

Supporting Information

Synthesis of Fullerooxazoles: Novel Reactions of [60]Fullerene with Nitriles Promoted by Ferric Perchlorate

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¹ H NMR spectrum of compound 2a	S2
¹³ C NMR spectrum of compound 2a	S3
¹ H NMR spectrum of compound 2b	S4
¹³ C NMR spectrum of compound 2b	S5
¹ H NMR spectrum of compound 2c	S6
¹ H NMR spectrum of compound 2d	S7
¹³ C NMR spectrum of compound 2d	S8
¹ H NMR spectrum of compound 2e	S9
¹ H NMR spectrum of compound 2f	S10
¹³ C NMR spectrum of compound 2f	S11
¹ H NMR spectrum of compound 2g	S12
¹³ C NMR spectrum of compound 2g	S13
¹ H NMR spectrum of compound 2h	S14
¹³ C NMR spectrum of compound 2h	S15

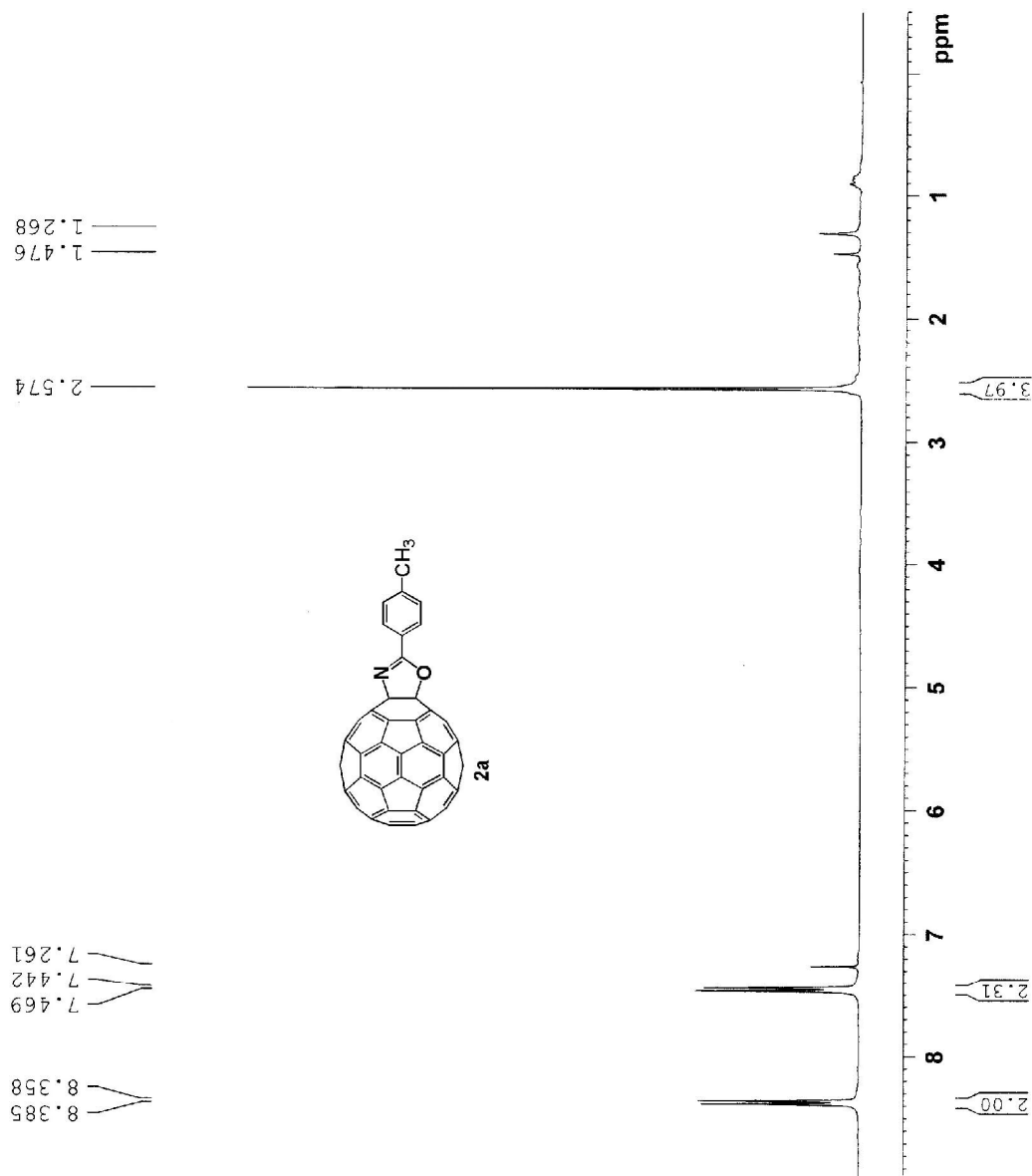
¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2a

Current Data Parameters
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 EXPNO 1
 PROCNO 1

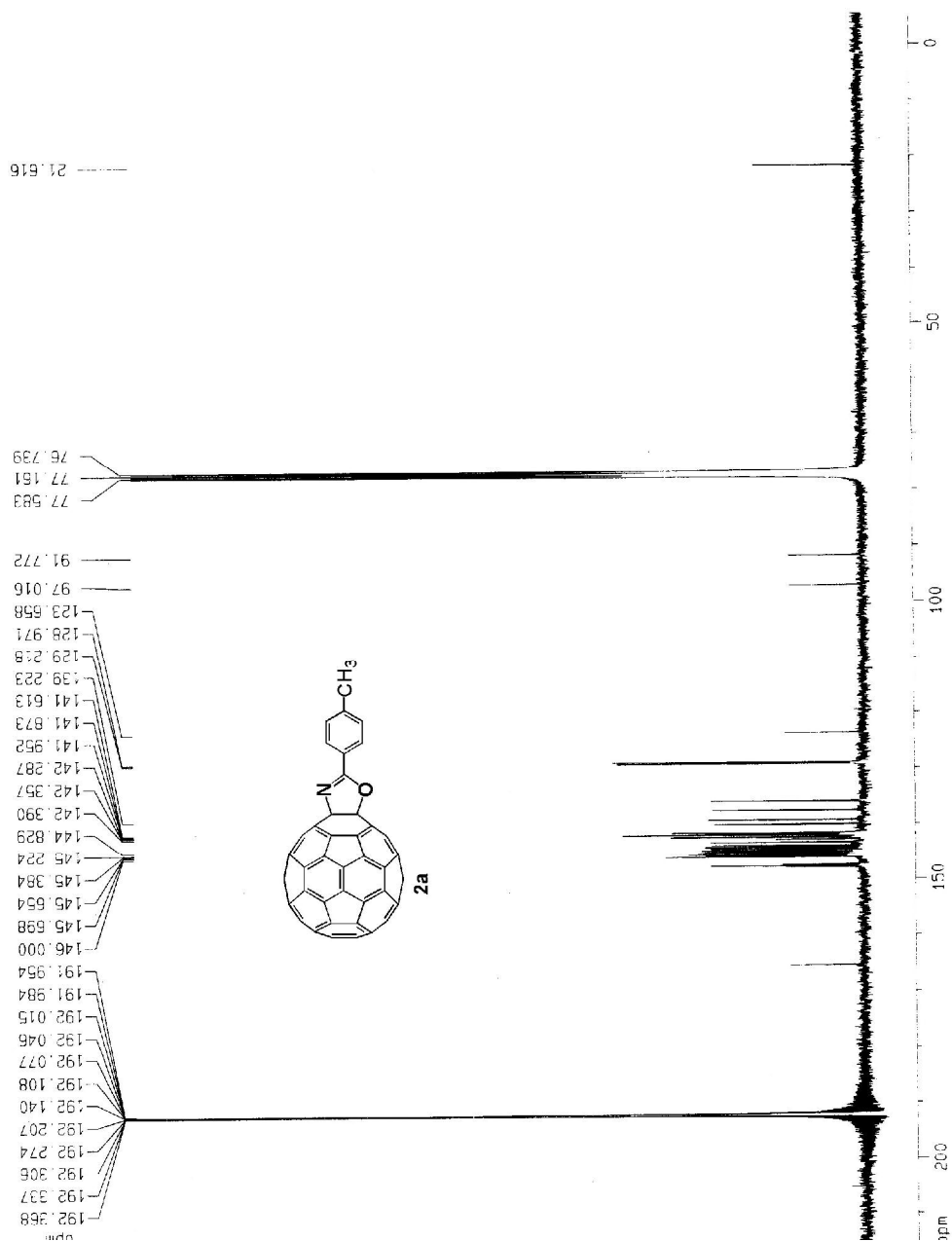
F2 - Acquisition Parameters
 Date_ 20071008
 Time 17.17
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl₃
 NS 32
 DS 1
 SWH 8992.806 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 55.600 usec
 DE 6.00 usec
 TE 300.0 K
 DI 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SFO1 300.1321009 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300060 MHz
 WDW ro
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2a



Current Data Parameters
NAME 17u07100801
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071009
Time 6.10
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT Acetone
NS 16432
DS 4
SWH 37878.789 Hz
FIDRES 1.455969 Hz
AQ 0.4325876 sec
RG 6502
DM 13.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCARRK 0.01500000 sec

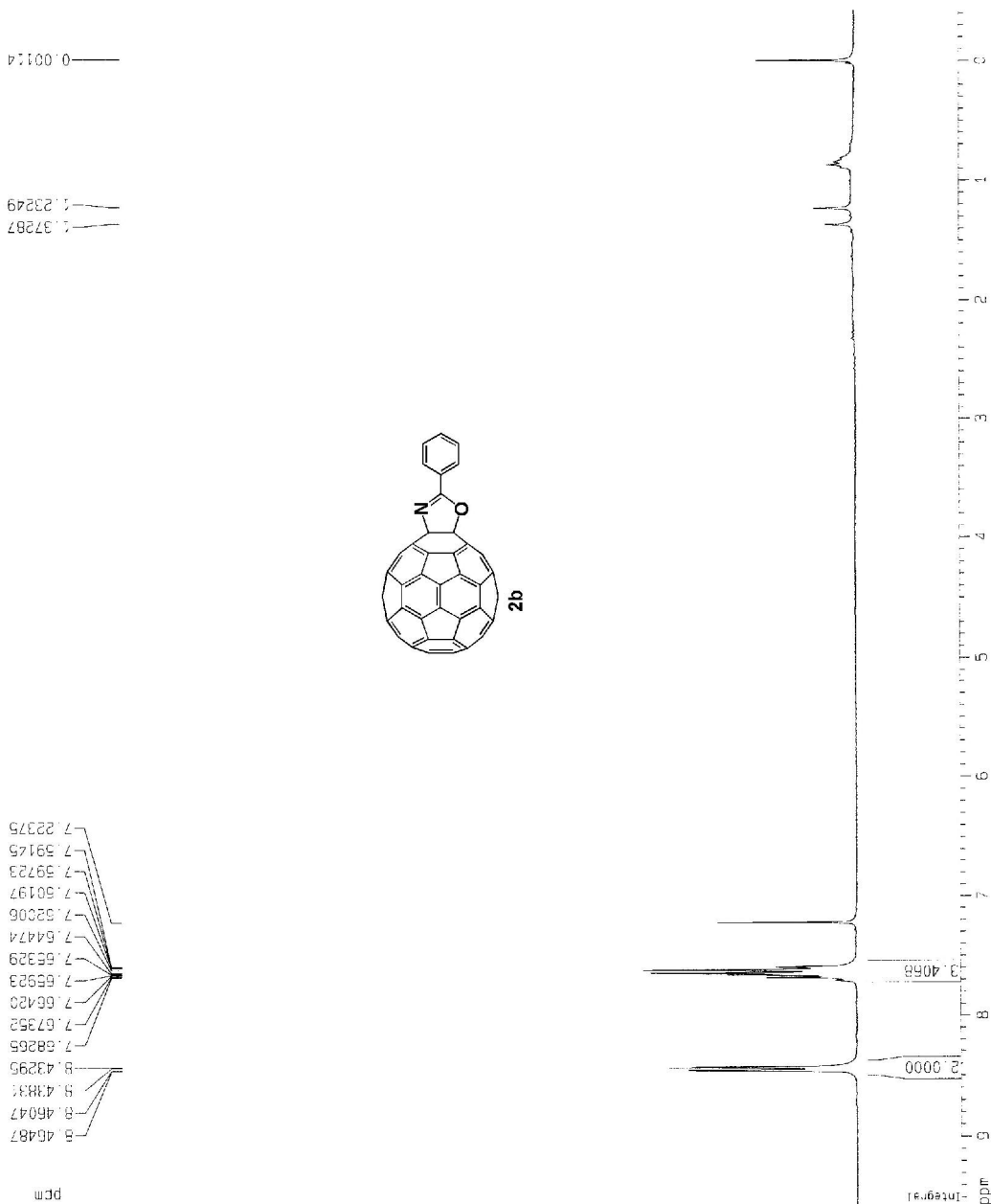
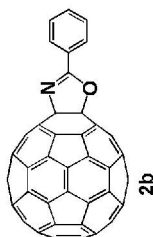
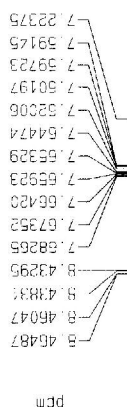
===== CHANNEL f1 =====
NUC1 13C
P1 3.00 usec
PL1 -1.00 dB
SF01 75.4758051 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SF02 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4577843 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 215.932 ppm
F1 16295.93 Hz
F2P -5.550 ppm
F2 -418.84 Hz
PPMCM 10.05/37 ppm/cm
HZCM 759.75208 Hz/cm

¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2b



Current Data Parameters
 NAME 1f06c1801
 EXNO 1
 PROCNO 1

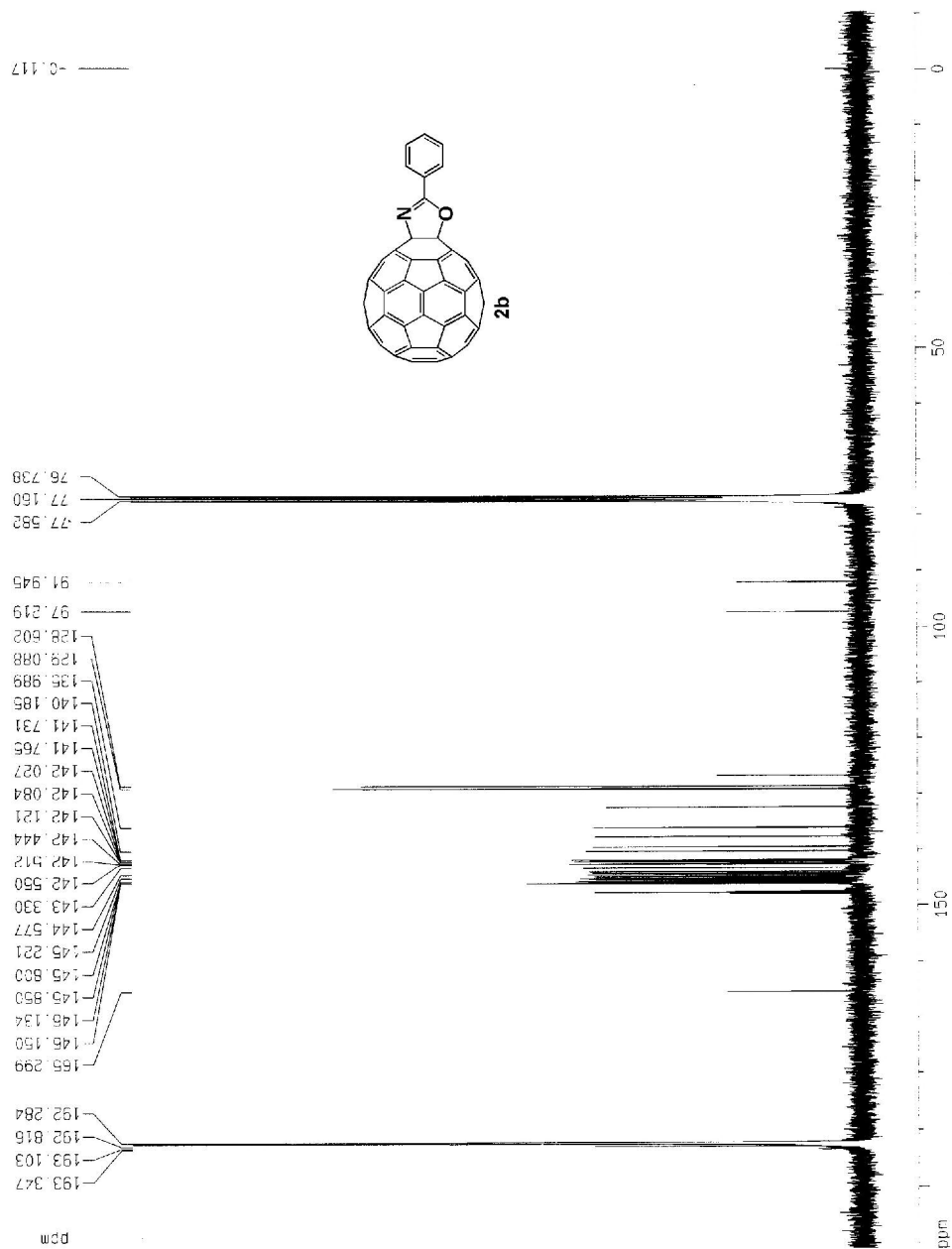
F2 - Acquisition Parameters
 Date_ 2006-018
 Time 16 52
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 65536
 SOLVENTI CDCl3
 NS 32
 DS 1
 SWH 8892.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 456.1
 CW 55.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 NUCREST 0.00000000 sec
 NUCNRC 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 3.00 dB
 SF01 300.1321009 MHz

F2 - Processing parameters
 SI 15384
 SF 300.1300174 MHz
 WDW to
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.20

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 9.571 ppm
 F1 2872.50 Hz
 F2P -0.426 ppm
 F2 -127.74 Hz
 PPMCM 0.45440 ppm/cm
 HZCM 136.37915 Hz/cm

¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2b



Current Data Parameters
NAME 1f061018C1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061019
Time 6.01
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15017
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451186 sec
RG 4597.6
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNMR 0.01500000 sec

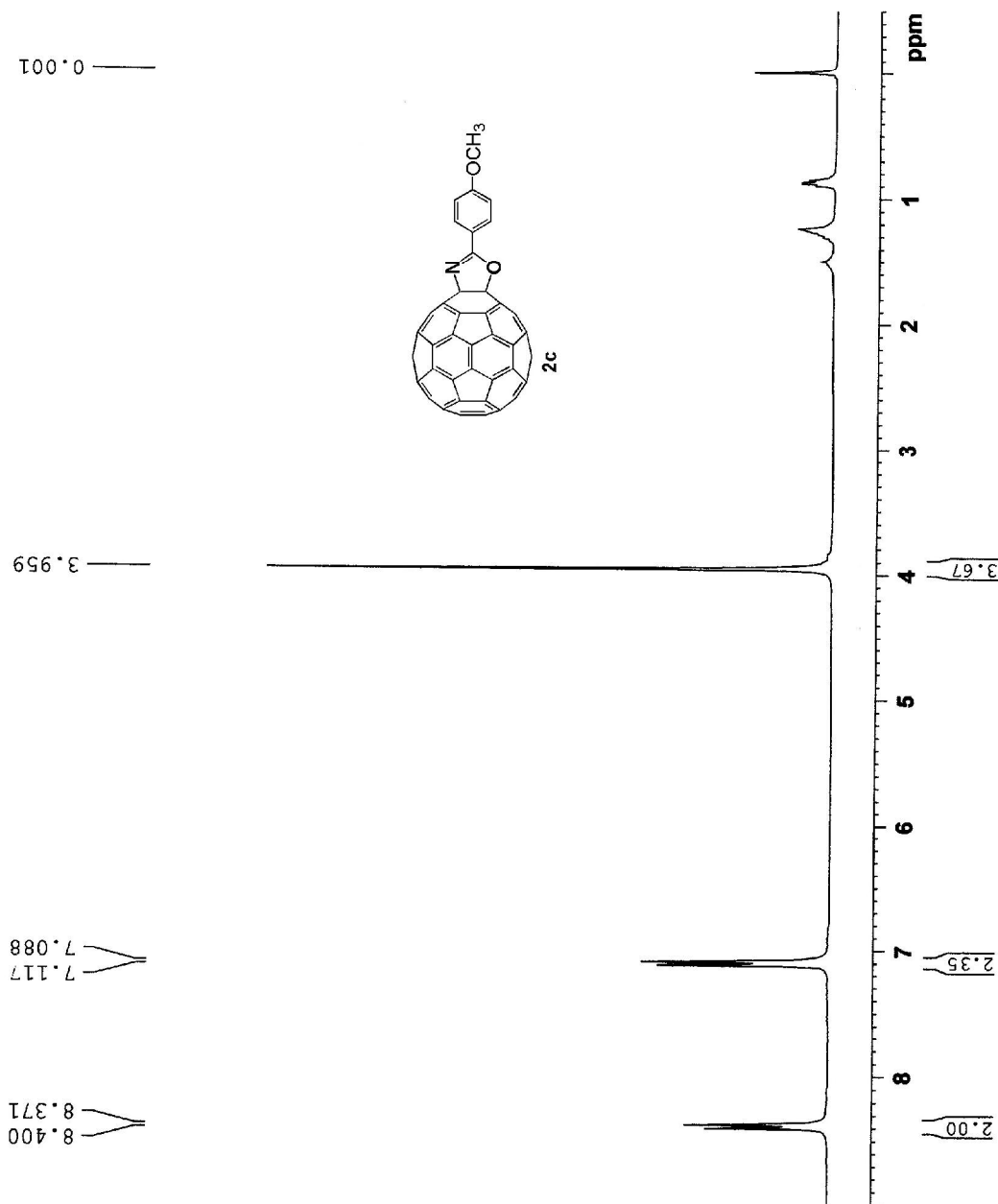
===== CHANNEL f1 =====
NUC1 13C
P1 3.00 usec
PL1 -4.00 dB
SF01 75.47756051 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SF02 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4677749 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40

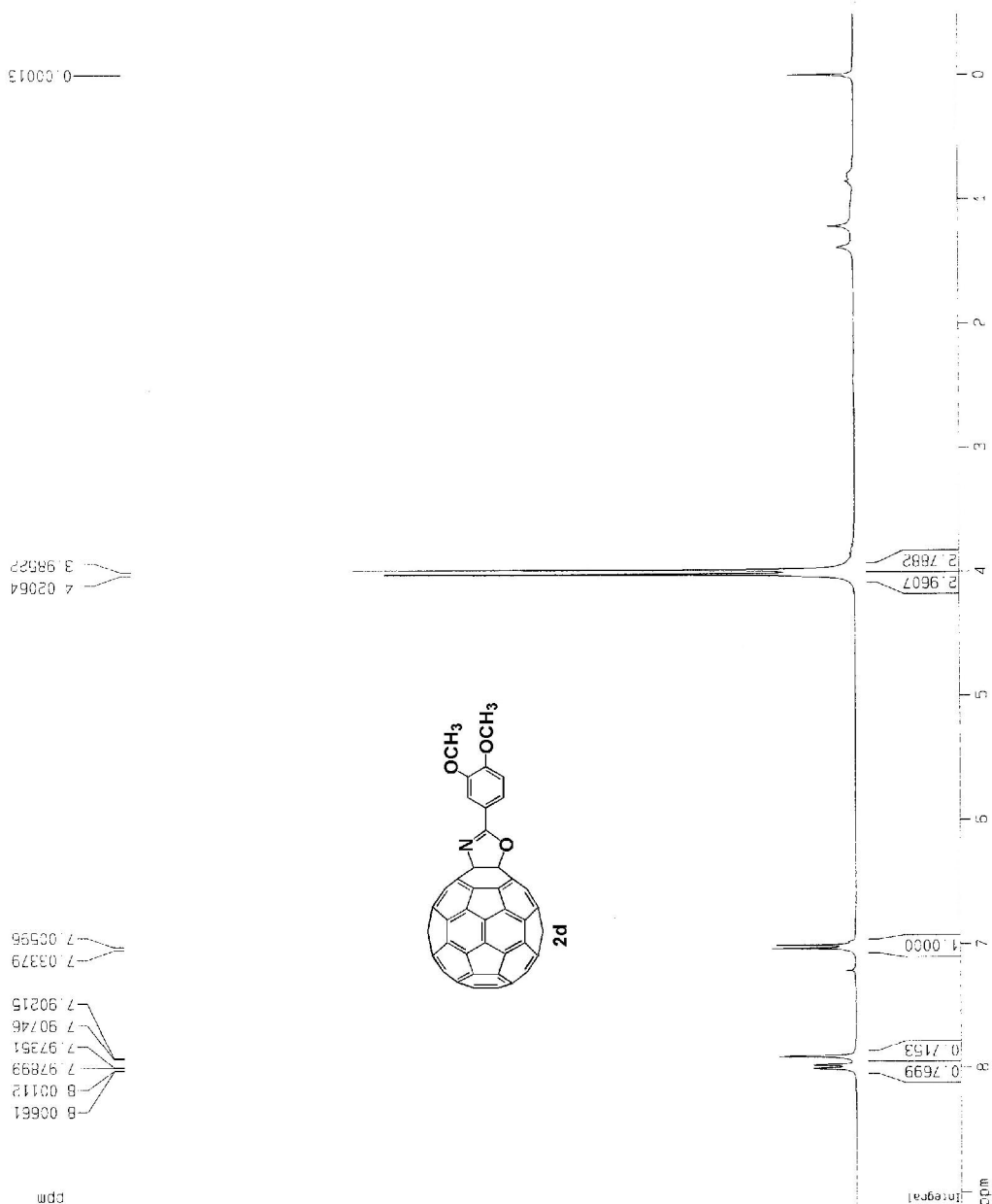
1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 211.175 ppm
F1 15937.19 Hz
F2P -10.349 ppm
F2 -781.05 Hz
PPHMM 10.56946 ppm/cm
HZCM 759.91966 Hz/cm

¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2c



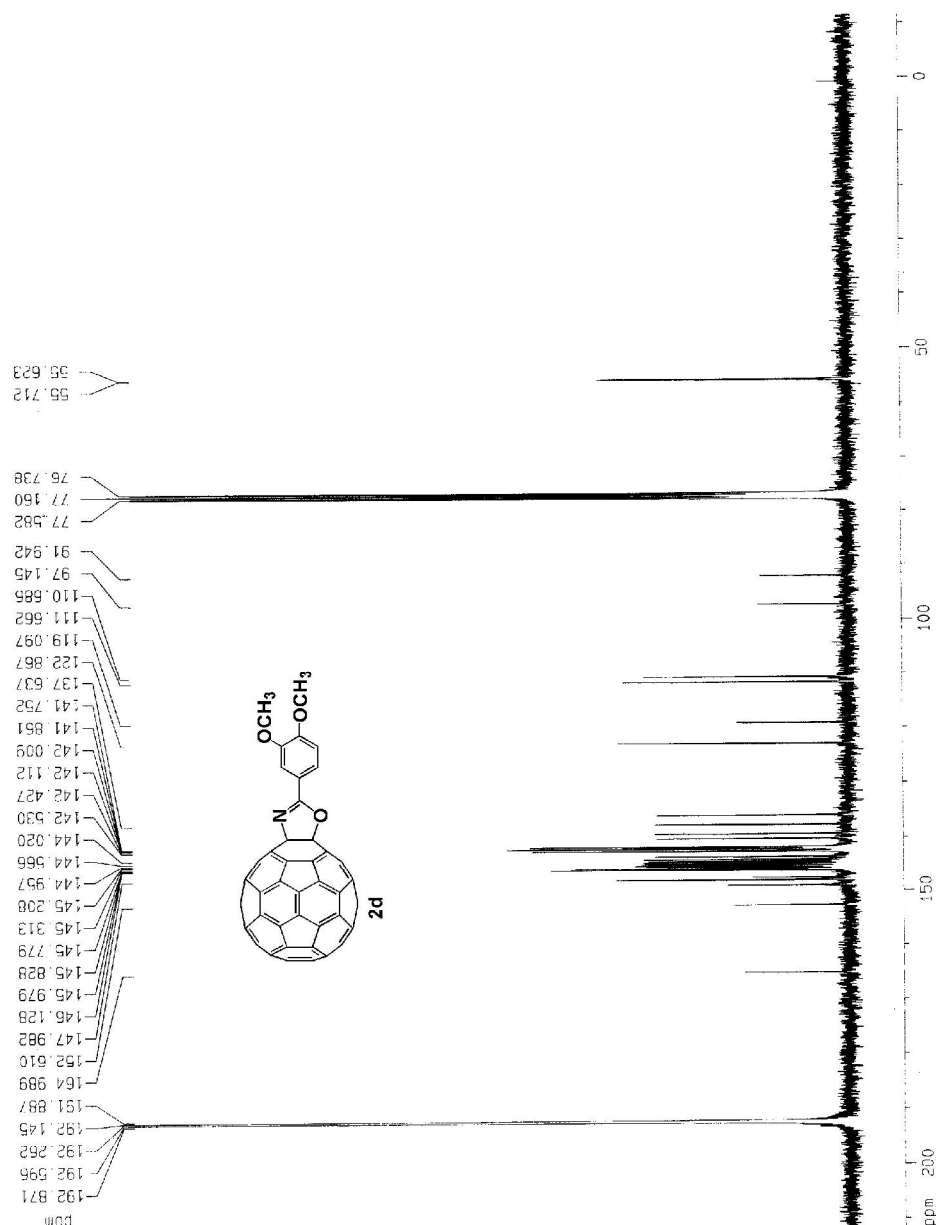
Current Data Parameters
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 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20080328
 Time 17.00
 INSTRUM av300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 1
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7339011 sec
 RG 287.4
 DW 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 DL 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec
 CHANNEL f1
 NUC1 1H
 P1 7.50 usec
 PL1 -3.00 dB
 SFO1 300.1321009 MHz
 F2 - Processing parameters
 SI 16384
 SF 300.1300161 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2d



Current Data Parameters
NAME _f00710100_
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071010
Time 17.02
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 1
SWH 6992.306 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 287.4
CW 55.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SF01 300.1321039 MHz
F2 - Processing parameters
SI 16384
SF 300.1300223 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
EC 1.00
ID NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1 9.113 ppm
F2 2735.22 Hz
F2P -0.494 ppm
F2 -148.19 Hz
PPMCM 0.43669 ppm/cm
HZCM 131.06400 Hz/cm

¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2d



Current Data Parameters
NAME 1f607101002
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071011
Time 7.45
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 13432
DS 4
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 9195.2
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
VCREST 0.00000000 sec
XCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 3.00 usec
PL1 -1.00 dB
SF01 75.4768051 MHz

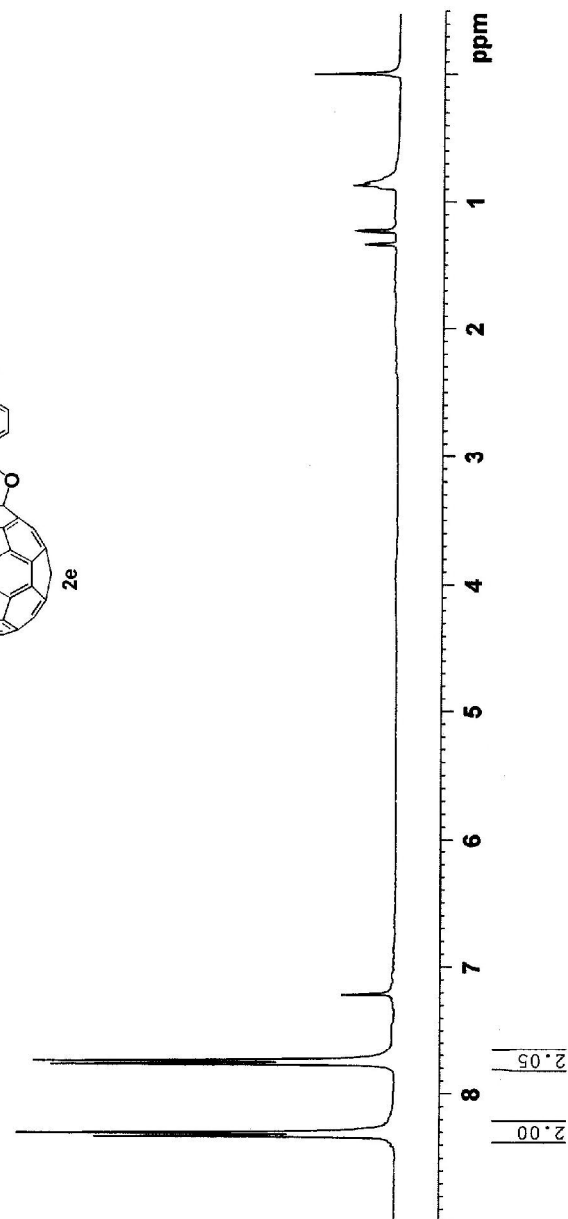
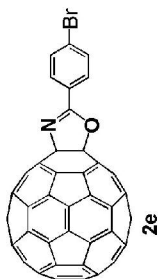
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SF02 300.1315007 MHz

F2 - Processing parameters
SI 131072
SF 75.4677253 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
FIP 211.700 ppm
F1 15976.55 Hz
F2 -11.505 ppm
F2 -888.26 Hz
FPMCM 10.14571 ppm/cm
GZCM 765.67419 Hz/cm

¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2e

8.333
8.305
7.772
7.744

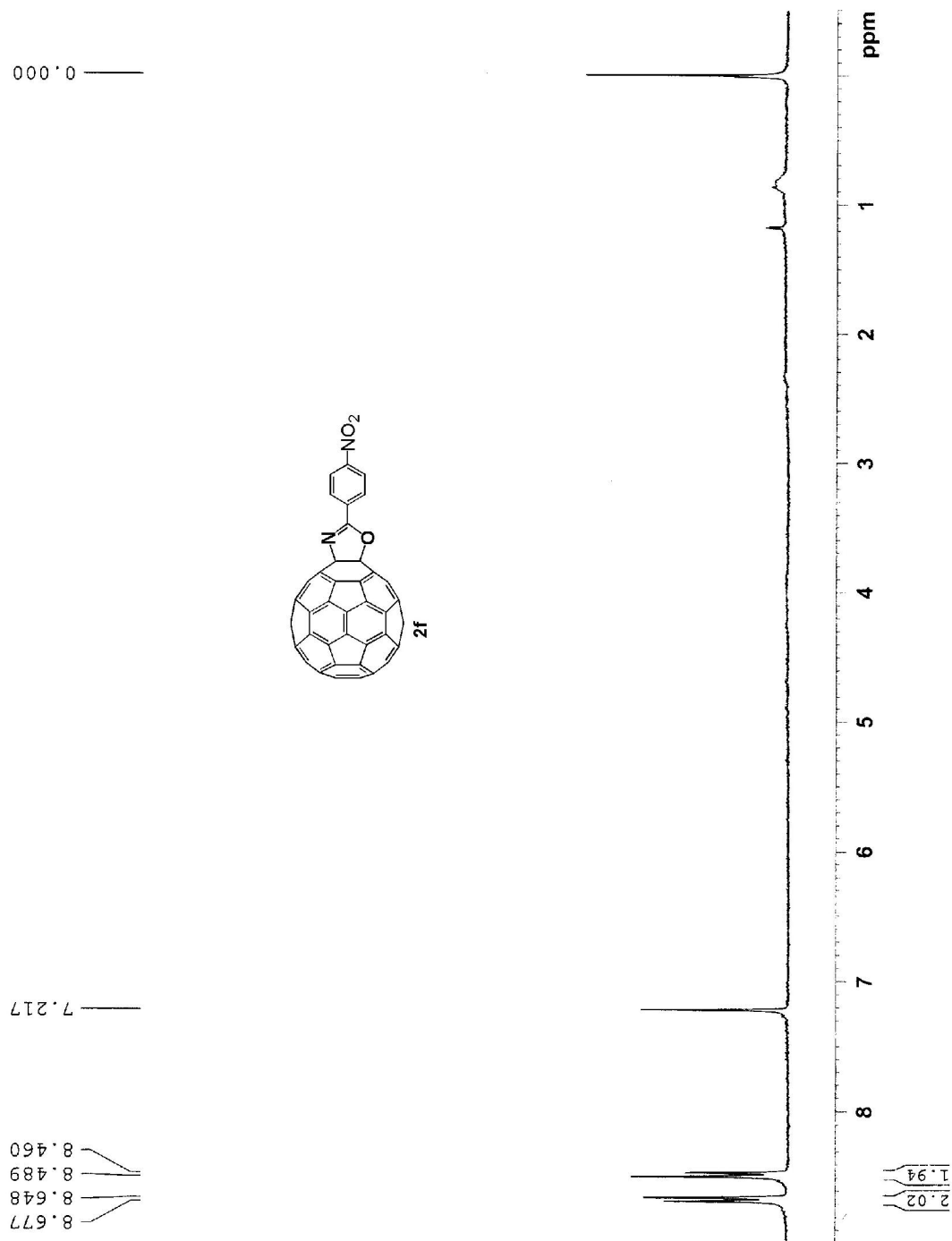


Current Data Parameters
NAME lfb08032801
EXPNO 1
PROCNO 1

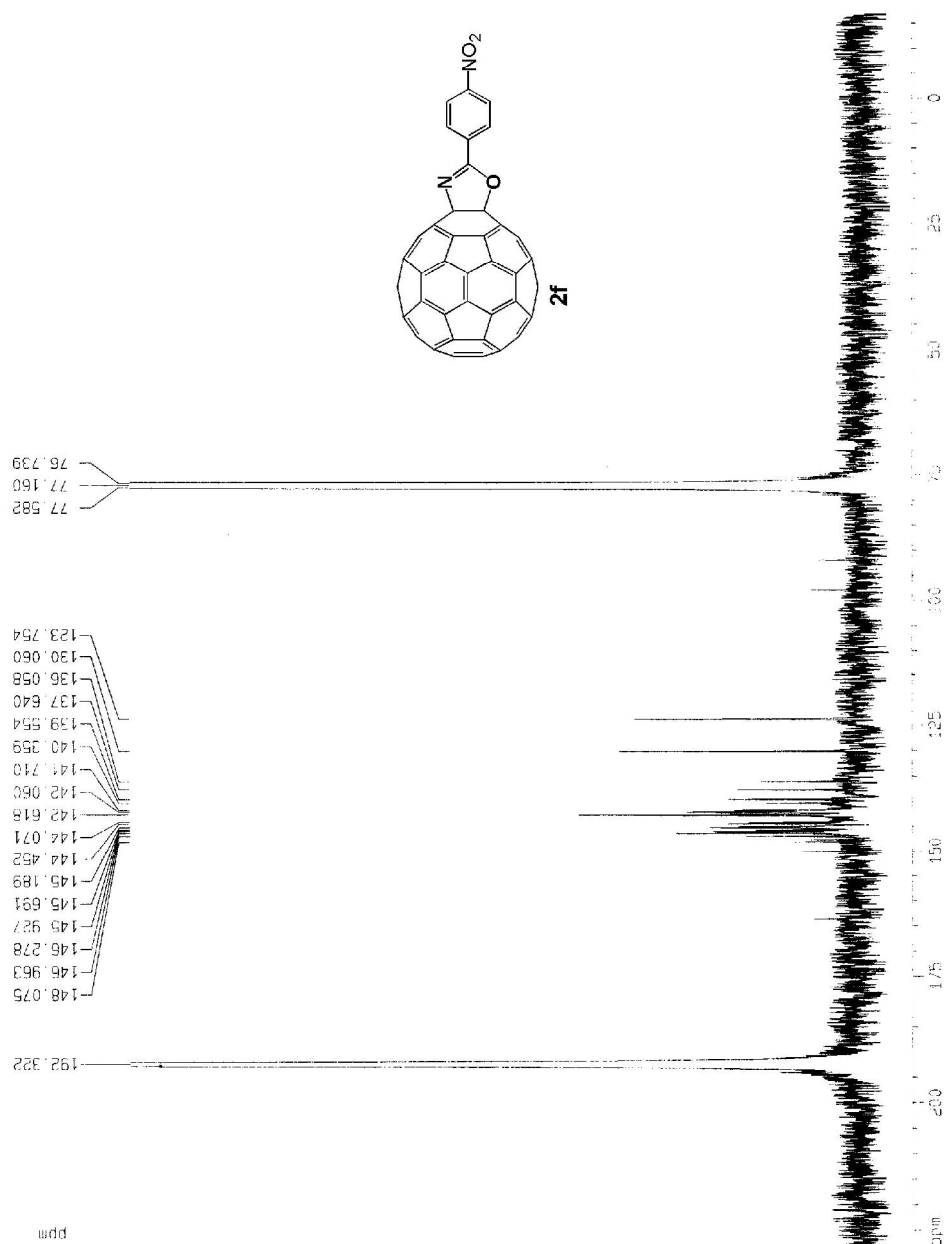
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Date_ 20080328
Time_ 17.05
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PROBHD av300
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 1
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 406.4
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
NCNCRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 -3.00 dB
SFO1 300.1321009 MHz

F2 - Processing parameters
SI 16384
SF 300.1300190 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00



¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2f



Current Data Parameters
NAME 1f607112901
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071128
Time 7.56
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 21163
DS 4
SWH 37878.799 Hz
FIDRES 1.155968 Hz
AQ 0.4325876 sec
RG 912.3
DK 13.200 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
wDRES1 0.00000000 sec
wDWRK 0.01500000 sec

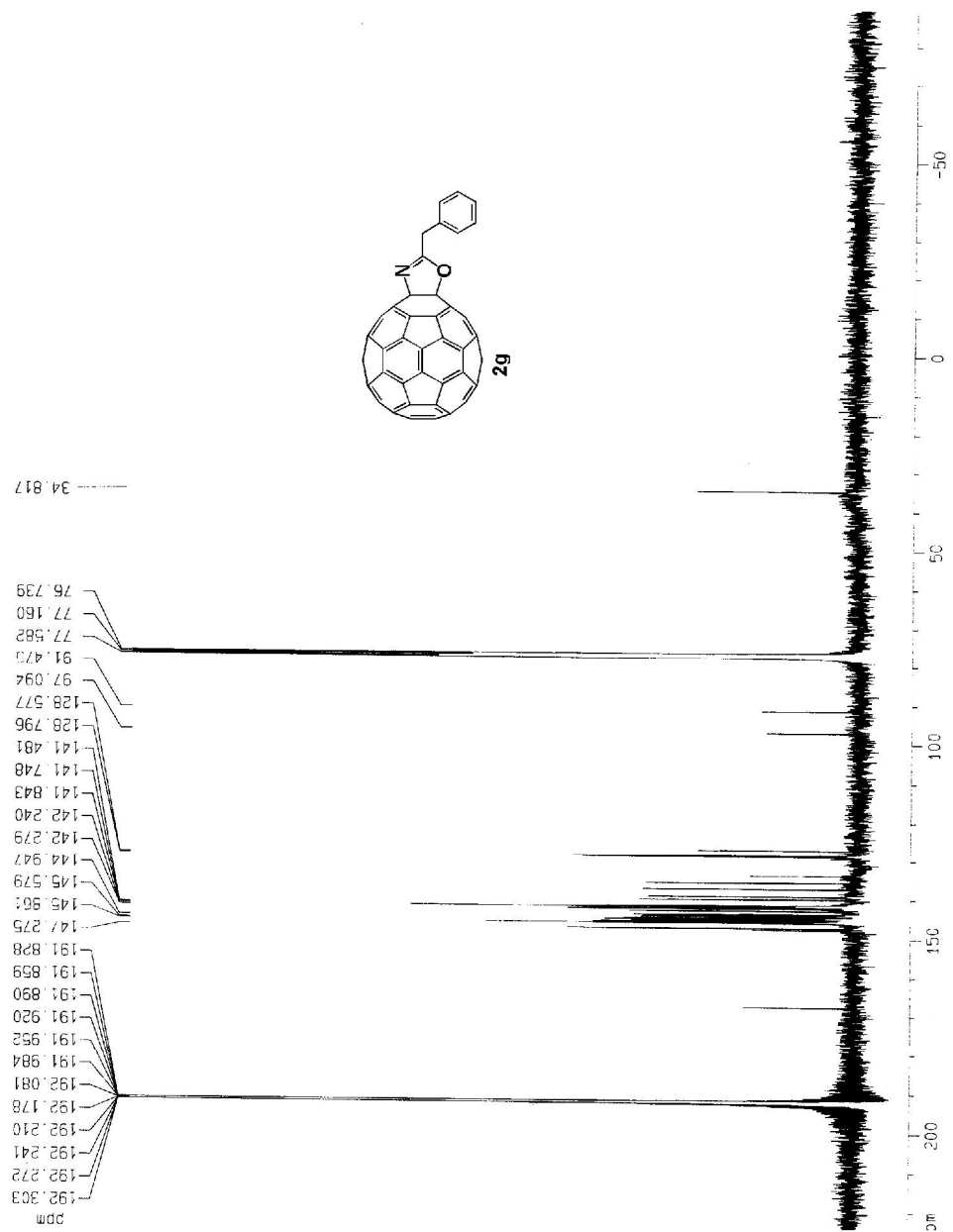
===== CHANNEL f1 =====
NUC1 ¹³C
P1 3.00 usec
PL1 -1.00 dB
SF01 75.4756051 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.00 dB
SF02 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 75.4677710 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
ZIP 228.068 mm
F1 17211.77 Hz
F2 -15.850 ppm
F2 -1271.62 Hz
SFOCM 11.13262 ppm/cm
AQCM 840.15411 Hz/cm

¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2g



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Current Data Parameters
NAME      1f007101501
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20071015
Time      7.12
INSTRUM   av300
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         20480
DS         4
SWH        37878.789 Hz
FIDRES     1.155969 Hz
AQ          0.4325676 sec
RG          728H-2
DM          13.200 usec
DE          5.00 usec
TE          300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
MCREST     0.00000000 sec
MCWRRK     0.01500000 sec

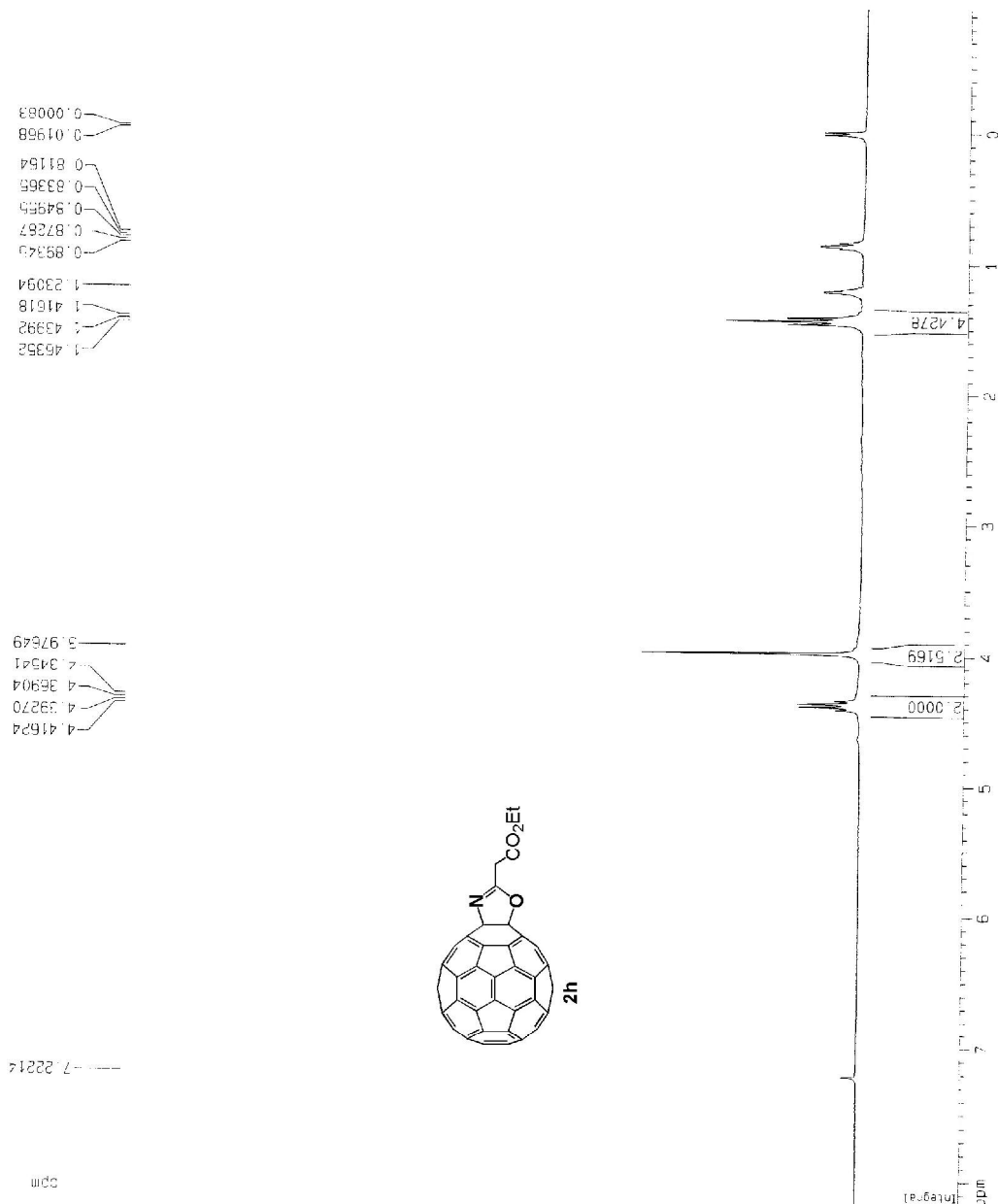
===== CHANNEL f1 =====
NUC1        13C
P1           3.00 usec
PL1         -1.00 dB
SFO1        75.4768051 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2        80.00 usec
PL2          -3.00 dB
PL12         16.00 dB
SFO2        300.1315007 MHz

F2 - Processing parameters
SI          131072
SF          75.4677942 MHz
RG          EM
WDW          0
SSB          0
LB           2.00 Hz
GB           0
PC           1.40

1D NMR plot parameters
CX          22.00 cm
CY           0.00 cm
F1P         226.956 ppm
F1          17127.85 Hz
F2P         -89.333 ppm
F2          -6741.80 Hz
SFOCM       14.37678 ppm/cm
F2CM        1084.98401 Hz/cm
    
```

¹H NMR (300 MHz, CS₂/CDCl₃) of compound 2h



Current Data Parameters
 NAME: 1f07101701
 EXPNO: 1
 PROCNO: 1

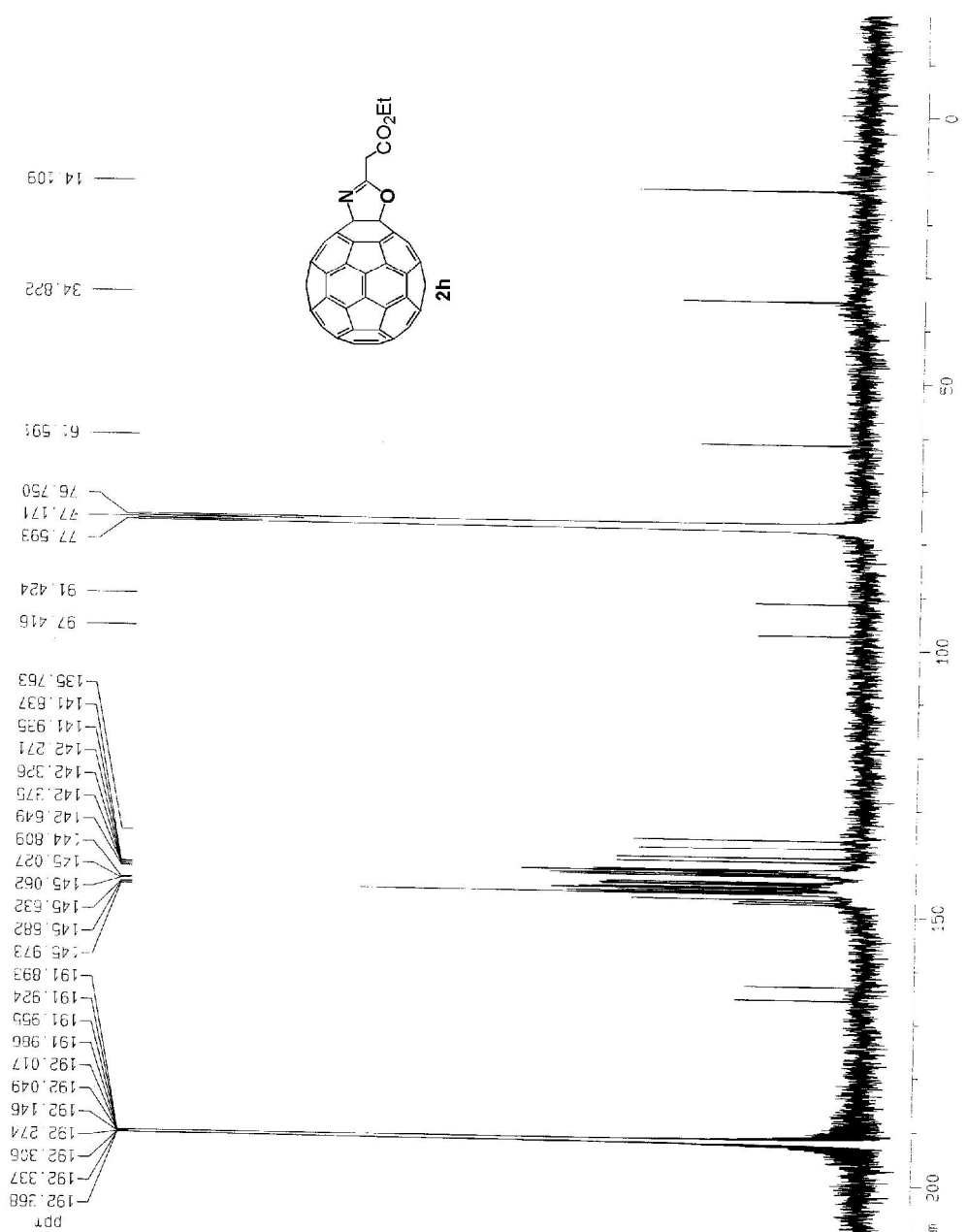
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 Date_: 20071017
 Time: 16.54
 INSTRUM: av300
 PROBHD: 5 mm BBO BB-1H
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 24
 DS: 4
 SWH: 8937.805 Hz
 FIDRES: 0.274439 Hz
 AQ: 0.1819568 sec
 RG: 322.5
 DW: 55.600 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 2.00000000 sec
 MCREST: 0.00000000 sec
 MCPR: 0.01500000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: -2.00 dB
 SFO: 300.1321009 MHz

F2 - Processing parameters
 SI: 16394
 SF: 300.1300175 MHz
 WDW: n0
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 0.00 cm
 F1p: 8.177 ppm
 F1: 2454.12 Hz
 F2p: -0.955 ppm
 F2: -286.54 Hz
 PHC: 0.41507 ppm/cm
 HZCM: 124.57567 Hz/cm

¹³C NMR (75 MHz, CS₂/CDCl₃) of compound 2h



Current Data Parameters
 NAME : /7607101701
 EXPNO : 4
 PROCNO : 1

F2 - Acquisition Parameters
 Date_ : 20071018
 Time : 7.28
 INSTRUM : av300
 PROBHD : 5 mm BBO BB-1H
 PULPROG : zgpg30
 TD : 32768
 SOLVENT : CDCl₃
 NS : 2048
 DS : 4
 SWH : 37878.769 Hz
 FIDRES : 1.155969 Hz
 AQ : 0.4325676 sec
 RG : 2048
 DW : 13.220 usec
 DE : 6.00 usec
 TE : 300.0 K
 D1 : 2.00000000 sec
 d11 : 0.03000000 sec
 MCHES : 0.00000000 sec
 MCWAK : 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 : ¹³C
 P1 : 3.00 usec
 PL1 : -1.00 dB
 SF01 : 75.4756051 MHz

===== CHANNEL f2 =====
 CPDPRG2 : waltz16
 NUC2 : ¹H
 PCPD2 : 80.00 usec
 PL2 : -3.00 dB
 PL12 : 15.00 dB
 SF02 : 300.1315007 MHz

F2 - Processing parameters
 SI : 131072
 SF : 75.4677975 MHz
 WDW : EM
 SSB : 0
 LB : 2.00 Hz
 GB : 0
 PC : 1.40

1D NMR plot parameters
 CX : 22.00 cm
 CY : 0.00 cm
 FIP : 211.907 ppm
 F1 : 15992.12 Hz
 F2P : -19.136 ppm
 F2 : -1444.15 Hz
 PP4CM : 10.50193 ppm/cm
 ZCM : 792.55762 Hz/cm