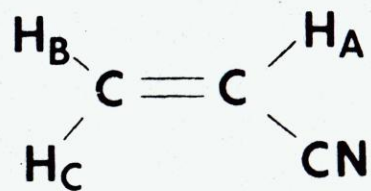
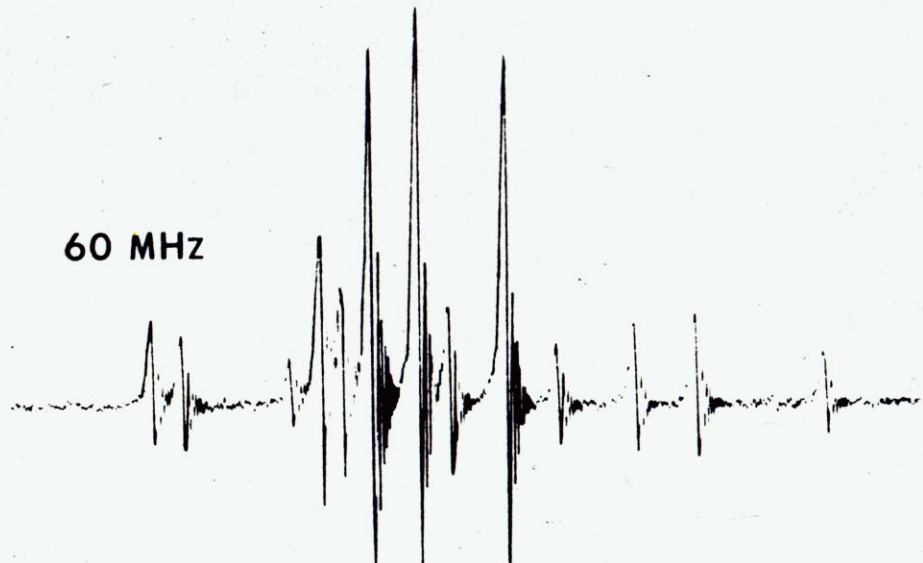


**RMN PULSADA,
COM
TRANSFORMADA
DE FOURIER.**



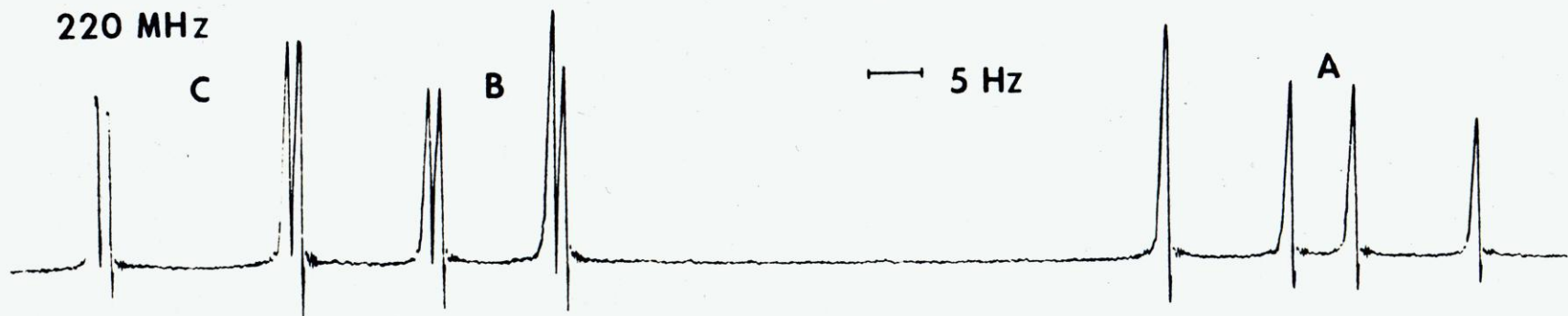
60 MHz

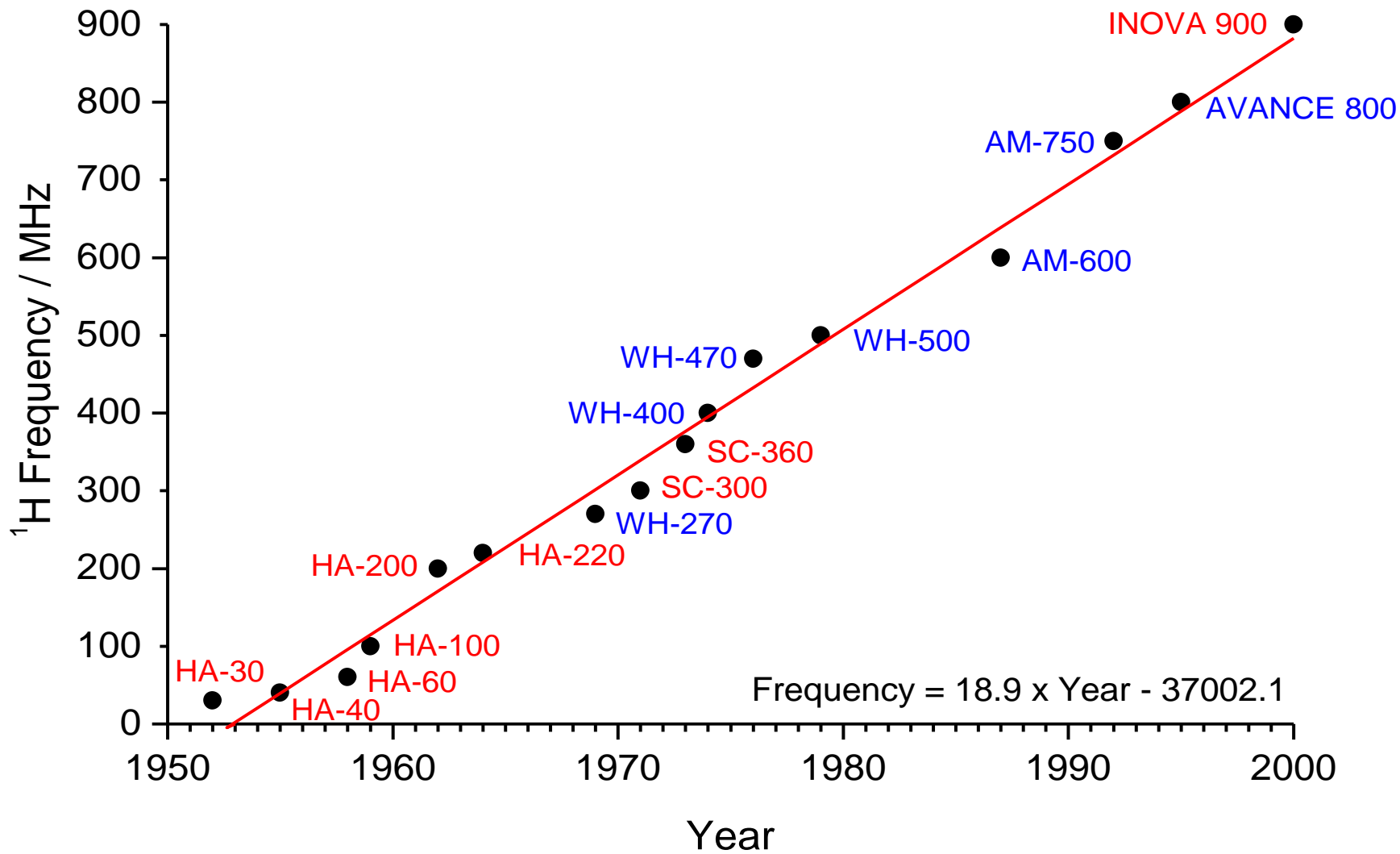


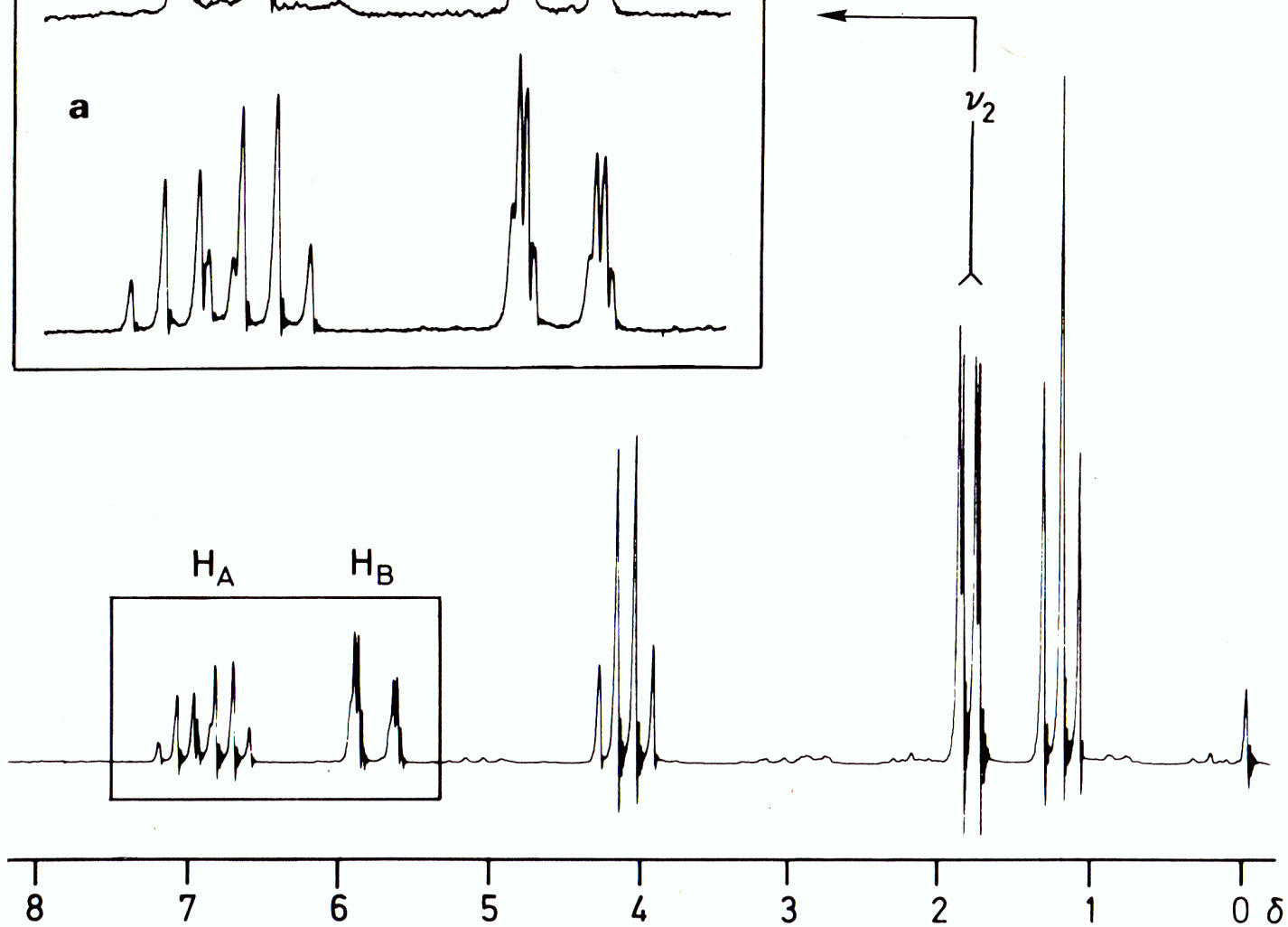
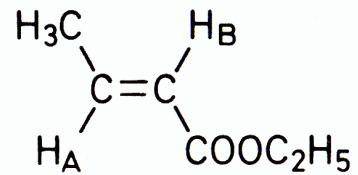
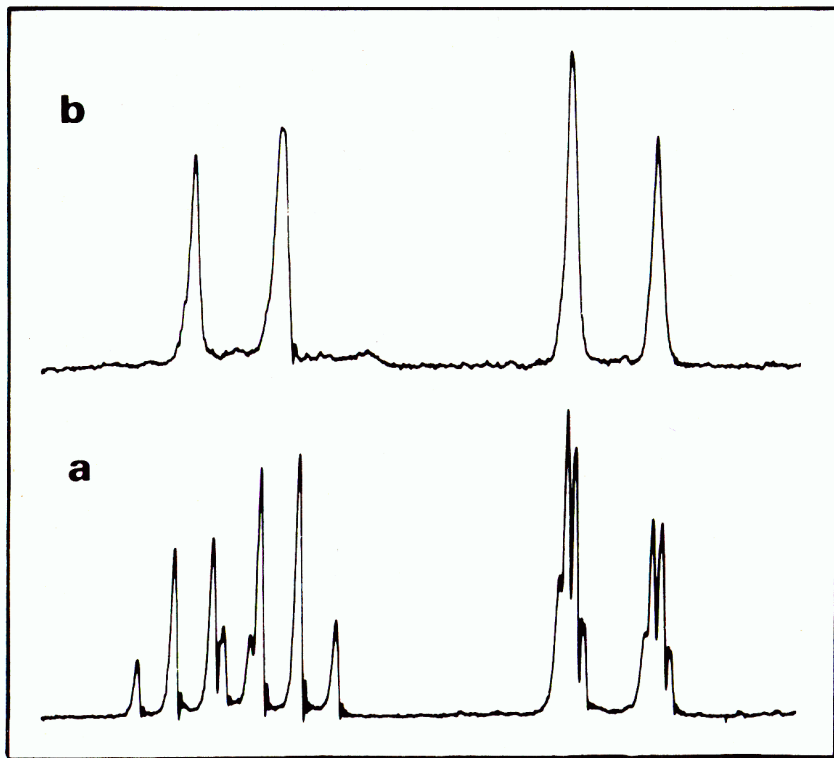
100 MHz

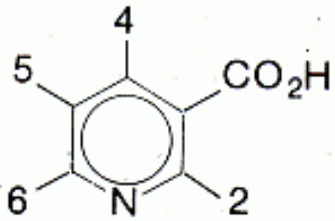


220 MHz

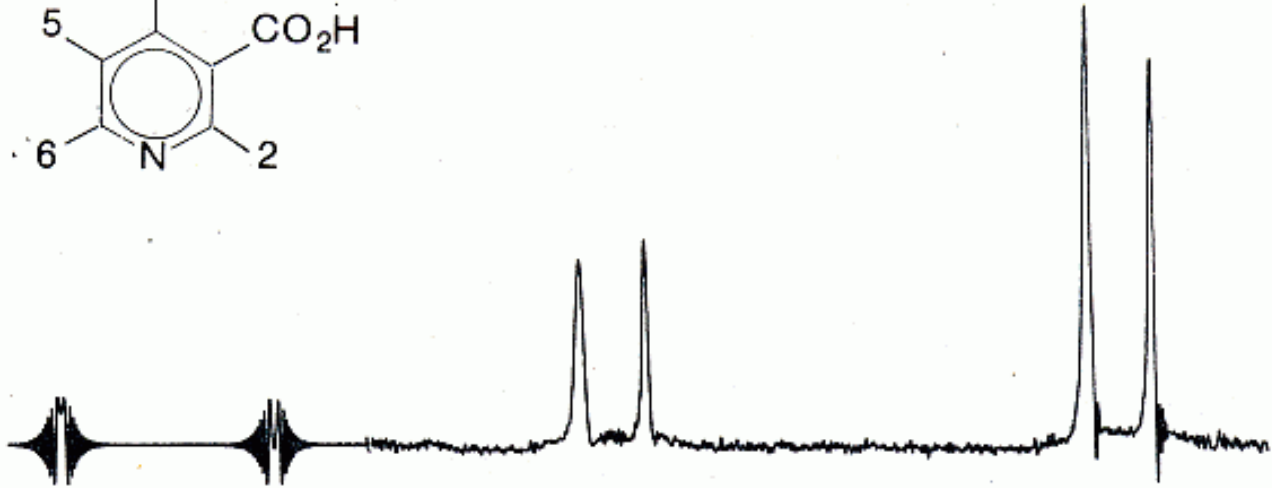




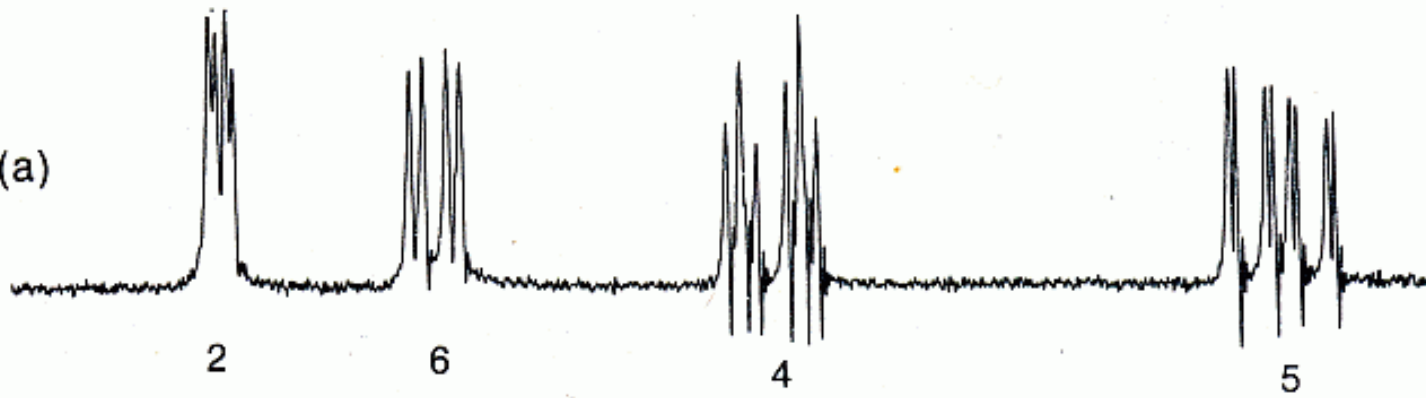


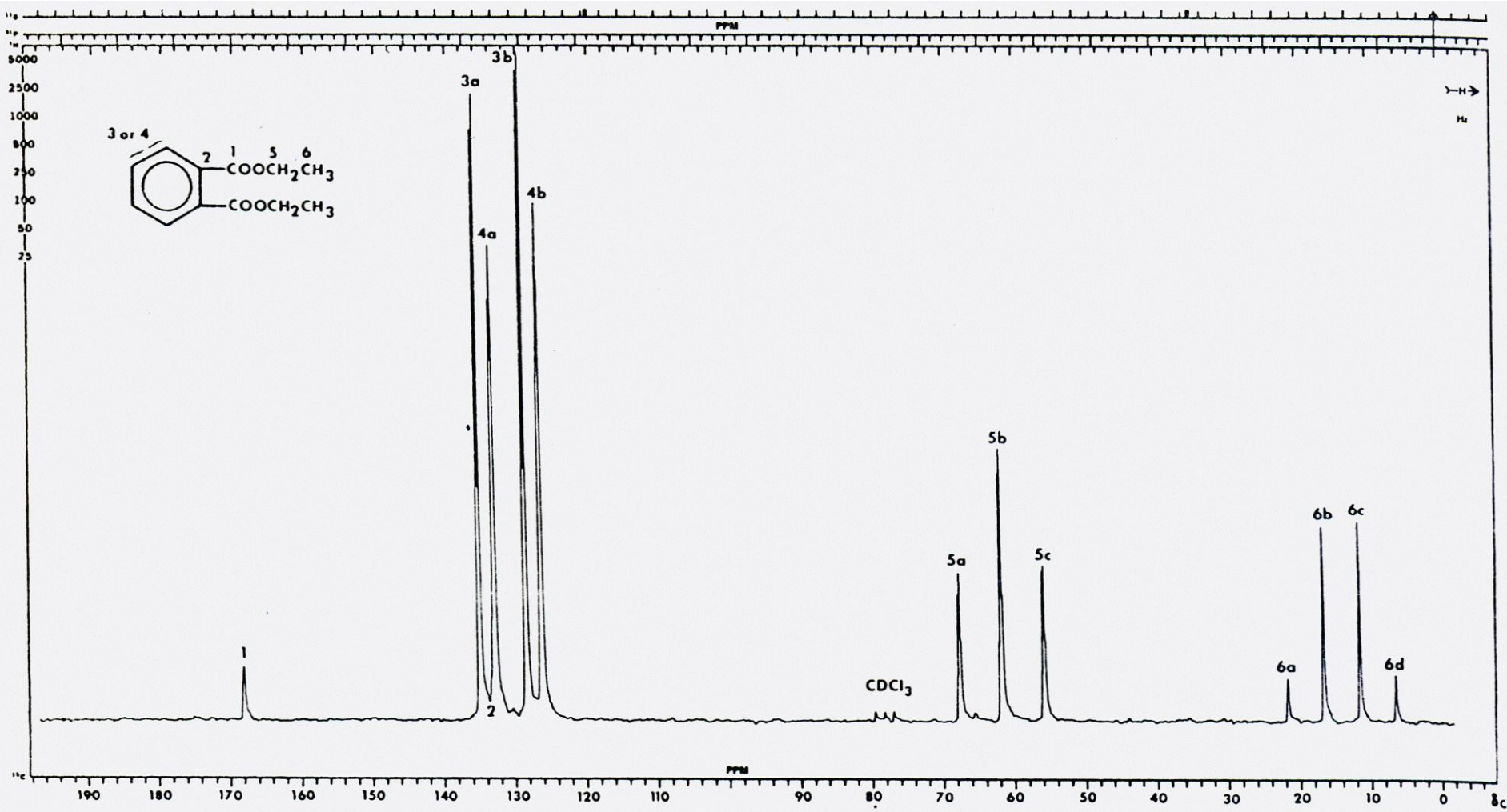


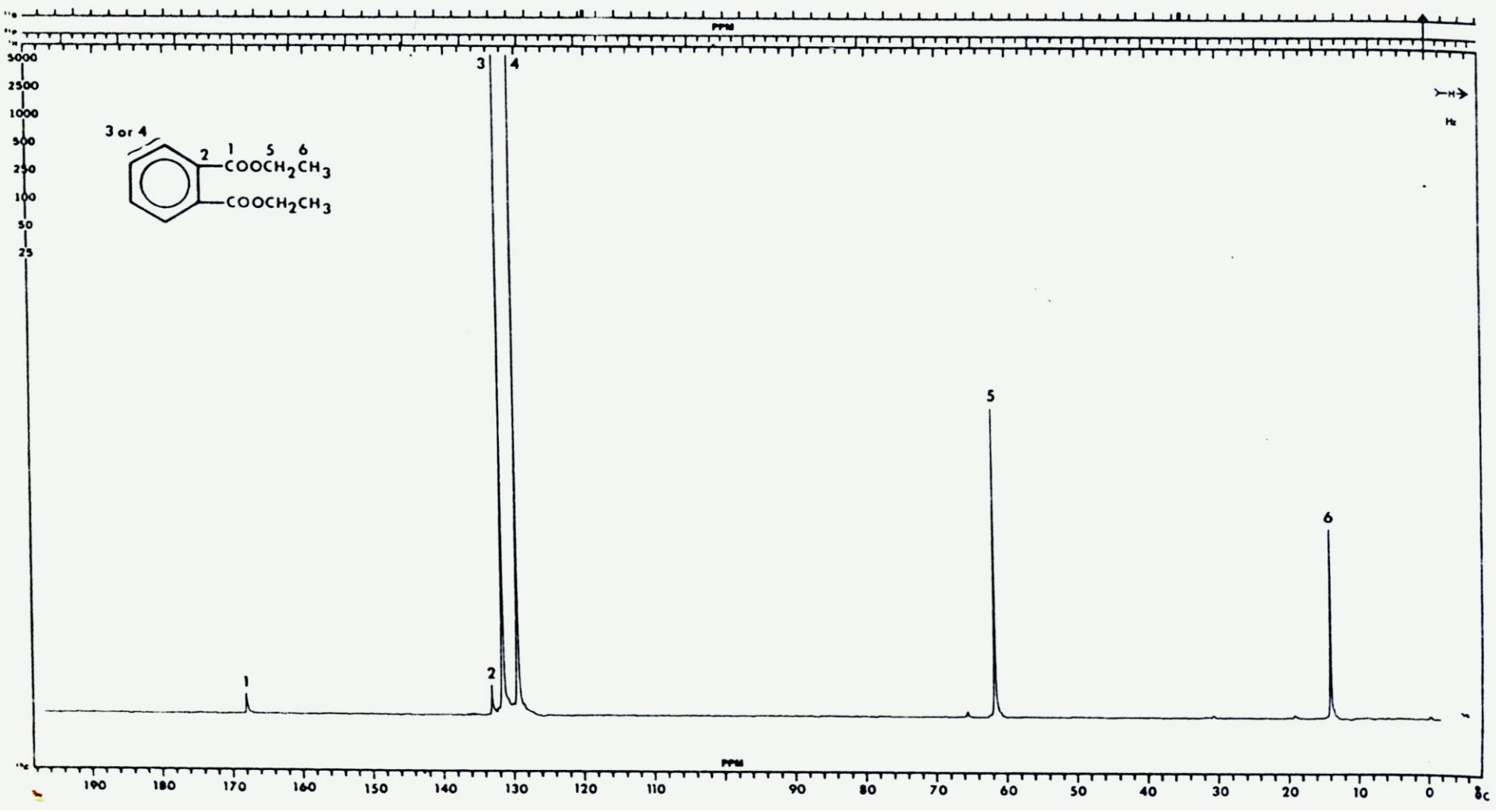
(b)



(a)







EXPERIMENTAL
PARAMETERS

Instr. HA-100
Mode CW
Time 15 min
Solv. Dioxane
Conc. .5ml/1ml soln

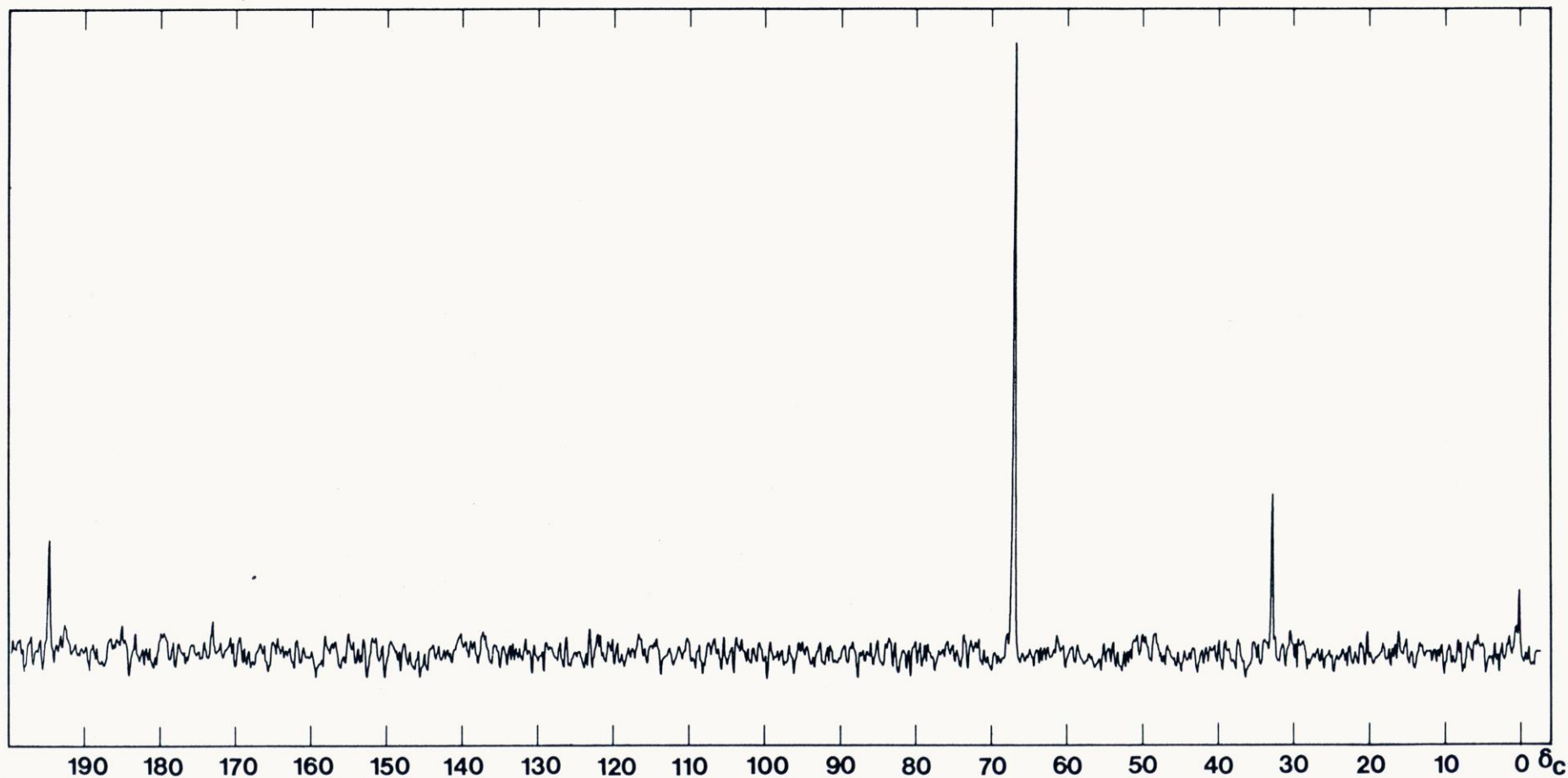
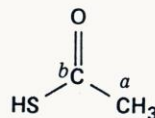
ASSIGNMENTS

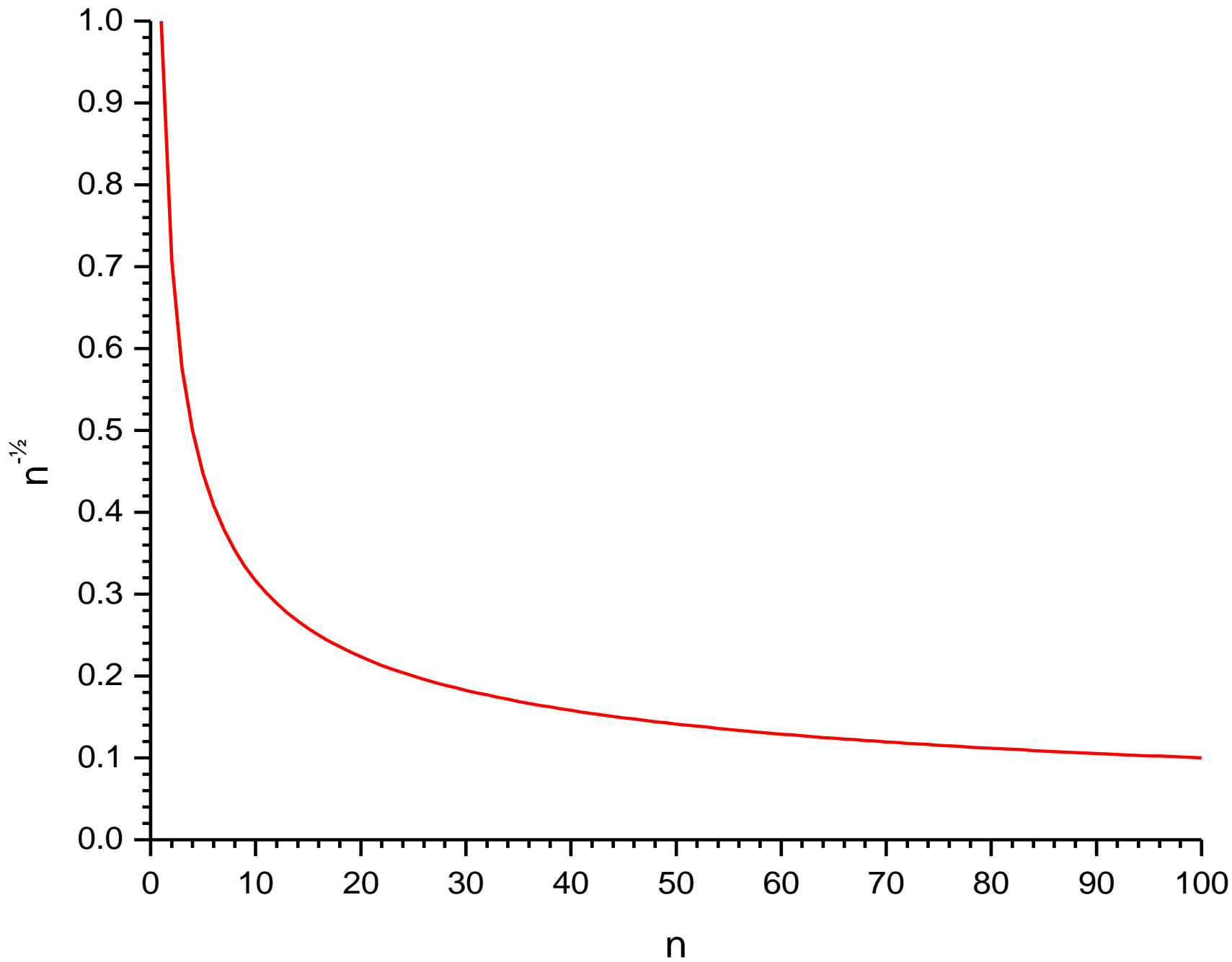
a 32.6
b 194.5

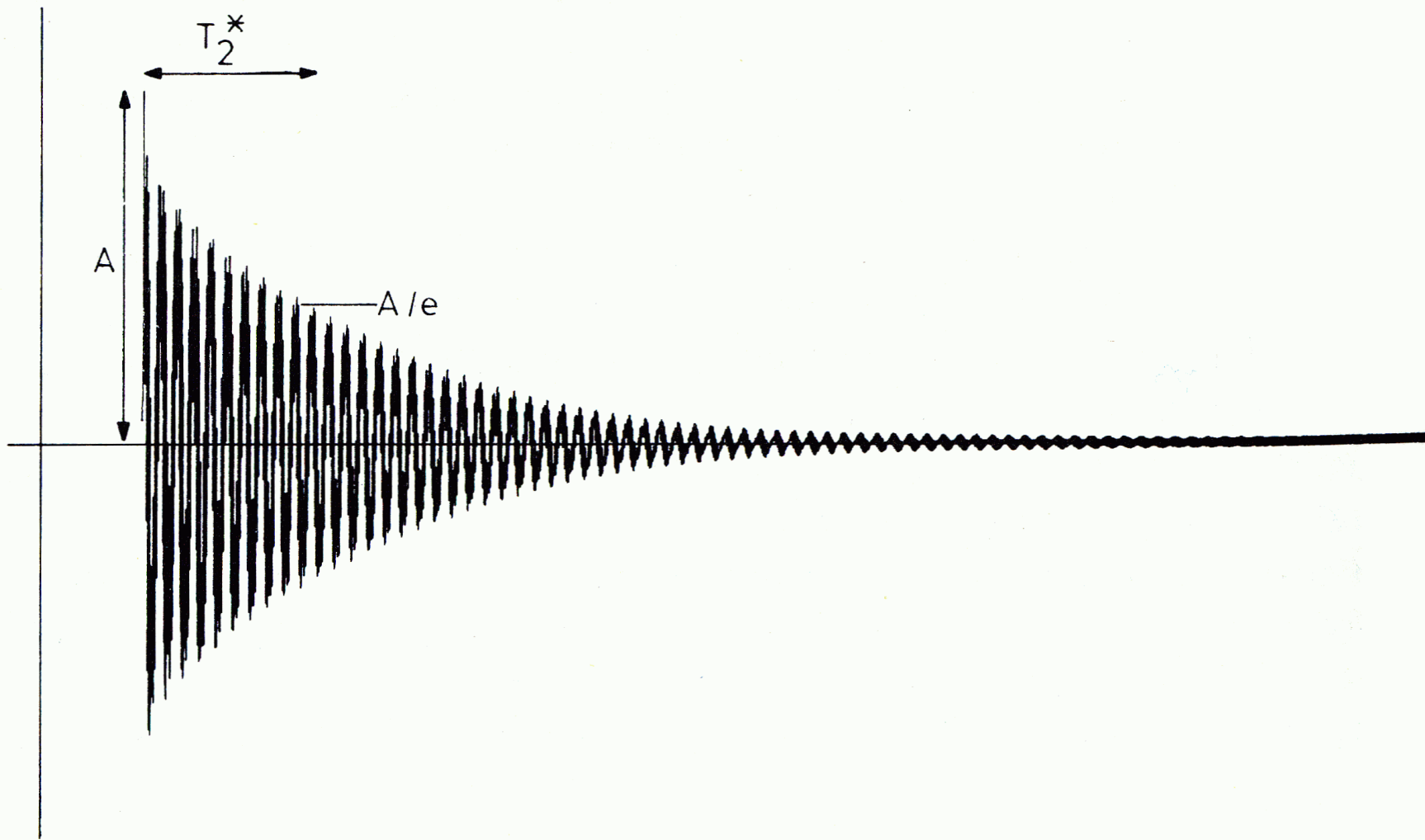
thioacetic acid

6

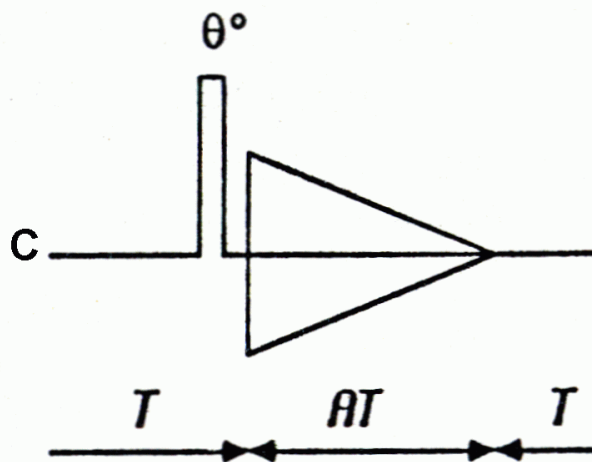
C₂H₄OS



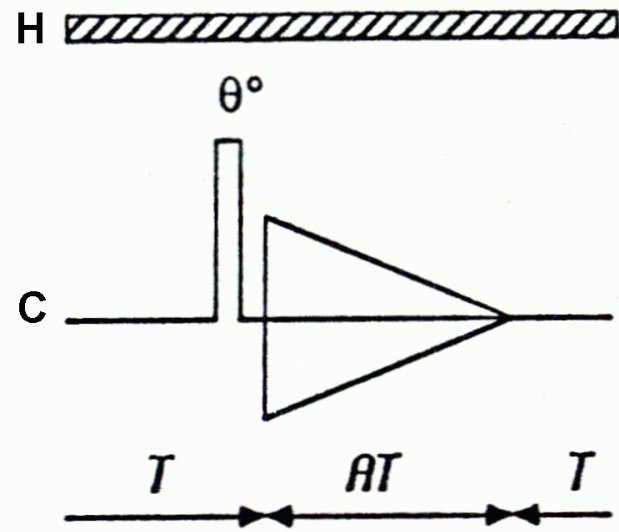




ACOPLADO



DESACOPLADO



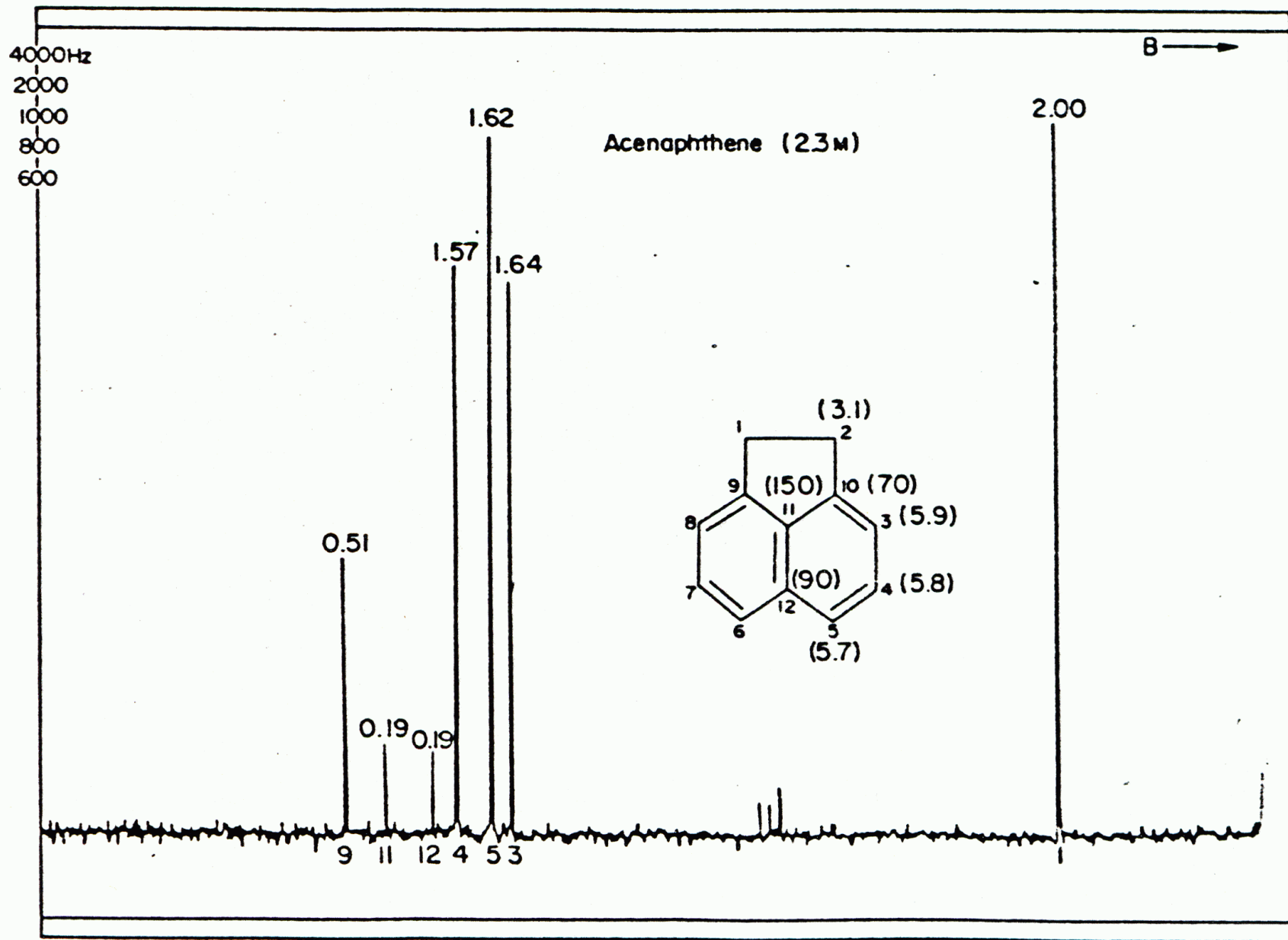
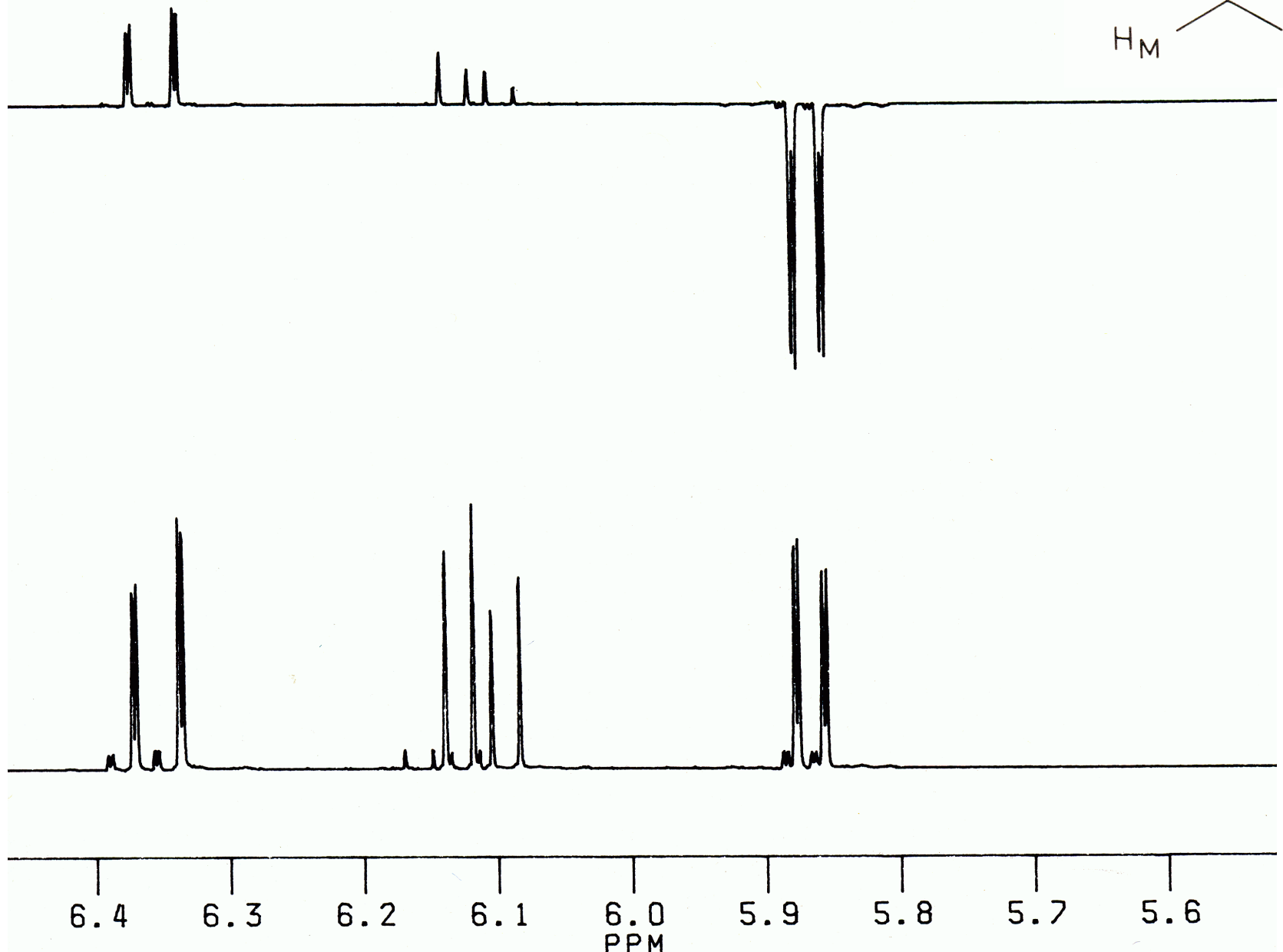
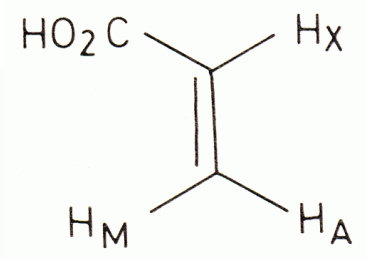
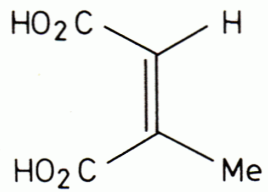
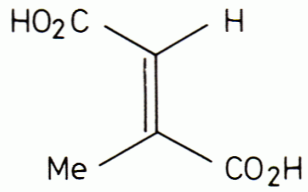


FIG. 1. Acenaphthene ^{13}C spectrum run under normal conditions showing assignments and T_1 relaxation times.

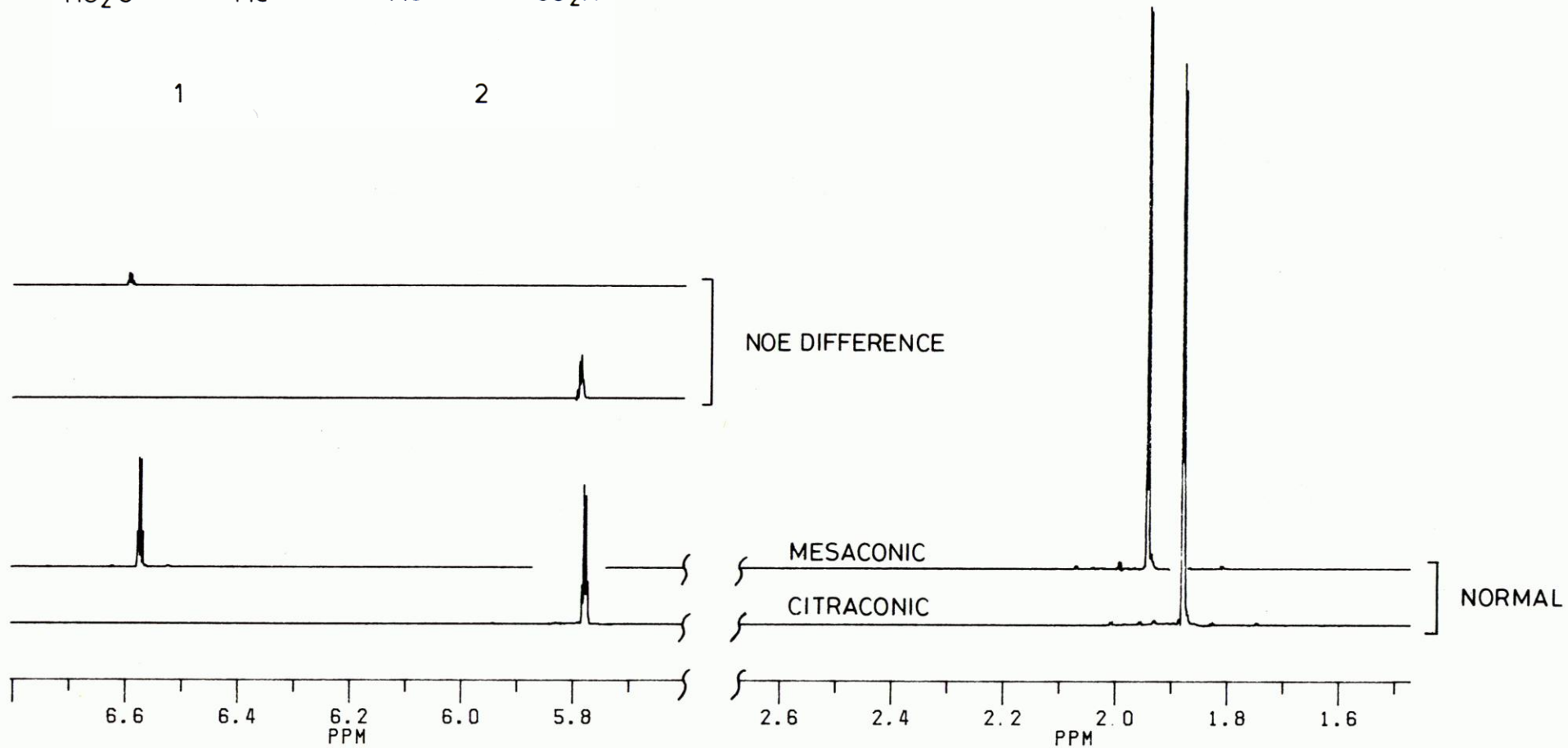




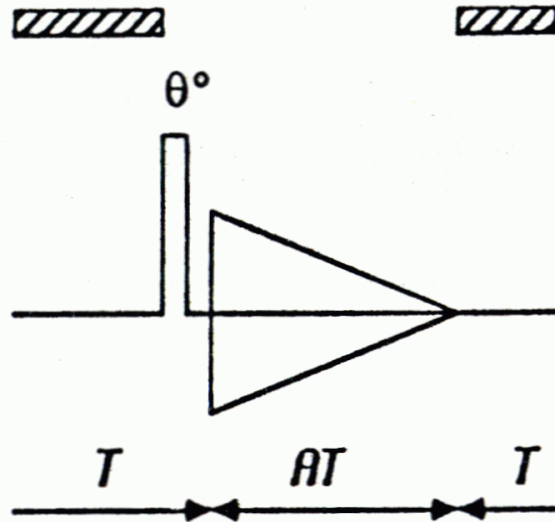
1



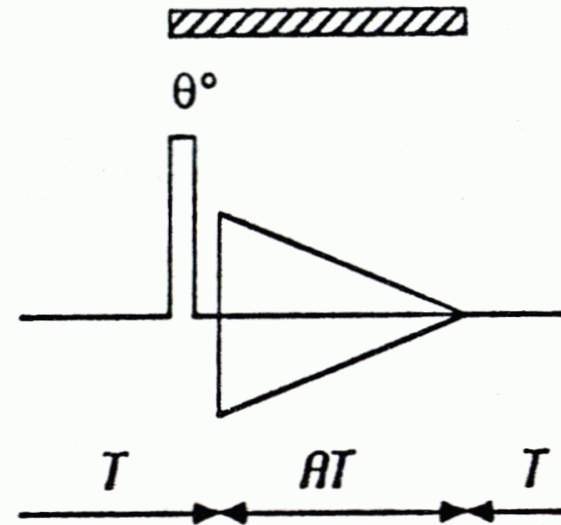
2



GATEDEC



INVGATE



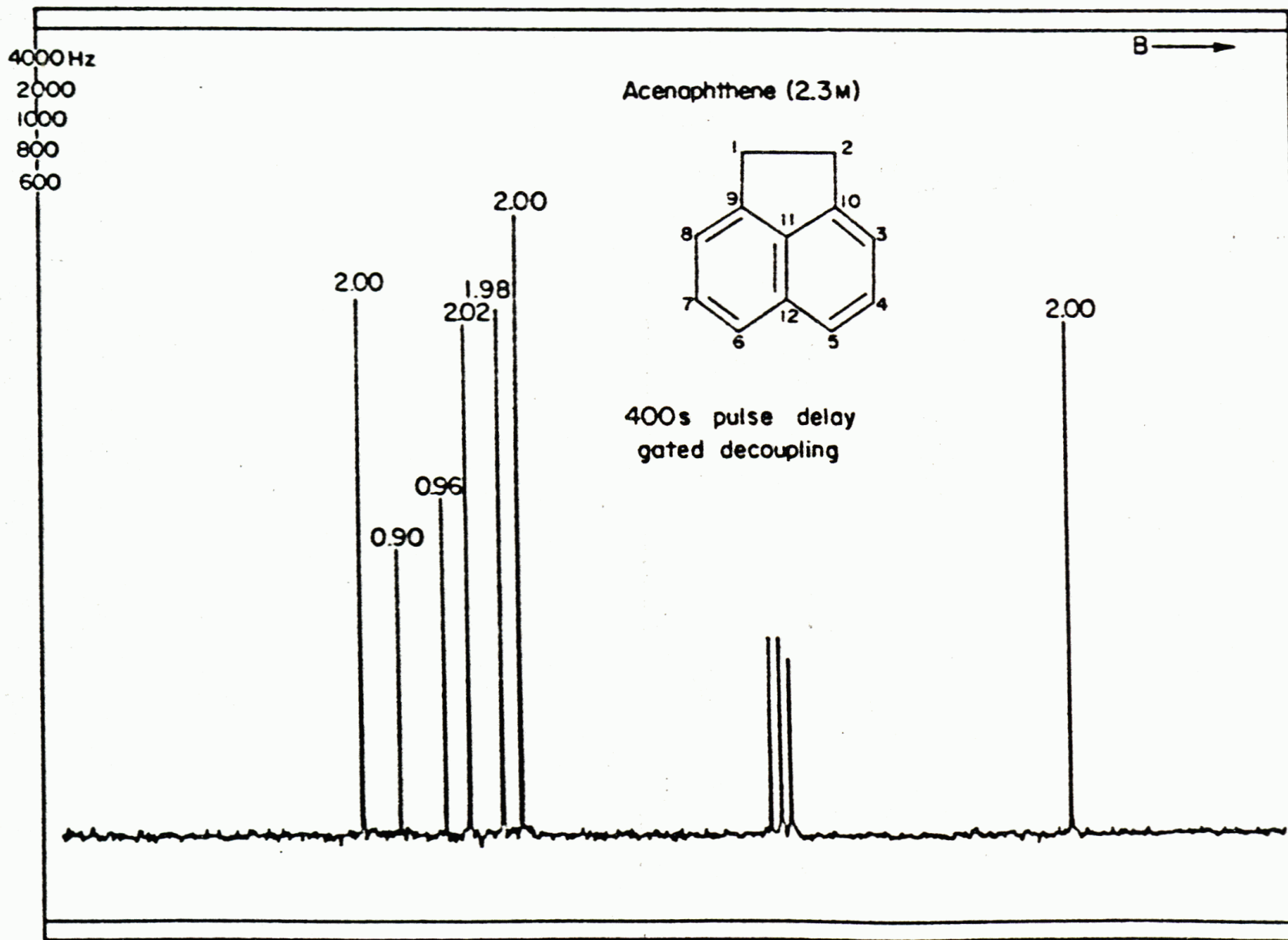
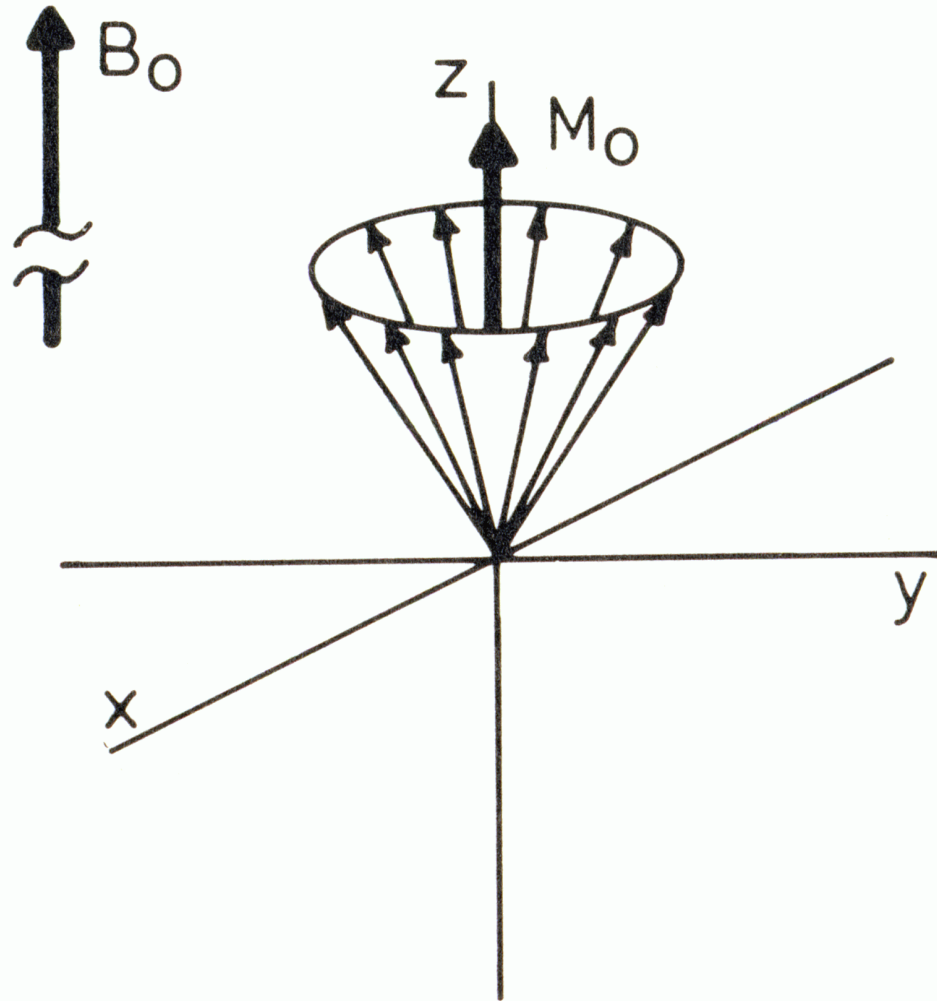
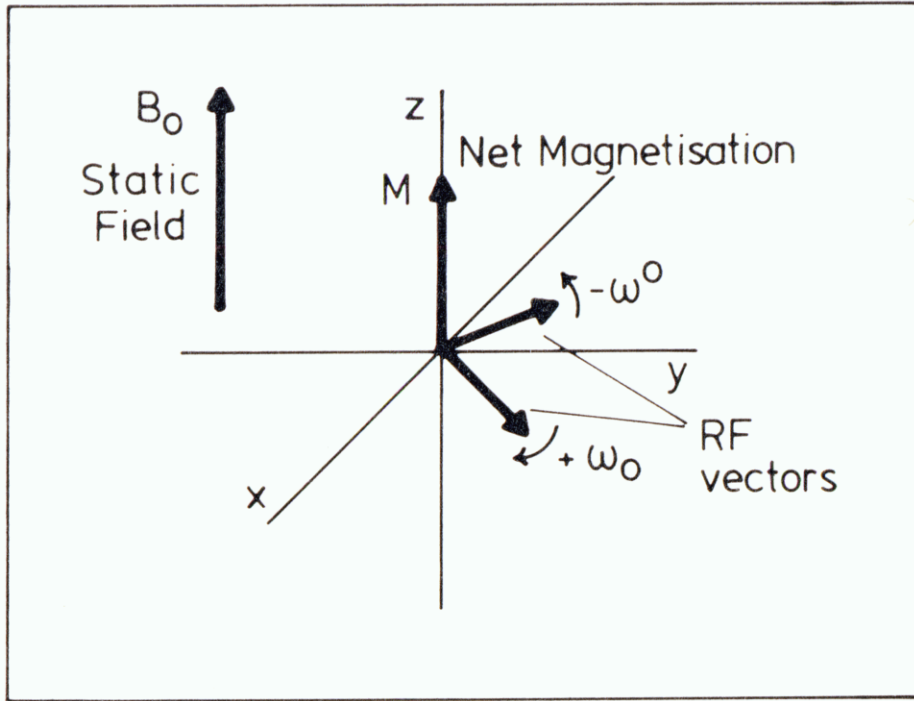
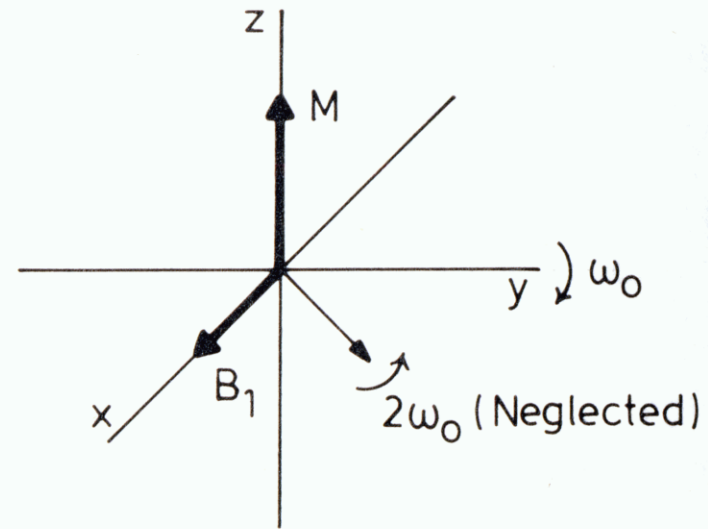


FIG. 3. Acenaphthene ^{13}C spectrum with 400 s pulse delay and decoupler gated 'off' during delay period.

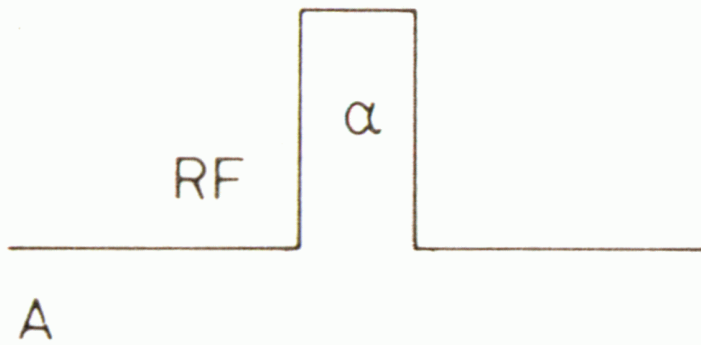
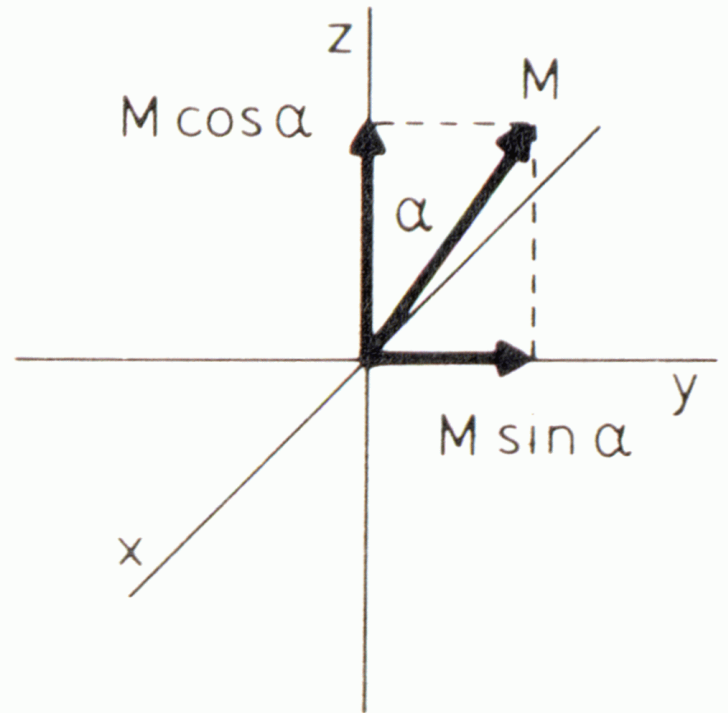
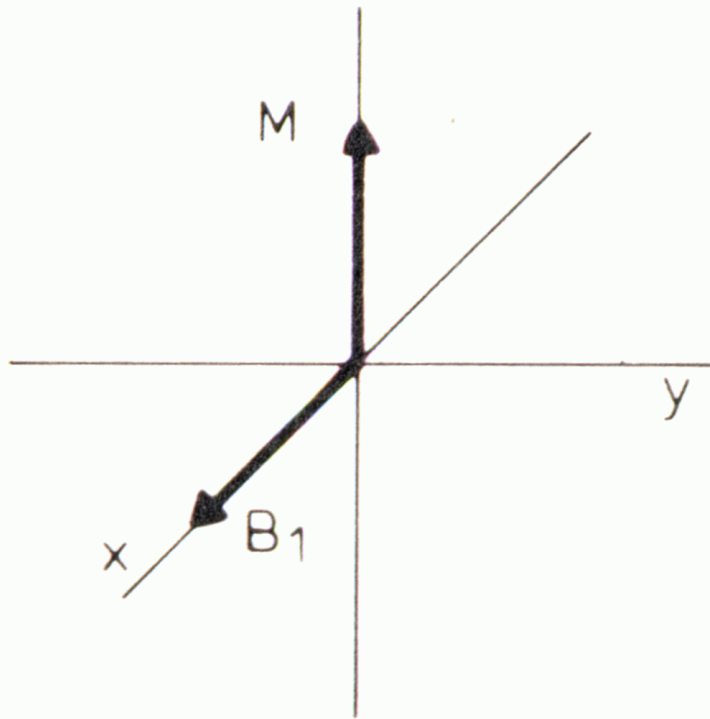


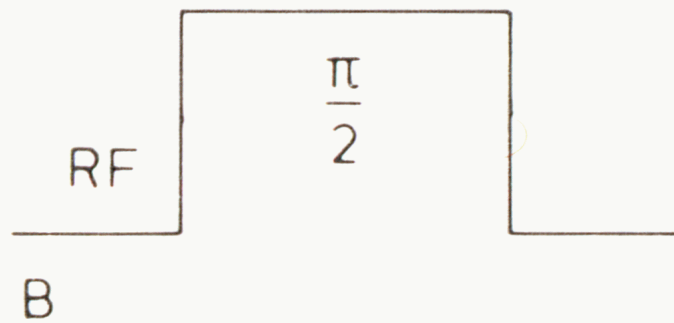
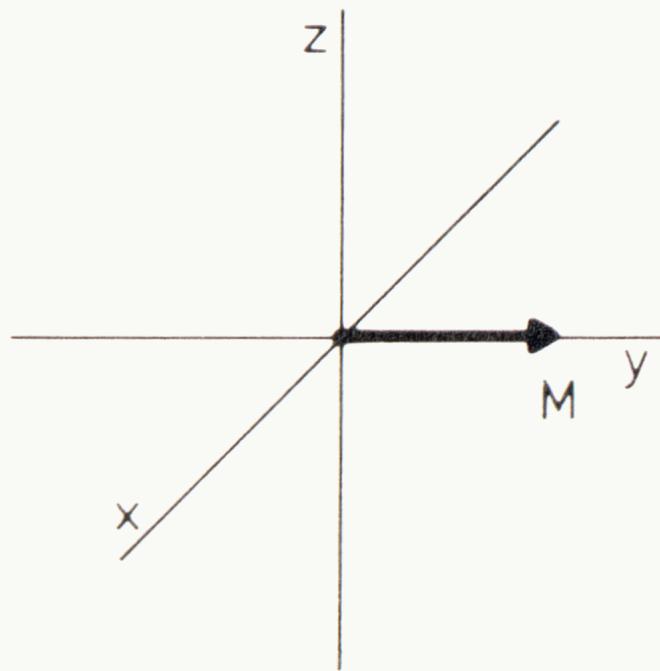
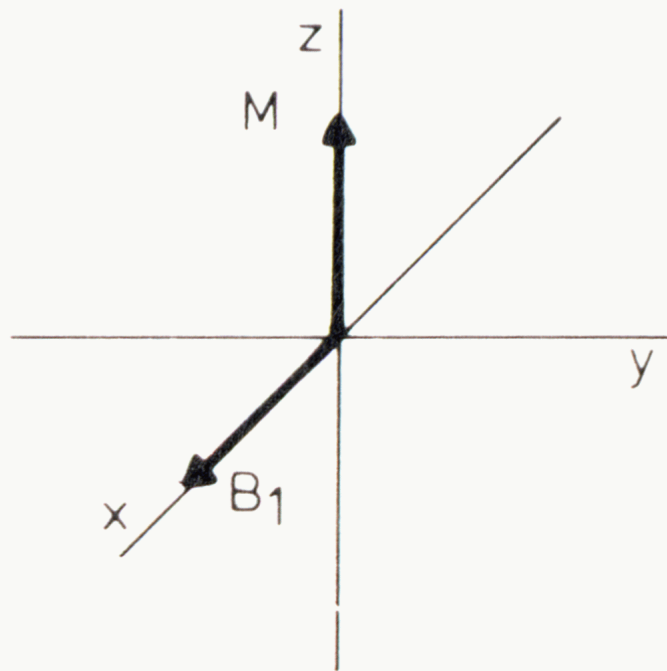


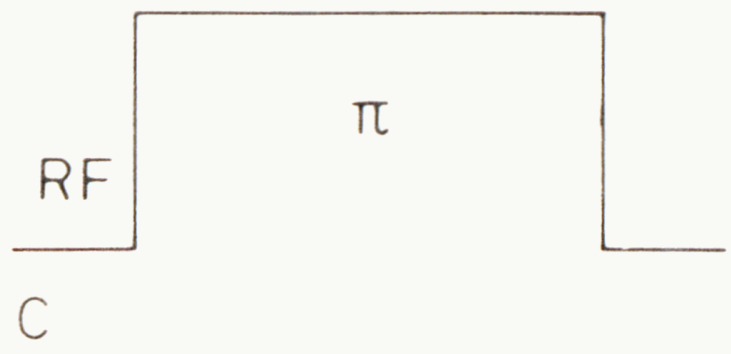
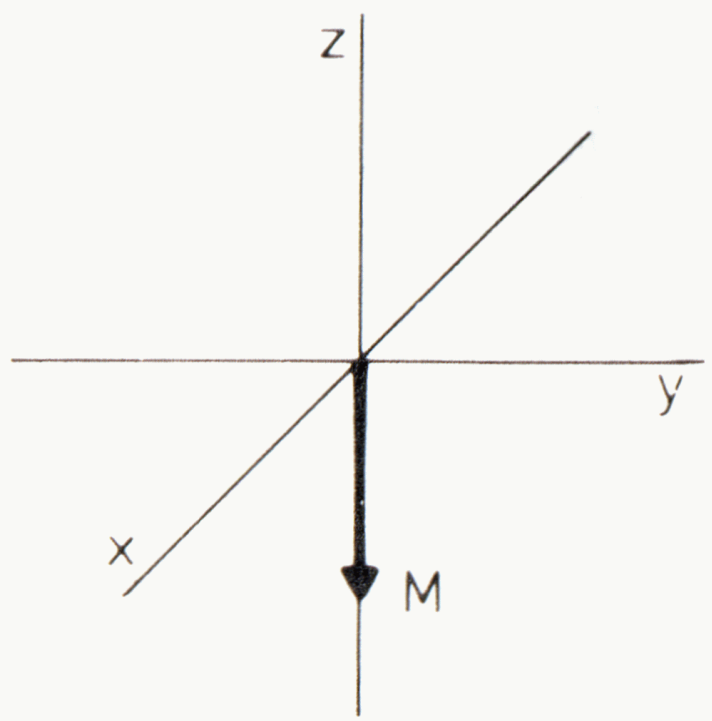
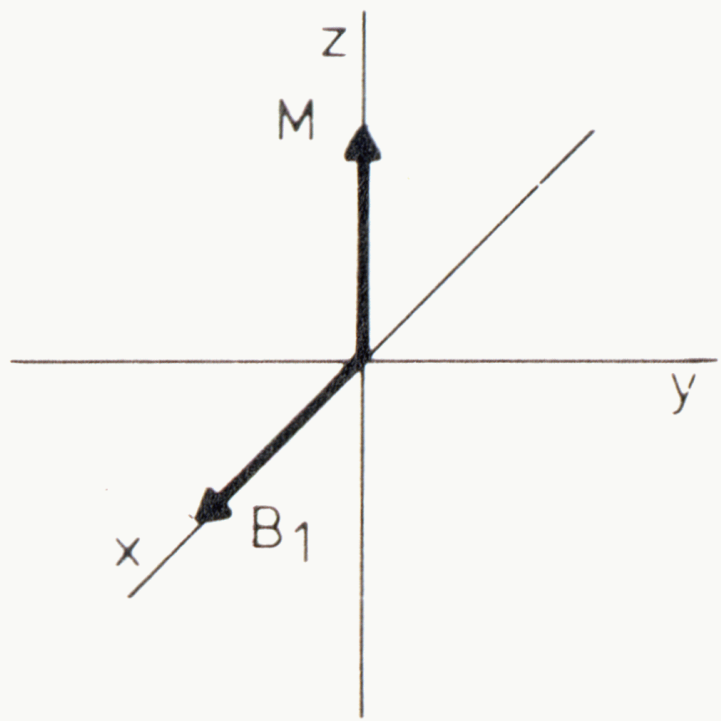
LAB. FRAME



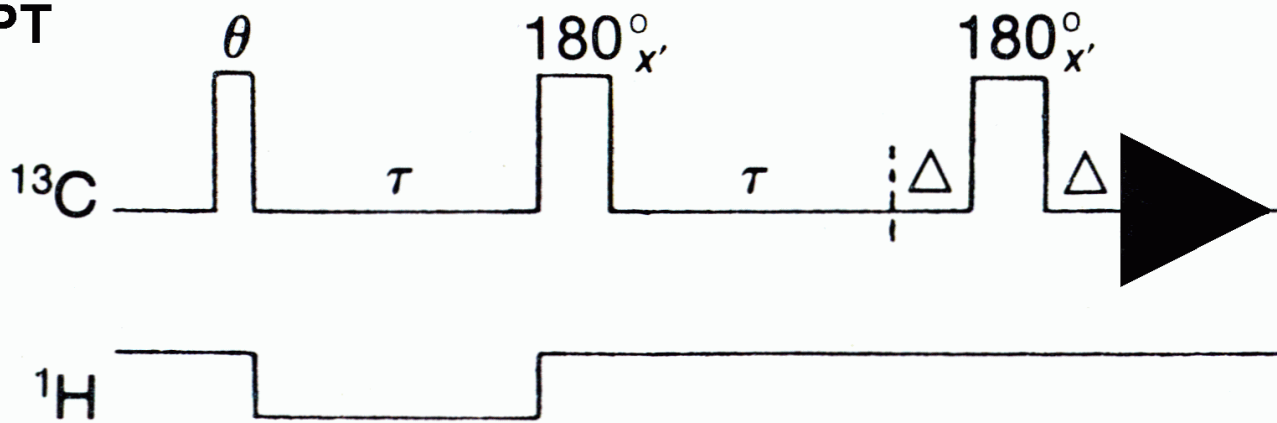
ROTATING FRAME

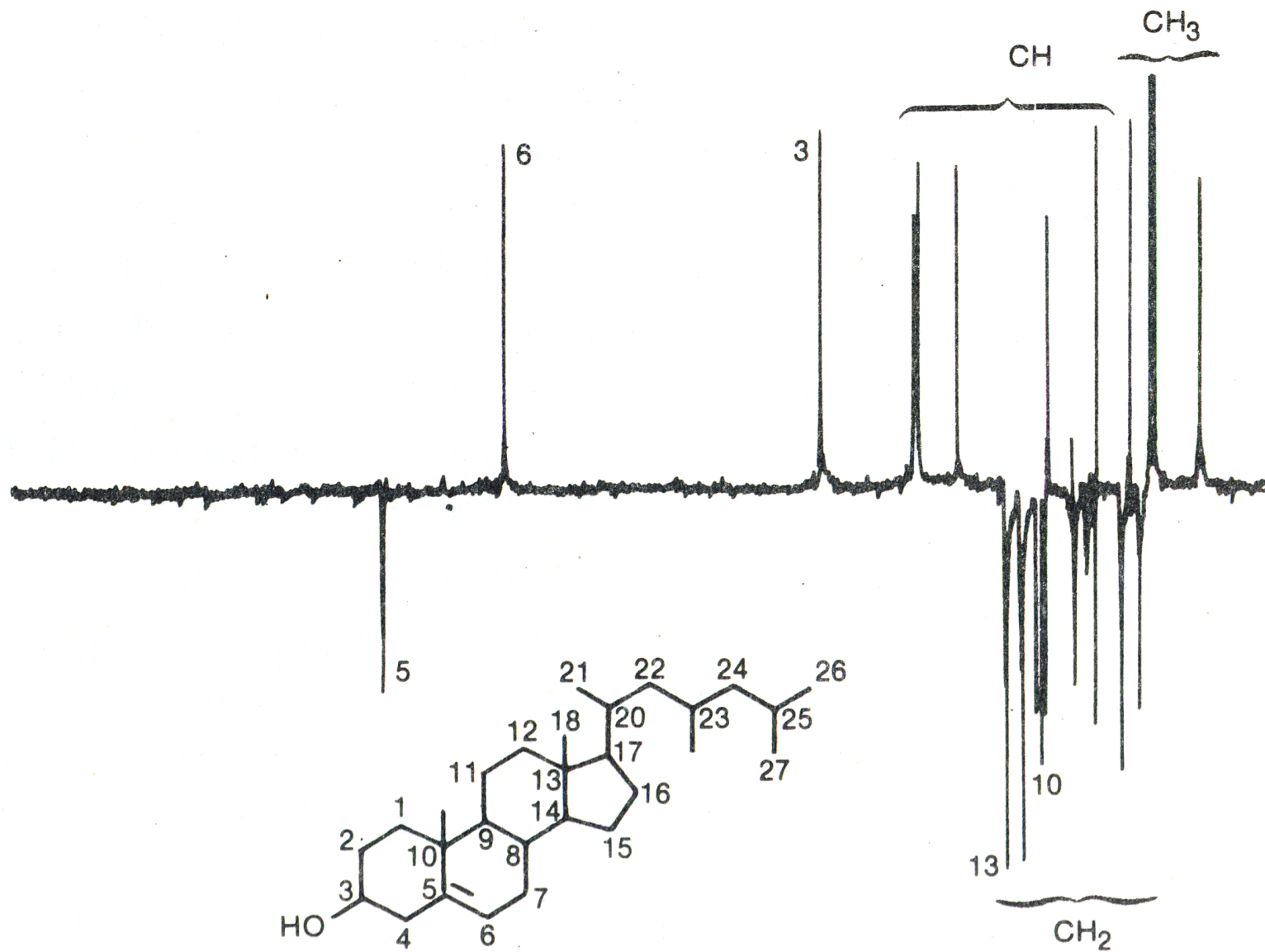




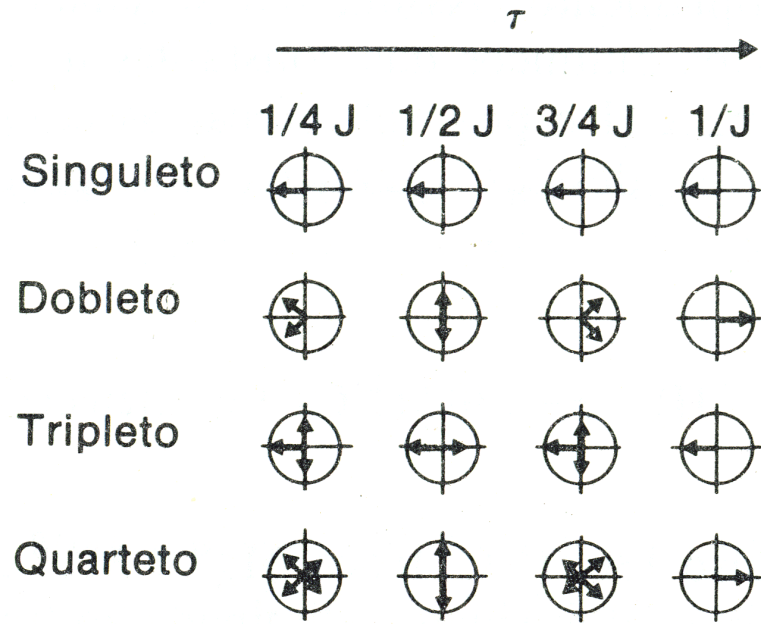


APT

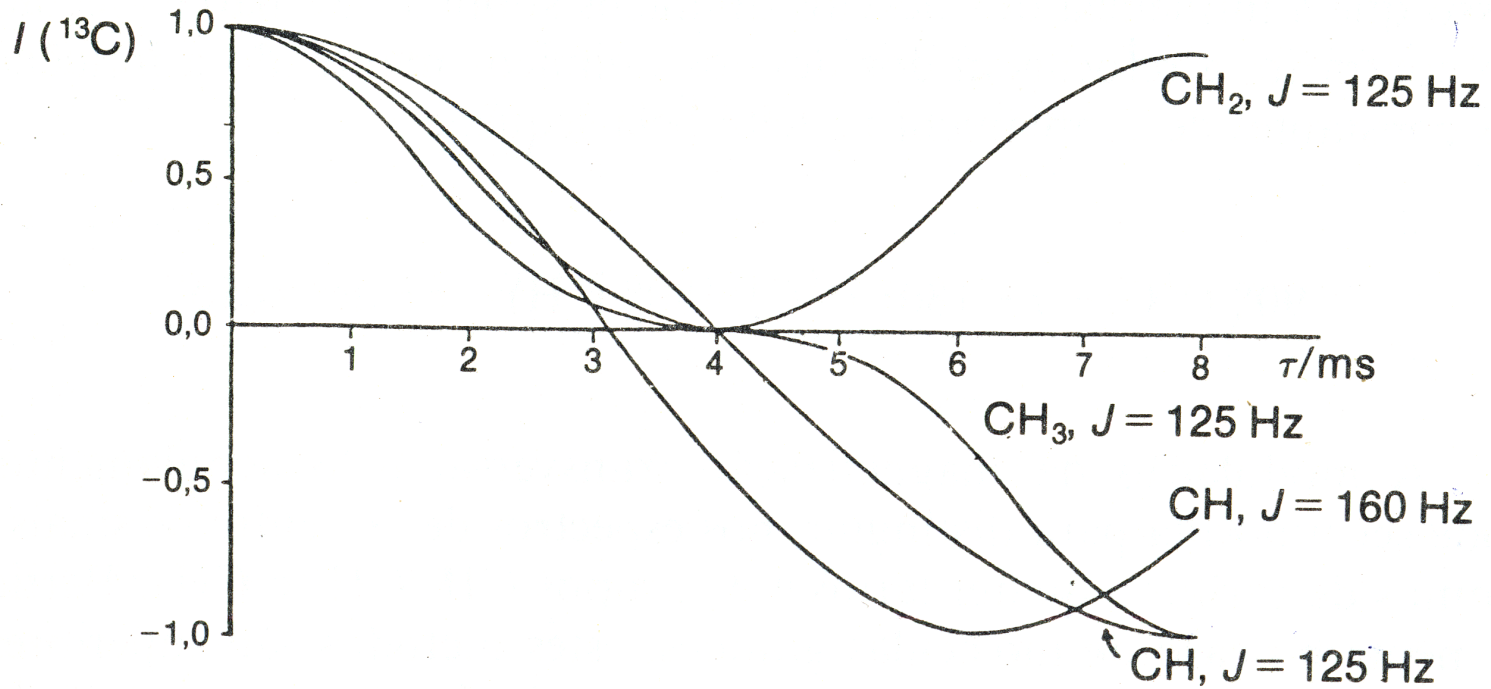


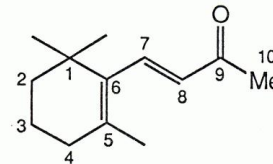


(a)

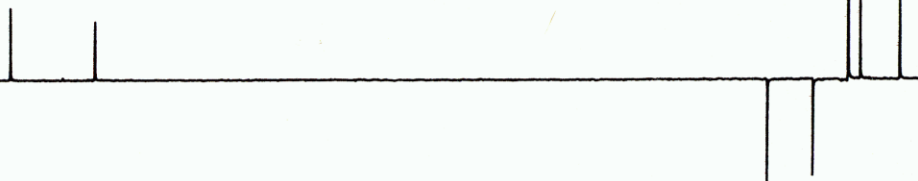


(b)





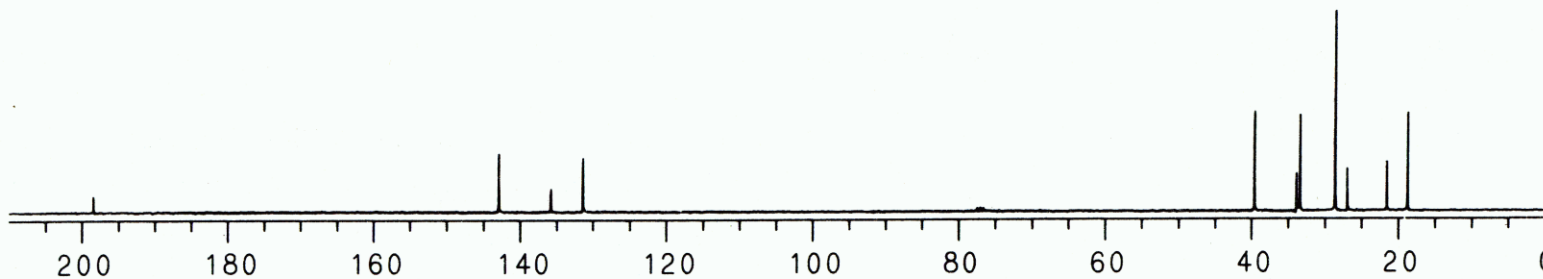
C ($\theta=135^\circ$)



B ($\theta=90^\circ$)



A ($\theta=45^\circ$)



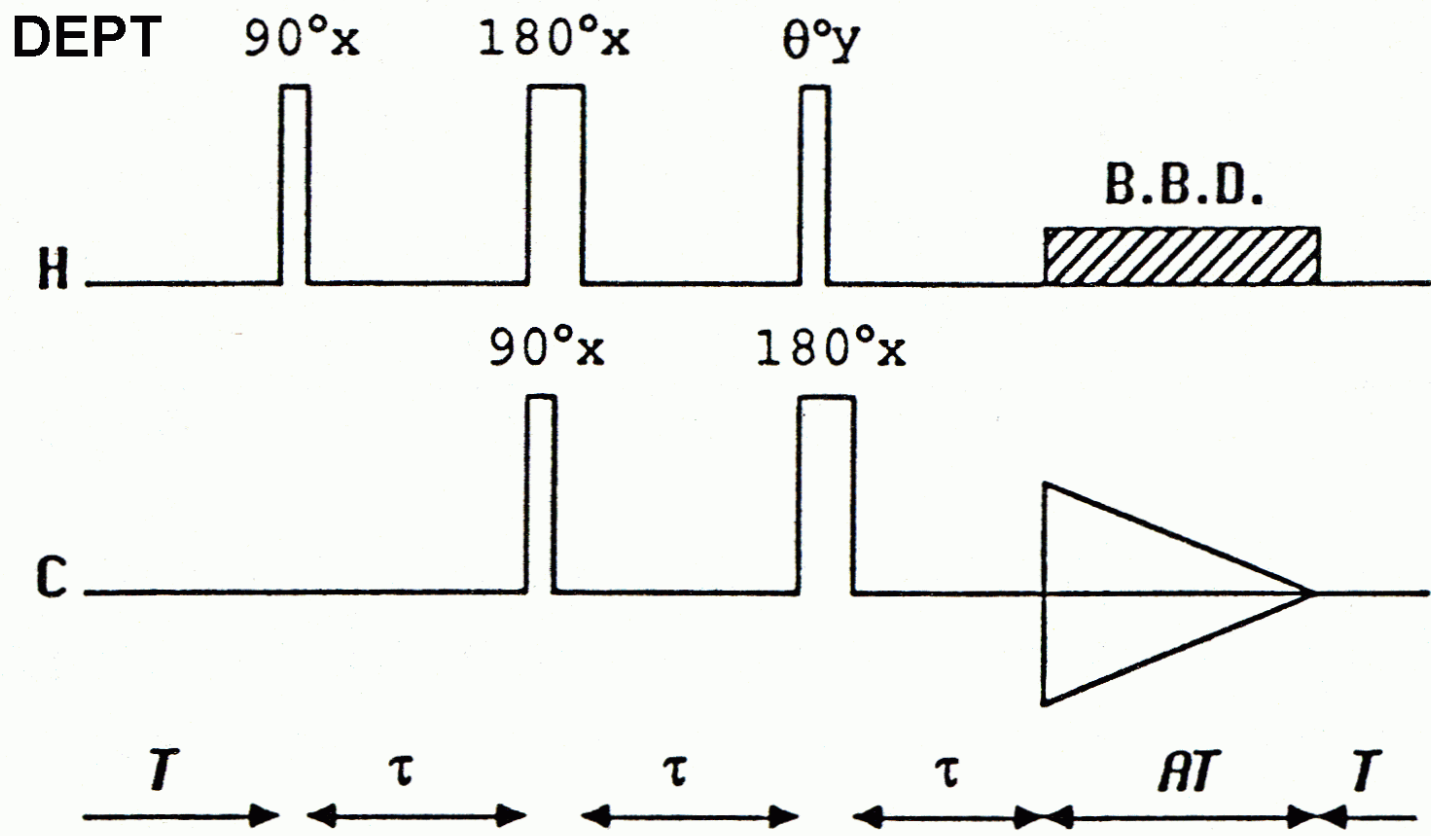
IONONE 100
SUNBOR 21DEC86
BETA-IONONE /CDCL3
DEPT 45 DEG.

D. ENHANCEMENT BY
POLARIZATION TRANSFER

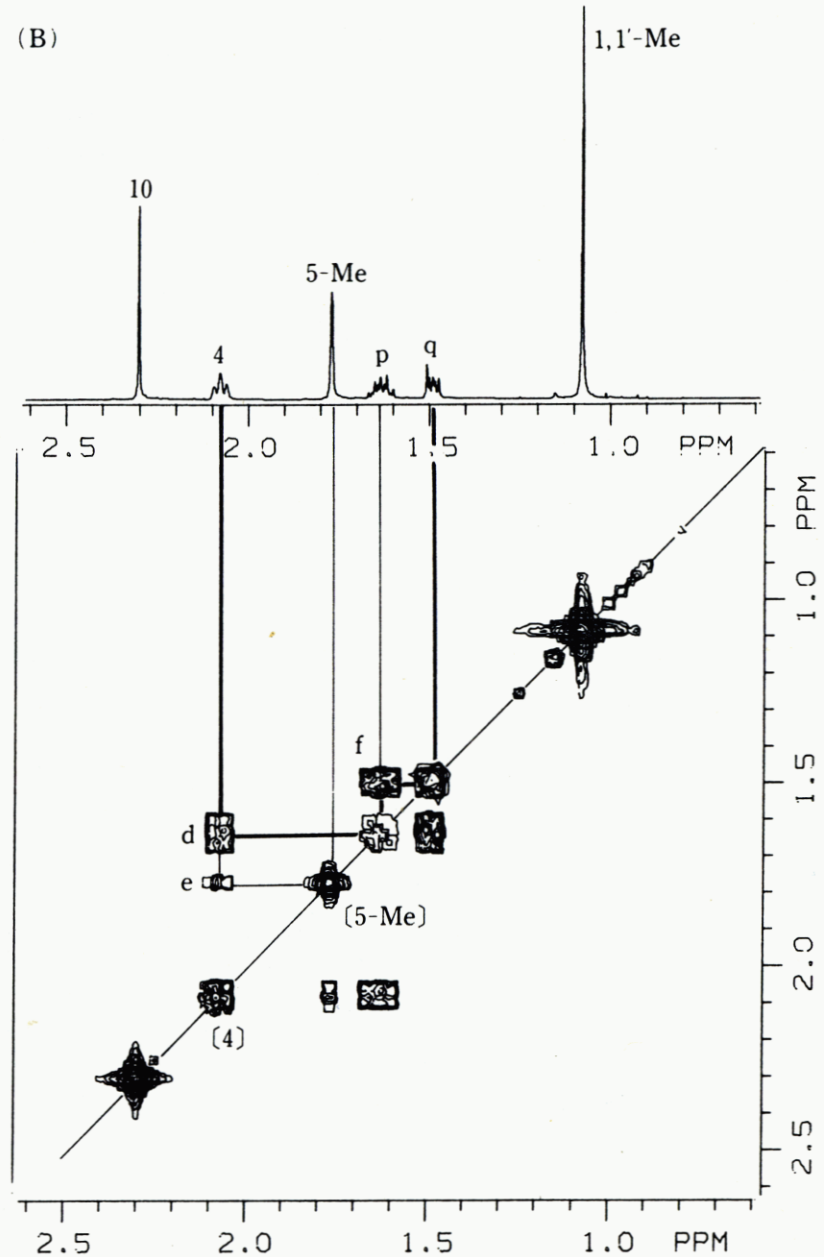
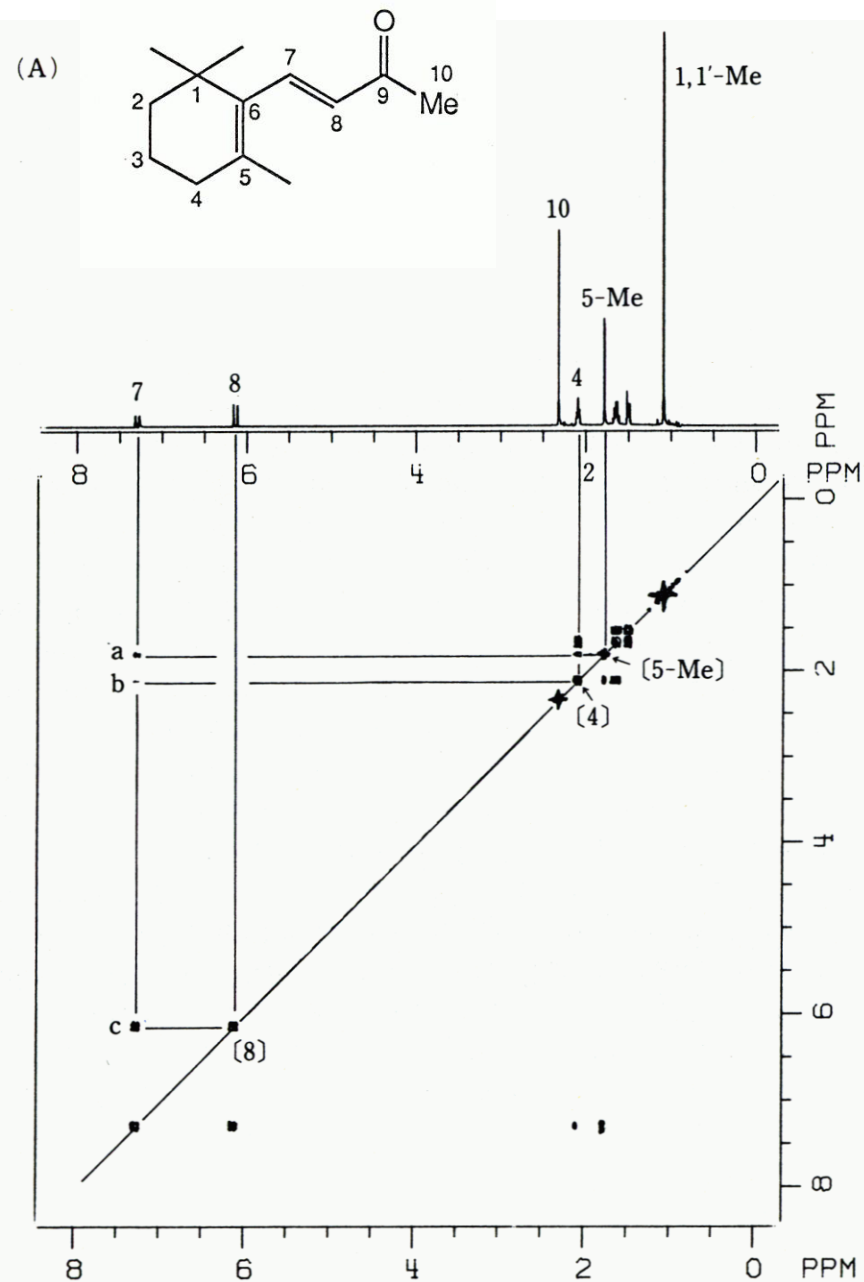
P2 = 11.20 USEC
P4 = 22.40 USEC
D2 = 19.00 USEC
D4 = 38.00 USEC
D5 = 10.00 SEC
D10 = 3.60 MSEC
L1 = 59
L2 = 72
NA = 64
SIZE = 32768
ADC = 12
AI = 8
RC = 10
EM = 1.00
PA = 5.2
PB = -142.6
LOCK = 7.26
OF = 9122.41
SW = +/- 10000.0 HZ
DW = 50 USEC
DE/DW = 50
AT = 819.20 MSEC
SF = 75.4689574
F2 = 300.0997336

OBS HI PWR = 63
OBS LO PWR = 0
DEC PWR = 59
DEC SCHEME = 3
SCALE = 528.32 HZ/CM
= 7.0004 PPM/CM
FROM 210.00
TO 00 PPM

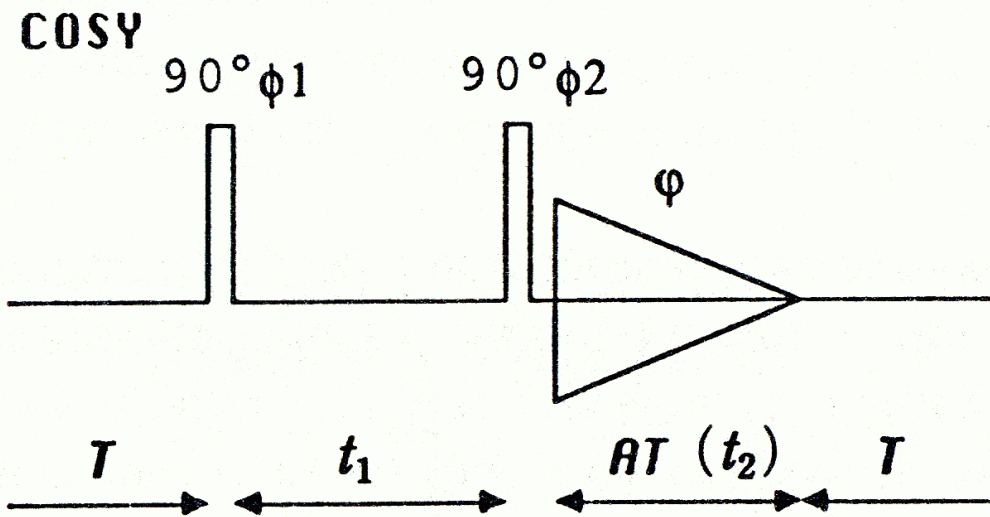
75 MHz ^{13}C -NMR (CDCl₃) [KM]



$$\tau = 1/2 \ ^1J_{CH}$$



360MHz $^1\text{H-NMR}$ (CDCl_3) [TI]



(1) Absolute value mode

ϕ_1	x	x	x	x
ϕ_2	x	y	-x	-y
ϕ	x	-x	x	-x

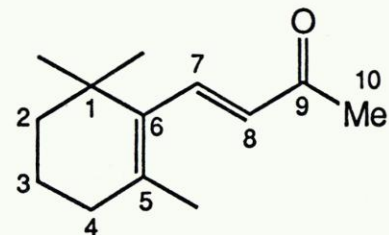
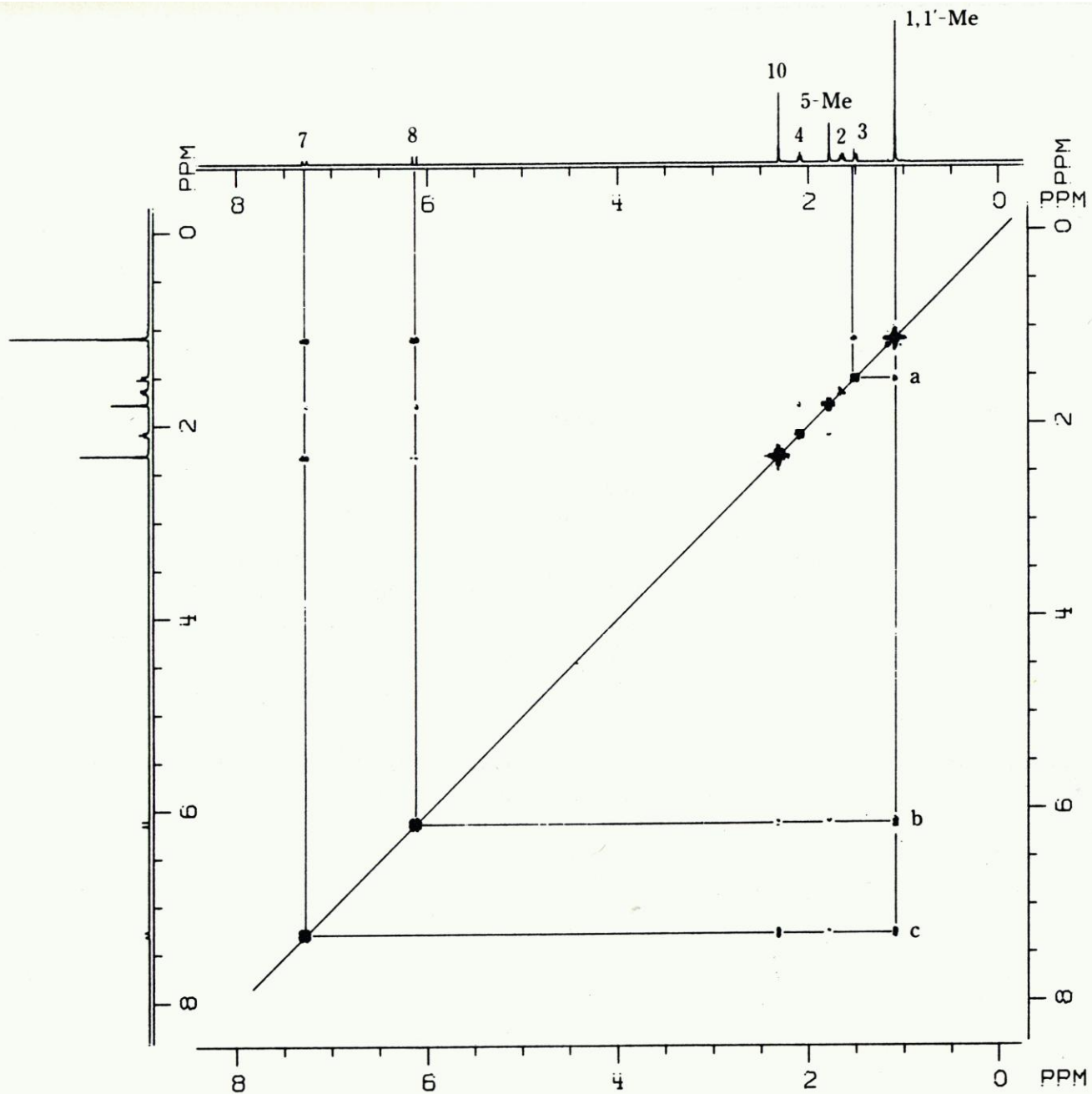
(2) Phase-sensitive mode

Real t_1

ϕ_1	x	x
ϕ_2	x	-x
ϕ	x	x

Imaginary t_1

ϕ_1	x	x
ϕ_2	y	-y
ϕ	y	y

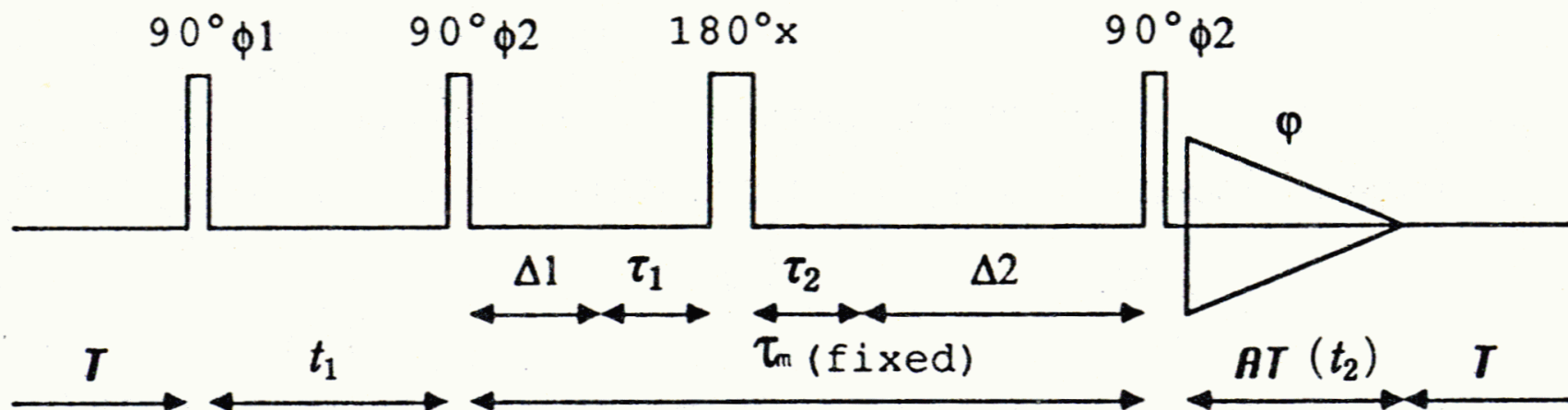


2DNOE
 MIN NA=16. DP=0. AB=-
 DB=DW/4. DB=TM/2
 SYM
 P1= 14.00 USEC
 P2= 7.00 USEC
 D5= 1.00 SEC
 D6= 2.00 SEC
 D8= 80.00 USEC
 I8= 80.00 USEC
 NA = 16
 SIZE = 1024
 AT = 163.84 MSEC
 QPD ON = 0
 ABC OFF
 BUTTERWORTH FILTER ON
 DB ATT. = 3
 ADC = 12 BITS
 A1 = 7
 SW = +/- 1582.50
 DW = 320
 RU = 10 USEC
 DE = 320 USEC
 TL HIGH POWER ON
 QF = 1488.87
 SF = 360.055455
 SCALE 156.25 HZ/CM
 = 4338 PPM/CM
 CONTOUR LEVEL=16
 (15=13688)

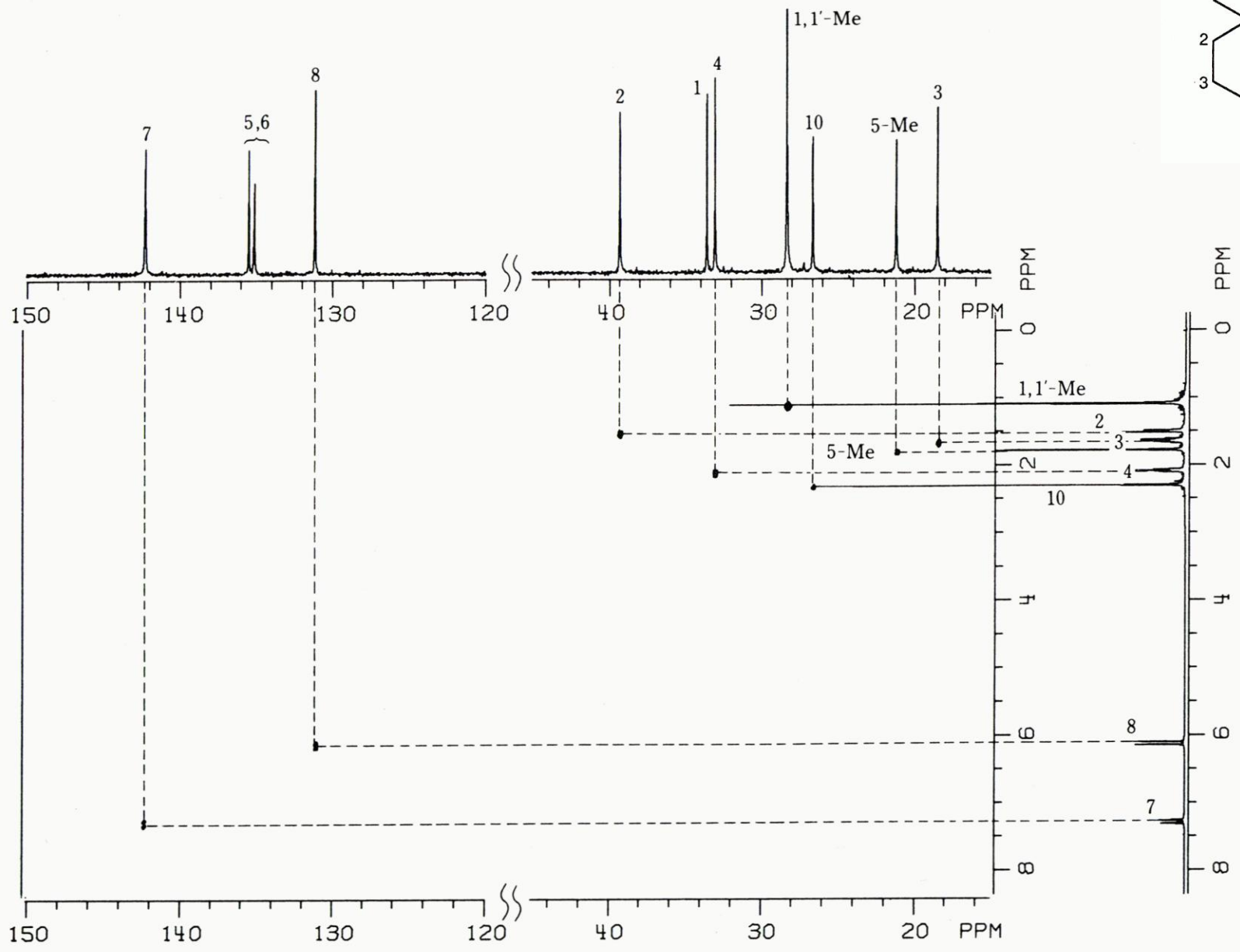
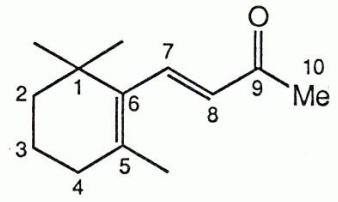
360MHz ¹H-NMR (CDCl₃) [TI]

NOESY

ϕ_1	x	x	x	x
ϕ_2	x	y	-x	-y
φ	x	-x	x	-x



$$\tau_1 = t_1/k, \tau_2 = \Delta - t_1/k \text{ or } \tau_1 = \Delta' \text{ (random), } \tau_2 = \Delta'' \text{ (random)}$$



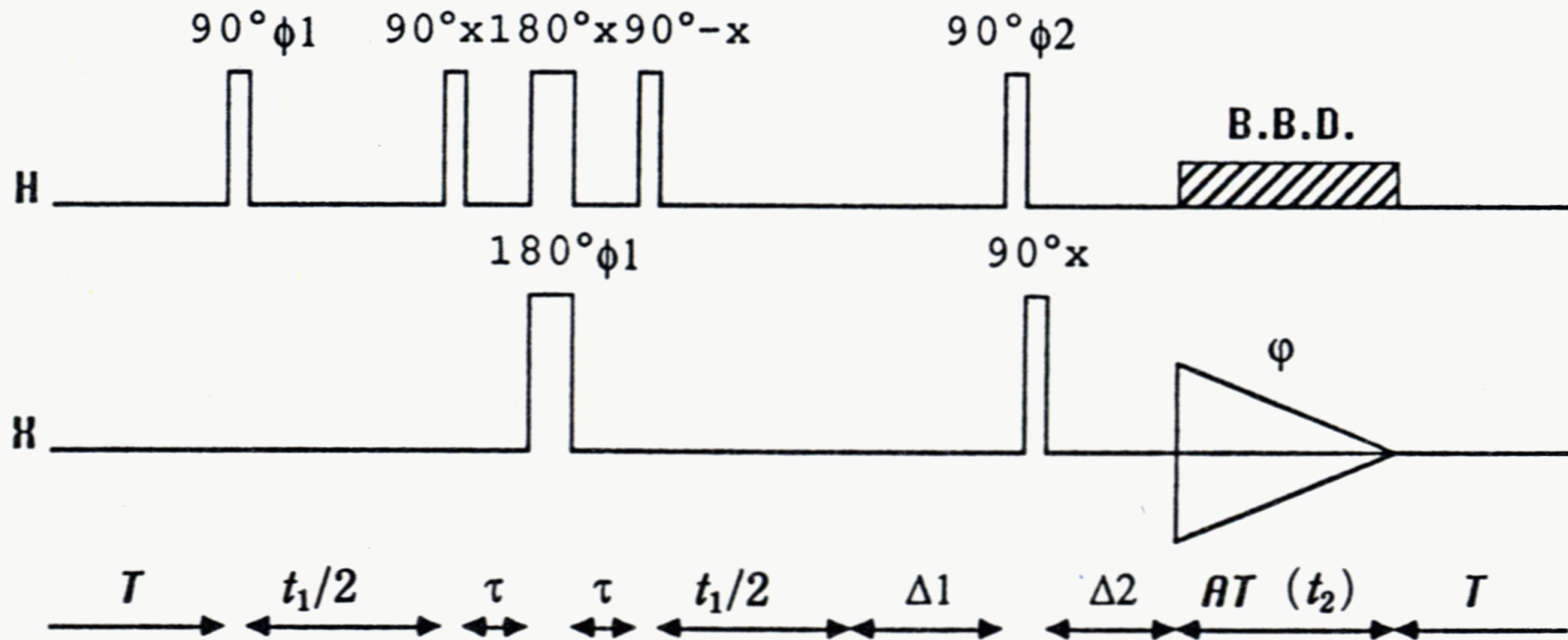
```

CSCM
NA=8.,QP=+0,AB=-
I8=DM/2(H)
P1= 46.00 USEC
P2= 29.00 USEC
D3= 3.30 MSEC
D4= 2.00 MSEC
D5= 1.00 SEC
D6= 94.00 USEC
D8= 160.00 USEC
I8= 160.00 USEC
NA = 128
SIZE = 4096
AT = 102.40 MSEC
QPD ON = 0
ABC OFF
BUTTERWORTH FILTER ON
DB ATT.= 3
ADC = 12 BITS
AI = 13
SW = +/- 10000.0
DM = 50
RG = 10 USEC
DE = 50 USEC
TL HIGH POWER ON
F2= 360.055380
BB MODULATION ON
OF= 9522.70
SF= 90.545201

SCALE 227.05 HZ/CM
      = 2.5075 PPM/CM
MATRIX(F1XF2)=256 X 4K
F1:DM=3
F2:DM=3
CONTOUR LEVEL=6
(YF=17000;Y9=15351)
  
```

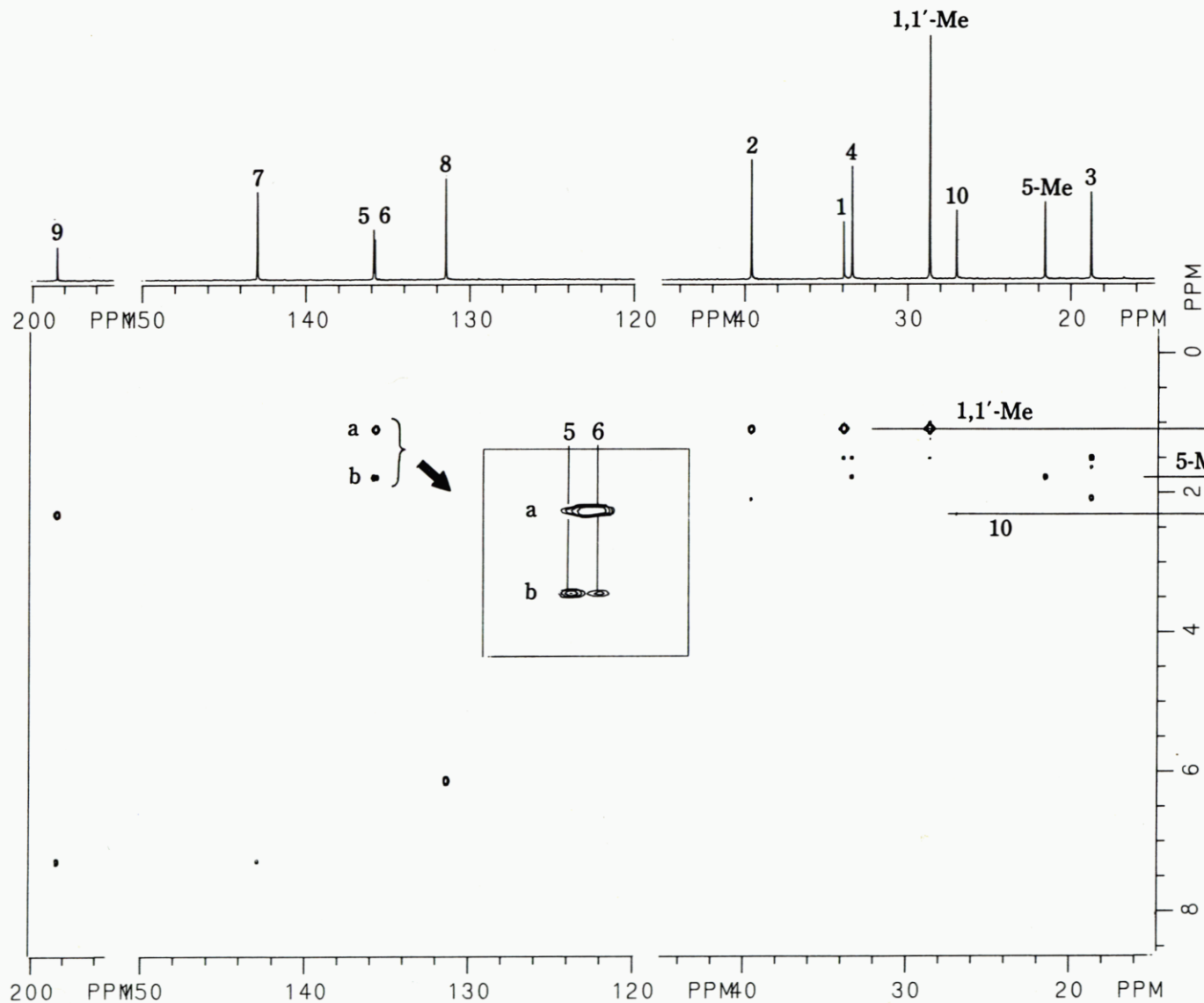
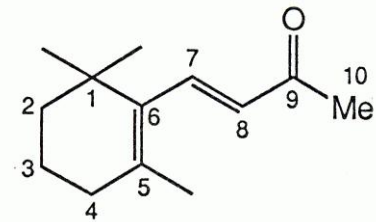
90MHz ¹³C-NMR (CDCl₃) [TI]

HETCOR with F1 decoupling



$$\Delta_1 = 1/2 {}^1J_{XH}, \Delta_2 = 1/3 {}^1J_{XH}, \tau = 1/2 {}^1J_{XH} \quad ({}^1J_{XH} \gg J_{HH})$$

ϕ_1	x	-x	x	-x	-x	x	-x	x
ϕ_2	x	y	-x	-y	-x	-y	x	y
ϕ	x	-y	-x	y	x	-y	-x	y



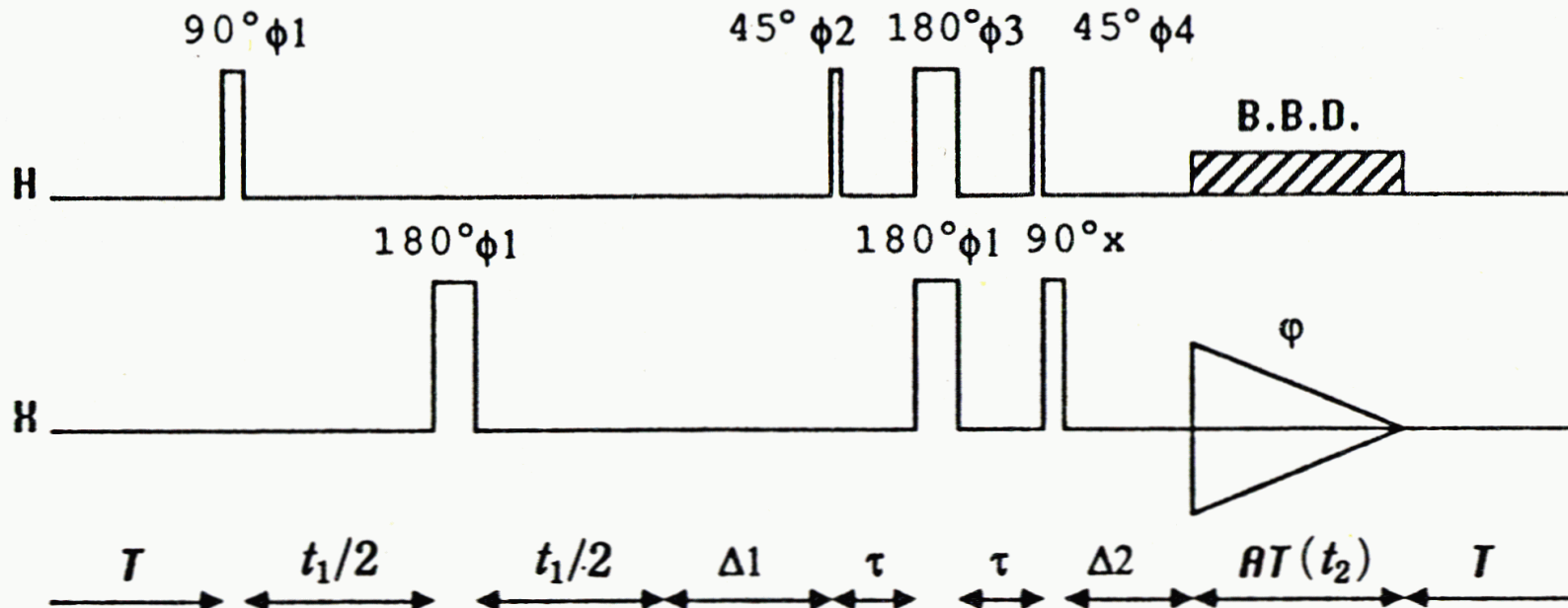
TONONS DAT
 SUNBOR 16OCT87
 BETA-IONONE /CDCl₃
 CSCMLR
 LONG RANGE CORRELATION
 QP+0 AB- NA=8*

P2	=	6.00	USEC
P4	=	12.00	USEC
D1	=	12.50	USEC
D2	=	25.00	USEC
D4	=	50.00	USEC
D5	=	2.00	SEC
D8	=	1.00	USEC
D10	=	50.00	MSEC
D11	=	3.60	MSEC
D12	=	34.00	MSEC
I8	=	112.00	USEC
L1	=	55	
L2	=	82	
NA	=	64	
DC	=	2	
SIZE	=	4096	
ADC	=	16	
AI	=	16	
RG	=	30	
LOCK	=	7.26	
T2	=	32	
OF	=	13833.82	
VOF	=	2060.92	
F1SW	=	27777.77	
F2SW	=	4464.28	
F1DW	=	36	
F2DW	=	224	
F1 ORIG SIZE	=	2048	
F2 ORIG SIZE	=	256	
F1 FINAL SIZE	=	2048	
F2 FINAL SIZE	=	512	
F1SF	=	125.7634616	
F2SF	=	500.099532	

OBS HI PWR = 63
 OBS-LO PWR = 2047
 DEC PWR = 55
 DEC SCHEME = 3
 SCALE = 315.34 HZ/CM
 = 2.5074 PPM/CM
 FROM 150.01
 TO 120.02 PPM
 CONTOUR LEVEL=5
 HEIGHT=3072
 MAX. HEIGHT=12288

125 MHz ¹³C-NMR (CDCl₃) [TI]

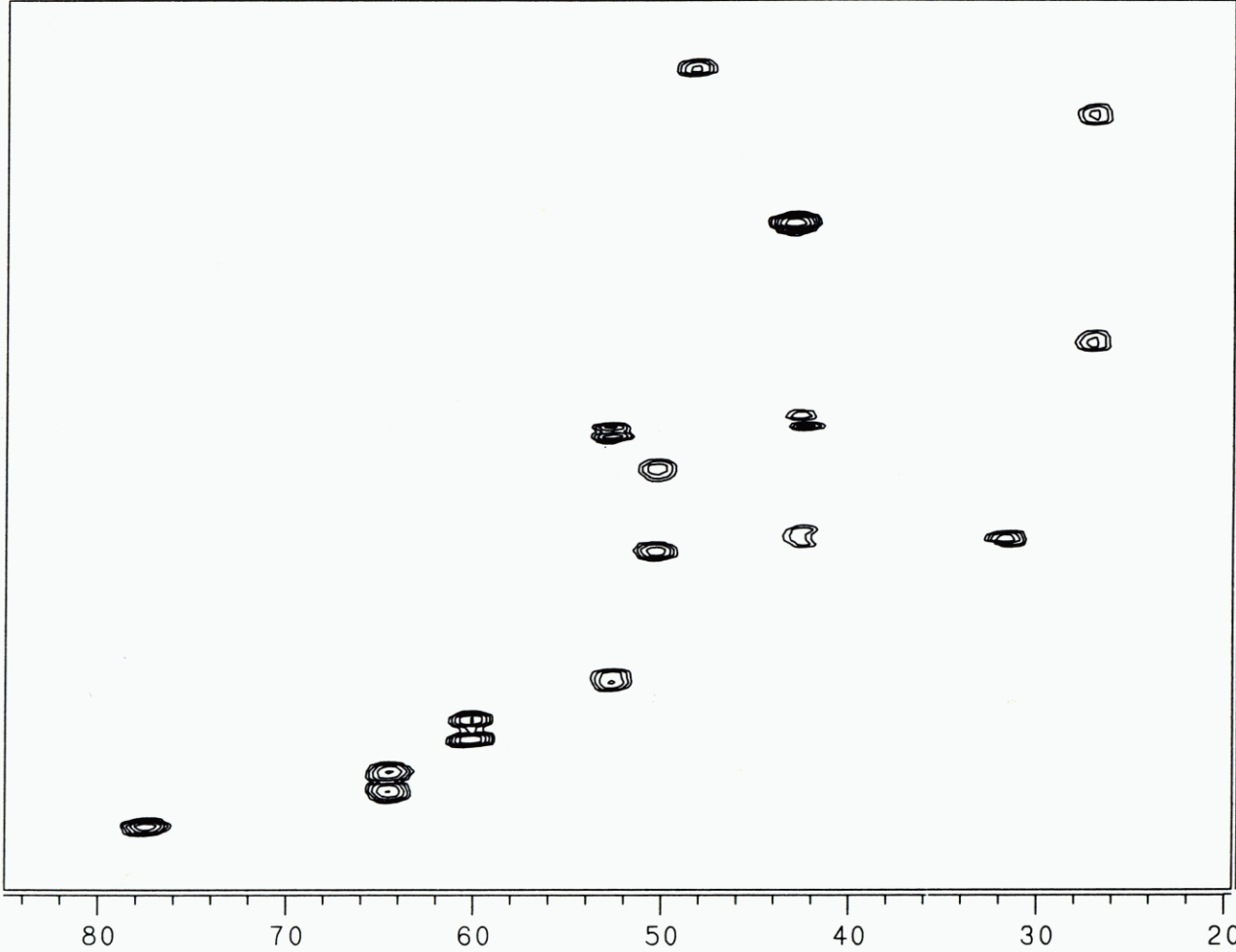
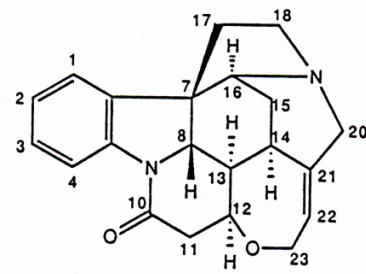
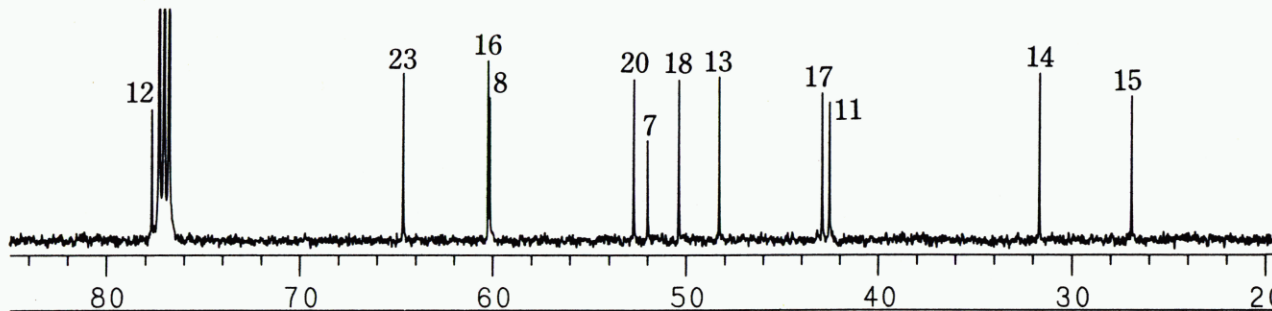
HETCOR-LR for long range spin-spin coupling



ϕ_1	x	-x	x	-x	-x	x	-x	x
ϕ_2	x	y	-x	-y	-x	-y	x	y
ϕ_3	y	-x	-y	x	-y	x	y	-x
ϕ_4	-x	-y	x	y	x	y	-x	-y
ϕ	x	-y	-x	y	x	-y	-x	y

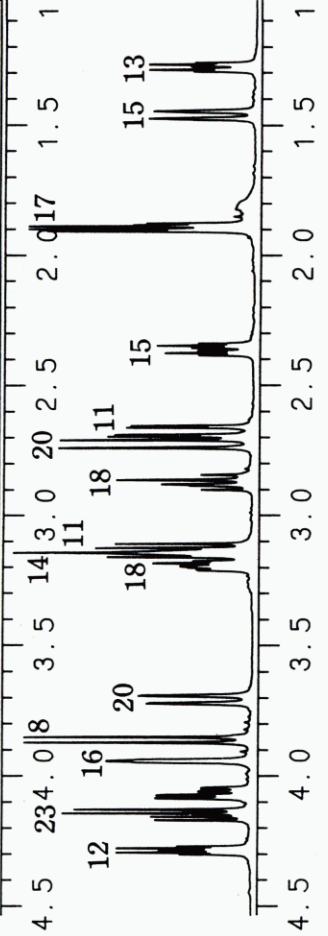
$$\Delta_1 = 1/2 {}^{\text{lr}}J_{\text{XH}}, \Delta_2 = 1/2 {}^{\text{lr}}J_{\text{XH}} \sim 1/3 {}^{\text{lr}}J_{\text{XH}}, \tau = 1/2 {}^1J_{\text{XH}}$$

(${}^{\text{lr}}J_{\text{XH}}$: long range spin-spin coupling between X and H)



PPM

1-D PPM



```

STRO3   DAT
SUNBOR  18NOV88

STRYCHNINE /CDCL3
HMQCSM  /NO SPIN

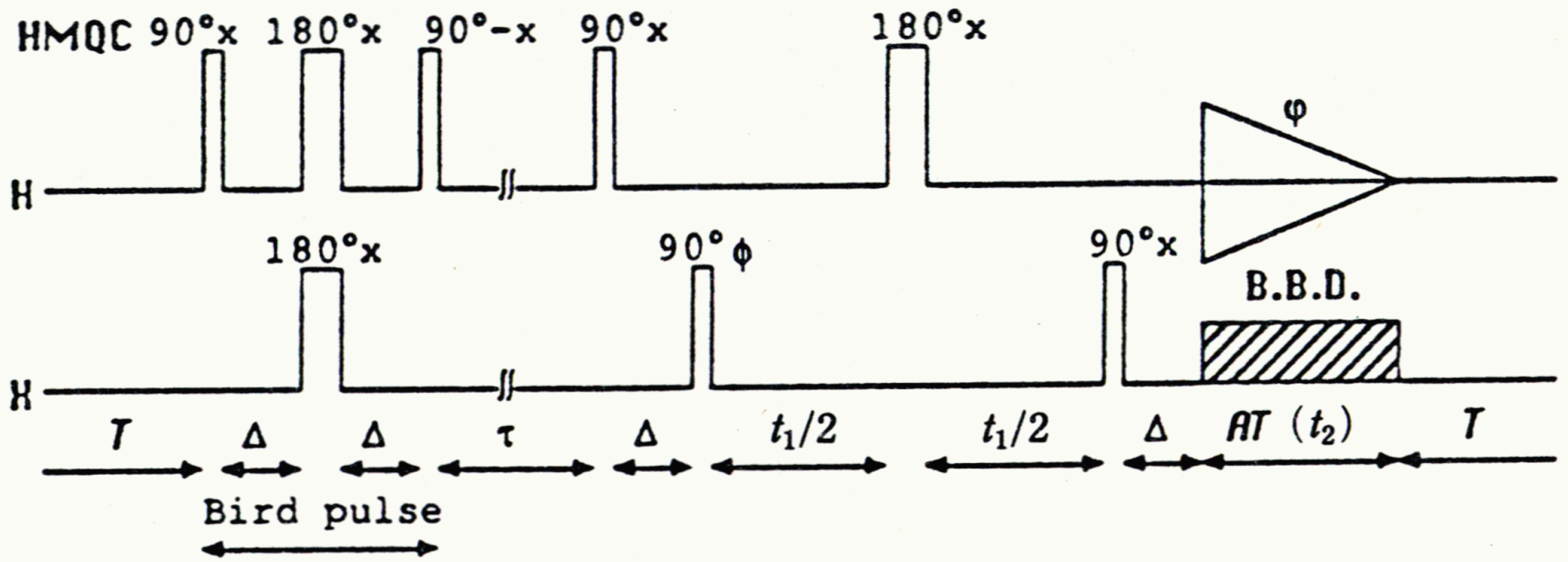
HMQC FOR SMALL MOL.
MB=2 QP+0 AB- NA=4+

P2      = 16.00 USEC
P4      = 32.00 USEC
D2      = 42.00 USEC
D4      = 84.00 USEC
D5      = 1.00 SEC
D8      = 1.00 USEC
D9      = 15.00 USEC
D10     = 30.00 USEC
D11     = 3.60 MSEC
D12     = 200.00 MSEC
I8      = 19.00 USEC
NA      = 16
DC      = 2
SIZE    = 1024
ADC     = 16
AI      = 4
RC      = 10
GM      = 205.76
PA      = -4.2
LOCK    = 7.26
OF      = 12485.09
VOF     = 1983.53
F1SW   = 5000.00
F2SW   = 26315.78
F1DW   = 200
F2DW   = 38
F1 ORIG SIZE = 1024
F2 ORIG SIZE = 128
F1 FINAL SIZE = 512
F2 FINAL SIZE = 512
F1SF   = 500.099498
F2SF   = 125.7621900

OBS HI PWR = 63
OBS LO PWR = 0
DEC PWR    = 0
DEC SCHEME = 4
SCALE     = 328.94 HZ/CM
          = 2.6156 PPM/CM

FROM      84.97
TO        19.98 PPM
CONTOUR LEVEL=6
MAX. HEIGHT=8968
  
```

500 MHz ¹H-NMR (CDCl₃) [TI]



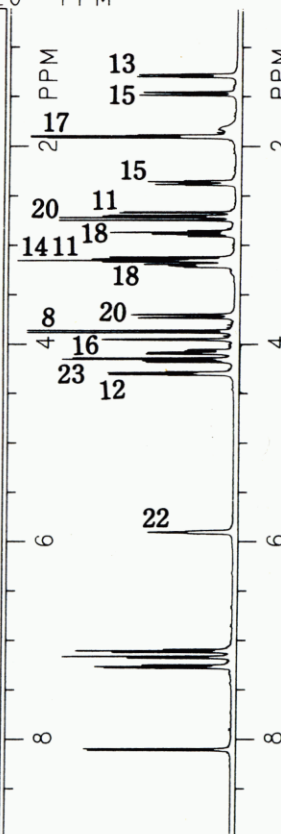
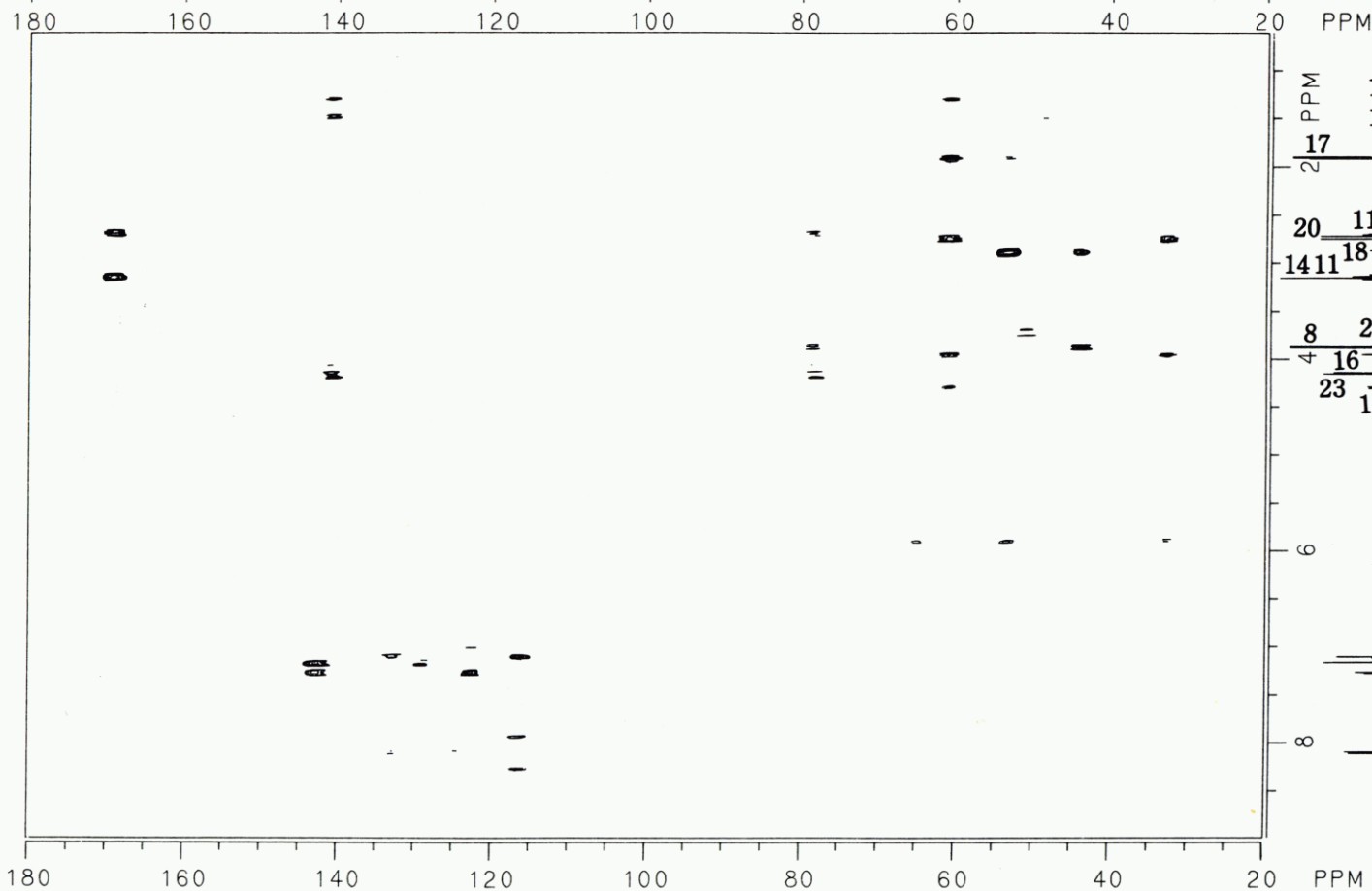
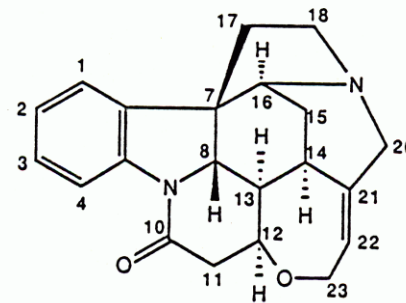
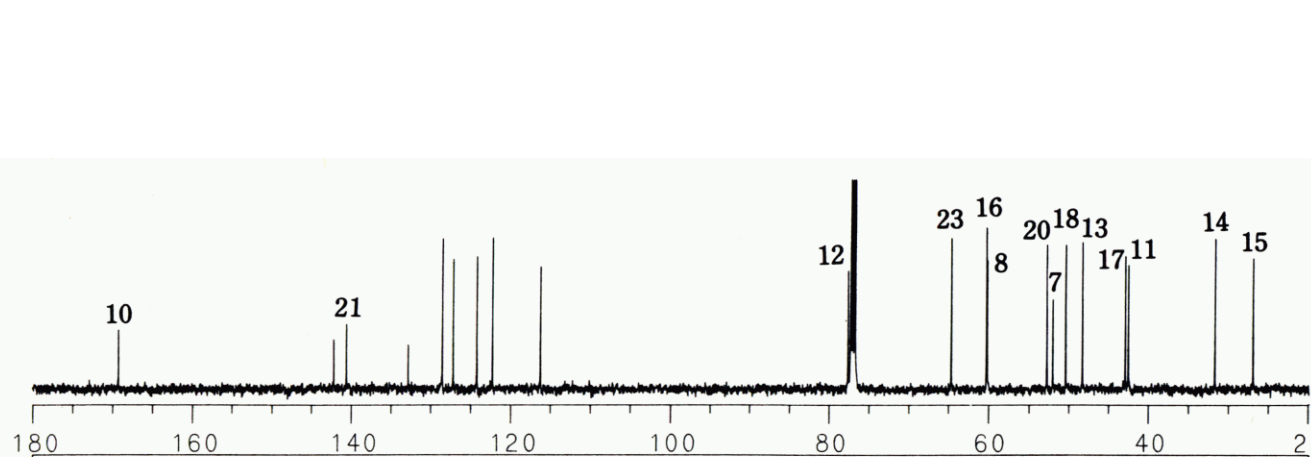
Real t_1 :

ϕ	x	-x	x	-x
ϕ	x	-x	x	-x

Imaginary t_1 :

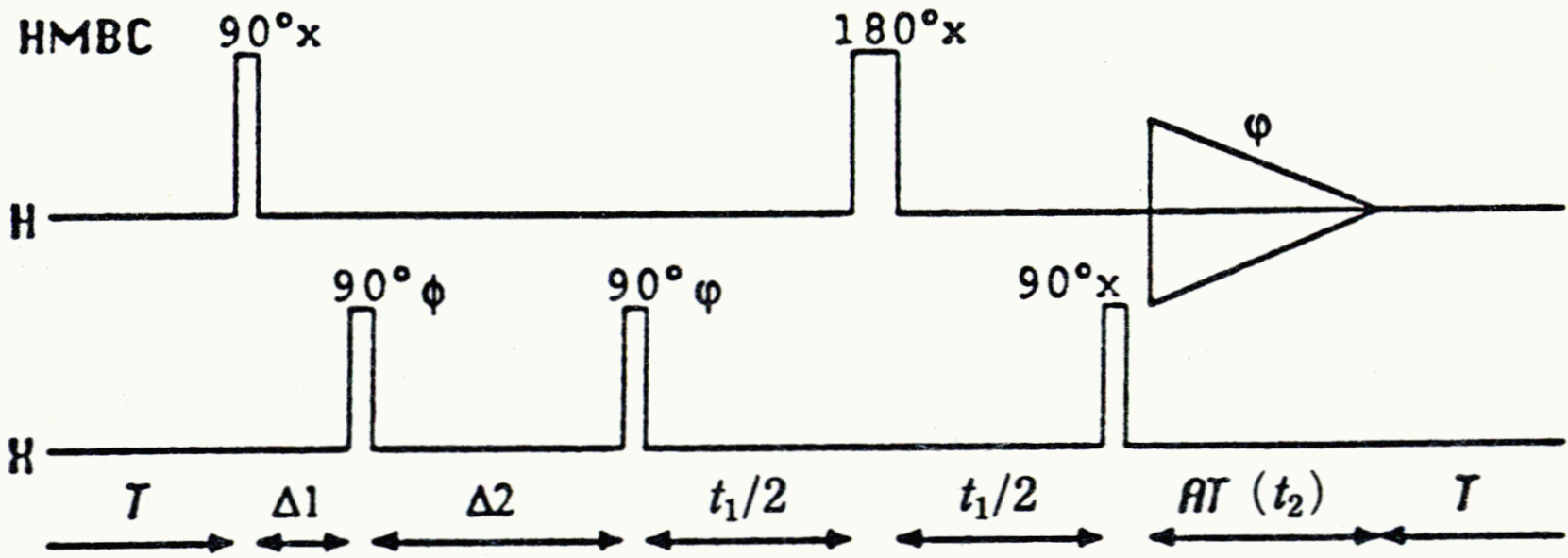
ϕ	y	-y	y	-y
ϕ	x	-x	x	-x

$\Delta_1 = 1/2 {}^1J_{XH}$, τ depends on T_1 of proton.



HMBC3 DAT
 SUNBOR 24DEC87
 STRYCHININE /CDCL3
 HMBC /NO SPIN
 HMBC QP+0 AB- MC NA=32*
 P2 = 14.00 USEC
 P4 = 28.00 USEC
 D5 = 2.50 SEC
 D8 = 1.00 USEC
 D9 = 14.50 USEC
 D11 = 3.60 MSEC
 D12 = 50.00 MSEC
 I8 = 19.00 USEC
 NA = 128
 DC = 4
 SIZE = 1024
 ADC = 16
 AI = 10
 RC = 10
 LOCK = 7.26
 OF = 12568.15
 VOF = 1992.01
 F1SW = 28315.78
 F2SW = 5000.00
 F1DW = 38
 F2DW = 200
 F1 ORIG SIZE = 1024
 F2 ORIG SIZE = 128
 F1 FINAL SIZE = 1024
 F2 FINAL SIZE = 512
 F1SF = 125.7621900
 F2SF = 500.099498
 OBS HI PWR = 63
 OBS LO PWR = 0
 DEC PWR = 0
 DEC SCHEME = 4
 SCALE = 939.84 HZ/CM
 = 7.4732 PPM/CM
 FROM 204.56
 TO -4.28 PPM
 CONTOUR LEVEL=6
 (HEIGHT=5000)
 MAX. HEIGHT=5491

500 MHz ¹H-NMR (CDCl₃) [TI]



ϕ	x	x	-x	-x	x	x	-x	-x
ψ	x	-x	x	-x	y	-y	y	-y

$\Delta_1 = 1/2 \ ^1J_{XH}$, Δ_2 is about 60 ms.