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Effects of Substituent Modification on Face Selection in Reduction
by
Cheryl D. J. Jones, Mira Kaselj, Ralph N. Salvatore and William J. le Noble
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	9.	----	C,D	47.	----	C,D
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	27.	----	H,d			
	28.	----	H,d			
	29.	----	C			
	30.	----	C,D			
	31.	----	C,d			
	32.	----	C,d,D			
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	34.	----	H,d			
	35.	----	C			
	36.	----	C,D			
	37.	----	C,d			
	38.	----	C,d,D			

* G = gas chromatogram

H = ¹H NMR

C = ¹³C NMR

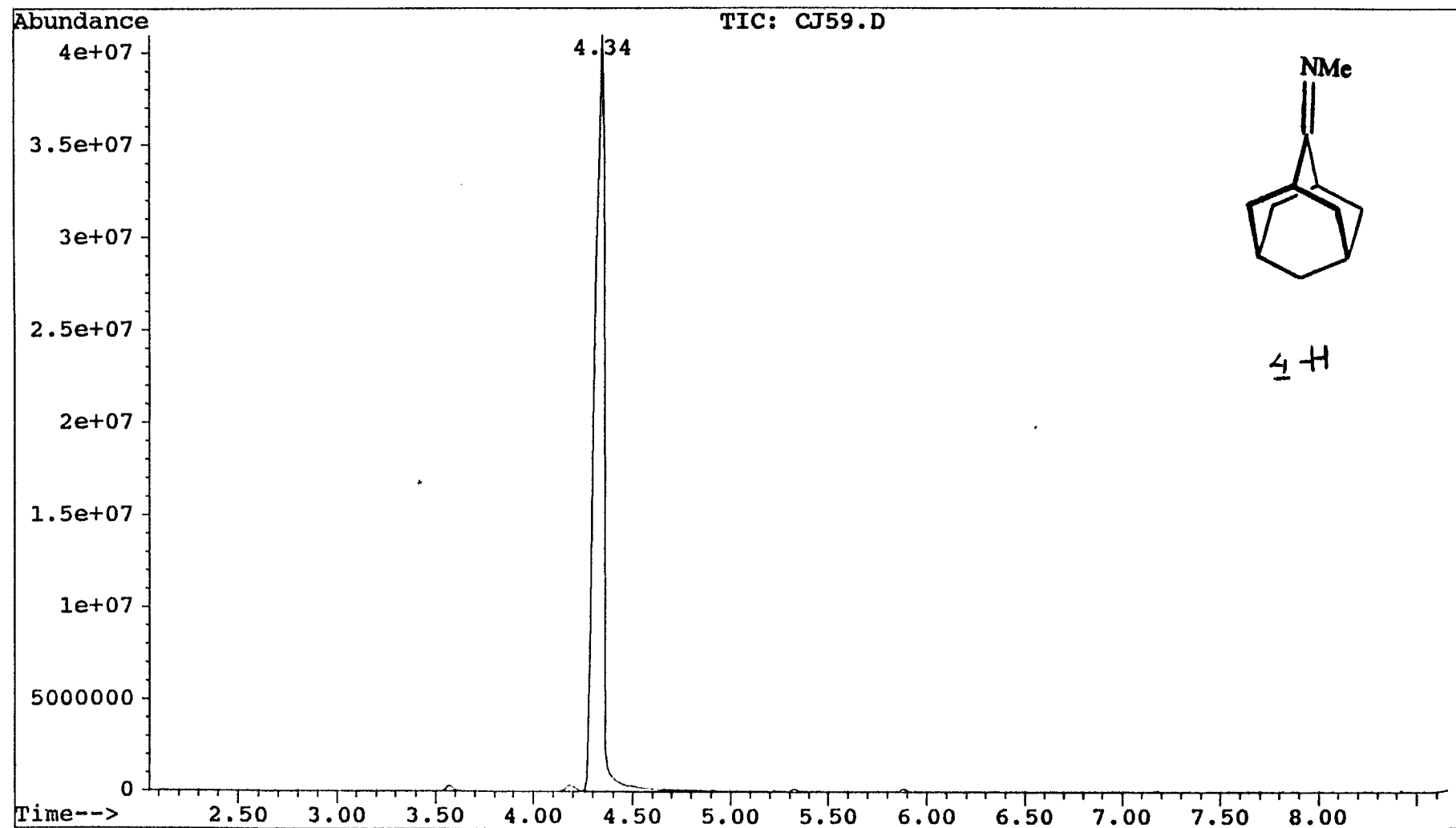
d = detail

D = DEPT spectrum

M = mass spectrum

Compound #'s 6 and 7 (not used in the paper) denote 2-*N*-methylamino- and 2-*N,N*-dimethylamino-5-phenyladamantane, respectively.

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Instrument : 5971 - In
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Vial Number: 1



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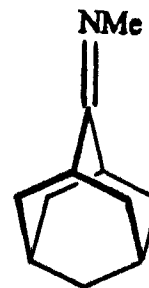
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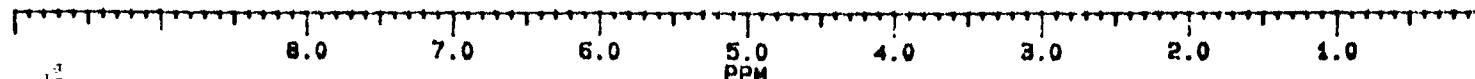


4-H



CJ53.H00
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TD 16384
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HZ/PT .365
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AQ 2.736
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D2 3210.000
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SR 2869.27

2



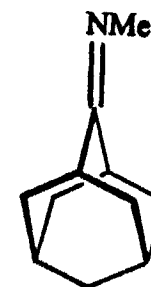
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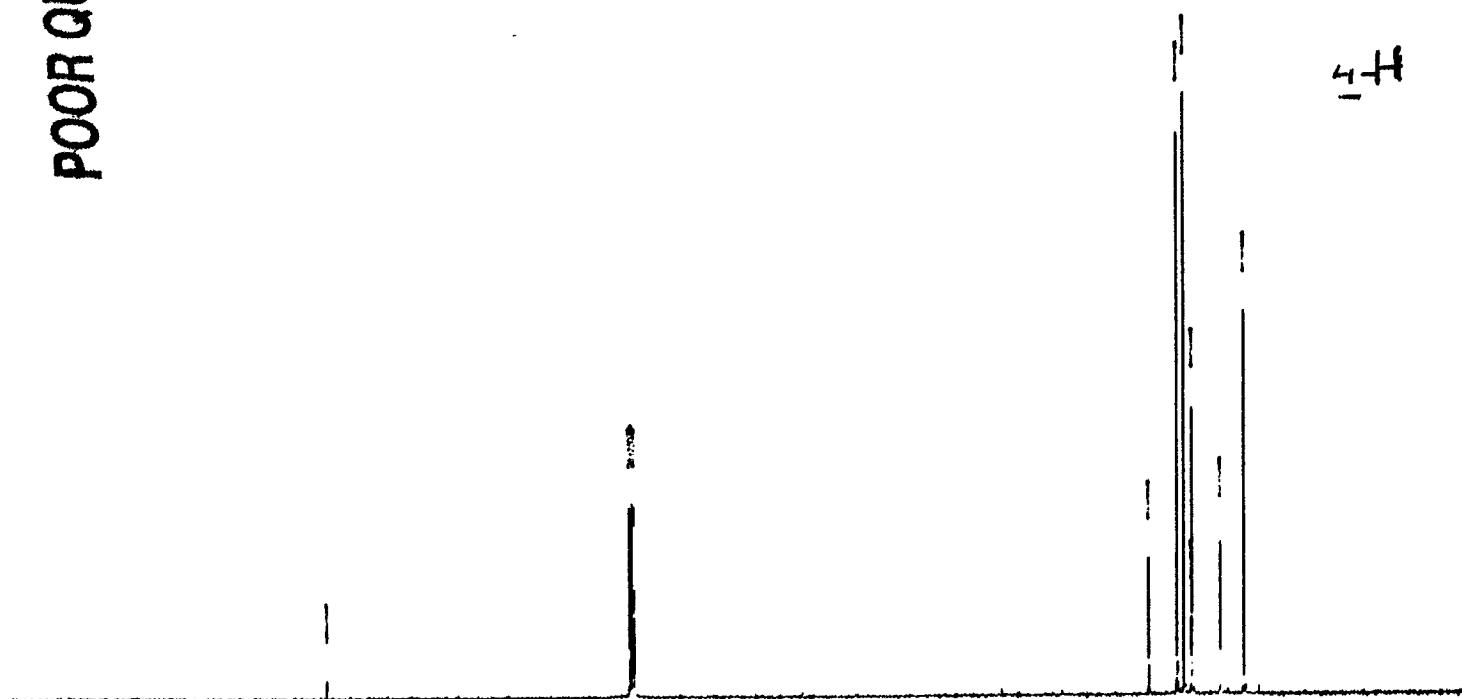
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TD 32768
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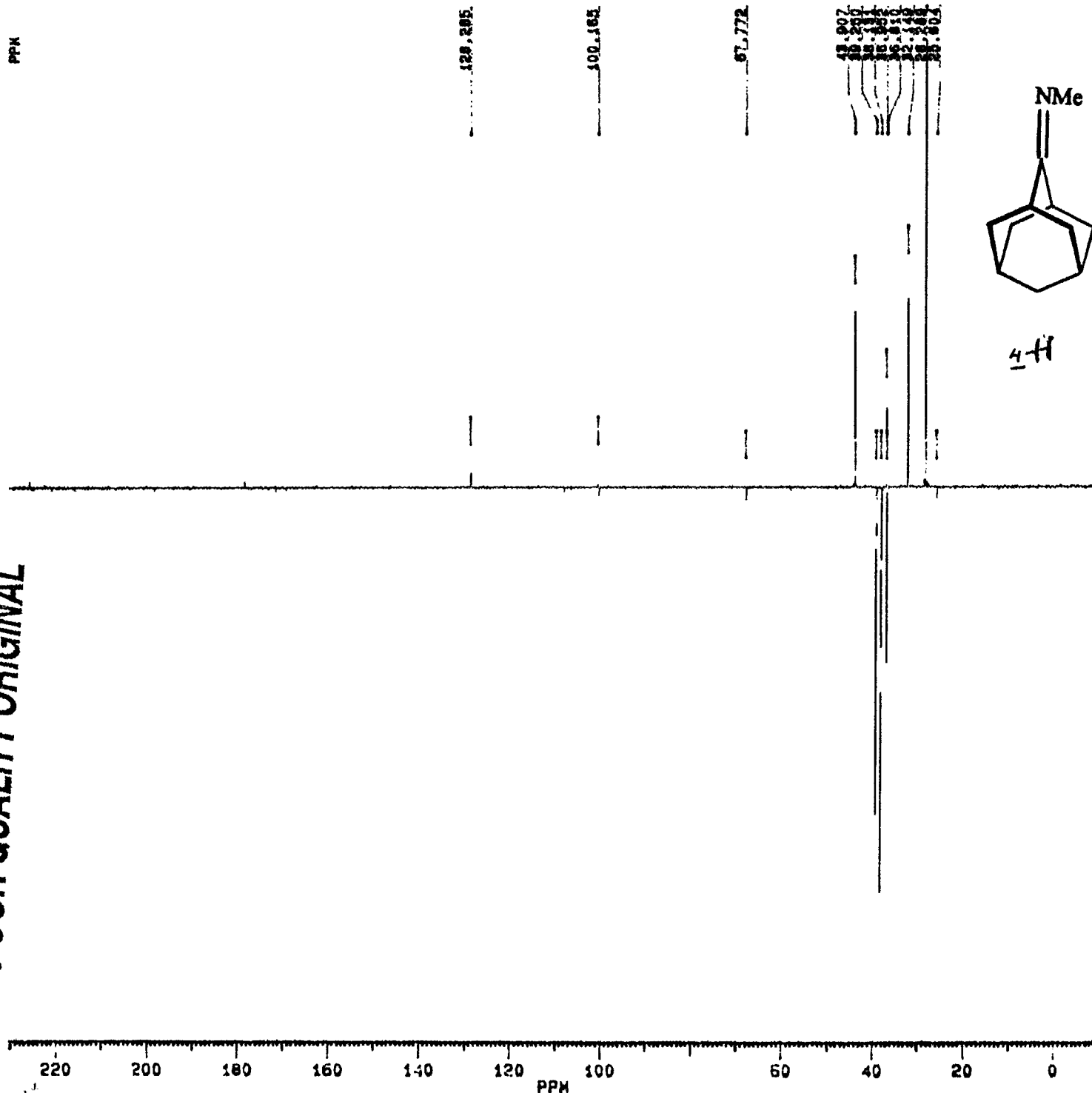
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PPM

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 AU PROG:
 DEPT1.AU
 DATE 8-5-96

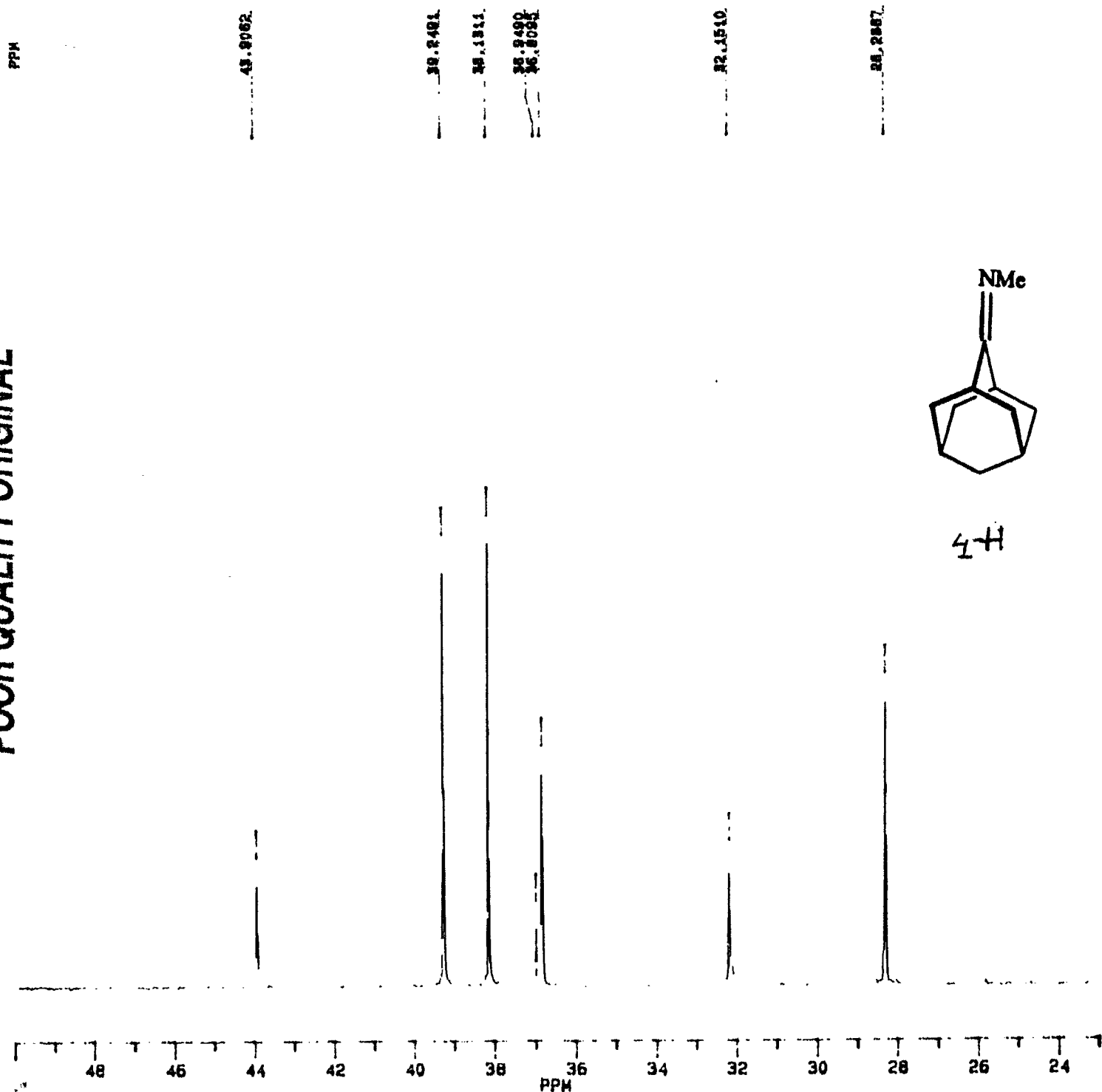
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DATE 8-5-96

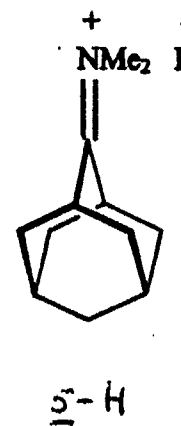
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HZ/PT	.954

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NOTES



CJ77.H00
DATE 25-6-96

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HZ/PT	.365

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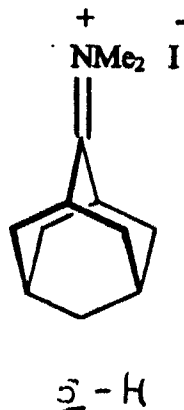
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SR	4181.57

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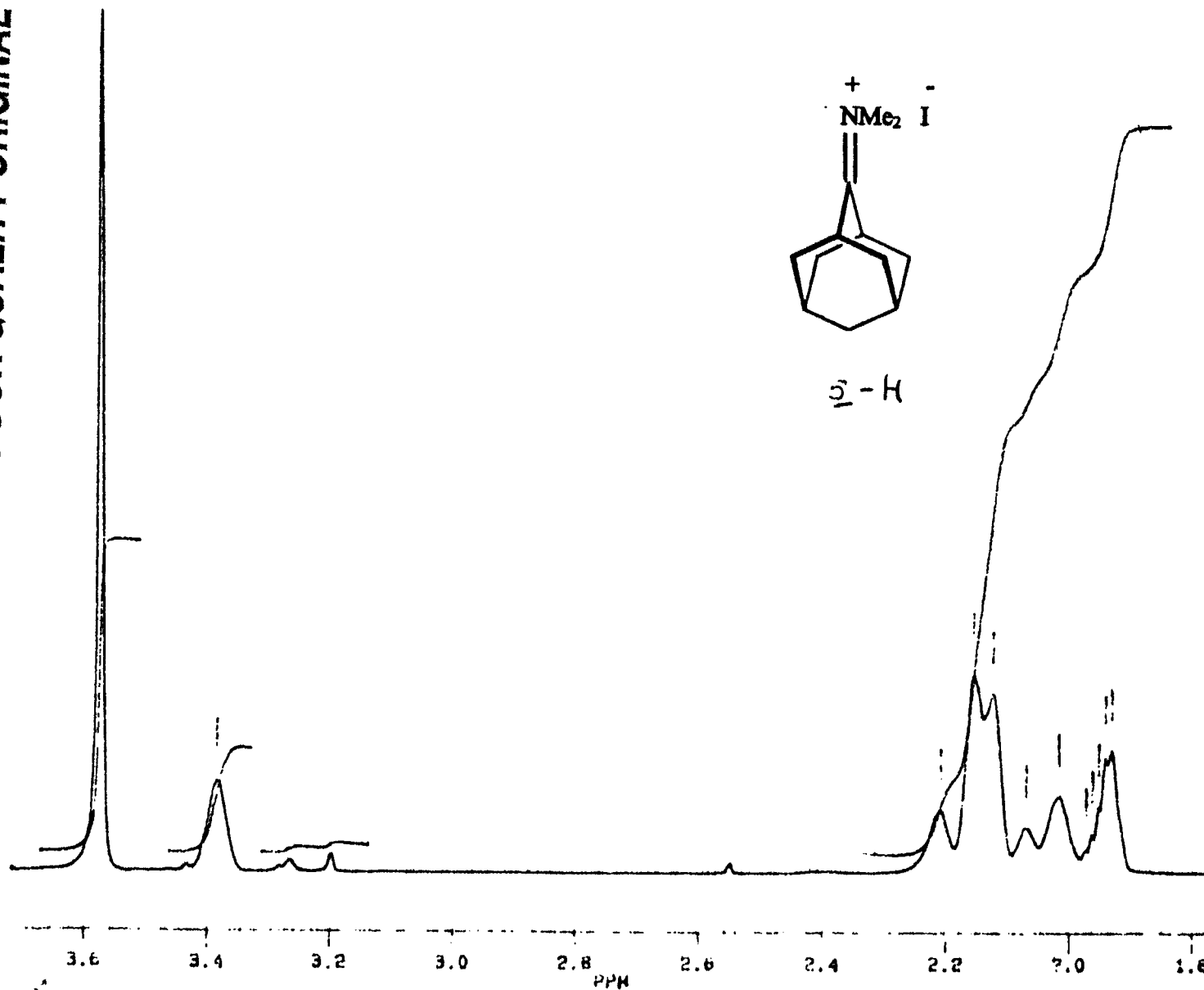


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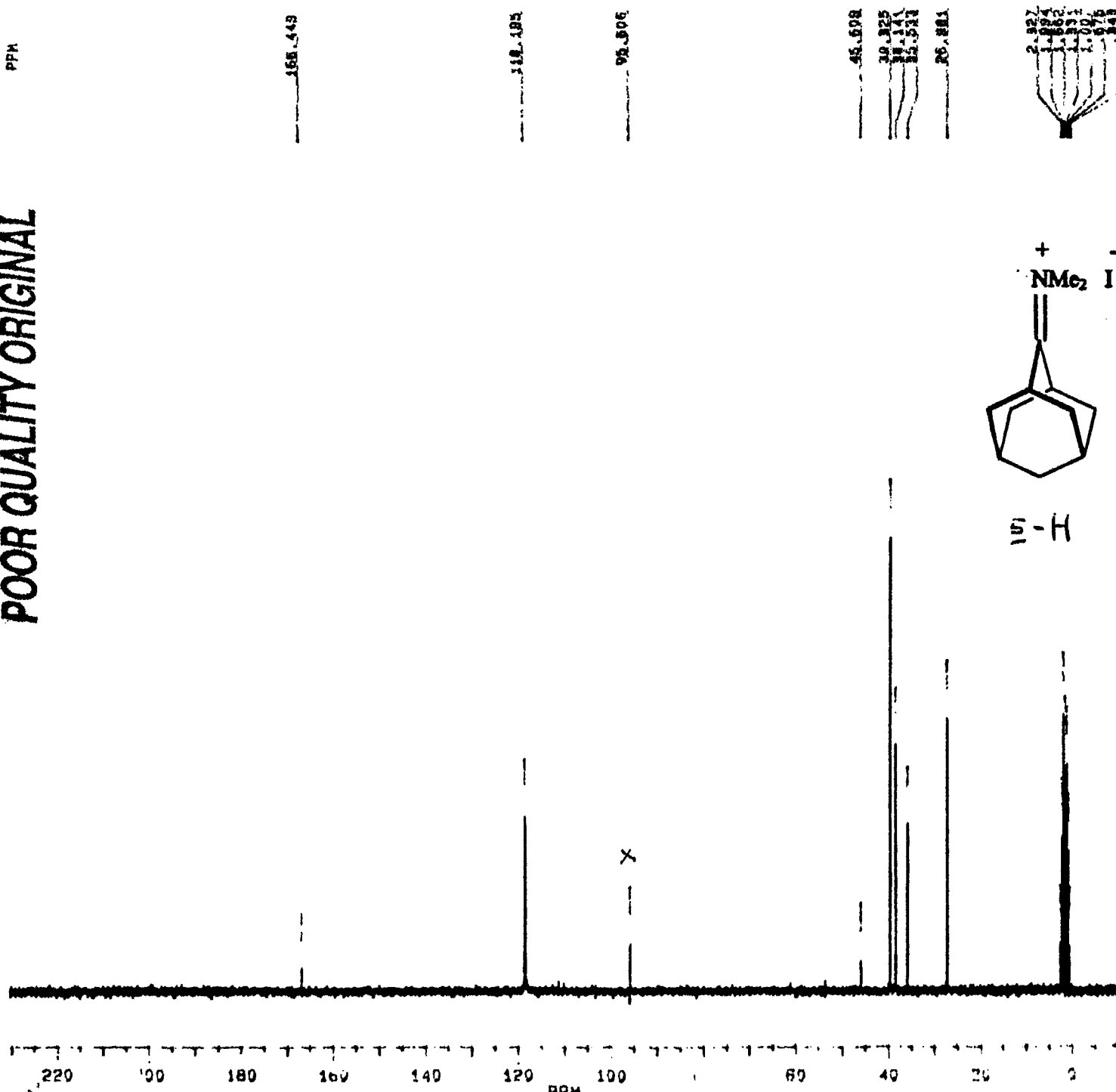
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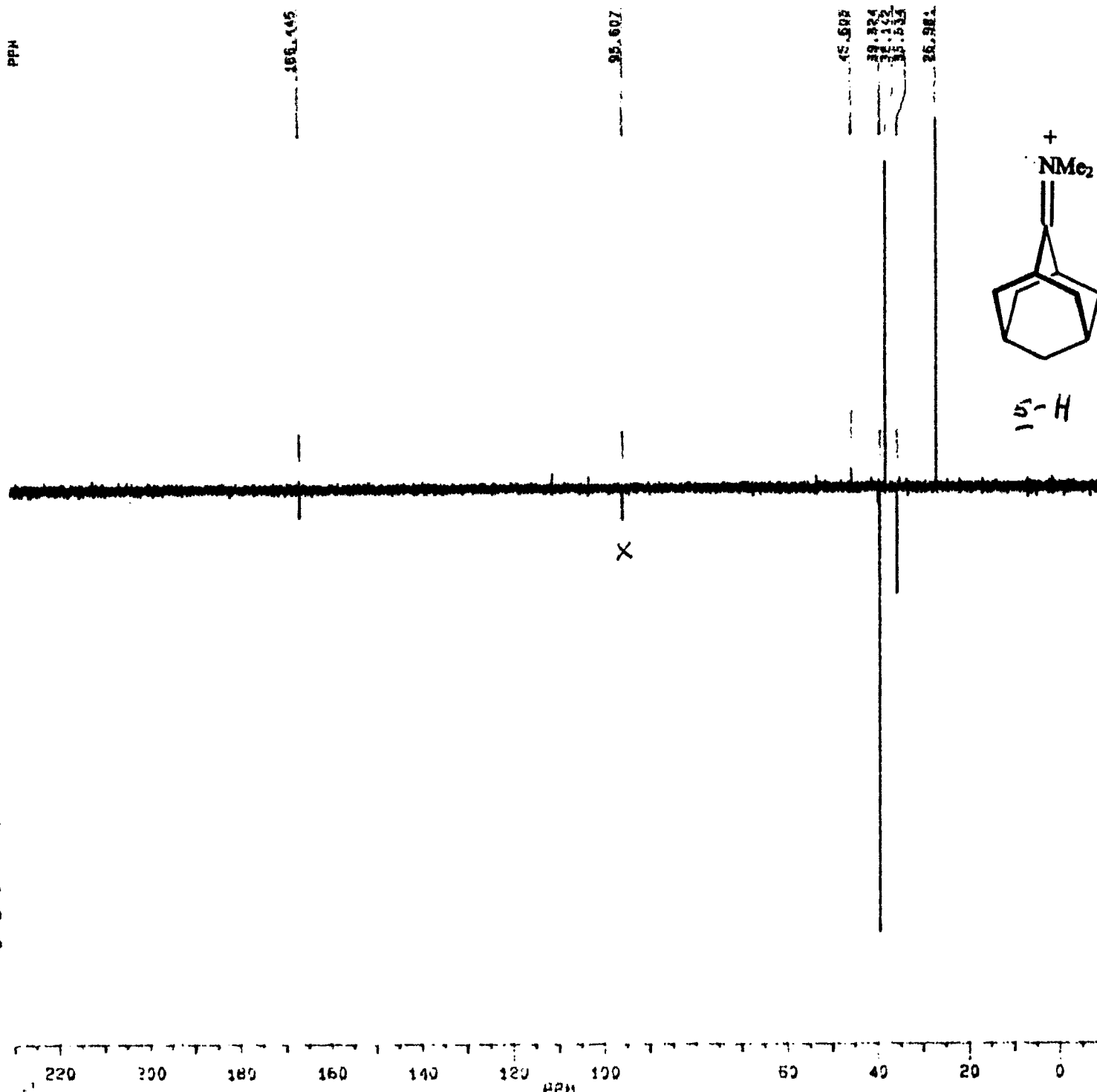


POOR QUALITY ORIGINAL

PPM



POOR QUALITY ORIGINAL



BRUKER

CJ77.D00
AU PROG:
DEPT1.AU
DATE 25-6-96

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TD 32768
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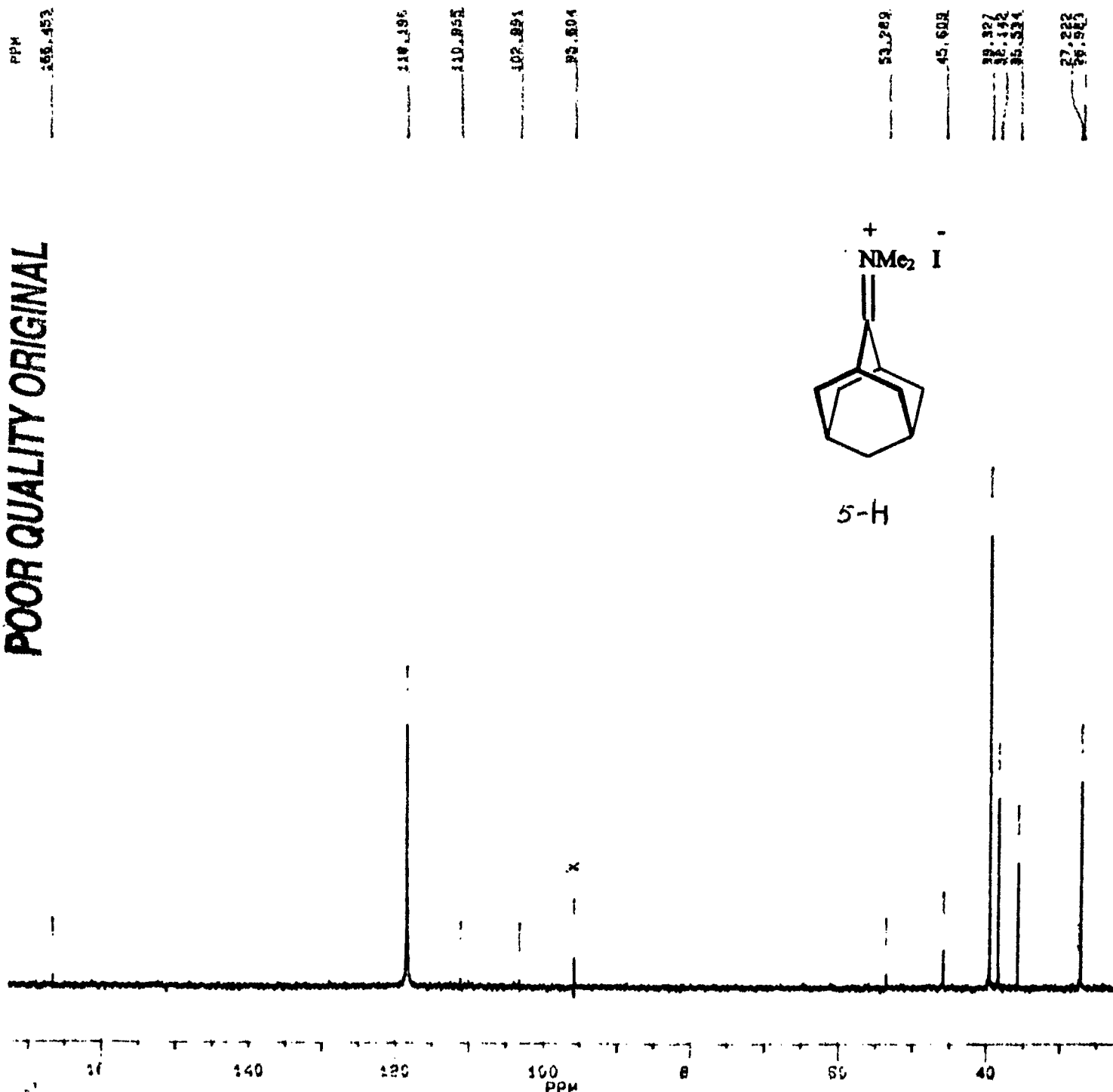
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9

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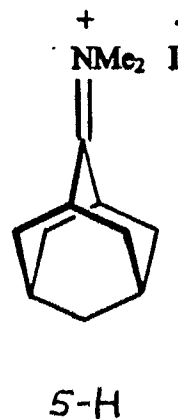
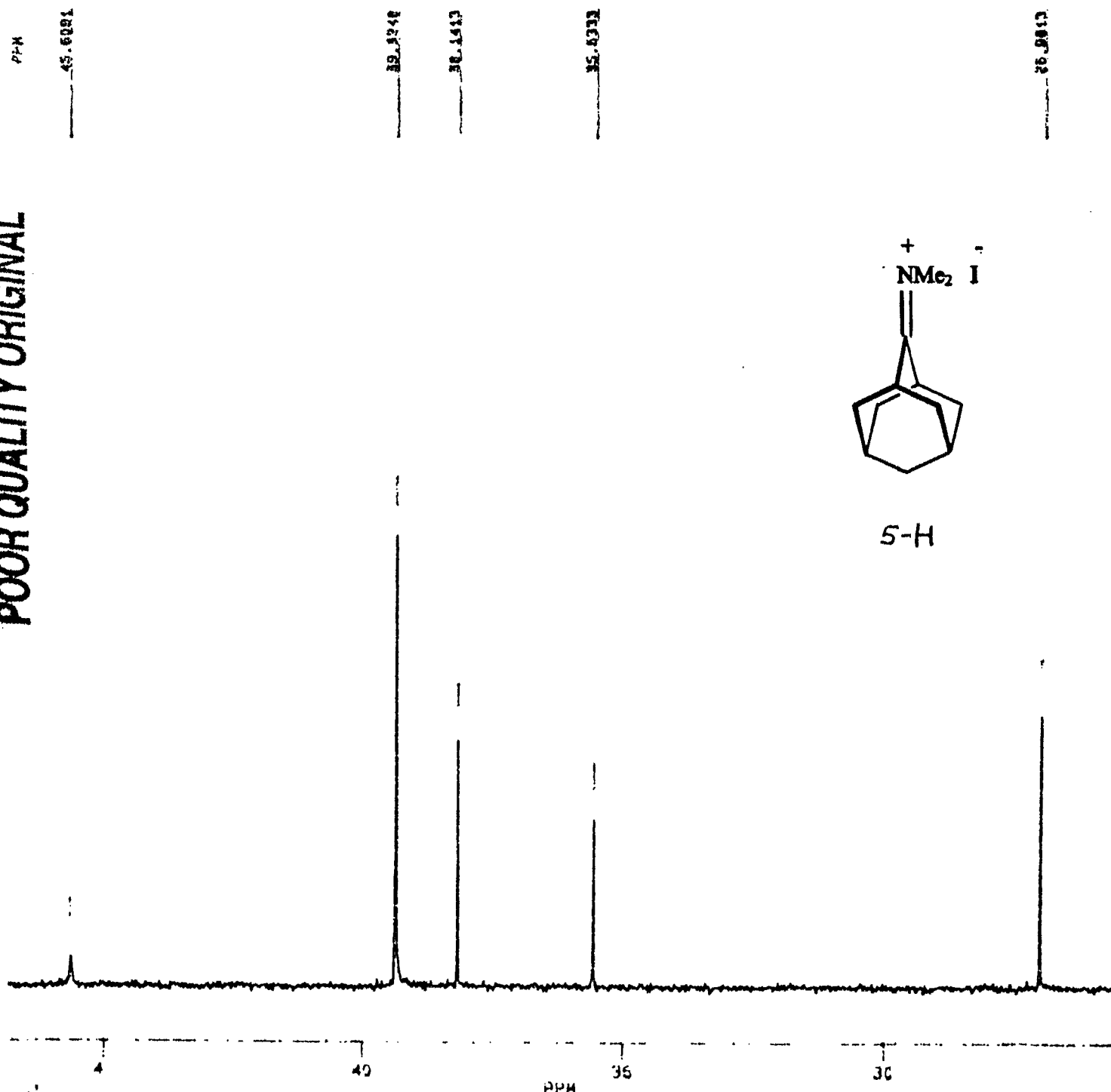
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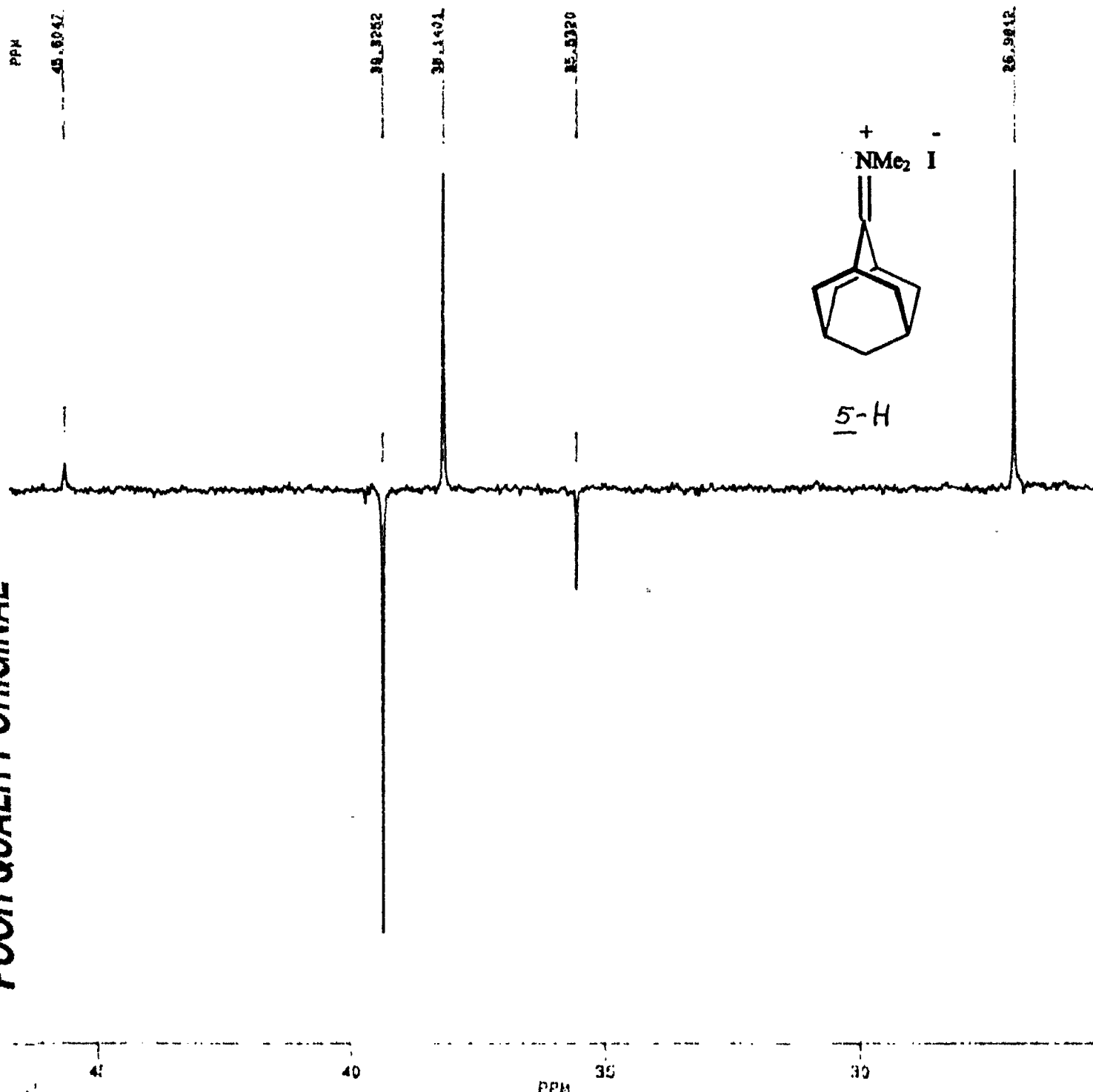
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POOR QUALITY ORIGINAL



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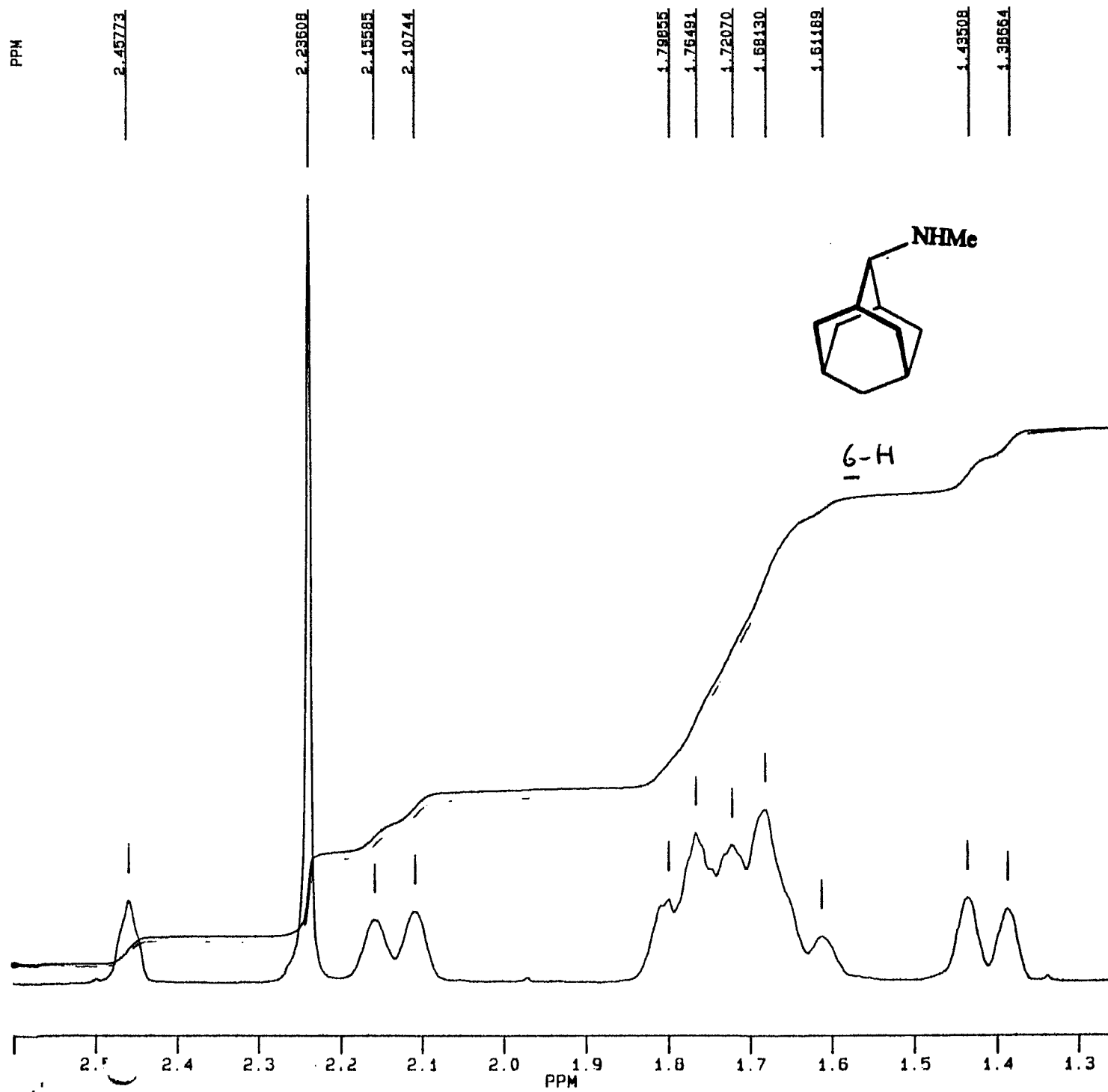
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(13)

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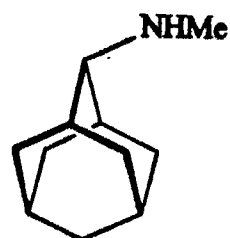
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6-H

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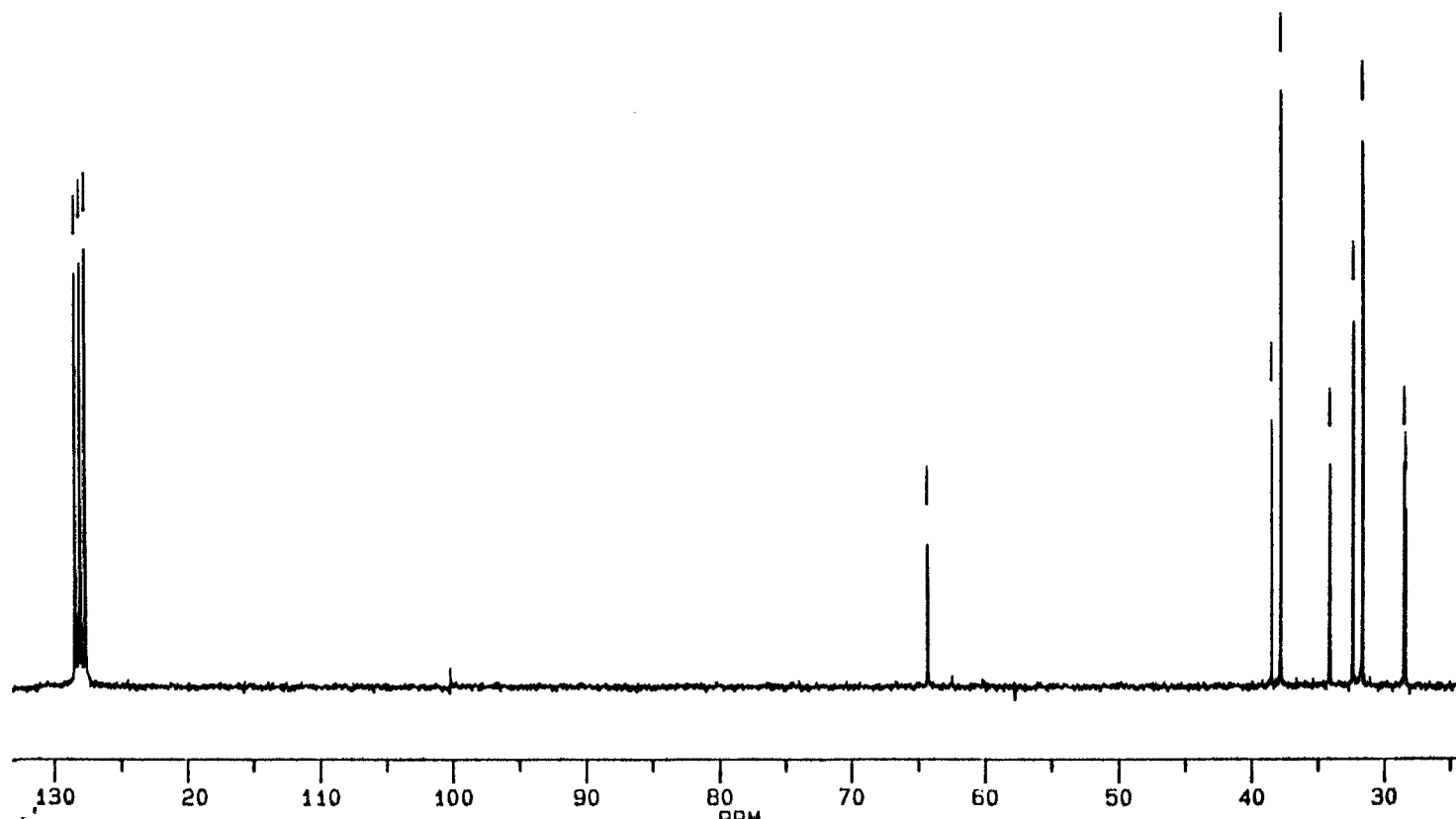
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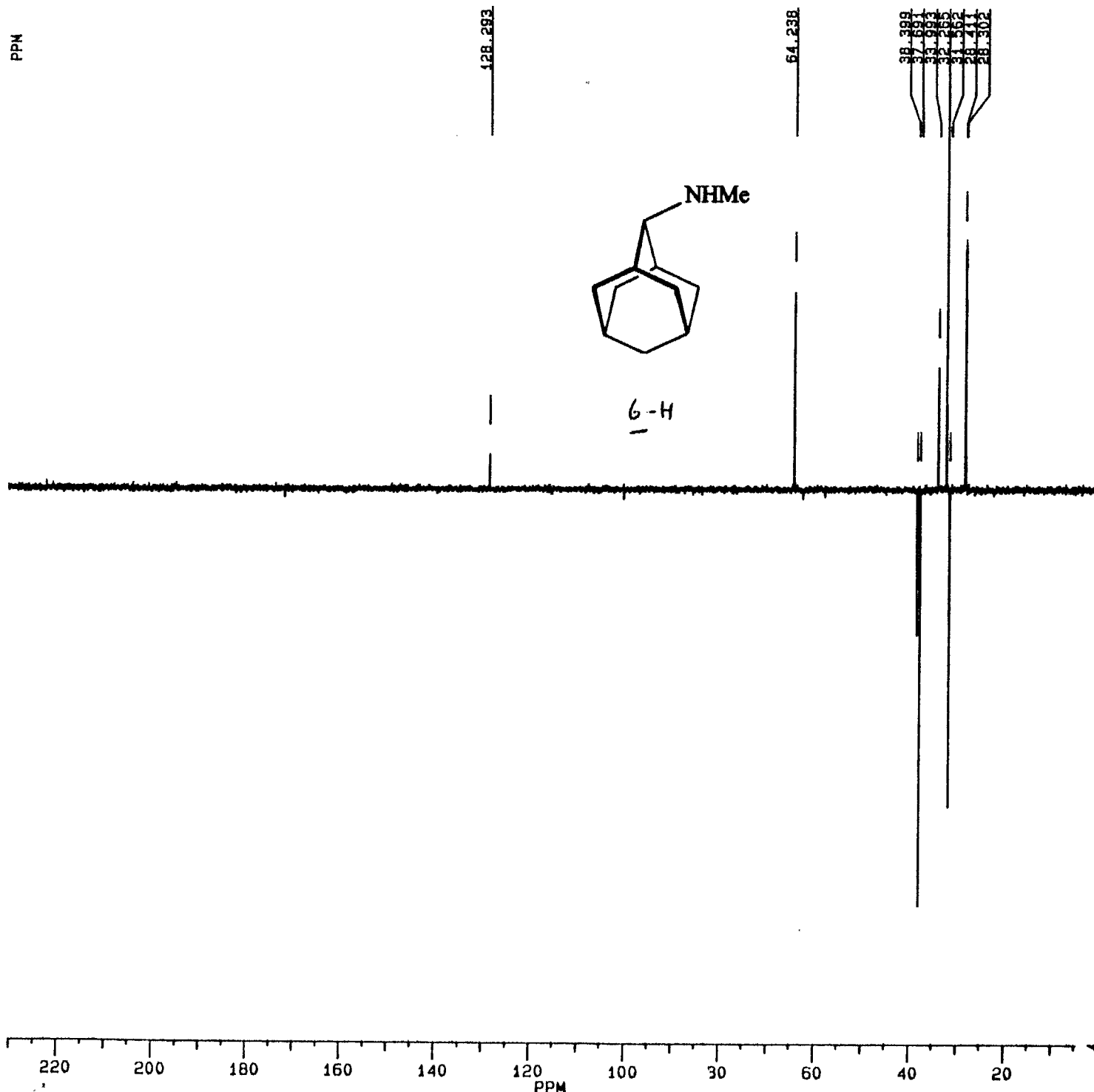
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14



15

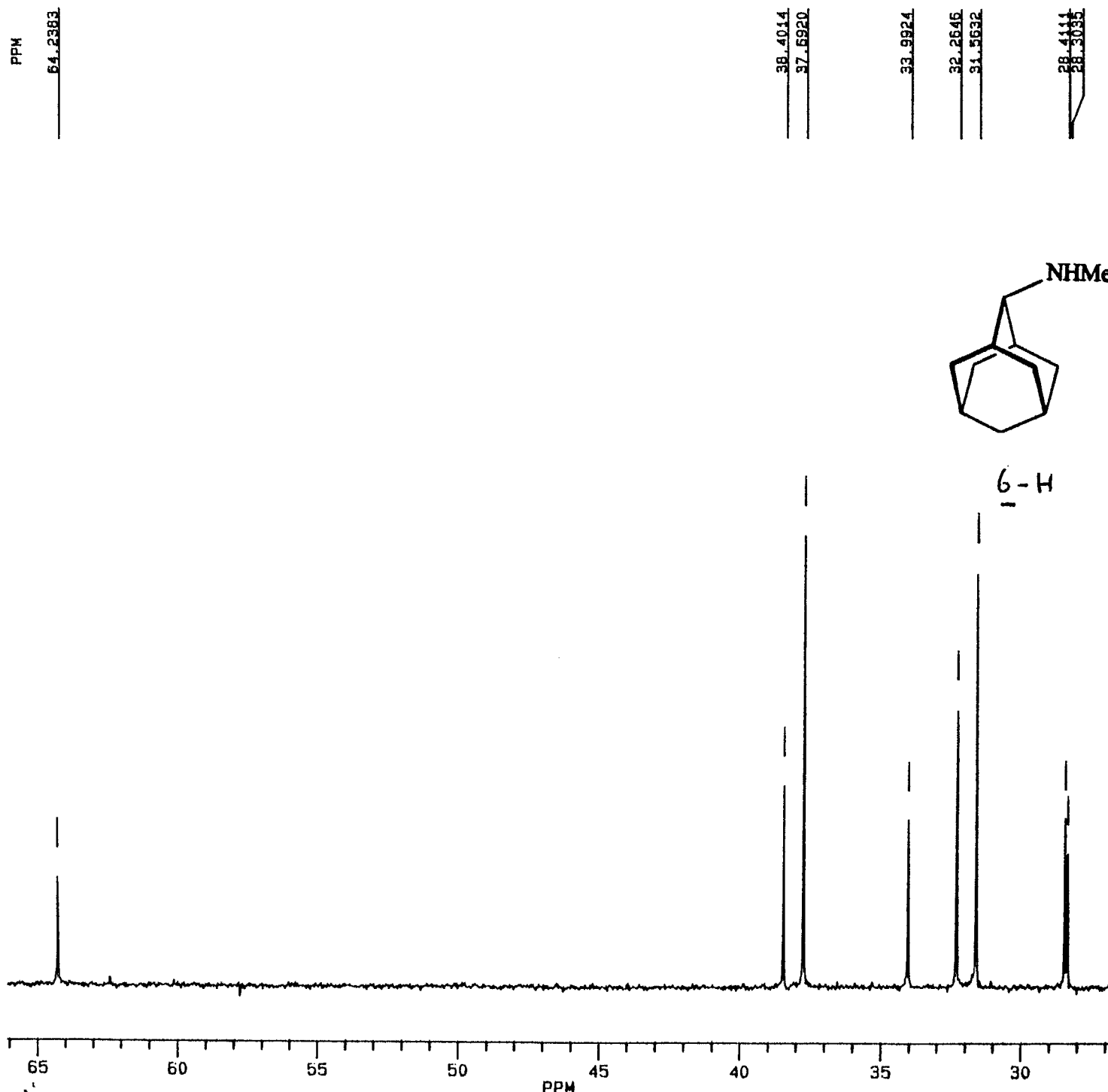
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DATE 25-5-96

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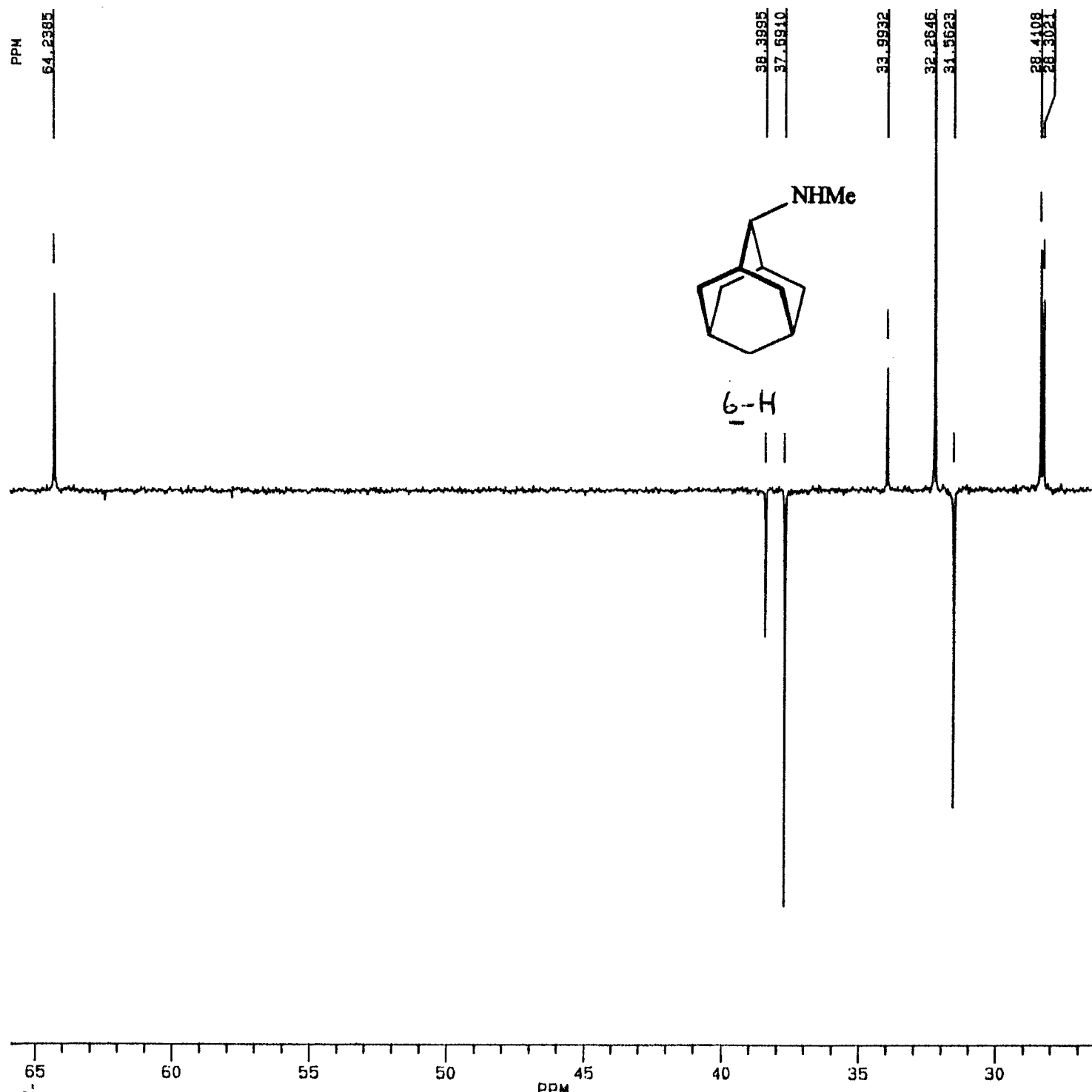
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TE 297

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BRUKER

17

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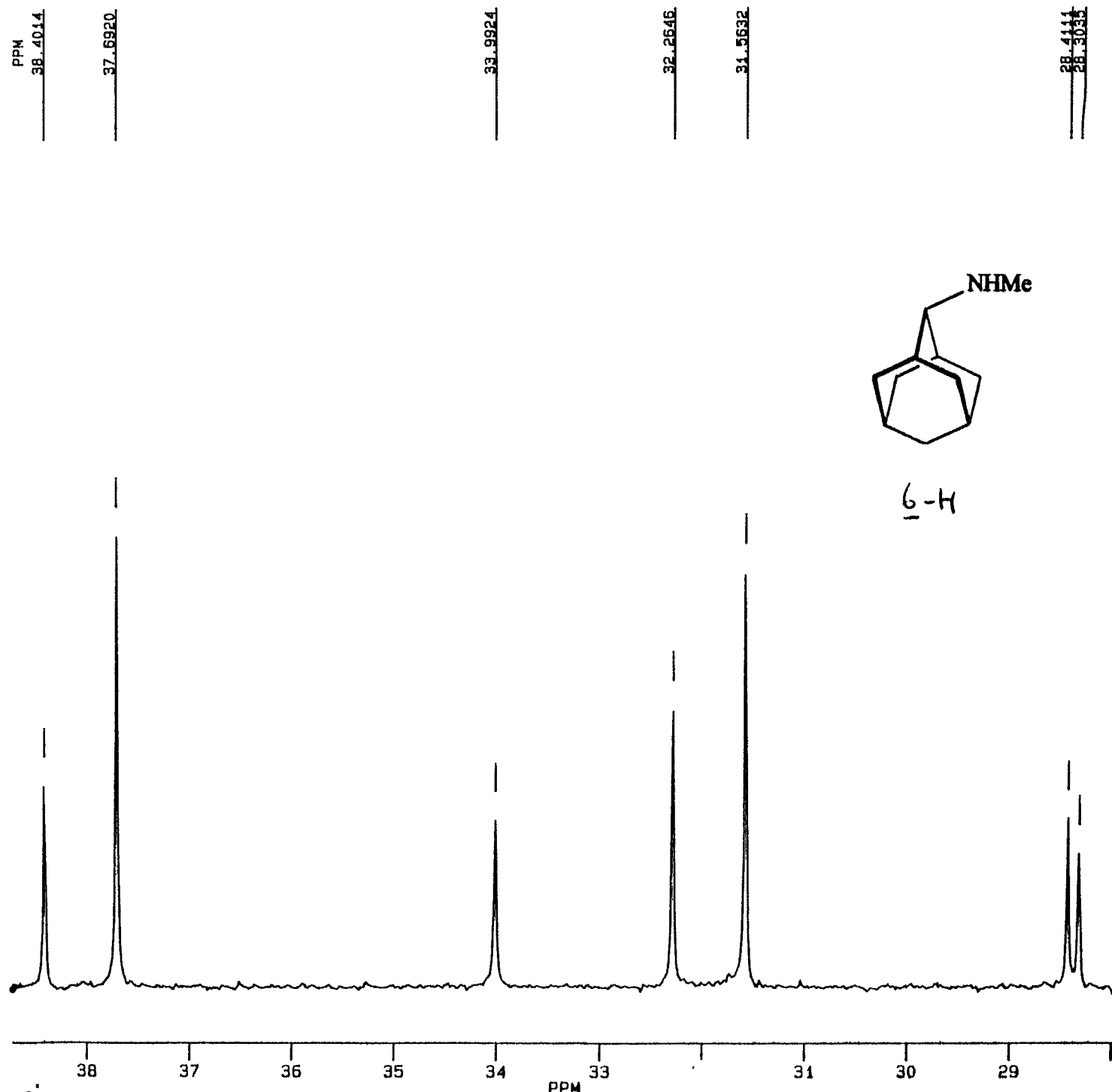
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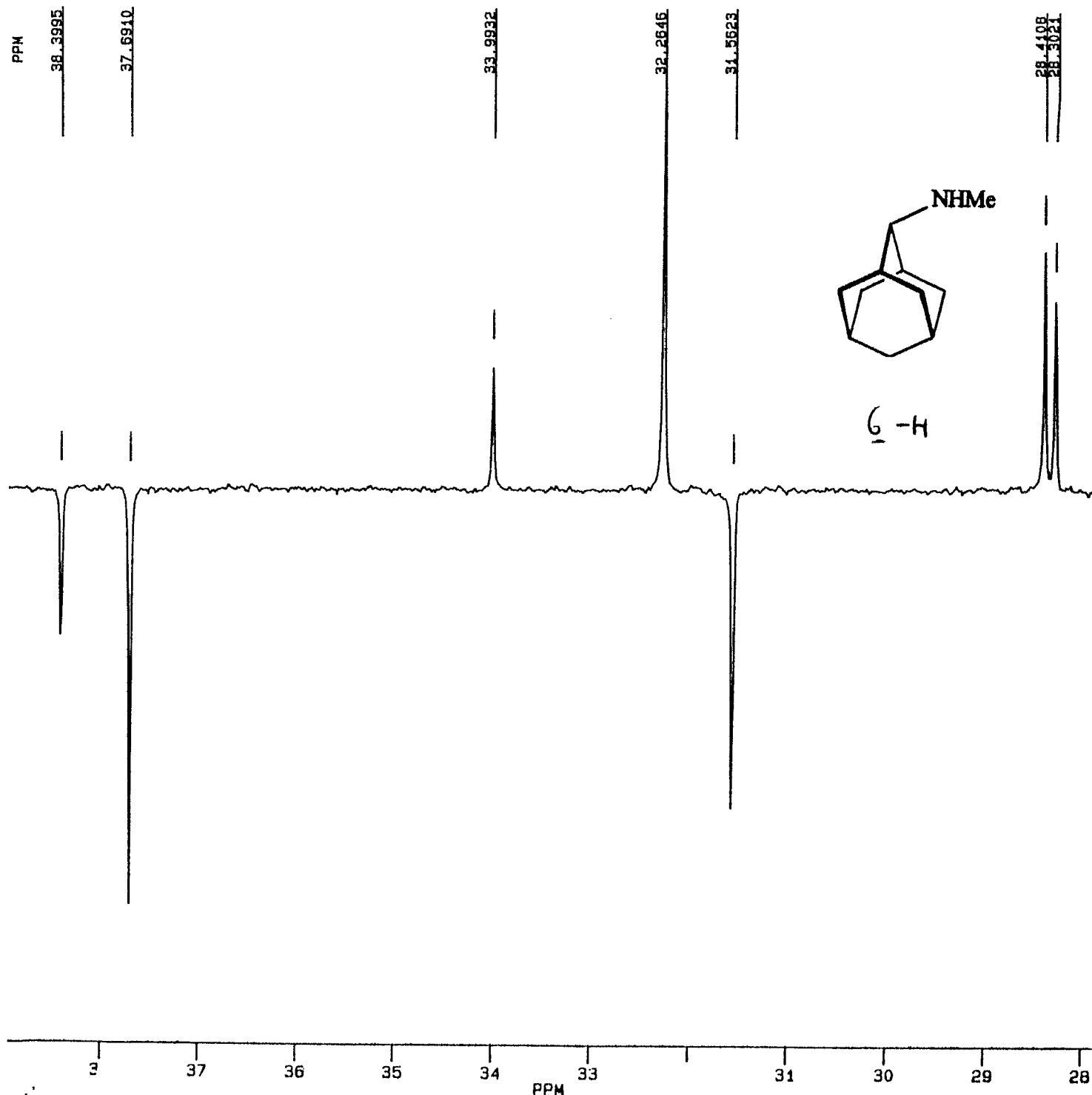
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12

~~BRUKER~~CJ59.C00
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~~BRUKER~~

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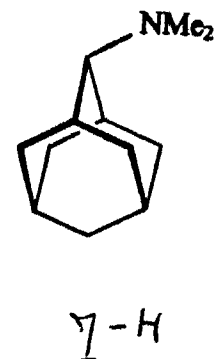
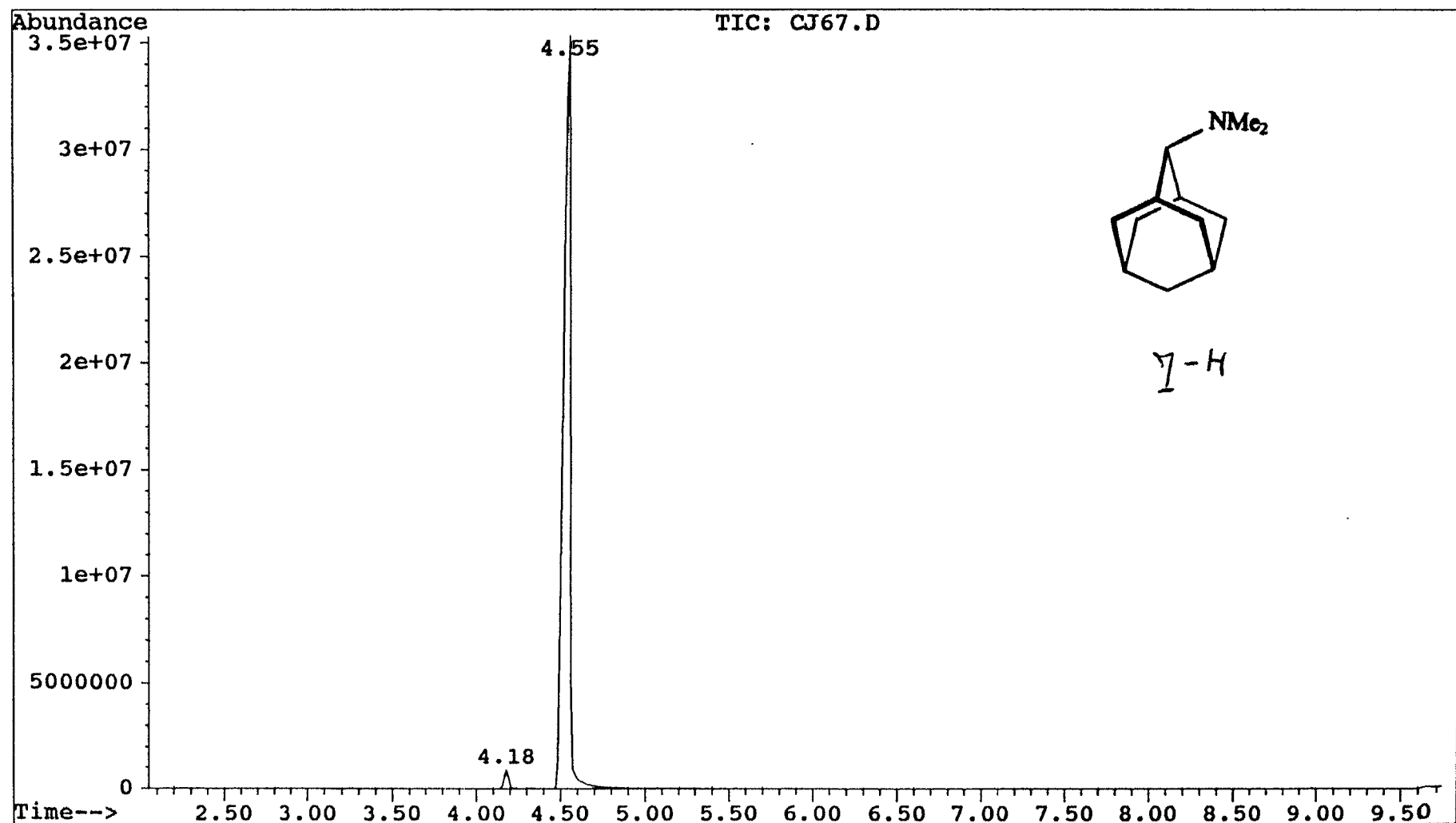
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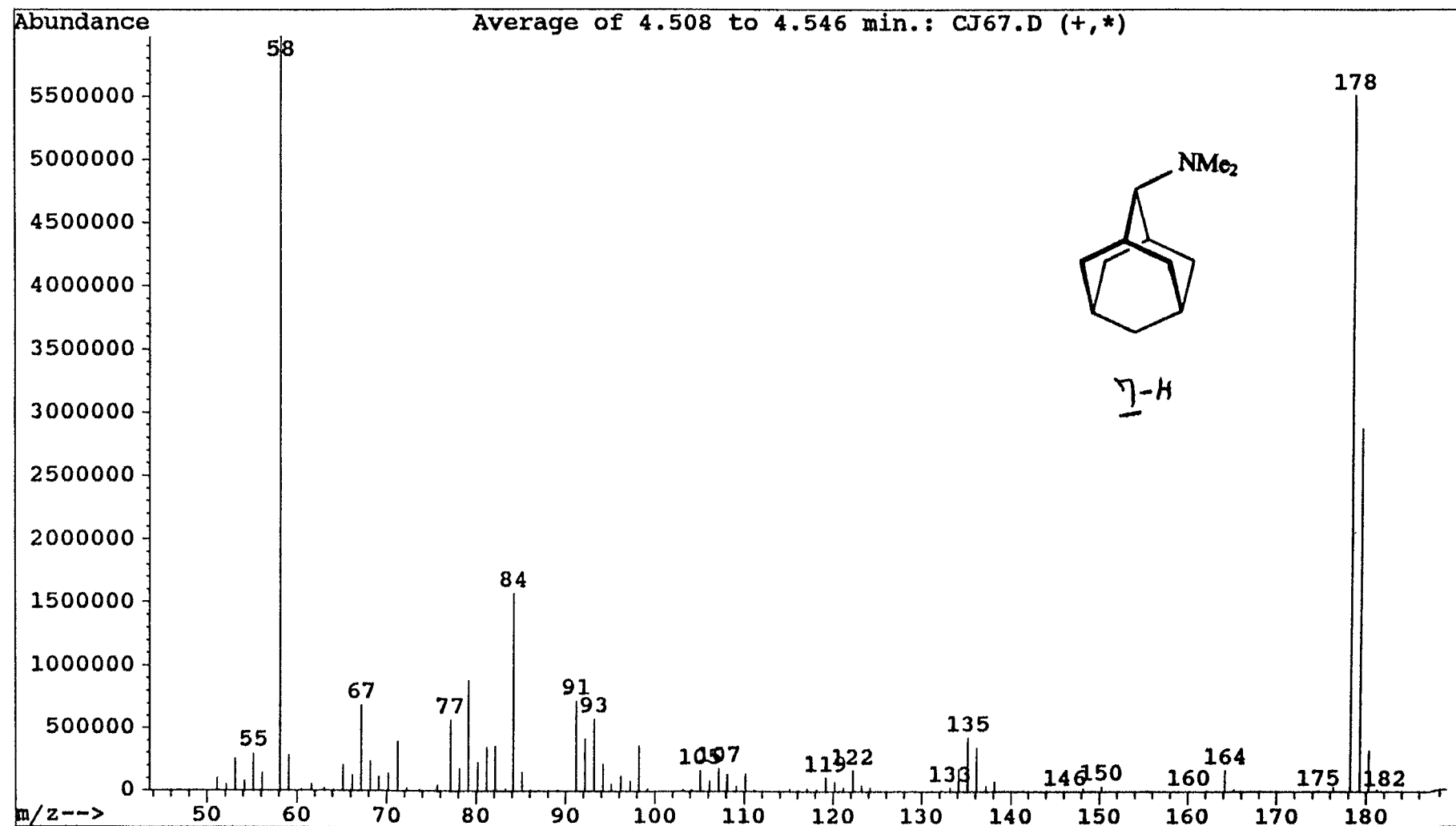
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Instrument : 5971 - In
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Vial Number: 1
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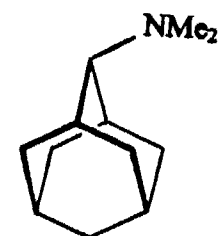
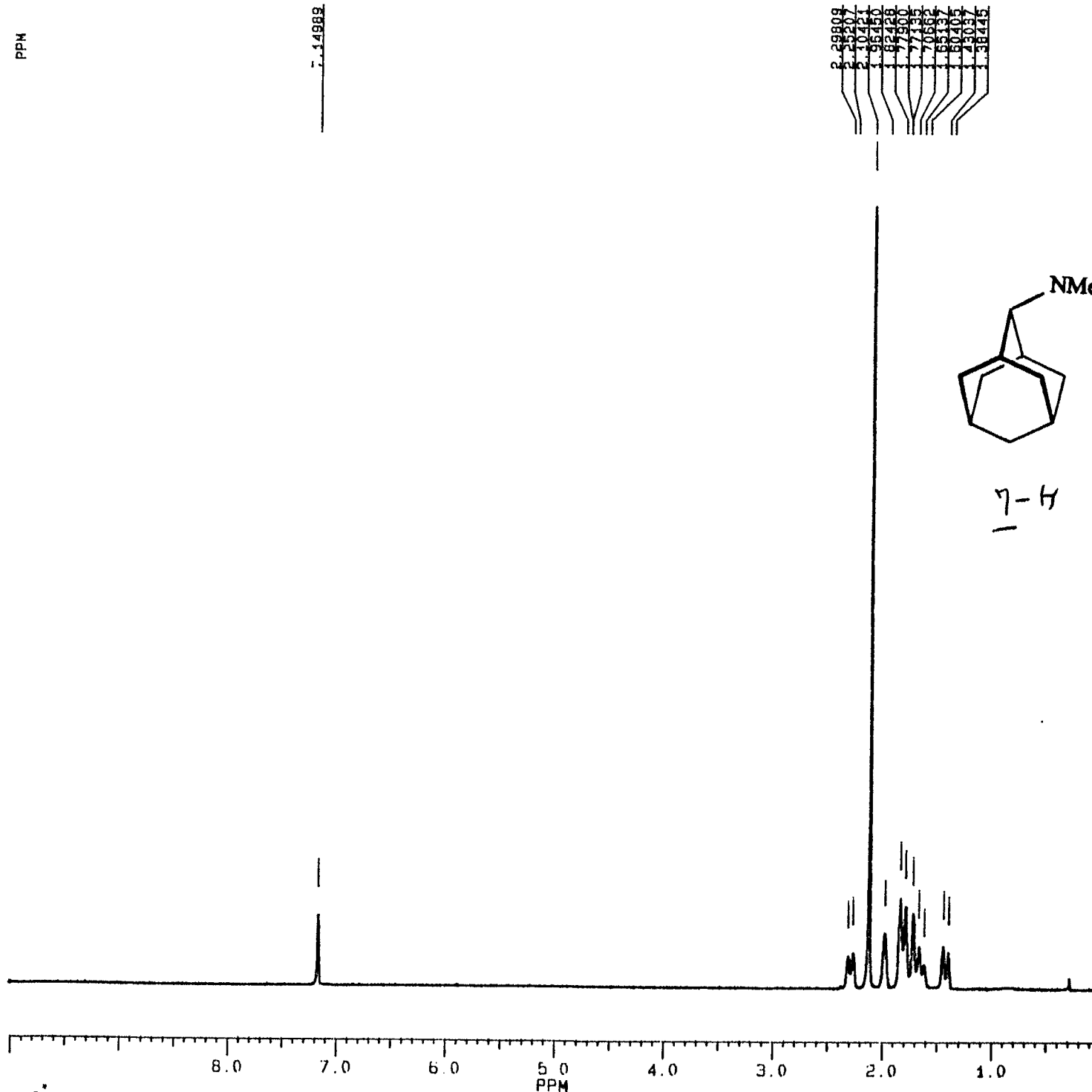


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Sample Name: cj-67
Misc Info : 140 hold 2 min 10/min to 220
Vial Number: 1



Mid

7.14989



7-4



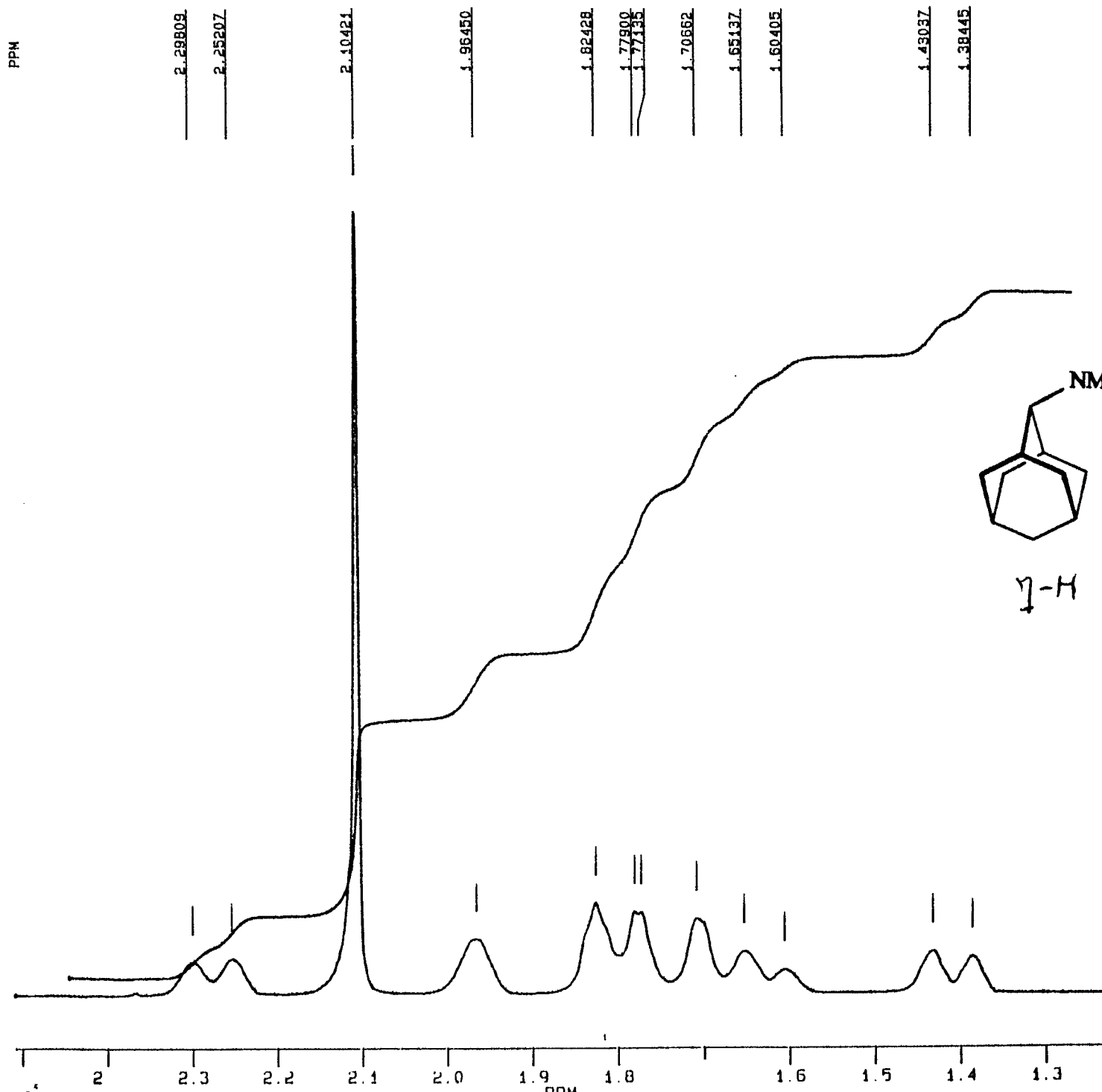
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SW	2994.012
HZ/PT	.365

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TE	297

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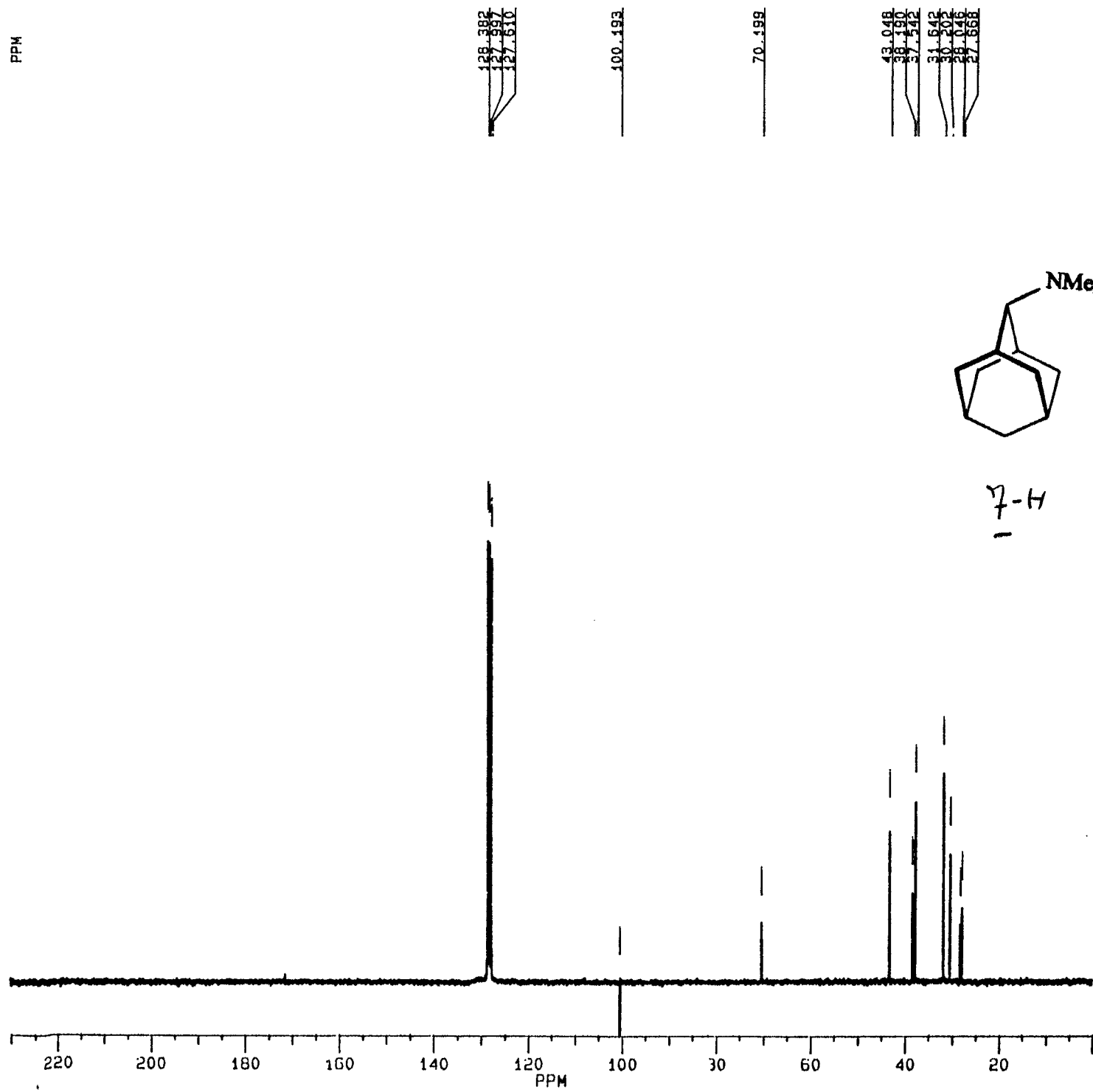
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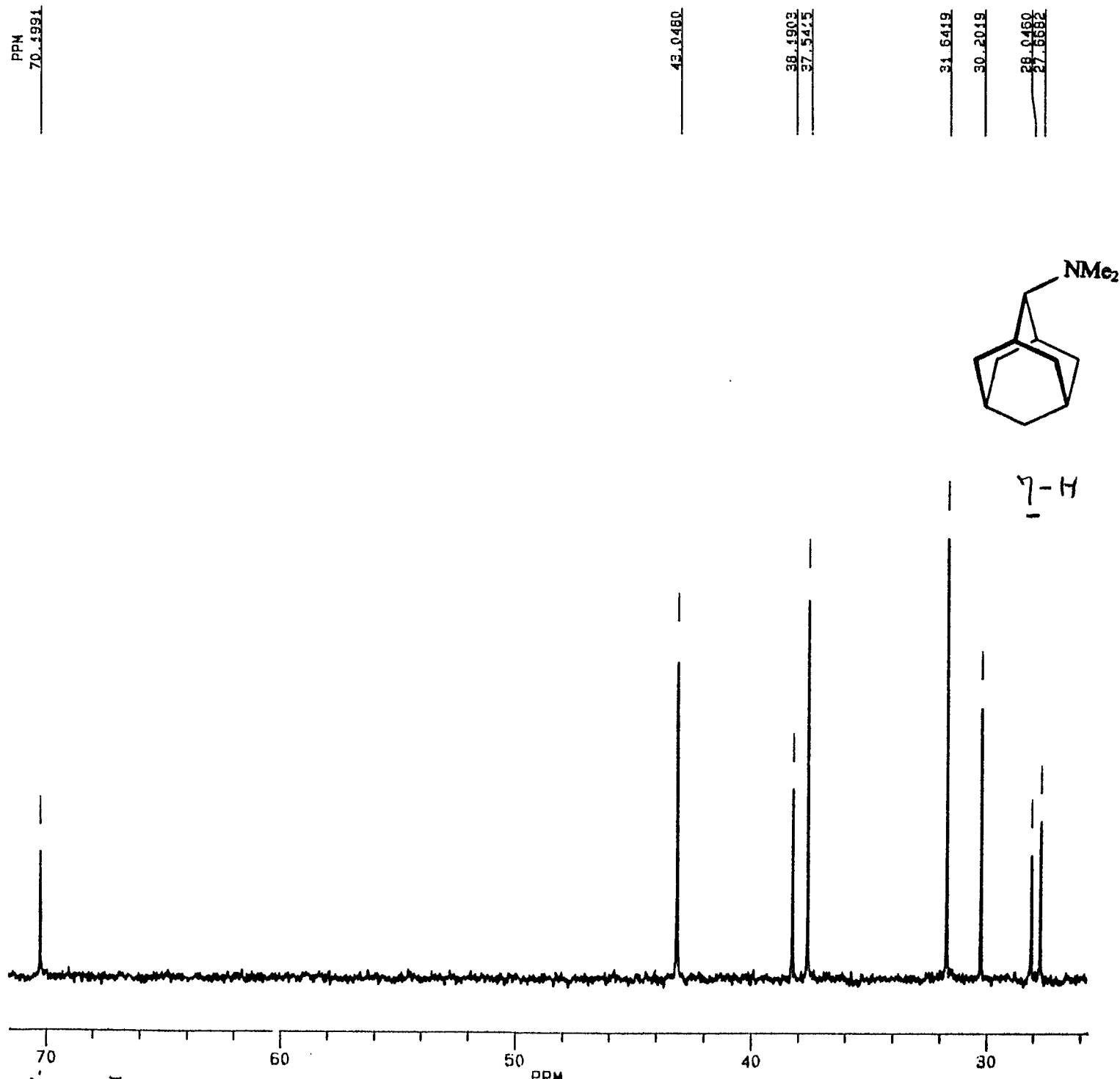
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CX 20.00
CY 8.00
F1 230.000P
F2 -.004P
HZ/CM 723.314
PPM/CM 11.500
SR -4059.23



BRUKER

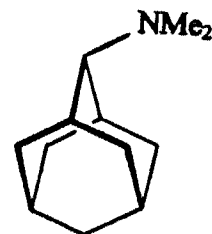
CJ67.C00
DATE 4-6-96

SF 62.896
SY 62.0
O1 3218.018
SI 32768
TD 32768
SW 15625.000
HZ/PT .954

PW 5.0
RD 1.000
AQ 1.049
RG 1600
NS 1017
TE 297

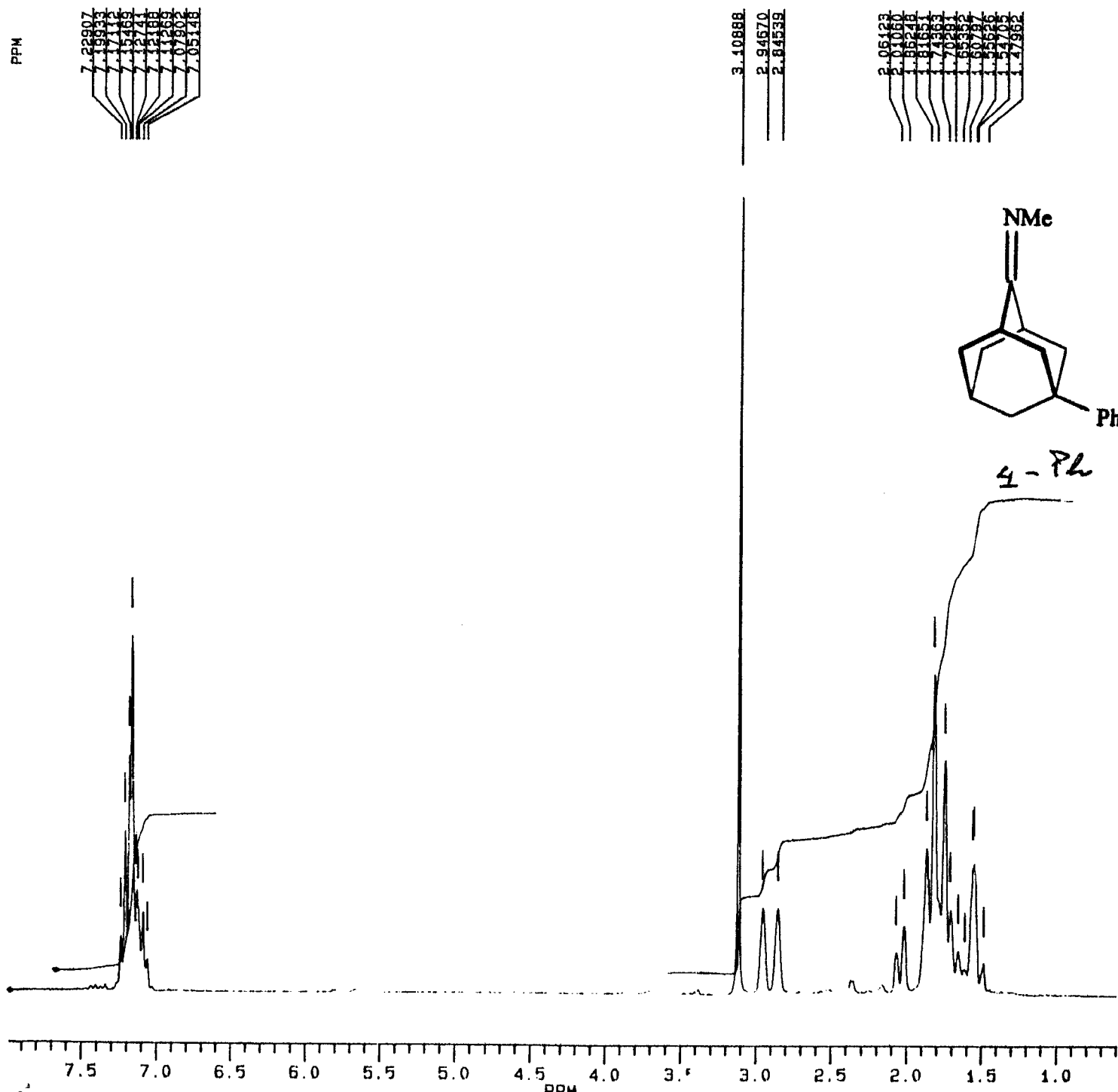
FW 19600
O2 4100.000
DP 20H CPD

LB 1.000
GB .100
CX 20.00
CY 8.00
F1 71.519P
F2 25.682P
HZ/CM 144.148
PPM/CM 2.292
SR -4059.23



7-H

26



CJ64.H00
DATE 28-5-96

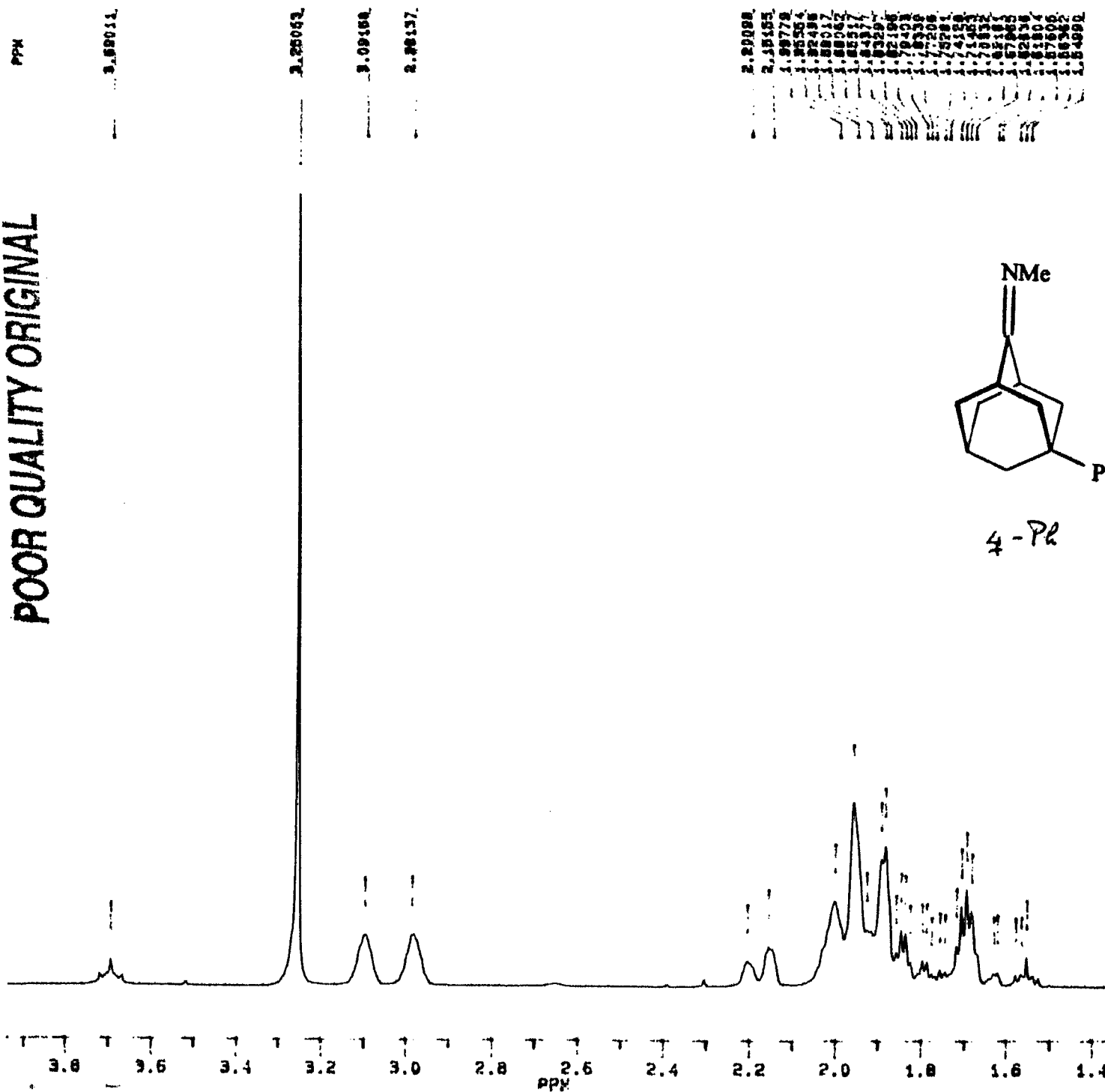
SF 250.133
SY 100.0
O1 4102.190
SI 16384
TD 16384
SW 2994.012
HZ/PT .365

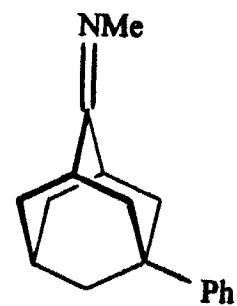
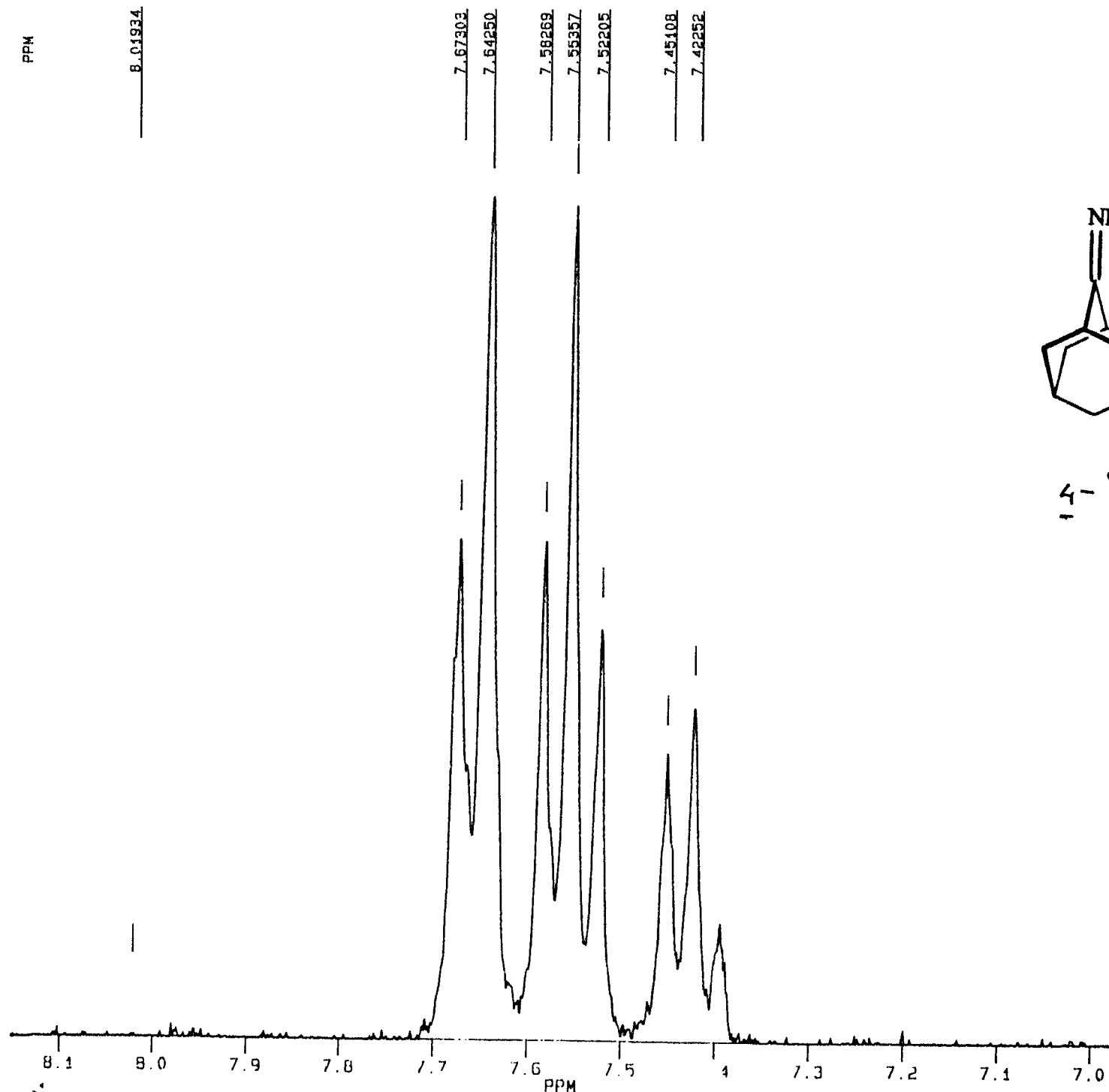
PW 3.0
RD 1.000
AQ 2.736
RG 16
NS 64
TE 297

FW 3000
O2 3210.000
DP 63L P0

LB .100
GB .100
CX 20.00
CY 14.00
F1 7.980P
F2 .594P
HZ/CM 92.375
PPM/CM .369
SR 2869.99

POOR QUALITY ORIGINAL

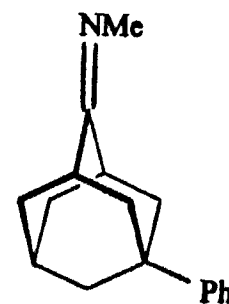
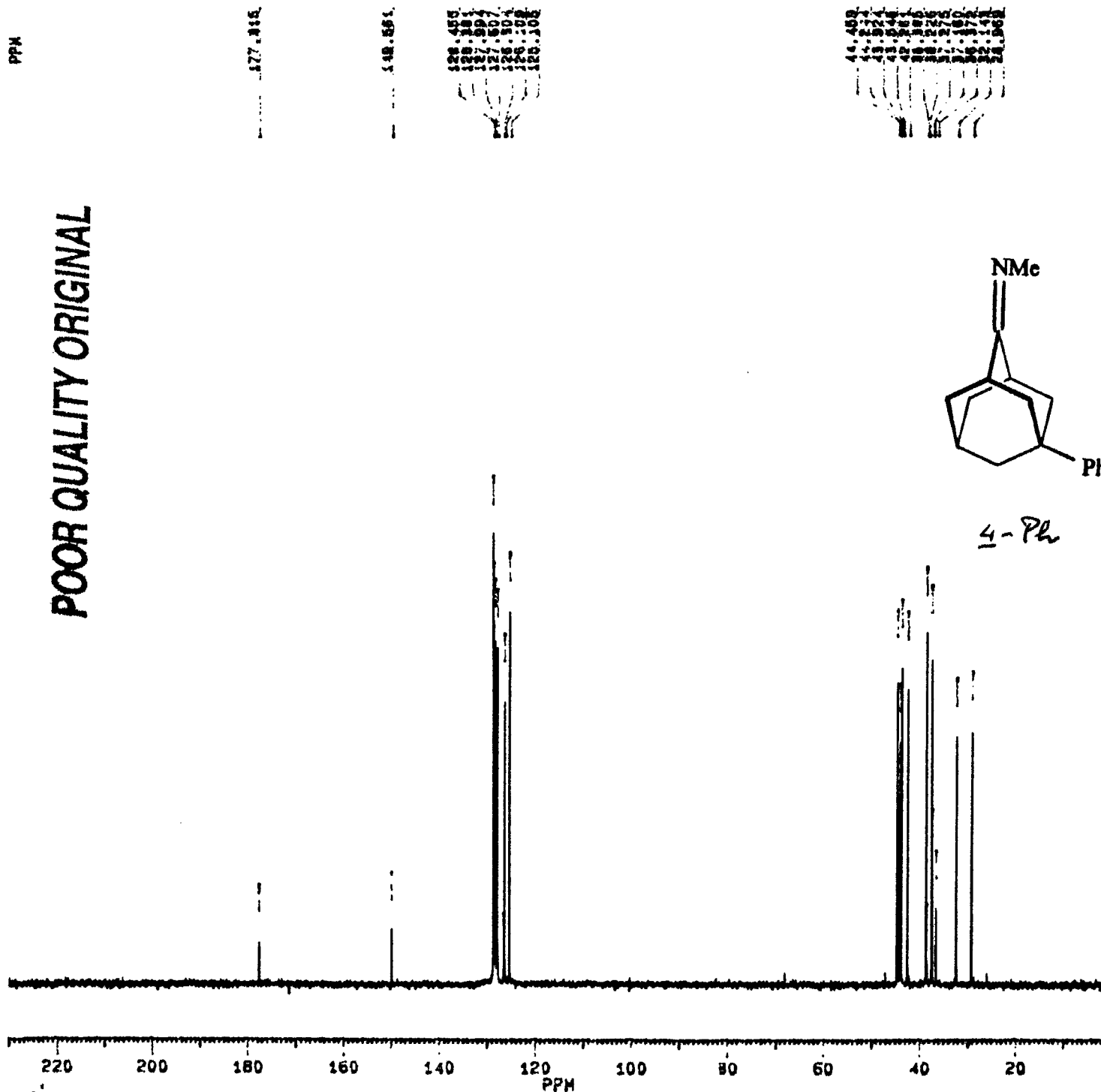




4-Ph

PPM

POOR QUALITY ORIGINAL

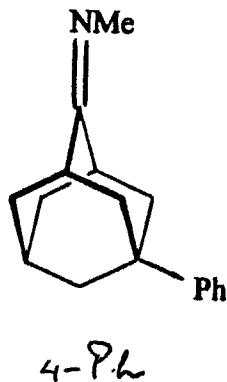


4-Ph

BRUKER

CJ54.C00
DATE 13-5-96SF 62.896
SY 62.0
O1 3218.018
SI 32768
TD 32768
SW 15625.000
HZ/PT .954PW 5.0
RD 1.000
AQ 1.049
RG 3200
NS 641
TE 297FW 19600
O2 4100.000
DP 20H CPDLB 1.000
GB .100
CX 20.00
CY 8.00
F1 230.000P
F2 -.004P
HZ/CM 723.314
PPM/CM 11.500
SR -4058.28

22X



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(30)

CJ54.D00
AU PROG:
DEPT1.AU
DATE 13-5-96

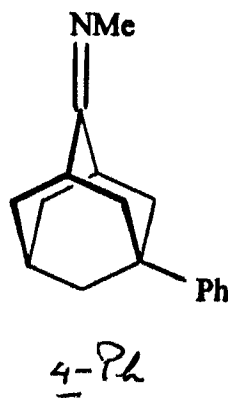
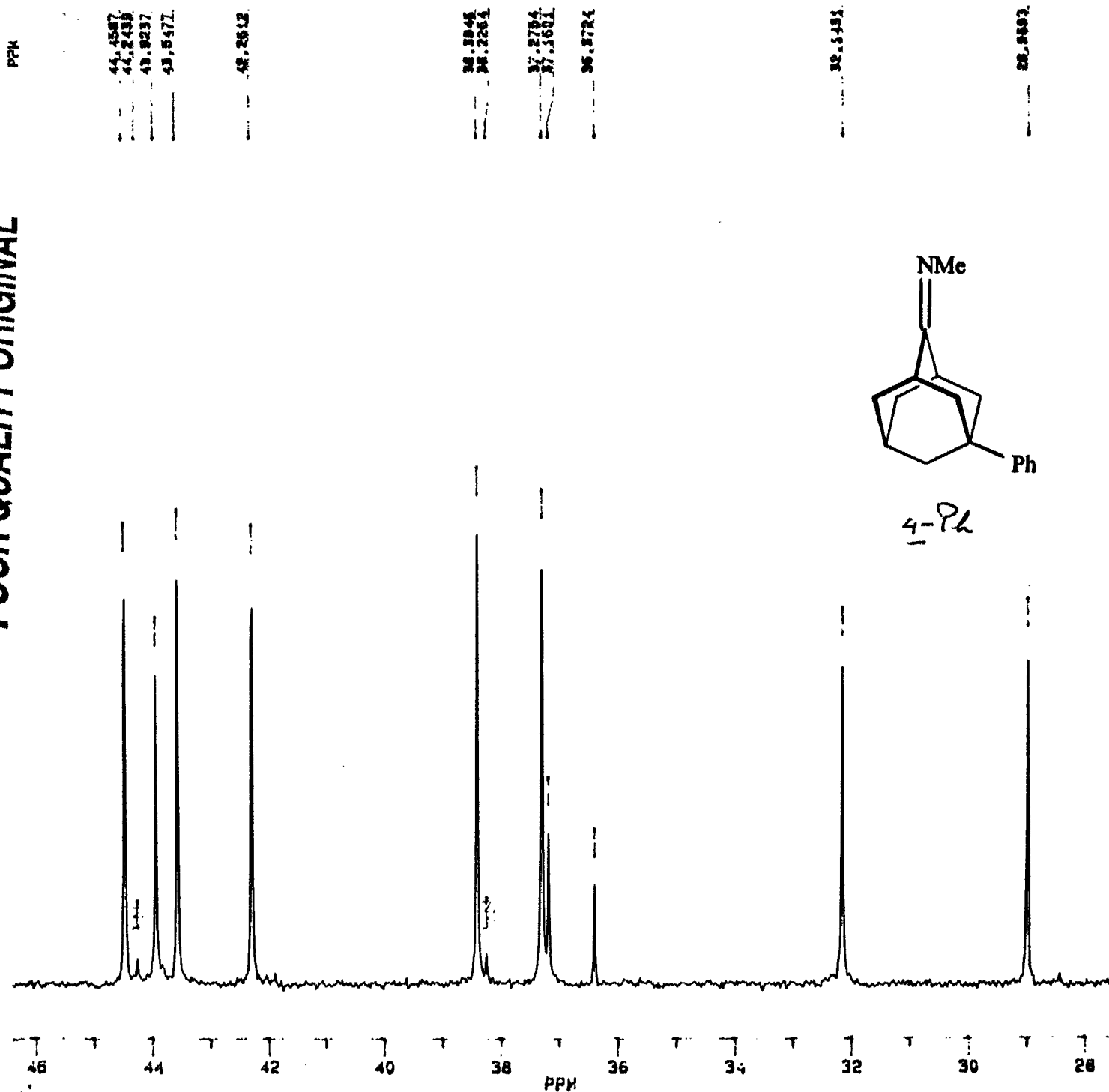
SF	62.896
SY	62.0
O1	3218.018
SI	32768
TD	32768
SW	15625.000
HZ/PT	.954

PW	0.0
RD	0.0
AQ	1.049
RG	3200
NS	453
TE	297

```
FW 19600
02 4100.000
DP 20H D0
```

LB	1.000
GB	.100
CX	20.00
CY	8.00
F1	230.000P
F2	-.004P
HZ/CM	723.314
PPM/CM	11.500
SR	-4058.28

POOR QUALITY ORIGINAL



~~BRUKER~~

CJ54.C00
DATE 13-5-96

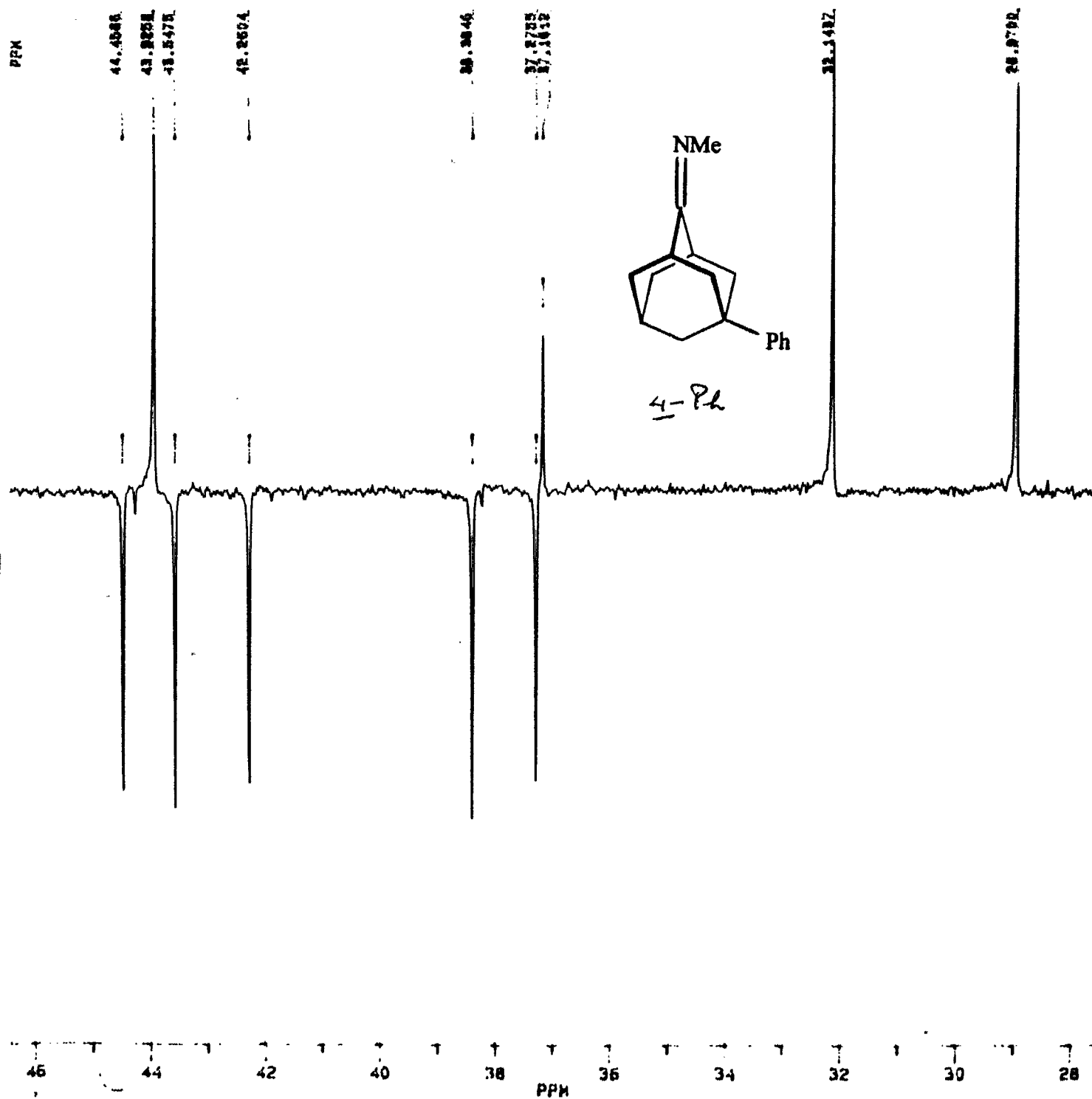
SF 62.896
SY 62.0
O1 3218.018
SI 32768
TD 32768
SW 15625.000
HZ/PT .954

PW 5.0
RD 1.000
AQ 1.049
RG 3200
NS 641
TE 297

FW 19600
O2 4100.000
DP 20H CPD

LB 1.000
GB .100
CX 20.00
CY 8.00
F1 46.424P
F2 27.517P
HZ/CM 59.462
PPM/CM .945
SR -4058.28

POOR QUALITY ORIGINAL



~~BRUKER~~

32

CJ54.D00
AU PROG.
DEPT1.AU
DATE 13-5-96

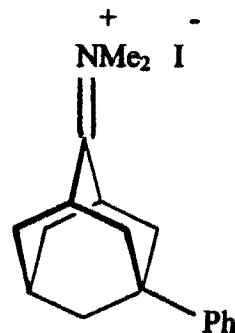
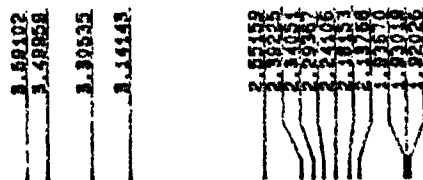
SF 62.896
SY 62.0
O1 3218.018
SI 32768
TD 32768
SW 15625.000
HZ/PT .954

PW 0.0
RD 0.0
AQ 1.049
RG 3200
NS 453
TE 297

FW 19600
O2 4100.000
DP 20H D0

LB 1.000
GB .100
CX 20.00
CY 8.00
F1 46.424P
F2 27.517P
HZ/CM 59.462
PPM/CM .945
SR -4058.28

Итого



5-72

BAUKER

CJ78ST.H00
DATE 24-6-96

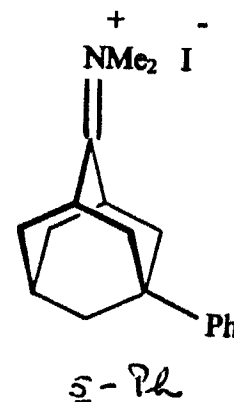
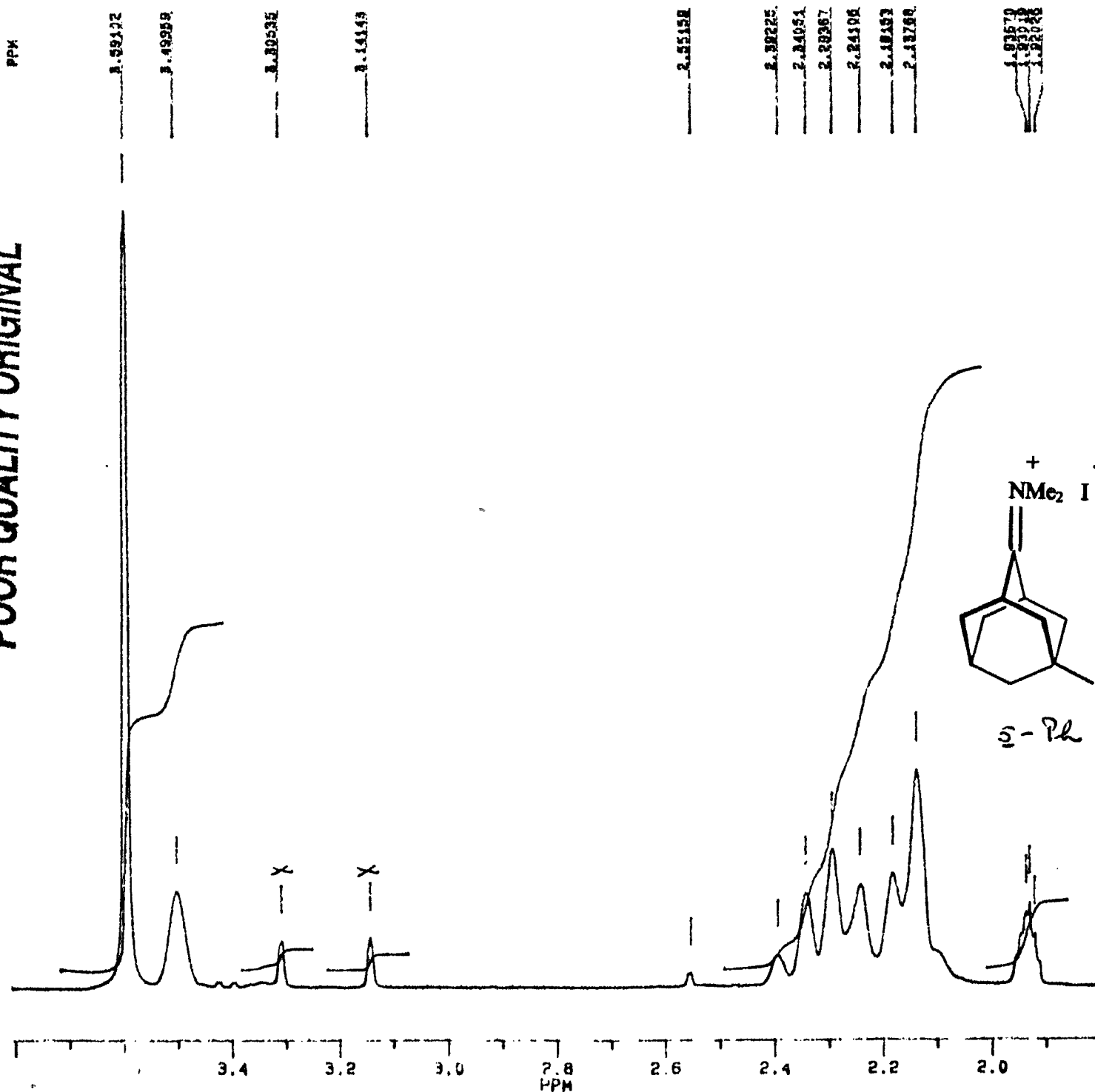
SF	250.134
SY	100.0
O1	5452.300
SI	16384
TD	16384
SW	2994.012
HZ/PT	.365

PW	3.0
RD	1.000
AQ	2.736
RG	80
NS	64
TE	297

FW 3000
02 3210.000
DP 63L P0

LB	.100
GB	.100
CX	20.00
CY	14.00
F1	7.903P
F2	1.432P
HZ/CM	80.936
PPM/CM	.324
SR	4186.32

POOR QUALITY ORIGINAL



~~BRUKER~~

CJ78ST.H00
DATE 24-6-96

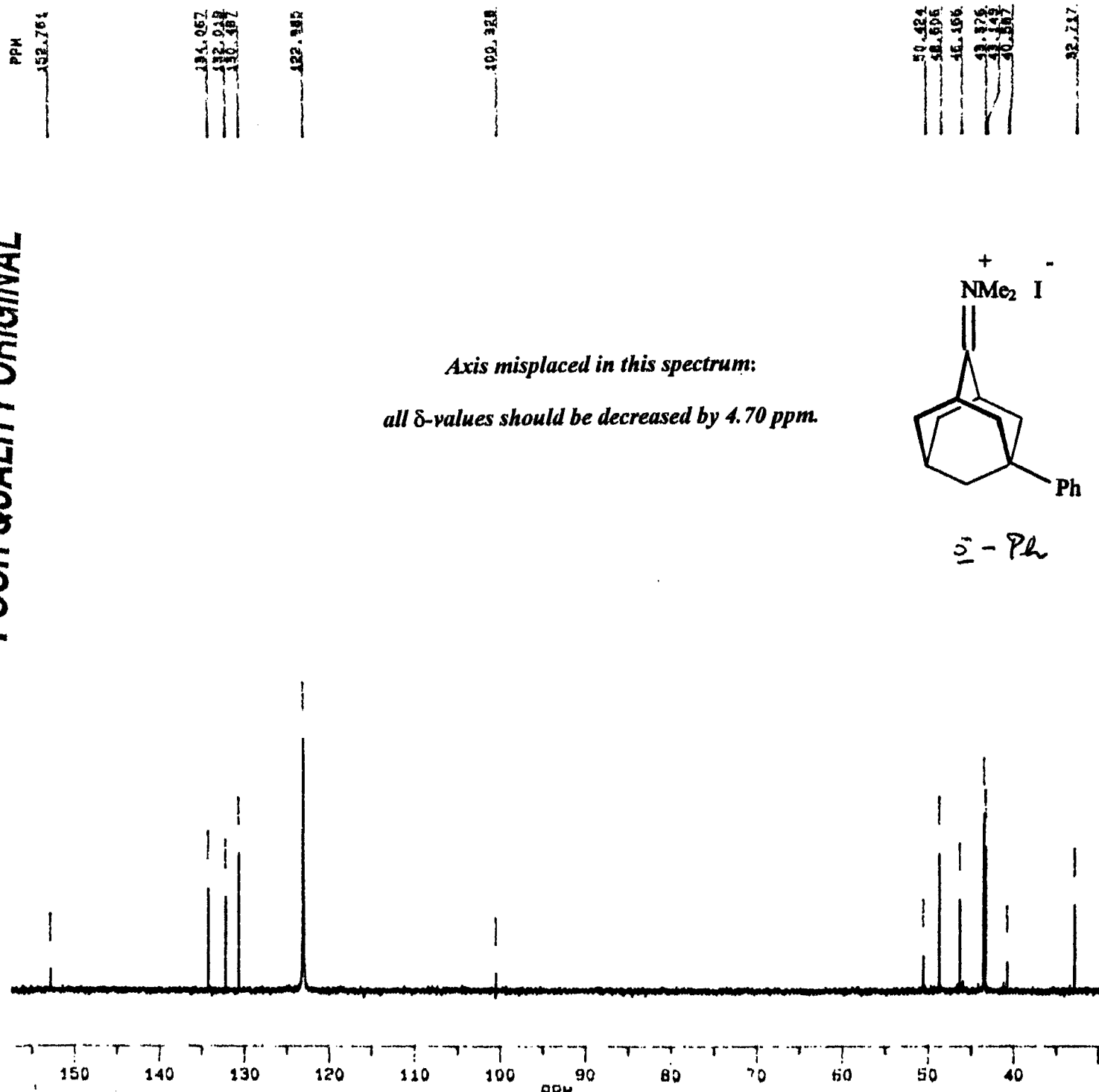
SF 250.134
SY 100.0
O1 5452.300
SI 16384
TD 16384
SW 2994.012
HZ/PT .365

PW 3.0
RD 1.000
AQ 2.736
RG 80
NS 64
TE 297

FW 3000
O2 3210.000
DP 63L PO

LB .100
GB .100
CX 20.00
CY 14.00
F1 3.805P
F2 1.798P
HZ/CM 25.090
PPM/CM .100
SR 4186.32

POOR QUALITY ORIGINAL



CJ78ST.C00
DATE 25-6-96

SF 62.896
SY 62.0
O1 3218.018
SI 32768
TO 32768
SW 15625.000
HZ/PT .954

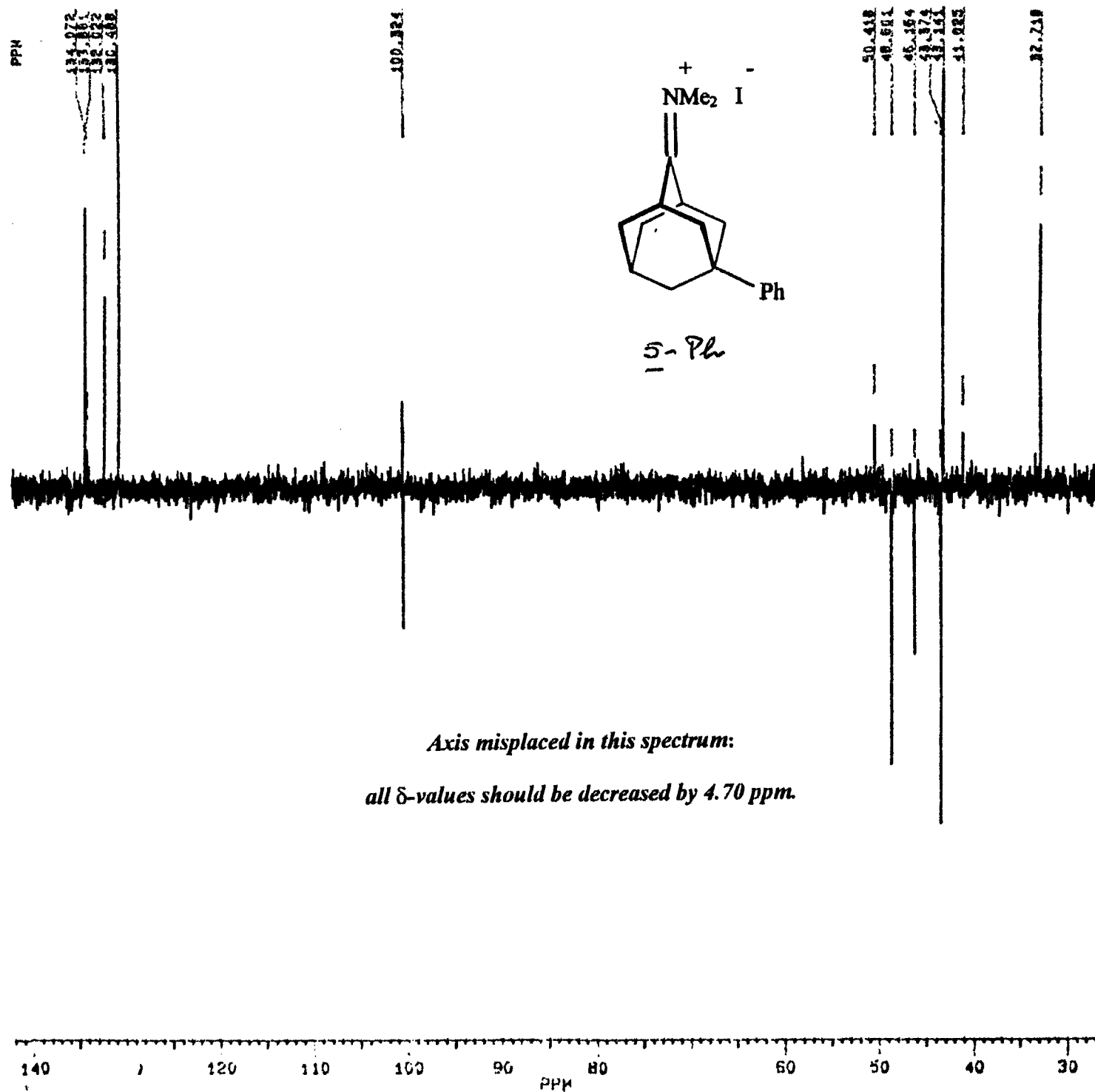
PW 5.0
RD 2.000
AQ 1.049
RG 1600
NS 2248
TE 297

FW 19600
O2 4100.000
DP 20H CPD

LB .100
GB .100
CX 20.00
CY 8.00
F1 157.264P
F2 29.184P
HZ/CM 402.784
PPM/CM 6.404
SR -4060.19

35

POOR QUALITY ORIGINAL



BRUKER

CJ78ST.D00
 AU PROG:
 DEPT1.AU
 DATE 25-6-96

SF 62.896
 SY 62.0
 O1 3218.018
 SI 32768
 TD 32768
 SW 15625.000
 HZ/PT .954

PW 0.0
 RD 0.0
 AQ 1.049
 RG 1600
 NS 711
 TE 297

FW 19600
 O2 4100.000
 DP 20H D0

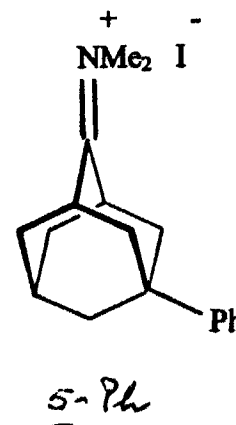
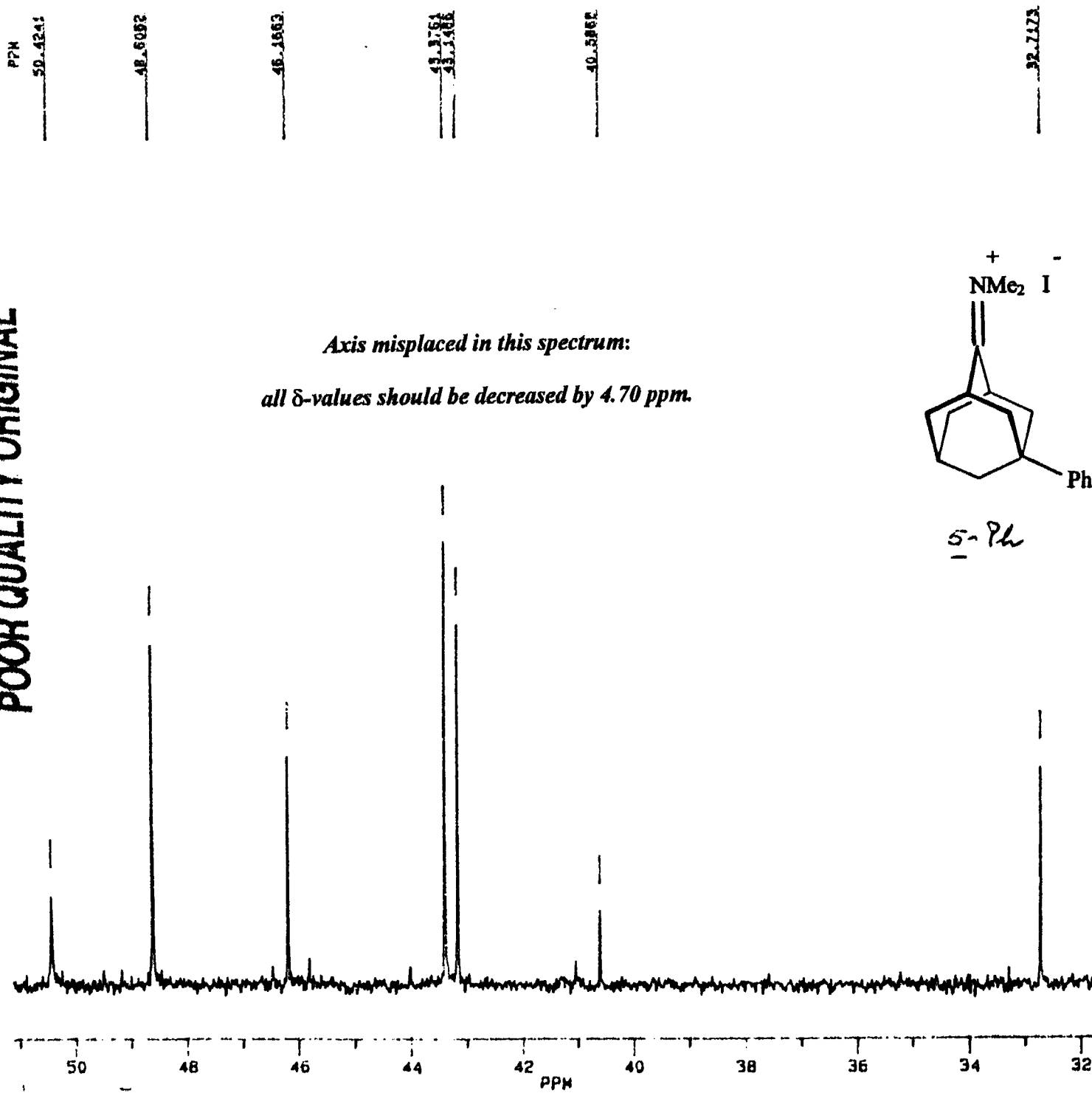
LB 1.000
 GB .100
 CX 20.00
 CY 8.00
 F1 142.071P
 F2 26.606P
 HZ/CM 363.111
 PPM/CM 5.773
 SR -4060.16

Axis misplaced in this spectrum:

all δ -values should be decreased by 4.70 ppm.

(36)

POOR QUALITY ORIGINAL



~~BRUKER~~

CJ78ST.C00
DATE 25-6-96

SF 62.896
SY 62.0
O1 3218.018
SI 32768
TD 32768
SW 15625.000
HZ/PT .954

PW 5.0
RD 2.000
AQ 1.049
RG 1600
NS 2248
TE 297

FW 19600
O2 4100.000
DP 20H CPD

LB .100
GB .100
CX 20.00
CY 8.00
F1 51.110P
F2 31.686P
HZ/CM 61.083
PPM/CM .971
SR -4060.19

37

PPM

50.4183

48.6207

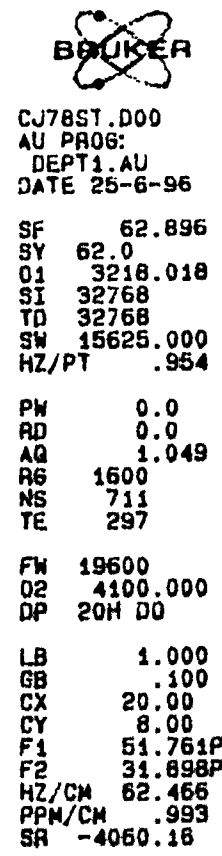
46.1643

43.2736
43.1407

41.0248

32.2101

CN(C)=C1C2C(C1)C3C2C(C3)C4C(C2)C(C4)C5C(C3)C(C5)C6C(C4)C(C6)C7C(C5)C(C7)C8C(C6)C(C8)C9C(C7)C(C9)C10C(C8)C(C10)C11C(C9)C(C11)C12C(C10)C(C12)C13C(C11)C(C13)C14C(C12)C(C14)C15C(C13)C(C15)C16C(C14)C(C16)C17C(C15)C(C17)C18C(C16)C(C18)C19C(C17)C(C19)C20C(C18)C(C20)C21C(C19)C(C21)C22C(C20)C(C22)C23C(C21)C(C23)C24C(C22)C(C24)C25C(C23)C(C25)C26C(C24)C(C26)C27C(C25)C(C27)C28C(C26)C(C28)C29C(C27)C(C29)C30C(C28)C(C30)C31C(C29)C(C31)C32C(C30)C(C32)C33C(C31)C(C33)C34C(C32)C(C34)C35C(C33)C(C35)C36C(C34)C(C36)C37C(C35)C(C37)C38C(C36)C(C38)C39C(C37)C(C39)C40C(C38)C(C40)C41C(C39)C(C41)C42C(C40)C(C42)C43C(C41)C(C43)C44C(C42)C(C44)C45C(C43)C(C45)C46C(C44)C(C46)C47C(C45)C(C47)C48C(C46)C(C48)C49C(C47)C(C49)C50C(C48)C(C50)C51C(C49)C(C51)C52C(C50)C(C52)C53C(C51)C(C53)C54C(C52)C(C54)C55C(C53)C(C55)C56C(C54)C(C56)C57C(C55)C(C57)C58C(C56)C(C58)C59C(C57)C(C59)C60C(C58)C(C60)C61C(C59)C(C61)C62C(C60)C(C62)C63C(C61)C(C63)C64C(C62)C(C64)C65C(C63)C(C65)C66C(C64)C(C66)C67C(C65)C(C67)C68C(C66)C(C68)C69C(C67)C(C69)C70C(C68)C(C70)C71C(C69)C(C71)C72C(C70)C(C72)C73C(C71)C(C73)C74C(C72)C(C74)C75C(C73)C(C75)C76C(C74)C(C76)C77C(C75)C(C77)C78C(C76)C(C78)C79C(C77)C(C79)C80C(C78)C(C80)C81C(C79)C(C81)C82C(C80)C(C82)C83C(C81)C(C83)C84C(C82)C(C84)C85C(C83)C(C85)C86C(C84)C(C86)C87C(C85)C(C87)C88C(C86)C(C88)C89C(C87)C(C89)C90C(C88)C(C90)C91C(C89)C(C91)C92C(C90)C(C92)C93C(C91)C(C93)C94C(C92)C(C94)C95C(C93)C(C95)C96C(C94)C(C96)C97C(C95)C(C97)C98C(C96)C(C98)C99C(C97)C(C99)C100C(C98)C(C100)C101C(C99)C(C101)C102C(C100)C(C102)C103C(C101)C(C103)C104C(C102)C(C104)C105C(C103)C(C105)C106C(C104)C(C106)C107C(C105)C(C107)C108C(C106)C(C108)C109C(C107)C(C109)C110C(C108)C(C110)C111C(C109)C(C111)C112C(C110)C(C112)C113C(C111)C(C113)C114C(C112)C(C114)C115C(C113)C(C115)C116C(C114)C(C116)C117C(C115)C(C117)C118C(C116)C(C118)C119C(C117)C(C119)C120C(C118)C(C120)C121C(C119)C(C121)C122C(C120)C(C122)C123C(C121)C(C123)C124C(C122)C(C124)C125C(C123)C(C125)C126C(C124)C(C126)C127C(C125)C(C127)C128C(C126)C(C128)C129C(C127)C(C129)C130C(C128)C(C130)C131C(C129)C(C131)C132C(C130)C(C132)C133C(C131)C(C133)C134C(C132)C(C134)C135C(C133)C(C135)C136C(C134)C(C136)C137C(C135)C(C137)C138C(C136)C(C138)C139C(C137)C(C139)C140C(C138)C(C140)C141C(C139)C(C141)C142C(C140)C(C142)C143C(C141)C(C143)C144C(C142)C(C144)C145C(C143)C(C145)C146C(C144)C(C146)C147C(C145)C(C147)C148C(C146)C(C148)C149C(C147)C(C149)C150C(C148)C(C150)C151C(C149)C(C151)C152C(C150)C(C152)C153C(C151)C(C153)C154C(C152)C(C154)C155C(C153)C(C155)C156C(C154)C(C156)C157C(C155)C(C157)C158C(C156)C(C158)C159C(C157)C(C159)C160C(C158)C(C160)C161C(C159)C(C161)C162C(C160)C(C162)C163C(C161)C(C163)C164C(C162)C(C164)C165C(C163)C(C165)C166C(C164)C(C166)C167C(C165)C(C167)C168C(C166)C(C168)C169C(C167)C(C169)C170C(C168)C(C170)C171C(C169)C(C171)C172C(C170)C(C172)C173C(C171)C(C173)C174C(C172)C(C174)C175C(C173)C(C175)C176C(C174)C(C176)C177C(C175)C(C177)C178C(C176)C(C178)C179C(C177)C(C179)C180C(C178)C(C180)C181C(C179)C(C181)C182C(C180)C(C182)C183C(C181)C(C183)C184C(C182)C(C184)C185C(C183)C(C185)C186C(C184)C(C186)C187C(C185)C(C187)C188C(C186)C(C188)C189C(C187)C(C189)C190C(C188)C(C190)C191C(C189)C(C191)C192C(C190)C(C192)C193C(C191)C(C193)C194C(C192)C(C194)C195C(C193)C(C195)C196C(C194)C(C196)C197C(C195)C(C197)C198C(C196)C(C198)C199C(C197)C(C199)C200C(C198)C(C200)C201C(C199)C(C201)C202C(C200)C(C202)C203C(C201)C(C203)C204C(C202)C(C204)C205C(C203)C(C205)C206C(C204)C(C206)C207C(C205)C(C207)C208C(C206)C(C208)C209C(C207)C(C209)C210C(C208)C(C210)C211C(C209)C(C211)C212C(C210)C(C212)C213C(C211)C(C213)C214C(C212)C(C214)C215C(C213)C(C215)C216C(C214)C(C216)C217C(C215)C(C217)C218C(C216)C(C218)C219C(C217)C(C219)C220C(C218)C(C220)C221C(C219)C(C221)C222C(C220)C(C222)C223C(C221)C(C223)C224C(C222)C(C224)C225C(C223)C(C225)C226C(C224)C(C226)C227C(C225)C(C227)C228C(C226)C(C228)C229C(C227)C(C229)C230C(C228)C(C230)C231C(C229)C(C231)C232C(C230)C(C232)C233C(C231)C(C233)C234C(C232)C(C234)C235C(C233)C(C235)C236C(C234)C(C236)C237C(C235)C(C237)C238C(C236)C(C238)C239C(C237)C(C239)C240C(C238)C(C240)C241C(C239)C(C241)C242C(C240)C(C242)C243C(C241)C(C243)C244C(C242)C(C244)C245C(C243)C(C245)C246C(C244)C(C246)C247C(C245)C(C247)C248C(C246)C(C248)C249C(C247)C(C249)C250C(C248)C(C250)C251C(C249)C(C251)C252C(C250)C(C252)C253C(C251)C(C253)C254C(C252)C(C254)C255C(C253)C(C255)C256C(C254)C(C256)C257C(C255)C(C257)C258C(C256)C(C258)C259C(C257)C(C259)C260C(C258)C(C260)C261C(C259)C(C261)C262C(C260)C(C262)C263C(C261)C(C263)C264C(C262)C(C264)C265C(C263)C(C265)C266C(C264)C(C266)C267C(C265)C(C267)C268C(C266)C(C268)C269C(C267)C(C269)C270C(C268)C(C270)C271C(C269)C(C271)C272C(C2



Axis misplaced in this spectrum:
all δ -values should be decreased by 4.70 ppm.

34

File : C:\CJ80B.D
Operator : cheryl jones
Acquired : 25 Jun 96 4:27 pm using AcqMethod CJONES
Instrument : 5971 - In
Sample Name: N-methyl-5-phenyladamantyl amine
Misc Info : 180 hold 2 min 5/min to 230
Vial Number: 1

