Supporting Information

Hypervalent Iodine Reagent-Mediated Reaction of [60]Fullerene with Amines

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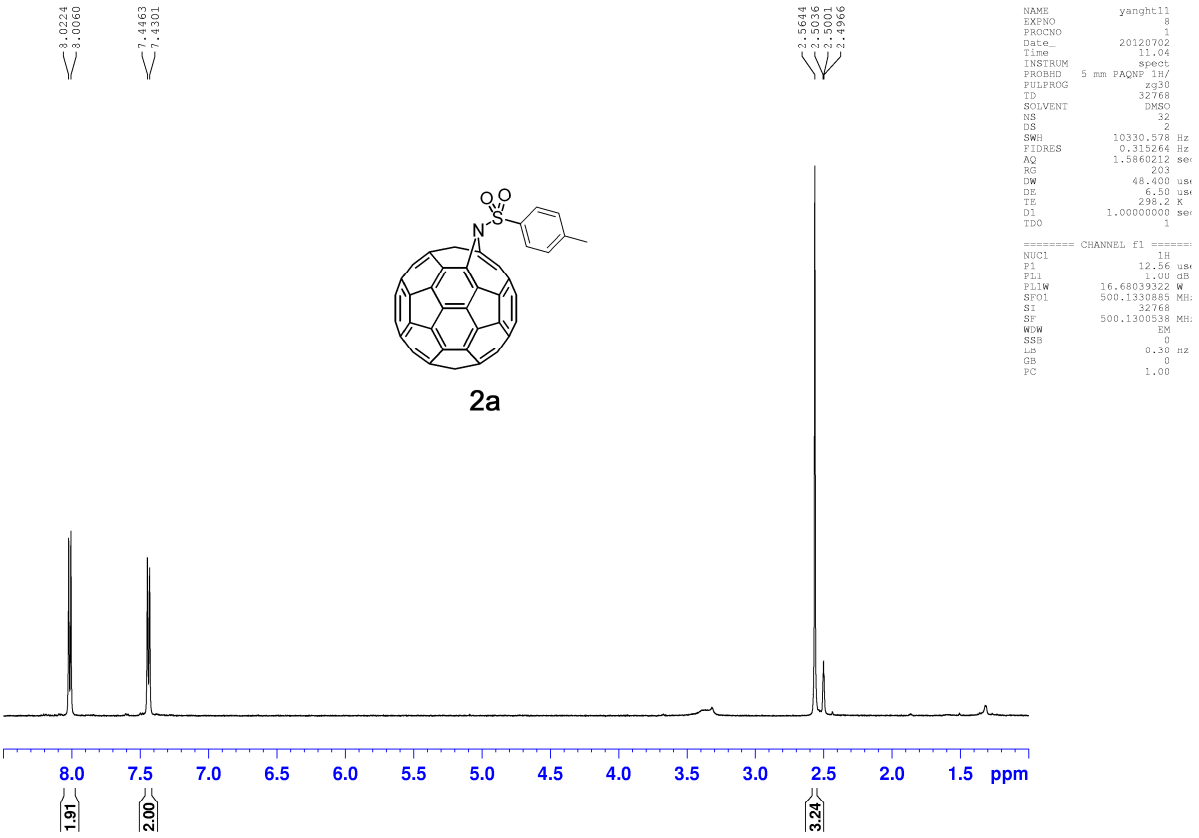
[1] Ulmer, L.; Mattay, J. *Eur. J. Org. Chem.* **2003**, 2933–2940. (Aziridinefullerenes **3** have a less polarity than azafulleroids **2** on TLC and the ^{1}H NMR spectrum of aziridinofullerenes **3** has a downfield shift compared to azafulleroids **2**.)

[2] Nagamachi, T.; Takeda, Y.; Nakayama, K.; Minakata, S. *Chem. Eur. J.* **2012**, *18*, 12035–12045.

[3] Ikuma, N.; Mikie, T.; Doi, Y.; Nakagawa, K.; Kokubo, K.; Oshima, T. *Org. Lett.* **2012**, *14*, 6040–6043.

[4] Gaussian 09 program (Revision C. 01, Gaussian, Inc., Wallingford, CT) was used in the theoretical calculations.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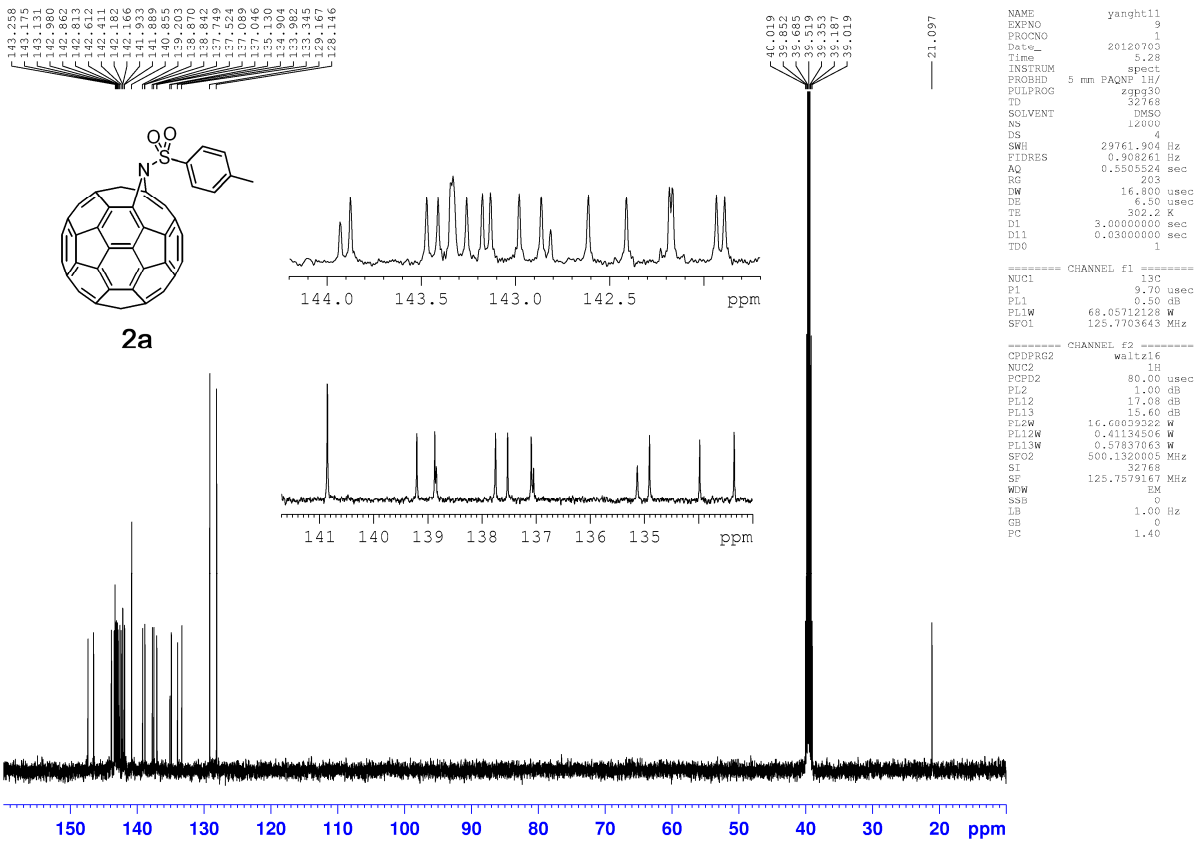
7.4463
7.4301
2.5644
2.5036
2.5001
2.4966
2a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.91
2.00
3.24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143.131
142.980
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142.612
142.411
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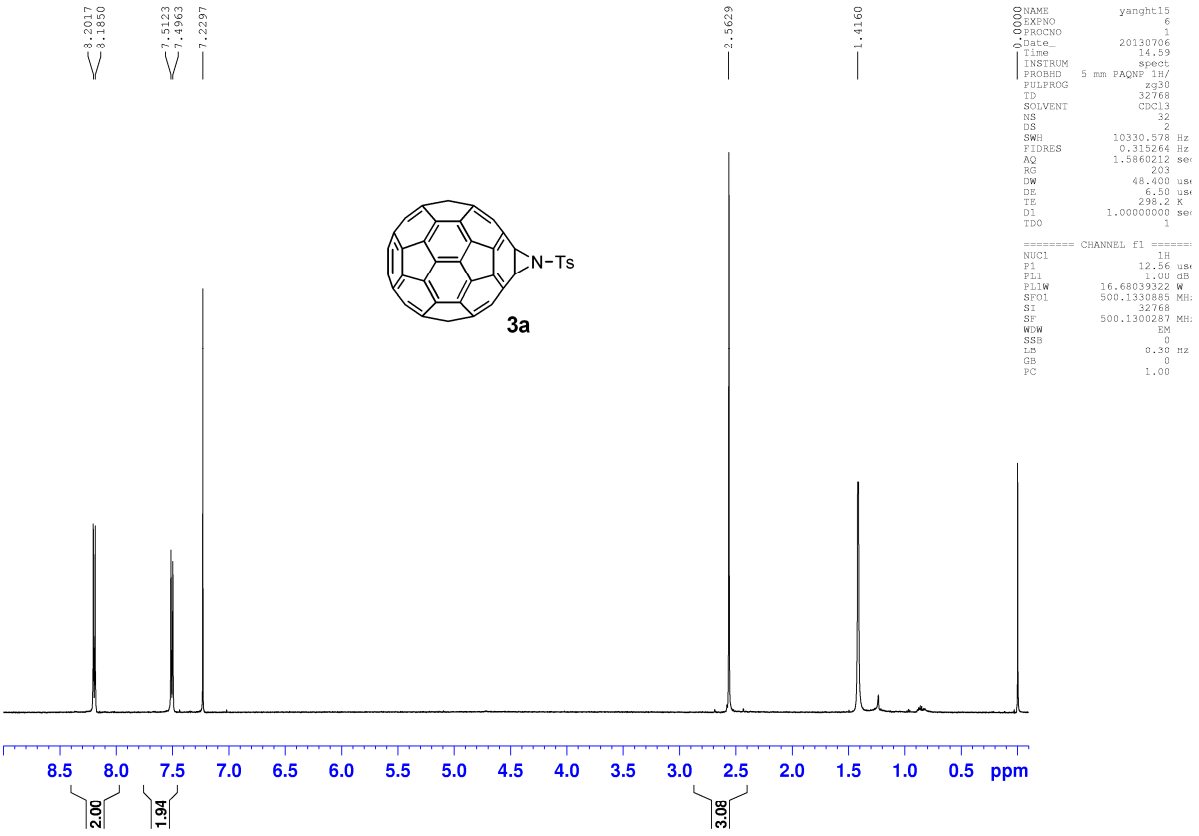
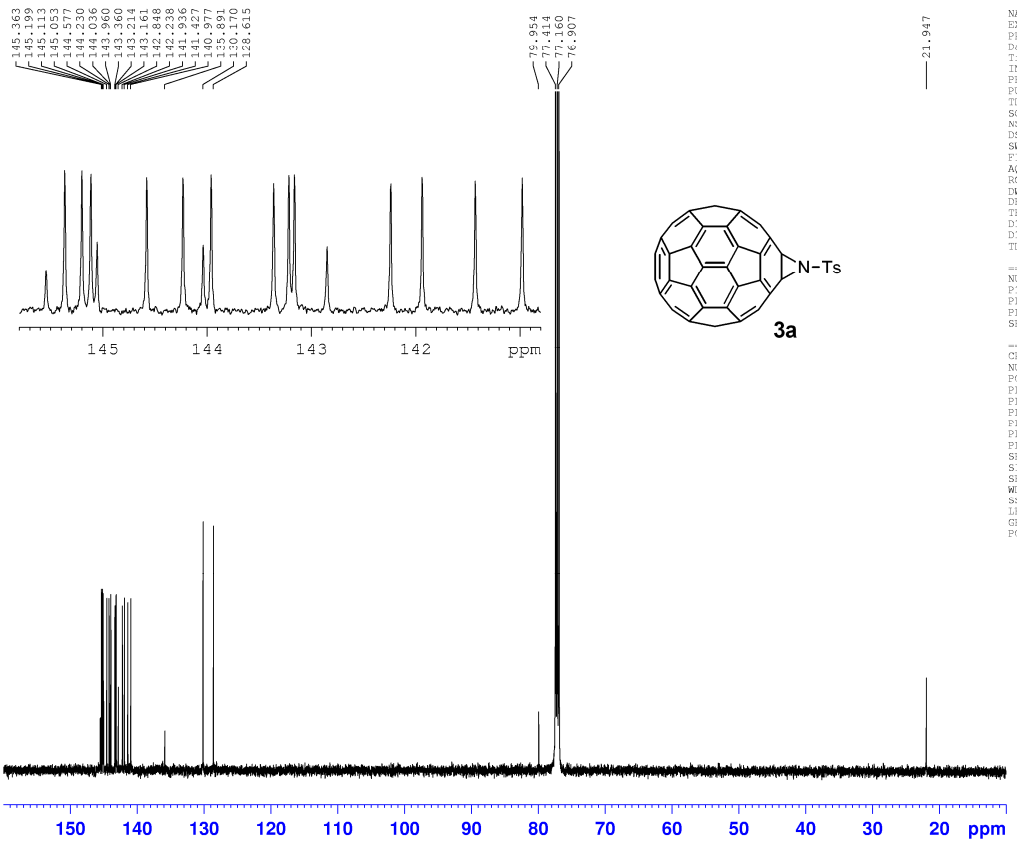
141.889
140.855
139.203
138.870
138.842
137.749
137.524
137.089
137.046
135.130
134.904
133.982
133.345
129.167
128.146
40.019
39.852
39.685
39.519
39.353
39.187
39.019
21.097
2a
144.0
143.5
143.0
142.5
ppm
141
140
139
138
137
136
135
ppm
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.2017
8.1850
7.5123
7.4963
7.2297
2.5629
1.4160
N-Ts
3a
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.94
3.08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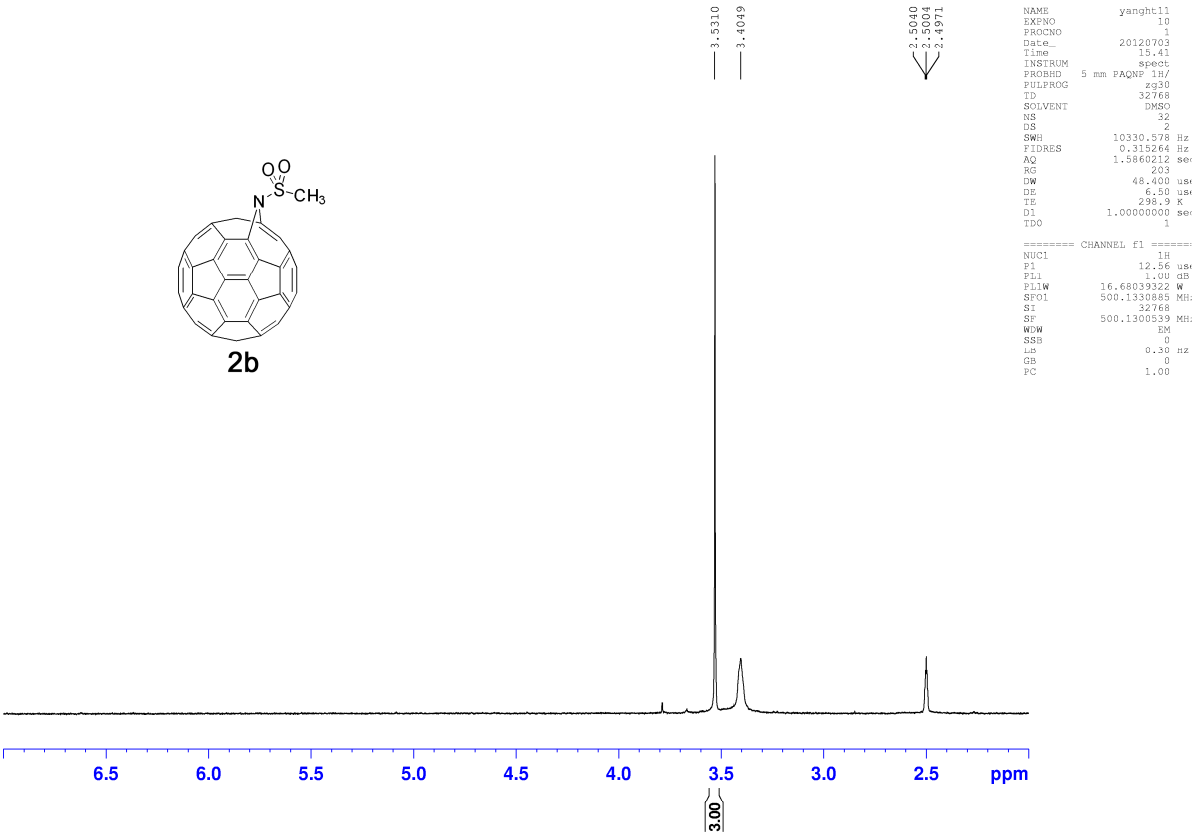
145.053
144.577
144.230
144.036
143.960
143.360
143.214
143.161
142.848
142.238
141.996
141.427
140.977
135.891
130.170
128.615
76.954
77.414
77.160
76.907
21.947
N-Ts
3a
145 144 143 142 ppm
150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm




```
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EXPNO                 10
PROCNO                 1
Date_           20120703
Time                15.41
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                     32
DS                      2
SWH            10330.578 Hz
FIDRES         0.315264 Hz
AQ             1.5860212 sec
RG                   203
DW                48.400 usec
DE                 6.50 usec
TE                298.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                  1H
P1                 12.56 usec
PL1                1.00 dB
PL1W          16.68039322 W
SFO1         500.1330885 MHz
SI                 32768
SF           500.1300539 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

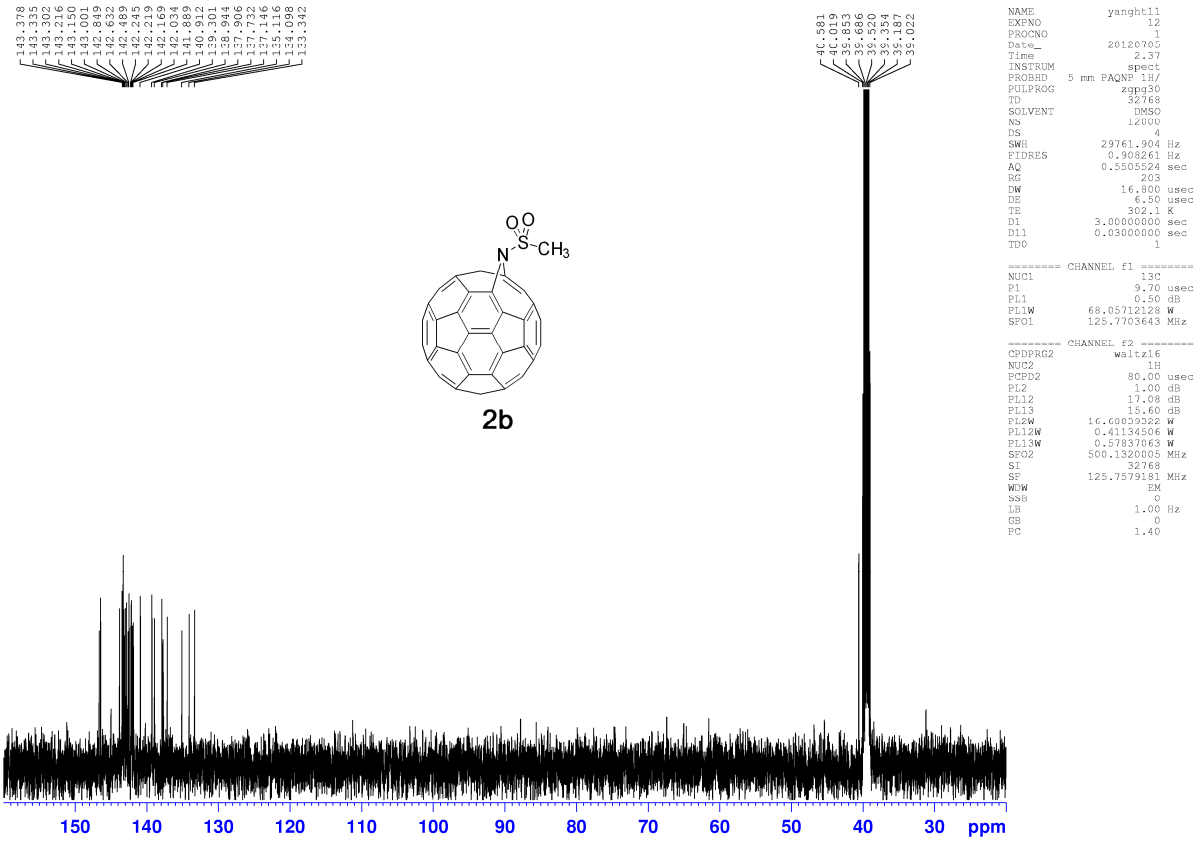


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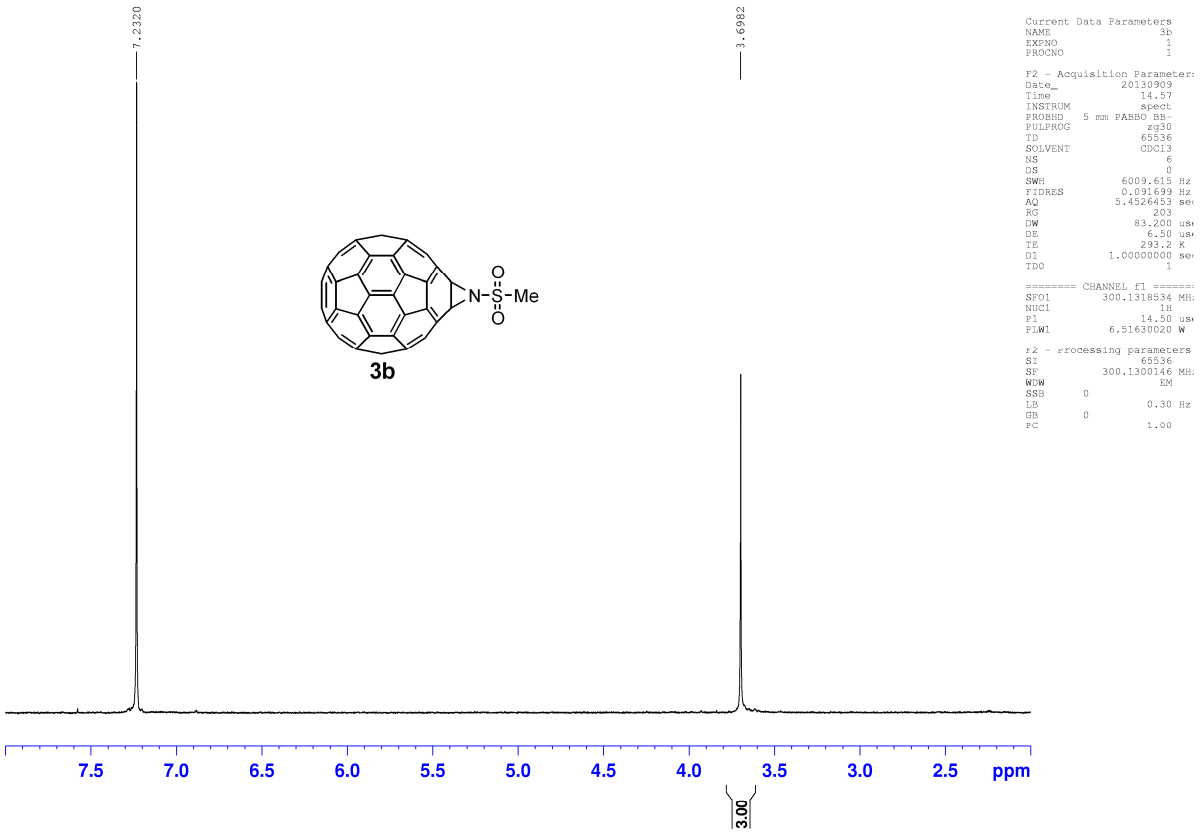
PROCNO                 1
Date_           20120705
Time                2.37
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                 12000
DS                     4
SWH            29761.904 Hz
FIDRES         0.908261 Hz
AQ             0.5505524 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                302.1 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.70 usec
PL1                0.50 dB
PL1W          68.05712128 W
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                1.00 dB
PL12               17.08 dB
PL13               15.60 dB
PL2W          16.68039222 W
PL12W          0.41134506 W
PL13W          0.57837063 W
SFO2         500.1320005 MHz
SI                 32768
SF           125.7579181 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME                      3b
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130909
Time                  14.57
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        6
DS                        0
SWH                6009.615 Hz
FIDRES             0.091699 Hz
AQ                 5.4526453 se
RG                      203
DW                   83.200 us
DE                    6.50 us
TE                   293.2 K
D1                 1.00000000 se
TD0                       1

======== CHANNEL f1 ======
SFO1             300.1318534 MH
NUC1                      1H
P1                    14.50 us
PLW1              6.51630020 W

F2 - Processing parameters
SI                    65536
SF               300.1300146 MH
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
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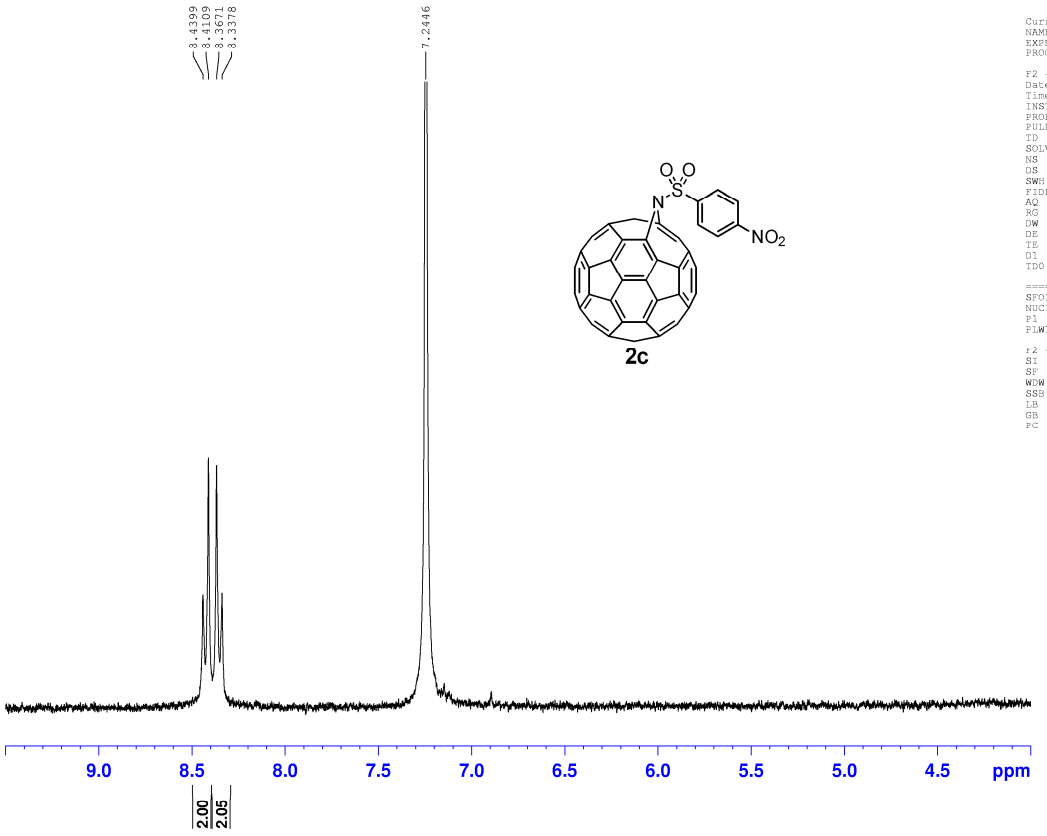
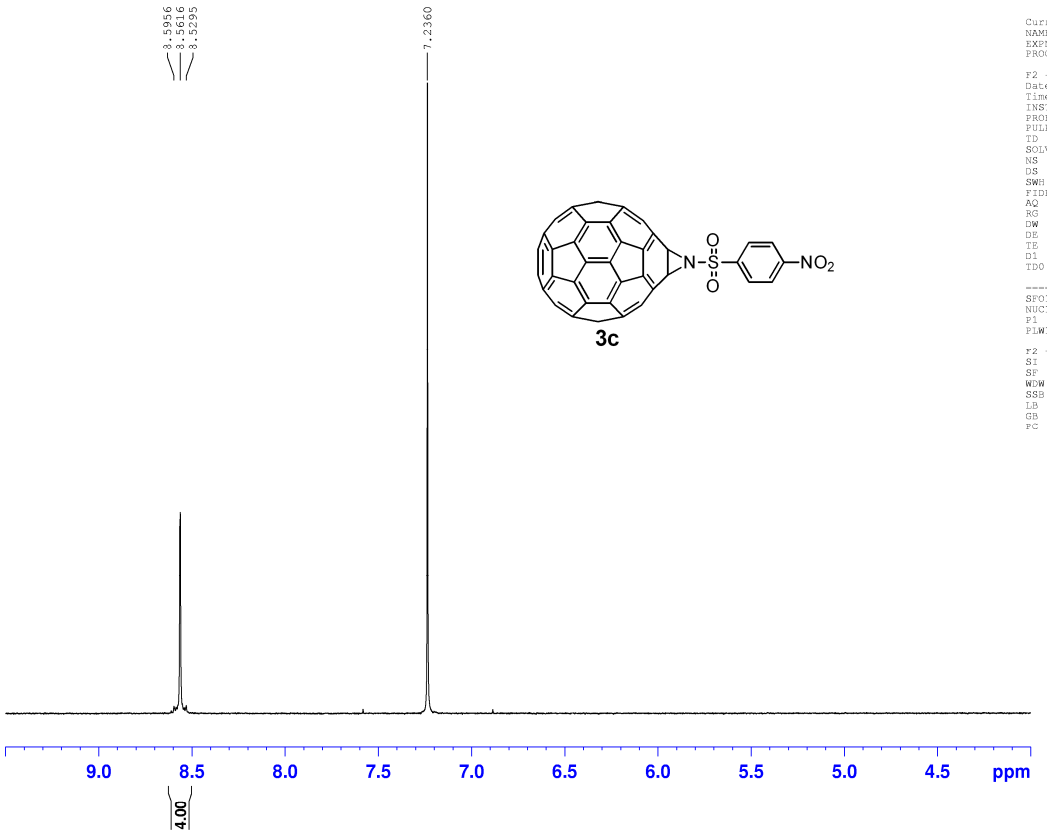



```
Current Data Parameters
NAME                  2c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130909
Time              15.52
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                     8
DS                     0
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4526453 se
RG                   203
DW              83.200 us
DE               6.50 us
TE              293.4 K
D1          1.00000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1        300.1318534 MH
NUC1                1H
P1                14.50 us
PLW1         6.51630020 W

F2 - Processing parameters
SI                 65536
SF          300.1300110 MH
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

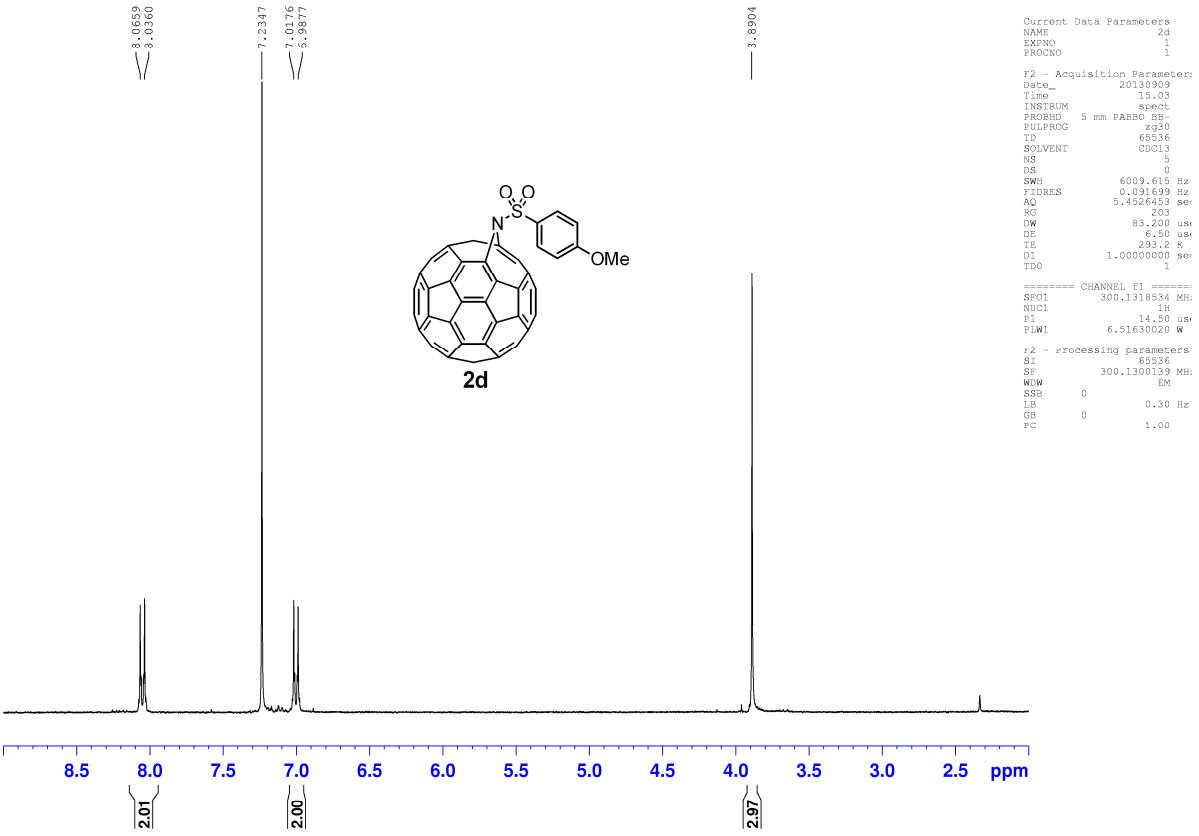



```
Current Data Parameters
NAME                  3c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130909
Time              15.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                     6
DS                     0
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4526453 se
RG                   203
DW              83.200 us
DE               6.50 us
TE              293.2 K
D1          1.00000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1        300.1318534 MH
NUC1                1H
P1                14.50 us
PLW1         6.51630020 W

F2 - Processing parameters
SI                 65536
SF          300.1300136 MH
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME                  2d
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130909
Time               15.03
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     0
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4526453 se
RG                   203
DW                83.200 us
DE                 6.50 us
TE                293.2 K
D1             1.00000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1         300.1318534 MH
NUC1                1H
P1                14.50 us
PLW1          6.51630020 W

F2 - Processing parameters
SI                 65536
SF          300.1300139 MH
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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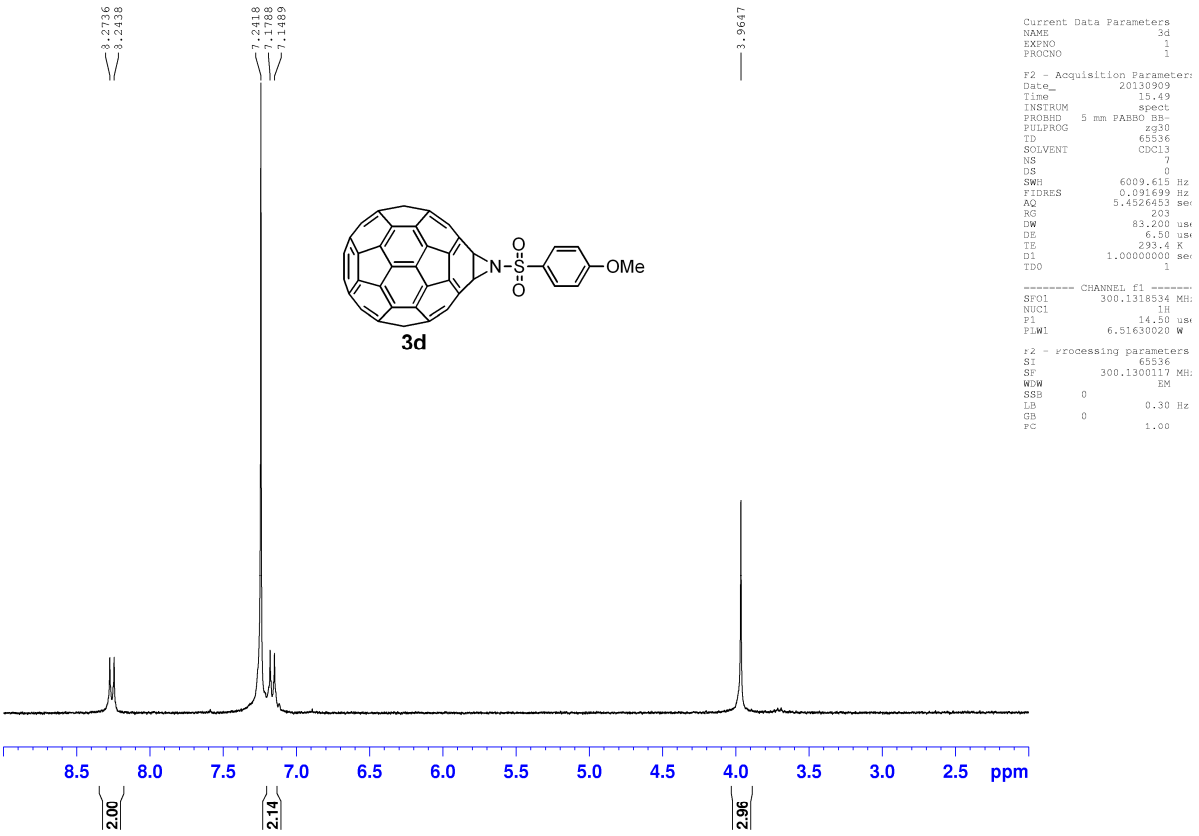
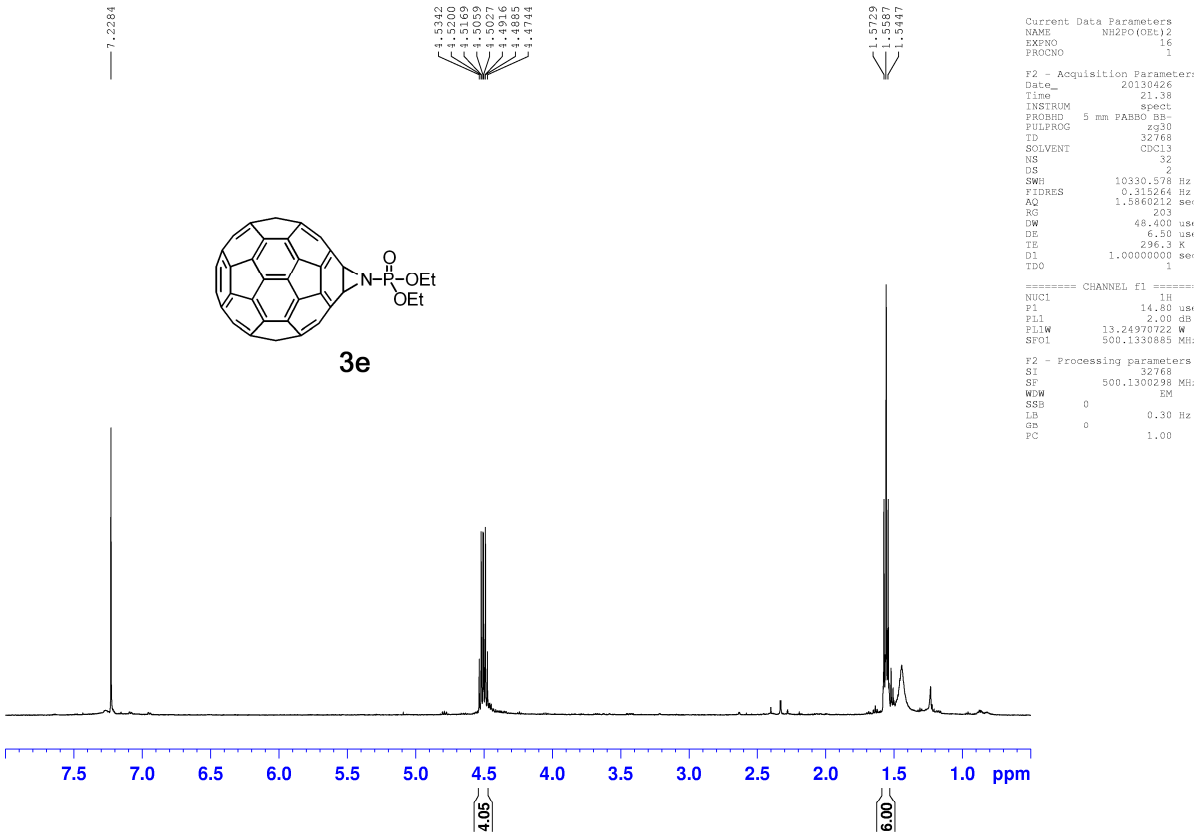



```
Current Data Parameters
NAME                  3d
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130909
Time               15.49
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     0
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4526453 se
RG                   203
DW                83.200 us
DE                 6.50 us
TE                293.4 K
D1             1.00000000 se
TD0                    1

======== CHANNEL f1 ======
SFO1         300.1318534 MH
NUC1                1H
P1                14.50 us
PLW1          6.51630020 W

F2 - Processing parameters
SI                 65536
SF          300.1300117 MH
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```


7.2284
4.5342
4.5200
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4.5027
4.4916
4.4885
4.4744
1.5729
1.5587
1.5447
O
N–P–OEt
OEt
3e
Current Data Parameters
NAME NH2PO(OEt)2
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130426
Time 21.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.80 usec
PL1 2.00 dB
PL1W 13.24970722 W
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300298 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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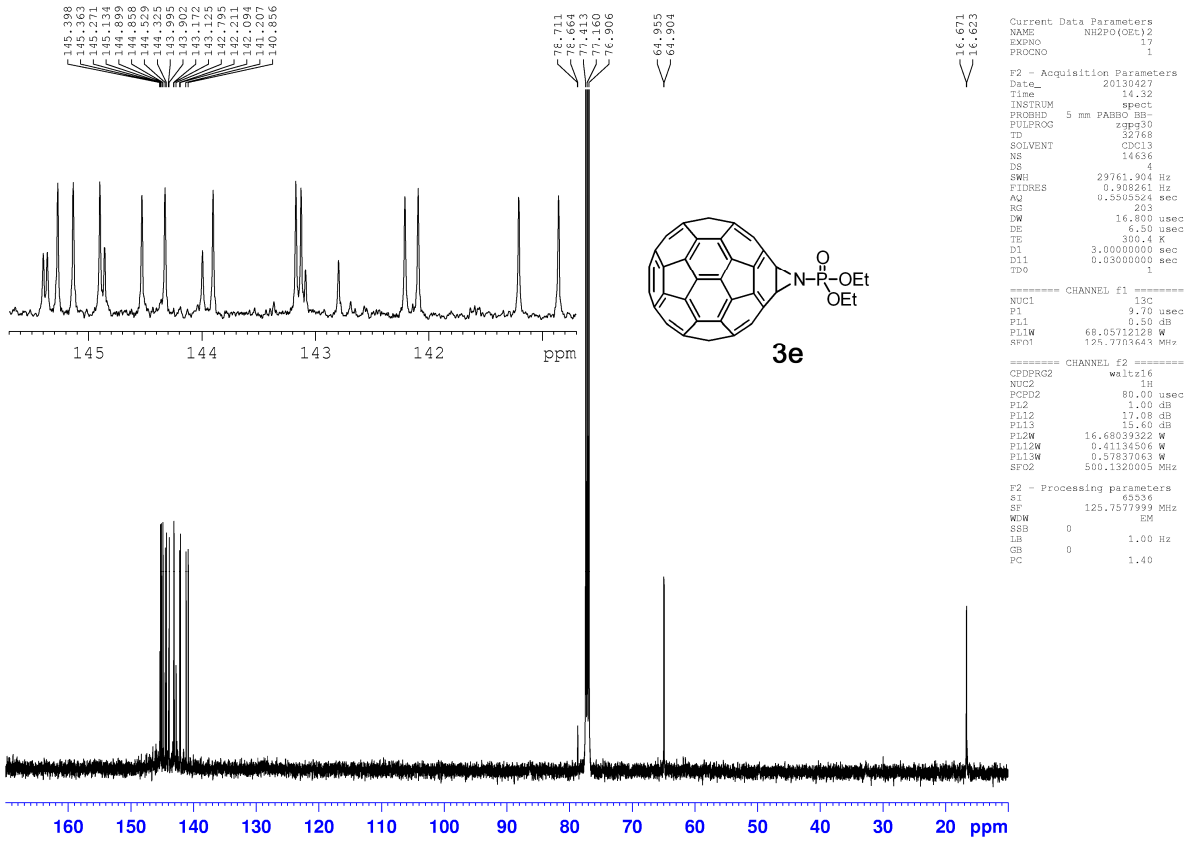
4.05
6.00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144.329
144.325
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143.902
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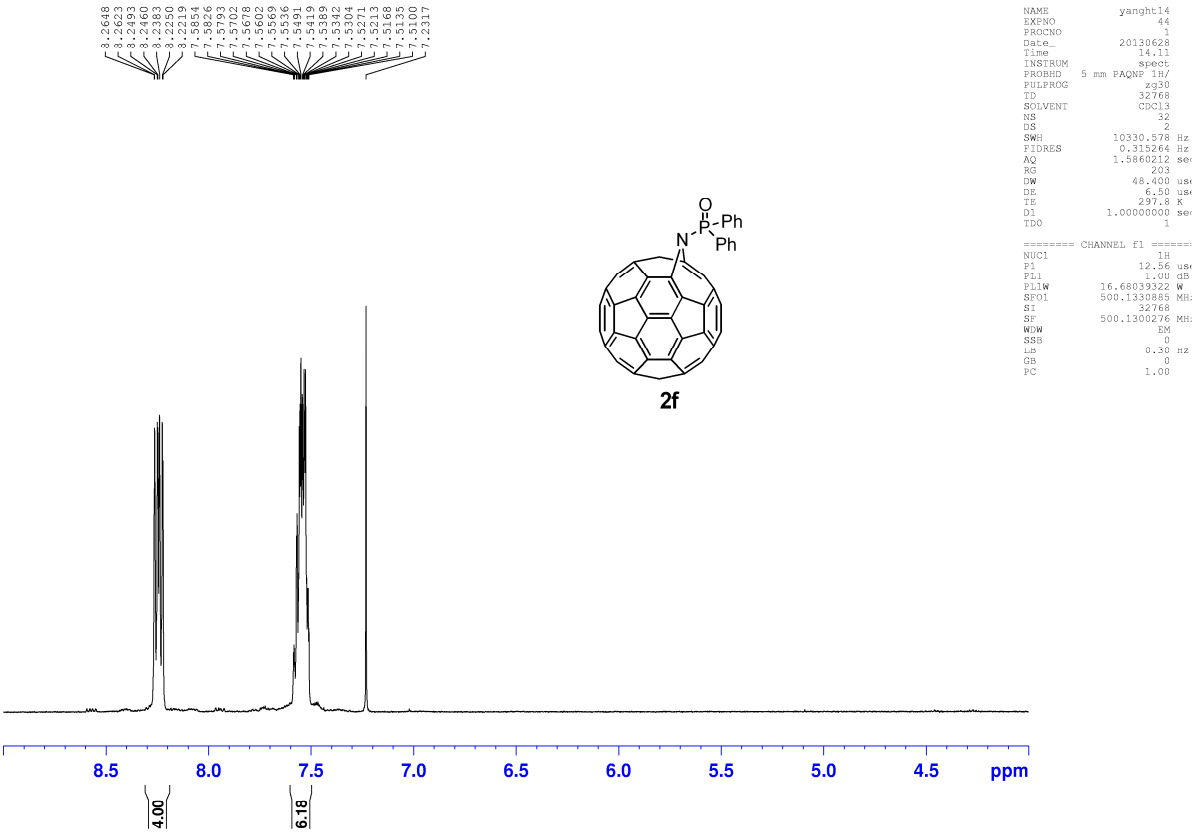
143.125
142.795
142.211
142.094
141.207
140.856
78.711
78.664
77.413
77.160
76.906
64.955
64.904
16.671
16.623
O
N–P–OEt
OEt
3e
Current Data Parameters
NAME NH2PO(OEt)2
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130427
Time 14.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 14636
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 0.50 dB
PL1W 68.05712128 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.08 dB
PL13 15.60 dB
PL2W 16.68039322 W
PL12W 0.41134506 W
PL13W 0.57837063 W
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577999 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
145 144 143 142 ppm
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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8.2383
8.2250
8.2219
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7.5826
7.5793
7.5702
7.5678
7.5602
7.5569
7.5536
7.5491
7.5419
7.5389
7.5342
7.5304
7.5271
7.5213
7.5168
7.5135
7.5100
7.2317
NAME yanght14
EXPNO 44
PROCNO 1
Date_ 20130628
Time 14.11
INSTRUM spect
PROBHD 5 mm PAQNP 1H/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 12.56 usec
PL1 1.00 dB
PL1W 16.68039322 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300276 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
P
Ph
Ph
N
2f
8.5
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7.5
7.0
6.5
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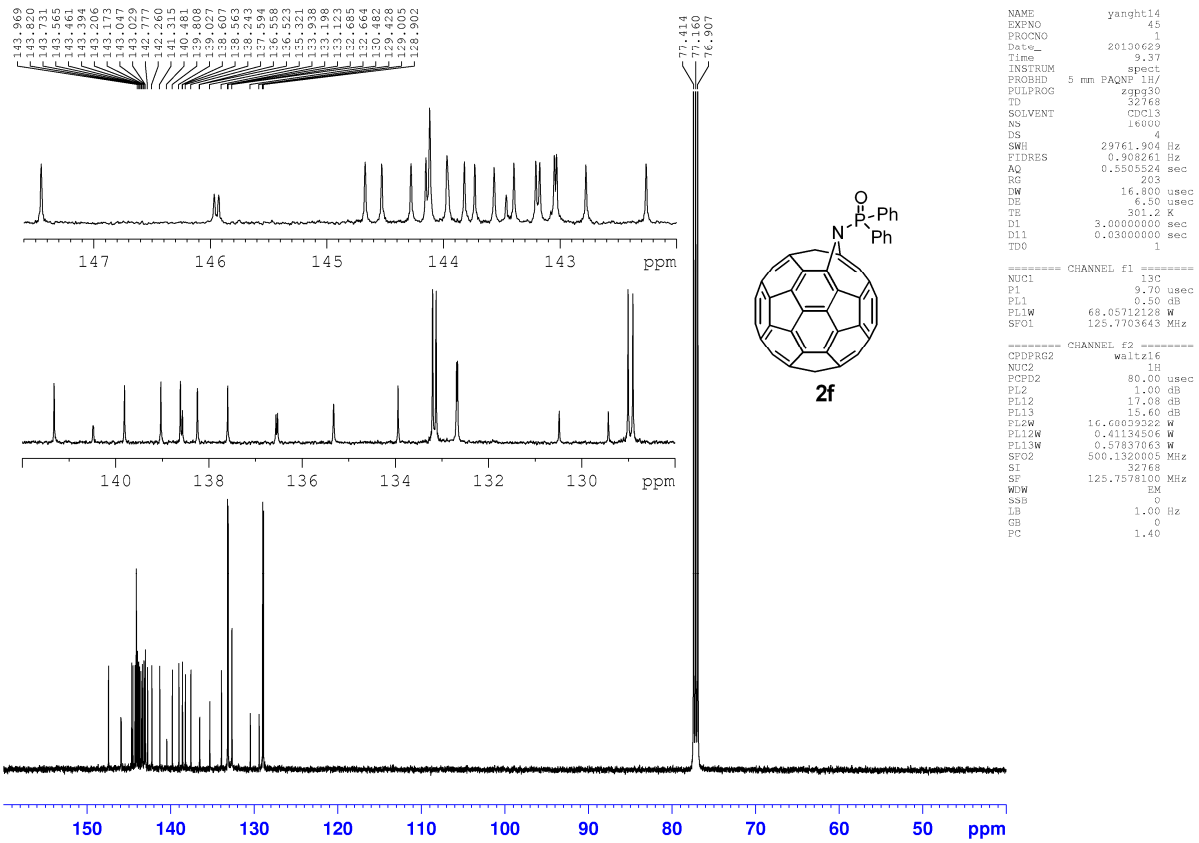
5.5
5.0
4.5
ppm
4.00
6.18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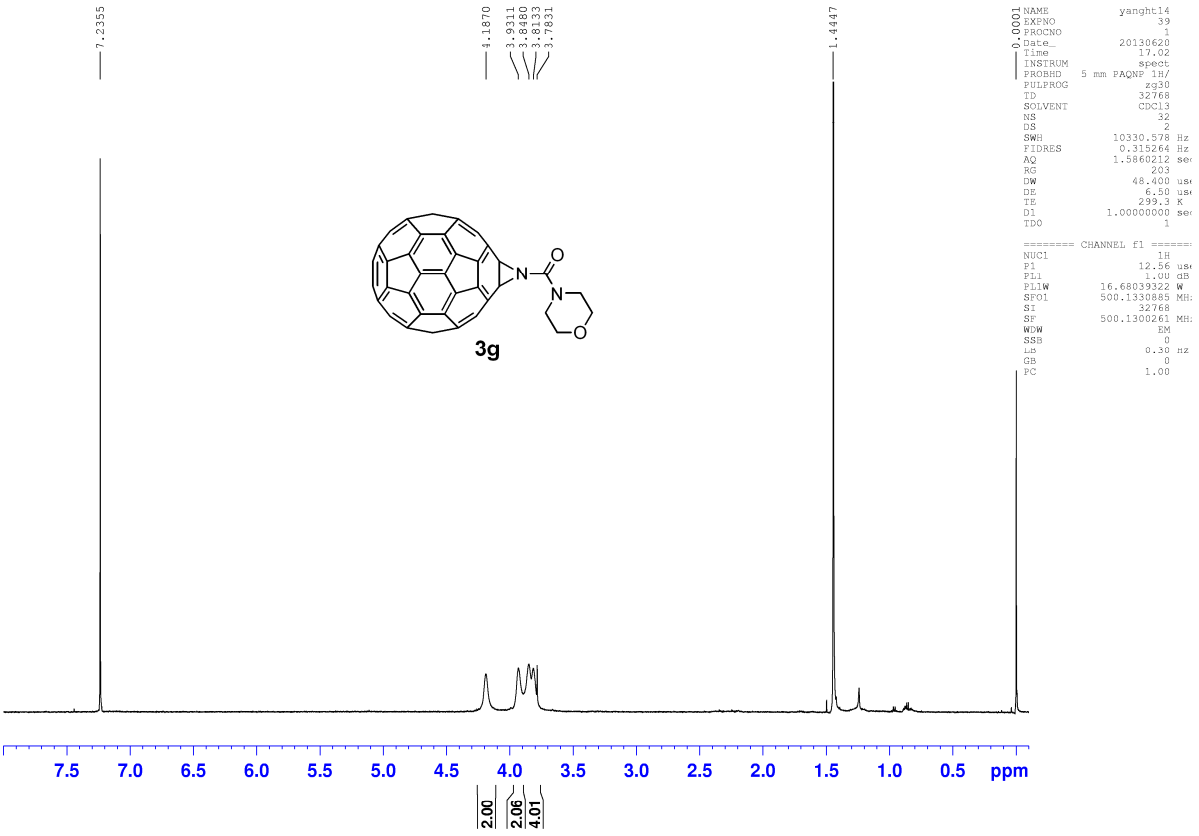
143.565
143.461
143.394
143.206
143.173
143.047
143.029
142.777
142.260
141.315
140.481
139.698
139.027
138.607
138.563
138.243
137.594
136.558
136.523
135.321
133.938
133.198
133.123
132.685
132.664
130.482
129.428
129.005
128.902
77.414
77.160
76.907
NAME yanght14
EXPNO 45
PROCNO 1
Date_ 20130629
Time 9.37
INSTRUM spect
PROBHD 5 mm PAQNP 1H/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 301.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 0.50 dB
PL1W 68.05712128 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.08 dB
PL13 15.60 dB
PL2W 16.68039222 W
PL12W 0.41134506 W
PL13W 0.57837063 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578100 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
P
Ph
Ph
N
2f
147
146
145
144
143
ppm
140
138
136
134
132
130
ppm
150
140
130
120
110
100
90
80
70
60
50
ppm




```
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EXPNO                 39
PROCNO                 1
Date_           20130620
Time                17.02
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            10330.578 Hz
FIDRES         0.315264 Hz
AQ             1.5860212 sec
RG                   203
DW                48.400 usec
DE                 6.50 usec
TE                299.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.56 usec
PL1                1.00 dB
PL1W         16.68039322 W
SFO1         500.1330885 MHz
SI                 32768
SF           500.1300261 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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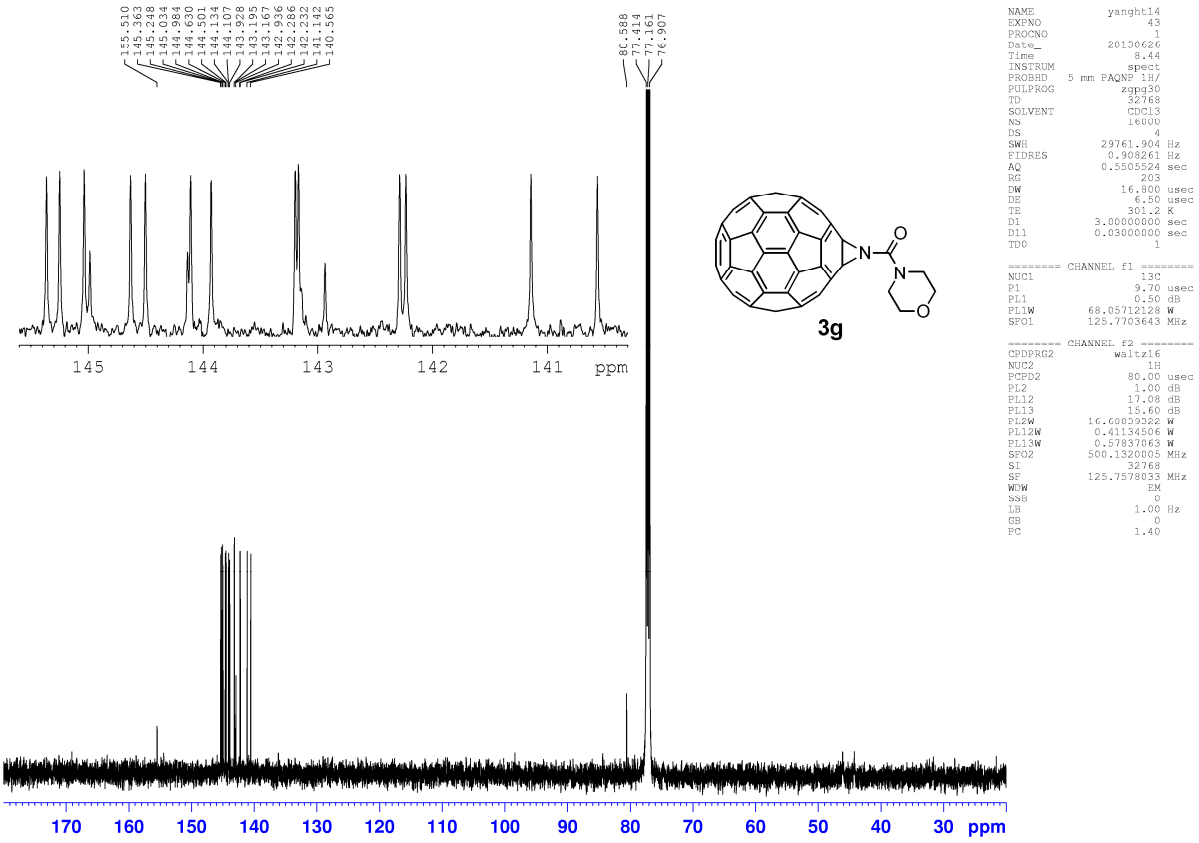
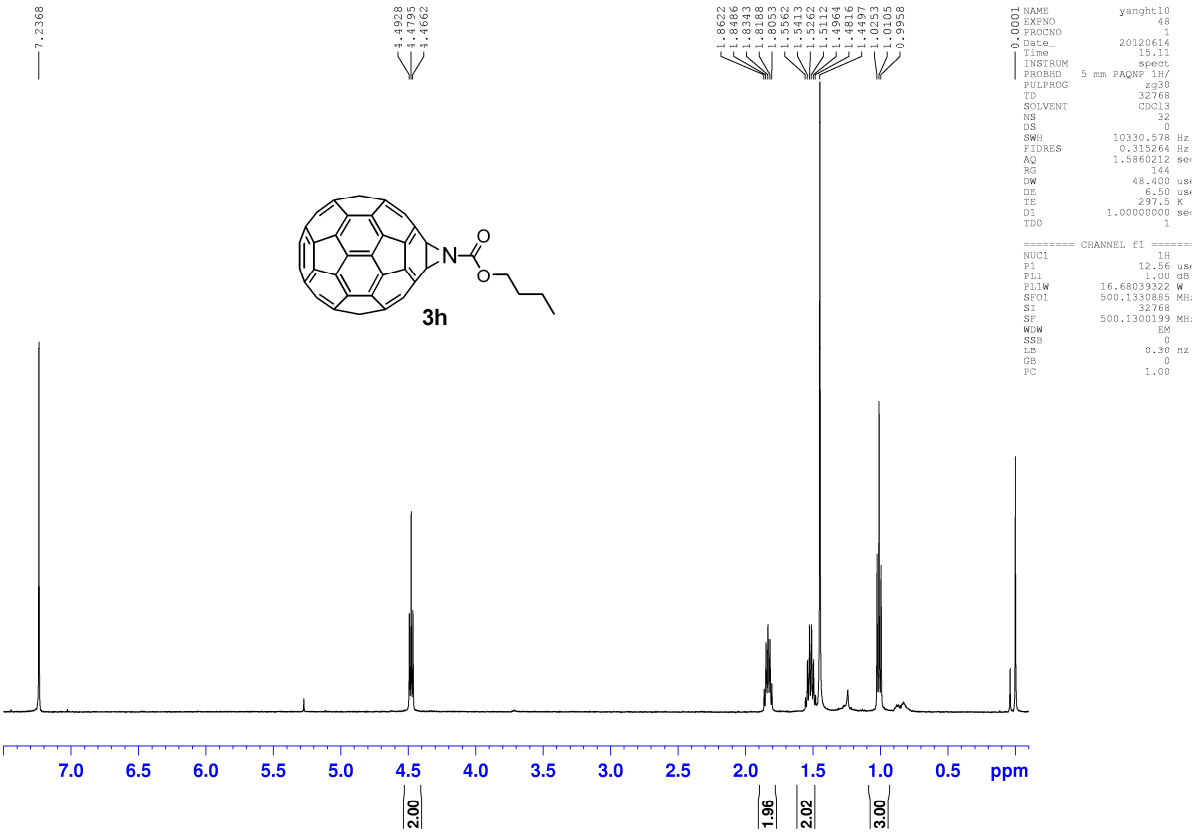
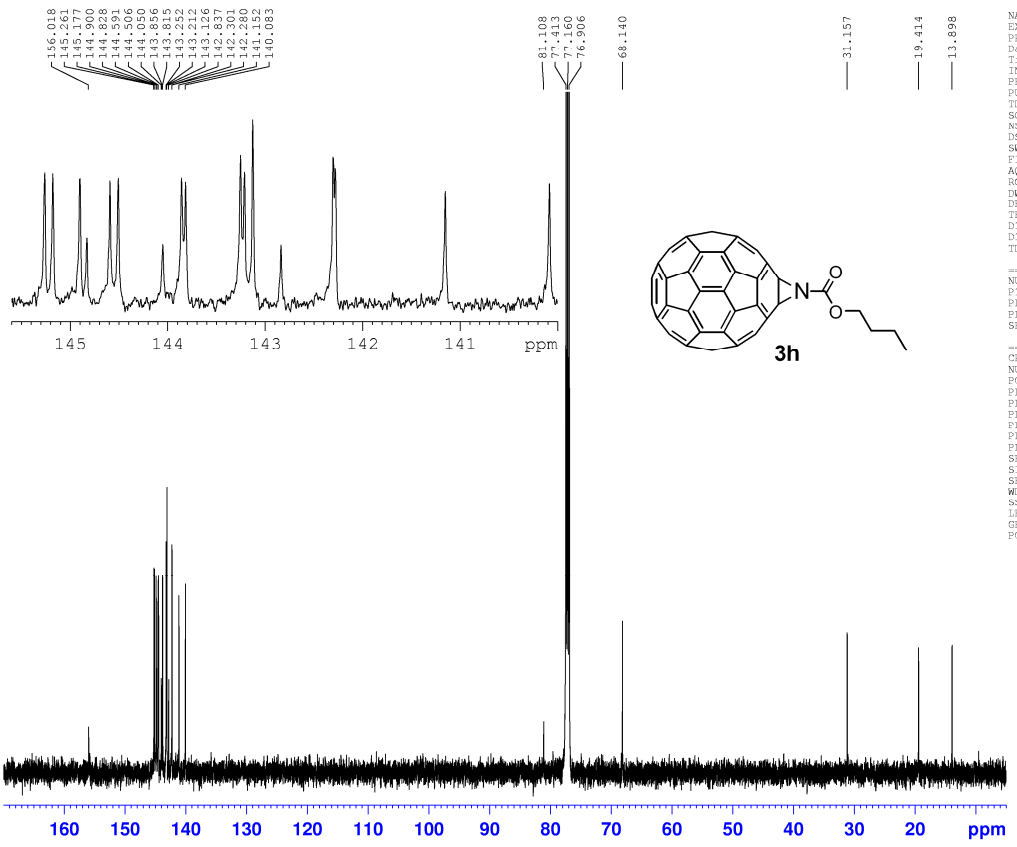
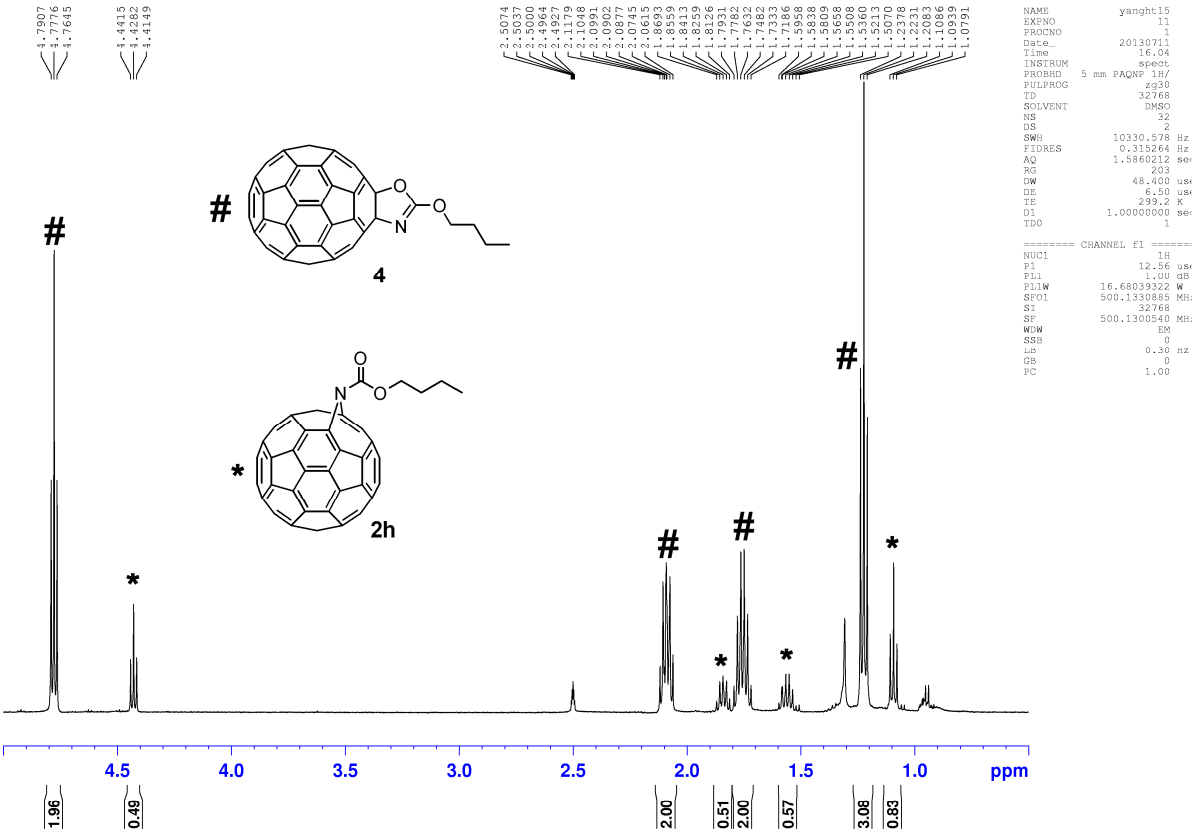
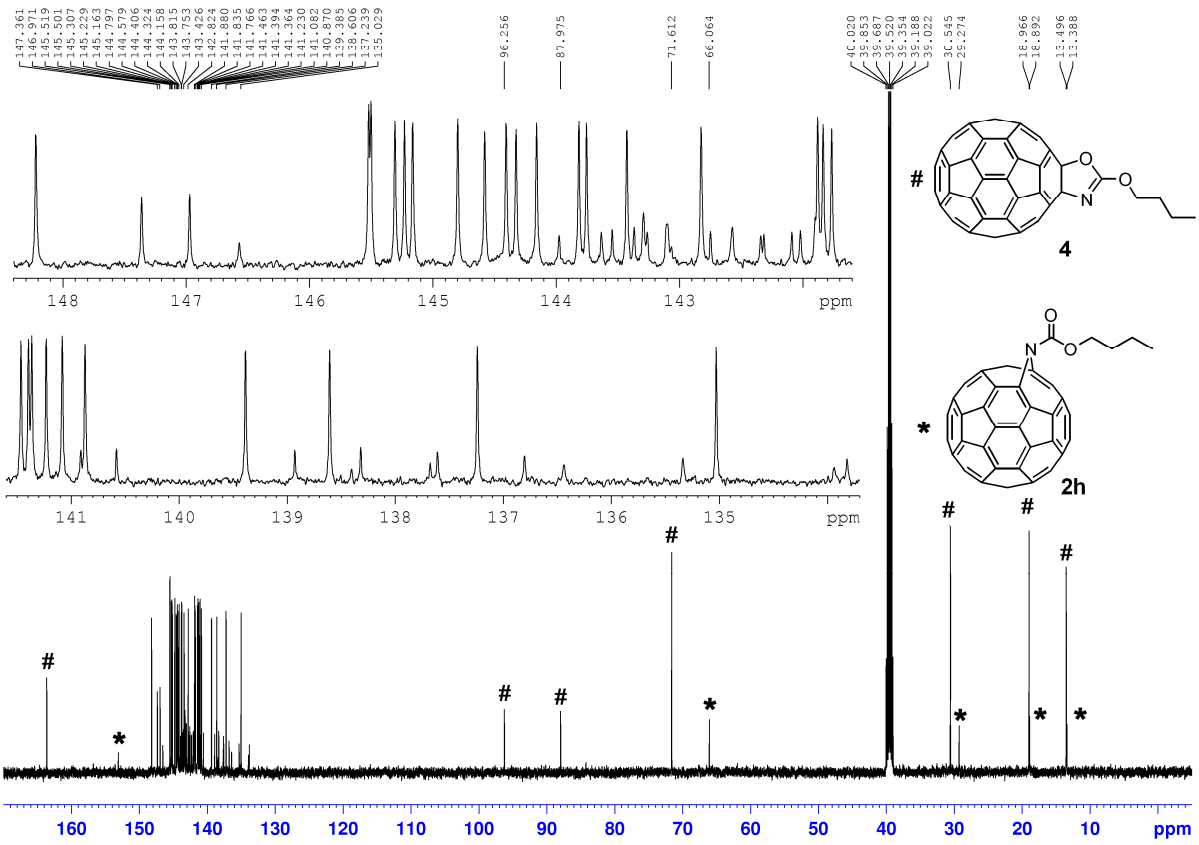


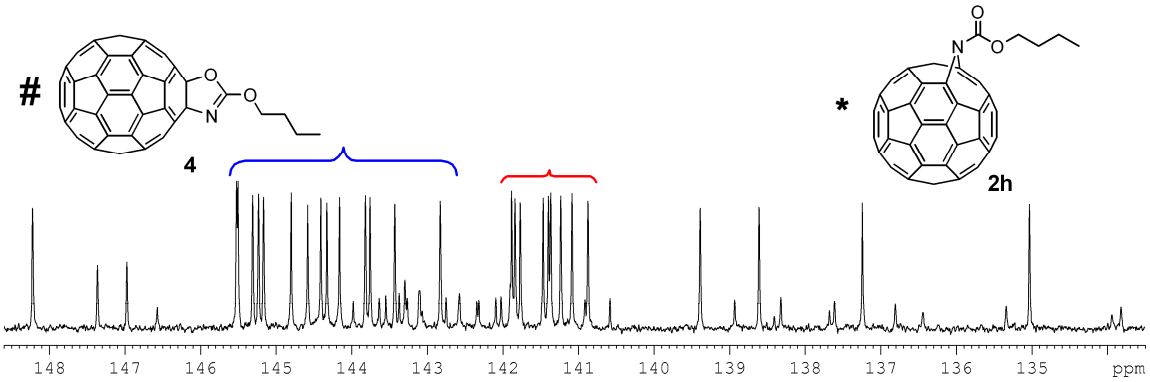

```
NAME            yanght14
EXPNO                 43
PROCNO                 1
Date_           20130626
Time                8.44
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 16000
DS                     4
SWH            29761.904 Hz
FIDRES         0.908261 Hz
AQ             0.5505524 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                301.2 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.70 usec
PL1                0.50 dB
PL1W         68.05712128 W
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                1.00 dB
PL12              17.08 dB
PL13              15.60 dB
PL2W         16.68039222 W
PL12W         0.41134506 W
PL13W         0.57837063 W
SFO2         500.1320005 MHz
SI                 32768
SF           125.7578033 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

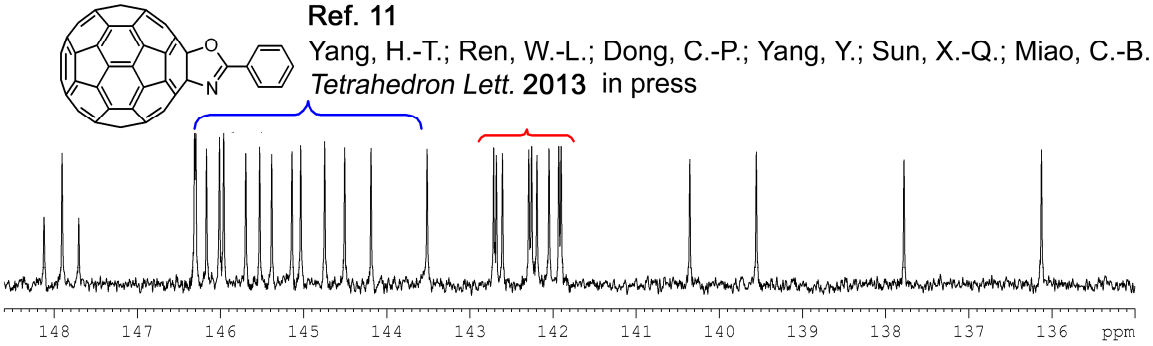

7.2368
4.4928
4.4795
4.4662
1.8622
1.8486
1.8343
1.8188
1.8053
1.5562
1.5413
1.5262
1.5112
1.4964
1.4816
1.4497
1.0253
1.0105
0.9958
3h
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.96
2.02
3.00


156.018
145.261
145.177
144.900
144.828
144.591
144.506
144.050
143.856
143.815
143.252
143.212
143.126
142.837
142.301
142.280
141.152
140.083
81.108
77.413
77.160
76.906
68.140
31.157
19.414
13.898
3h
145 144 143 142 141 ppm
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

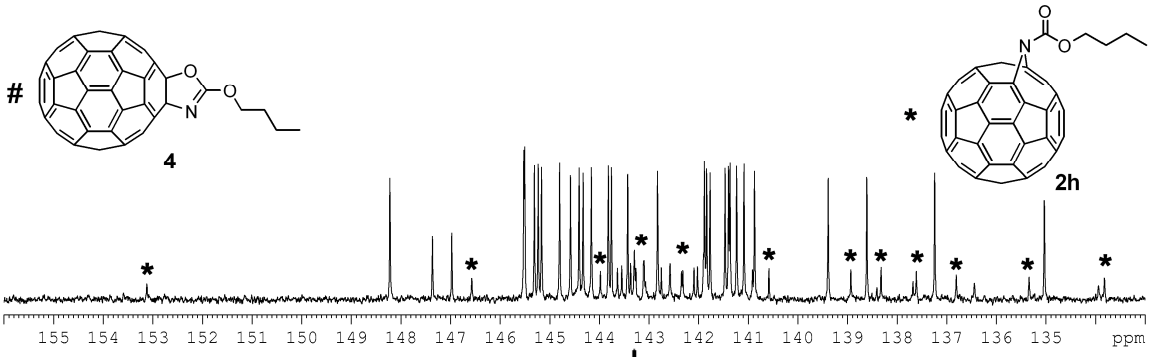

4
2h
ppm

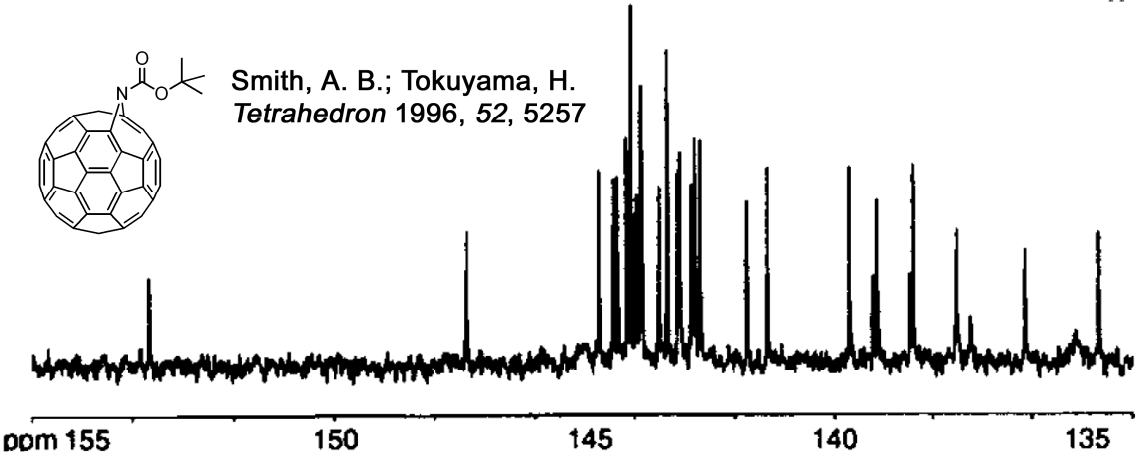

4
2h
ppm

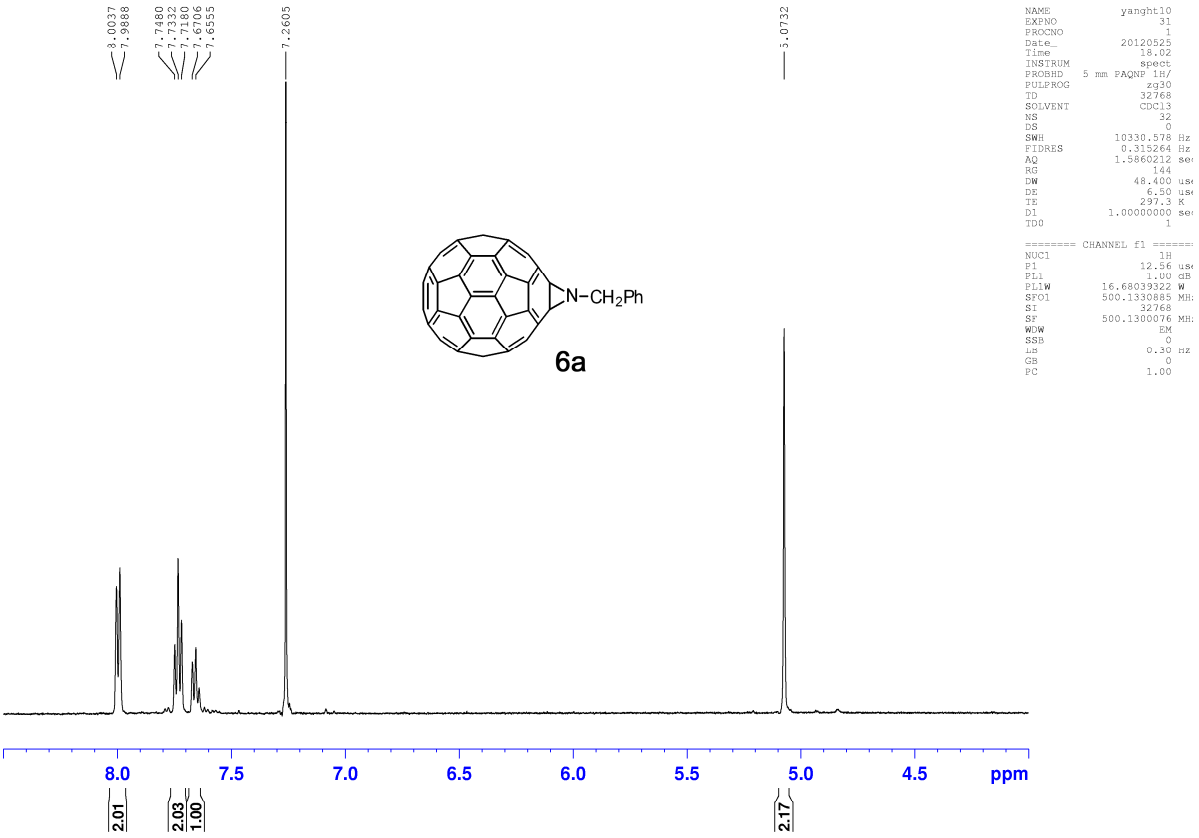


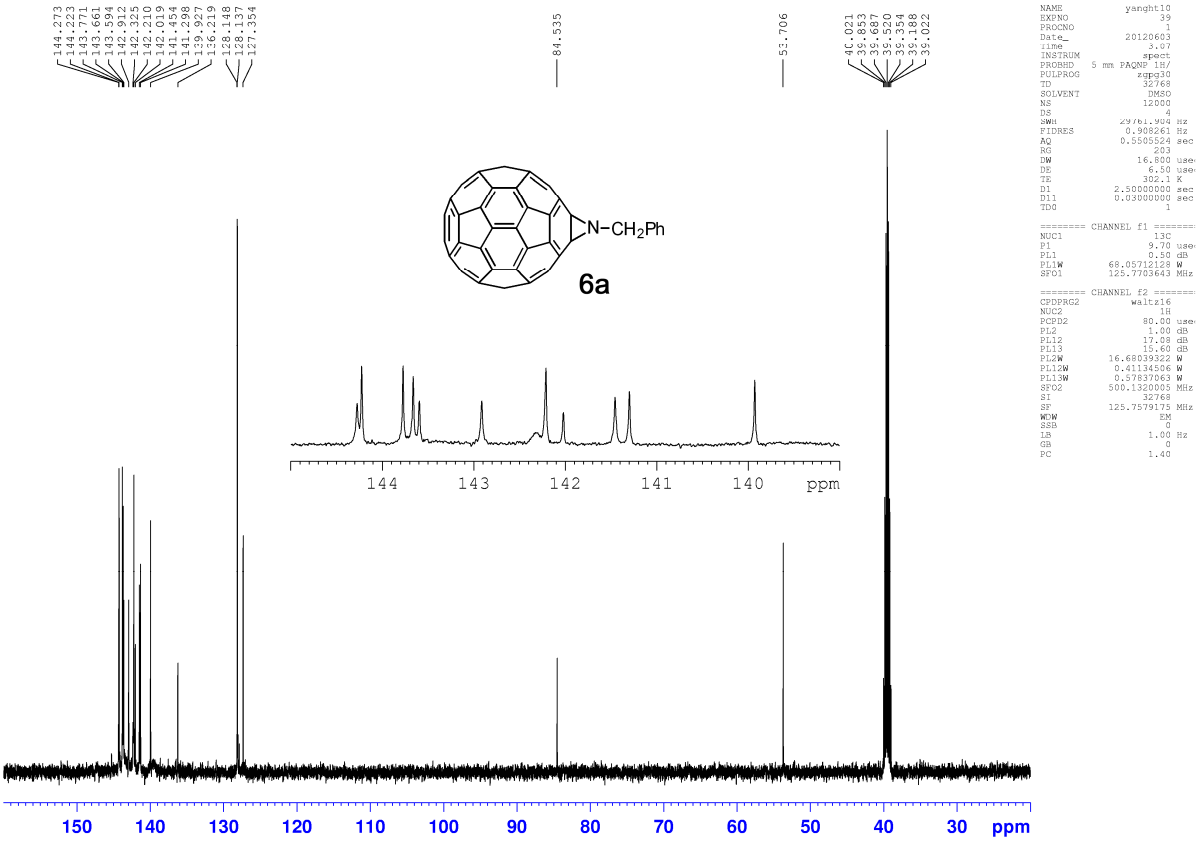


Ref. 11
Yang, H.-T.; Ren, W.-L.; Dong, C.-P.; Yang, Y.; Sun, X.-Q.; Miao, C.-B.
Tetrahedron Lett. **2013** in press






8.0037
7.9888
7.7480
7.7332
7.7180
7.6006
7.6555
7.2605
5.0732
N–CH2Ph
6a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
2.01
2.03
1.00
2.17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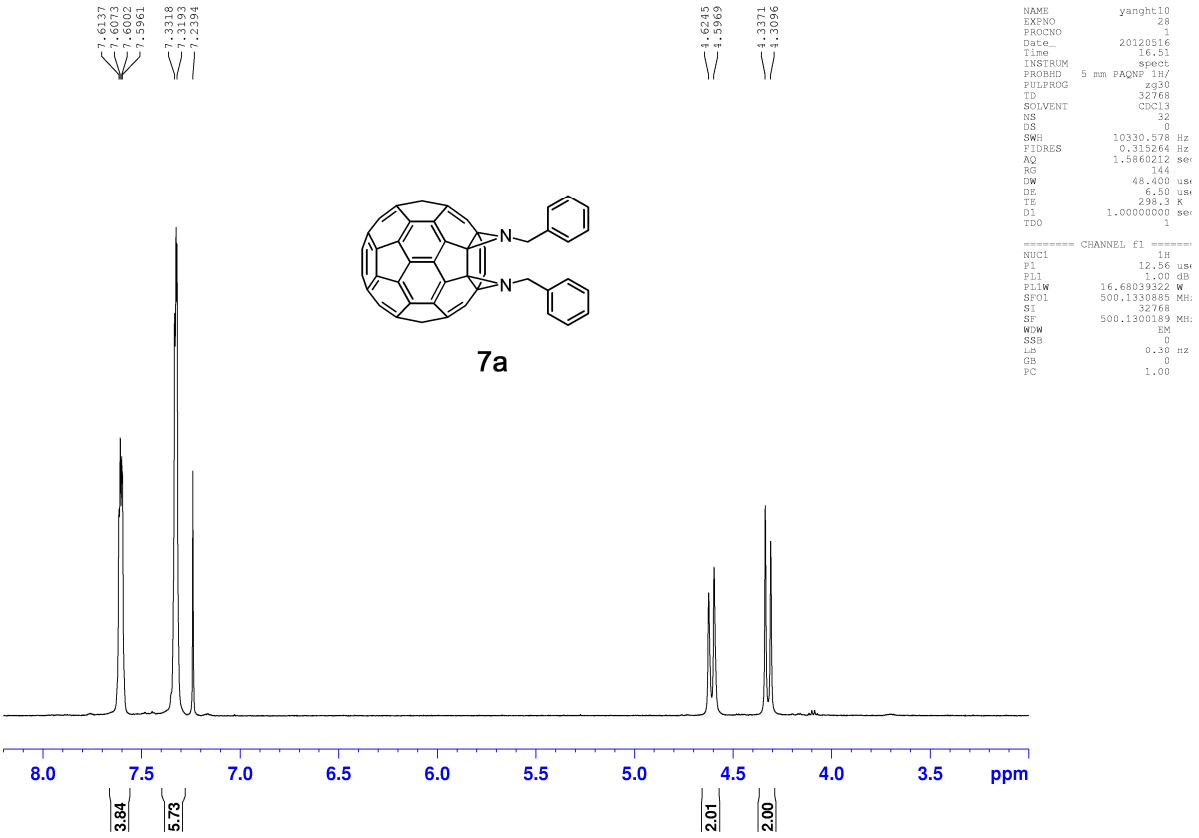
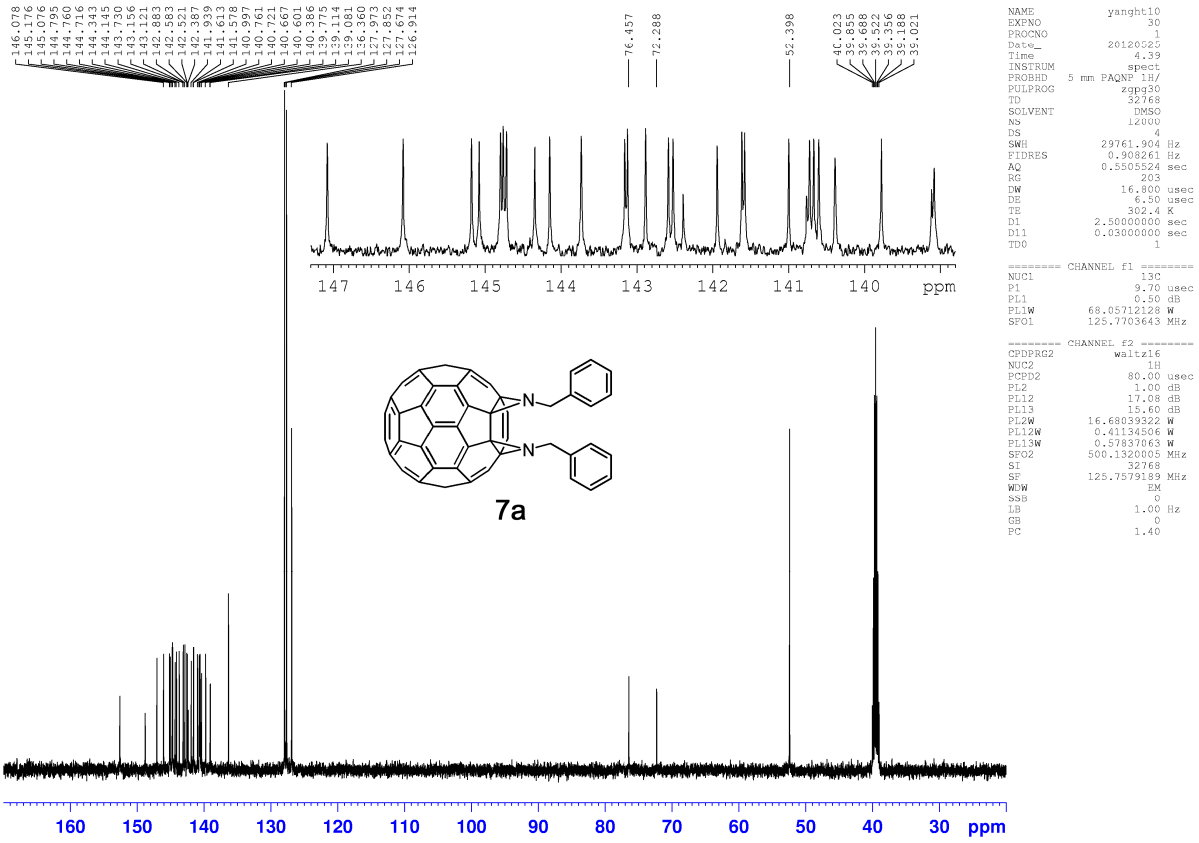
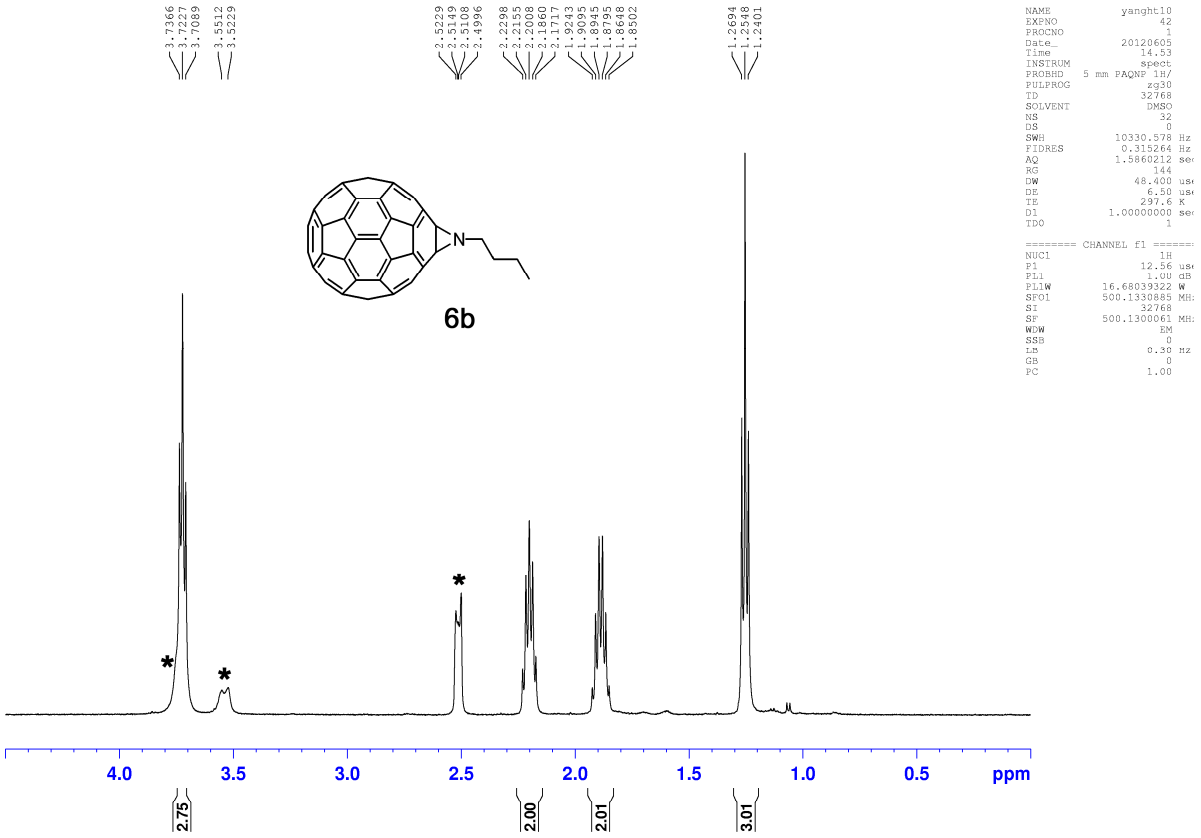
144.223
143.771
143.661
143.594
142.912
142.325
142.210
142.019
141.454
141.298
139.927
136.219
128.148
128.137
127.354
84.535
53.706
40.021
39.853
39.687
39.520
39.354
39.188
39.022
N–CH2Ph
6a
144
143
142
141
140
ppm
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm



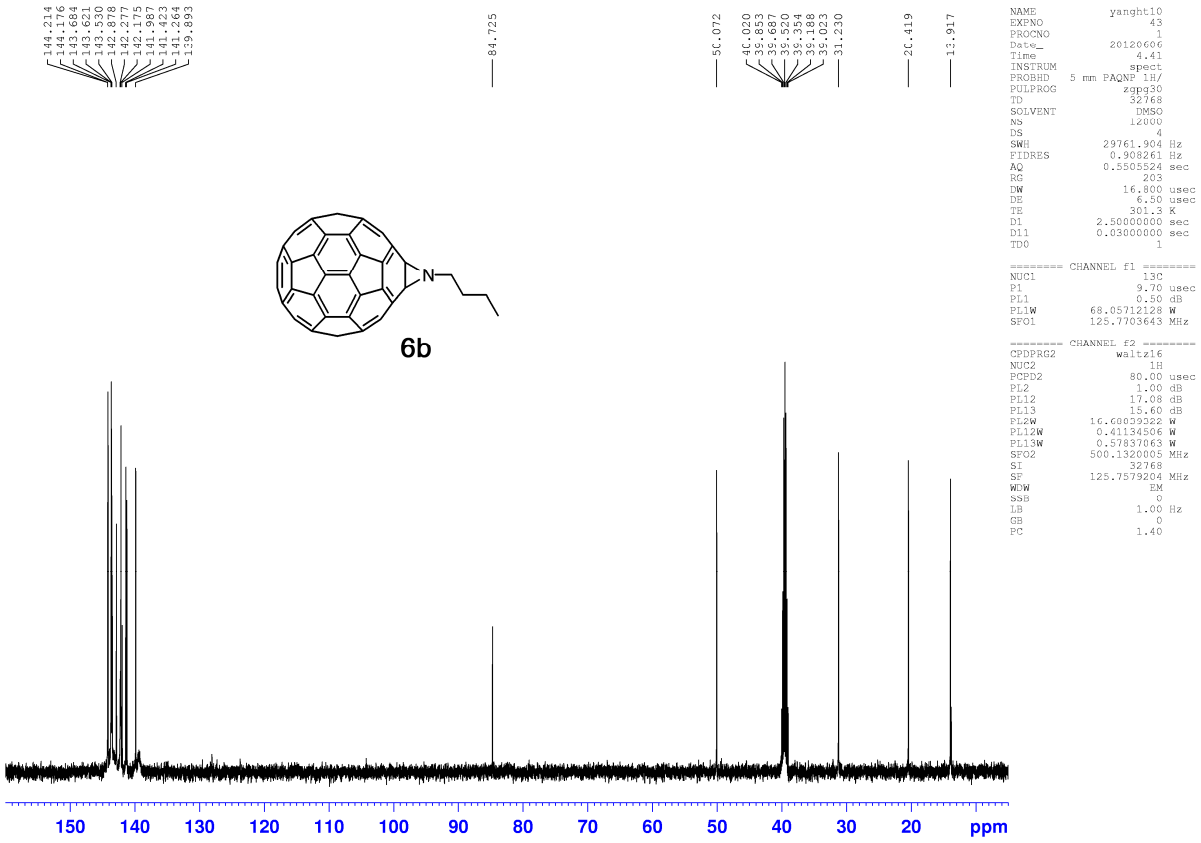

```
NAME            yanght10
EXPNO                28
PROCNO                1
Date_          20120516
Time               16.51
INSTRUM            spect
PROBHD   5 mm PAQNP 1H/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    0
SWH           10330.578 Hz
FIDRES        0.315264 Hz
AQ            1.5860212 sec
RG                  144
DW               48.400 usec
DE                6.50 usec
TE               298.3 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1                12.56 usec
PL1                1.00 dB
PL1W         16.68039322 W
SFO1        500.1330885 MHz
SI                32768
SF          500.1300189 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



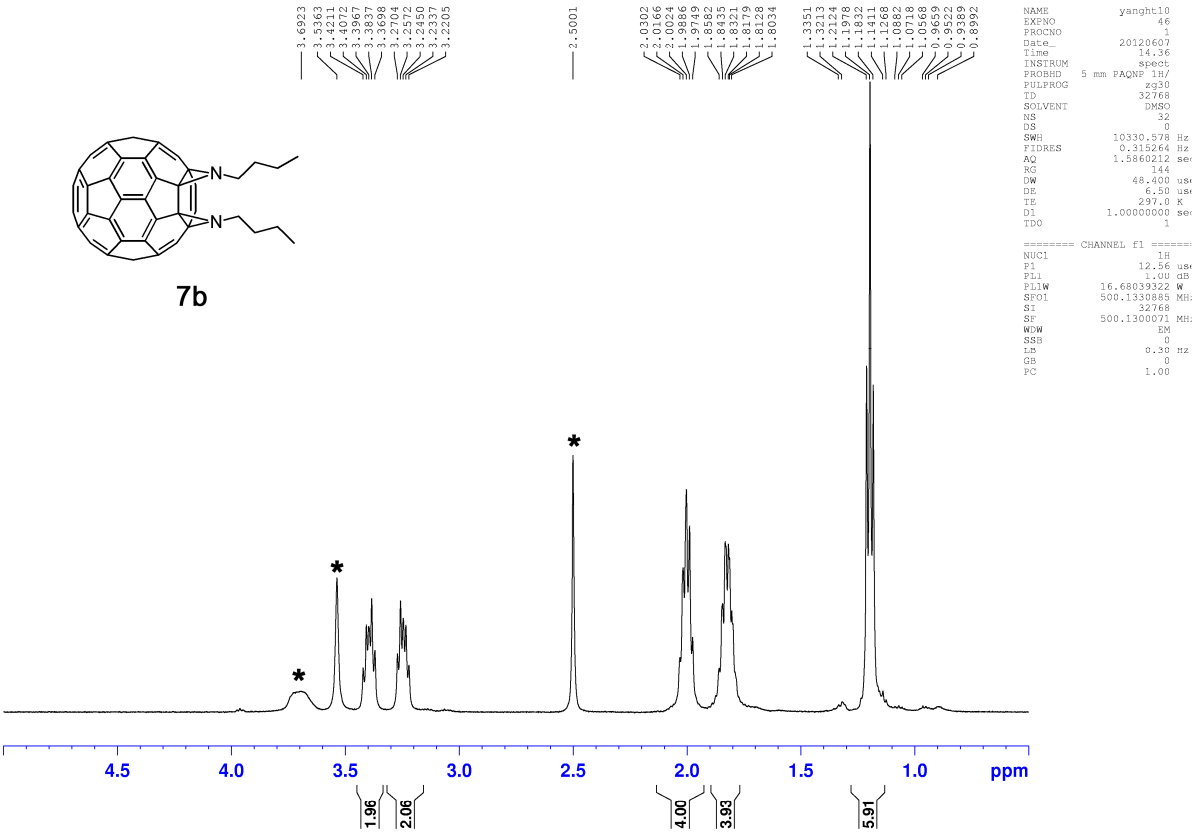

```
NAME            yanght10
EXPNO                30
PROCNO                1
Date_          20120525
Time               4.39
INSTRUM            spect
PROBHD   5 mm PAQNP 1H/
PULPROG          zgpg30
TD                32768
SOLVENT           DMSO
NS                12000
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE               302.4 K
D1            2.50000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.70 usec
PL1                0.50 dB
PL1W         68.05712128 W
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                1.00 dB
PL12              17.08 dB
PL13              15.60 dB
PL2W         16.68039322 W
PL12W         0.41134506 W
PL13W         0.57837063 W
SFO2        500.1320005 MHz
SI                32768
SF          125.7579189 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

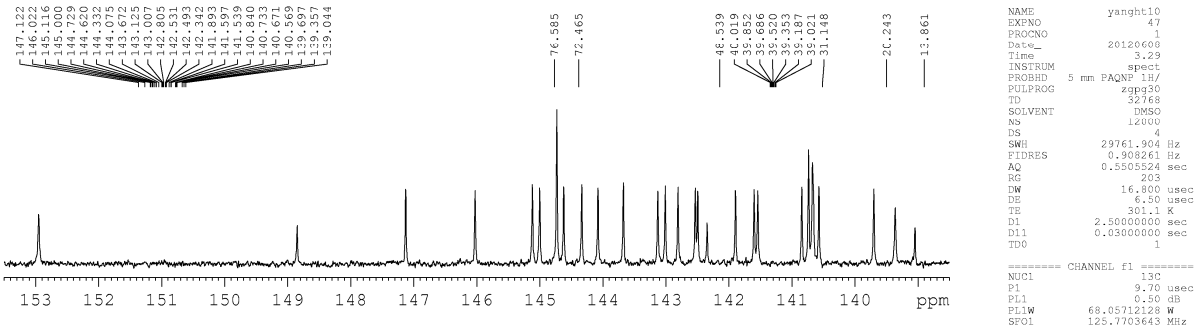


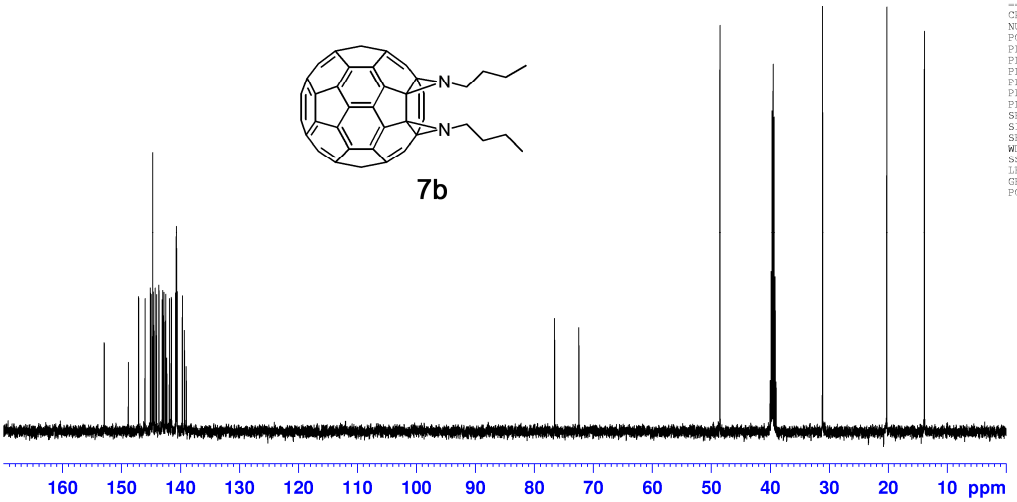

```
NAME            yanght10
EXPNO                 42
PROCNO                 1
Date_           20120605
Time                14.53
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     0
SWH           10330.578 Hz
FIDRES        0.315264 Hz
AQ            1.5860212 sec
RG                   144
DW               48.400 usec
DE                6.50 usec
TE               297.6 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                1H
P1              12.56 usec
PL1              1.00 dB
PL1W        16.68039322 W
SFO1        500.1330885 MHz
SI                 32768
SF          500.1300061 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

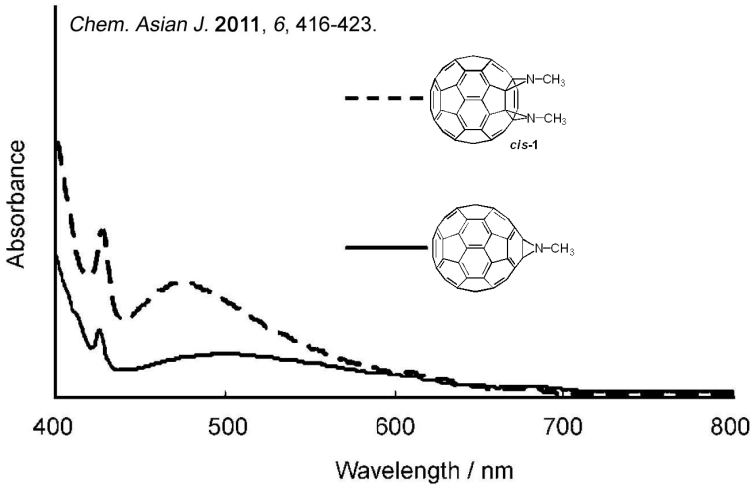


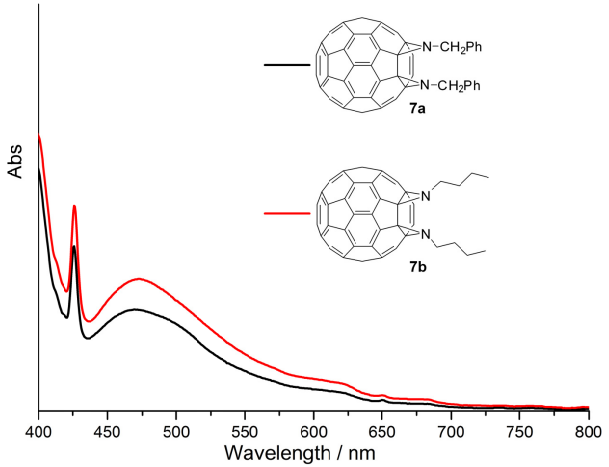

```
NAME            yanght10
EXPNO                 43
PROCNO                 1
Date_           20120606
Time                4.41
INSTRUM             spect
PROBHD   5 mm PAQNP 1H/
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                 12000
DS                     4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG                   203
DW               16.800 usec
DE                6.50 usec
TE               301.3 K
D1            2.50000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1               9.70 usec
PL1              0.50 dB
PL1W        68.05712128 W
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              1.00 dB
PL12            17.08 dB
PL13            15.60 dB
PL2W        16.68039222 W
PL12W        0.41134506 W
PL13W        0.57837063 W
SFO2        500.1320005 MHz
SI                 32768
SF          125.7579204 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

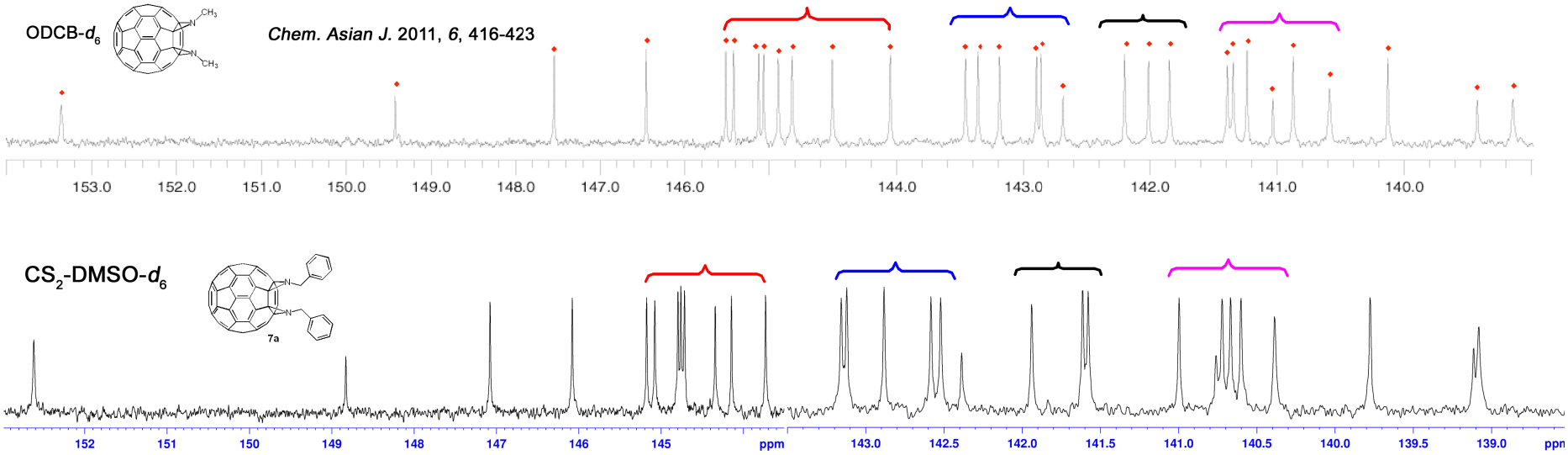

7b
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.96
2.06
4.00
3.93
5.91


153
152
151
150
149
148
147
146
145
144
143
142
141
140
ppm


7b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Chem. Asian J. 2011, 6, 416-423.
Absorbance
400
500
600
700
800
Wavelength / nm
N–CH3
N–CH3
cis-1
N–CH3

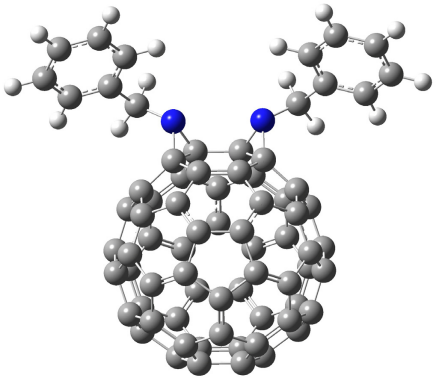

Abs
400
450
500
550
600
650
700
750
800
Wavelength / nm
N–CH2Ph
N–CH2Ph
7a
N
N
7b


ODCB-d6
Chem. Asian J. 2011, 6, 416-423
153.0
152.0
151.0
150.0
149.0
148.0
147.0
146.0
144.0
143.0
142.0
141.0
140.0
CS2-DMSO-d6
7a
152
151
150
149
148
147
146
145
ppm
143.0
142.5
142.0
141.5
141.0
140.5
140.0
139.5
139.0
ppm

Relative energies of the eight isomers of 7a at the level of B3LYP/6-31G*//AM1 (Energies are given in kcal/mol)

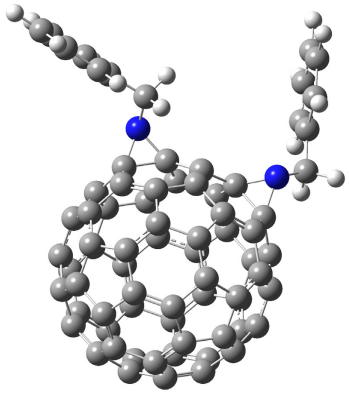
Species	Energies (kcal/mol)
cis-1	0.00
cis -2	7.80
cis -3	6.81
e	4.34
trans-1	5.16
trans-2	4.89
trans-3	4.59
trans-4	5.15

As seen from the Table, *cis*-1 isomer is the most stable product, which is more stable than the second stable *e*-isomer by lower 4.34 kcal/mol, thus explaining the preferred formation of *cis*-1 isomer.



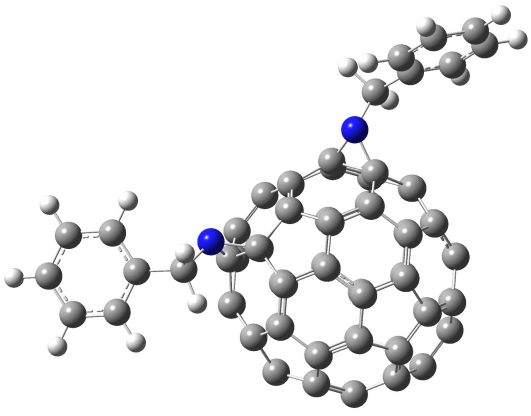
cis-1 isomer

Total energy = -2937.5286073 Hartrees



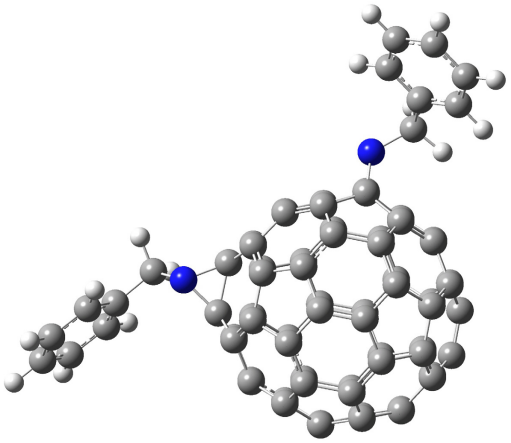
cis -2 isomer

Total energy = -2937.5161808 Hartrees



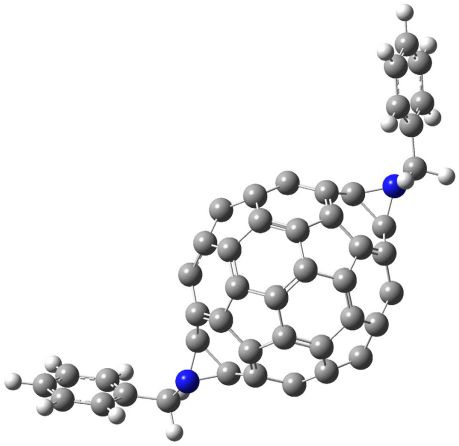
cis-3 isomer

Total energy = -2937.5177545 Hartrees



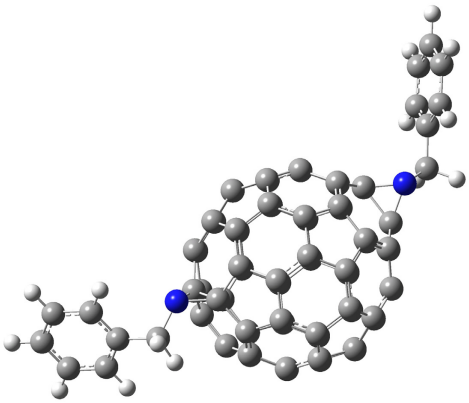
e- isomer

Total energy = -2937.5216861 Hartrees



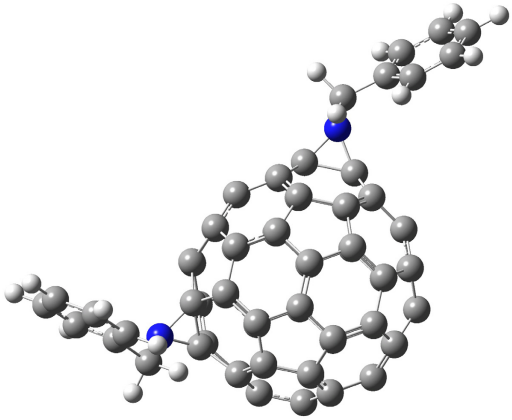
trans-1 isomer

Total energy = -2937.5203884 Hartrees



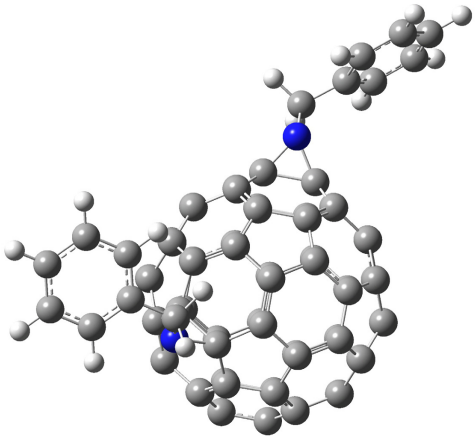
trans-2 isomer

Total energy = -2937.5208125 Hartrees



trans-3 isomer

Total energy = -2937.5212916 Hartrees



trans-4 isomer

Total energy = -2937.5203975 Hartrees