
 148.669
 129.788
 128.372
 128.052
 124.952
 124.548
 121.661
 121.341
 120.920
 114.695
 111.951

77.214
 77.002
 76.790
 69.310
 69.072

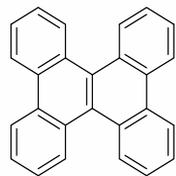
31.811
 30.908
 29.387
 29.365
 29.265
 29.200
 29.100
 26.031
 25.991
 22.658
 14.081



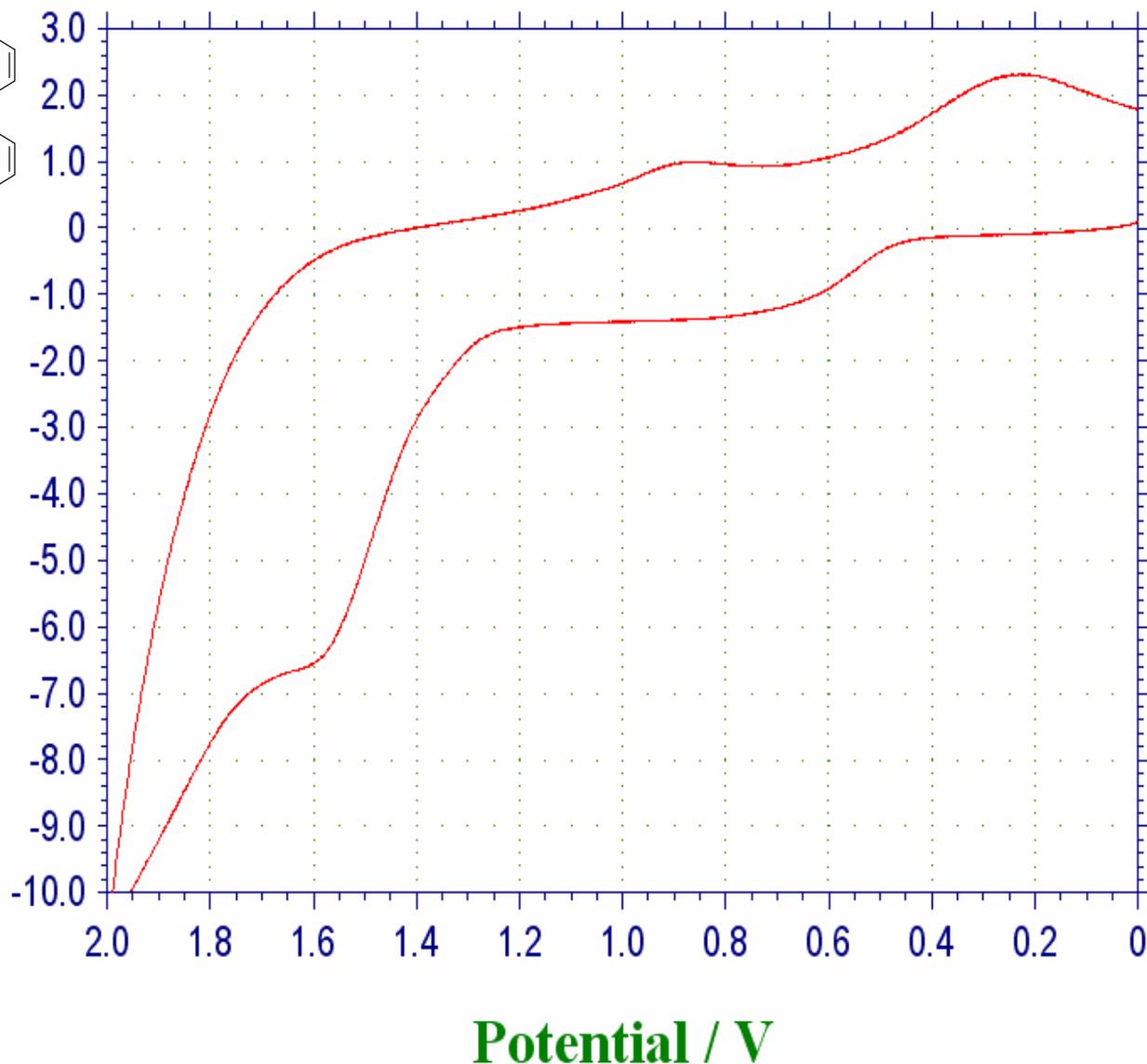
4



S36



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:

Potential / V

Figure S1. Cyclic voltammetry of **1**: (Sample concentration was 1*10⁻³M in CH₂Cl₂ 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)

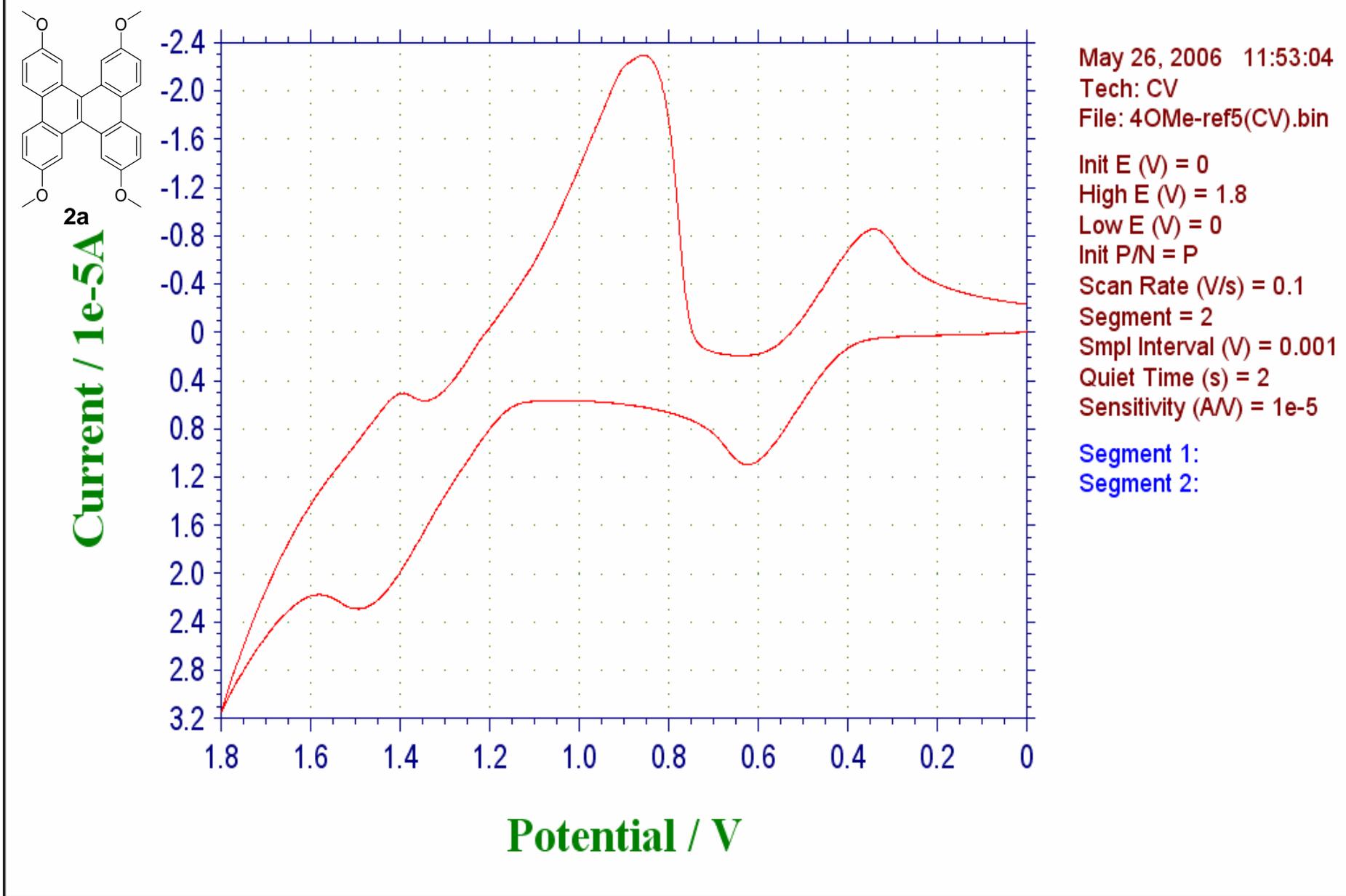
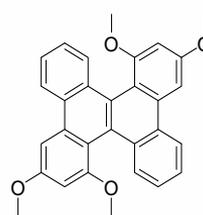
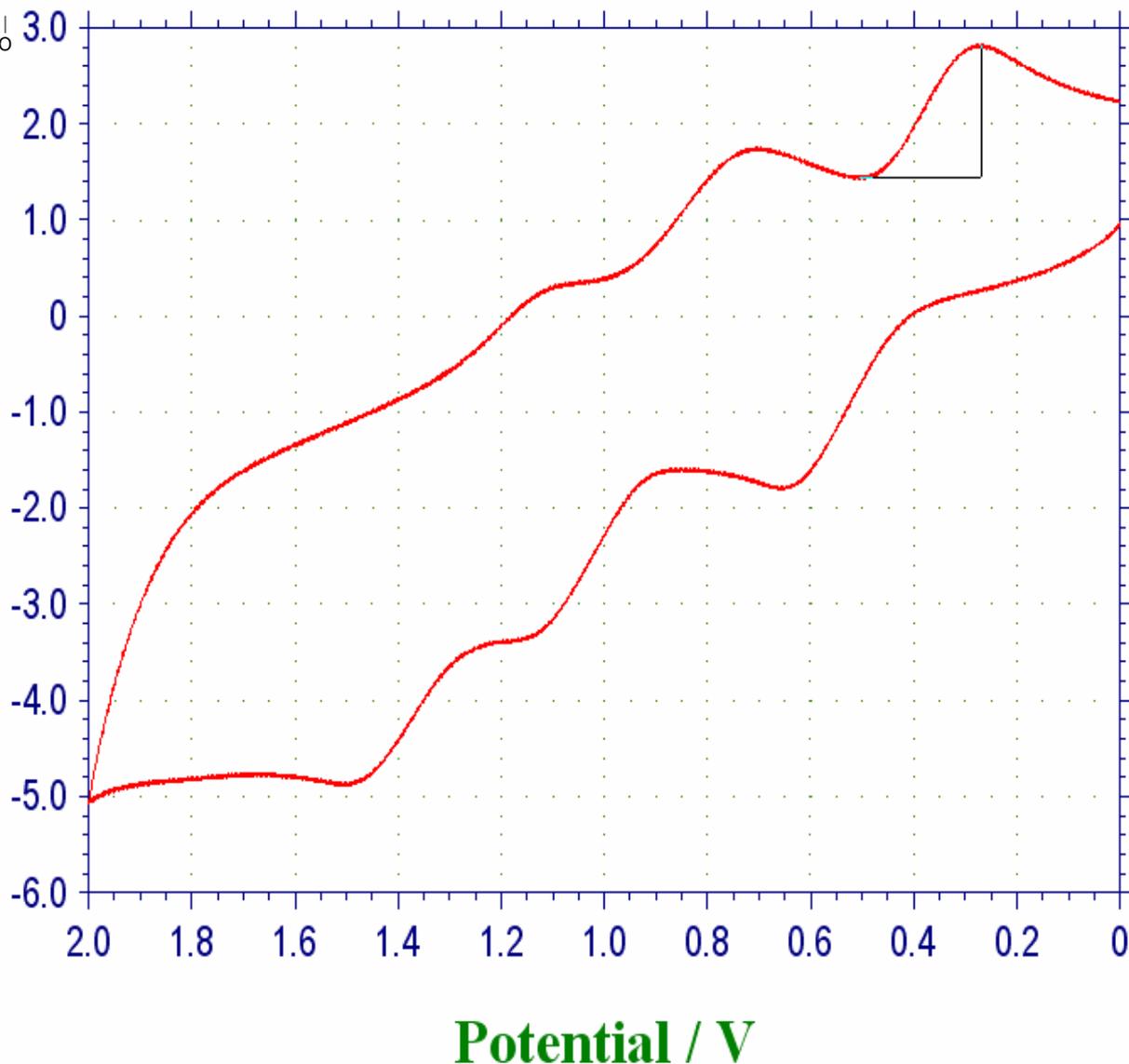


Figure S2. Cyclic voltammetry of **2a**: (Sample concentration was $1 \times 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)



2b

Current / 1e-6A



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:

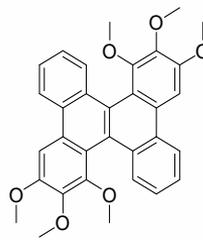
Segment 2:

Ep = 0.269V

ip = 1.384e-6A

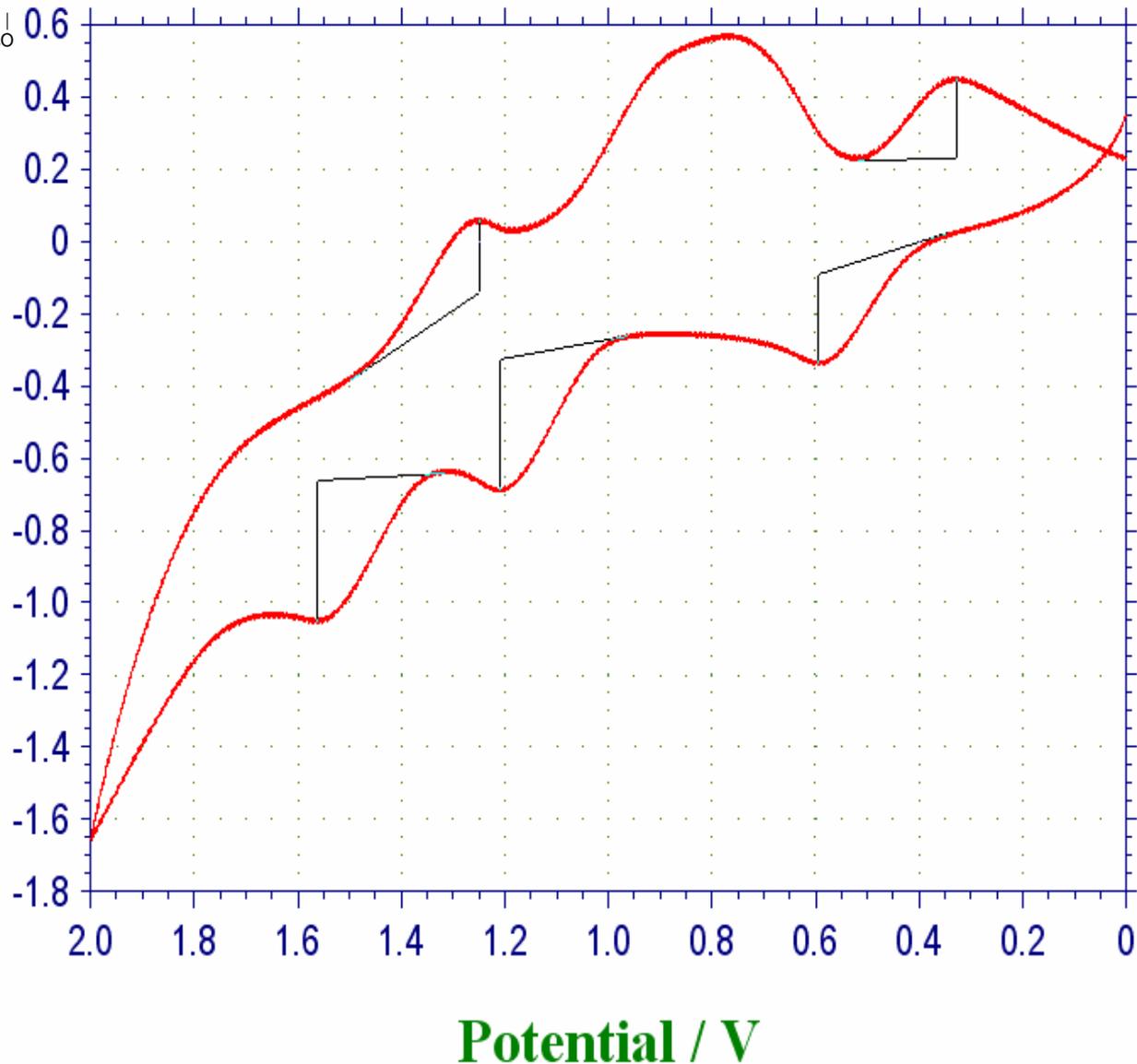
Ah = 1.584e-6C

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

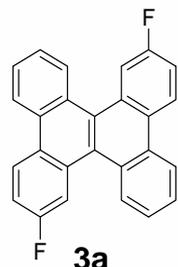
Ep = 1.564V

ip = -3.943e-6A

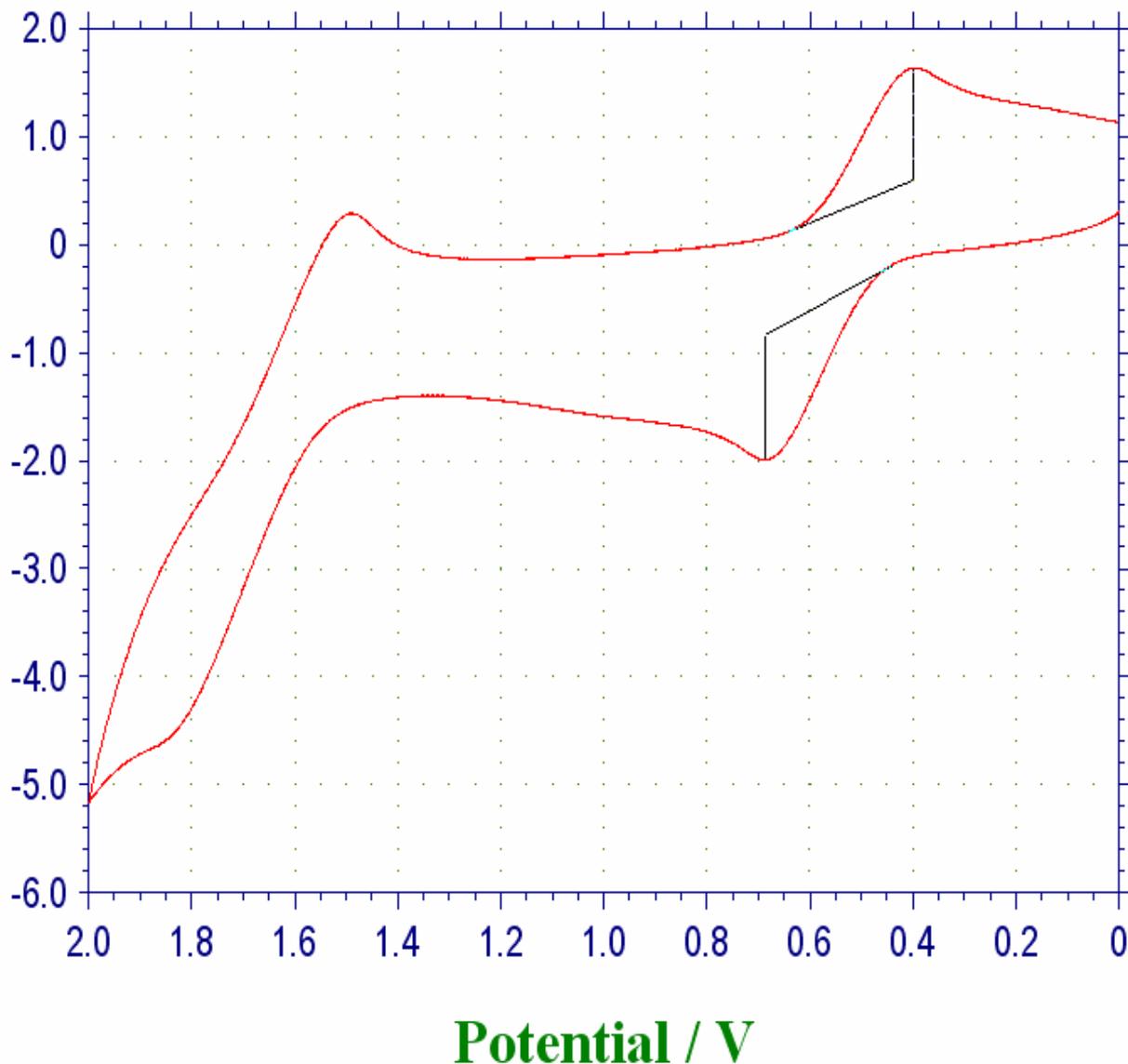
Ah = -4.571e-6C

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)



3a
Current / 1e-6A



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

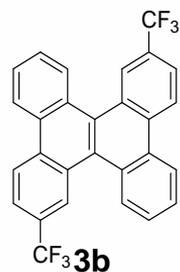
Segment 2:

Ep = 0.398V

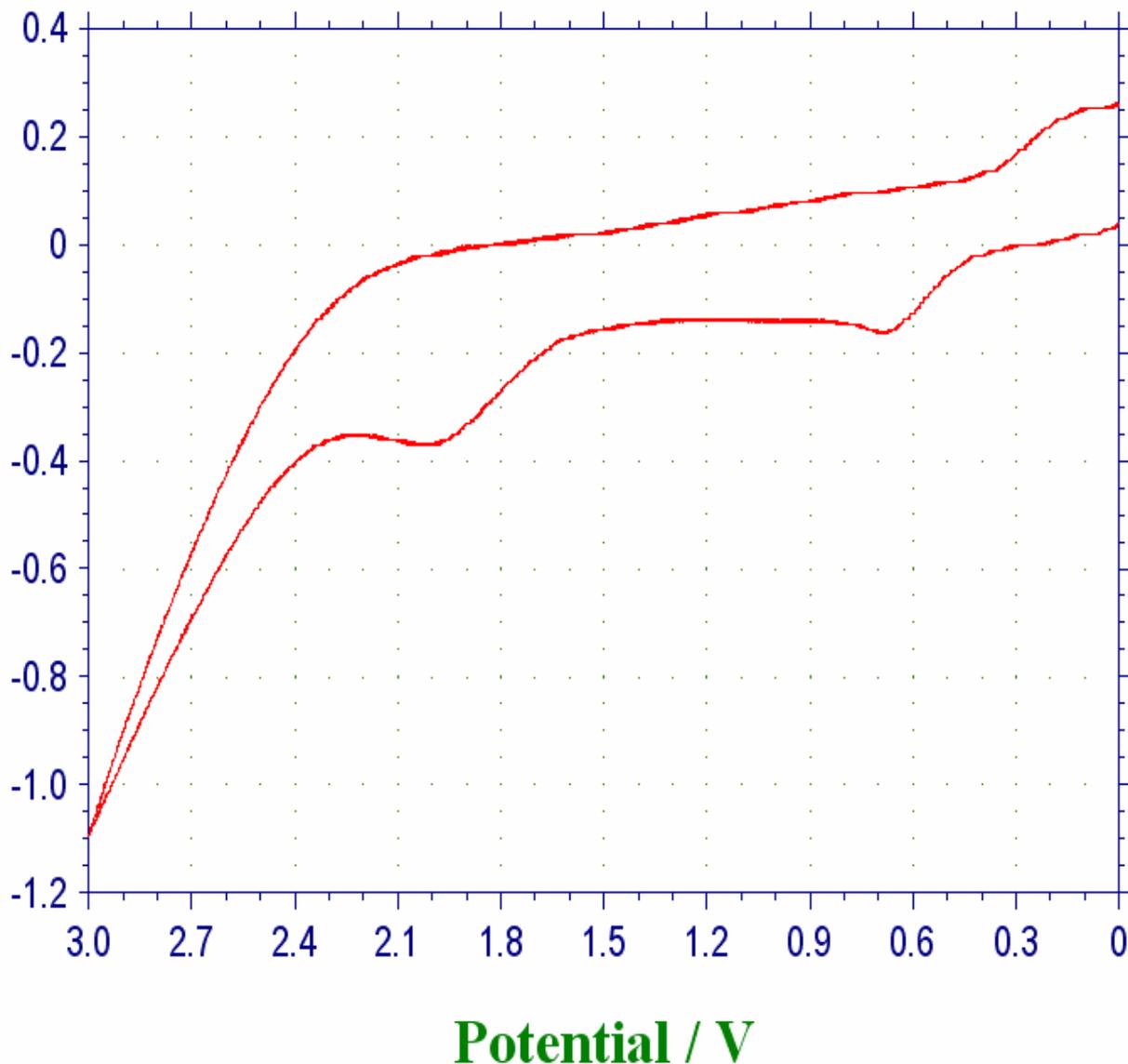
ip = 1.046e-6A

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)

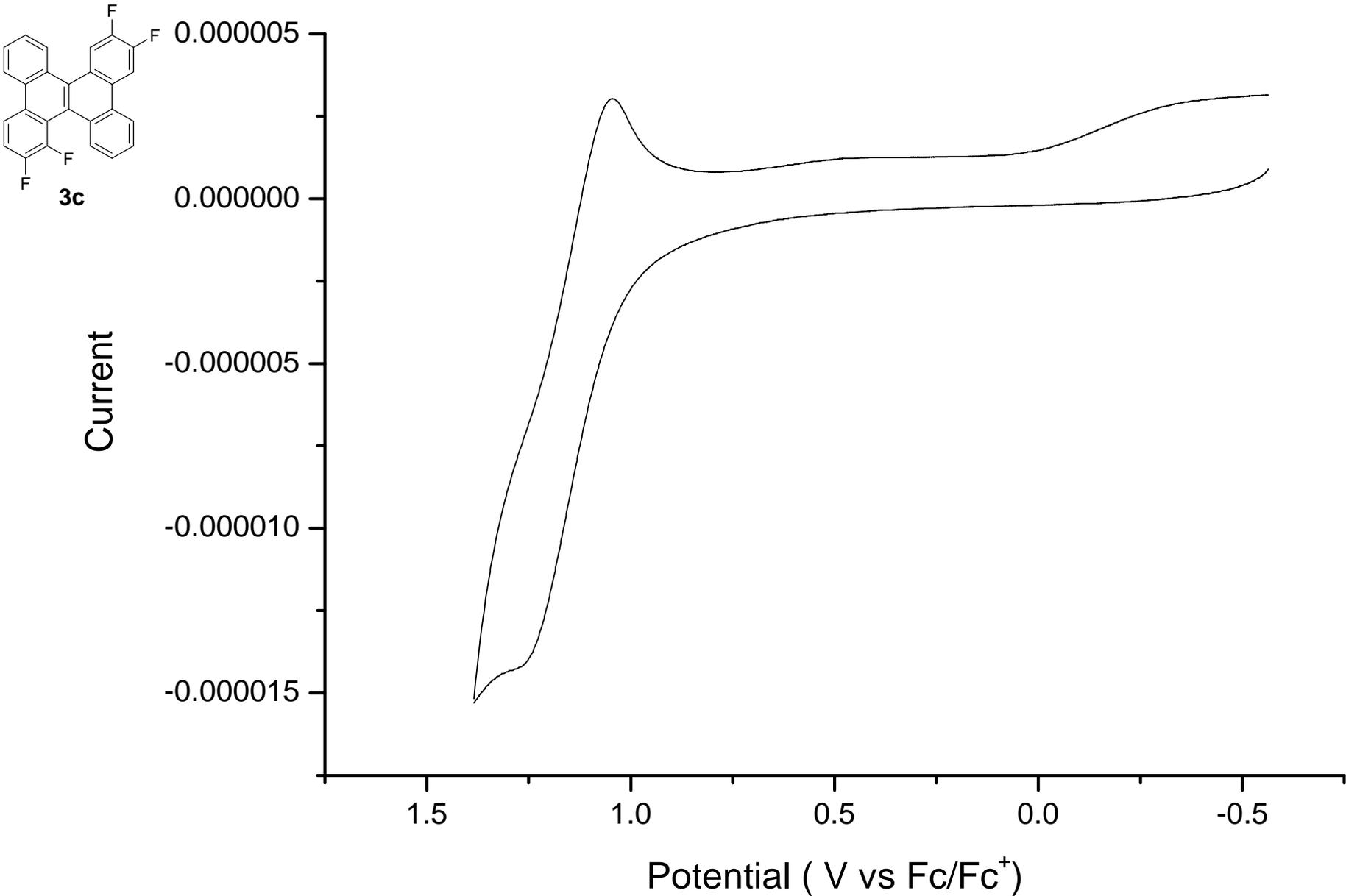


Figure S7. Cyclic voltammetry of **3c**: (Sample concentration was $1 \cdot 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

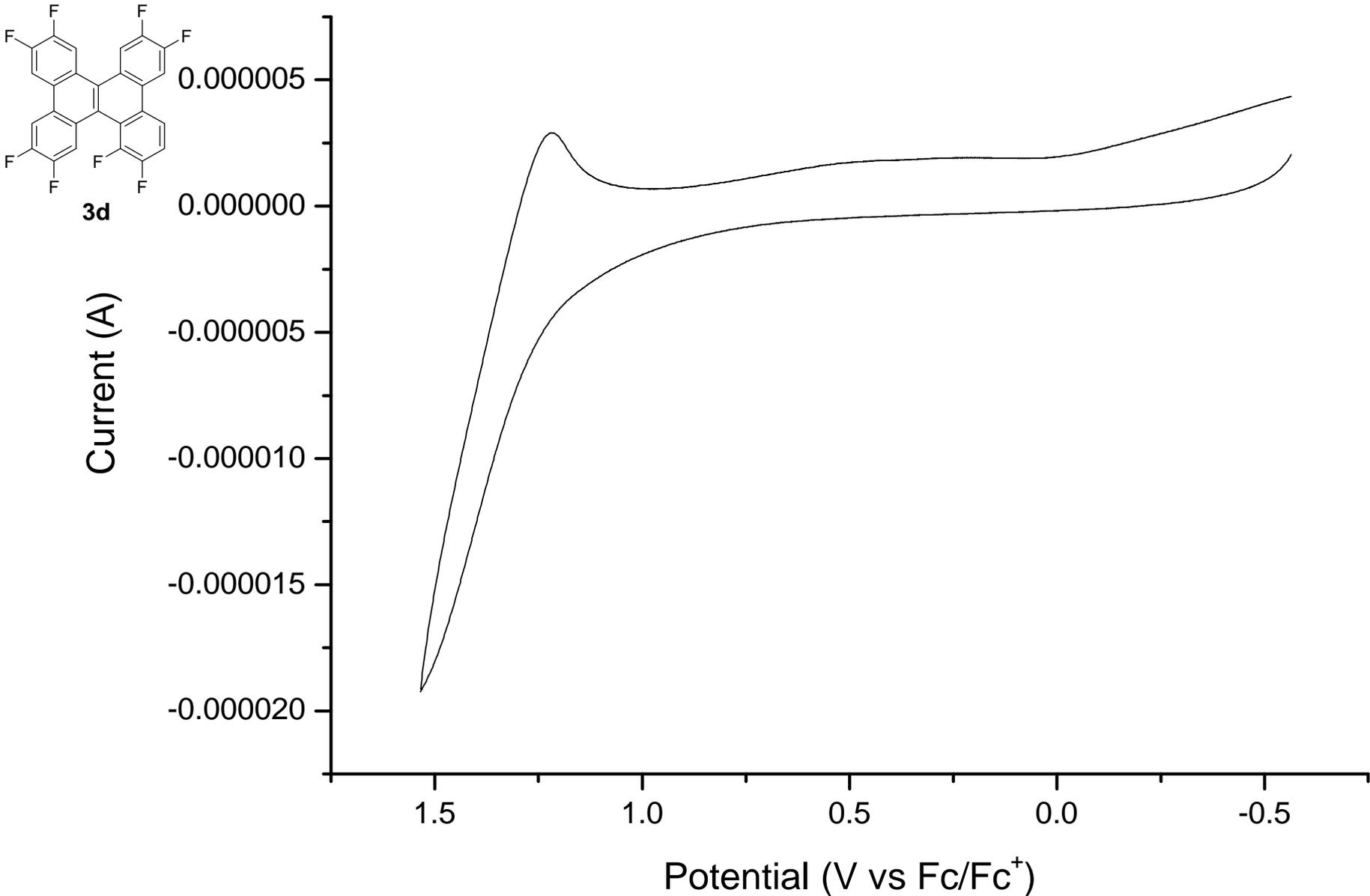


Figure S8. Cyclic voltammetry of **3d**: (Sample concentration was $1 \cdot 10^{-3} \text{M}$ in CH_2Cl_2 for oxidation, with Ag/AgCl as reference electrolyte, Pt as the support electrolyte and glassy carbon electrode as working electrode. The scan rate was 0.1 V/s)

TG/DTA

<Name>
080602A
<Date>
86/08/01 10:54

<Sample>
1
3.485 mg
(3.485 mg)
<Reference>
Pt
0.000 mg

<Comment>

<Sampling>
0.5 sec

<Temp.program[C] [C/min] [min]>
1* 25.0- 900.0 5.00 0.00
<Gas>
N2 100.0 ml/min
no 0.0 ml/min

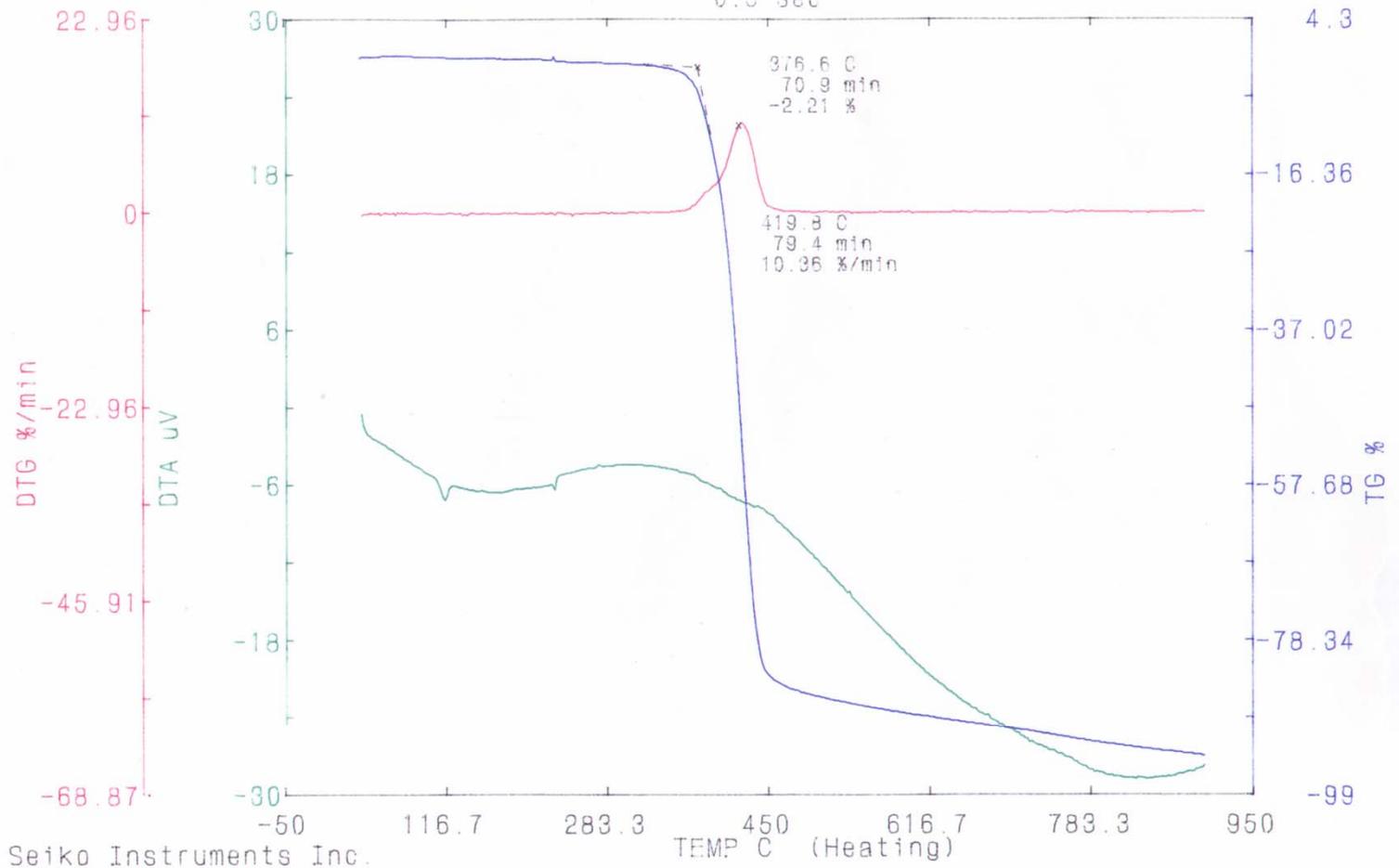


Figure S8. The TGA measurement of 4