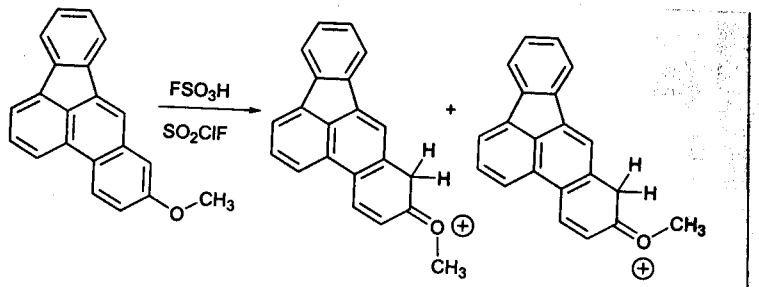
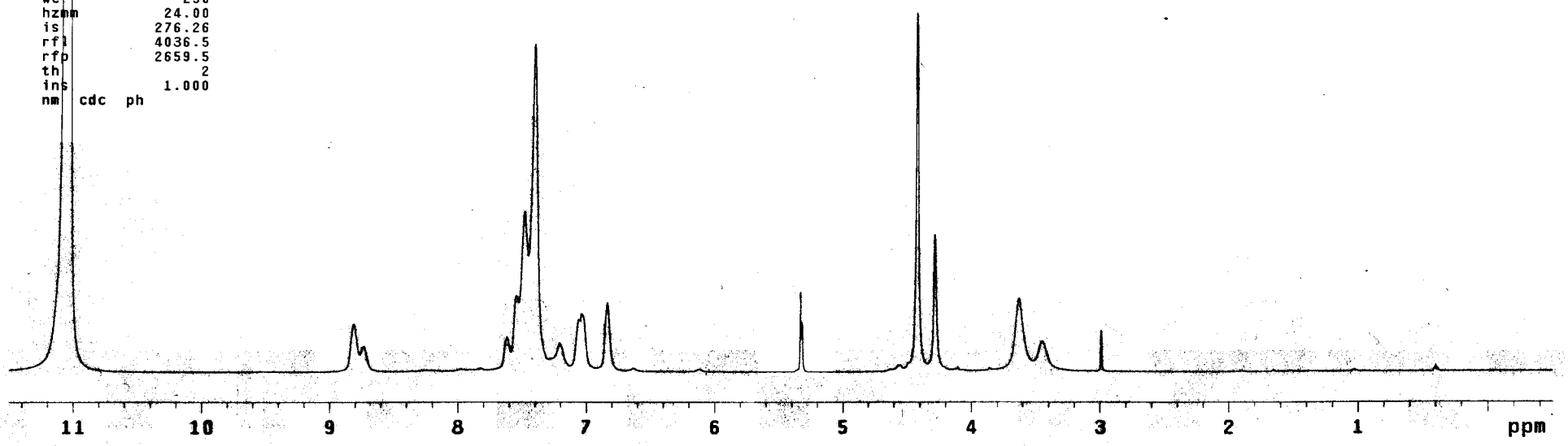
```
5mmsw,H lineshape
spin,7-8-98

exp9  s2pul

      SAMPLE                DEC. & VT
date   May 11 2000   dfrq        499.910
solvent     CD2CL2   dn               H1
file /export/home/~  dpwr             30
laali/okazaki05/to~  dof          1198.4
00051107-H70-CD2Cl~  dm                n
          2-5.fid    dmm               c
   ACQUISITION       dmf             200
sfrq       499.910   dseq
tn              H1   dres           1.0
at           1.384   homo             n
np           32000   temp         -70.0
sw         11562.4                DEC2
fb            6000   dfrq2            0
bs               4   dn2
tpwr            55   dpwr2            1
pw            12.0   dof2             0
d1           1.000   dm2              n
tof         1918.9   dmm2             c
nt              16   dmf2           200
ct              16   dseq2
alock            n   dres2          1.0
gain      not used   homo2            n
     FLAGS                 PROCESSING
il               n   wtfile
in               n   proc             ft
dp               y   fn           65536
hs              nn   math             f
    DISPLAY
sp          -250.3   werr
wp          5998.7   wexp
vs             277   wbs
sc               0   wnt            wft
wc             250
hzmm         24.00
is          276.26
rfl         4036.5
rfp         2659.5
th               2
ins          1.000
nm   cdc  ph
```



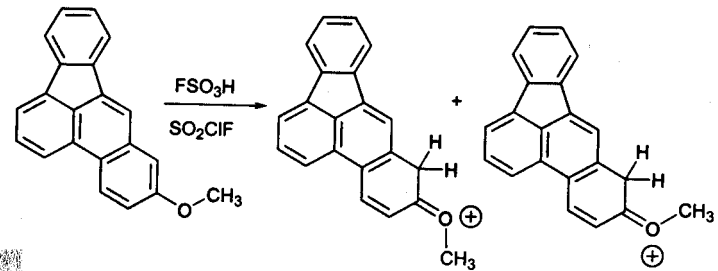

$^1$H NMR at -70°C



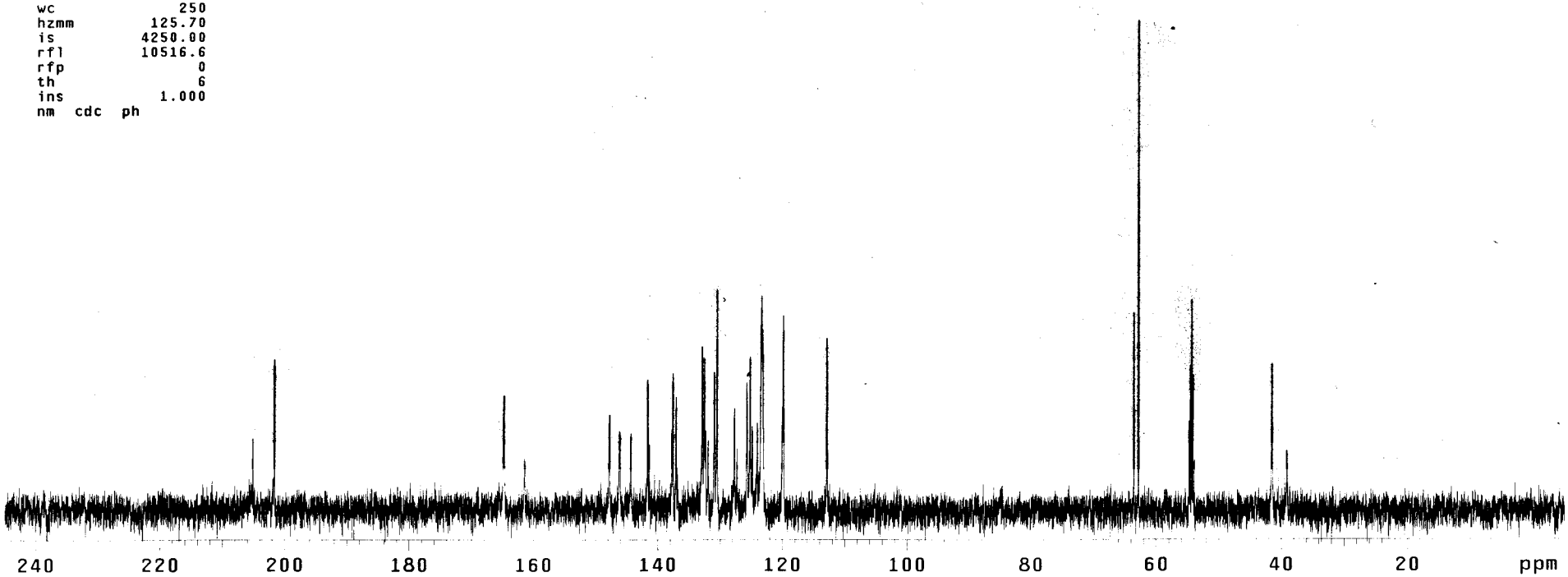
STANDARD CARBON PARAMETERS

exp8 s2pul

| SAMPLE | | DEC. & VT | |
|---|---|---|---|
| date | May 11 2000 | dfrq | 499.908 |
| solvent | CD2CL2 | dn | H1 |
| file | /export/home/~ | dpwr | 35 |
| laali/okazaki05/to~ | | dof | 0 |
| 00051107-C70-CD2Cl~ | | dm | nyy |
| | 2-5.fid | dmm | w |
| ACQUISITION | | dmf | 10800 |
| sfrq | 125.716 | dseq | |
| tn | C13 | dres | 1.0 |
| at | 0.640 | homo | n |
| np | 64000 | temp | -70.0 |
| sw | 50000.0 | DEC2 | |
| fb | not used | dfrq2 | 0 |
| bs | 4 | dn2 | |
| tpwr | 52 | dpwr2 | 1 |
| pw | 16.0 | dof2 | 0 |
| d1 | 0.500 | dm2 | n |
| d2 | 0.500 | dmm2 | c |
| tof | 2423.4 | dmf2 | 10000 |
| nt | 10000 | dseq2 | |
| ct | 288 | dres2 | 1.0 |
| alock | n | homo2 | n |
| gain | 60 | PROCESSING | |
| FLAGS | | lb | 2.00 |
| il | n | wtfile | |
| in | n | proc | ft |
| dp | y | fn | 131072 |
| hs | nn | math | f |
| DISPLAY | | | |
| sp | -628.8 | werr | |
| wp | 31425.2 | wexp | |
| vs | 78 | wbs | |
| sc | 0 | wnt | |
| wc | 250 | | |
| hzmm | 125.70 | | |
| is | 4250.00 | | |
| rfl | 10516.6 | | |
| rfp | 0 | | |
| th | 6 | | |
| ins | 1.000 | | |
| nm cdc ph | | | |



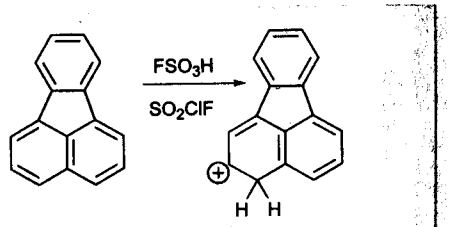

$^{13}$C NMR at -70°C



5mmsw,H lineshape
spin,7-8-98

exp9 s2pul

| SAMPLE | | DEC. & VT | |
|---|---|---|---|
| date | May 17 2000 | dfrq | 499.910 |
| solvent | CD2CL2 | dn | H1 |
| file | /export/home/~ | dpwr | 30 |
| | laali/okazaki05/to~ | dof | 1198.4 |
| | 00051702-H50-CD2CL~ | dm | n |
| | 2-5.fid | dmm | c |
| ACQUISITION | | dmf | 200 |
| sfrq | 499.910 | dseq | |
| tn | H1 | dres | 1.0 |
| at | 1.384 | homo | n |
| np | 32000 | temp | -50.0 |
| sw | 11562.4 | DEC2 | |
| fb | 6000 | dfrq2 | 0 |
| bs | 4 | dn2 | |
| tpwr | 55 | dpwr2 | 1 |
| pw | 12.0 | dof2 | 0 |
| d1 | 1.000 | dm2 | n |
| tof | 1918.9 | dmm2 | c |
| nt | 16 | dmf2 | 200 |
| ct | 16 | dseq2 | |
| alock | n | dres2 | 1.0 |
| gain | not used | homo2 | n |
| FLAGS | | PROCESSING | |
| il | n | wtfile | |
| in | n | proc | ft |
| dp | y | fn | 65536 |
| hs | nn | math | f |
| DISPLAY | | | |
| sp | -250.1 | werr | |
| wp | 6998.4 | wexp | |
| vs | 1747 | wbs | |
| sc | 0 | wnt | wft |
| wc | 250 | | |
| hzmm | 27.99 | | |
| is | 276.26 | | |
| rfl | 1379.6 | | |
| rfp | 0 | | |
| th | 2 | | |
| ins | 1.000 | | |
| nm cdc ph | | | |



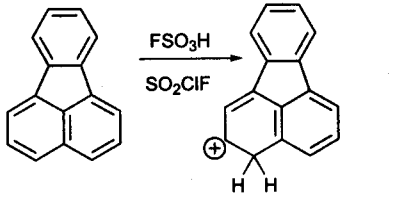

$^1$H NMR at -50°C

okazaki/cation

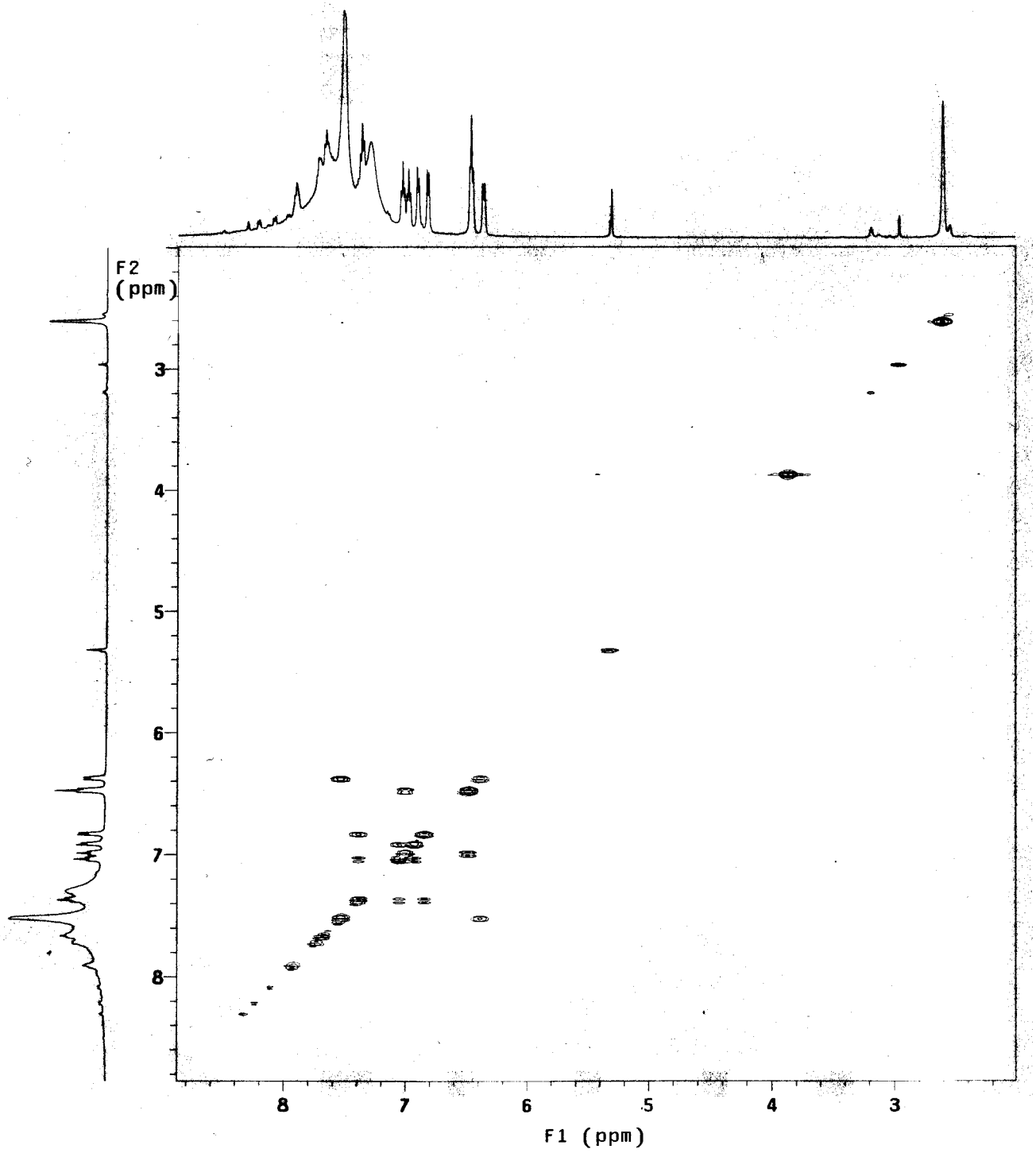
Pulse Sequence: relayh

Solvent: CD2CL2
Temp. -50.0 C / 223.2 K
File: to00051702-COSY50-CD2Cl2-5
INOVA-500 "ksu500"

PULSE SEQUENCE: relayh
Relax. delay 0.780 sec
COSY 90-90
Acq. time 0.345 sec
Width 3429.9 Hz
2D Width 3429.9 Hz
4 repetitions
128 increments
OBSERVE H1, 499.9058775 MHz
DATA PROCESSING
Sine bell 0.150 sec
F1 DATA PROCESSING
Sine bell 0.019 sec
FT size 2048 x 512
Total time 9 min, 53 sec



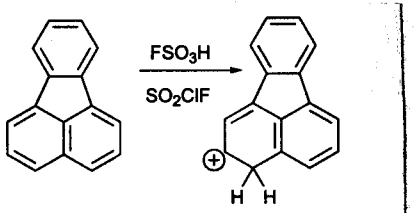

H/H COSY at -50°C



STANDARD CARBON PARAMETERS

exp8 s2pul

| SAMPLE | | DEC. & VT | |
|---|---|---|---|
| date | May 17 2000 | dfrq | 499.908 |
| solvent | CD2CL2 | dn | H1 |
| file | /export/home/~ | dpwr | 35 |
| | laali/okazaki05/to~ | dof | 0 |
| | 00051702-C50-CD2Cl~ | dm | nyy |
| | 2-5.fid | dmm | w |
| ACQUISITION | | dmf | 10800 |
| sfrq | 125.716 | dseq | |
| tn | C13 | dres | 1.0 |
| at | 0.640 | homo | n |
| np | 64000 | temp | -50.0 |
| sw | 50000.0 | DEC2 | |
| fb | not used | dfrq2 | 0 |
| bs | 4 | dn2 | |
| tpwr | 52 | dpwr2 | 1 |
| pw | 16.0 | dof2 | 0 |
| d1 | 0.500 | dm2 | n |
| d2 | 0.500 | dmm2 | c |
| tof | 2423.4 | dmf2 | 10000 |
| nt | 10000 | dseq2 | |
| ct | 300 | dres2 | 1.0 |
| alock | n | homo2 | n |
| gain | 60 | PROCESSING | |
| FLAGS | | lb | 2.00 |
| il | n | wtfile | |
| in | n | proc | ft |
| dp | y | fn | 131072 |
| hs | nn | math | f |
| DISPLAY | | | |
| sp | -628.9 | werr | |
| wp | 25140.0 | wexp | |
| vs | 91 | wbs | |
| sc | 0 | wnt | |
| wc | 250 | | |
| hzmm | 100.56 | | |
| is | 4250.00 | | |
| rfl | 17313.0 | | |
| rfp | 6787.9 | | |
| th | 6 | | |
| ins | 1.000 | | |
| nm cdc ph | | | |




$^{13}$C NMR at -50°C

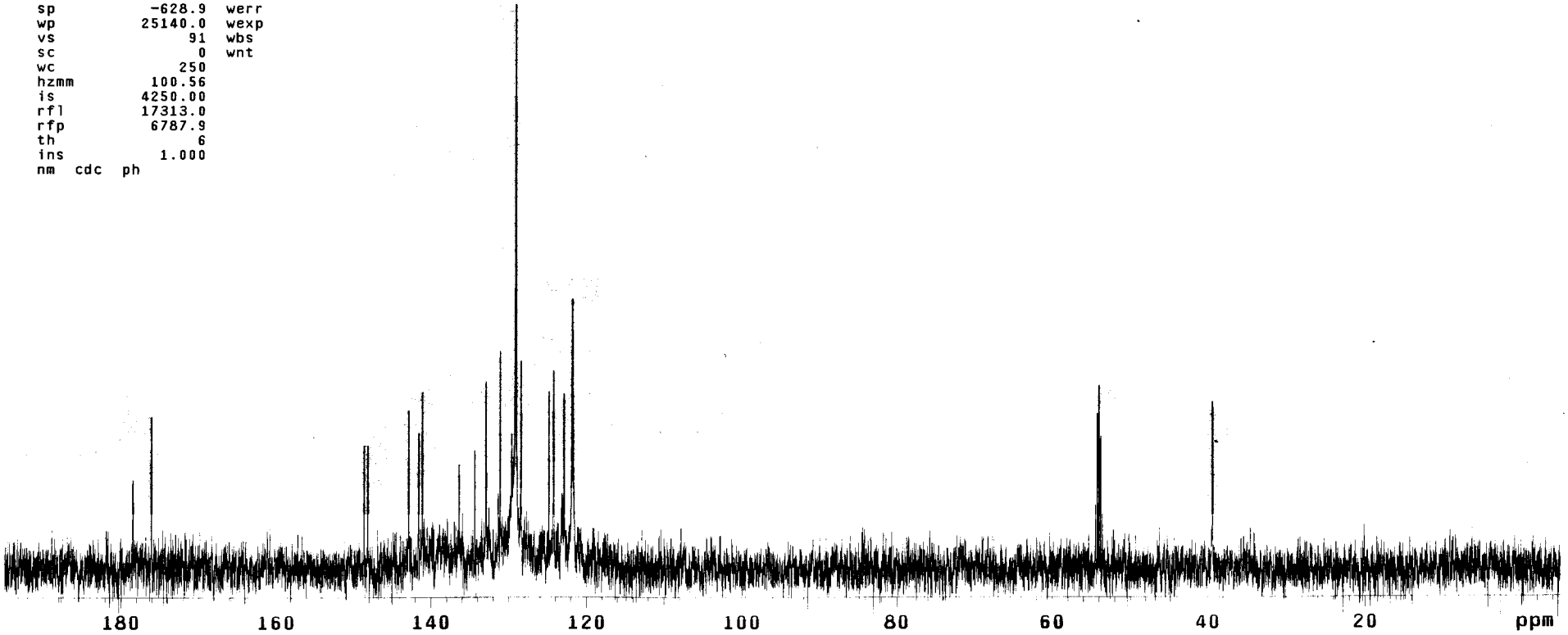


Table 1. Heat of Formation, Zero Point Energy, Number of Imaginary frequency for Protonated Fluorathene and Neutral compound by AM1 Calculations.

| Protonated Site | Heat of Formation (kcal/mol) | Zero Point Energy (kcal/mol) | Number of Imaginary frequency | file name for AM1 | file name of frequency calculations |
|---|---|---|---|---|---|
| Neutral | 87.921516 | 134.366 | 0 | fl00 | fl00f |
| C-1 | 259.333140 | 139.782 | 0 | fl01 | fl01f |
| C-2 | 262.594594 | 139.938 | 0 | fl02 | fl02f |
| C-3 | 255.192101 | 139.967 | 0 | fl03 | fl03f |
| C-3a | 278.186639 | 139.676 | 0 | fl03a | fl03af |
| C-3b | 265.191086 | 139.587 | 0 | fl03b | fl03bf |
| C-6a | 266.450445 | 140.073 | 0 | fl06a | fl06af |
| C-6b | 264.651860 | 140.065 | 0 | fl06b | fl06bf |
| C-7 | 259.470740 | 139.950 | 0 | fl07 | fl07f |
| C-8 | 257.168863 | 140.098 | 0 | fl08 | fl08f |

Table 2. Heat of Formation, Zero Point Energy, Number of Imaginary frequency for 3,3'-bifluorathene by AM1 Calculations.

| Protonated Site | Heat of Formation (kcal/mol) | Zero Point Energy (kcal/mol) | Number of Imaginary frequency | file name for AM1 | file name of frequency calculations |
|---|---|---|---|---|---|
| 182.035224 | 256.459 | 0 | dfl01 | dfl01f | |

Table 3. Heat of Formation, Zero Point Energy, Number of Imaginary frequency for Protonated benz[e]acephenanthrylene and Neutral compound by AM1 Calculations.

| Protonated Site | Heat of Formation (kcal/mol) | Zero Point Energy (kcal/mol) | Number of Imaginary frequency | file name for AM1 | file name of frequency calculations |
|---|---|---|---|---|---|
| Neutral, | 103.243671 | 165.091 | 0 | bfl00 | bfl00f |
| C-1, | 269.254096 | 170.767 | 0 | bfl01 | bfl01f |
| C-2, | 273.912814 | 170.730 | 0 | bfl02 | bfl02f |
| C-3, | 271.828435 | 170.640 | 0 | bfl03 | bfl03f |
| C-4, | 273.591820 | 170.682 | 0 | bfl04 | bfl04f |
| C-5, | 271.533168 | 170.835 | 0 | bfl05 | bfl05f |
| C-6, | 271.456968 | 170.846 | 0 | bfl06 | bfl06f |
| C-7, | 273.976860 | 170.667 | 0 | bfl07 | bfl07f |

C-8, 269.626818, 170.593, 0, bfl08, bfl08f
C-9, 272.386842, 170.745, 0, bfl09, bfl09f
C-10, 276.306555, 170.789, 0, bfl10, bfl10f
C-11, 273.291129, 170.775, 0, bfl11, bfl11f
C-12, 275.137026, 170.734, 0, bfl12, bfl12f

---

Table 4.
Heat of Formation, Zero Point Energy,
Number of Imaginary frequency for Protonated
10-Methoxybenz[e]acephenanthrylene and Neutral
compound by AM1 Calculations.

---

Direction of Methoxy, Protonated Site, Heat of Formation
(kcal/mol), Zero Point Energy (kcal/mol),
Nember of Imaginary Frequency

---

Out, Neutral, 65.406888, 185.953, 0
In, Neutral, 65.823833, 185.937, 0
Out, C-1, 229.481508, 191.671, 0
In, C-1, 229.765655, 191.652, 0
Out, C-2, 235.962869, 191.543, 0
In, C-2, 236.036433, 191.537, 0
Out, C-3, 231.677030, 191.600, 0
In, C-3, 231.702214, 191.581, 0
Out, C-4, 235.708767, 191.543, 0
In, C-4, 235.719360, 191.518, 0
Out, C-5, 233.982587, 191.658, 0
In, C-5, 234.064375, 191.623, 0
Out, C-6, 233.573645, 191.696, 0
In, C-6, 233.556045, 191.680, 0
Out, C-7, 236.444736, 191.503, 0
In, C-7, 236.500910, 191.452, 0
Out, C-8, 229.967737, 191.566, 0
In, C-8, 229.486345, 191.535, 0
Out, C-9, 227.414822, 191.707, 0
In, C-9, 225.303474, 191.725, 0
*, C-10, 246.169427, 191.807, 0
*, C-10, 245.966811, 191.822, 0
*, C-10, 245.848030, 191.792, 0
Out, C-11, 228.707303, 191.723, 0
In, C-11, 231.046820, 191.686, 0
Out, C-12, 240.245358, 191.359, 0
In, C-12, 238.691417, 191.488, 0

---

* Three isomers on C-OME conformation

Table 5. Heat of Formation, Zero Point Energy, and Number of Imaginary Frequency for Neutral and Protonated 10-Fluorobenz[e]acephenanthrylene by AM1.

---

Protonated Site, Heat of Formation (kcal/mol), Zero Point Energy (kcal/mol), Number of Imaginery Frequency

---

Neutral, 58.340653, 160.421, 0
C-1, 226.497763, 166.169, 0
C-2, 232.297760, 166.064, 0
C-3, 228.965695, 166.055, 0
C-4, 231.080823, 166.052, 0
C-5, 229.557548, 166.160, 0
C-6, 228.838122, 166.202, 0
C-7, 232.086990, 166.004, 0
C-8, 226.774093, 166.003, 0
C-9, 228.499945, 166.214, 0
C-10, 244.989676, 166.432, 0
C-11, 230.152421, 166.221, 0
C-12, 236.980781, 166.037, 0

---

Table 6. Heat of Formation, Zero Point Energy, and Number of Imaginary Frequency for Neutral and protonated Indeno[1,2,3-cd]pyrene (9) by AM1.

---

Protonated Site, Heat of Formation (kcal/mol), Zero Point Energy (kcal/mol), Number of Imaginary Frequency

---

Neutral, 116.340753, 174.000, 0
C-1, 283.909190, 179.823, 0
C-2, 280.819605, 179.844, 0
C-3, 277.148864, 179.839, 0
C-4, 290.158457, 179.680, 0
C-5, 277.267671, 179.835, 0
C-6, 281.708328, 179.551, 0
C-7, 331.415940, 178.789, 0
C-8, 280.962145, 179.919, 0
C-9, 329.373407, 179.068, 0
C-10, 282.693414, 179.792, 0
C-11, 286.006361, 179.596, 0
C-12, 275.193767, 179.937, 0

---

Cartesian coordinates for 3-protonated fluoranthenium optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Thursday, June 28 2001

1 1

| | | | |
|---|---|---|---|
| C | -0.670506 | -2.404633 | -0.000022 |
| C | -2.037449 | -2.472876 | -0.000025 |
| C | -2.948934 | -1.290534 | 0.000036 |
| C | -2.911020 | 1.305490 | -0.000015 |
| C | -2.137951 | 2.463258 | -0.000022 |
| C | -0.715148 | 2.441120 | -0.000009 |
| C | 2.528801 | 1.422509 | 0.000013 |
| C | 3.723650 | 0.669713 | 0.000006 |
| C | 3.714183 | -0.727574 | -0.000005 |
| C | 2.501228 | -1.422727 | -0.000010 |
| C | -2.274129 | 0.048180 | 0.000004 |
| C | -0.083972 | 1.215665 | 0.000009 |
| C | 1.325714 | 0.746829 | 0.000010 |
| C | 1.311189 | -0.686866 | -0.000001 |
| C | -0.064009 | -1.121488 | 0.000004 |
| C | -0.884637 | 0.051698 | 0.000016 |
| H | -0.072322 | -3.309990 | -0.000050 |

| | | | |
|---|---|---|---|
| H | -2.518396 | -3.448225 | -0.000052 |
| H | -3.630783 | -1.384758 | 0.863604 |
| H | -3.630999 | -1.384746 | -0.863352 |
| H | -3.994526 | 1.378014 | -0.000027 |
| H | -2.638451 | 3.426919 | -0.000042 |
| H | -0.165604 | 3.377340 | -0.000017 |
| H | 2.572586 | 2.507207 | 0.000019 |
| H | 4.674343 | 1.194599 | 0.000009 |
| H | 4.651235 | -1.274131 | -0.000009 |
| H | 2.490855 | -2.508813 | -0.000016 |

Cartesian coordinates for 1-protonated benz[e]acephenanthrylenium optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Friday, June 29 2001

1 1

| | | | |
|---|---|---|---|
| C | 4.666977 | -0.632514 | 0.000009 |
| C | 4.108217 | -1.920042 | 0.000004 |
| C | 3.844966 | 0.491058 | 0.000007 |

| | | | |
|---|---|---|---|
| C | 2.719083 | -2.125288 | -0.000003 |
| C | 2.454488 | 0.301984 | 0.000000 |
| C | 1.886728 | -1.017101 | -0.000005 |
| C | 1.380273 | 1.257159 | -0.000005 |
| C | 0.418856 | -0.880631 | -0.000008 |
| C | 1.358422 | 2.680200 | -0.000007 |
| C | 0.153504 | 0.523847 | -0.000007 |
| C | -0.638294 | -1.742414 | -0.000003 |
| C | 0.145795 | 3.303084 | -0.000009 |
| C | -1.103631 | 1.090961 | -0.000003 |
| C | -1.983697 | -1.217515 | -0.000002 |
| C | -1.168962 | 2.589566 | 0.000012 |
| C | -2.232201 | 0.202374 | -0.000002 |
| C | -3.085035 | -2.095300 | 0.000000 |
| C | -3.567805 | 0.664052 | 0.000001 |
| C | -4.385525 | -1.611157 | 0.000003 |
| C | -4.628289 | -0.226678 | 0.000004 |
| H | 5.745568 | -0.515216 | 0.000013 |
| H | 4.767949 | -2.782754 | 0.000006 |
| H | 4.274867 | 1.488375 | 0.000009 |
| H | 2.318788 | -3.134416 | -0.000006 |
| H | 2.278570 | 3.255389 | -0.000013 |
| H | -0.506654 | -2.821136 | -0.000002 |
| H | 0.100151 | 4.389171 | -0.000015 |

| | | | |
|---|---|---|---|
| H | -1.750569 | 2.951499 | -0.864809 |
| H | -2.904127 | -3.166486 | -0.000001 |
| H | -3.768812 | 1.731091 | 0.000002 |
| H | -5.220232 | -2.305315 | 0.000005 |
| H | -5.648214 | 0.144457 | 0.000006 |
| H | -1.750499 | 2.951464 | 0.864897 |

Cartesian coordinates for 9-protonated 10-methoxybenz[e]acephenanthrylenium (**6aH$^+$**) optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Saturday, Jun 30 2001

1 1

| | | | |
|---|---|---|---|
| C | 5.031191 | -1.588876 | -0.000001 |
| C | 4.165606 | -2.686419 | -0.000001 |
| C | 4.539260 | -0.273497 | -0.000002 |
| C | 2.779183 | -2.498296 | 0.000000 |
| C | 3.166668 | -0.076301 | -0.000001 |
| C | 2.281604 | -1.196516 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 2.347536 | 1.155674 | -0.000001 |
| C | 0.910273 | -0.687793 | 0.000000 |
| C | 2.609976 | 2.509216 | -0.000001 |
| C | 0.996145 | 0.735129 | 0.000000 |
| C | -0.343398 | -1.284209 | 0.000000 |
| C | 1.510793 | 3.410923 | -0.000001 |
| C | -0.103897 | 1.596033 | 0.000000 |
| C | -1.485992 | -0.466006 | 0.000001 |
| C | 0.191460 | 2.986635 | 0.000000 |
| C | -1.405232 | 0.956296 | 0.000000 |
| C | -2.841780 | -1.134217 | 0.000001 |
| C | -2.607625 | 1.698745 | 0.000000 |
| C | -4.034060 | -0.232533 | 0.000001 |
| C | -3.886040 | 1.146024 | 0.000001 |
| H | 6.104346 | -1.754721 | -0.000002 |
| H | 4.572403 | -3.692733 | -0.000001 |
| H | 5.228648 | 0.565763 | -0.000002 |
| H | 2.111342 | -3.355455 | 0.000000 |
| H | 3.622899 | 2.900679 | -0.000001 |
| H | -0.456002 | -2.365487 | 0.000001 |
| H | 1.716181 | 4.477178 | -0.000001 |
| H | -2.539270 | 2.782547 | 0.000000 |
| O | -5.259950 | -0.711210 | 0.000002 |
| H | -4.769959 | 1.773714 | 0.000000 |

| | | | |
|---|---|---|---|
| C | -5.527820 | -2.129495 | 0.000002 |
| H | -0.597840 | 3.731427 | -0.000001 |
| H | -2.913964 | -1.805399 | -0.870344 |
| H | -2.913964 | -1.805400 | 0.870345 |
| H | -5.117558 | -2.597532 | 0.899524 |
| H | -6.613209 | -2.210464 | 0.000003 |
| H | -5.117559 | -2.597533 | -0.899519 |

Cartesian coordinates for 9-protonated 10-methoxybenz[e]acephenanthrylenium (**6bH$^+$**) optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Saturday, Jun 30 2001

1 1

| | | | |
|---|---|---|---|
| C | 5.199332 | -1.313256 | 0.000138 |
| C | 4.419560 | -2.473331 | 0.000086 |
| C | 4.609683 | -0.038074 | 0.000125 |
| C | 3.022947 | -2.390746 | 0.000018 |
| C | 3.226626 | 0.054690 | 0.000058 |
| C | 2.428875 | -1.129672 | 0.000004 |
| C | 2.316111 | 1.221327 | 0.000027 |
| C | 1.024093 | -0.727090 | -0.000058 |

| | | | |
|---|---|---|---|
| C | 2.474733 | 2.590977 | 0.000058 |
| C | 1.000931 | 0.699034 | -0.000042 |
| C | -0.180037 | -1.420590 | -0.000126 |
| C | 1.309618 | 3.405335 | 0.000022 |
| C | -0.161510 | 1.472362 | -0.000077 |
| C | -1.382193 | -0.695950 | -0.000179 |
| C | 0.026304 | 2.880768 | -0.000051 |
| C | -1.410583 | 0.732091 | -0.000134 |
| C | -2.681767 | -1.459872 | -0.000367 |
| C | -2.662931 | 1.375474 | -0.000064 |
| C | -3.941068 | -0.654873 | -0.000105 |
| C | -3.905184 | 0.729349 | -0.000026 |
| H | 6.281955 | -1.397670 | 0.000191 |
| H | 4.901583 | -3.445815 | 0.000100 |
| H | 5.233990 | 0.850633 | 0.000165 |
| H | 2.421132 | -3.295426 | -0.000020 |
| H | 3.454645 | 3.058873 | 0.000116 |
| H | -0.208116 | -2.507118 | -0.000145 |
| H | 1.432378 | 4.484280 | 0.000047 |
| H | -2.677811 | 2.461624 | 0.000002 |
| O | -5.023231 | -1.401498 | 0.000036 |
| H | -4.812873 | 1.319750 | 0.000116 |
| C | -6.335945 | -0.792773 | 0.000489 |
| H | -0.817638 | 3.563078 | -0.000107 |

| | | | |
|---|---|---|---|
| H | -2.718963 | -2.134543 | -0.869133 |
| H | -2.718909 | -2.135259 | 0.867831 |
| H | -6.468382 | -0.186618 | -0.899604 |
| H | -7.034504 | -1.627382 | 0.000150 |
| H | -6.468209 | -0.187506 | 0.901205 |

Cartesian coordinates for 1-protonated 10-fluorobenz[e]acephenanthrylenium optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Wednesday, Jul 4 2001

1 1

| | | | |
|---|---|---|---|
| C | 4.883052 | -1.064872 | -0.000009 |
| C | 4.180849 | -2.279147 | 0.000005 |
| C | 4.195509 | 0.146768 | -0.000016 |
| C | 2.776688 | -2.322039 | 0.000011 |
| C | 2.793480 | 0.119023 | -0.000005 |
| C | 2.078995 | -1.125167 | 0.000008 |
| C | 1.834353 | 1.192760 | 0.000004 |

| | | | |
|---|---|---|---|
| C | 0.635340 | -0.820390 | 0.000003 |
| C | 1.976642 | 2.609474 | -0.000002 |
| C | 0.534045 | 0.606531 | 0.000003 |
| C | -0.511209 | -1.556796 | 0.000001 |
| C | 0.844335 | 3.367655 | -0.000001 |
| C | -0.652034 | 1.313428 | 0.000001 |
| C | -1.788979 | -0.879989 | 0.000001 |
| C | -0.544694 | 2.810537 | 0.000009 |
| C | -1.870907 | 0.561211 | 0.000001 |
| C | -2.977281 | -1.629293 | 0.000000 |
| C | -3.147544 | 1.173265 | -0.000001 |
| C | -4.199253 | -0.977137 | 0.000000 |
| C | -4.306012 | 0.421211 | -0.000002 |
| H | 5.968010 | -1.072452 | -0.000013 |
| H | 4.737052 | -3.211913 | 0.000006 |
| H | 4.737755 | 1.087788 | -0.000022 |
| H | 2.261662 | -3.277751 | 0.000016 |
| H | 2.957174 | 3.074314 | -0.000012 |
| H | -0.503713 | -2.643251 | 0.000003 |
| H | 0.923293 | 4.451829 | -0.000009 |
| H | -1.079127 | 3.237372 | -0.865597 |
| H | -2.954043 | -2.714112 | -0.000002 |
| H | -3.226362 | 2.255933 | -0.000002 |
| F | -5.318492 | -1.700841 | -0.000008 |

| | | | |
|---|---|---|---|
| H | -5.288434 | 0.880256 | -0.000005 |
| H | -1.079087 | 3.237346 | 0.865655 |

Cartesian coordinates for 8-protonated 10-fluorobenz[e]acephenanthrylenium optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Thursday, Jul 5 2001

1 1

| | | | |
|---|---|---|---|
| C | -4.895187 | -1.061611 | -0.000002 |
| C | -4.191639 | -2.265757 | -0.000001 |
| C | -4.228177 | 0.184985 | -0.000002 |
| C | -2.790031 | -2.267102 | 0.000001 |
| C | -2.849342 | 0.192450 | -0.000001 |
| C | -2.123332 | -1.040435 | 0.000001 |
| C | -1.855415 | 1.294461 | -0.000001 |
| C | -0.711947 | -0.722786 | 0.000002 |
| C | -1.919684 | 2.661373 | -0.000002 |
| C | -0.570955 | 0.667547 | 0.000002 |
| C | 0.486372 | -1.587396 | 0.000003 |

| | | | |
|---|---|---|---|
| C | -0.685079 | 3.386253 | 0.000000 |
| C | 0.660601 | 1.359047 | 0.000003 |
| C | 1.811208 | -0.845303 | 0.000002 |
| C | 0.557876 | 2.776203 | 0.000002 |
| C | 1.886519 | 0.580703 | 0.000002 |
| C | 2.984685 | -1.595410 | 0.000000 |
| C | 3.160147 | 1.194686 | 0.000000 |
| C | 4.214425 | -0.947109 | -0.000001 |
| C | 4.322321 | 0.445965 | -0.000001 |
| H | -5.980854 | -1.077920 | -0.000003 |
| H | -4.731751 | -3.206702 | -0.000001 |
| H | -4.802670 | 1.106358 | -0.000004 |
| H | -2.243791 | -3.206144 | 0.000002 |
| H | -2.859433 | 3.204484 | -0.000003 |
| H | -0.729412 | 4.471564 | 0.000000 |
| H | 2.963537 | -2.680968 | 0.000000 |
| H | 3.239165 | 2.275825 | 0.000000 |
| F | 5.326256 | -1.680820 | -0.000004 |
| H | 5.302991 | 0.908584 | -0.000003 |
| H | 1.444811 | 3.398499 | -0.000006 |
| H | 0.440452 | -2.265389 | 0.867877 |
| H | 0.440452 | -2.265392 | -0.867868 |

Cartesian coordinates for 12-protonated indeno[1,2,3-cd]pyrenium optimized by B3LYP/6-31G(d)

#B3LYP/6-31G* NMR

Thursday, Jul 5 2001

1 1

| | | | |
|---|---|---|---|
| C | -5.024712 | -0.191940 | 0.000000 |
| C | -4.647928 | -1.539847 | -0.000001 |
| C | -4.062079 | 0.822544 | 0.000001 |
| C | -3.299131 | -1.908346 | -0.000001 |
| C | -2.717041 | 0.466381 | 0.000001 |
| C | -2.333169 | -0.905742 | 0.000000 |
| C | -1.493163 | 1.292146 | 0.000002 |
| C | -0.859635 | -0.978536 | -0.000001 |
| C | -1.203891 | 2.617867 | 0.000003 |
| C | -0.396829 | 0.359809 | 0.000000 |
| C | 0.079968 | -1.995405 | -0.000003 |
| C | 0.216283 | 3.112157 | 0.000003 |
| C | 0.956296 | 0.713532 | 0.000000 |
| C | 1.482611 | -1.686345 | -0.000002 |
| C | 1.314565 | 2.079033 | 0.000000 |

| | | | |
|---|---|---|---|
| C | 1.916521 | -0.325871 | 0.000000 |
| C | 2.474104 | -2.687450 | -0.000002 |
| C | 3.292151 | 0.015200 | 0.000005 |
| C | 3.835522 | -2.359591 | 0.000001 |
| C | 4.247114 | -1.030533 | 0.000004 |
| H | -6.078171 | 0.070270 | 0.000001 |
| H | -5.412964 | -2.310104 | -0.000001 |
| H | -4.367214 | 1.865143 | 0.000002 |
| H | -3.019643 | -2.958115 | -0.000002 |
| H | -1.981699 | 3.377228 | 0.000003 |
| H | 2.175322 | -3.732382 | -0.000004 |
| C | 3.641902 | 1.395580 | 0.000011 |
| H | 5.306556 | -0.789021 | 0.000007 |
| C | 2.683704 | 2.401332 | -0.000012 |
| H | -0.219682 | -3.040541 | -0.000004 |
| H | 2.998445 | 3.440954 | -0.000044 |
| H | 4.694530 | 1.666099 | -0.000030 |
| H | 4.575824 | -3.152836 | 0.000001 |
| H | 0.354859 | 3.783732 | -0.864458 |
| H | 0.354860 | 3.783728 | 0.864468 |