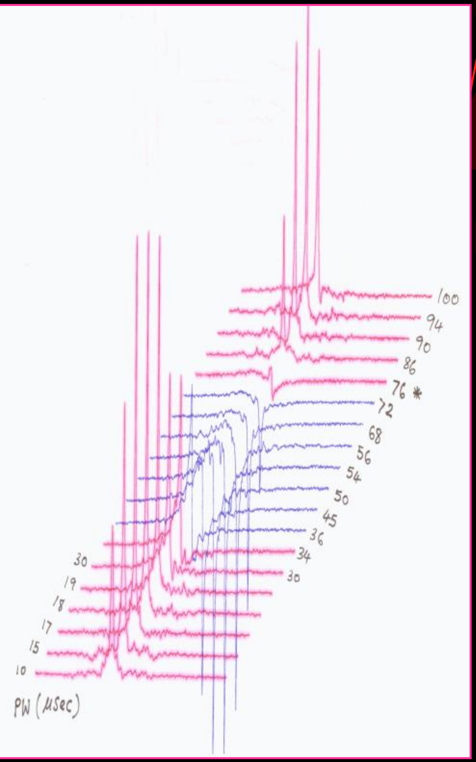
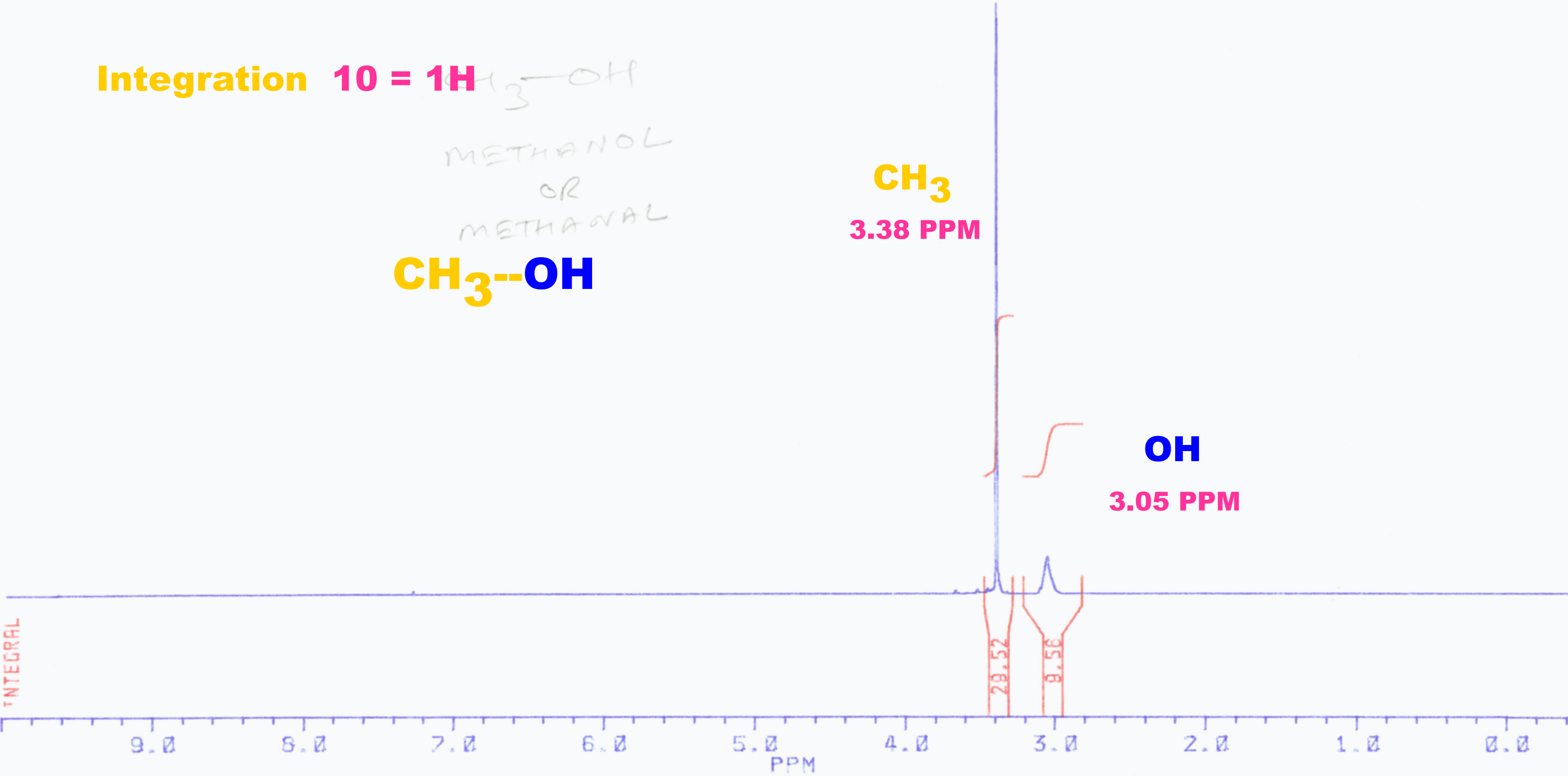
NMR SPECTROSCOPY



DR. M. KANJIA

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Methanal or Methanol

^{1}H NMR of CH_3--OH



Integration 10 = 1H

CH_3--OH

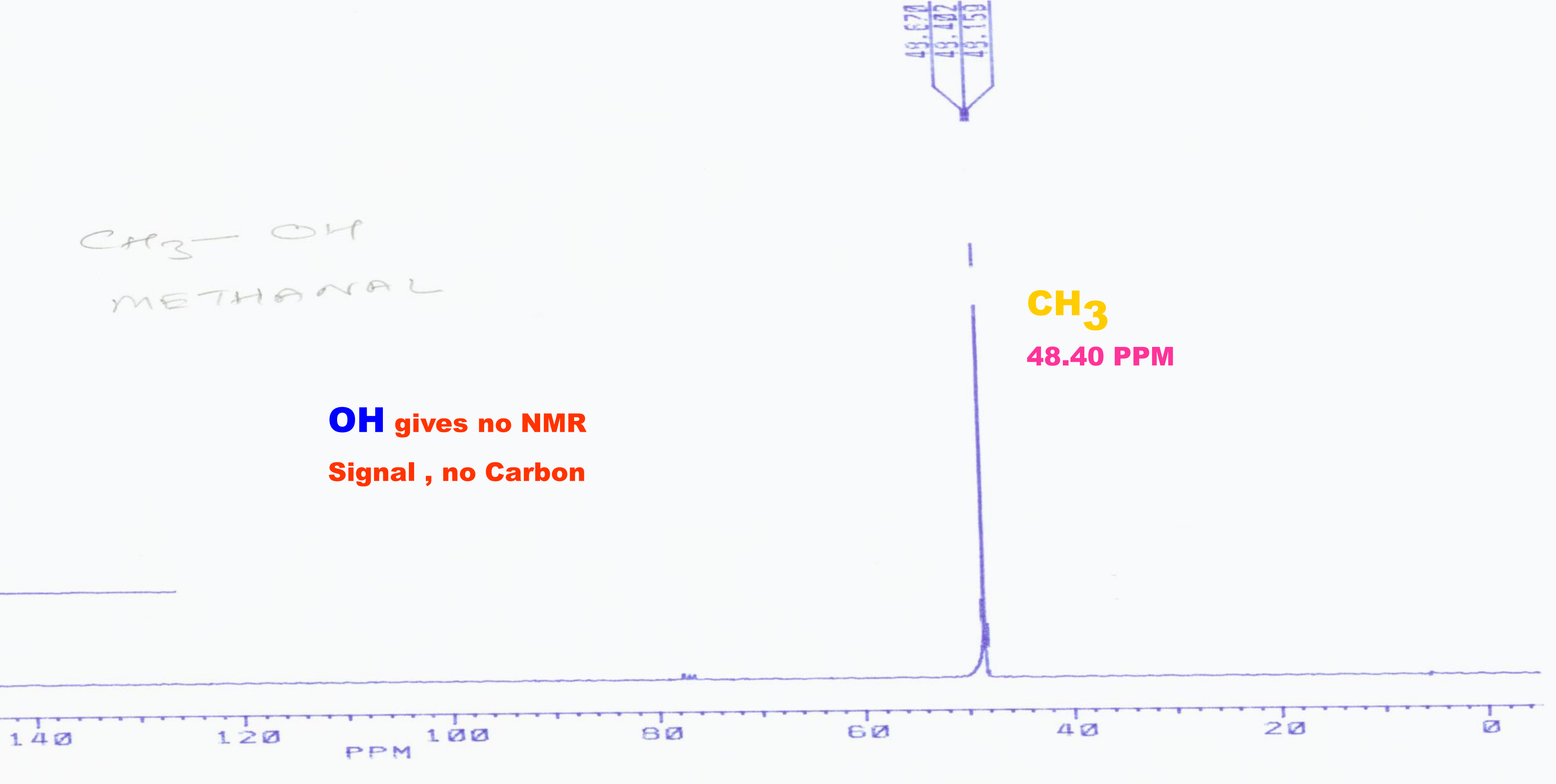
CH_3

3.38 PPM

OH

3.05 PPM

^{13}C NMR Spectrum of Methanal
CH_3OH



CH_3

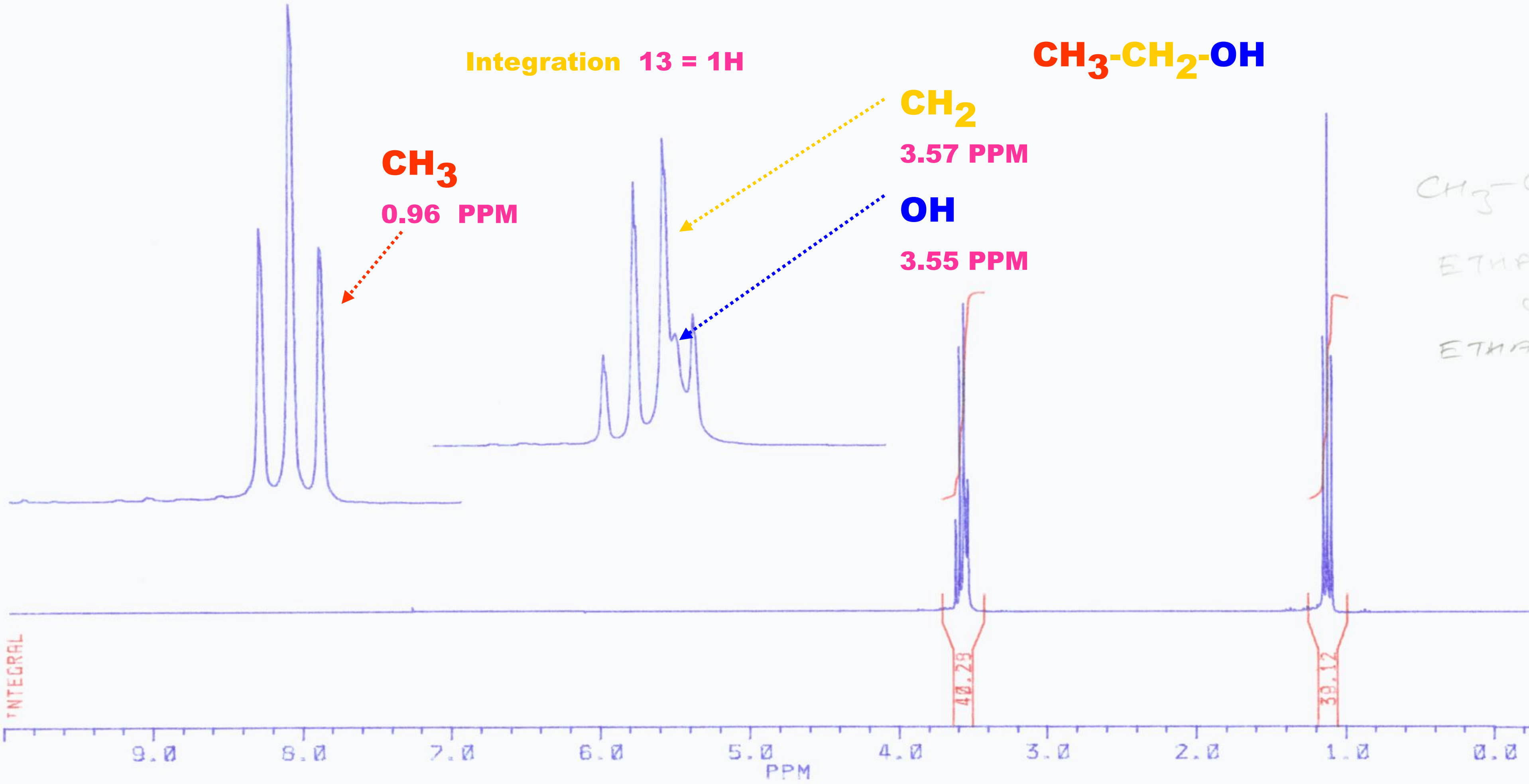
48.40 PPM

OH gives no NMR

Signal , no Carbon

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Ethanal or Ethanol CH_3--CH_2--OH

^{1}H NMR Spectrum



Integration 13 = 1H

CH_3-CH_2-OH

CH_3

0.96 PPM

CH_2

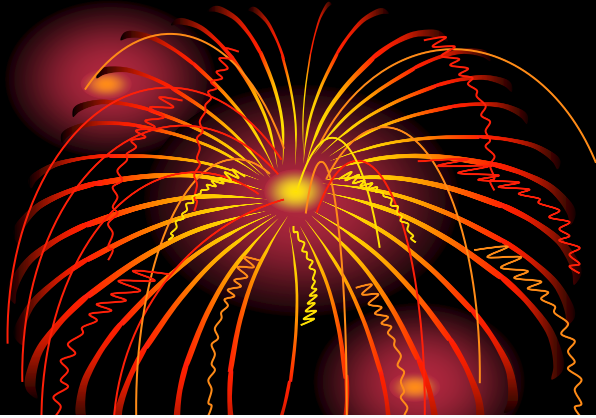
3.57 PPM

OH

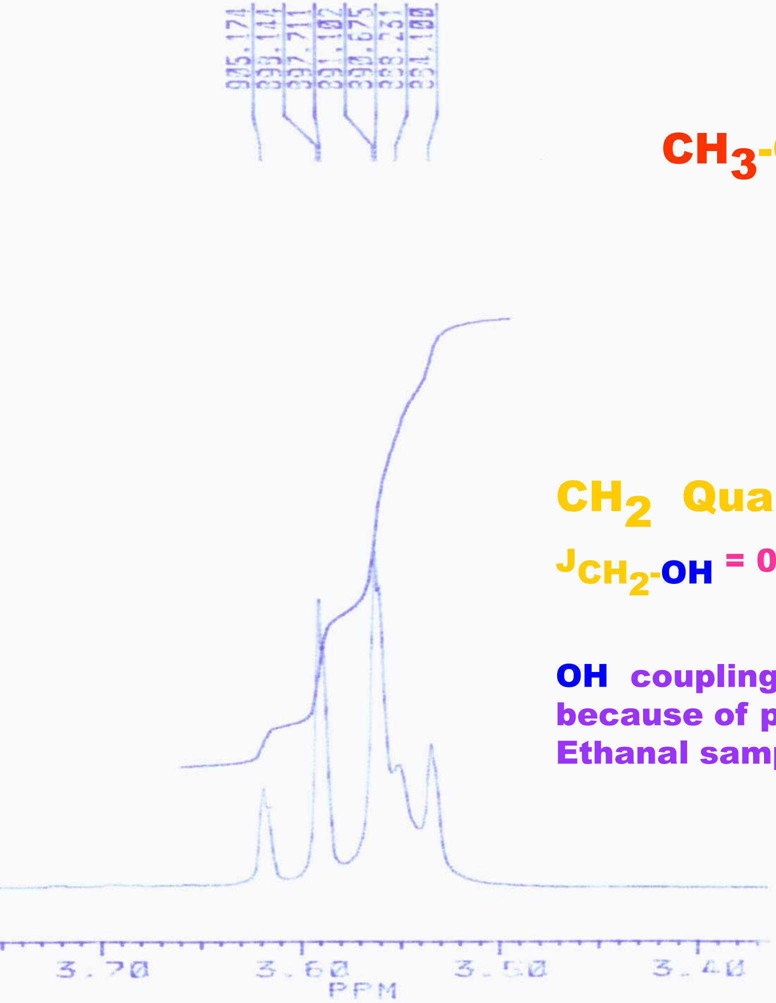
3.55 PPM

Expansion of ^{1}H NMR of Ethanal

CH_3—CH_2--OH



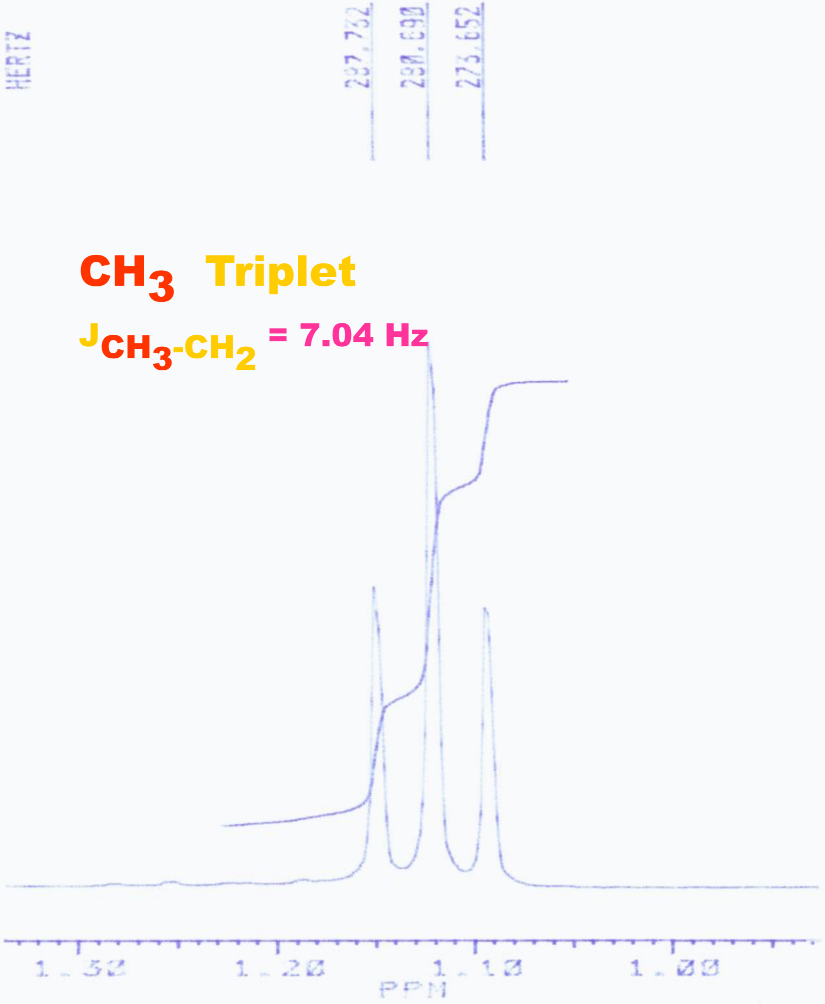
CH_3-CH_2-OH



CH_2 Quartet

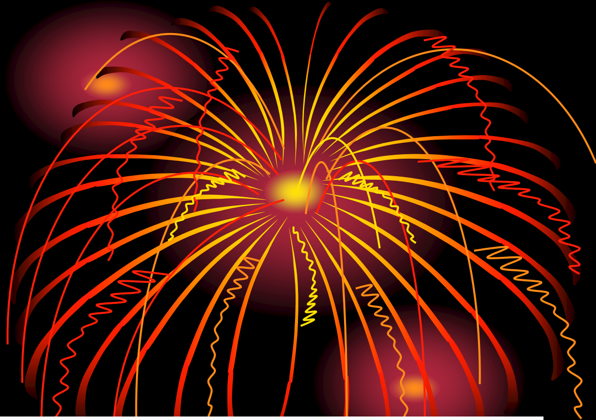
$J_{CH_2\text{-}OH}$ = 0.43 Hz

OH coupling is visible because of purity of Ethanal sample.



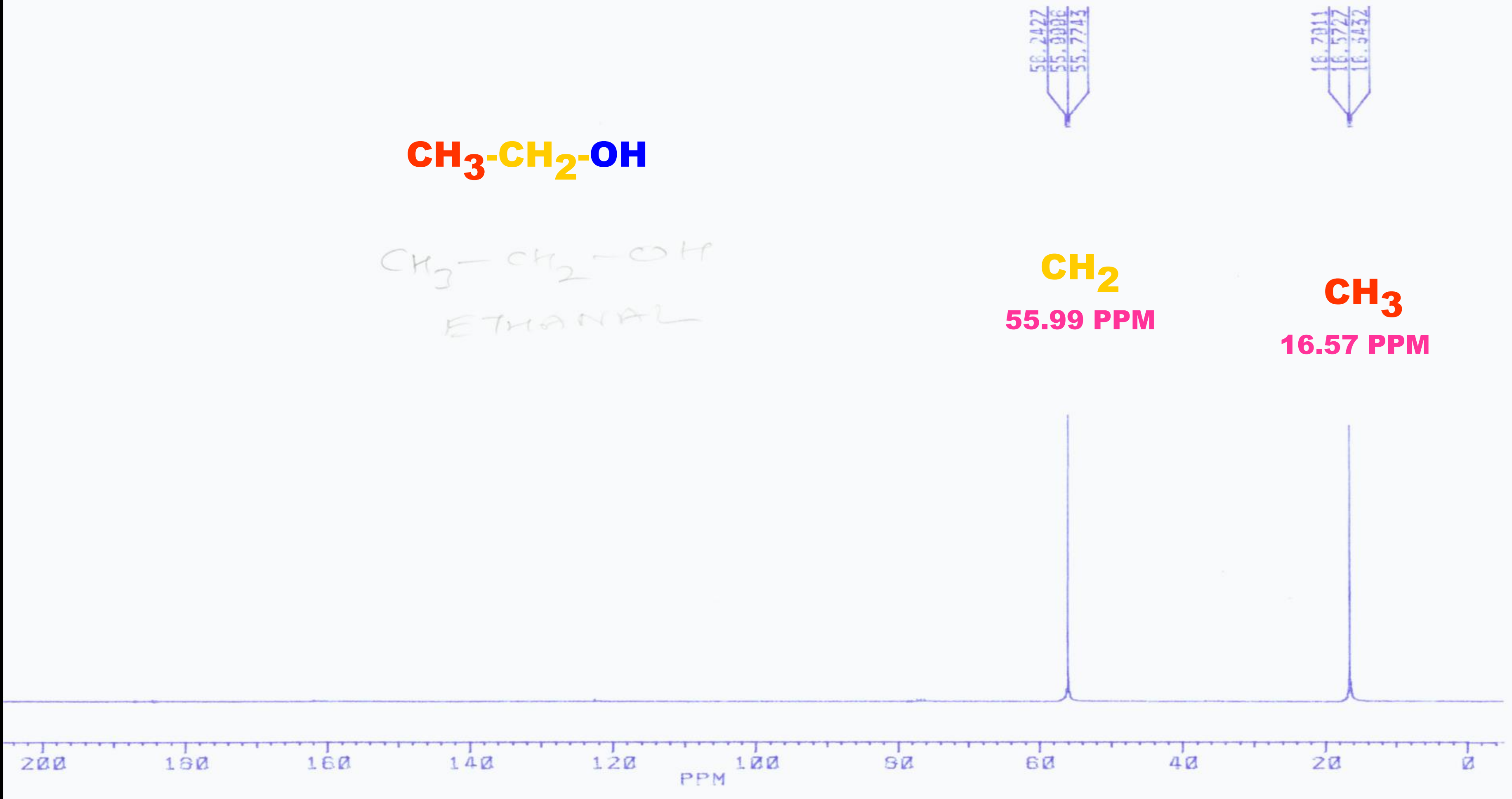
CH_3 Triplet

$J_{CH_3\text{-}CH_2}$ = 7.04 Hz

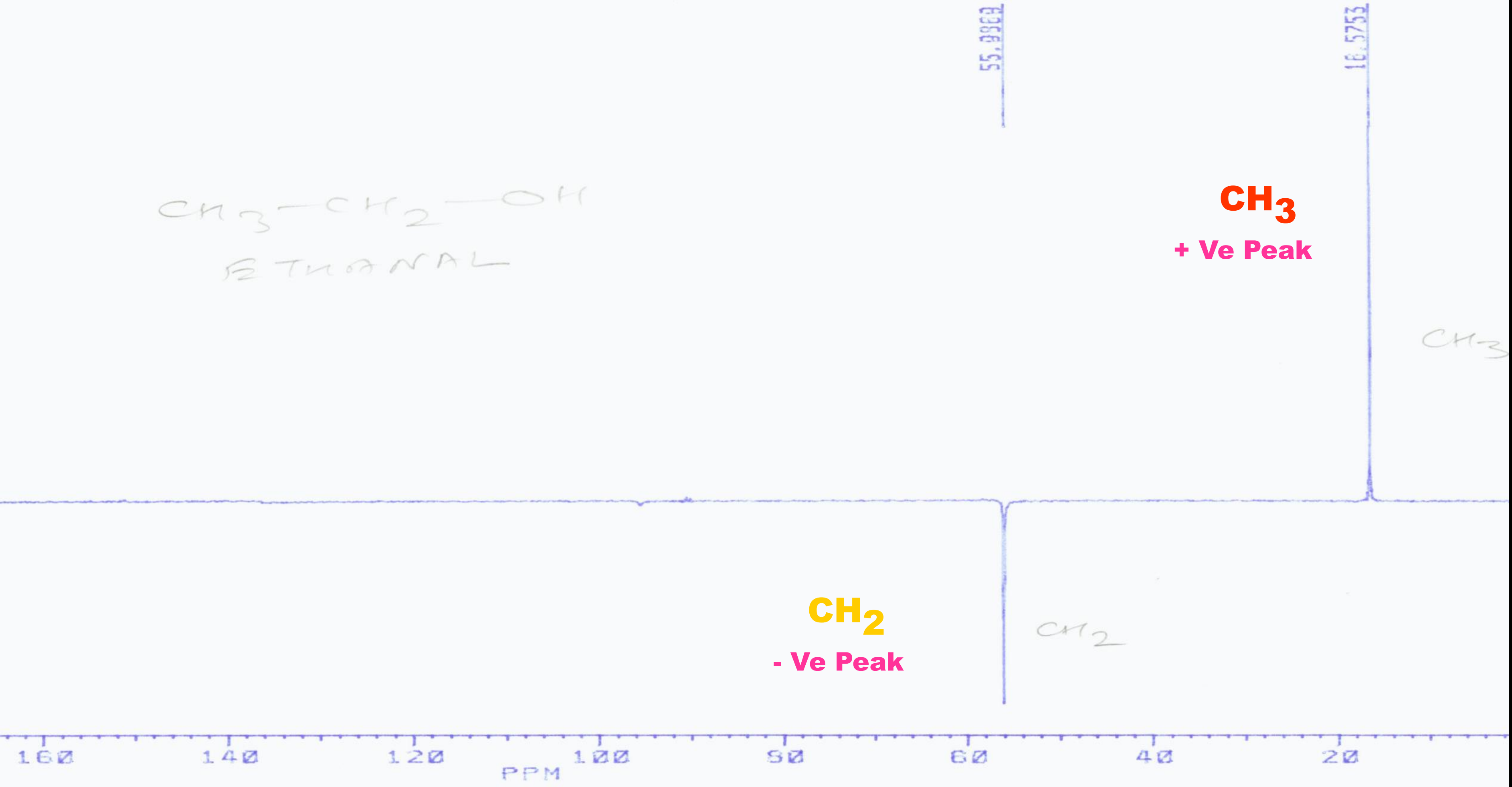


^{13}C NMR Spectrum of Ethanal

CH_3—CH_2--OH



^{13}C Dept 135 NMR Spectrum of Ethanal



CH_3

+ Ve Peak

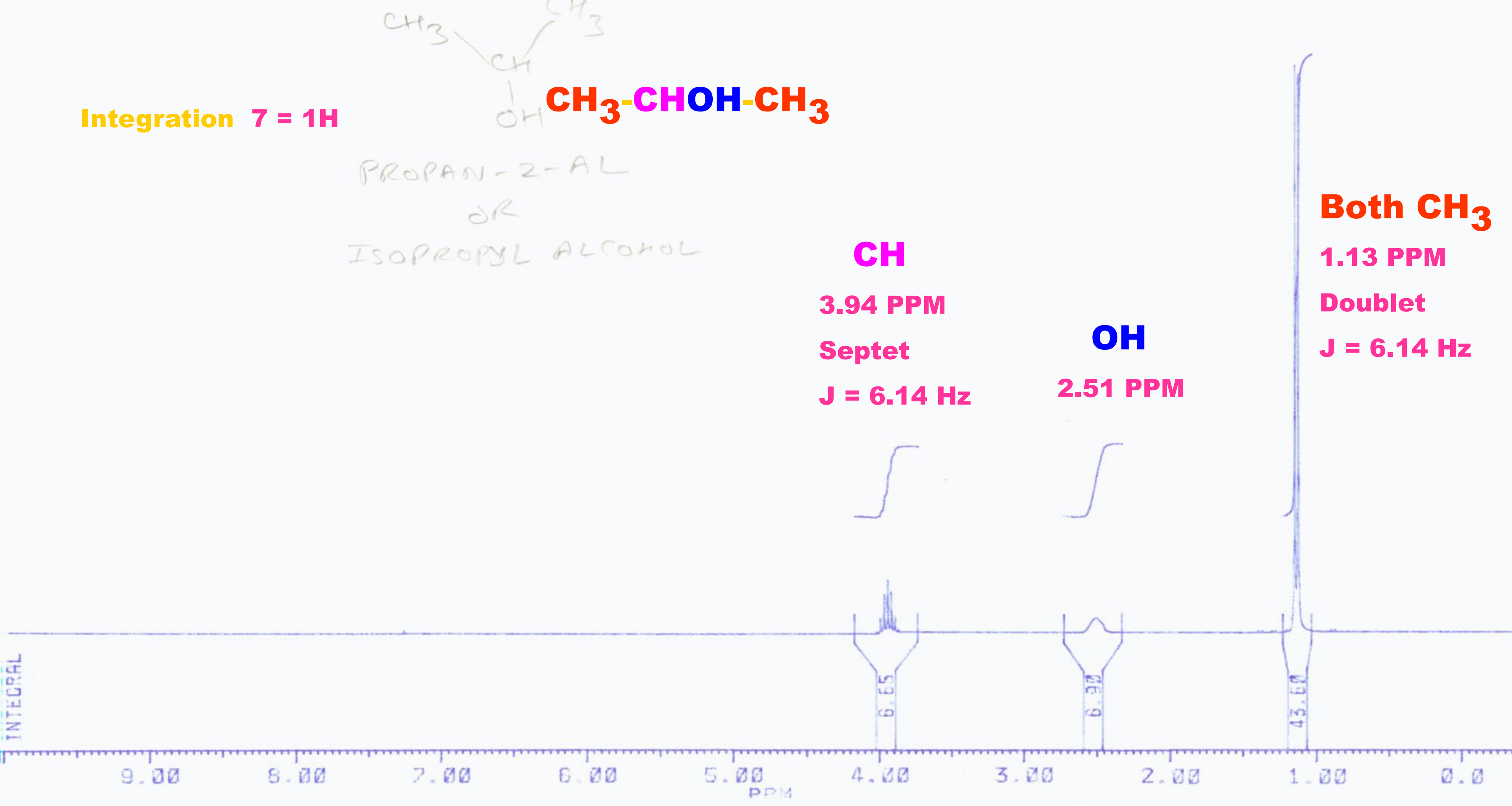
CH_2

- Ve Peak

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Propan-2-al

$CH_3—CHOH—CH_3$

^{1}H NMR Spectrum



Integration 7 = 1H

CH_3-CHOH-CH_3

CH

3.94 PPM

Septet

J = 6.14 Hz

OH

2.51 PPM

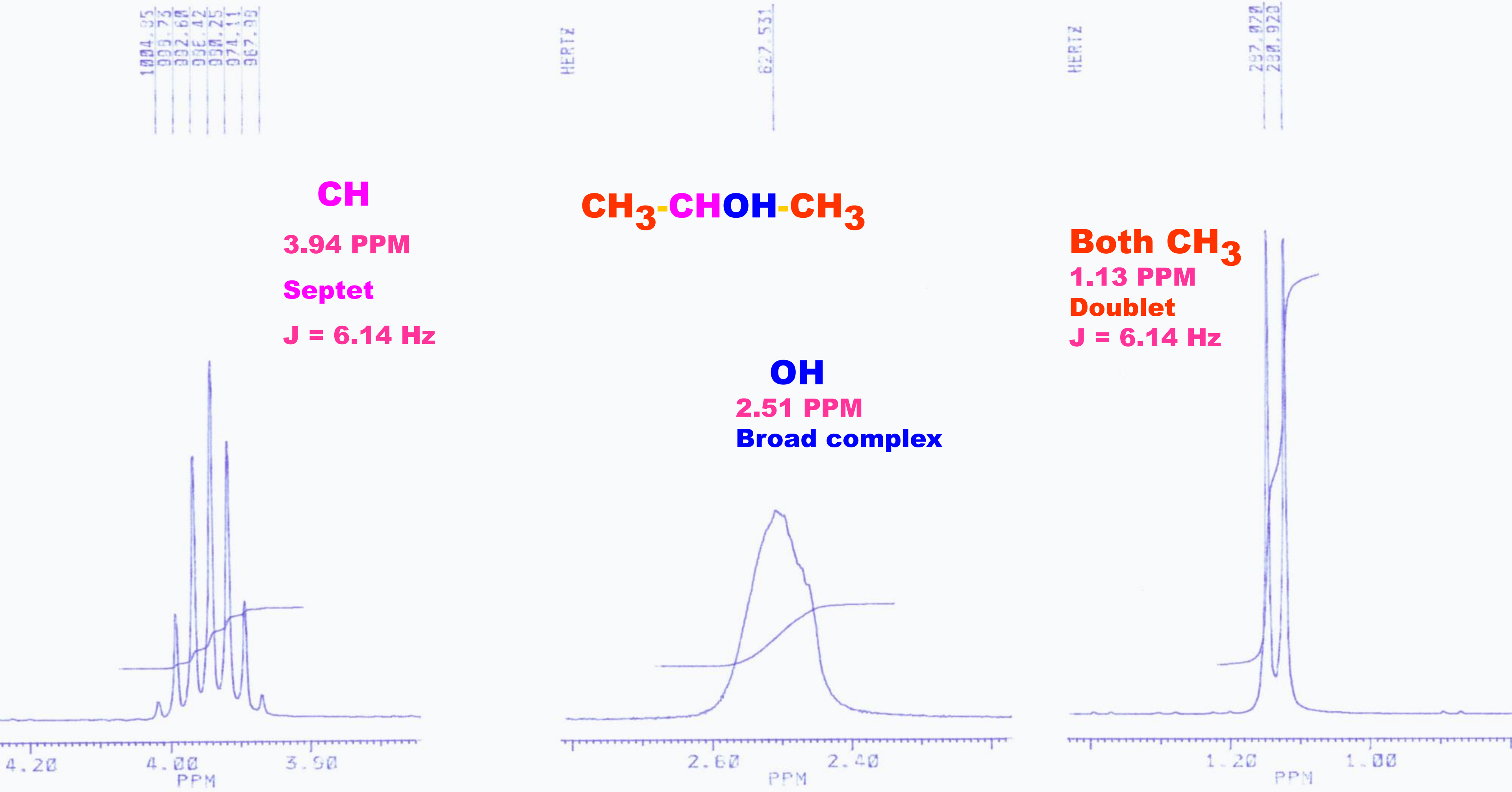
Both CH_3

1.13 PPM

Doublet

J = 6.14 Hz

Expansion of ^{1}H NMR Spectrum of Propan-2-al



CH

3.94 PPM

Septet

J = 6.14 Hz

CH_3-CHOH-CH_3

OH

2.51 PPM

Broad complex

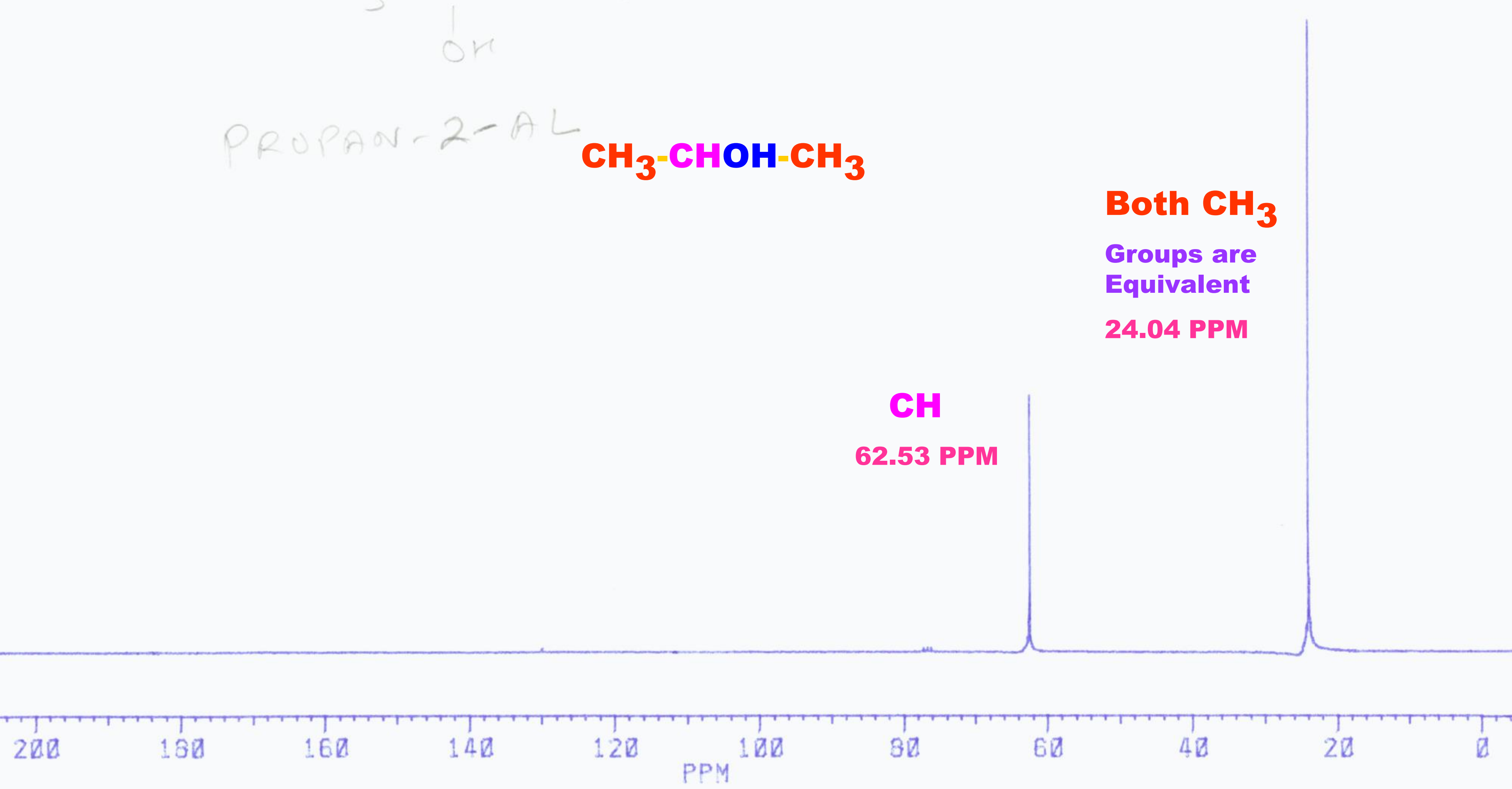
Both CH_3

1.13 PPM

Doublet

J = 6.14 Hz

^{13}C NMR Spectrum of Propan-2-al



CH_3-CHOH-CH_3

Both CH_3

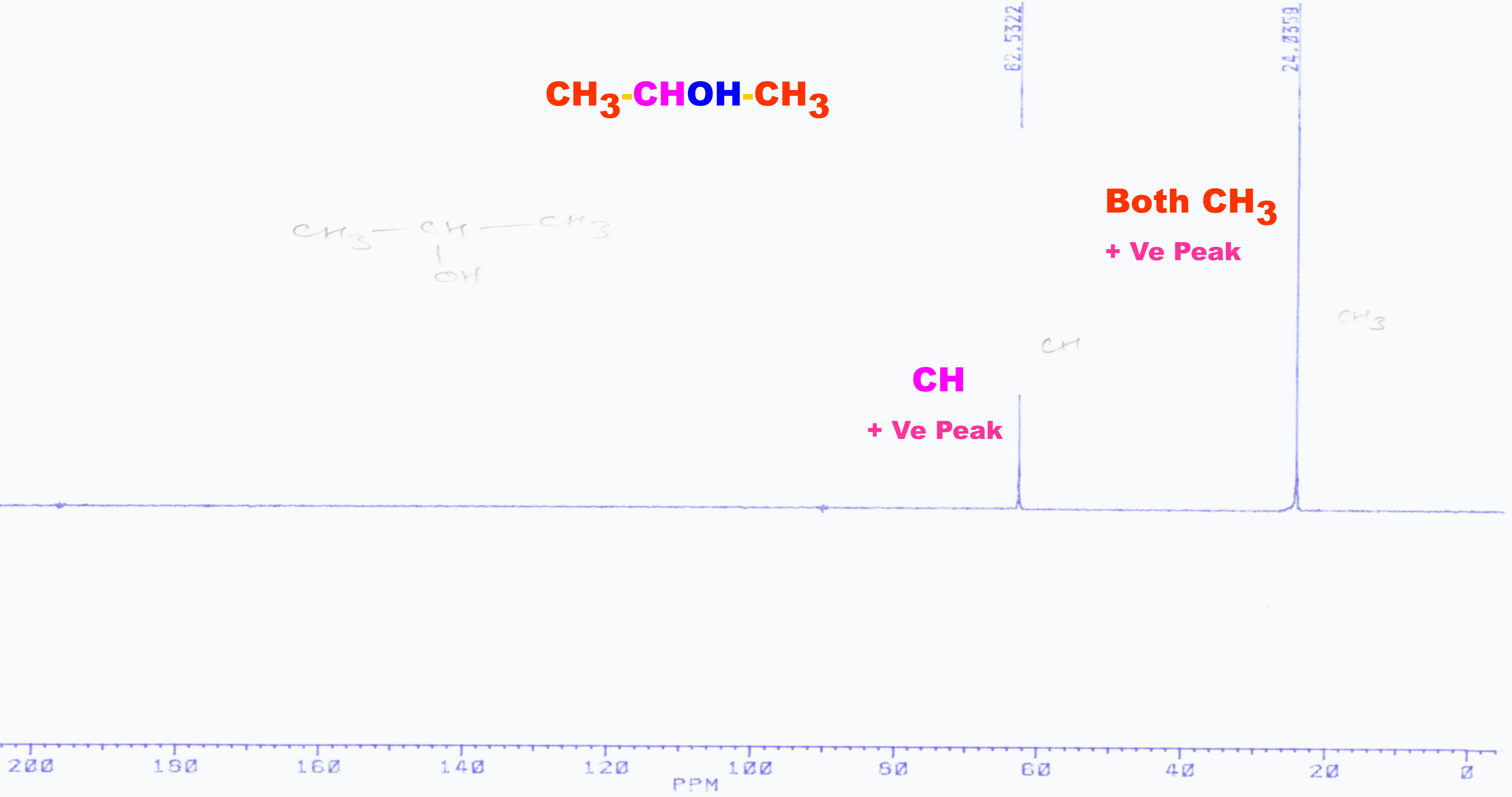
Groups are Equivalent

24.04 PPM

CH

62.53 PPM

^{13}C Dept 135 NMR Spectrum of Propan-2-al



CH_3-CHOH-CH_3

Both CH_3

+ Ve Peak

CH

+ Ve Peak

Analysis and interpretation of ^{1}H NMR Spectrum Of Butan-2-al

CH_3-$CHOH$-CH_2-CH_3
1 2 3 4

Integration 12 = 1H

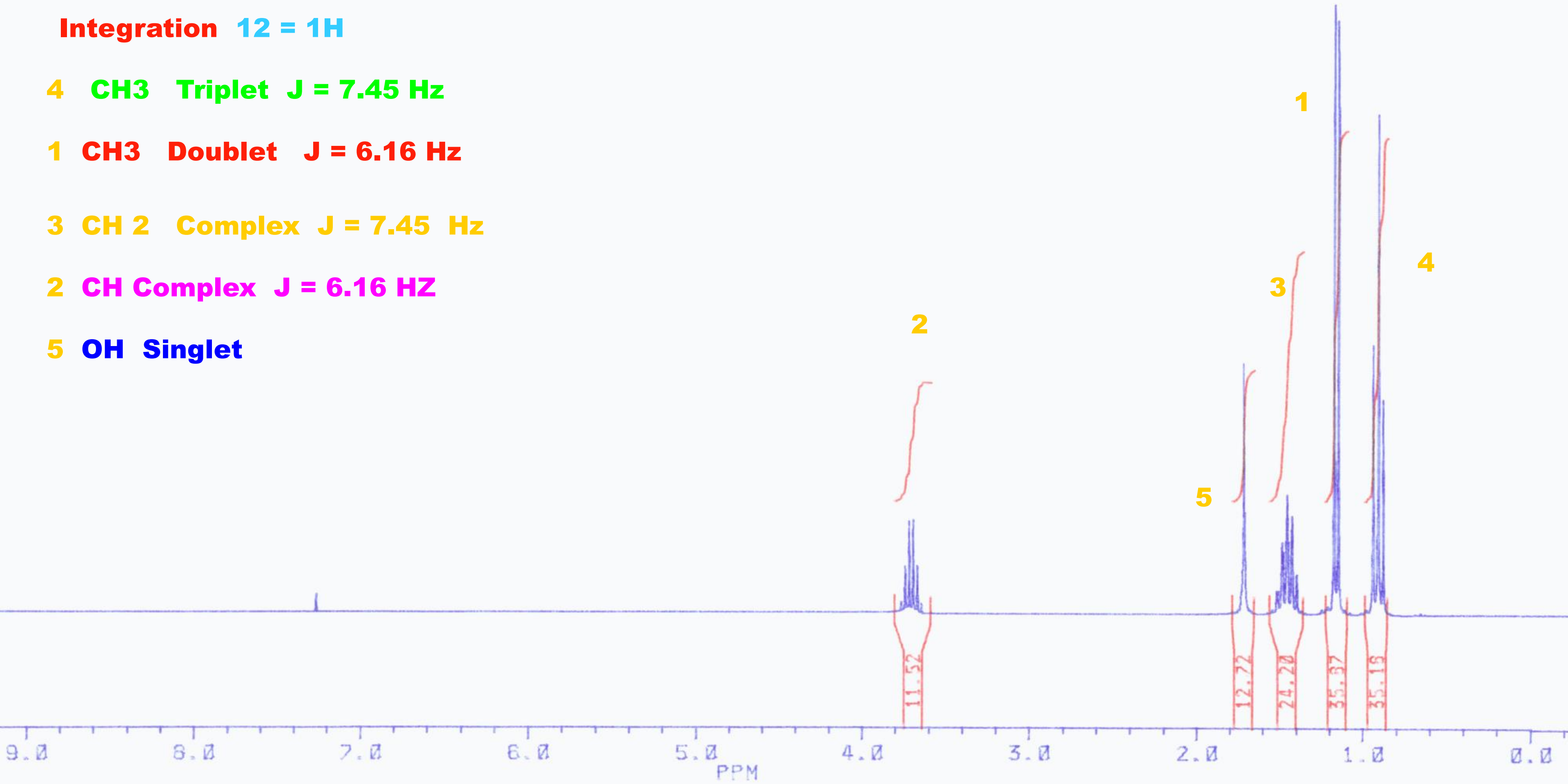
4 CH3 Triplet J = 7.45 Hz

1 CH3 Doublet J = 6.16 Hz

3 CH 2 Complex J = 7.45 Hz

2 CH Complex J = 6.16 HZ

5 OH Singlet

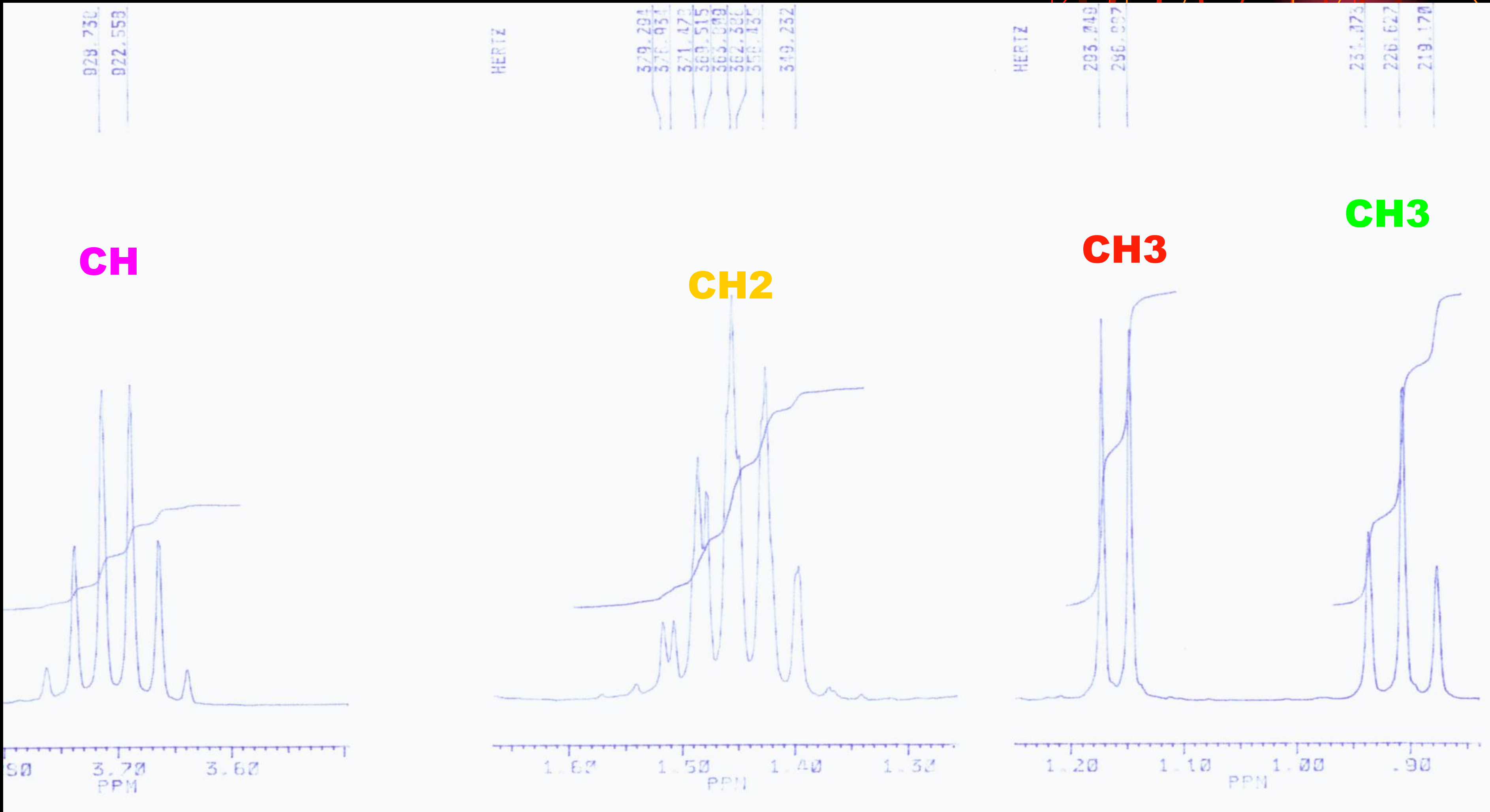


Analysis and interpretation of ^{1}H NMR Spectrum

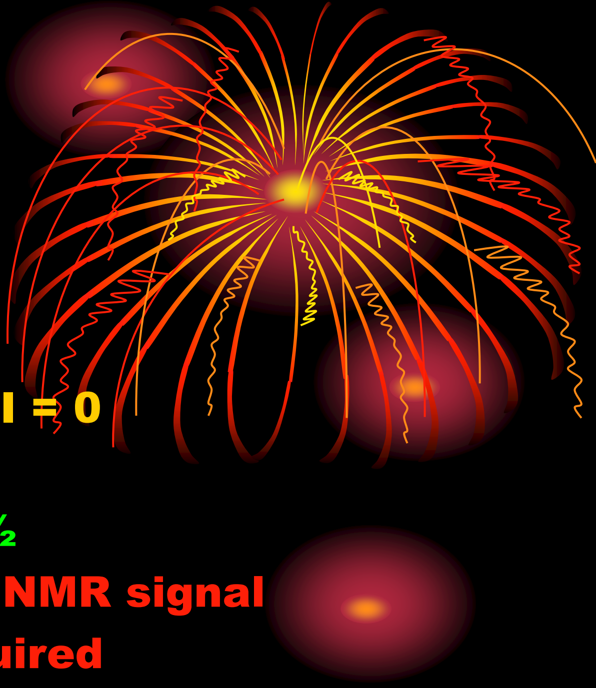
Of Butan-2-al

CH_3-CHOH-CH_2-CH_3

1 2 3 4



Facts about Carbon Atom



- Carbon ^{12}C is in most abundance 98.89 %
- Carbon ^{12}C is non NMR active as spin number I = 0
- Carbon ^{13}C is in less abundance 1.108 %
- Carbon ^{13}C is NMR active as spin number I = ½
- ^{13}C NMR signal is 6000 times weaker than ^{1}H NMR signal
- To see ^{13}C NMR signals Pulsed FT NMR is required

- Chemical Shift Range
- ^{1}H 0 to 12.00 PPM
- ^{13}C 0 to 220.00 PPM
- Resonance Frequency and Applied Field Strength

Applied Field	^{1}H	RF	^{13}C
1.41 Tesla	60.00 MHz		15.10 MHz
2.35 T	100.00 MHz		25.00 MHz
5.88 T	250.00 MHz		62.90 MHz
7.05 T	300.00 MHz		75.00 MHz

Spin Spin Coupling In ^{13}C NMR Spectroscopy

$^{13}C—^{13}C$ is not seen because the probability of two ^{13}C nuclei being in the same molecule is very small.

$^{13}C—^{1}H$ splitting is not seen in normal ^{13}C NMR Spectra because they are measured under broad band decoupling conditions which suppress these splitting.

Normally ^{13}C NMR signal is a singlet but if ^{13}C is attached to a spin active nuclei like ^{2}H (D), ^{19}F, ^{31}P then coupling are present from these nuclei. $CDCl_3$ solvent gives triplet in NMR spectrum due to ^{2}H coupling to ^{13}C.(^{2}H, I = 1)

^{13}C NMR
$CDCl_3$

Distortion less Enhancement of Polarization Transfer

DEPT is useful technique to differentiate how many ^{1}H attached to ^{13}C atom.

DEPT 135 gives CH_3 & CH as positive signals
CH_2 as negative signal
C (Quaternary) as null signal

	No. of Peaks	Terminology	Intensity Ratio
n=0	One Peak	Singlet	1
n=1	Two Peaks	Doublet	1 1
n=2	Three Peaks	Triplet	1 2 1
n=3	Four Peaks	Quartet	1 3 3 1
n=4	Five Peaks	Quintet	1 4 6 4 1
n=5	Six Peaks	Sextet	1 5 10 10 5 1
n=6	Seven Peaks	Septet	1 6 15 20 15 6 1
n=7	Eight Peaks	Octet	1 7 21 35 35 21 7 1

$I = \frac{1}{2}$ ^{1}H , ^{13}C , ^{19}F

Pascal's Triangle $I = \frac{1}{2}$

The relative intensities of multiplet are given by the coefficients of the binomial expansion.

In mathematics, the binomial theorem is an important formula giving the expansion of powers of sums. Its simplest version says

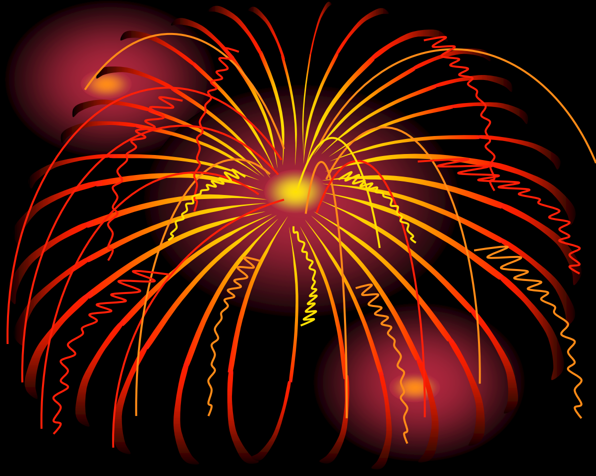
$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k \qquad (1)$$

$$\binom{n}{k} = \frac{n!}{k!\,(n-k)!}$$

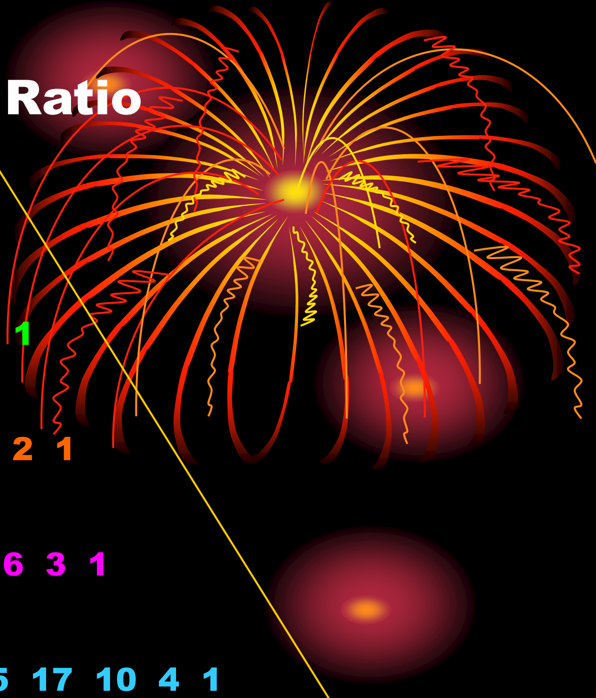
whenever *n* is any non-negative integer, the number is the binomial coefficient

Read the intensity ratio directly from Pascal Triangle.

Pascal Triangle and Binomial Coefficient



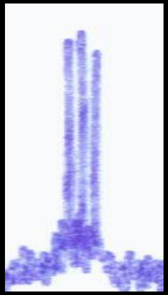
- No. Of Peaks = $2nI + 1$ Where n = spin active nuclei , I = Spin Number ^{1}H , $I = \frac{1}{2}$
- $(X + Y)^{0} = 0X + 0Y$ $(2nI + 1 = 2 \times 0 \times \frac{1}{2} + 1 = 1)$ 1
- $(X + Y)^{1} = 1X + 1Y$ 1   1
- $(X + Y)^{2} = 1X^{2} + 2XY + 1Y^{2}$ 1   2   1
- $(X + Y)^{3} = 1X^{3} + 3X^{2}Y + 3XY^{2} + 1Y^{3}$ 1   3   3   1
- $(X + Y)^{4} = 1X^{4} + 4X^{3}Y + 6X^{2}Y^{2} + 4XY^{3} + 1Y^{4}$ 1   4   6   4   1



	No. of Peaks	Terminology	Intensity Ratio
n=0	One Peak	Singlet	1
n=1	Three Peaks	Triplet	1 1 1
n=2	Five Peaks	Quintet	1 2 3 2 1
n=3	Seven Peaks	Septet	1 3 6 7 6 3 1
n=4	Nine Peaks	Nonet	1 4 10 17 25 17 10 4 1

I = 1 Deuterium ^{2}H (D) , ^{14}N

Pascal ' s Triangle I = 1



^{13}C NMR of $CDCl_3$

I = 1 ^{2}H to ^{13}C

Intensity ratio 1 : 1 : 1

Read the intensity ratio directly from Pascal Triangle.

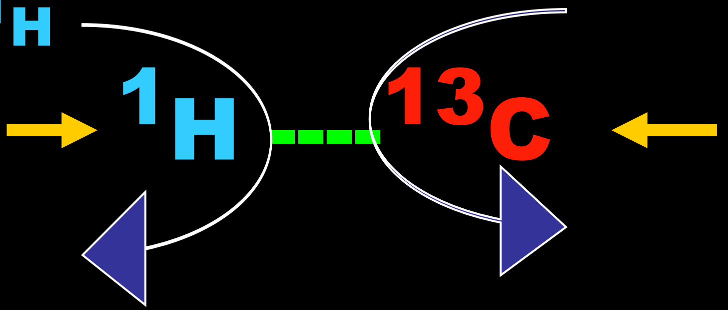
Broad Band ^{1}H Decoupled ^{13}C NMR Spectra

In this method all the ^{1}H are irradiated at certain RF and at the same time ^{13}C signals are measured at different RF.

Secondary RF source is required To decouple ^{1}H

(Decoupler) →

Continuously Saturates ^{1}H



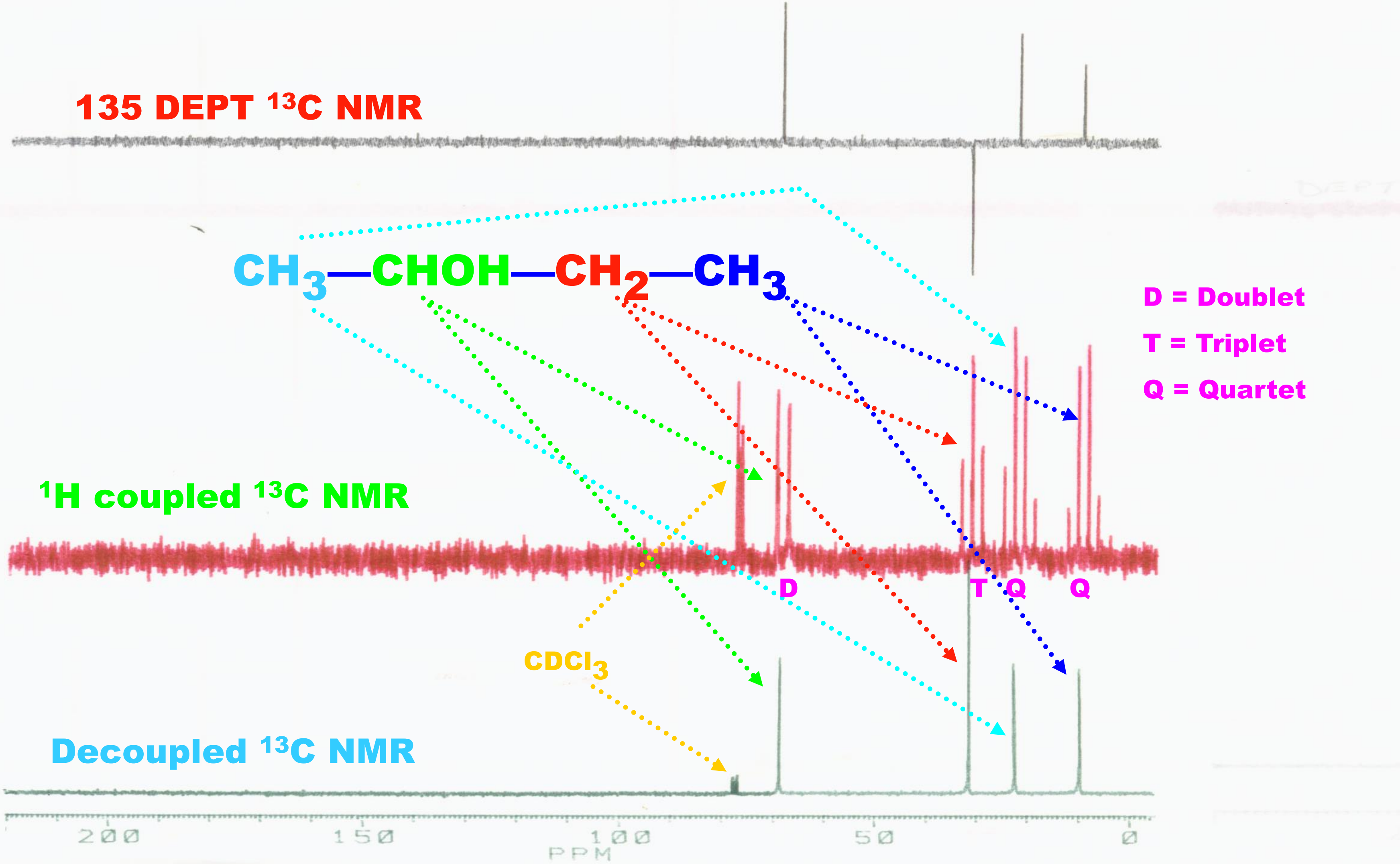
← Primary RF source is tuned to measure ^{13}C NMR signals

Which gives ^{13}C FID

Saturation means there are rapid and equal transitions from upward spin state to the downward spin state. No NMR signal from ^{1}H hence ^{13}C NMR signals are all singlet.

^{13}C NMR Spectra of Butan-2-ol

$CH_3—CHOH—CH_2—CH_3$



135 DEPT ^{13}C NMR

$CH_3—CHOH—CH_2—CH_3$

D = Doublet

T = Triplet

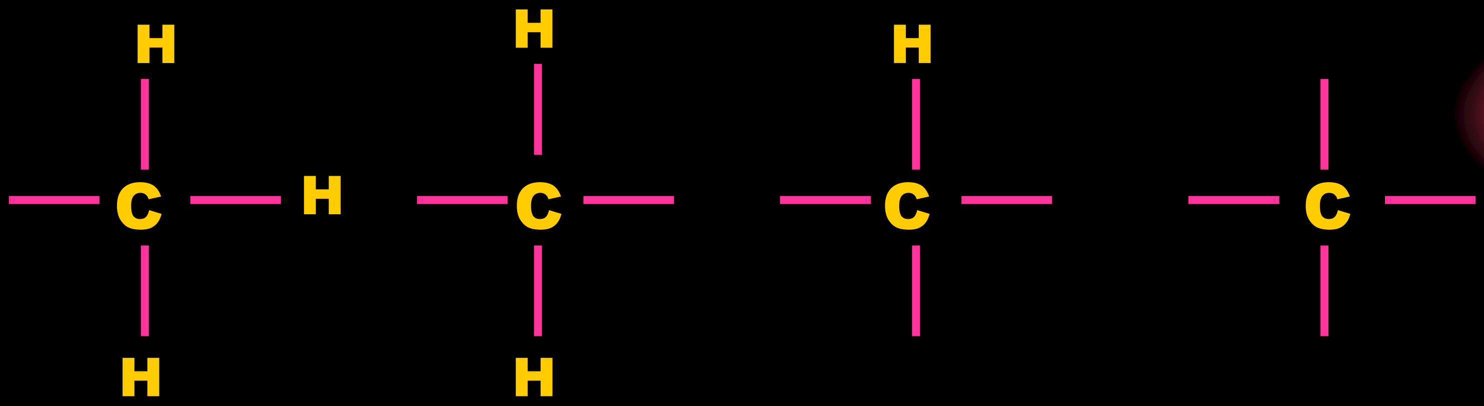
Q = Quartet

^1H coupled ^{13}C NMR

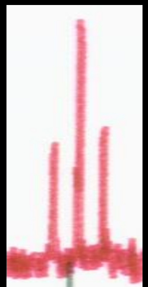
Decoupled ^{13}C NMR

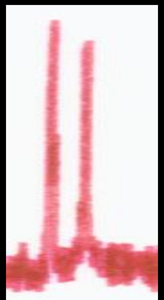
^{1}H coupling to ^{13}C in ^{13}C NMR Spectra

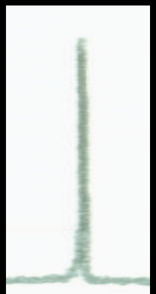
No. of peaks = 2nI + 1
n is No of spin active nuclei (^{1}H) [Neighbours]
I is Spin number of the active nucleus (^{1}H = ½)



Methyl ^{13}C	**Methylene ^{13}C**	**Methine ^{13}C**	**Quaternary ^{13}C**
Quartet	**Triplet**	**Doublet**	**Singlet**



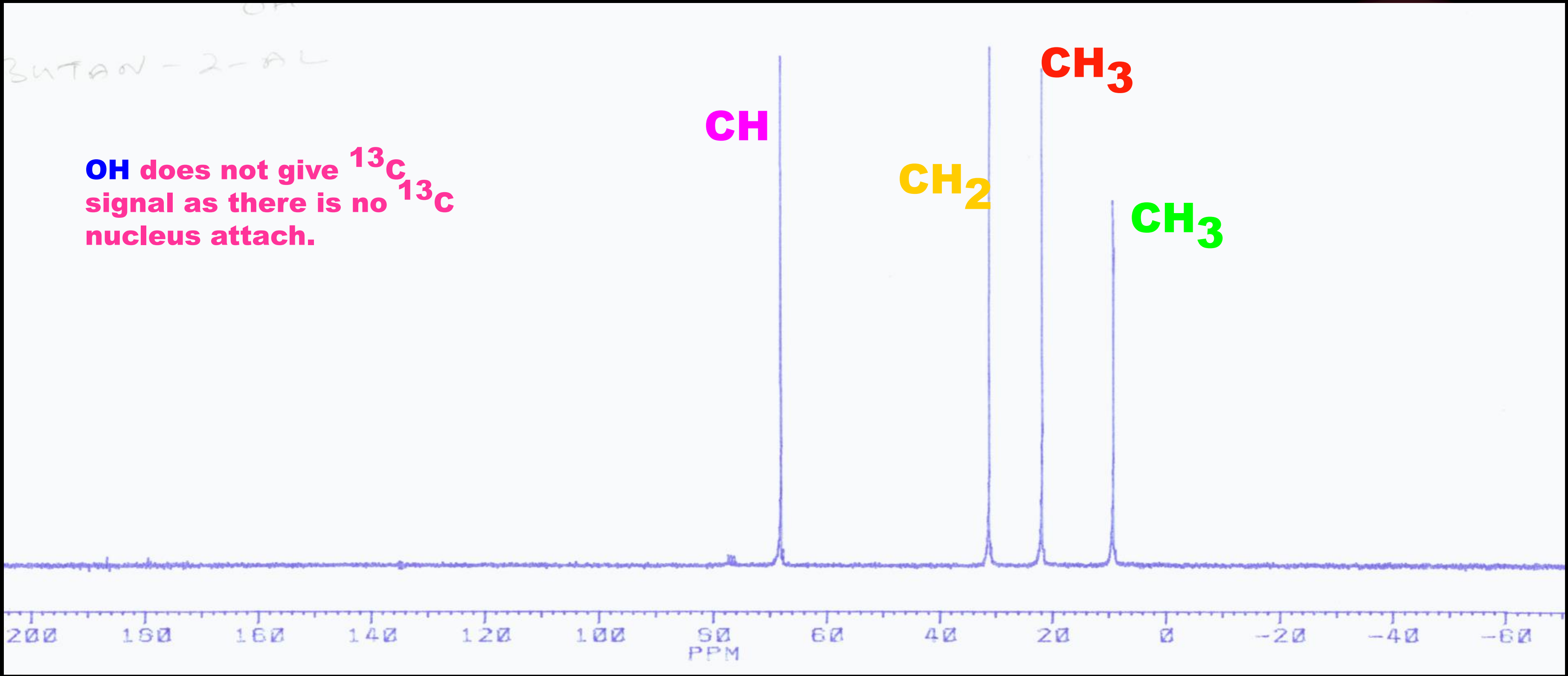




^{13}C NMR spectrum. Most of the ^{13}C NMR spectra are recorded as ^{1}H decoupled hence $CH/CH_2/CH_3$ give sharp singlet.

^{13}C NMR spectrum of Butan-2-al

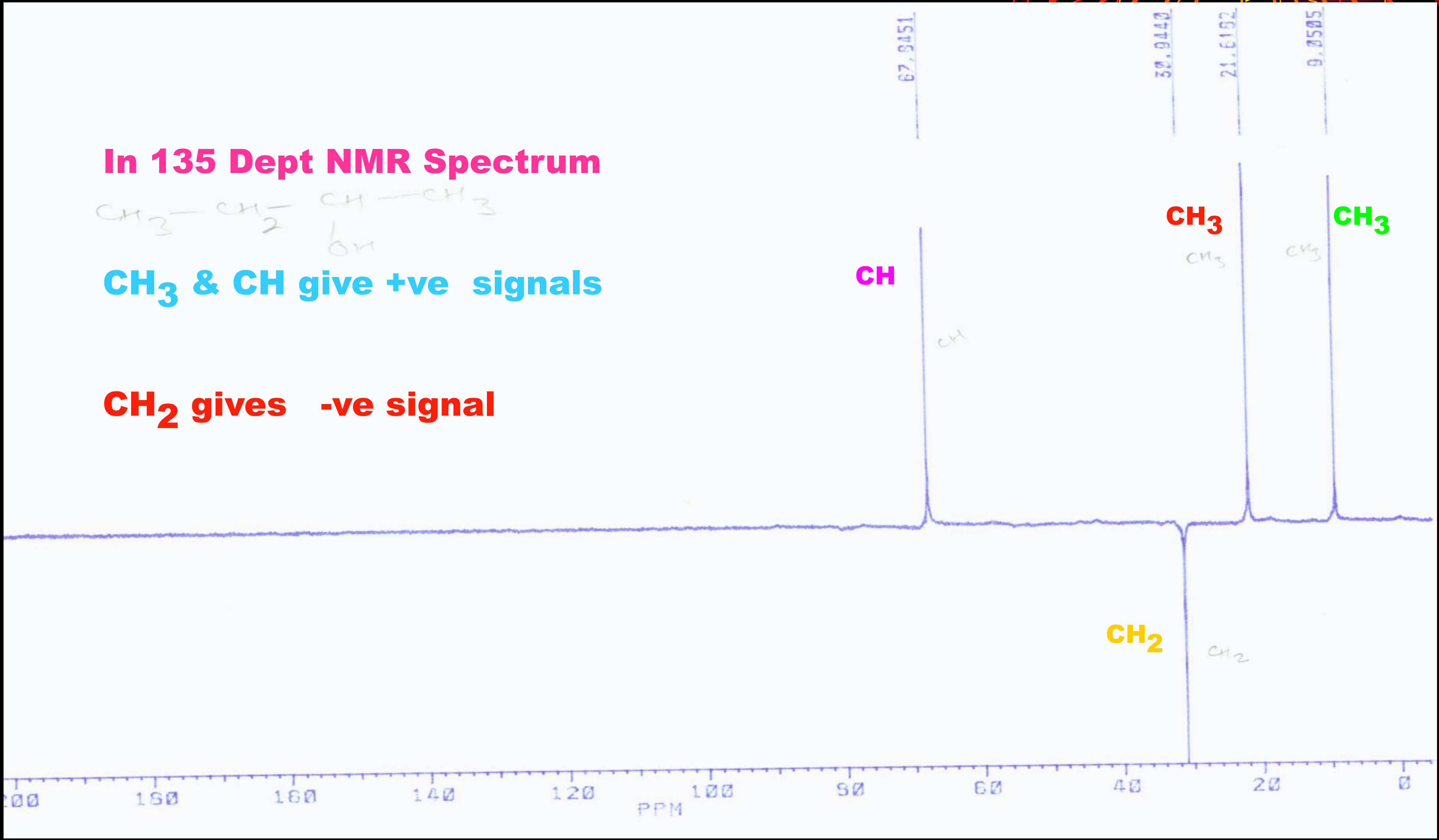
CH_3--$CHOH$—CH_2—CH_3



OH does not give ^{13}C signal as there is no ^{13}C nucleus attach.

^{13}C Dept 135 NMR spectrum of Butan-2-al

CH_3—CHOH—CH_2—CH_3



In 135 Dept NMR Spectrum

CH_3 & CH give +ve signals

CH_2 gives -ve signal

Analysis of ^{1}H and ^{13}C NMR Spectra Butan-2-al

CH_3-CH_2-CHOH-CH_3

CH_3	CH_3	CH_2	OH	CH	^{1}H NMR
0.91 PPM Triplet J= 7.45 Hz	1.16 Doublet J= 6.16 Hz	1.45 D of Q Complex	1.71 Singlet	3.70 T of Q Complex	D= Doublet T= Triplet Q= Quartet
CH_3	CH_3	CH_2	OH	CH	^{13}C NMR
9.03 PPM	21.63	30.96	No Signal	67.88	

Analysis and interpretation of ^{1}H NMR Spectrum of n-Butanal CH_3-CH_2-CH_2-CH_2OH

4 3 2 1

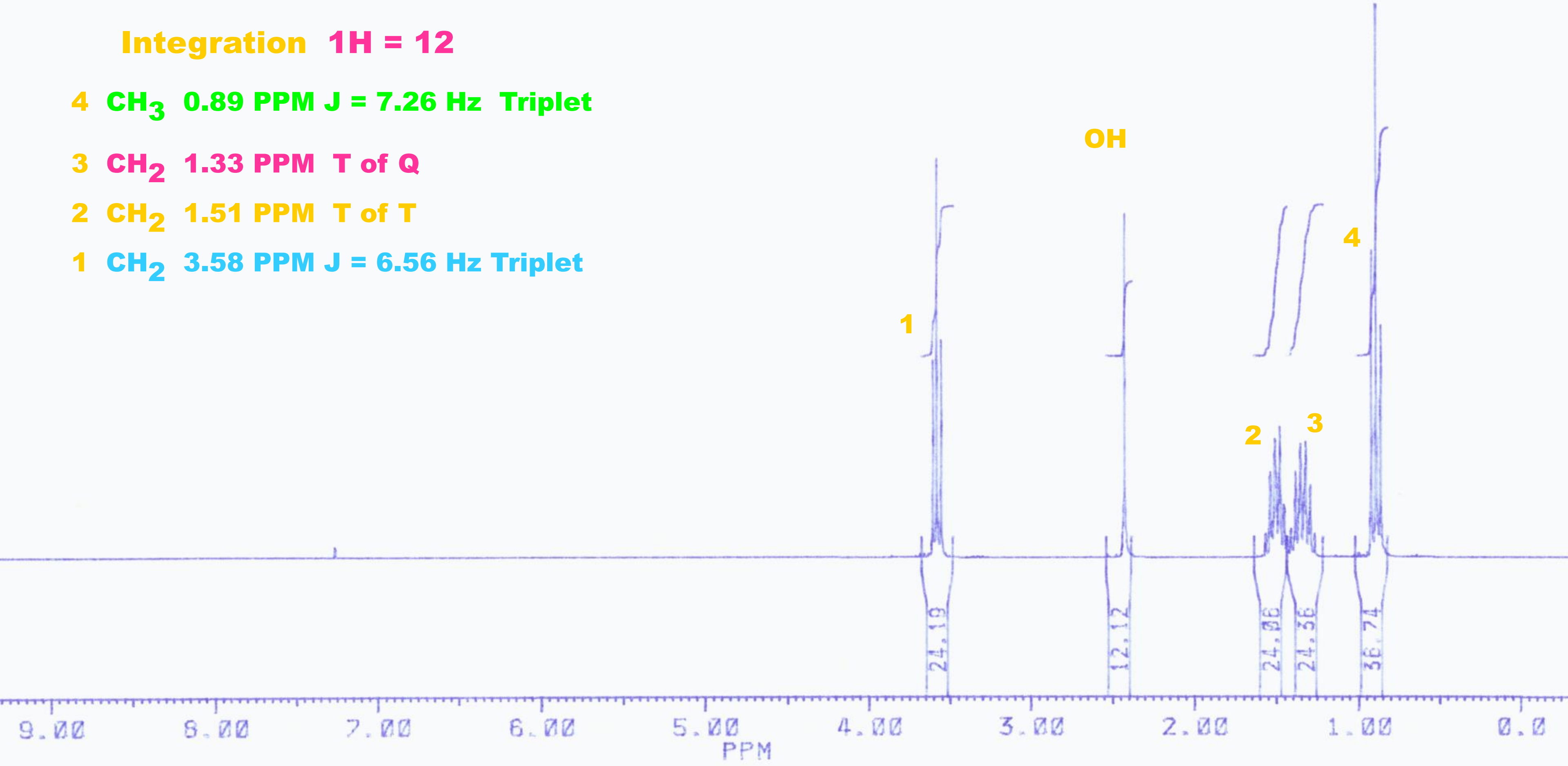
Integration 1H = 12

4 CH_3 0.89 PPM J = 7.26 Hz Triplet

3 CH_2 1.33 PPM T of Q

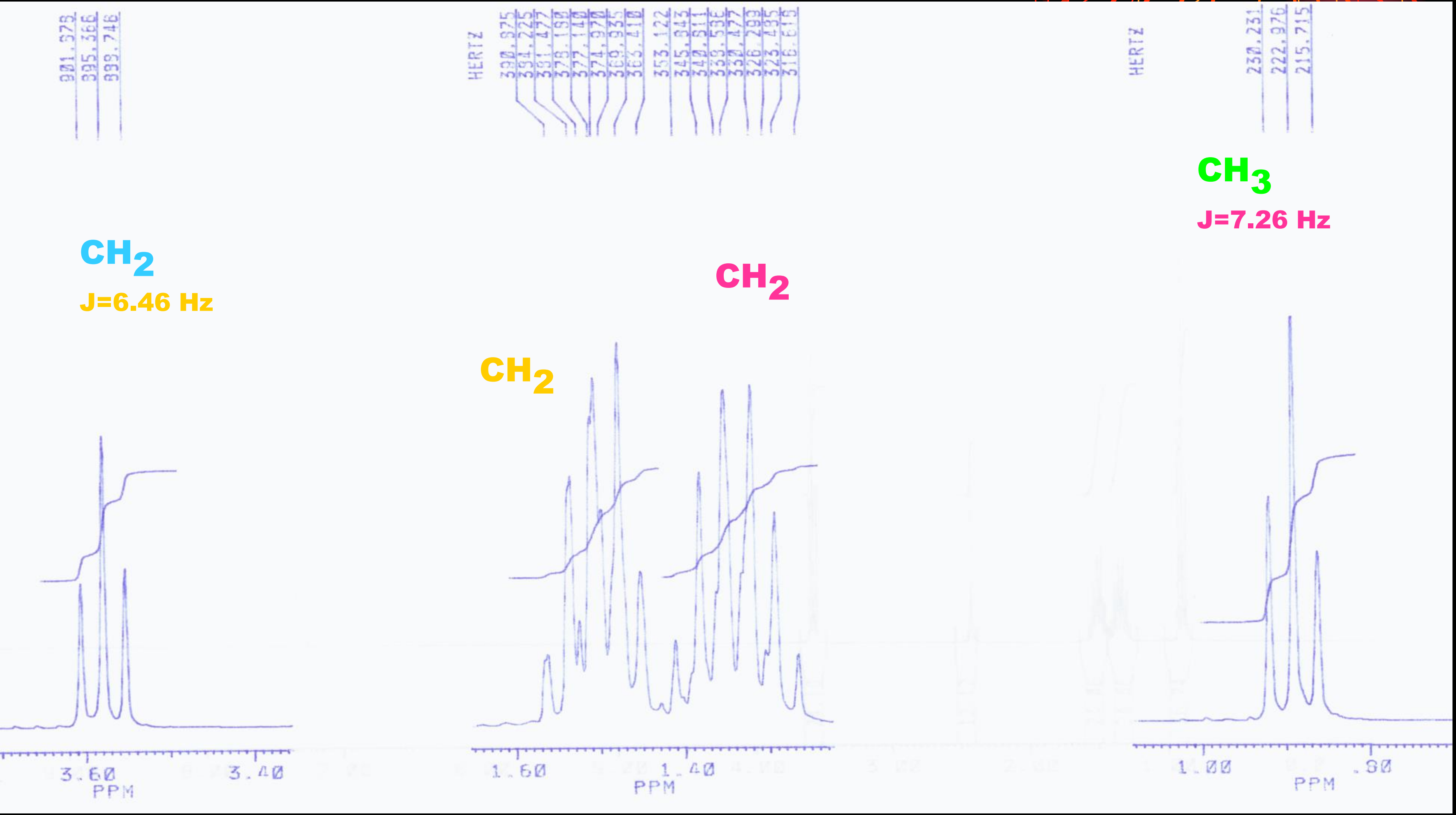
2 CH_2 1.51 PPM T of T

1 CH_2 3.58 PPM J = 6.56 Hz Triplet



Analysis and interpretation of ^{1}H NMR Spectrum of n-Butanal

CH_3-CH_2-CH_2-CH_2OH
4 3 2 1

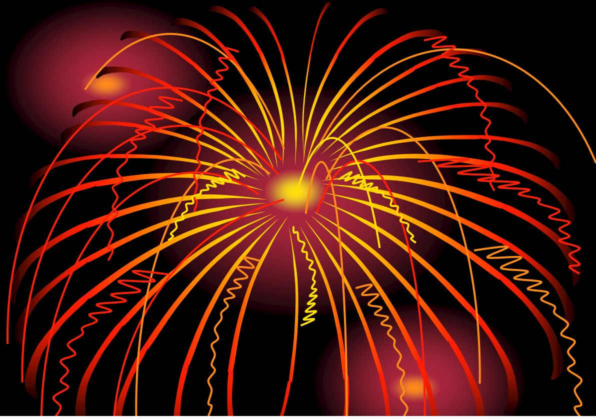


CH_2
J=6.46 Hz

CH_2

CH_2

CH_3
J=7.26 Hz



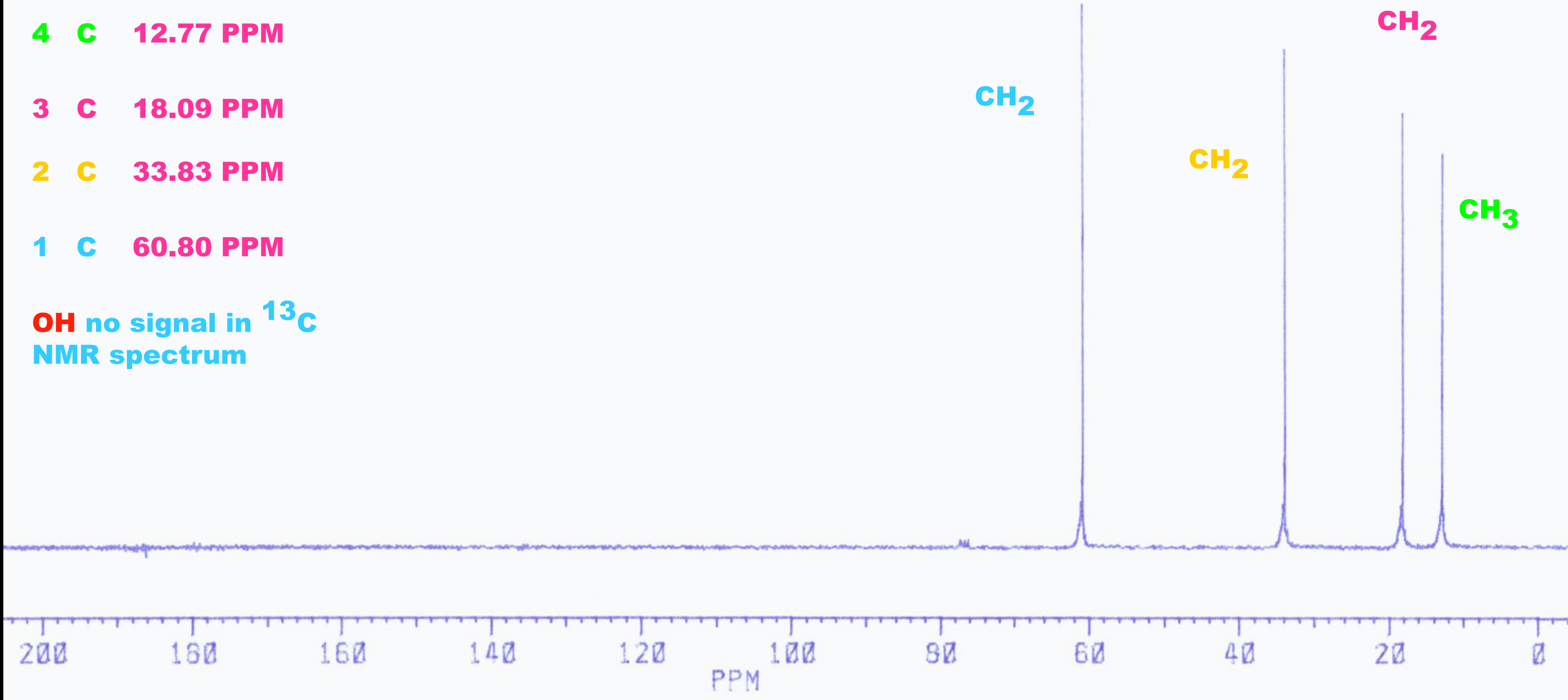
^{13}C NMR Spectrum of n-Butanal

CH_3-CH_2-CH_2-CH_2OH
4 3 2 1

Chemical Shifts

4	C	12.77 PPM
3	C	18.09 PPM
2	C	33.83 PPM
1	C	60.80 PPM

OH no signal in ^{13}C NMR spectrum



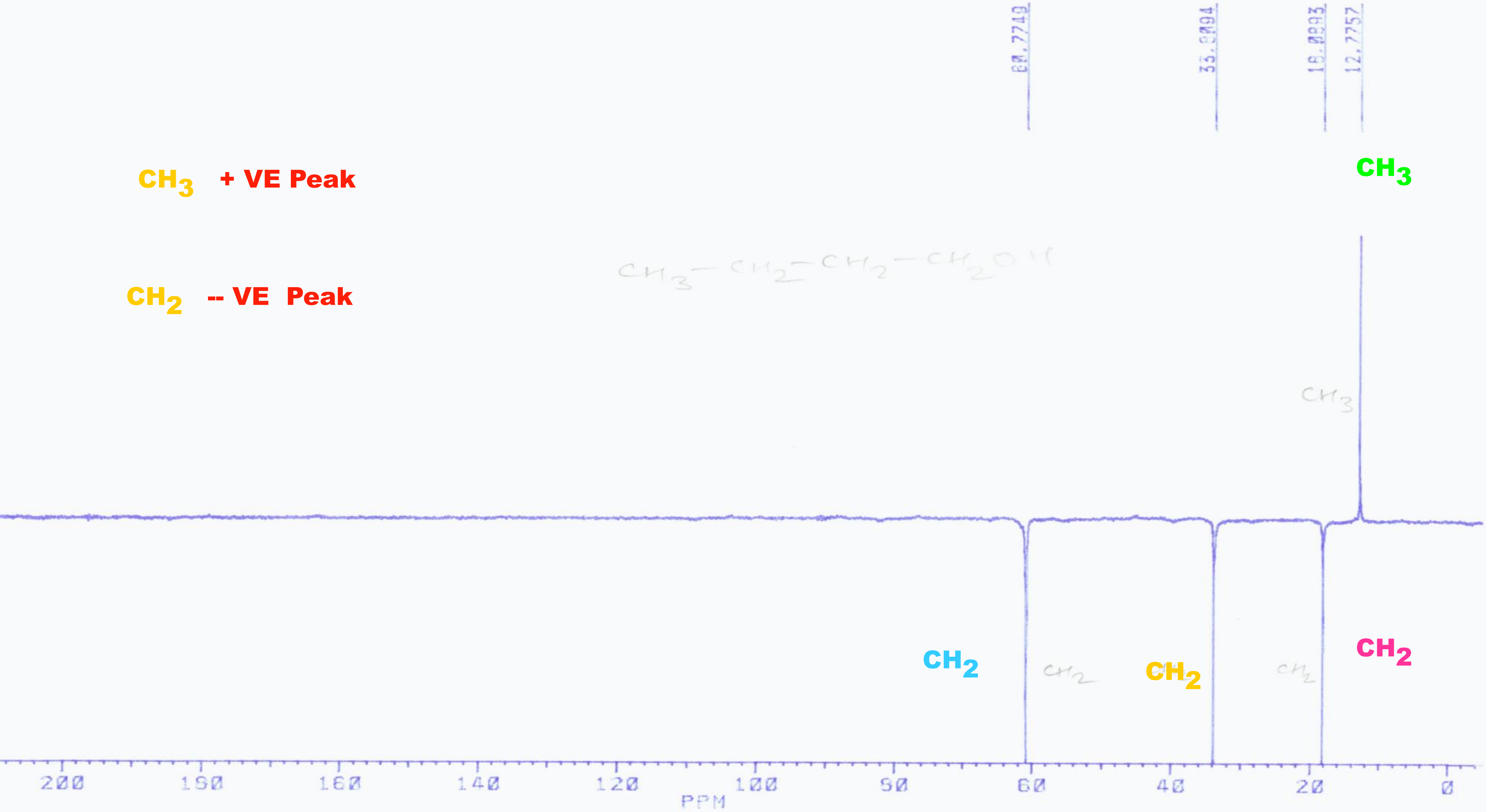
^{13}C Dept 135 NMR Spectrum of n-Butanal

CH_3-CH_2-CH_2-CH_2OH

4 3 2 1

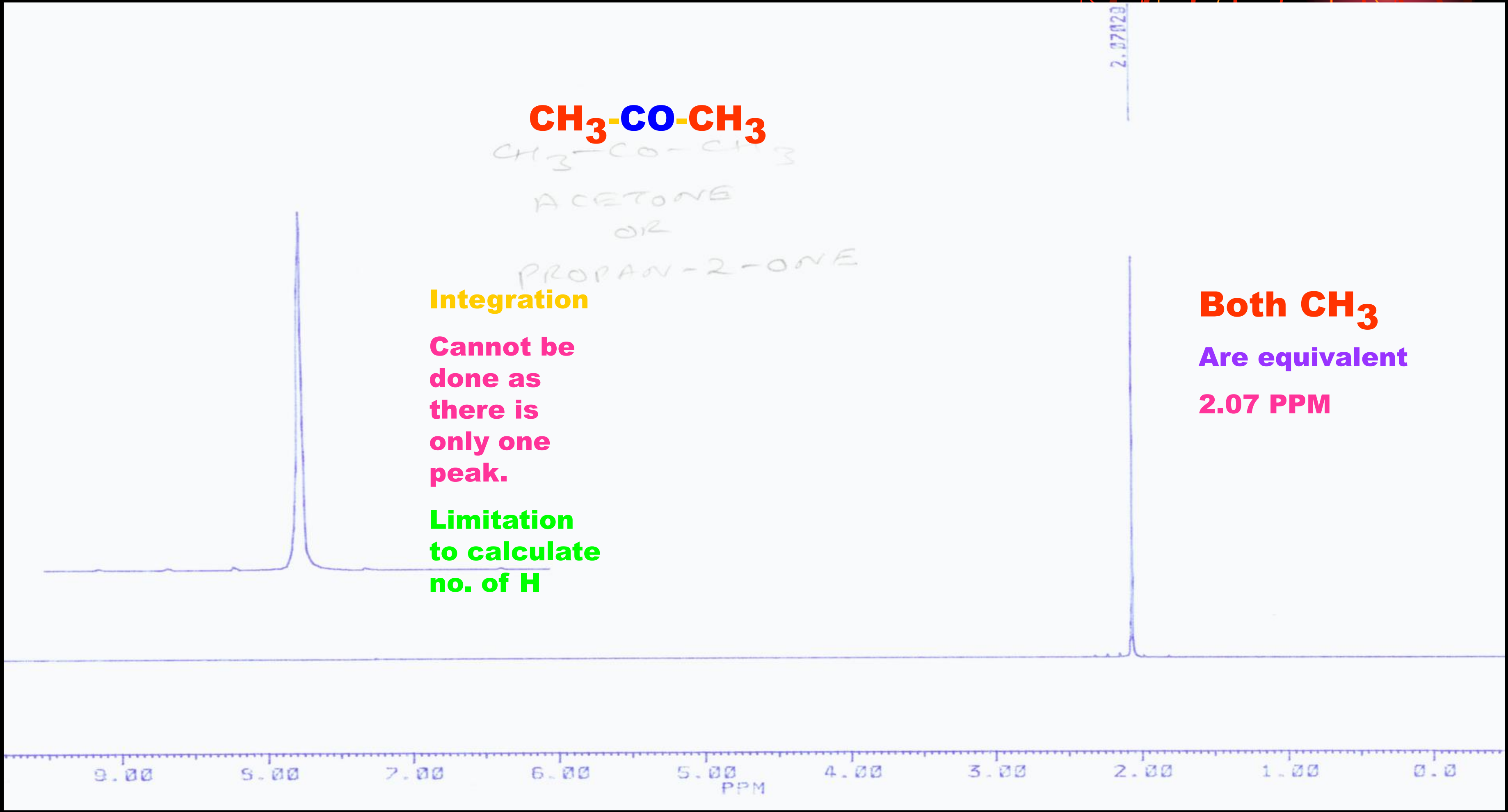
CH_3 + VE Peak

CH_2 -- VE Peak



Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Propan-2-one or Acetone

^{1}H NMR Spectrum $CH_3—CO—CH_3$



CH_3-CO-CH_3

Integration

Cannot be done as there is only one peak.

Limitation to calculate no. of H

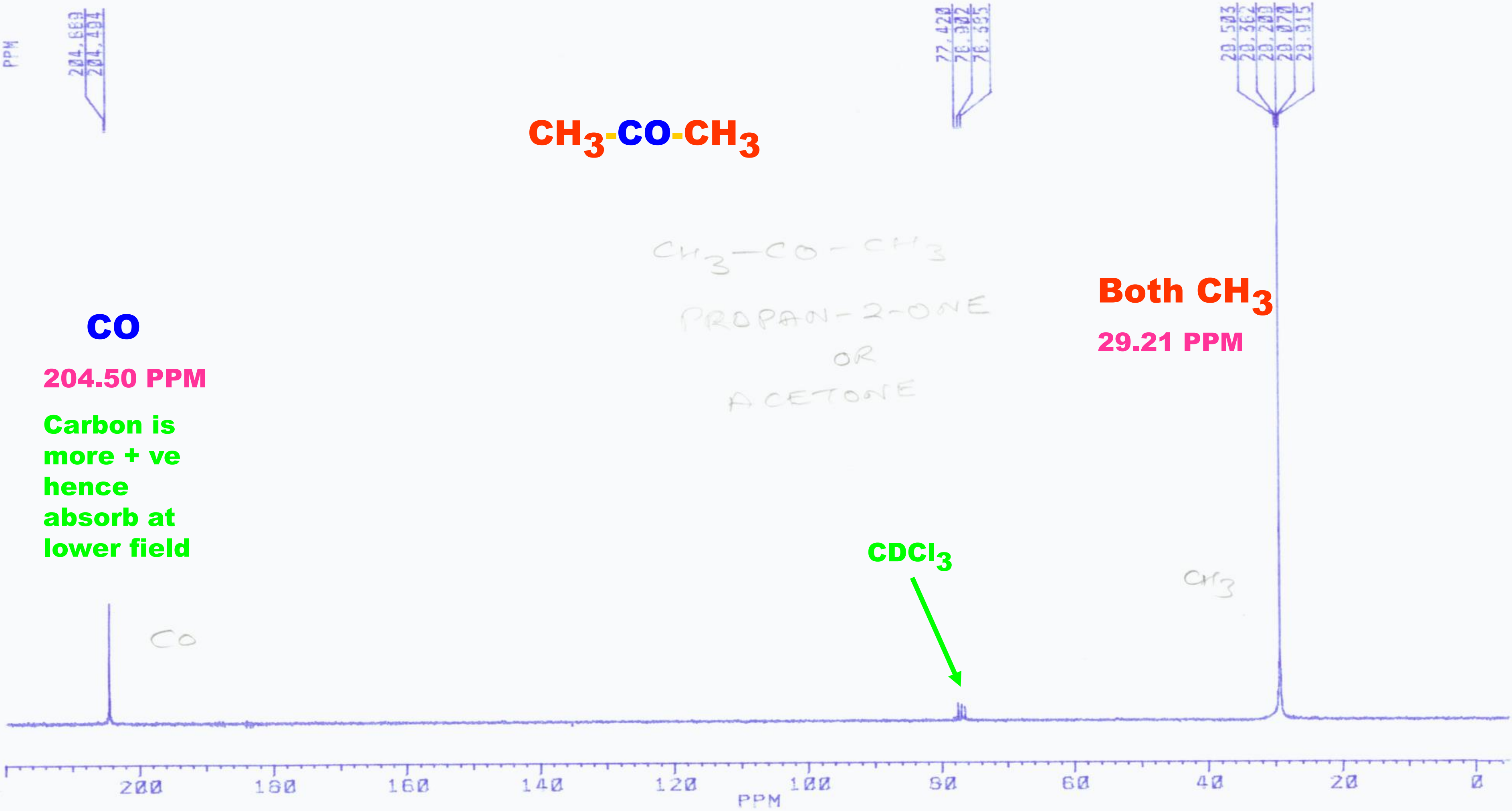
Both CH_3

Are equivalent

2.07 PPM

^{13}C NMR Spectrum of Propan-2one (Acetone)

$CH_3—CO—CH_3$



CH_3-CO-CH_3

CO

204.50 PPM

Carbon is more + ve hence absorb at lower field

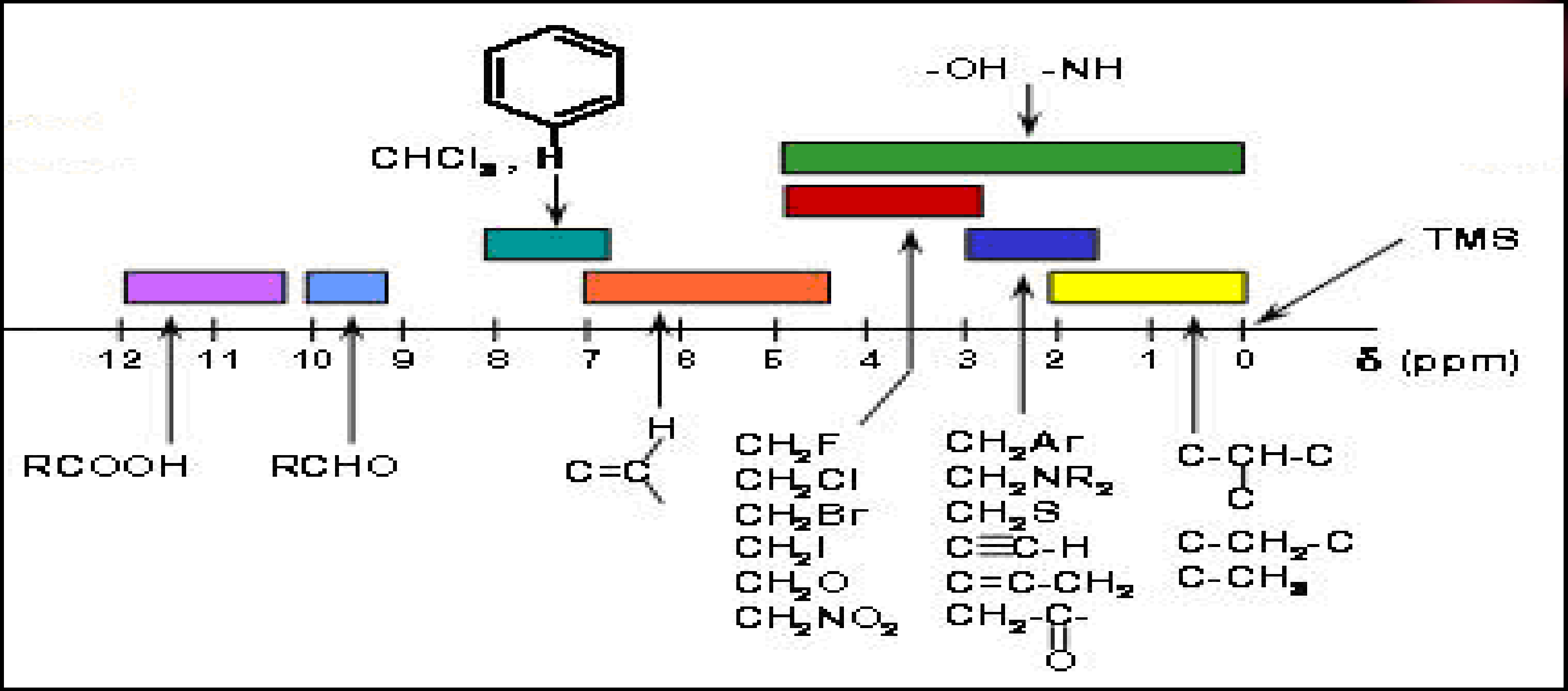
Both CH_3

29.21 PPM

$CDCl_3$

^{1}H Chemical Shift in PPM

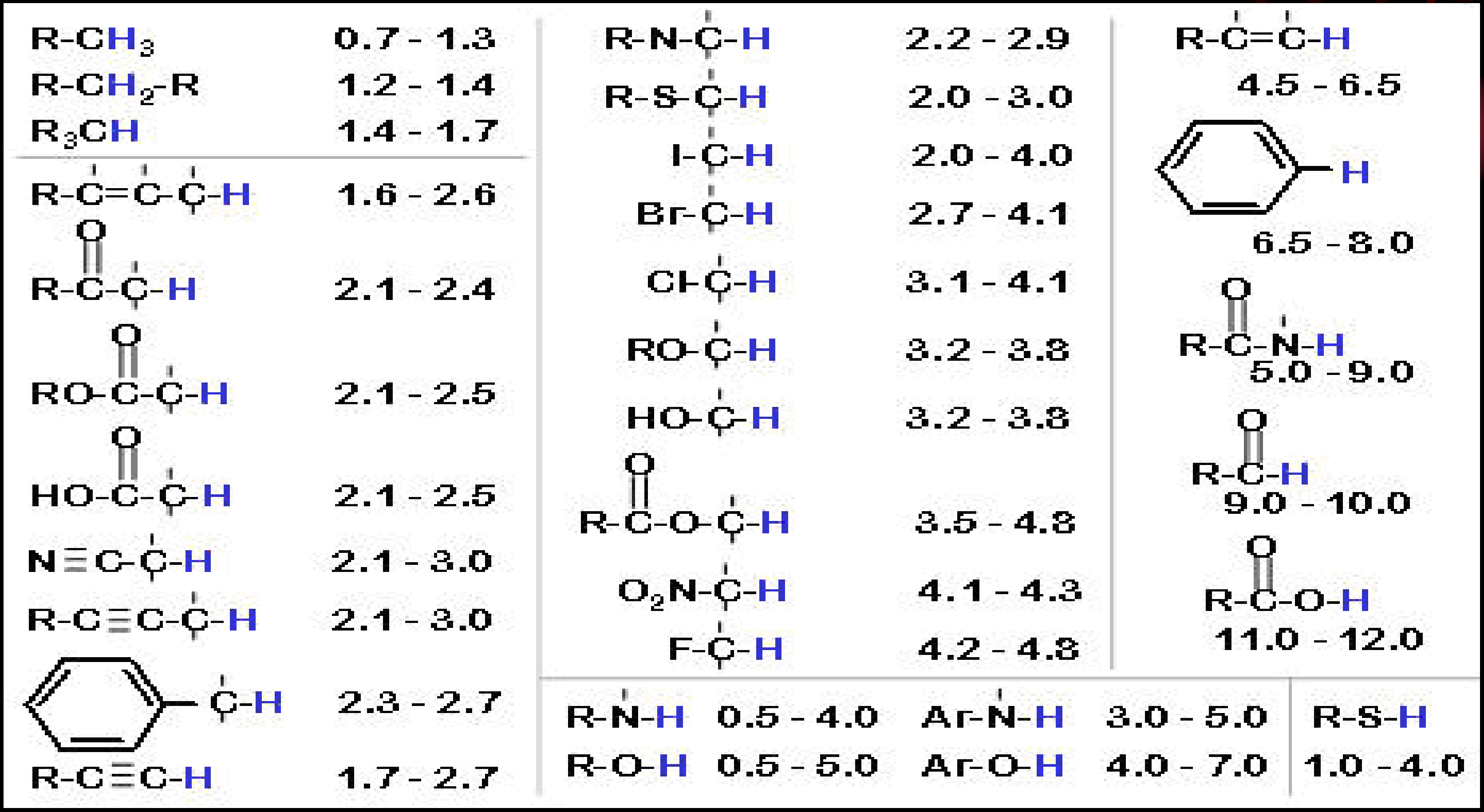
- **General Correlation Chart ^{1}H NMR Spectra**



Lower Field ⟷ **Higher Field**

^{1}H Chemical Shift in more details

- **^{1}H Chemical Shift Range Table**



R-CH$_3$	0.7 - 1.3
R-CH$_2$-R	1.2 - 1.4
R$_3$CH	1.4 - 1.7
R-C=C-C-H	1.6 - 2.6
R-$\overset{O}{\overset{\Vert}{C}}$-C-H	2.1 - 2.4
RO-$\overset{O}{\overset{\Vert}{C}}$-C-H	2.1 - 2.5
HO-$\overset{O}{\overset{\Vert}{C}}$-C-H	2.1 - 2.5
$N\equiv C$-C-H	2.1 - 3.0
R-$C\equiv C$-C-H	2.1 - 3.0
C-H	2.3 - 2.7
R-$C\equiv C$-H	1.7 - 2.7
R-N-C-H	2.2 - 2.9
R-S-C-H	2.0 - 3.0
I-C-H	2.0 - 4.0
Br-C-H	2.7 - 4.1
Cl-C-H	3.1 - 4.1
RO-C-H	3.2 - 3.8
HO-C-H	3.2 - 3.8
R-$\overset{O}{\overset{\Vert}{C}}$-O-C-H	3.5 - 4.8
O$_2$N-C-H	4.1 - 4.3
F-C-H	4.2 - 4.8
R-C=C-H	4.5 - 6.5
H	6.5 - 8.0
R-$\overset{O}{\overset{\Vert}{C}}$-N-H	5.0 - 9.0
R-$\overset{O}{\overset{\Vert}{C}}$-H	9.0 - 10.0
R-$\overset{O}{\overset{\Vert}{C}}$-O-H	11.0 - 12.0

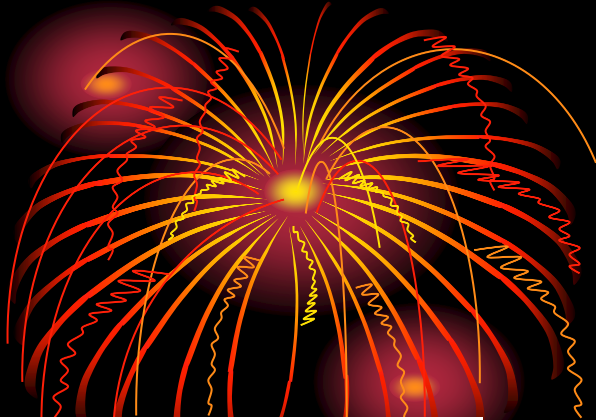
R-N-H	0.5 - 4.0	Ar-N-H	3.0 - 5.0	R-S-H
R-O-H	0.5 - 5.0	Ar-O-H	4.0 - 7.0	1.0 - 4.0

^{13}C Chemical Shift in PPM

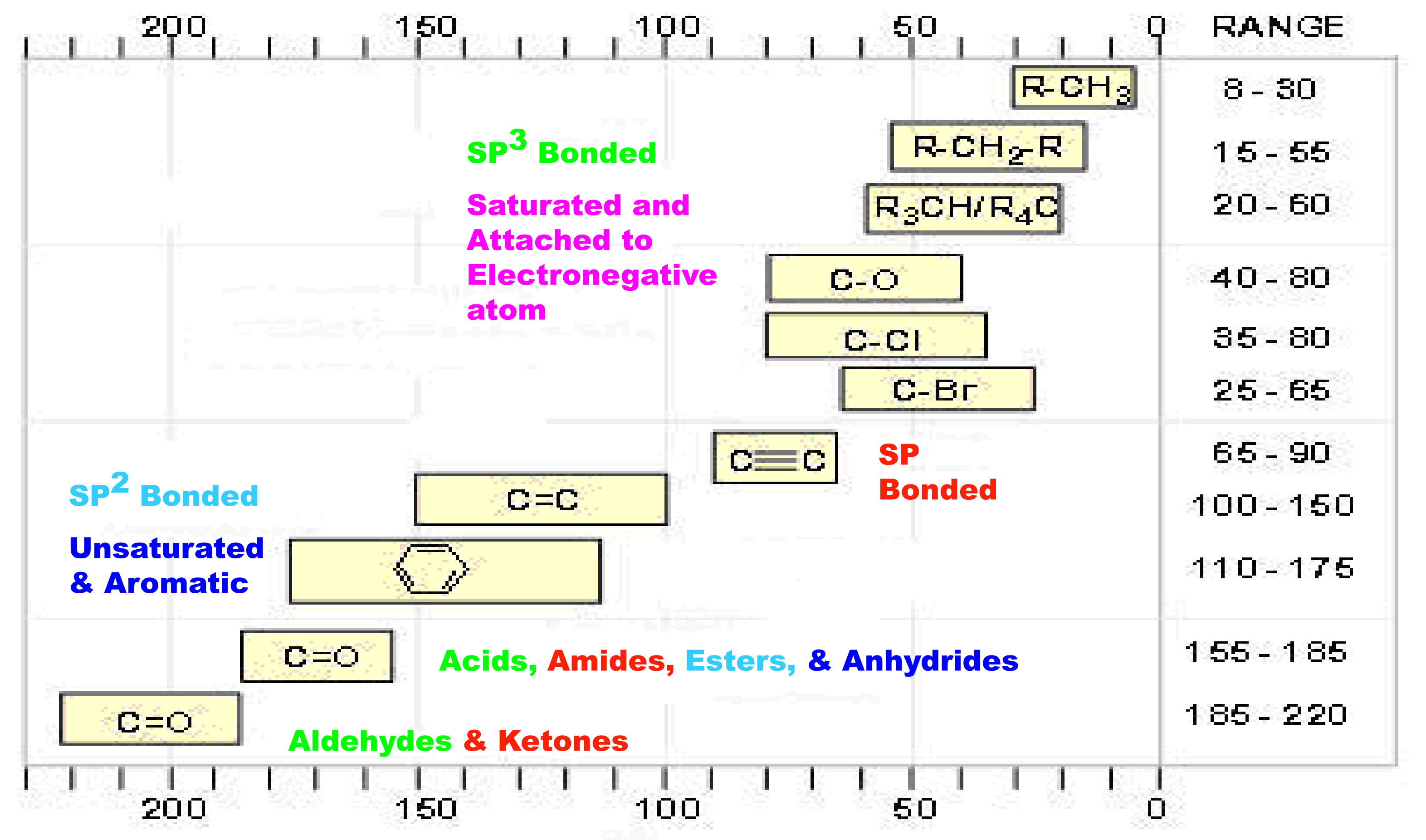
In FT NMR Spectroscopy, the intensities of the signal get distorted hence peak heights and areas under the peak can be deceptive.

RCH_3	0.0	to	35	PPM
$R2CH_2$	15	to	40	PPM
R3CH	25	to	50	PPM
R4C	30	to	40	PPM
RC = CR	65	to	90	PPM
R2C ≡ CR2	100	to	150	PPM
C_6H_6 (Aromatic)	110	to	175	PPM
R-CO-OR	160	to	185	PPM
R-CO-R	190	to	220	PPM
RCH_2Br	20	to	40	PPM
RCH_2Cl	25	to	50	PPM
RCH_2NH_2	35	to	50	PPM
RCH_2OH	50	to	65	PPM
RCH_2OR	50	to	65	PPM

^{13}C Chemical Shift in PPM



- ^{13}C Chemical Shift Range Table

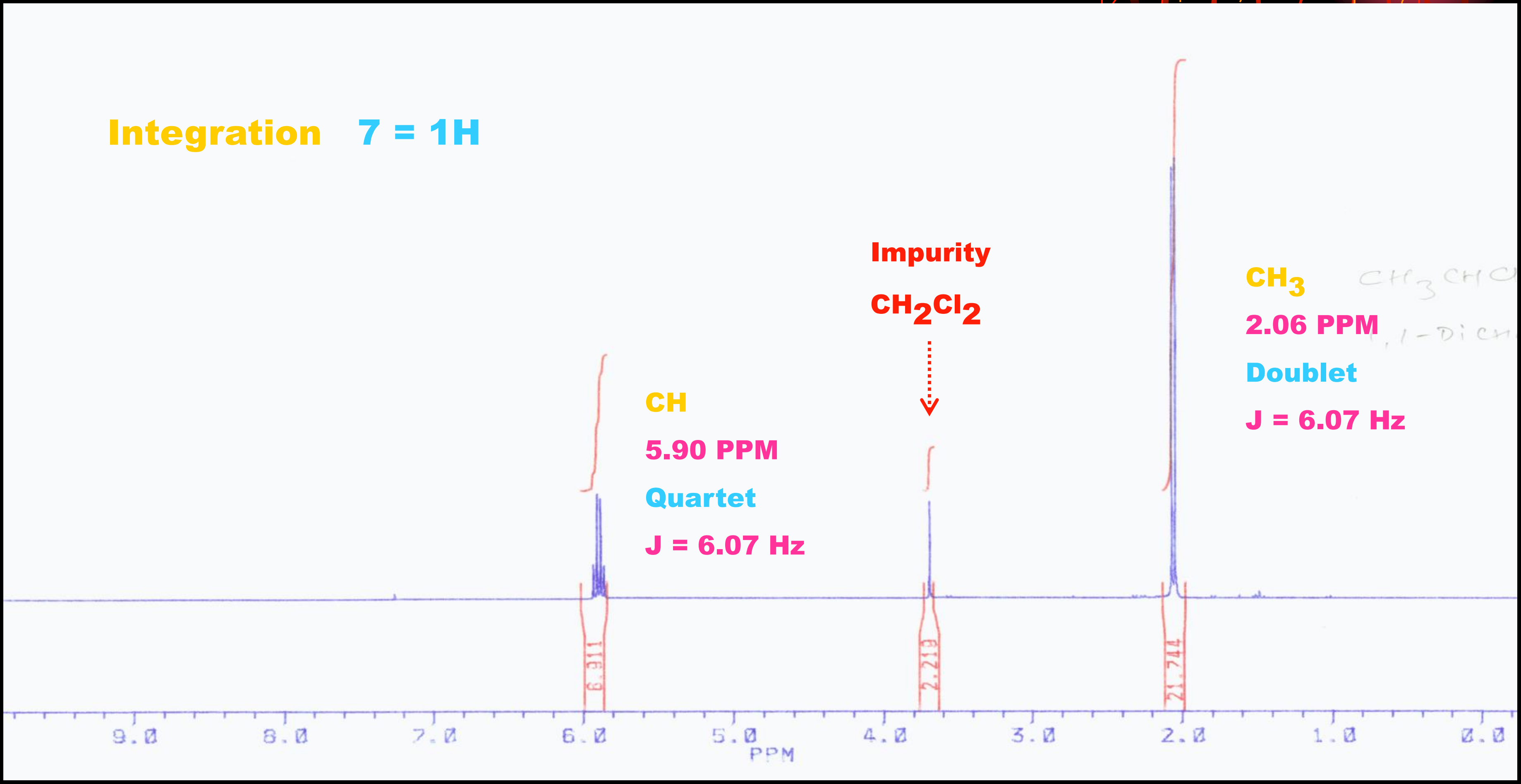


Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra

Of 1,1-Dichloroethane

$CH_3—CHCl_2$

2 1



Integration **7 = 1H**

Impurity

CH_2Cl_2

CH

5.90 PPM

Quartet

J = 6.07 Hz

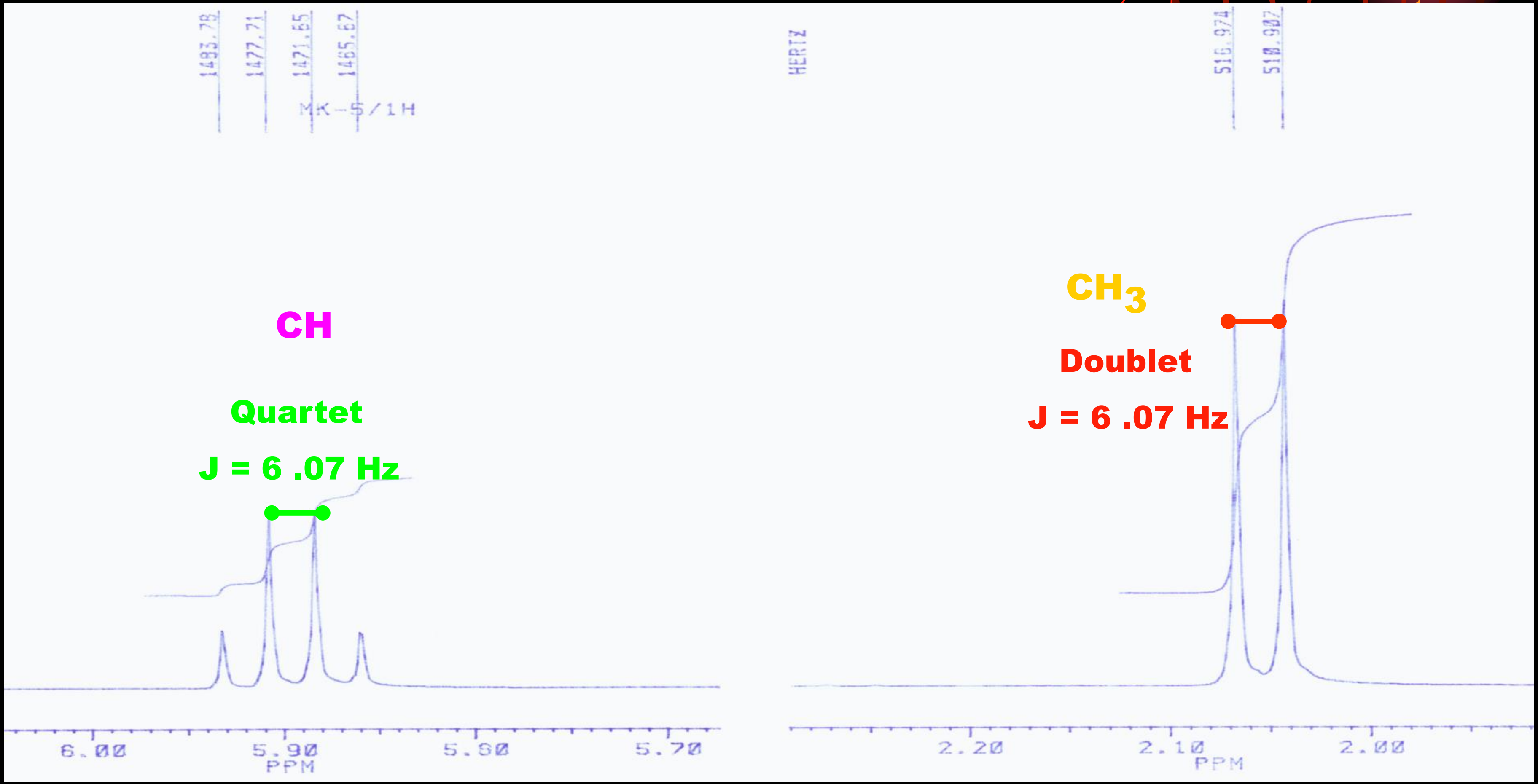
CH_3

2.06 PPM

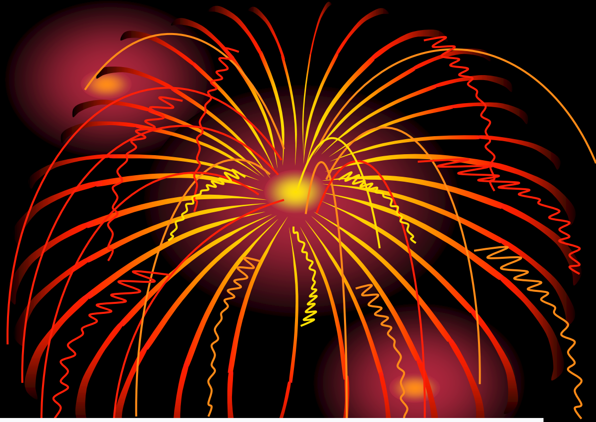
Doublet

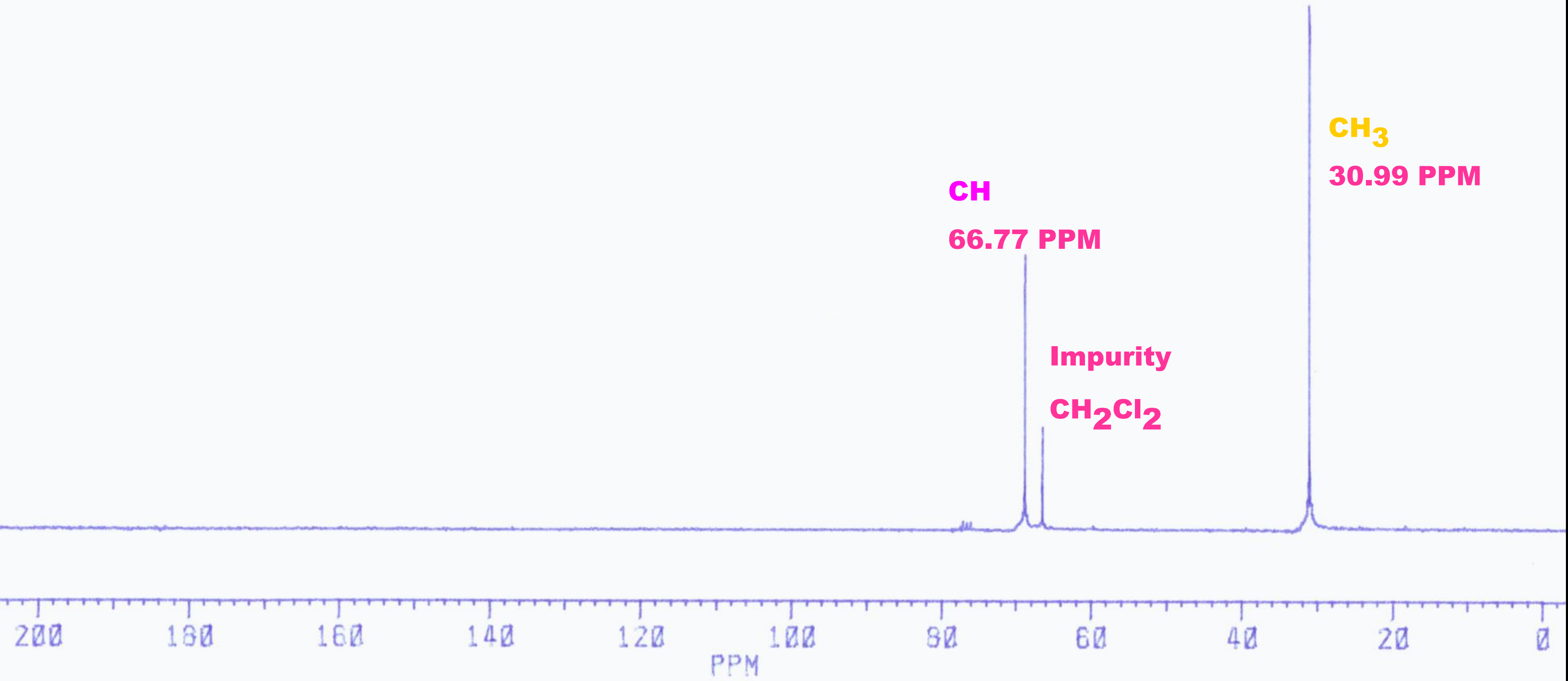
J = 6.07 Hz

Expansion of 1H NMR of 1,1-Dichloroethane
CH_3—$CHCl_2$



^{13}C NMR OF 1,1-Dichloroethane
$CH_3—CHCl_2$




CH

66.77 PPM

Impurity

CH_2Cl_2

CH_3

30.99 PPM

Factors affecting ^{1}H Chemical Shifts Shielding and Deshielding effects

1. The electro negativity of the atoms within the molecule.

2. The hybridization of the adjacent atoms.

3. The diamagnetic effects from adjacent Pi bonds.

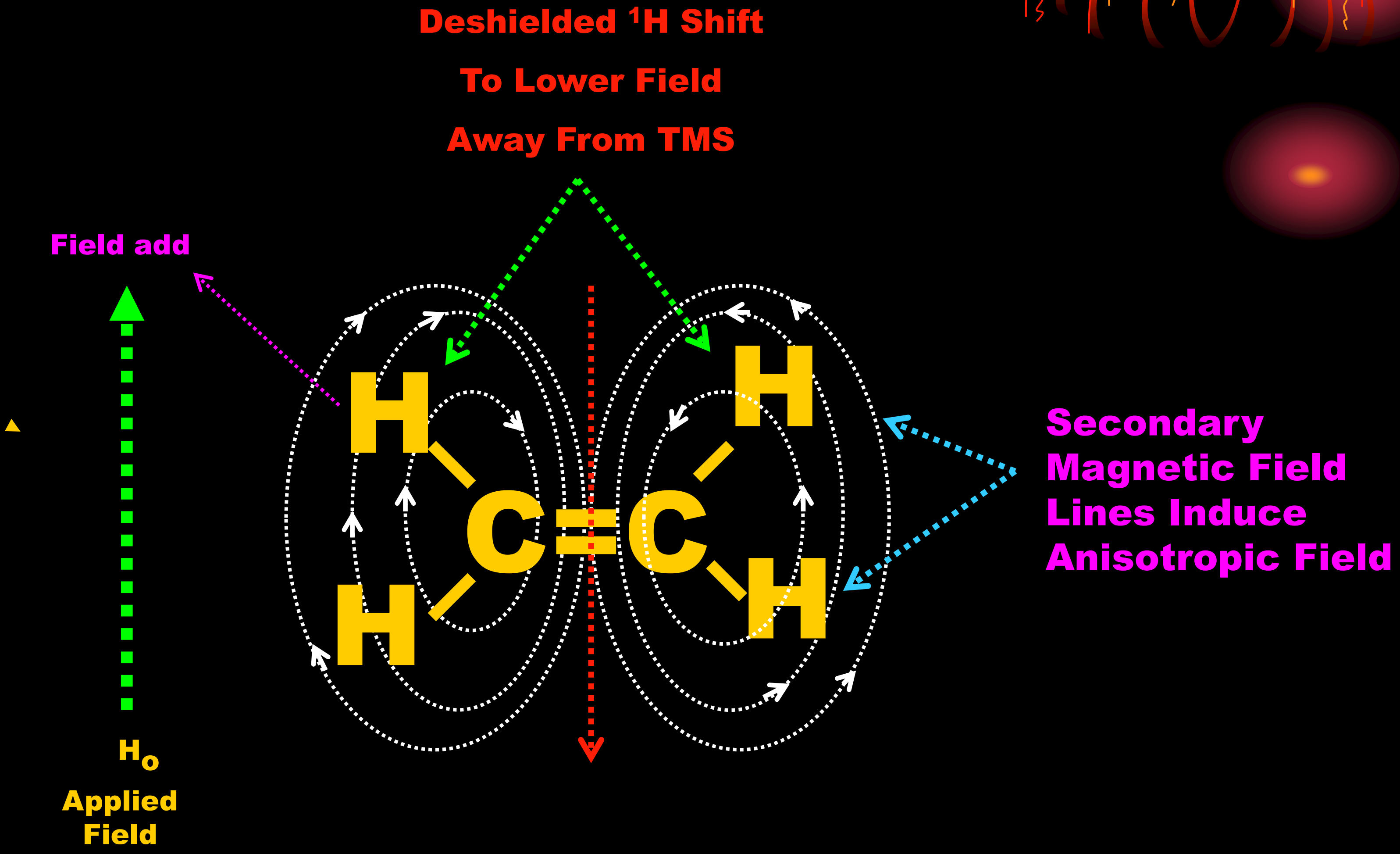
CH_3—X	Electro negativity of X	PPM
CH_3—F	4 .00	4 .26
CH_3—OH	3 .50	3 .57
CH_3—Cl	3 .10	3 .05
CH_3—Br	2 .80	2 .68
CH_3—I	2 .50	2 .16
$(CH_3)_4$—C	2 .10	0 .86
$(CH_3)_4$—Si	1 .80	0 .00

Type of ^{1}H R = Alkyl	Hybridization	PPM
$R-CH_3$, R_2-CH_2	Alkyl	0 .80 To 1 .70
R_3-CH		
$R_2C=C(R)CHR_2$	Allylic	1 .60 To 2 .60
$RC\equiv CH$	Acetylenic	2 .00 To 3 .00
$R_2C=CHR$	Vinynlic	4 .60 To 5 .70
$R_2C=CH_2$		
RCHO	Aldehydic	9 .50 To 10 .10

Type of ^{1}H	Name	PPM	Bonding (Diamagnetic effects)
RCH_3	Alkyl	0 .8 To 1 .0	SP^3
$RC\equiv CH$	Acetylenic	2 .0 To 3 .0	SP
$R_2C=CH_2$	Vinylic	4 .6 To 5 .7	SP^2

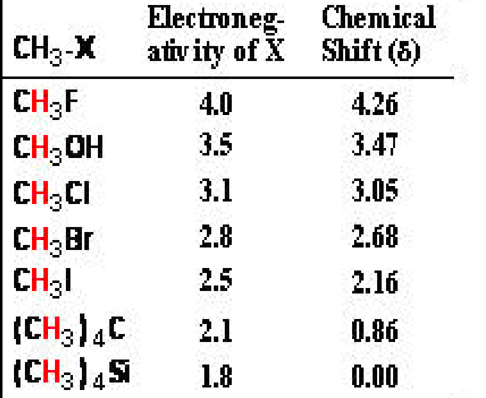
Anisotropic Field in an Alkenes (SP^2)

- **Anisotropic Field Effect**

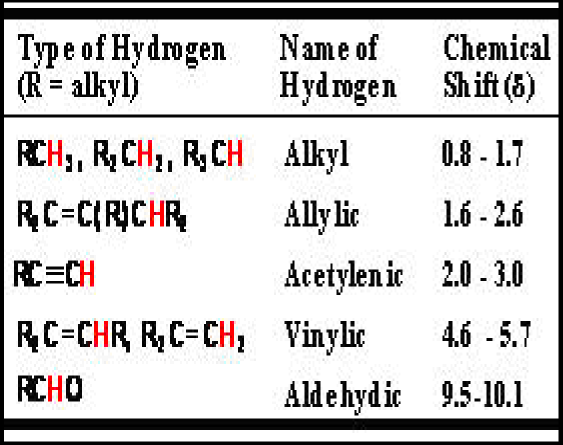


Factors affecting Chemical Shifts
Shielding and Deshielding effects

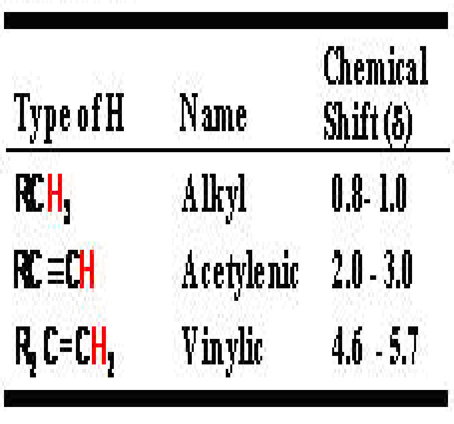
- 1. The electro negativity of the atoms within the molecule.
- 2. The hybridization of the adjacent atoms.
- 3. The diamagnetic effects from adjacent Pi bonds.



CH_3-X	Electronegativity of X	Chemical Shift (δ)
CH_3F	4.0	4.26
CH_3OH	3.5	3.47
CH_3Cl	3.1	3.05
CH_3Br	2.8	2.68
CH_3I	2.5	2.16
$(CH_3)_4C$	2.1	0.86
$(CH_3)_4Si$	1.8	0.00



Type of Hydrogen (R = alkyl)	Name of Hydrogen	Chemical Shift (δ)
RCH_3, R_2CH_2, R_3CH	Alkyl	0.8 - 1.7
$R_2C=C(R)CHR_2$	Allylic	1.6 - 2.6
RC≡CH	Acetylenic	2.0 - 3.0
$R_2C=CHR$, $R_2C=CH_2$	Vinylic	4.6 - 5.7
RCHO	Aldehydic	9.5-10.1



Type of H	Name	Chemical Shift (δ)
RCH_3	Alkyl	0.8- 1.0
RC≡CH	Acetylenic	2.0 - 3.0
$R_2C=CH_2$	Vinylic	4.6 - 5.7

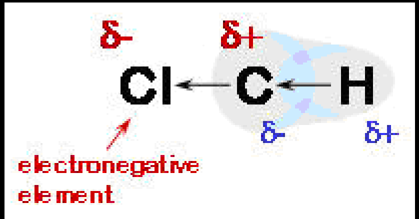
Hybridization

SP^3

SP

SP^2

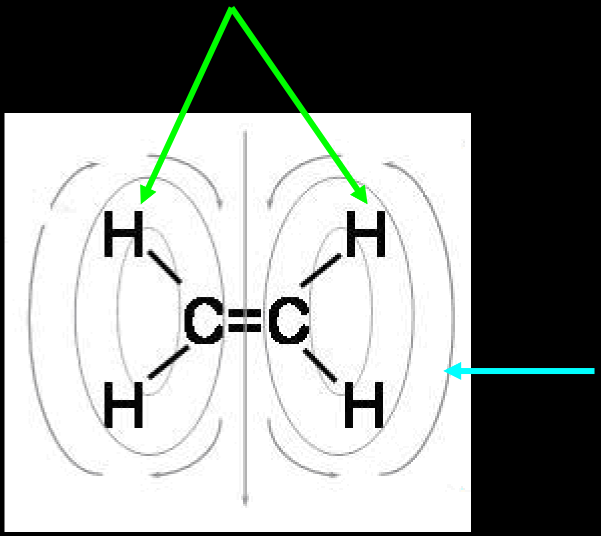
The most Deshielded atoms absorb at Lower Field (@ Higher PPM)



Chlorine takes the valence electro density away from Carbon which in turn takes more density from adjacent Hydrogen atoms causes Deshielding.

Anisotropic Field in an Alkenes (SP^2)

Anisotropic Field Effect



Deshielded ^1H

Shift To Lower Field

Fields Add

Secondary Magnetic

Field Lines Induce

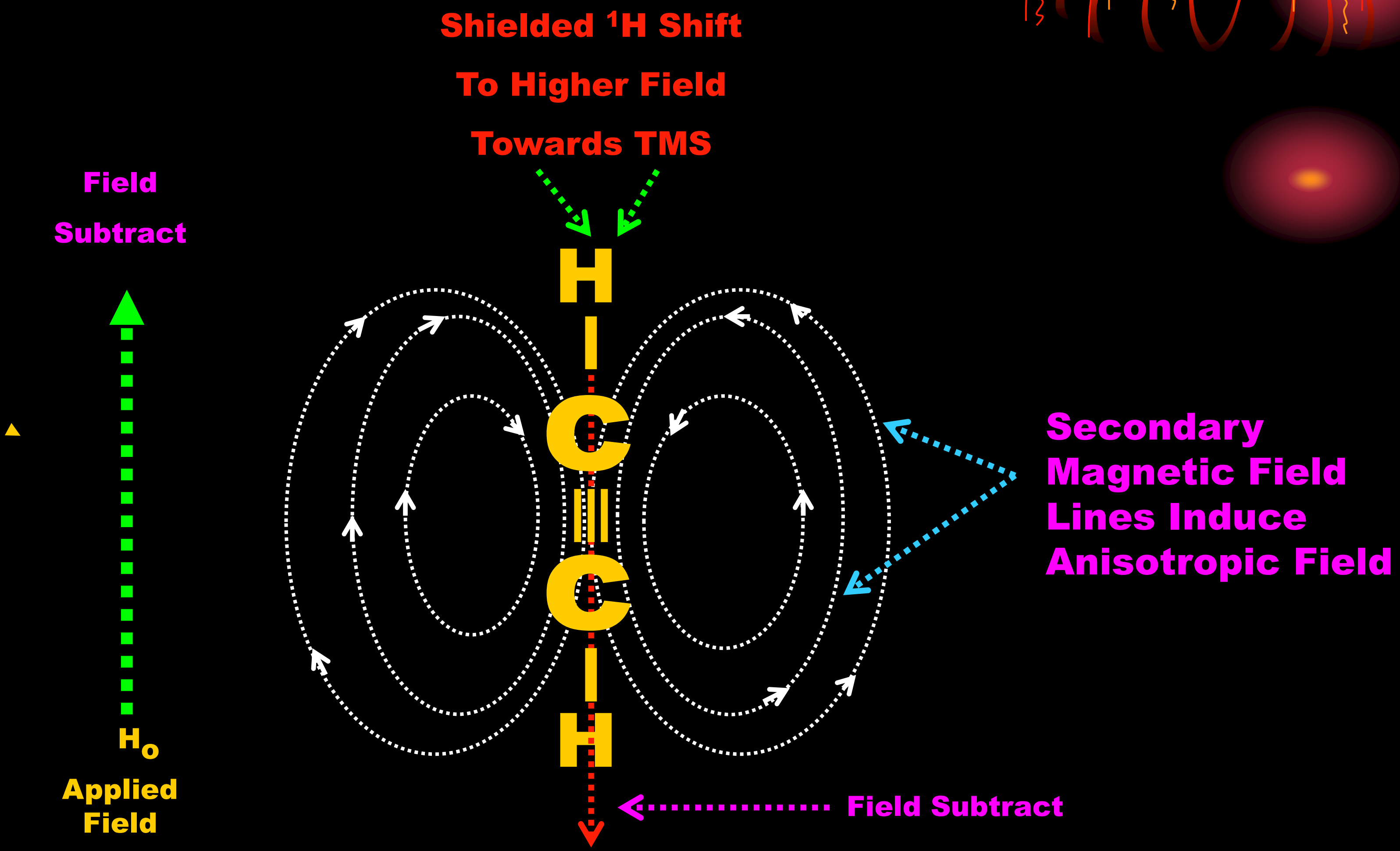
Anisotropic Field

H_0

Applied Field

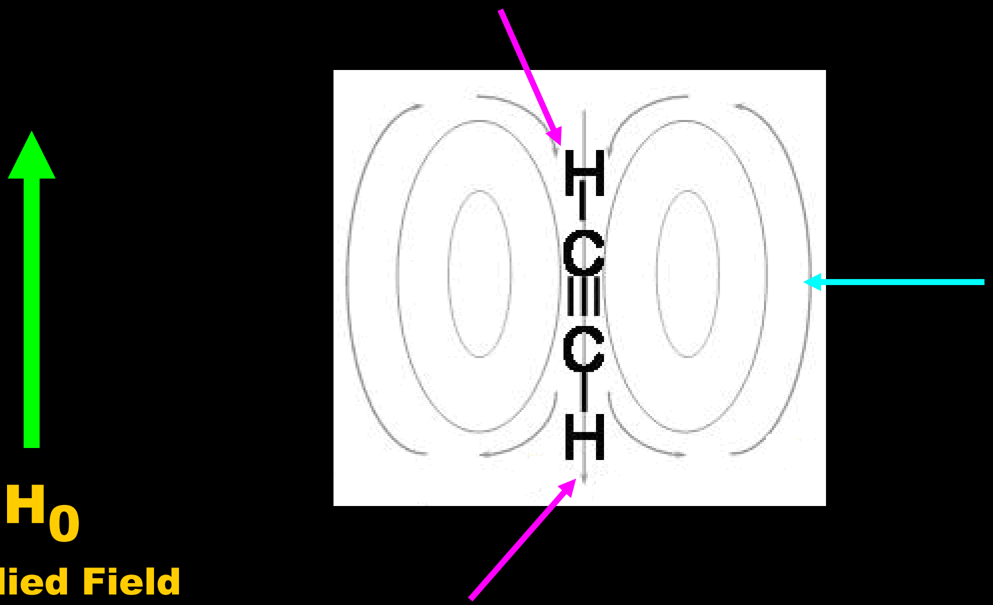
Anisotropic Field in an Alkynes (SP)

- **Anisotropic Field Effect**



Anisotropic Field in an Alkynes (SP)

- **Anisotropic Field Effect**



Shielded ^{1}H Shift

To Higher Field

Secondary
Magnetic Field
Lines Induce

Anisotropic Field

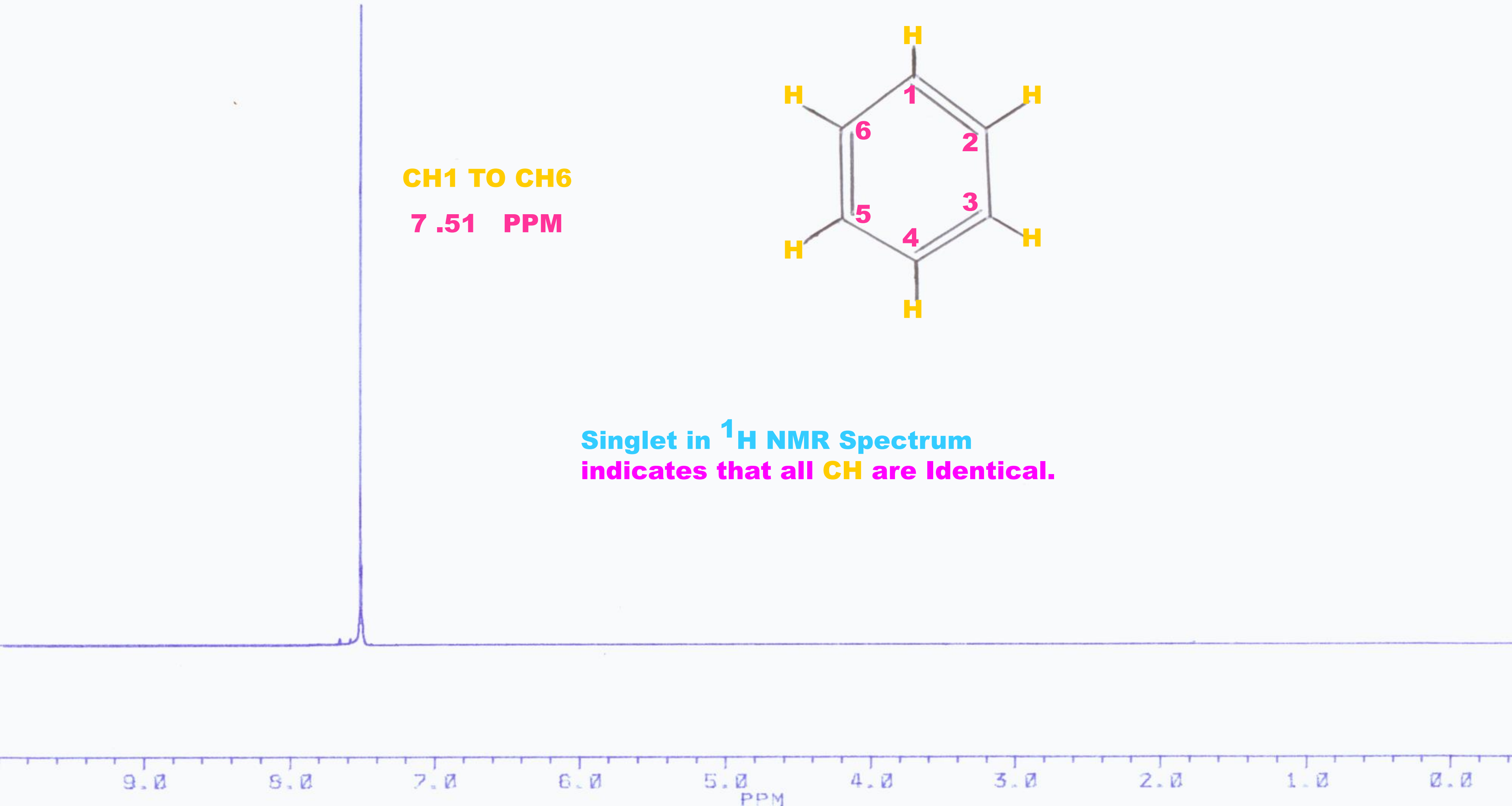
H_0

Applied Field

Fields
Subtract

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Benzene C_6H_6

^{1}H NMR Spectrum

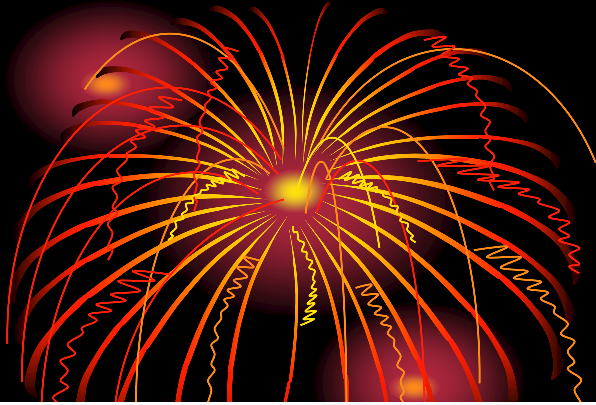


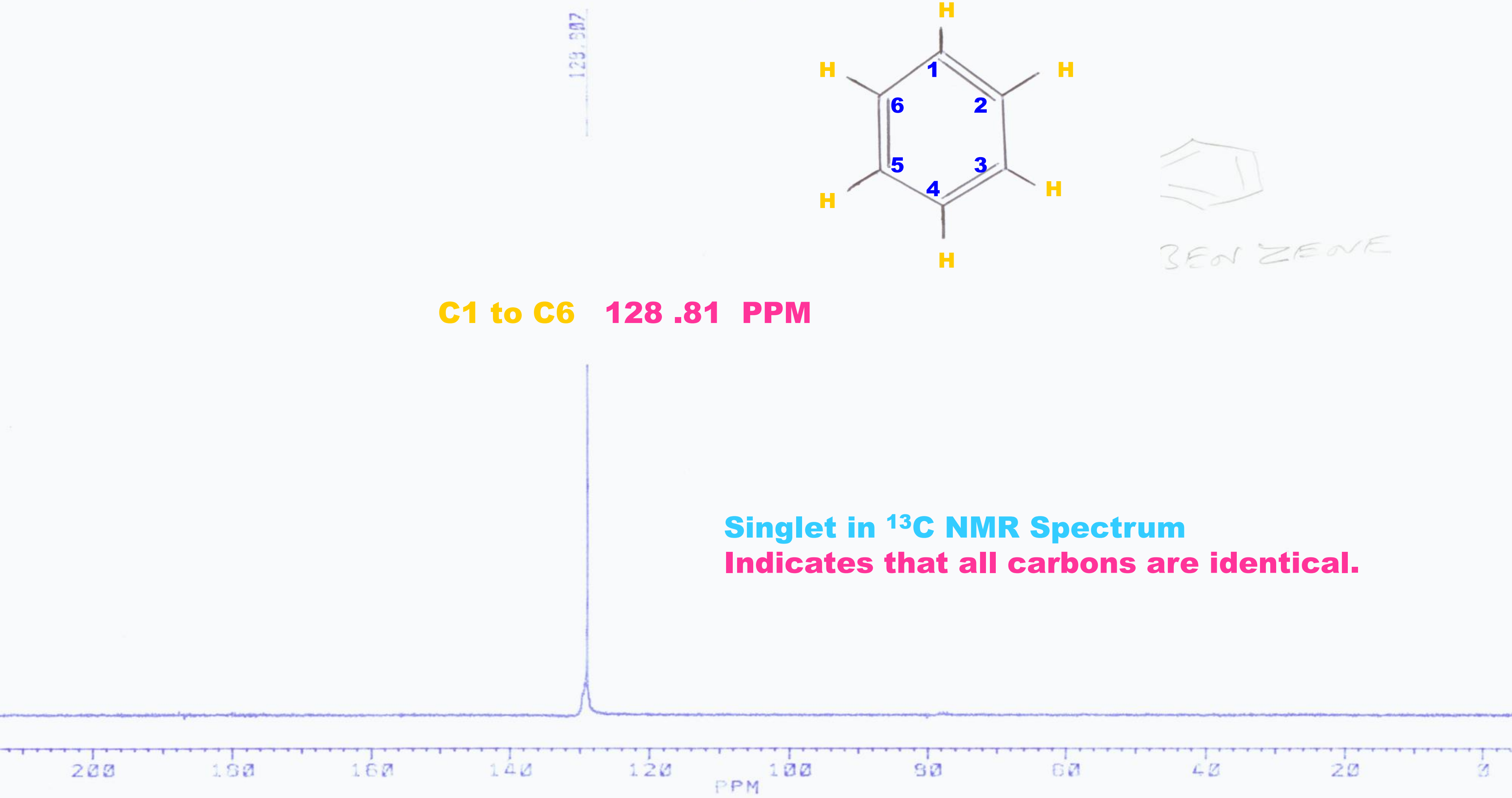
CH1 TO CH6

7 .51 PPM

Singlet in ^{1}H NMR Spectrum indicates that all CH are Identical.

^{13}C NMR Spectrum of Benzene C_6H_6



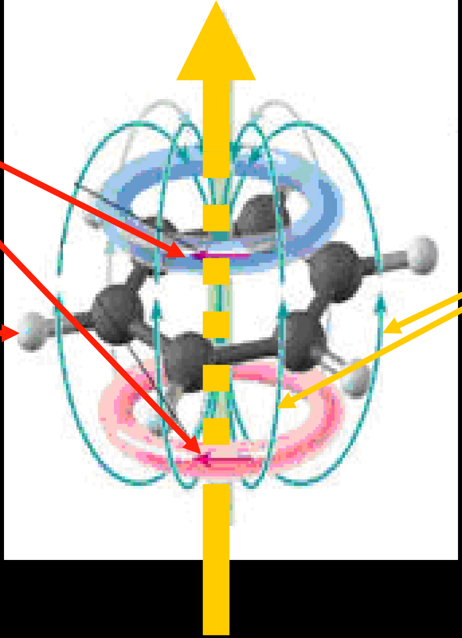


C1 to C6 128 .81 PPM

Singlet in ^{13}C NMR Spectrum
Indicates that all carbons are identical.

Magnetic Induction of the pi electrons in Aromatic Ring

- **Effect on Chemical Shift**



Induced circulation of pi electrons in the aromatic ring

^{1}H of Aromatic ring are Deshielded hence

absorb at Lower Field.

(Away from TMS)

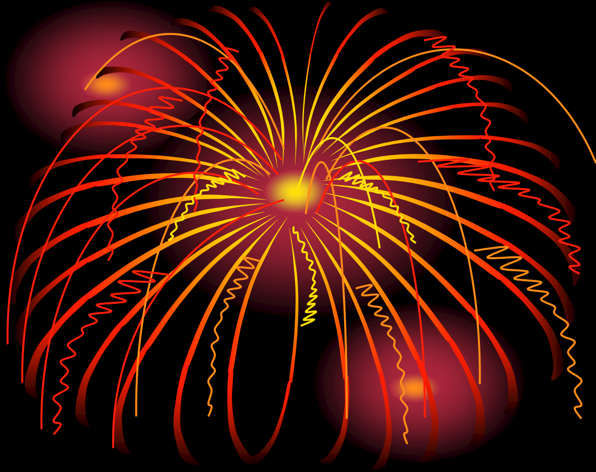
Circulating pi electrons generate secondary field lines which reinforces the applied field

(Adding Effect)

H_0

Applied Field

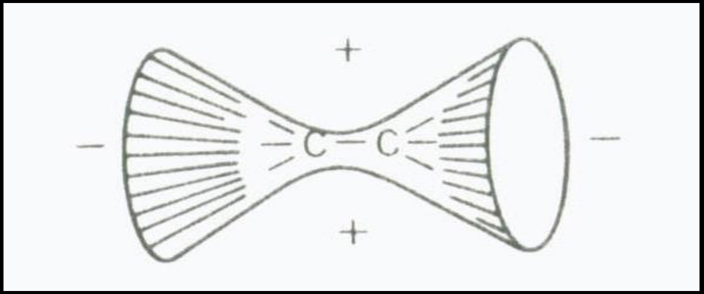
Anisotropic field effect of Various Bonds



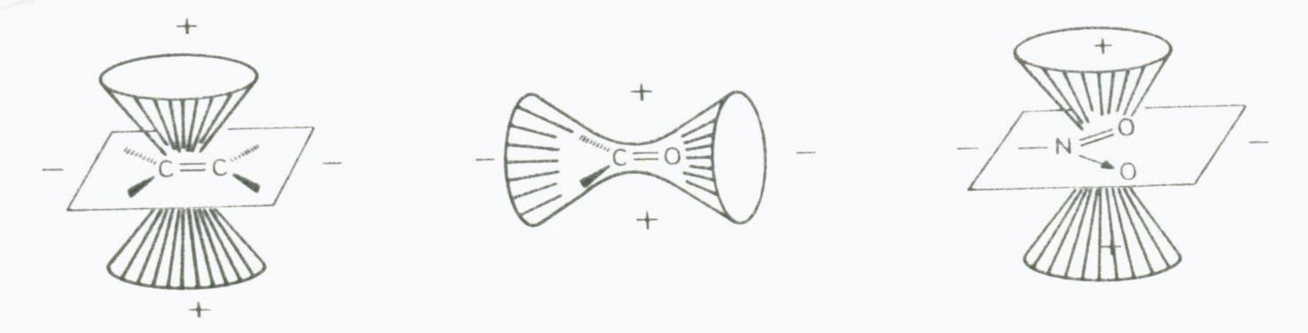
Shielded ^{1}H Shift to Higher Field (Towards TMS)

Deshieled ^{1}H Shift to Lower Field (Away from TMS)

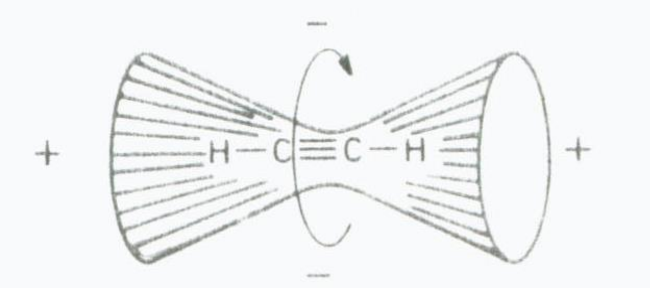
Single Bond



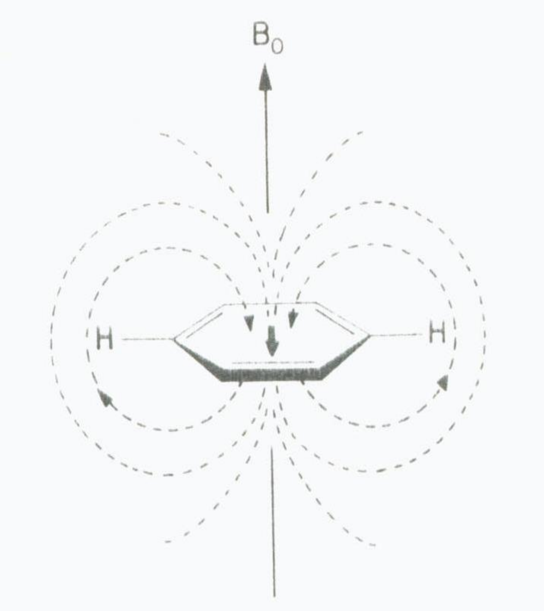
Double Bond



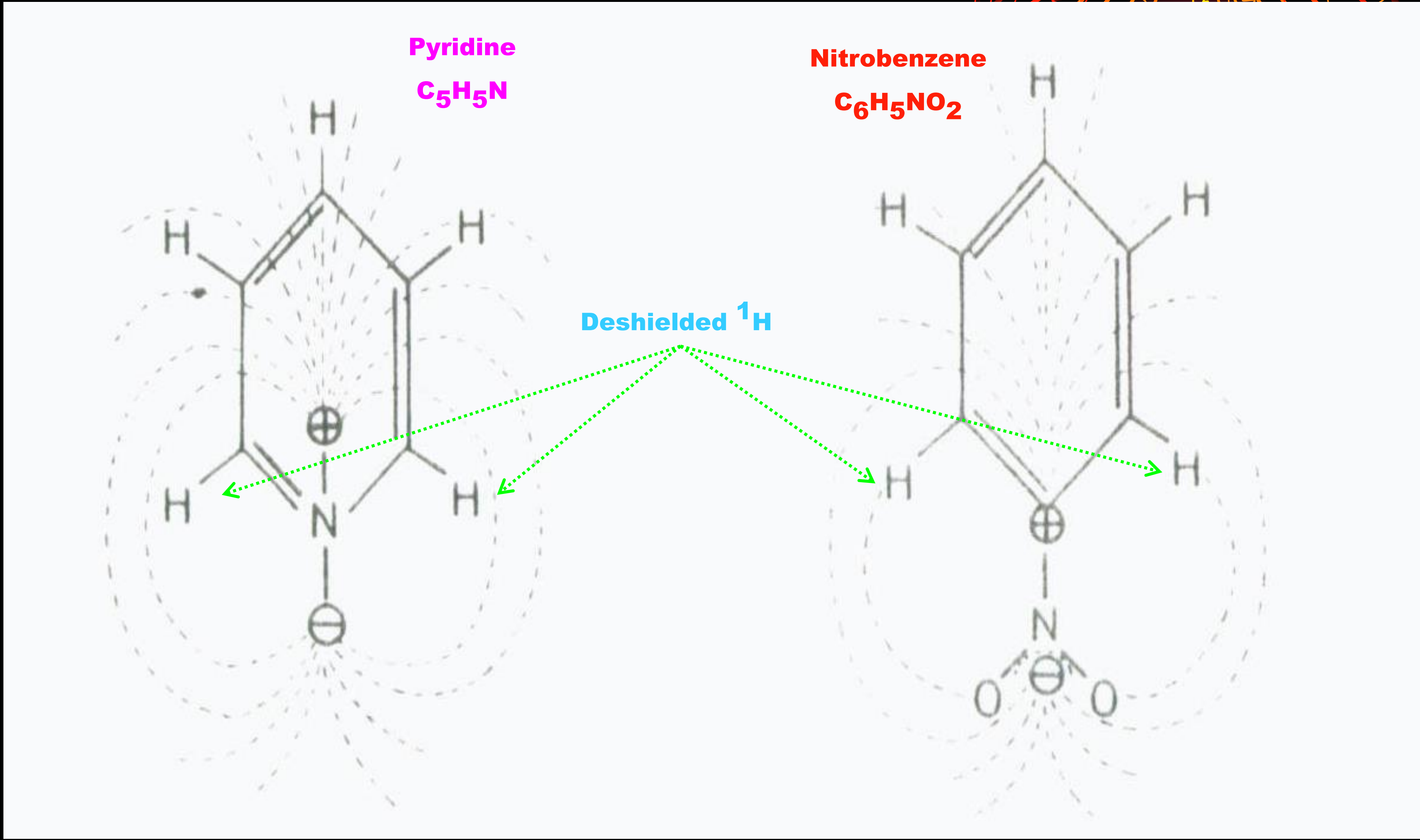
Triple Bond



Aromatic Double Bond



The Electric Field Effect on Pyridine & Nitrobenzene



Pyridine

C_5H_5N

Nitrobenzene

$C_6H_5NO_2$

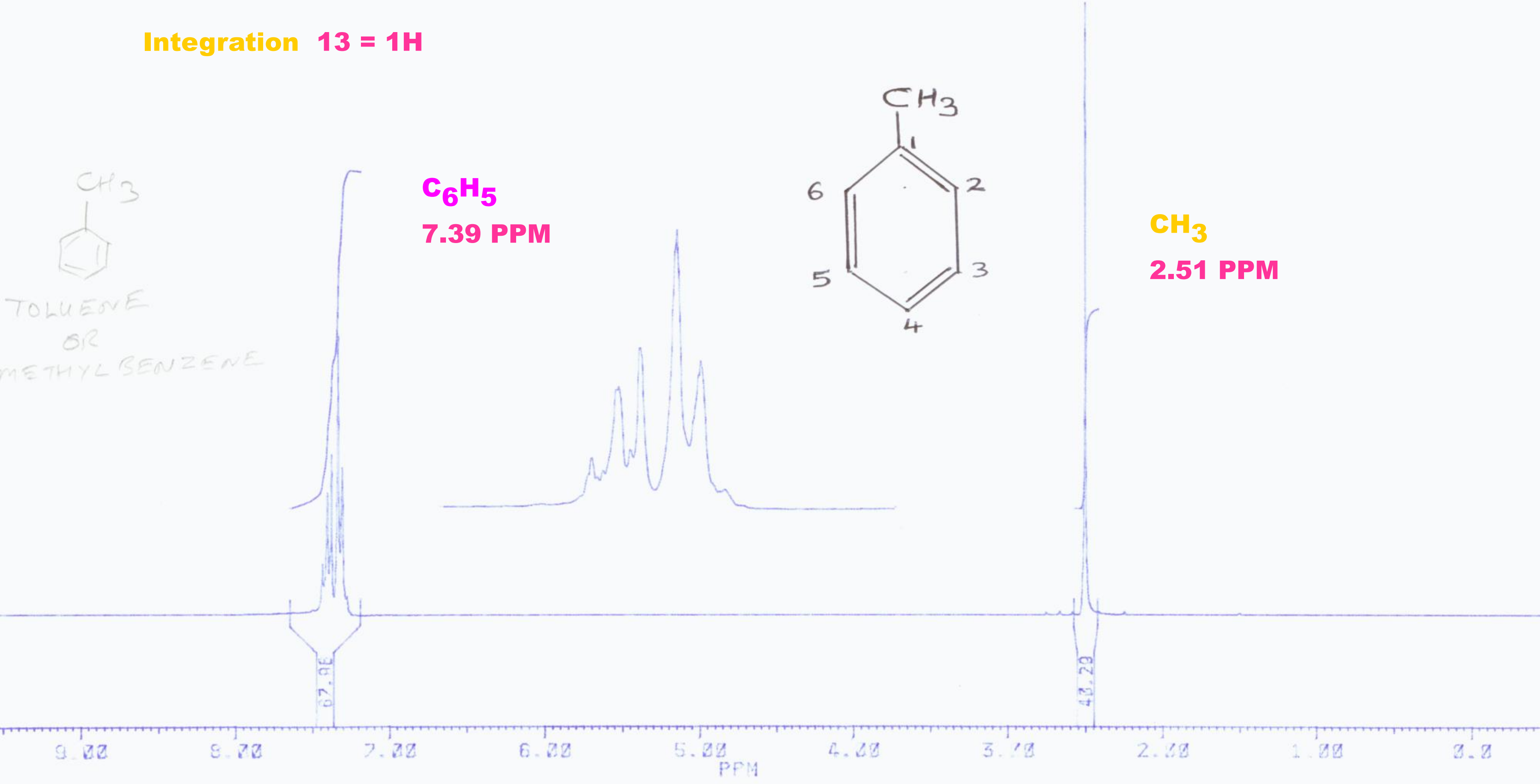
Deshielded ^1H

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra

of Methyl Benzene or Toluene

^{1}H NMR Spectrum $C_6H_5—CH_3$

Integration 13 = 1H

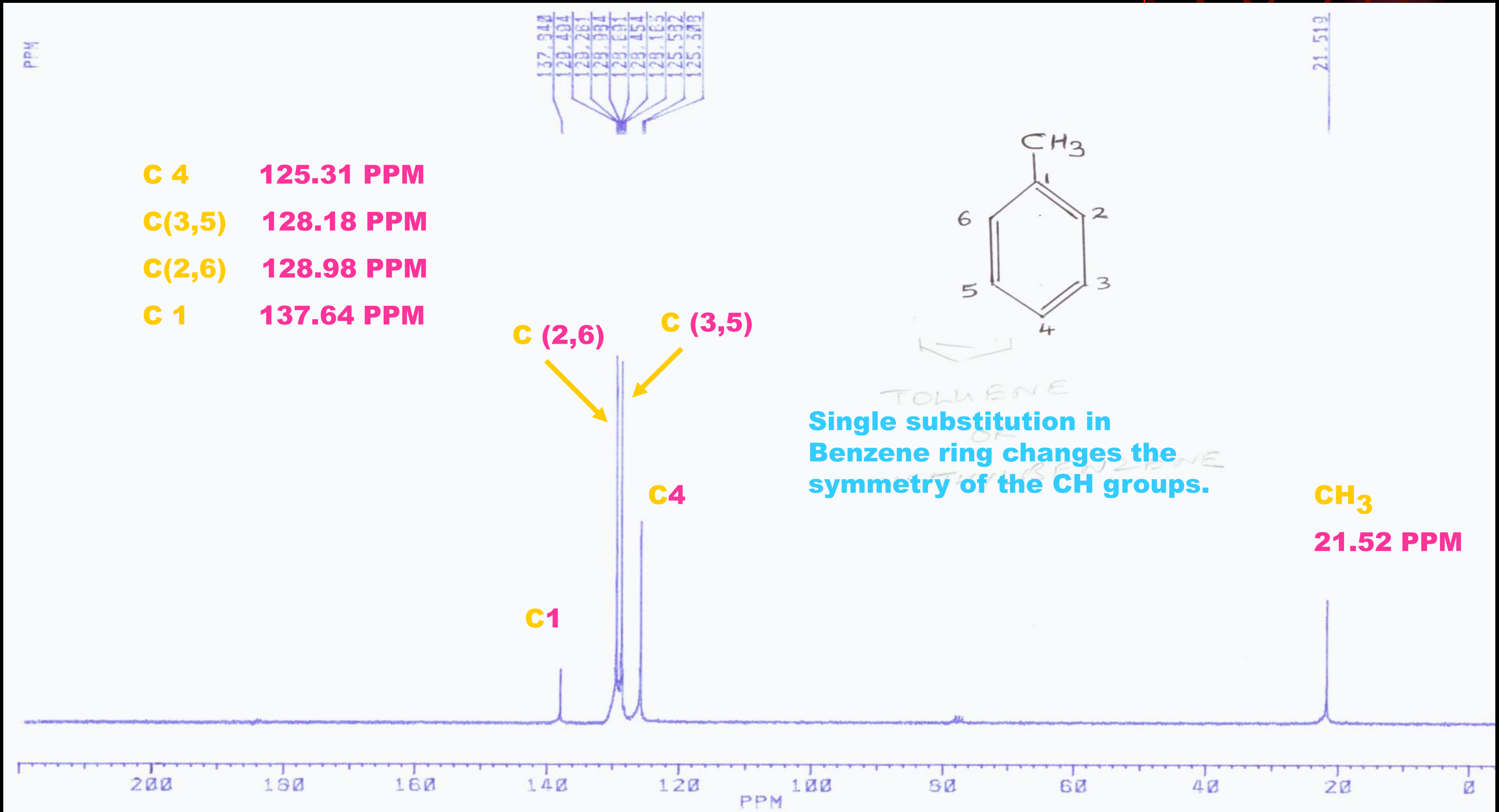


C_6H_5
7.39 PPM

CH_3
2.51 PPM

^{13}C NMR Spectrum of Methyl Benzene (Toluene)

$C_6H_5—CH_3$

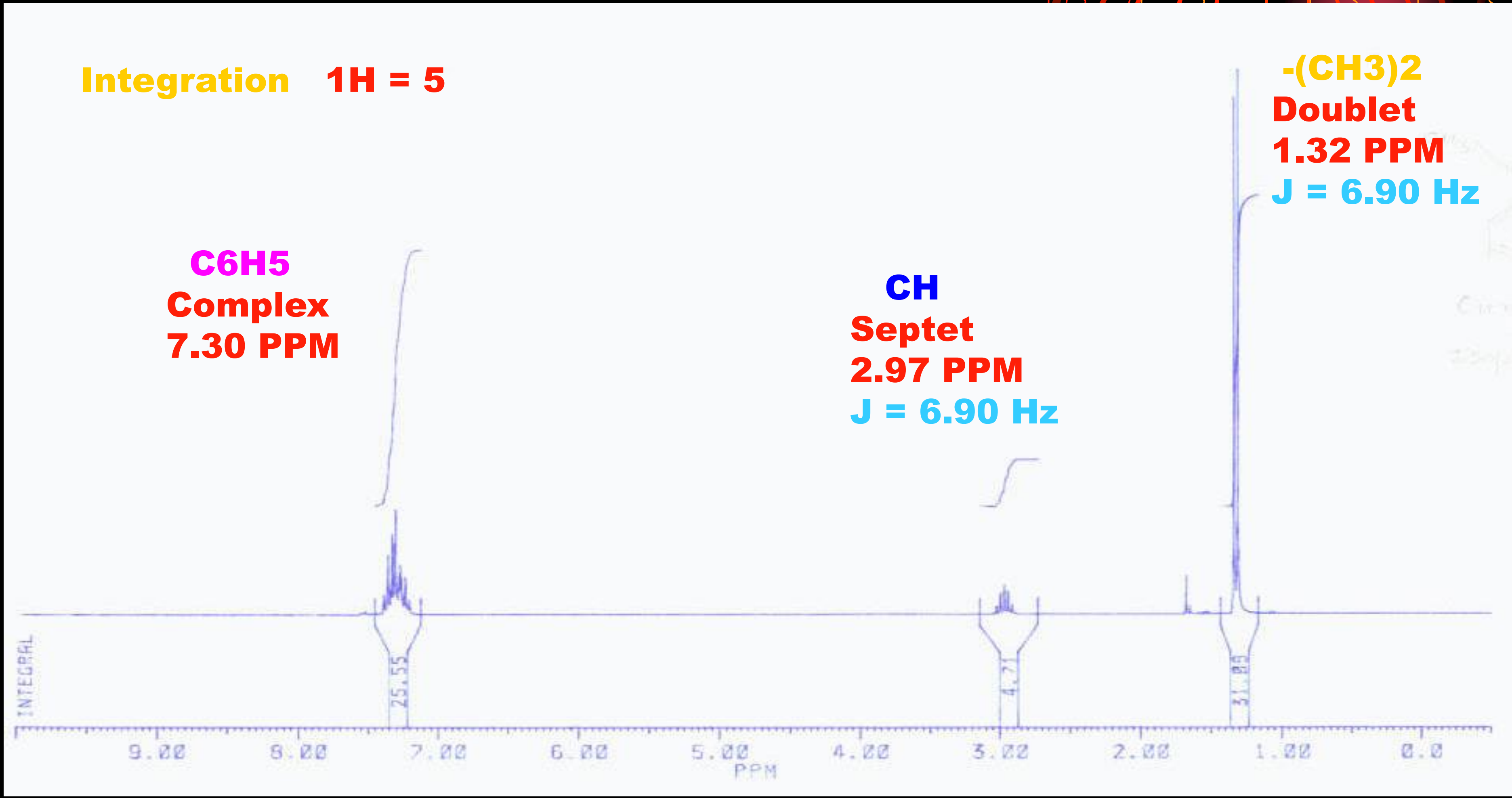


C 4	125.31 PPM
C(3,5)	128.18 PPM
C(2,6)	128.98 PPM
C 1	137.64 PPM

Single substitution in Benzene ring changes the symmetry of the CH groups.

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Cumene (Isopropyl Benzene)

^{1}H NMR $C_6H_5—CH(CH_3)_2$



Integration 1H = 5

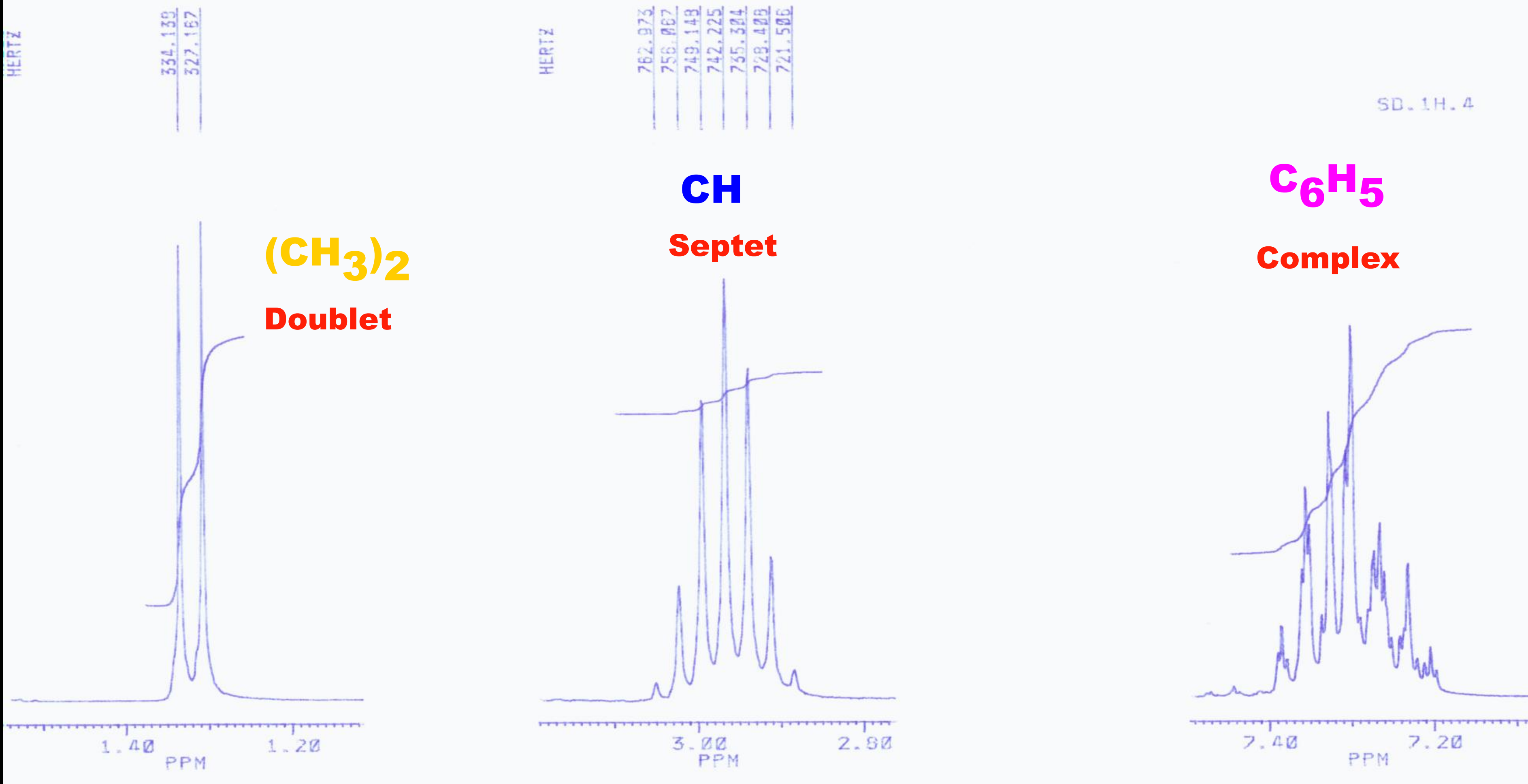
C6H5
Complex
7.30 PPM

CH
Septet
2.97 PPM
J = 6.90 Hz

-(CH3)2
Doublet
1.32 PPM
J = 6.90 Hz

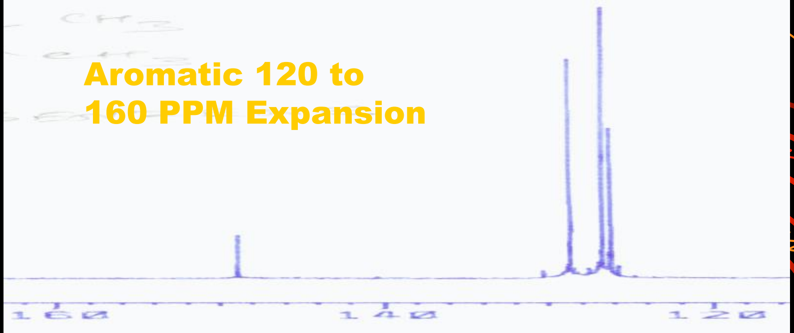
Expansion of ^{1}H NMR of Cumene (Isopropyl Benzene)

$C_6H_5—CH(CH_3)_2$

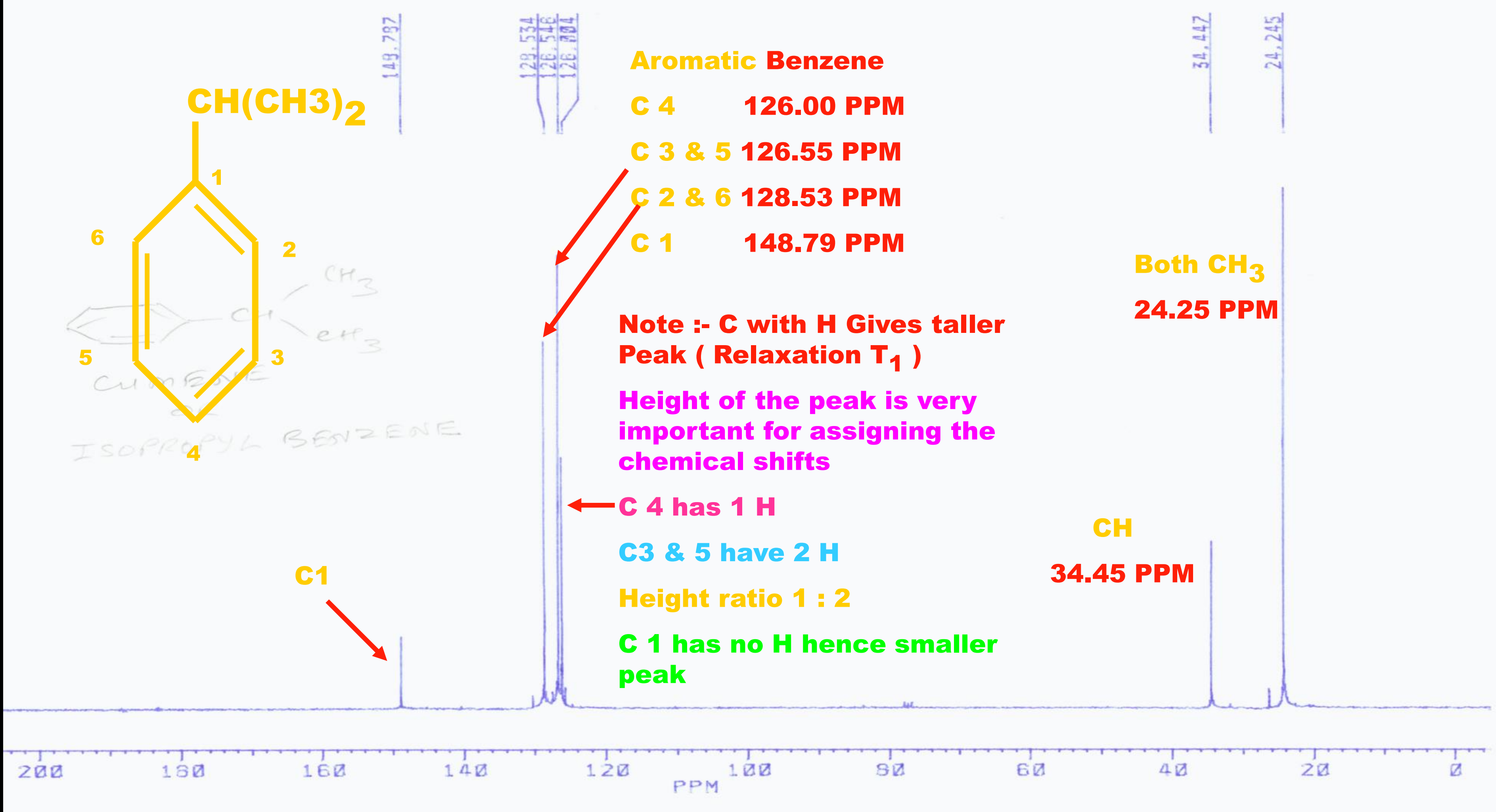


^{13}C NMR Spectrum of Cumene

$C_6H_5—CH(CH_3)_2$



Aromatic 120 to 160 PPM Expansion



Aromatic Benzene

C 4 126.00 PPM

C 3 & 5 126.55 PPM

C 2 & 6 128.53 PPM

C 1 148.79 PPM

Note :- C with H Gives taller Peak (Relaxation T_1)

Height of the peak is very important for assigning the chemical shifts

C 4 has 1 H

C3 & 5 have 2 H

Height ratio 1 : 2

C 1 has no H hence smaller peak

C1

Both CH_3

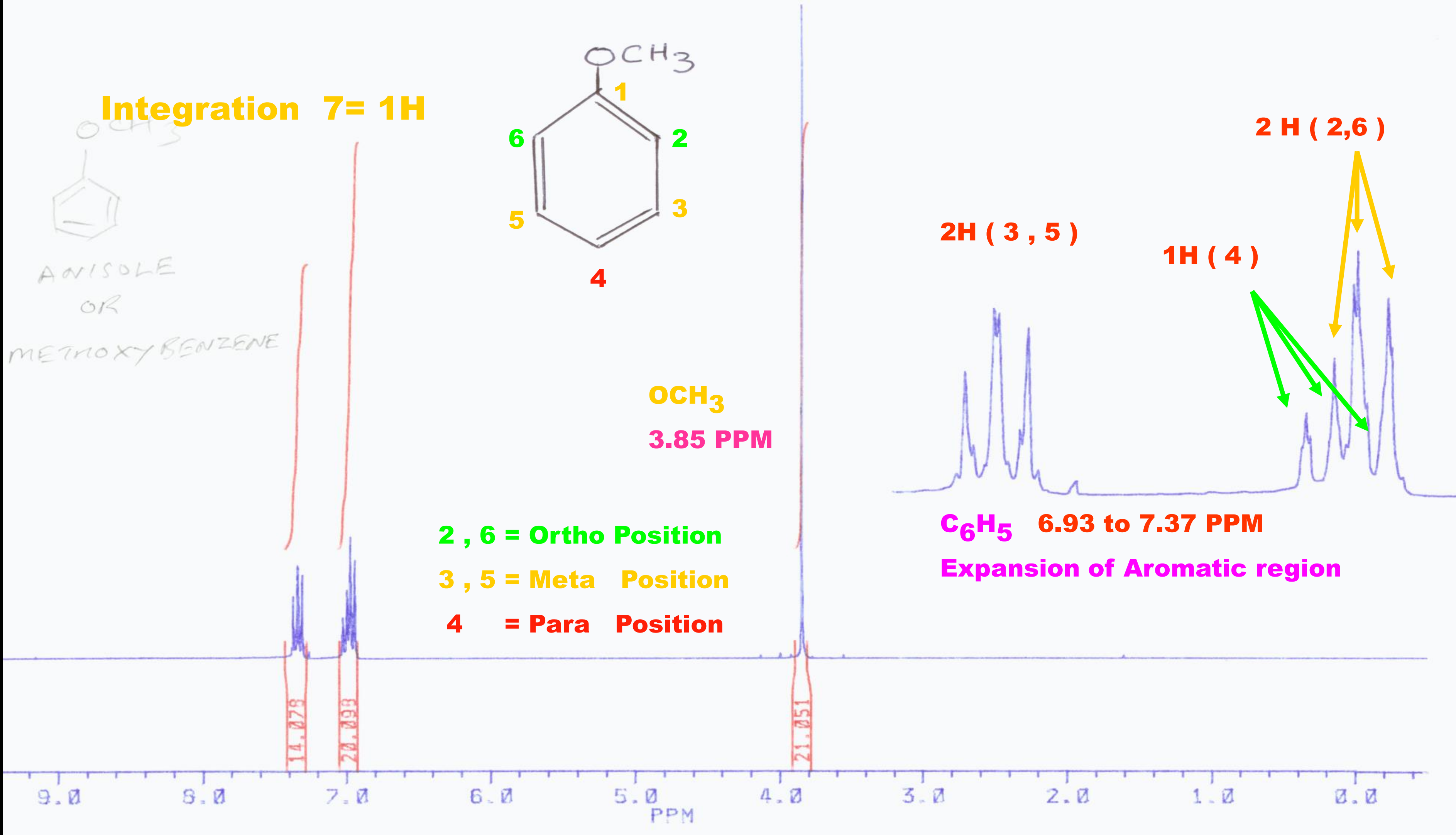
24.25 PPM

CH

34.45 PPM

Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Anisole (Methoxy Benzene) $C_6H_5—OCH_3$

^1H NMR Spectrum



Integration 7= 1H

OCH_3

3.85 PPM

2 , 6 = Ortho Position

3 , 5 = Meta Position

4 = Para Position

2H (3 , 5)

1H (4)

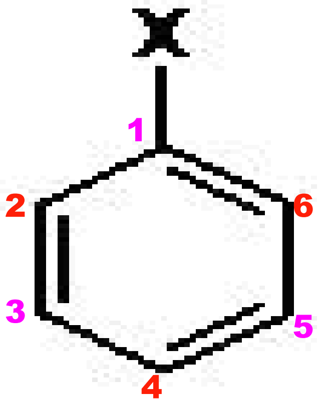
2 H (2,6)

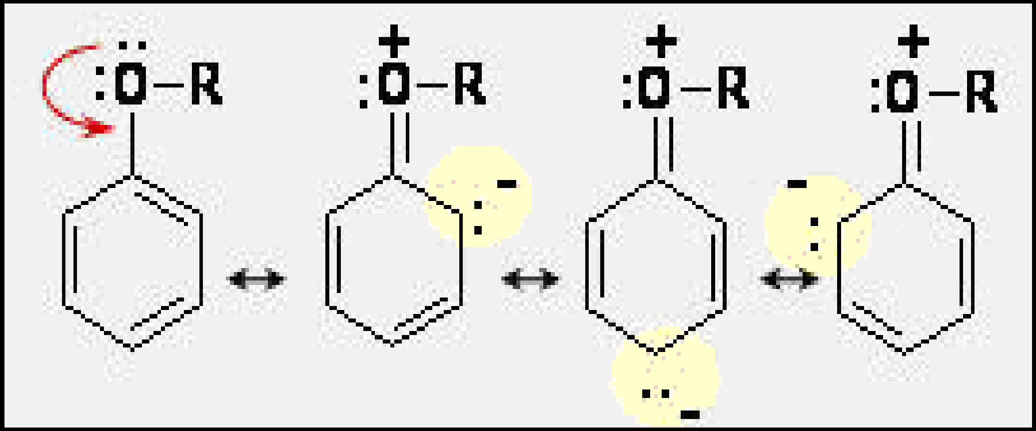
C_6H_5 6.93 to 7.37 PPM

Expansion of Aromatic region

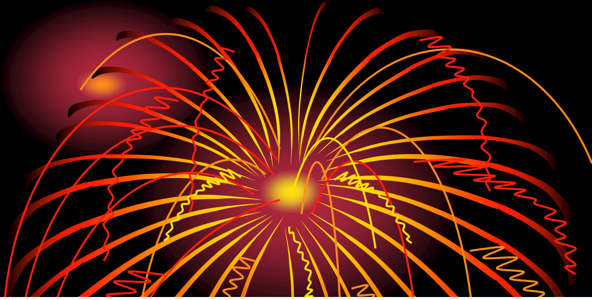
Shielding Effects on ^{1}H Ortho and Para Positions in Mono Substitution of Benzene.

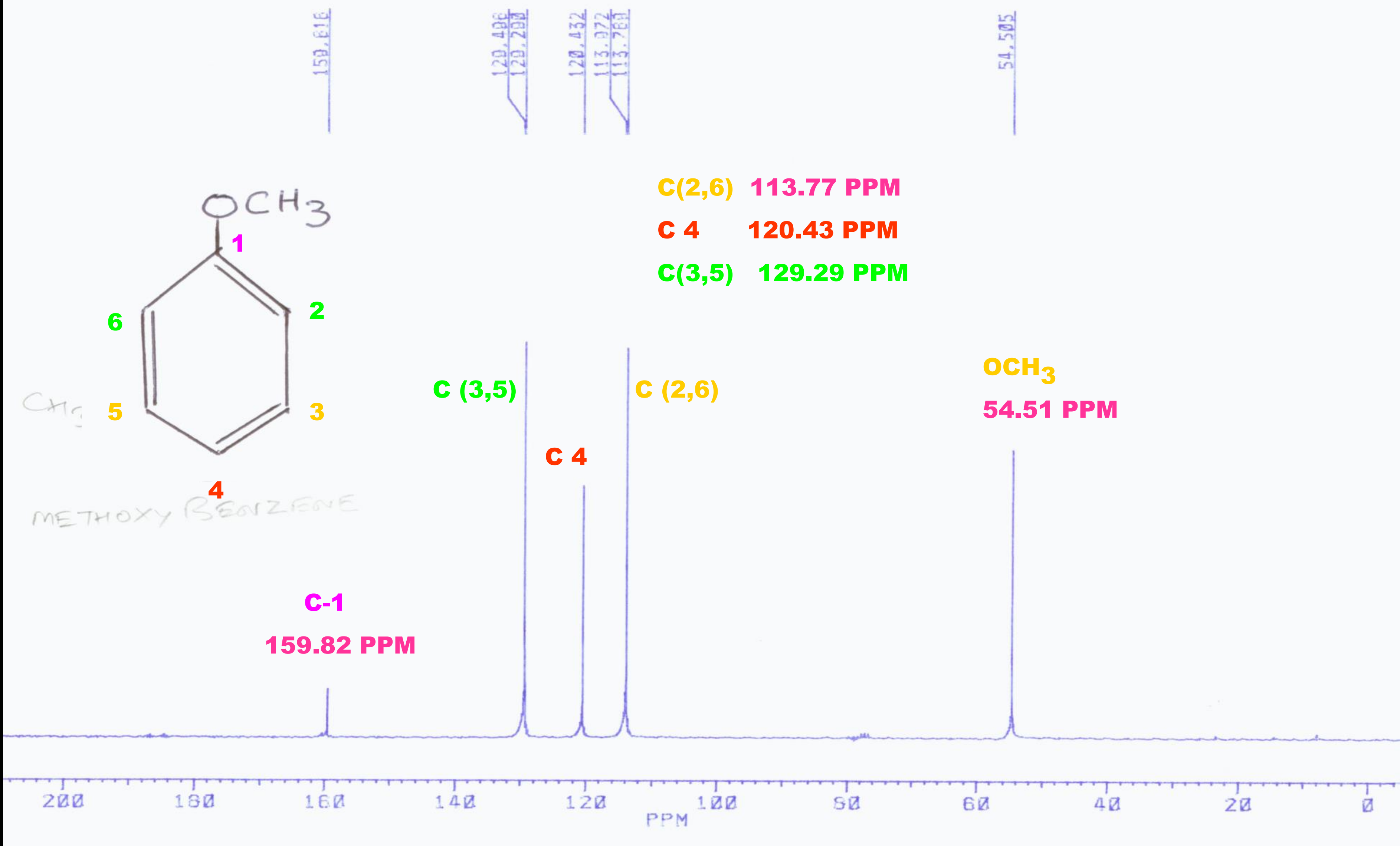
- Ortho and Para positions are shielded by mono substitution of electronegative group in benzene.
- X = OH, OR, NH_2, NR_2, $O\text{-}CO\text{-}CH_3$ Groups
  ^{1}H attached to Positions 2 , 4 and 6 are affected.
- Shift towards to TMS (To Right or Higher Field)





^{13}C NMR Spectrum of Anisole (Methoxy Benzene) $C_6H_5—OCH_3$





C(2,6) 113.77 PPM

C 4 120.43 PPM

C(3,5) 129.29 PPM

C (3,5)

C 4

C (2,6)

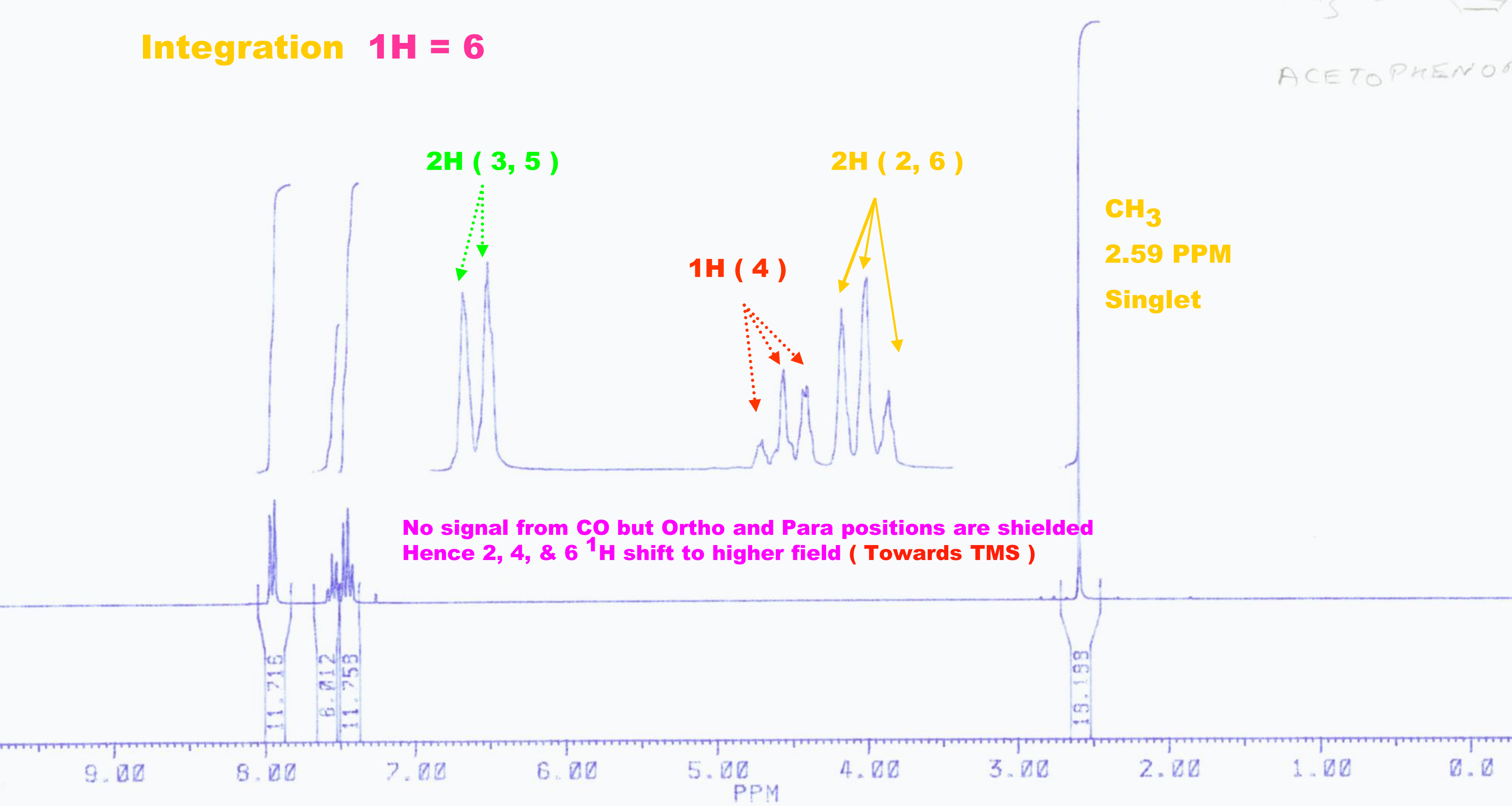
OCH_3

54.51 PPM

C-1

159.82 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Acetophenone $C_6H_5—CO—CH_3$



Integration 1H = 6

2H (3, 5)

1H (4)

2H (2, 6)

CH_3

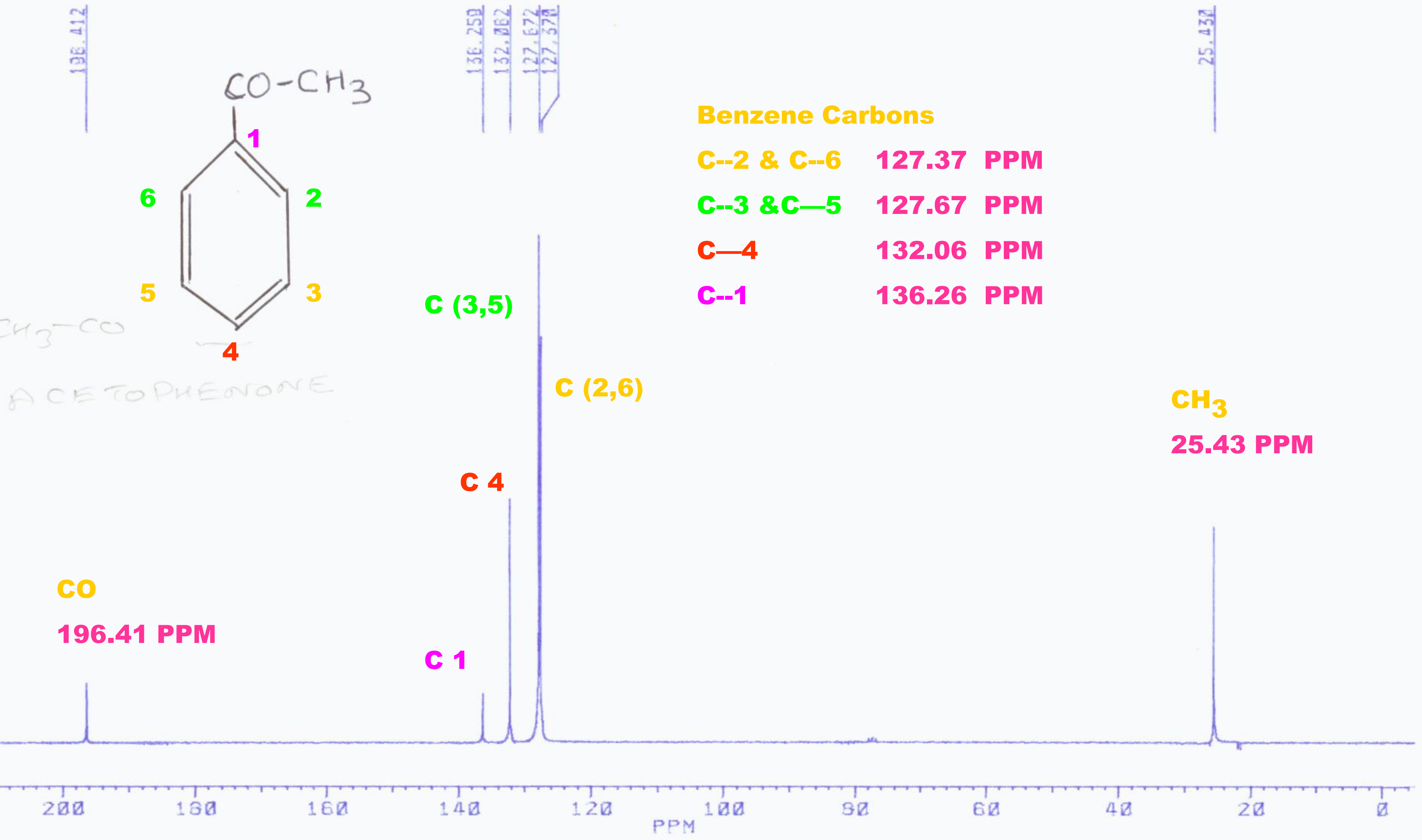
2.59 PPM

Singlet

No signal from CO but Ortho and Para positions are shielded
Hence 2, 4, & 6 ^{1}H shift to higher field (Towards TMS)

^{13}C NMR Spectrum of Acetophenone

$C_6H_5—CO—CH_3$

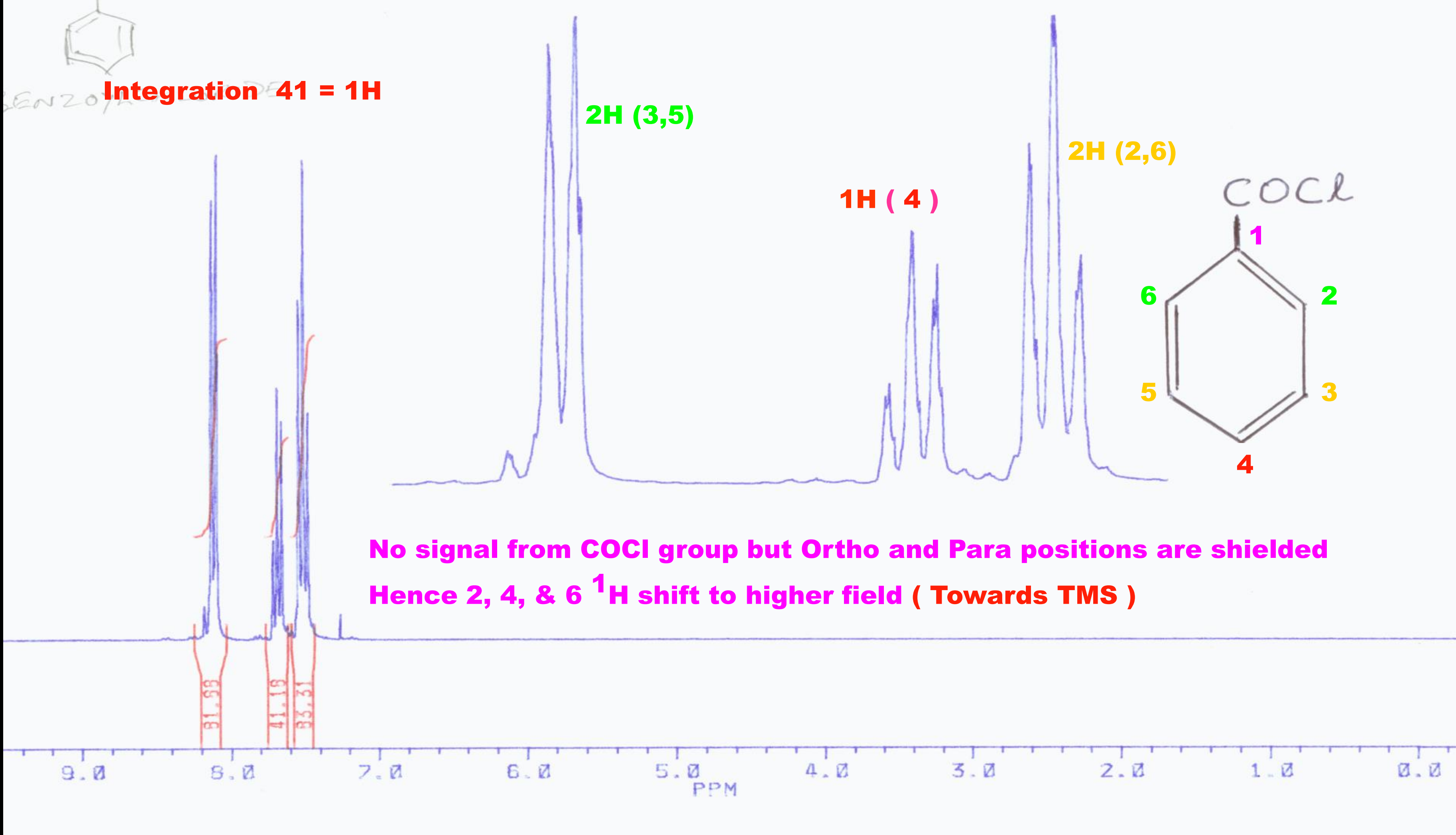


Benzene Carbons

C--2 & C--6	127.37 PPM
C--3 &C—5	127.67 PPM
C—4	132.06 PPM
C--1	136.26 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Benzoylchloride C_6H_5—COCl

^{1}H NMR Spectrum

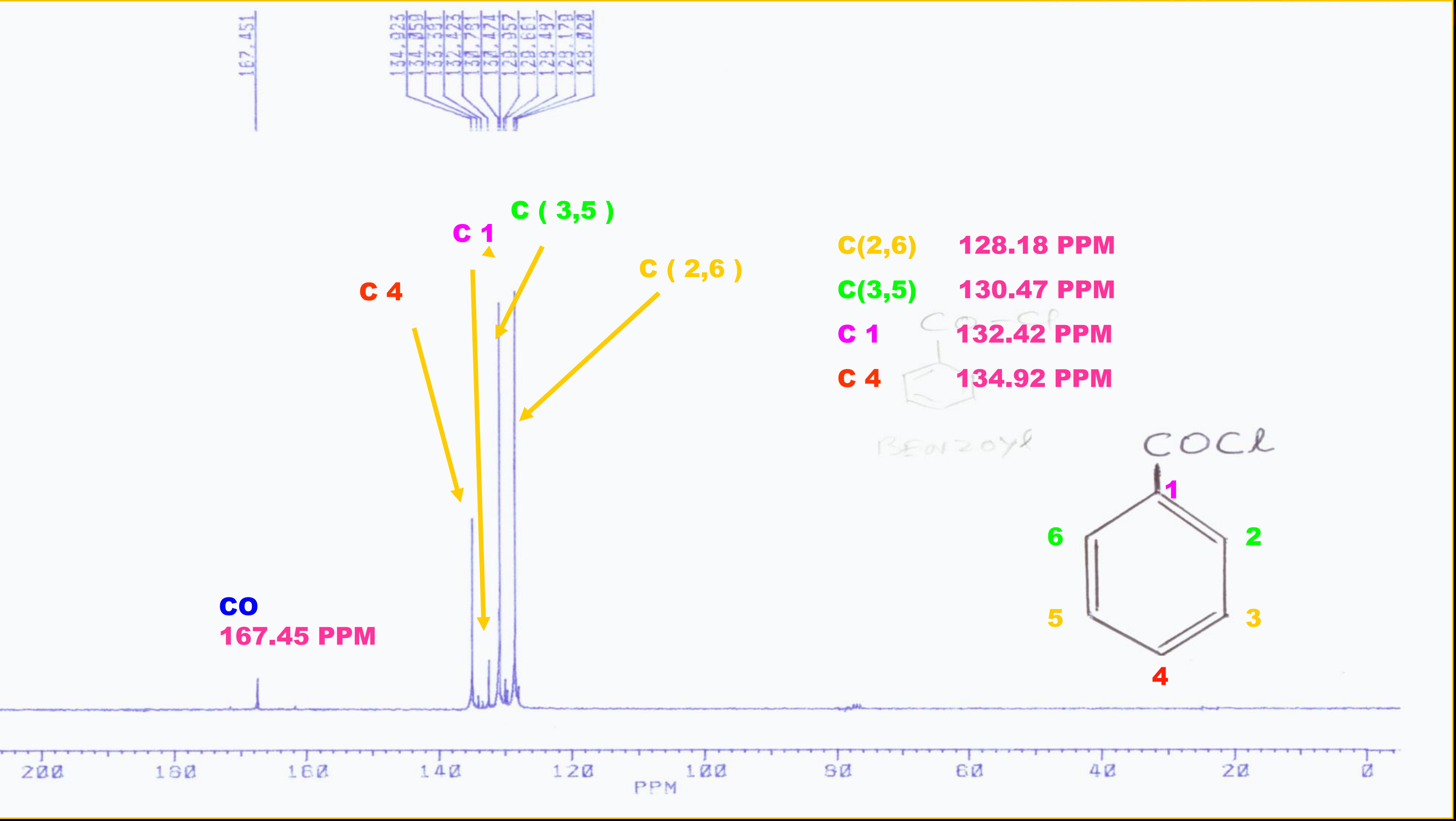


No signal from COCl group but Ortho and Para positions are shielded

Hence 2, 4, & 6 ^{1}H shift to higher field (Towards TMS)

^{13}C NMR Spectrum of Benzoylchloride

C_6H_5--COCl

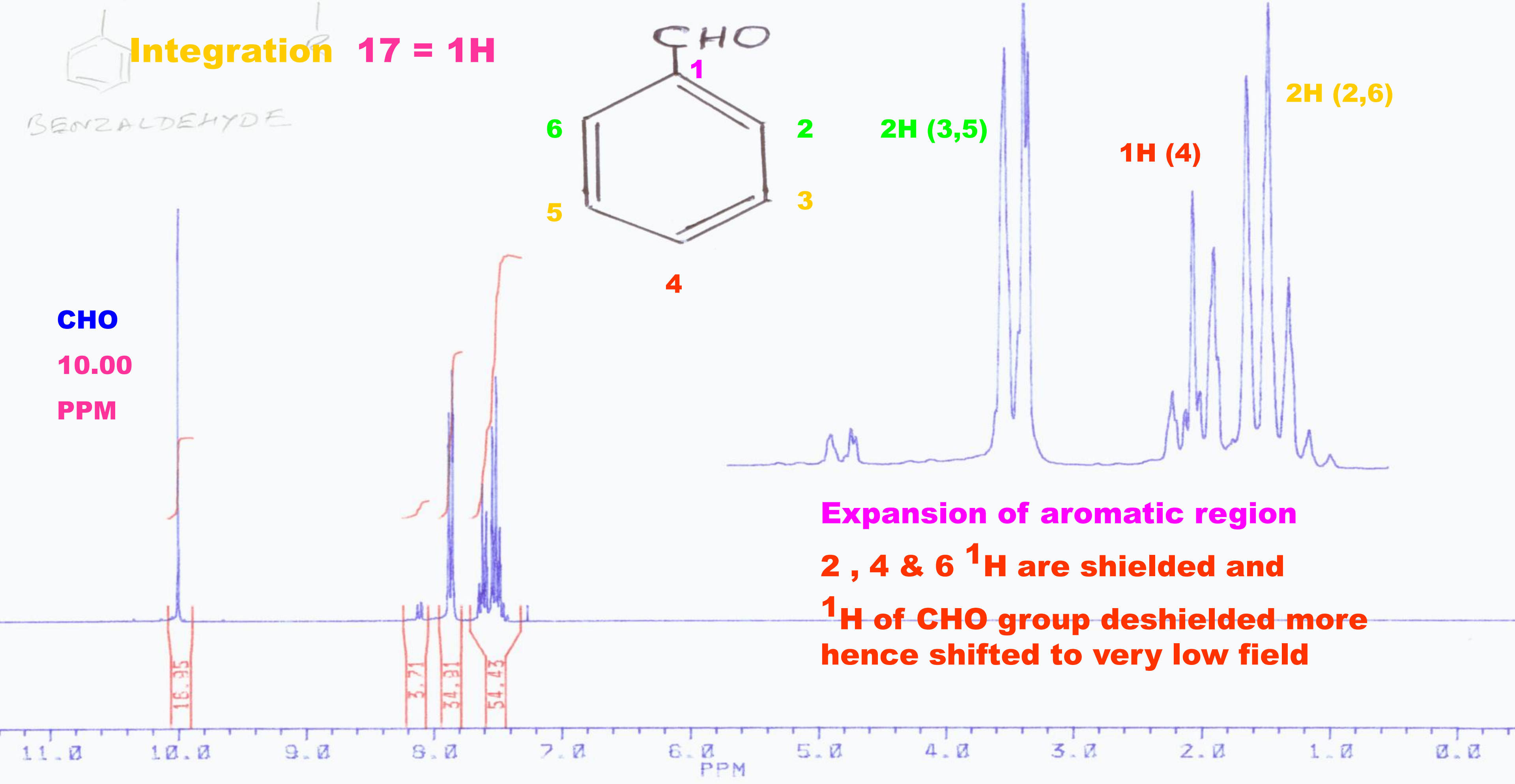


C(2,6)	128.18 PPM
C(3,5)	130.47 PPM
C 1	132.42 PPM
C 4	134.92 PPM

CO
167.45 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Benzaldehyde C_6H_5—CHO

^{1}H NMR Spectrum



Integration 17 = 1H

CHO

10.00

PPM

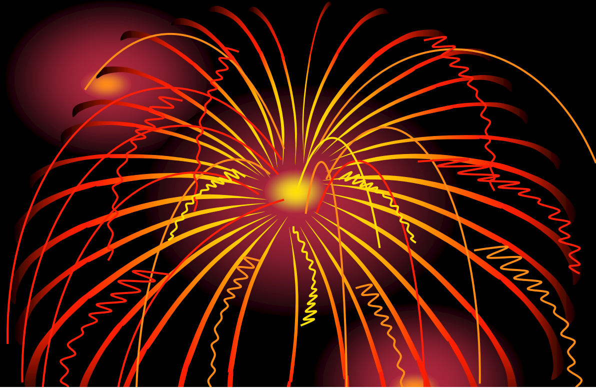
Expansion of aromatic region

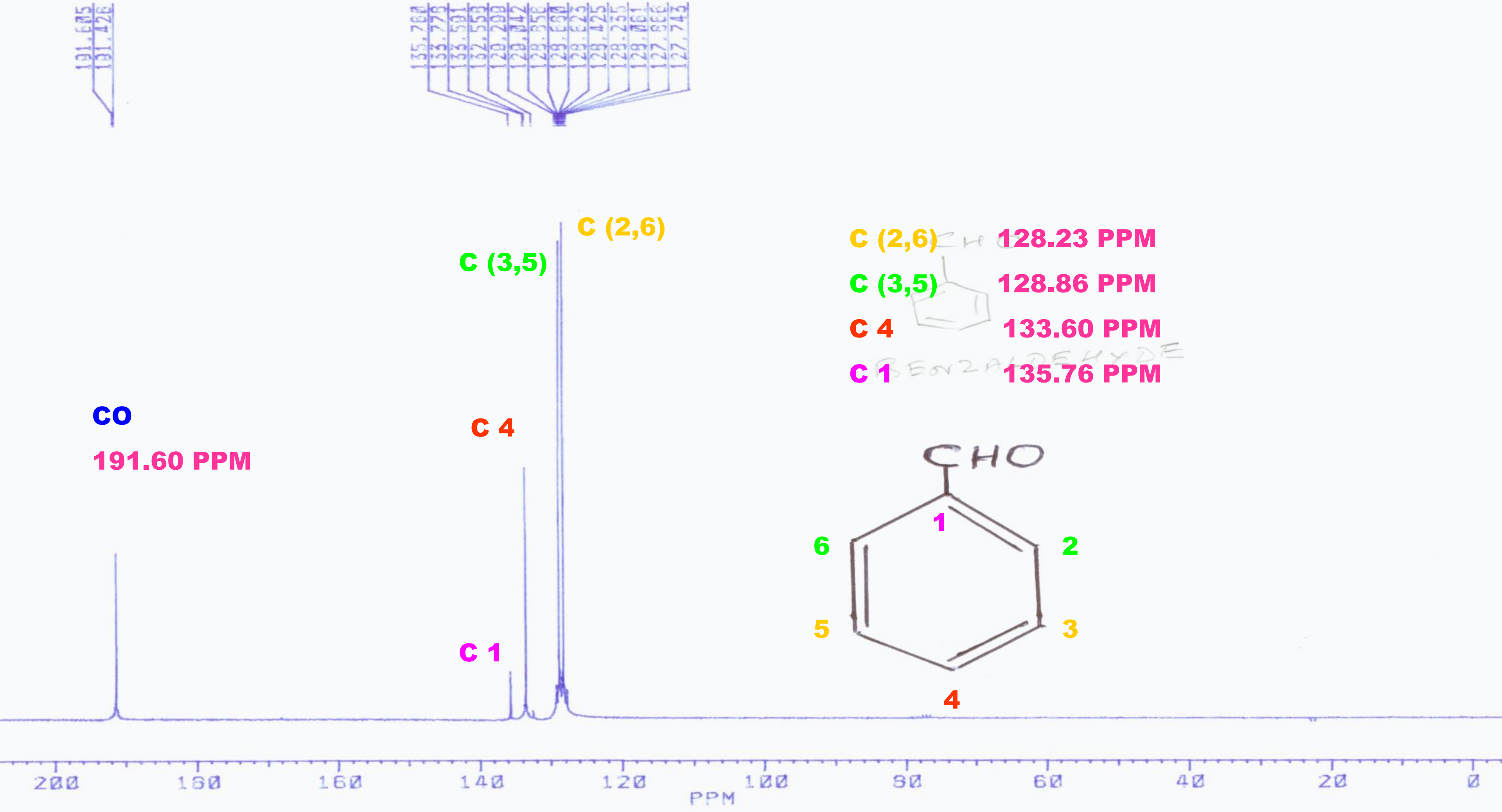
2 , 4 & 6 ^{1}H are shielded and

^{1}H of CHO group deshielded more hence shifted to very low field

^{13}C NMR Spectrum of Benzaldehyde

C_6H_5--CHO





CO

191.60 PPM

C 1

C 4

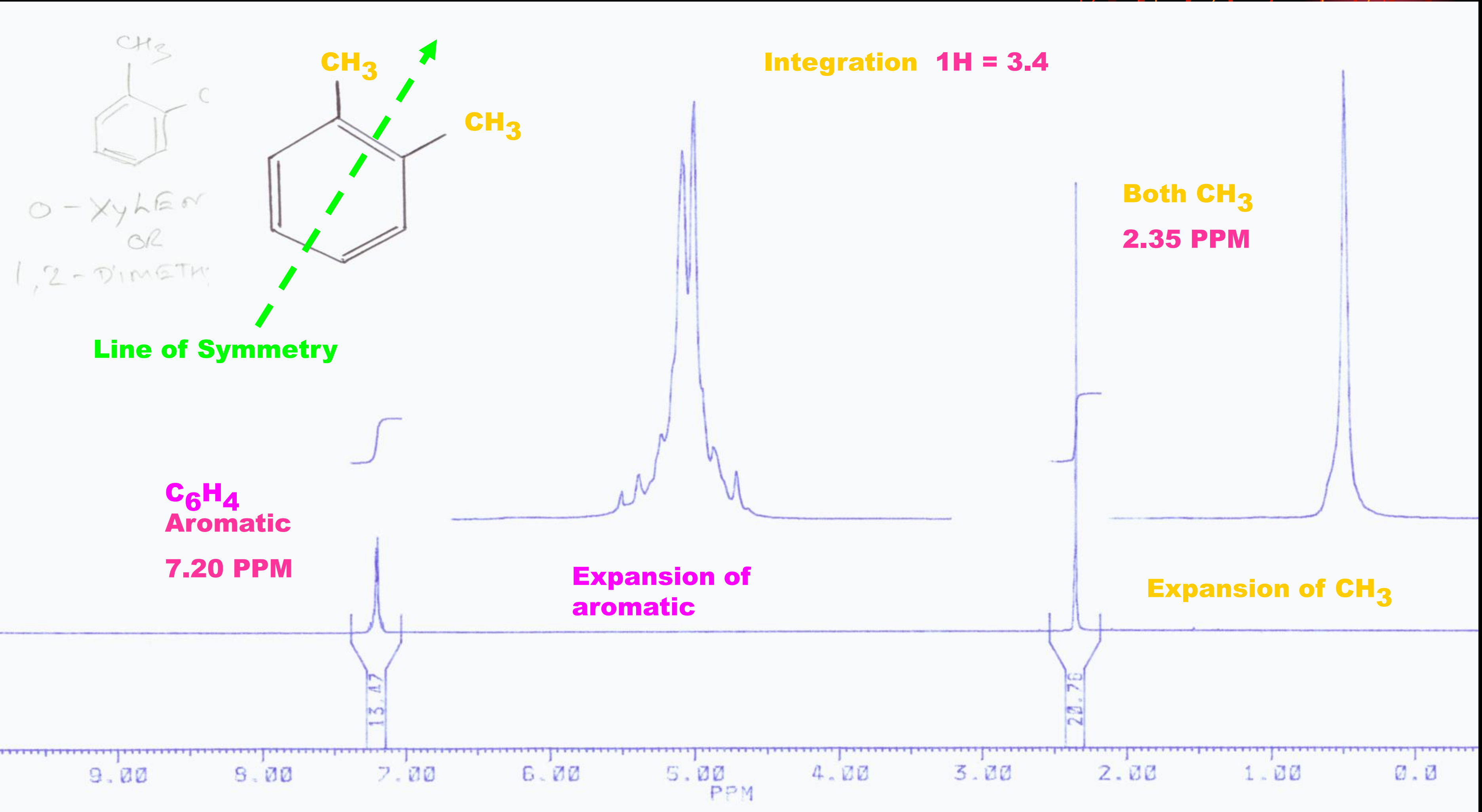
C (3,5)

C (2,6)

C (2,6)	**128.23 PPM**
C (3,5)	**128.86 PPM**
C 4	**133.60 PPM**
C 1	**135.76 PPM**

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,2-Dimethylbenzene (O-Xylene)

C_6H_4-$(CH_3)_2$ ^{1}H NMR Spectrum



CH_3

CH_3

Line of Symmetry

Integration 1H = 3.4

Both CH_3

2.35 PPM

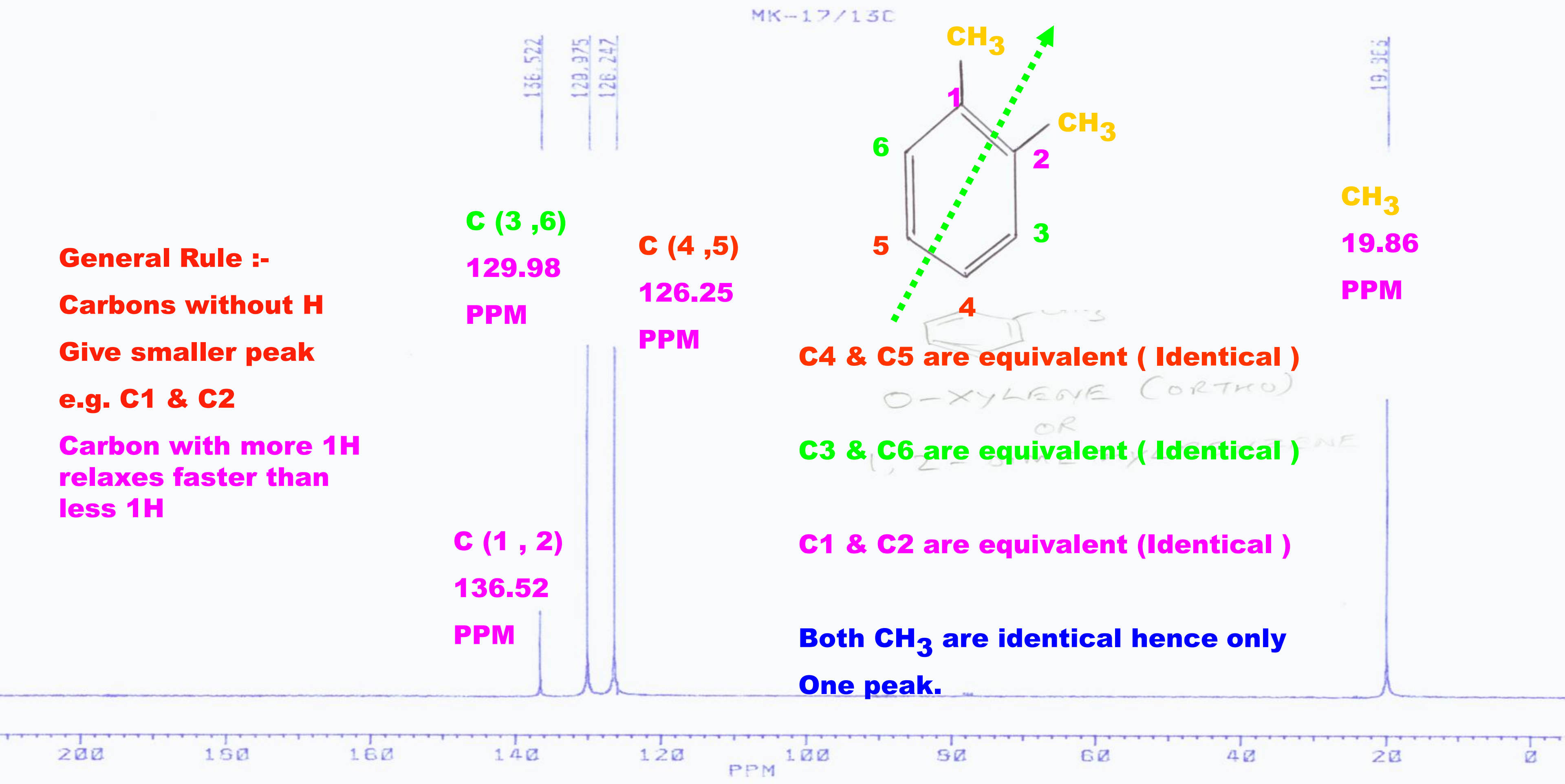
C_6H_4
Aromatic

7.20 PPM

Expansion of aromatic

Expansion of CH_3

^{13}C NMR Spectrum of 1,2-Dimethylbenzene (O-Xylene)



General Rule :-

Carbons without H

Give smaller peak

e.g. C1 & C2

Carbon with more 1H relaxes faster than less 1H

C (3 ,6)

129.98

PPM

C (4 ,5)

126.25

PPM

C (1 , 2)

136.52

PPM

CH_3

19.86

PPM

C4 & C5 are equivalent (Identical)

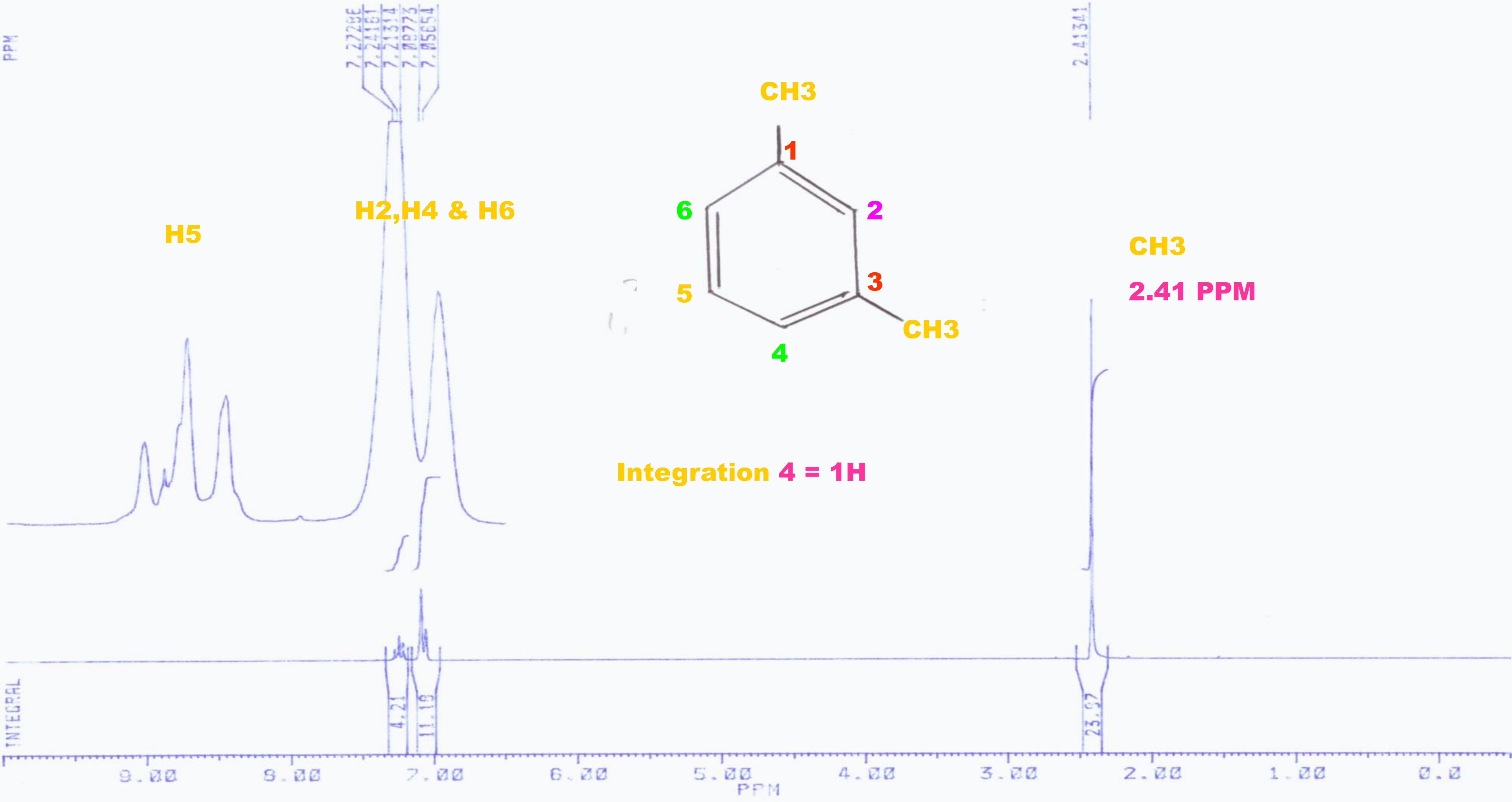
C3 & C6 are equivalent (Identical)

C1 & C2 are equivalent (Identical)

Both CH_3 are identical hence only One peak.

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,3-Dimethylbenzene (m-Xylene)

$C_6H_4\text{-}(CH_3)_2$ ^{1}H NMR Spectrum

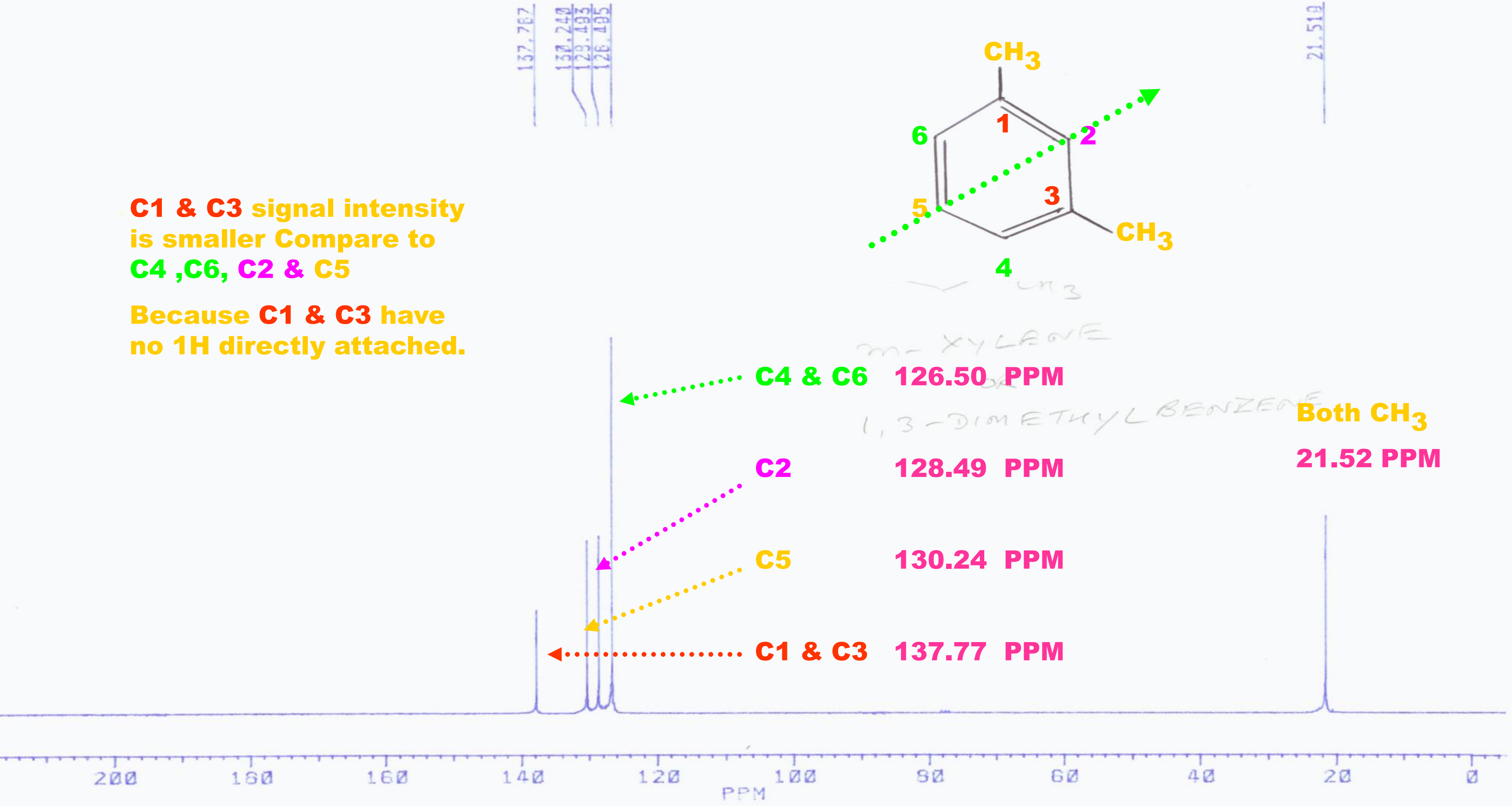


CH3

2.41 PPM

Integration 4 = 1H

^{13}C NMR Spectrum of 1,3-Dimethylbenzene (m-Xylene)



C1 & C3 signal intensity is smaller Compare to **C4 ,C6, C2 & C5**

Because **C1 & C3** have no 1H directly attached.

C4 & C6	126.50 PPM
C2	128.49 PPM
C5	130.24 PPM
C1 & C3	137.77 PPM

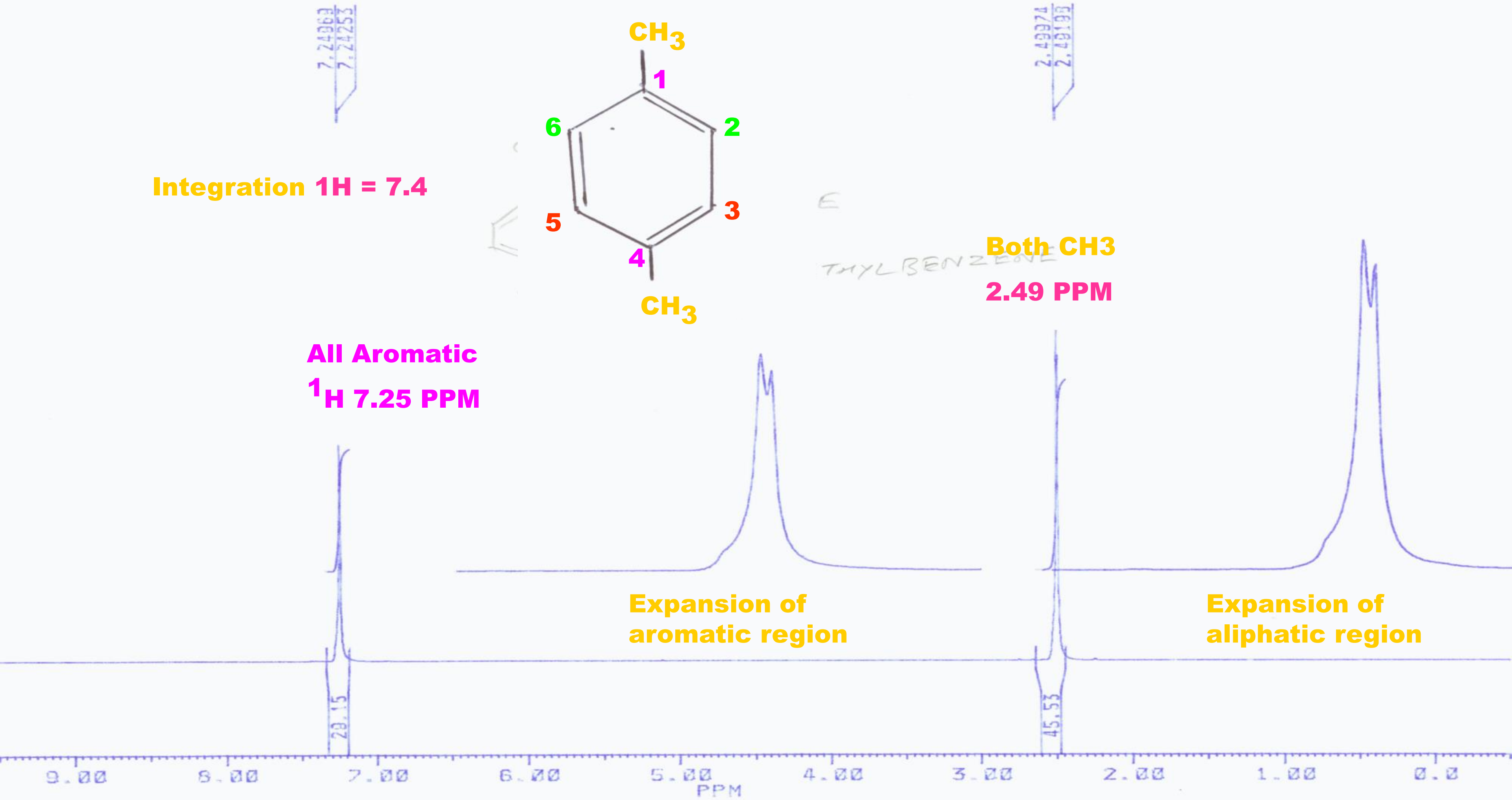
Both CH$_3$

21.52 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,3-Dimethylbenzene (p-Xylene)

C_6H_4-$(CH_3)_2$

^{1}H NMR Spectrum



Integration 1H = 7.4

All Aromatic ^{1}H 7.25 PPM

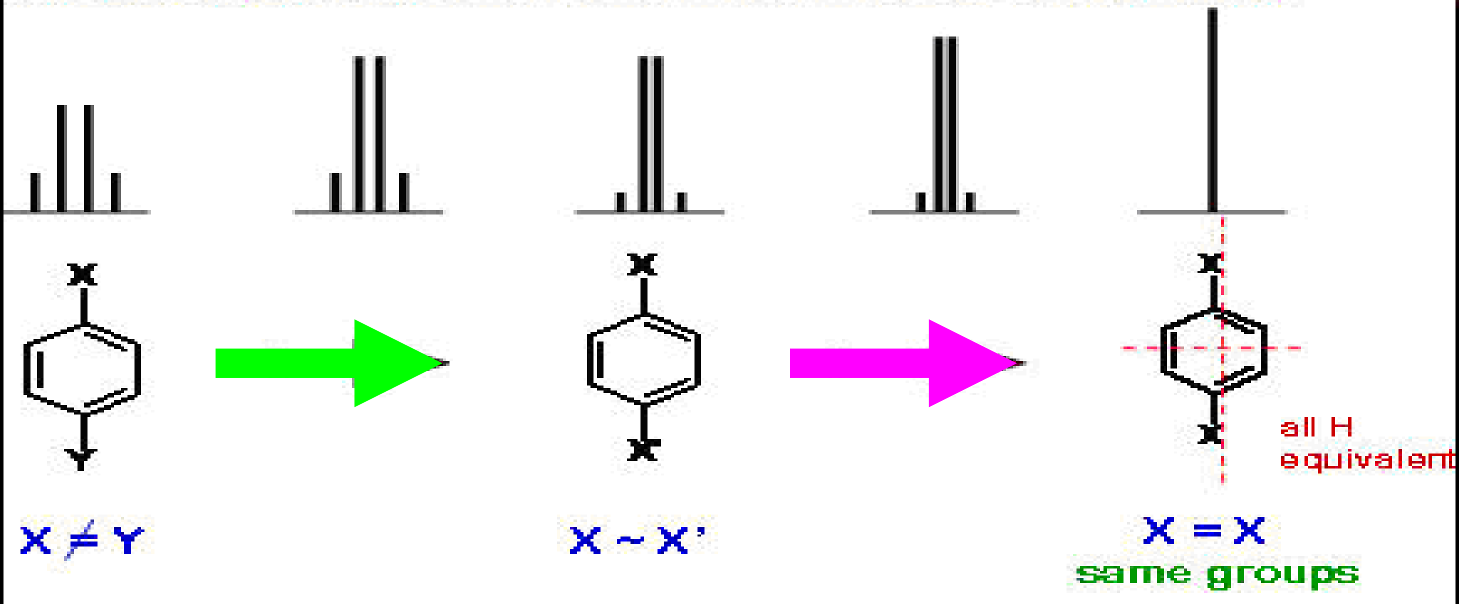
Both CH3 2.49 PPM

Expansion of aromatic region

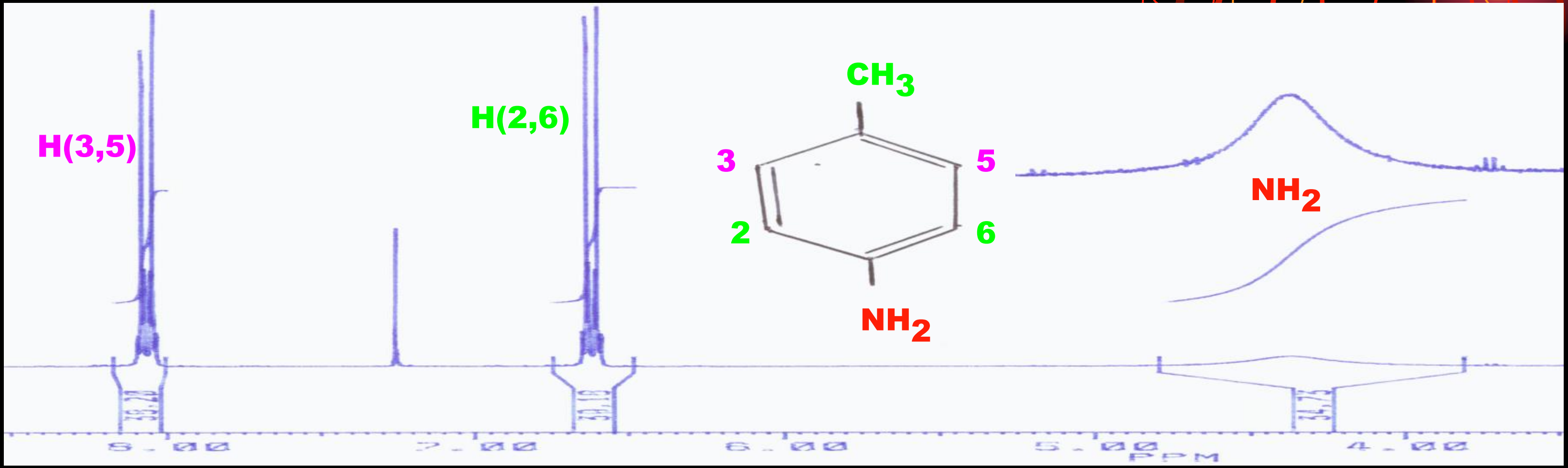
Expansion of aliphatic region

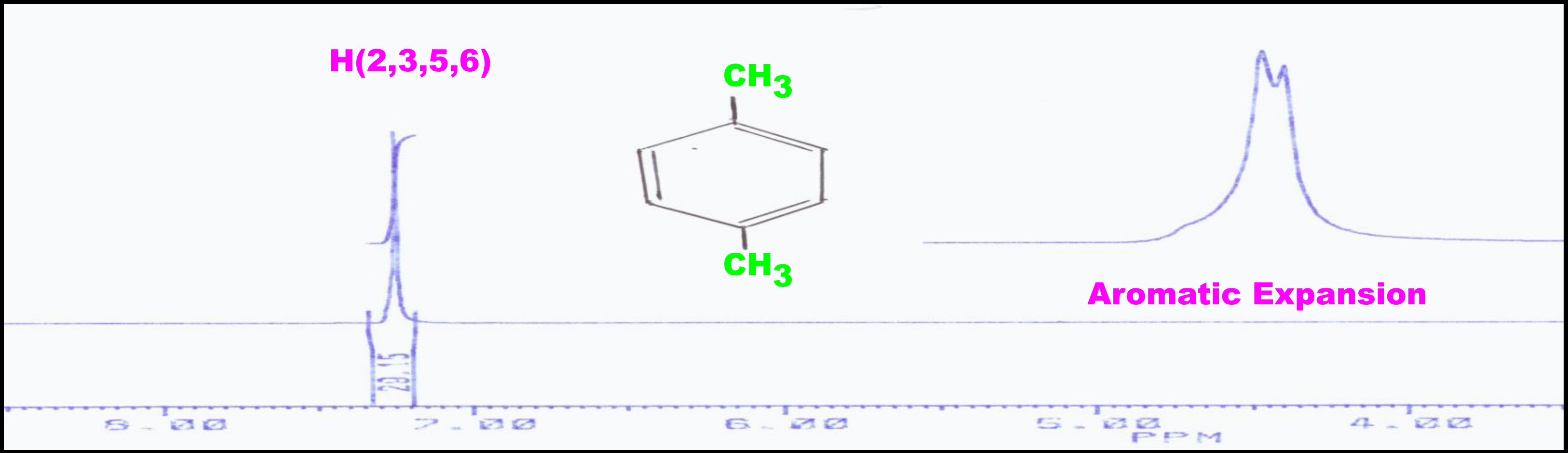
^{1}H NMR Patter of Para Disubstituted Benzene

- When two groups X & Y become more similar then
- All NMR Peaks move closer hence
- Outer peaks get smaller and finally disappear but
- Inner peaks get taller and finally merge into single peak.

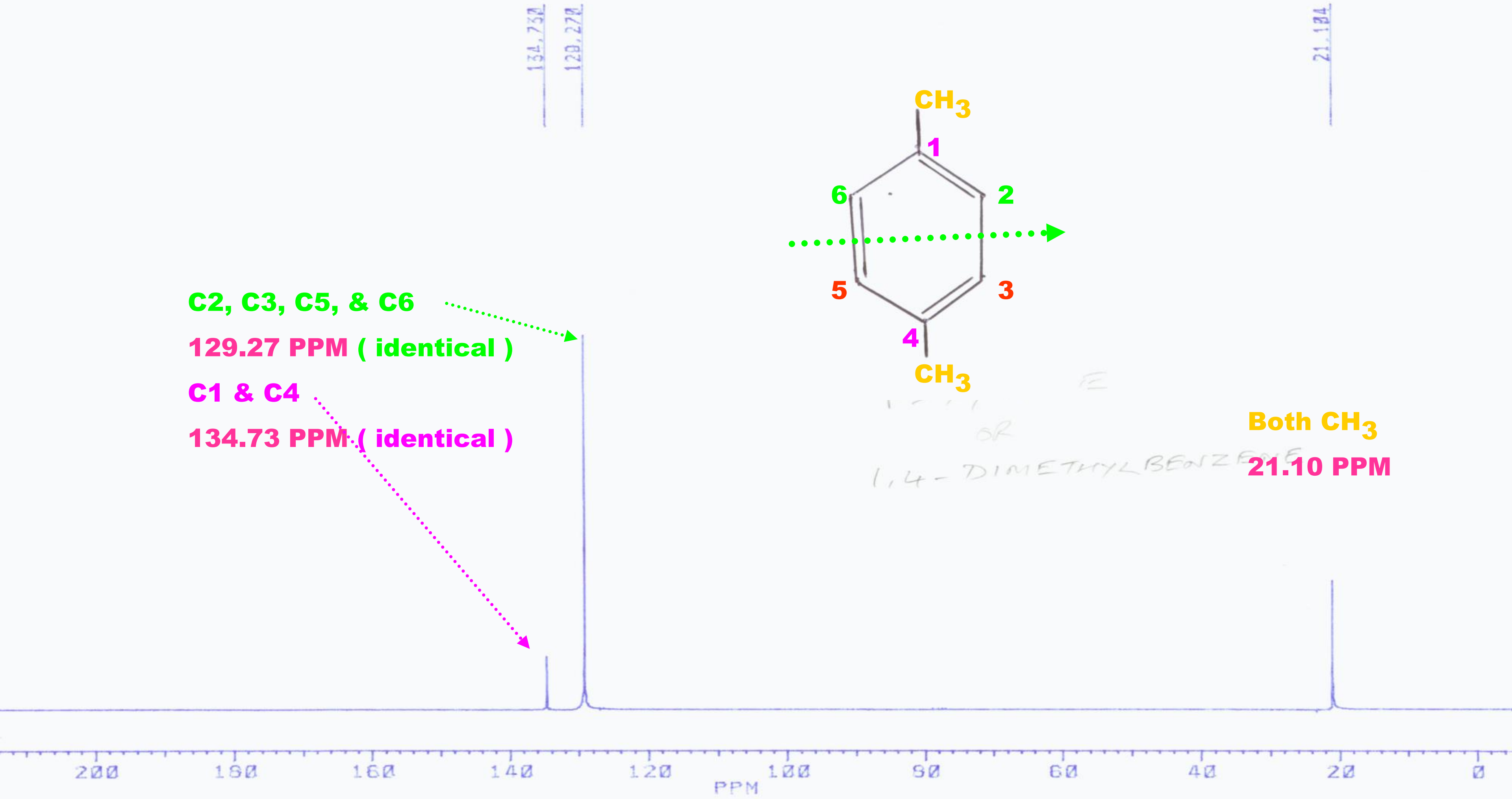


^{1}H NMR Spectra of 4-Methyl Aniline and p-Xylene only 8.5 to 4.5 PPM Region shown





^{13}C NMR Spectrum of 1,4-Dimethylbenzene (p-Xylene)



C2, C3, C5, & C6

129.27 PPM (identical)

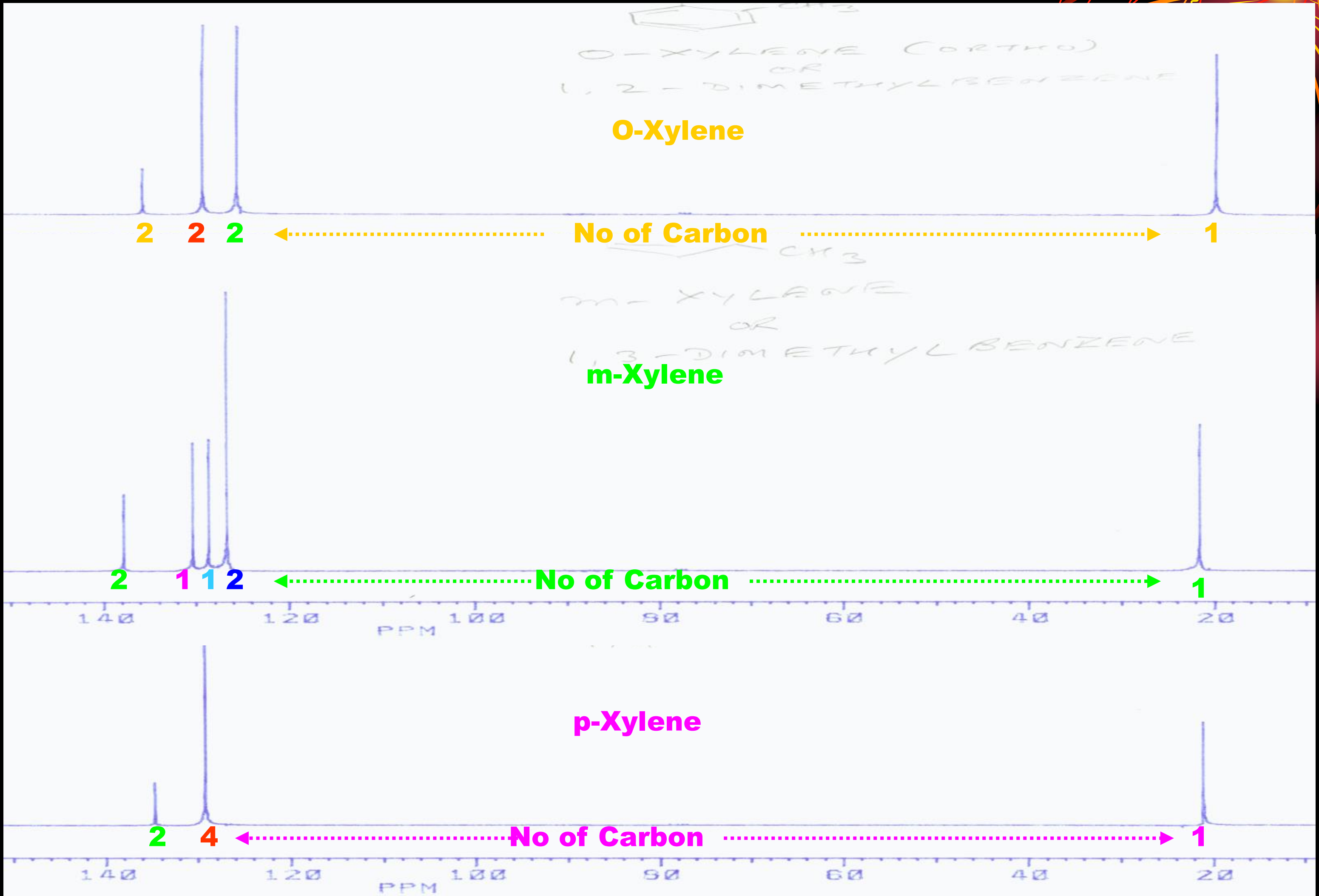
C1 & C4

134.73 PPM (identical)

Both CH_3

21.10 PPM

O, M, & P- Xylene ^{13}C NMR Spectra



O-Xylene

2 2 2 ← No of Carbon → 1

m-Xylene

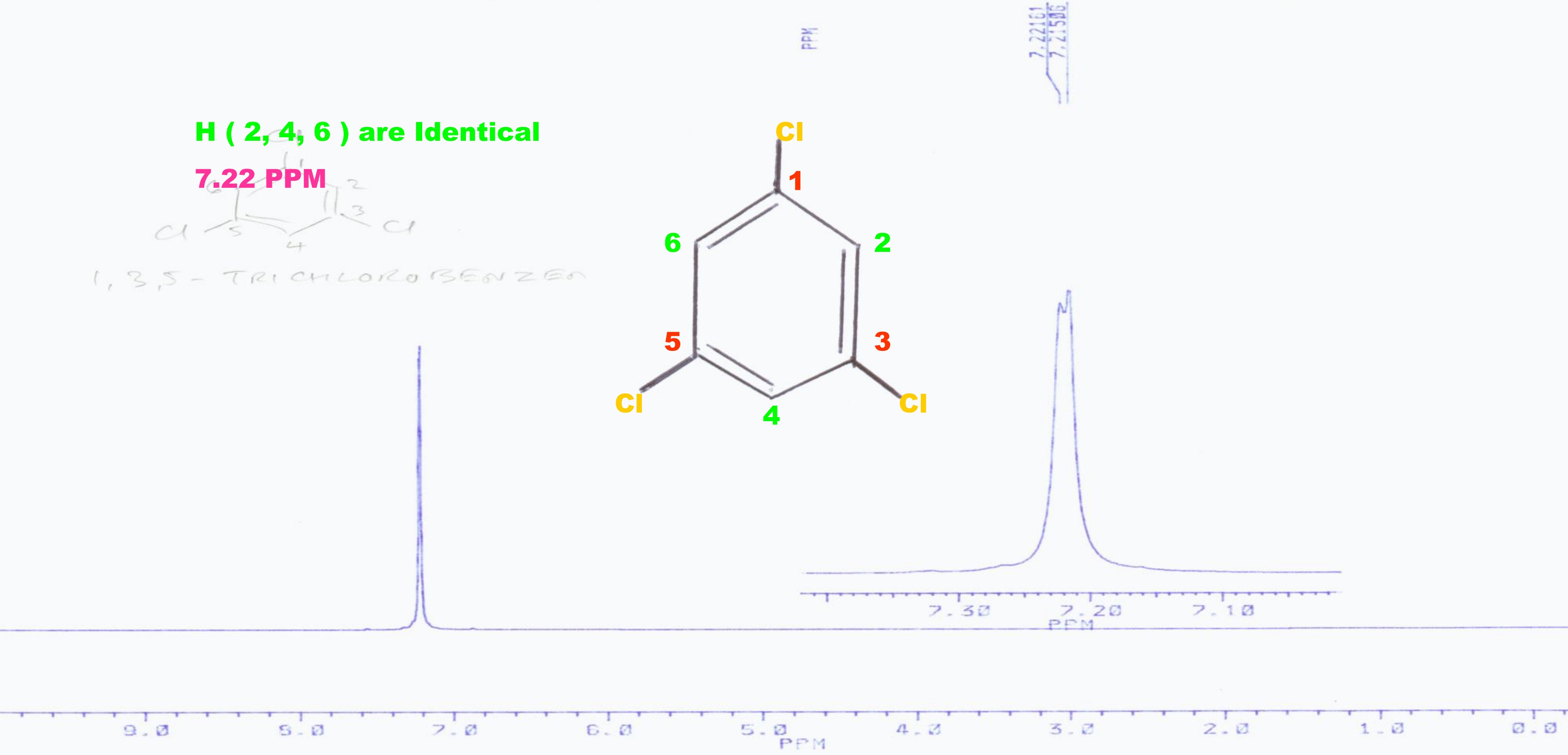
2 1 1 2 ← No of Carbon → 1

p-Xylene

2 4 ← No of Carbon → 1

Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,3,5-Trichlorobenzene

$C_6H_3Cl_3$ ^1H NMR Spectrum

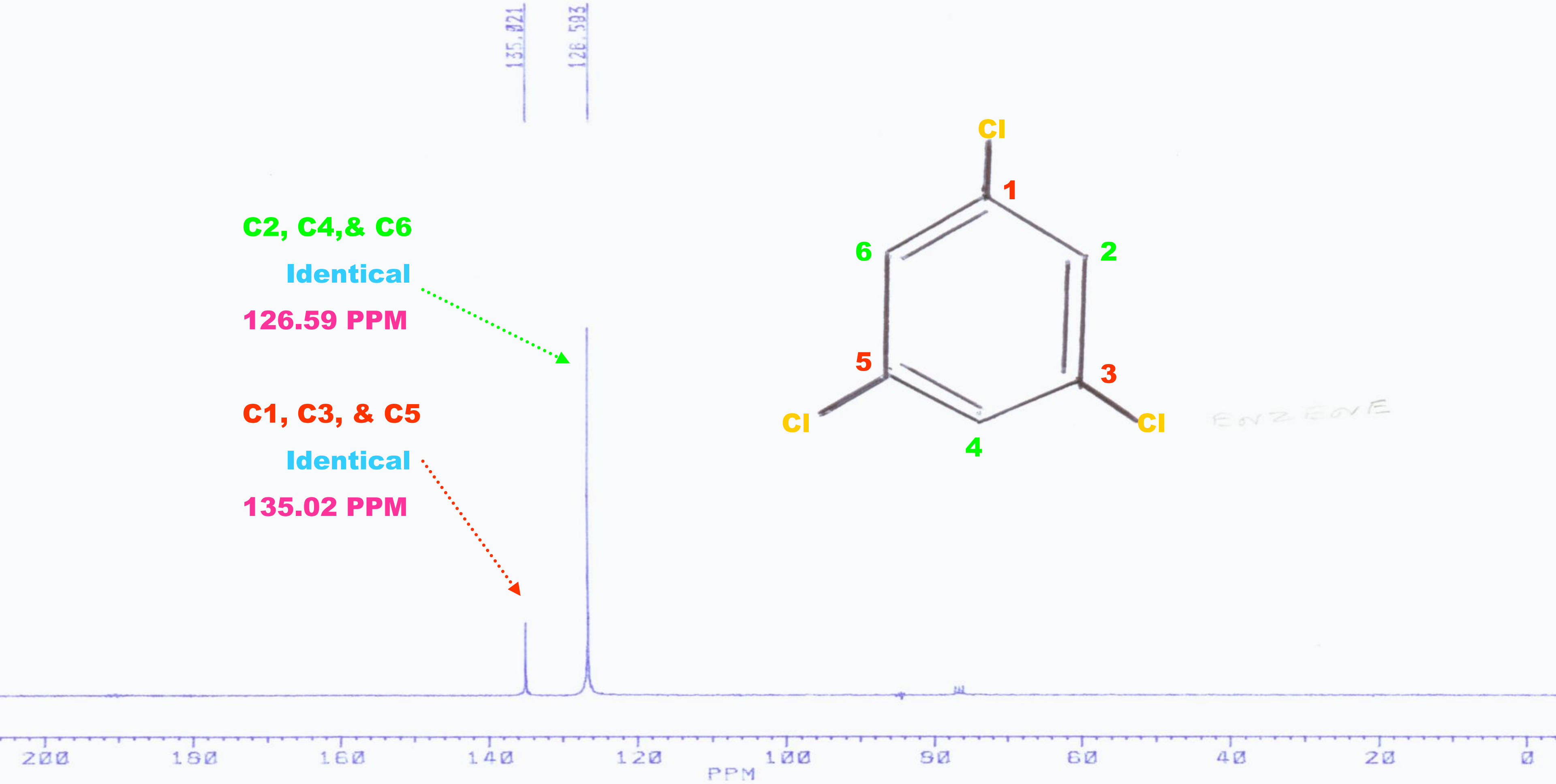


H (2, 4, 6) are Identical

7.22 PPM

^{13}C NMR Spectrum 1,3,5-Trichlorobenzene

$C_6H_3Cl_3$



C2, C4,& C6

Identical

126.59 PPM

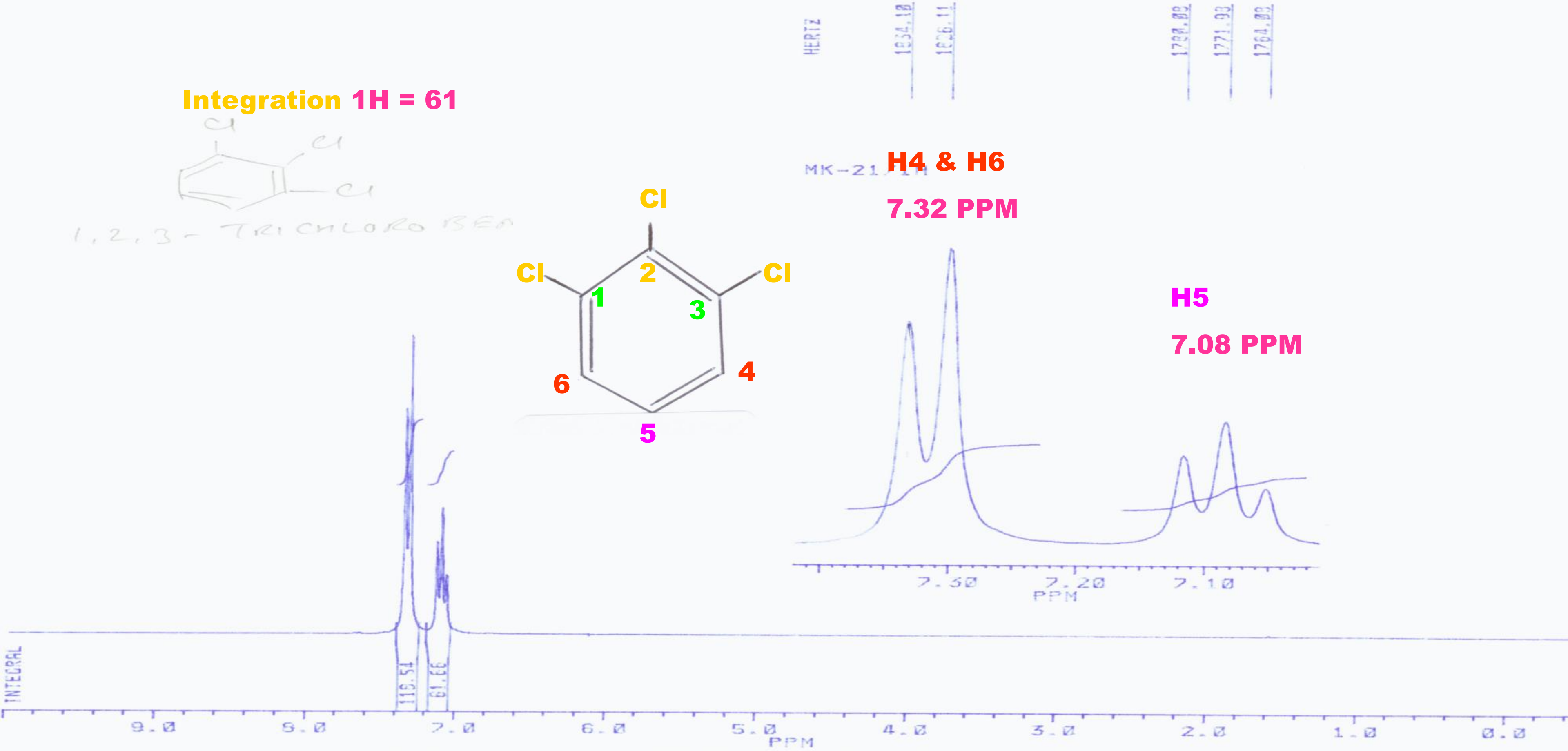
C1, C3, & C5

Identical

135.02 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,2,3-Trichlorobenzene

$C_6H_3Cl_3$ ^{1}H NMR Spectrum


Integration 1H = 61

H4 & H6

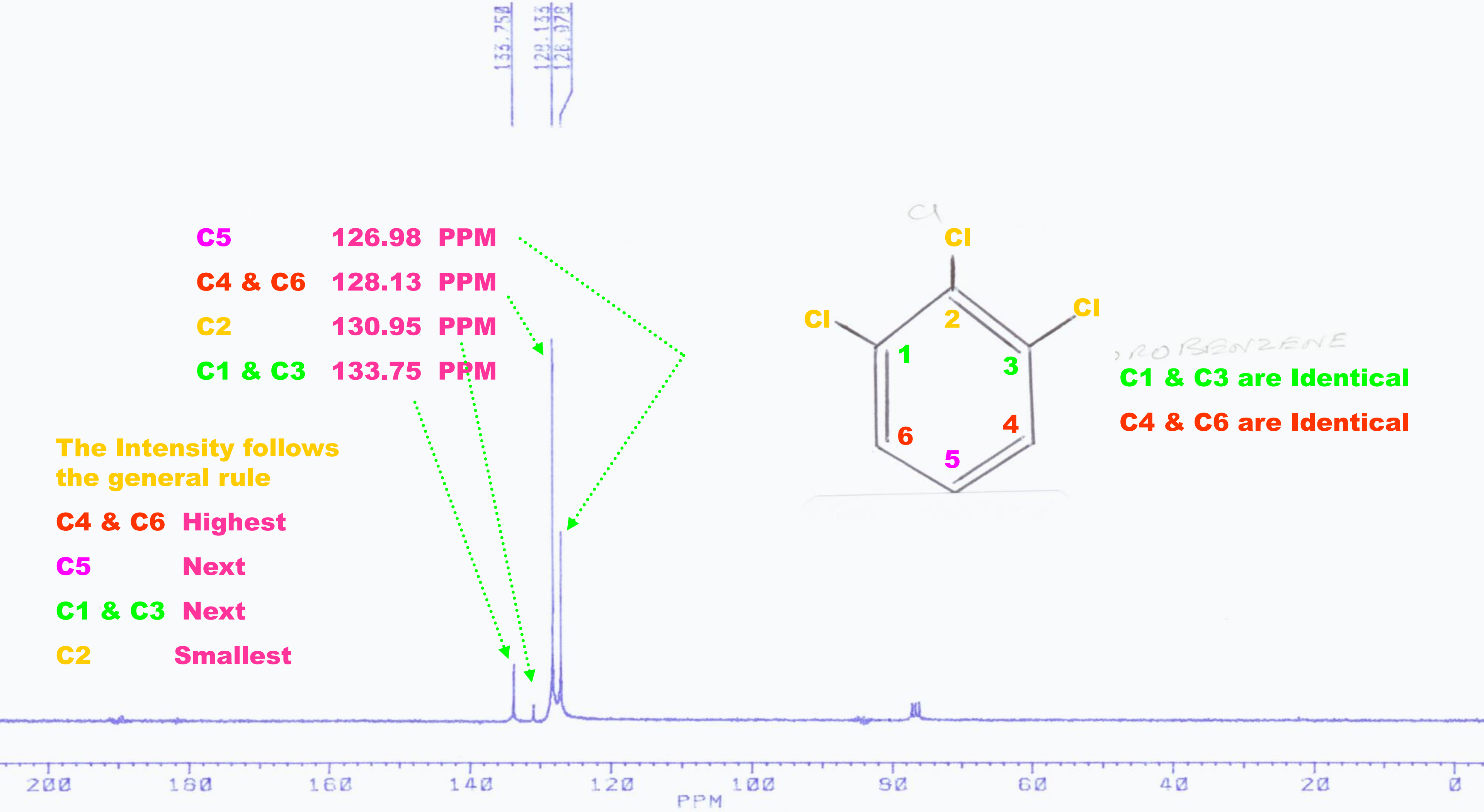
7.32 PPM

H5

7.08 PPM

^{13}C NMR Spectrum 1,2,3-Trichlorobenzene

$C_6H_3Cl_3$



C5	126.98 PPM
C4 & C6	128.13 PPM
C2	130.95 PPM
C1 & C3	133.75 PPM

C1 & C3 are Identical

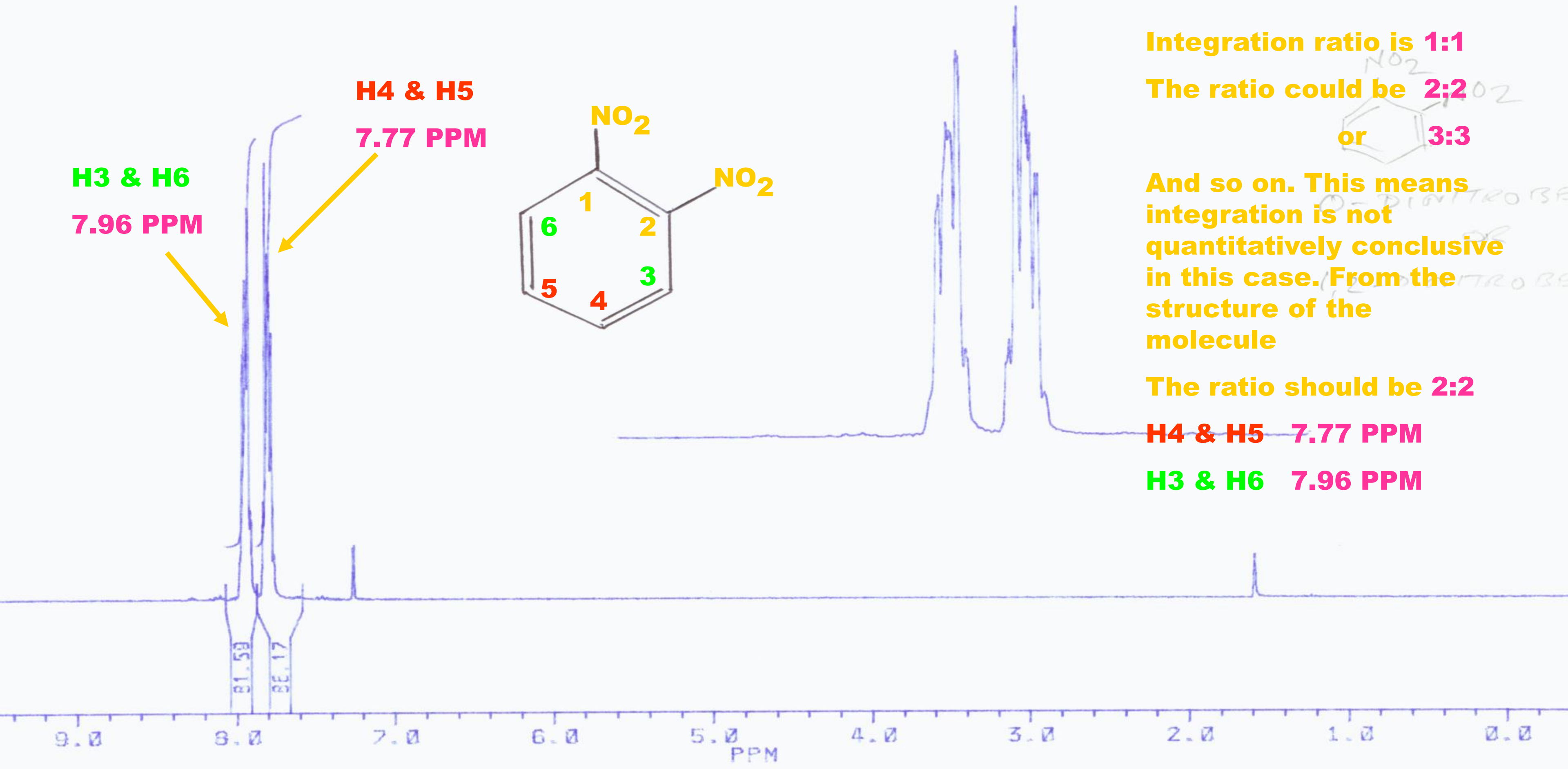
C4 & C6 are Identical

The Intensity follows the general rule

C4 & C6	Highest
C5	Next
C1 & C3	Next
C2	Smallest

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,2-Dinitrobenzene

$C_6H_4(NO_2)_2$ ^{1}H NMR Spectrum



Integration ratio is 1:1

The ratio could be 2:2

or 3:3

And so on. This means integration is not quantitatively conclusive in this case. From the structure of the molecule

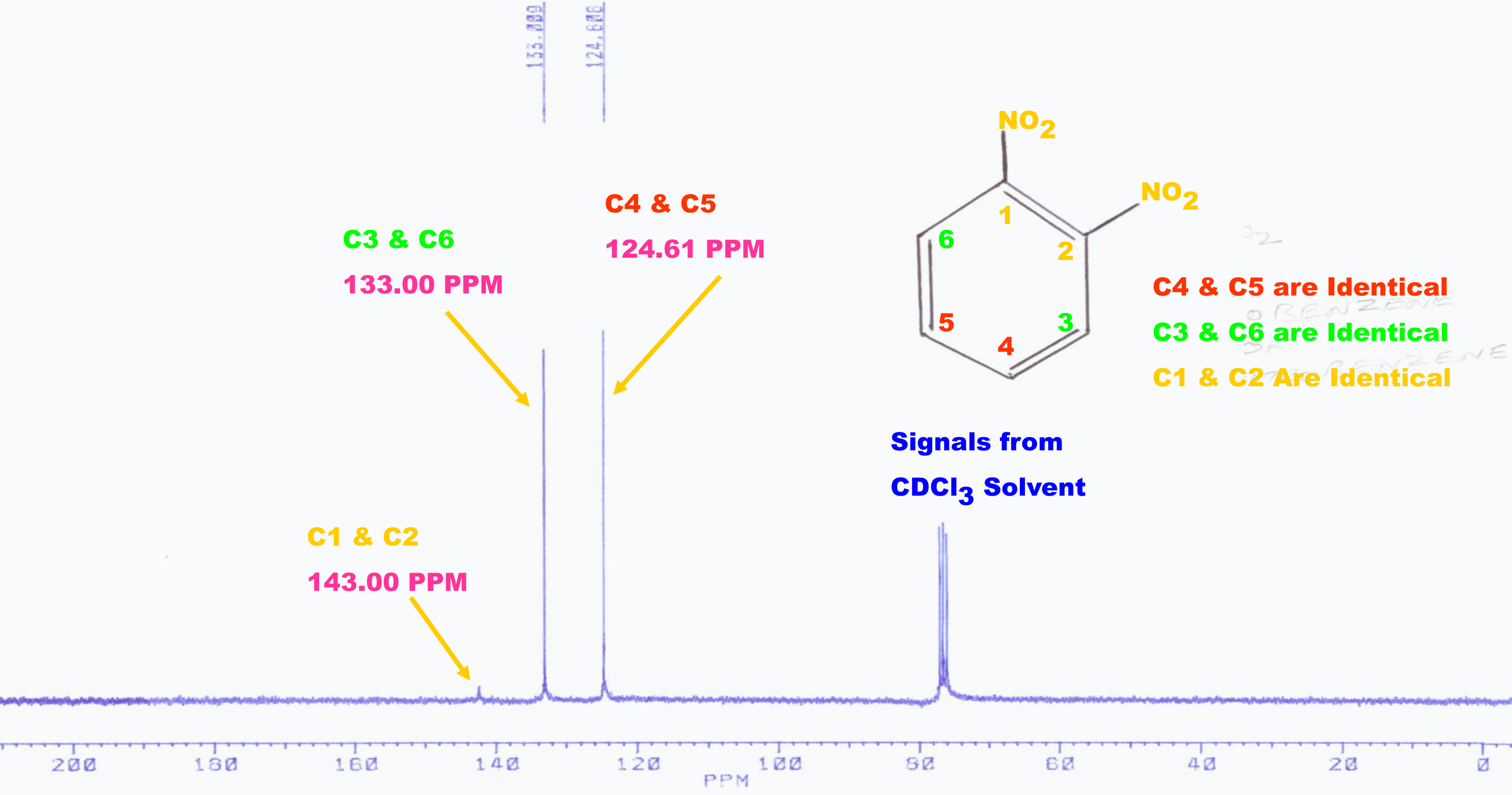
The ratio should be 2:2

H4 & H5 7.77 PPM

H3 & H6 7.96 PPM

^{13}C NMR Spectrum of 1,2-Dinitrobenzene

$C_6H_4(NO_2)_2$



C3 & C6

133.00 PPM

C4 & C5

124.61 PPM

C1 & C2

143.00 PPM

Signals from

$CDCl_3$ Solvent

C4 & C5 are Identical

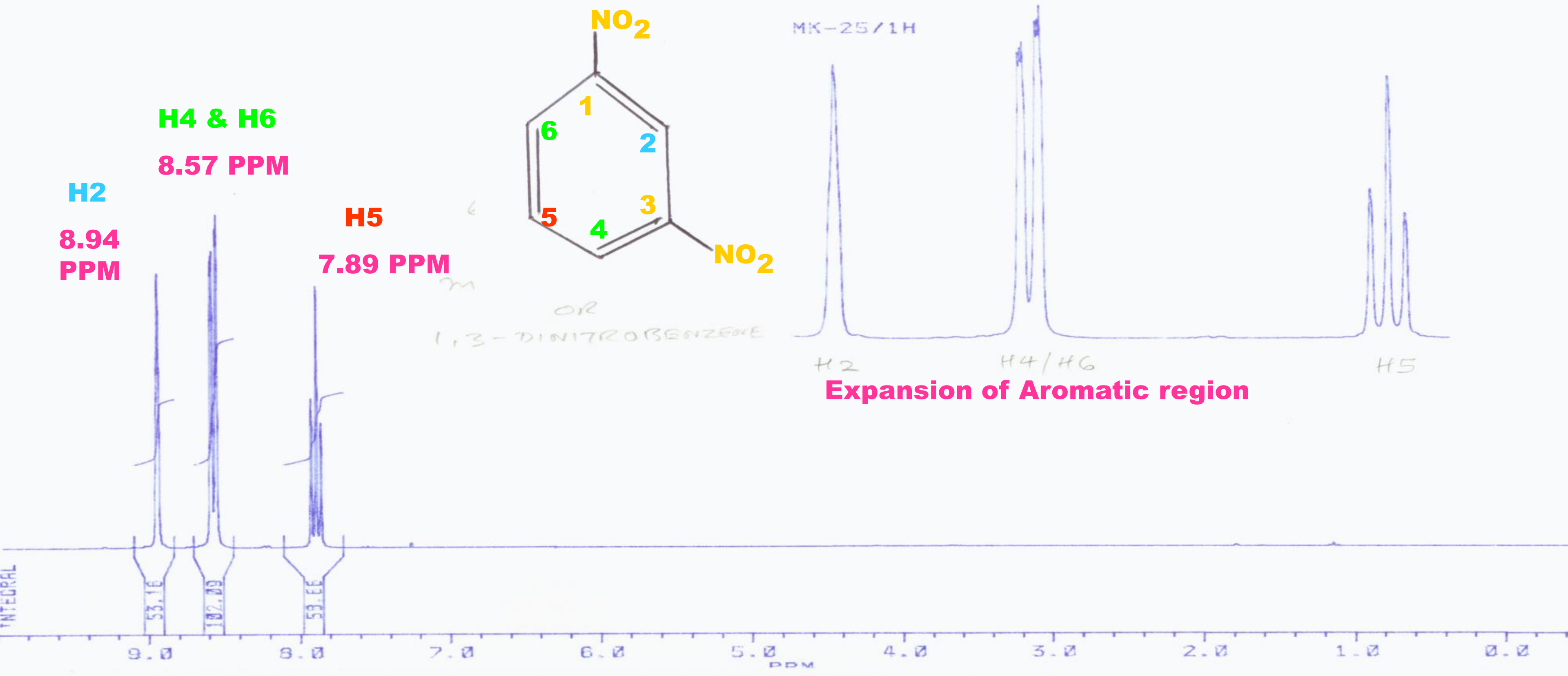
C3 & C6 are Identical

C1 & C2 Are Identical

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,3-Dinitrobenzene

$C_6H_4(NO_2)_2$ ^{1}H NMR Spectrum

Integration 1H = 54



H4 & H6

8.57 PPM

H2

8.94 PPM

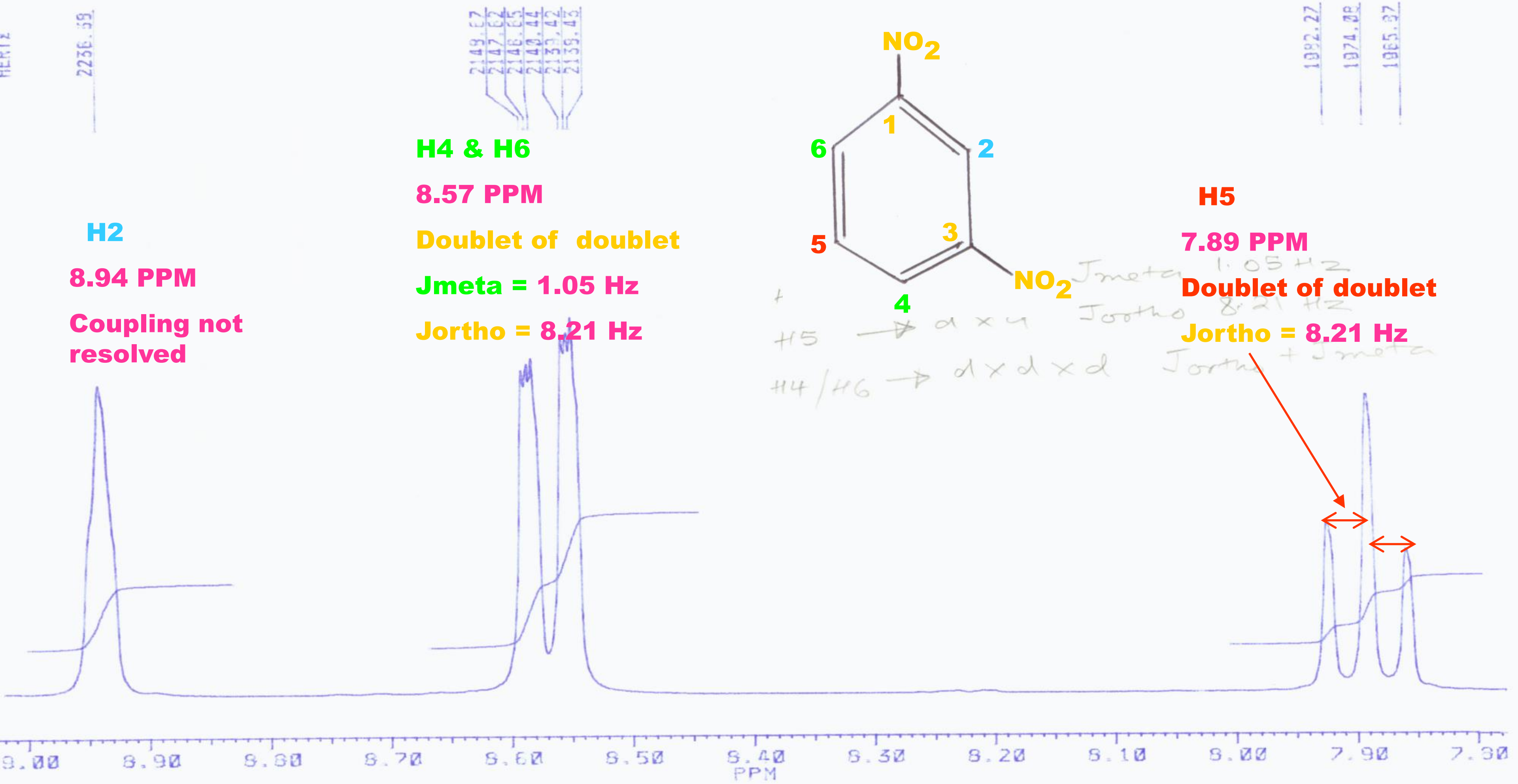
H5

7.89 PPM

Expansion of Aromatic region

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 1,3-Dinitrobenzene

$C_6H_4(NO_2)_2$ ^{1}H NMR Spectrum



H2

8.94 PPM

Coupling not resolved

H4 & H6

8.57 PPM

Doublet of doublet

Jmeta = 1.05 Hz

Jortho = 8.21 Hz

H5

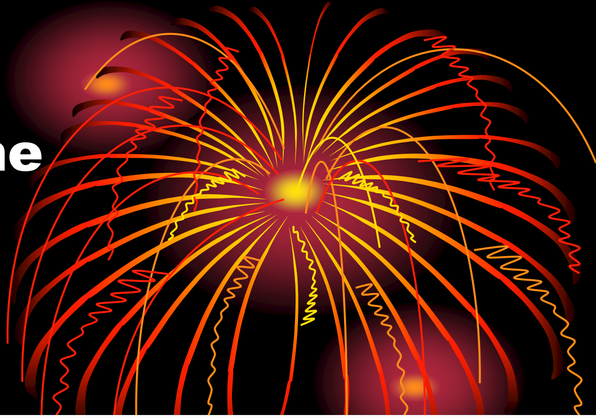
7.89 PPM

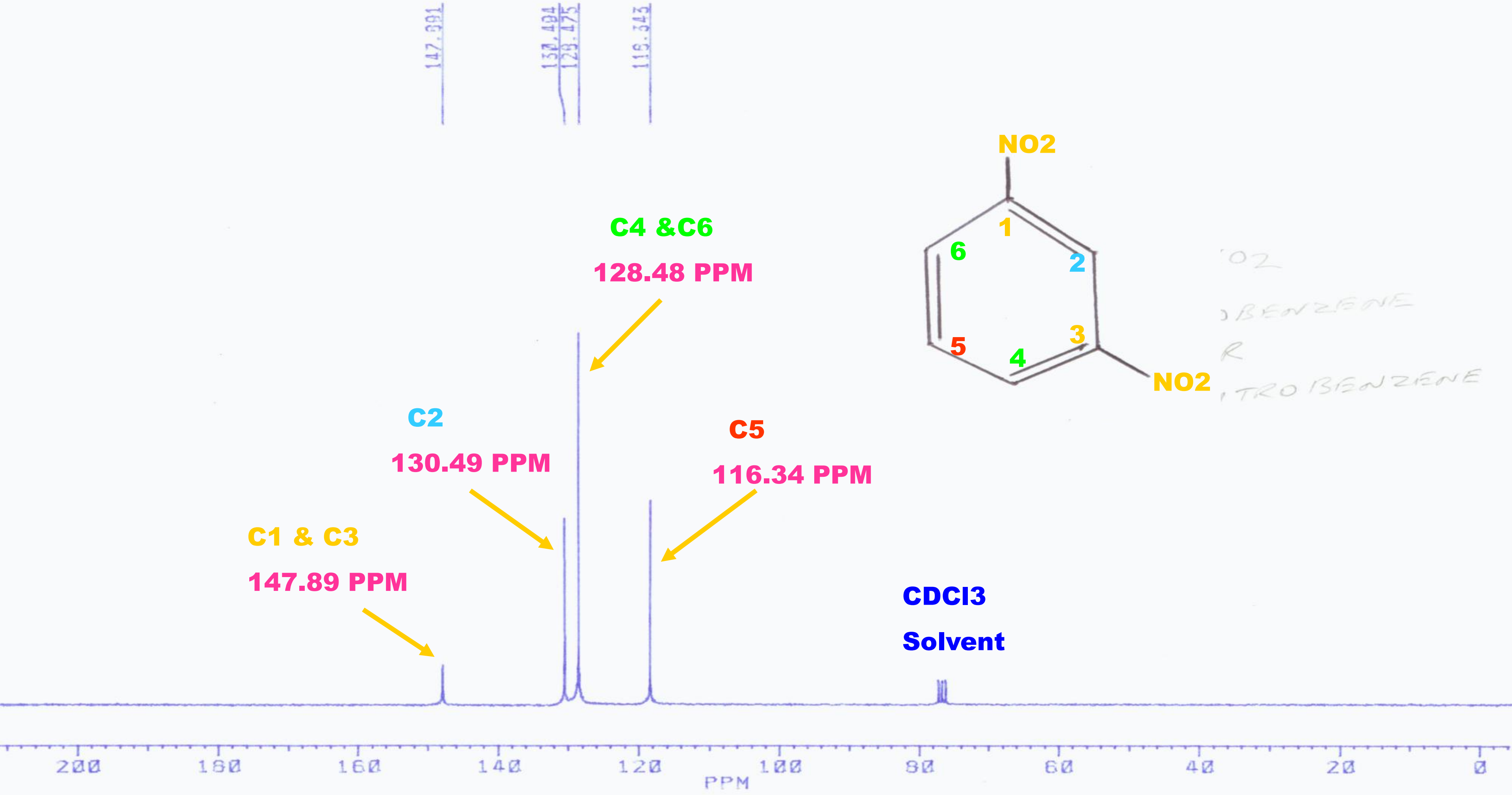
Doublet of doublet

Jortho = 8.21 Hz

^{13}C NMR Spectrum of 1,3-Dinitrobenzene

$C_6H_4(NO_2)_2$





C4 &C6

128.48 PPM

C2

130.49 PPM

C5

116.34 PPM

C1 & C3

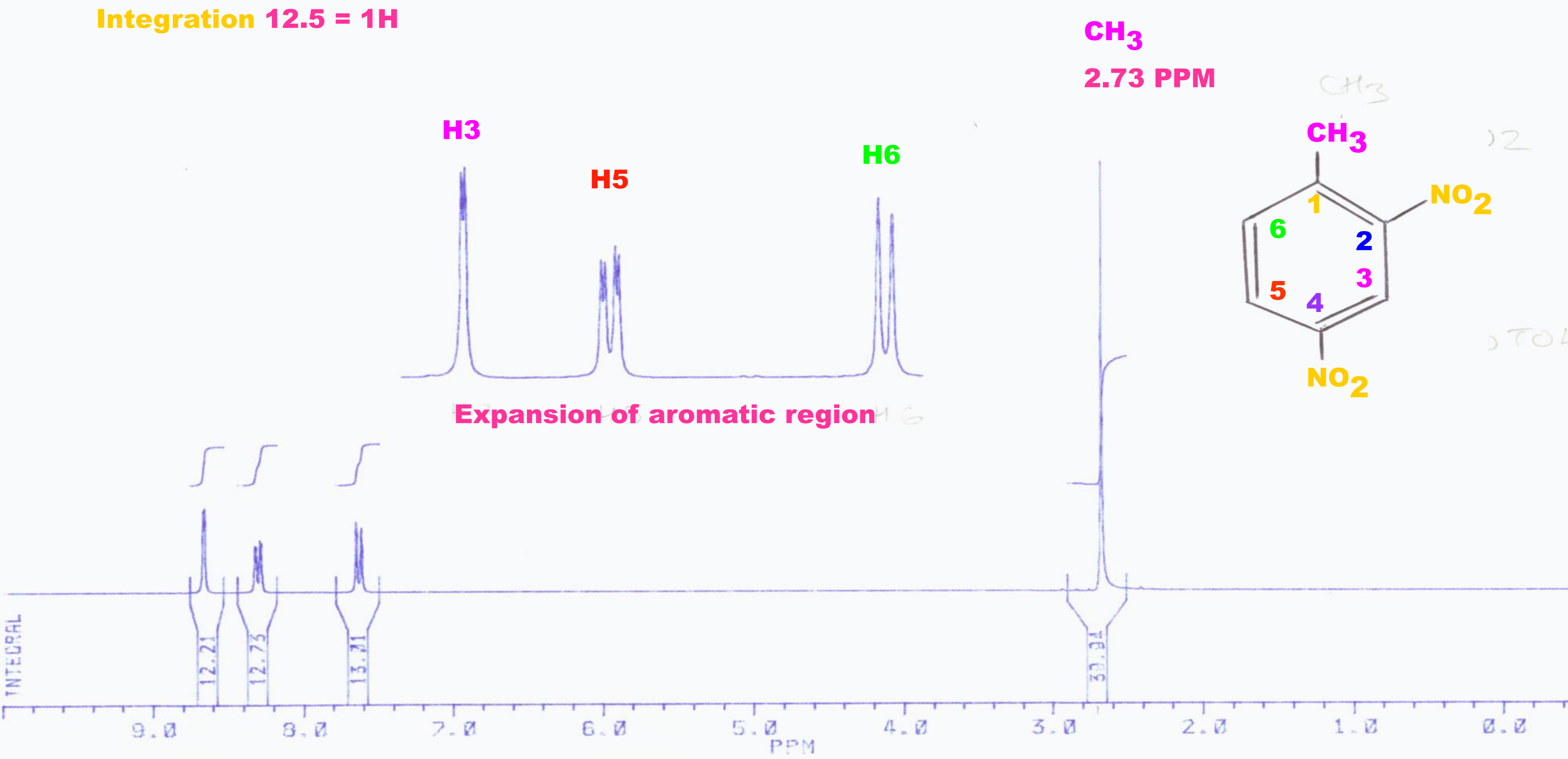
147.89 PPM

CDCl3

Solvent

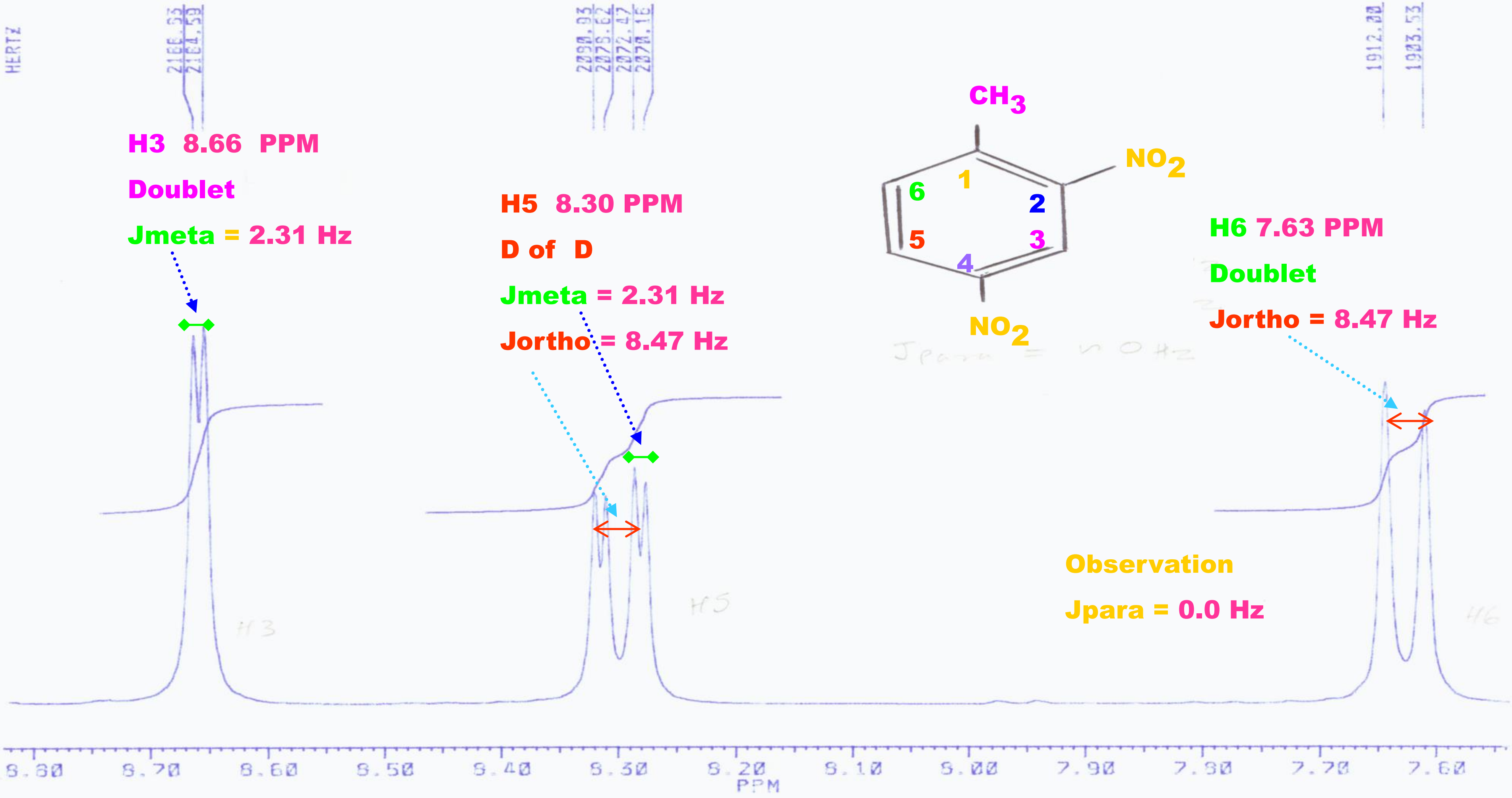
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

$C_6H_3CH_3(NO_2)_2$ ^1H NMR Spectrum



Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

$C_6H_3CH_3(NO_2)_2$ ^{1}H NMR Spectrum



H3 8.66 PPM

Doublet

Jmeta = 2.31 Hz

H5 8.30 PPM

D of D

Jmeta = 2.31 Hz

Jortho = 8.47 Hz

H6 7.63 PPM

Doublet

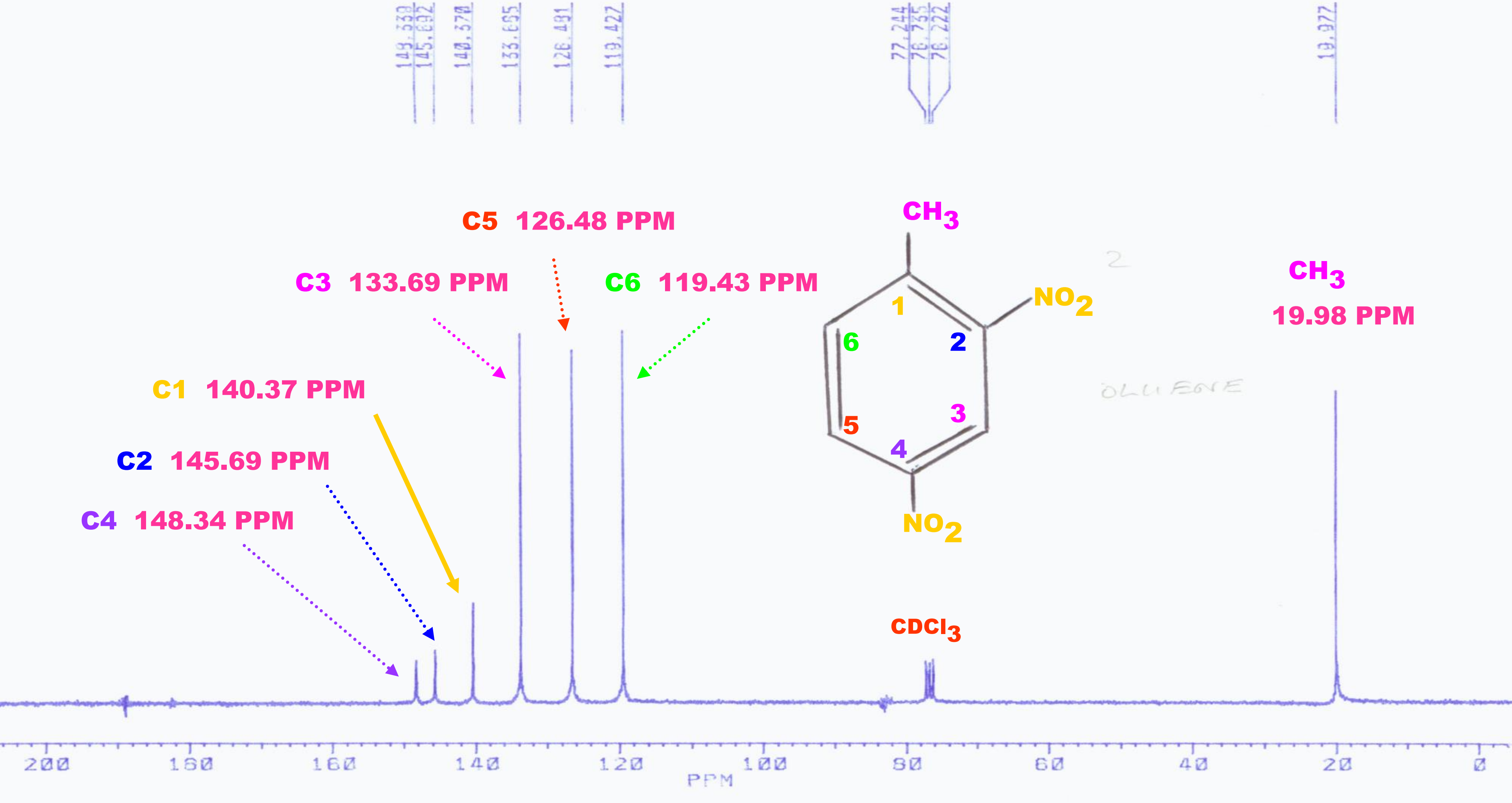
Jortho = 8.47 Hz

Observation

Jpara = 0.0 Hz

^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

$C_6H_3CH_3(NO_2)_2$



C5 126.48 PPM

C3 133.69 PPM

C6 119.43 PPM

C1 140.37 PPM

C2 145.69 PPM

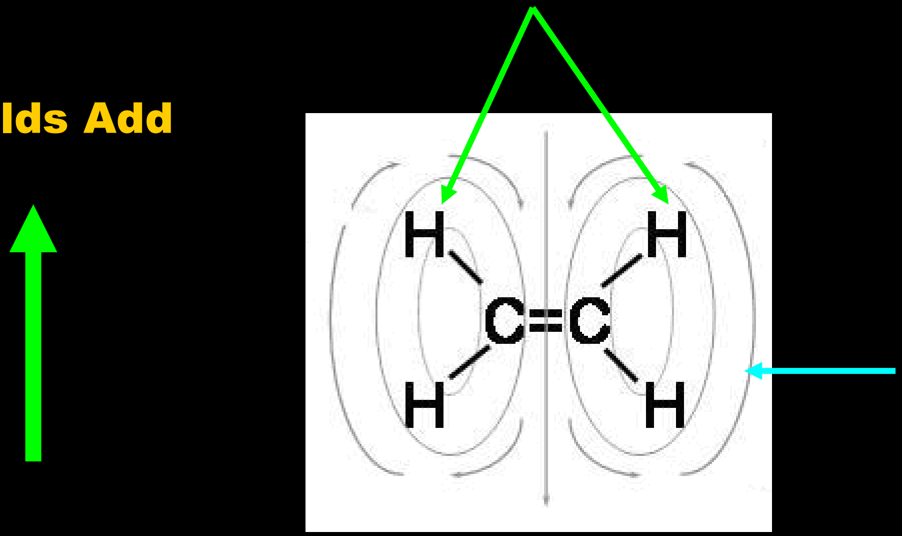
C4 148.34 PPM

CH_3
19.98 PPM

$CDCl_3$

Anisotropic Field in an Alkenes (SP^2)

Anisotropic Field Effect



Deshielded ^1H

Shift To Lower Field

Fields Add

Secondary Magnetic

Field Lines Induce

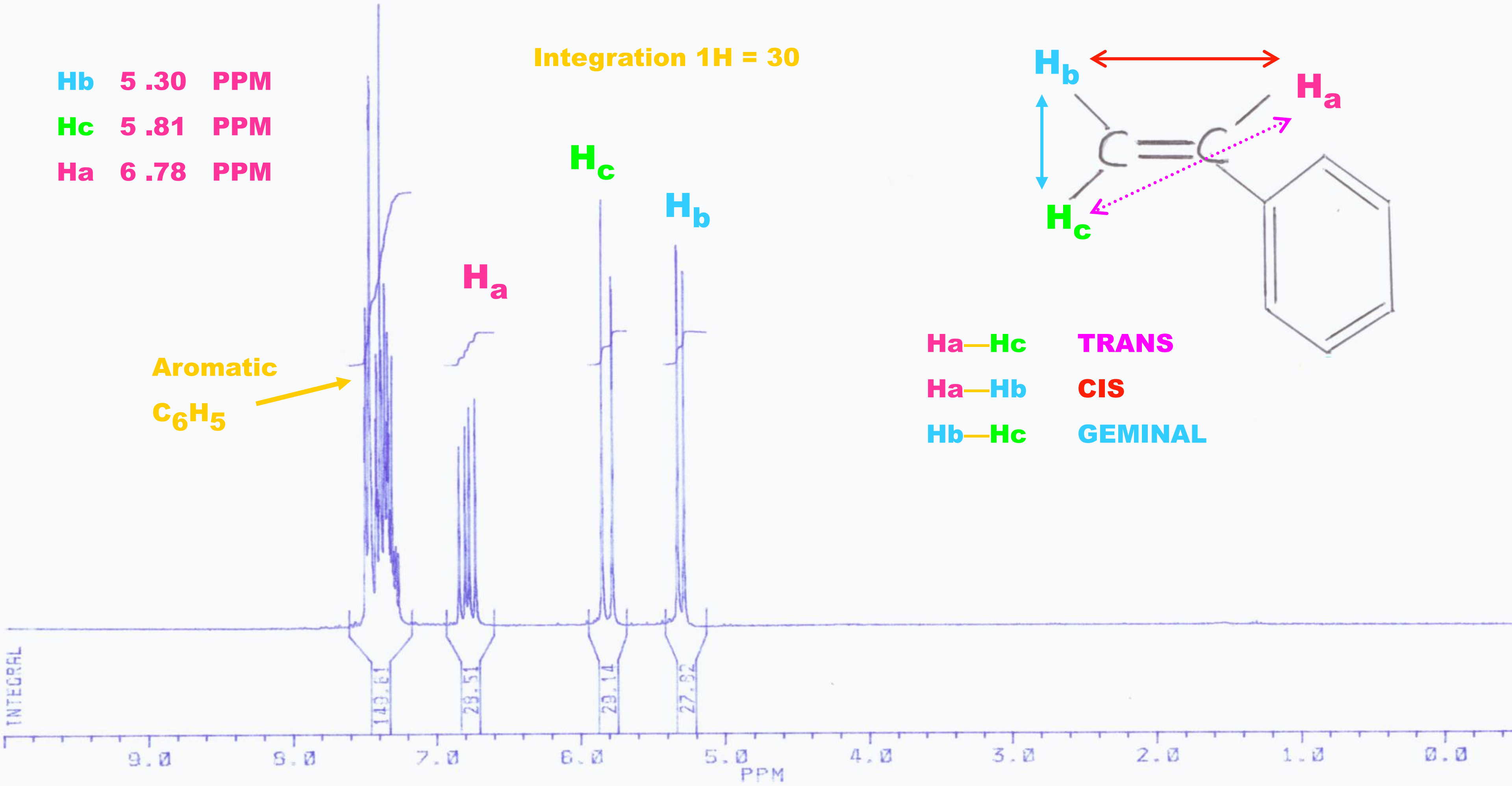
Anisotropic Field

H_0

Applied Field

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Styrene

C_6H_5-CH=CH_2 ^{1}H NMR Spectrum



Integration 1H = 30

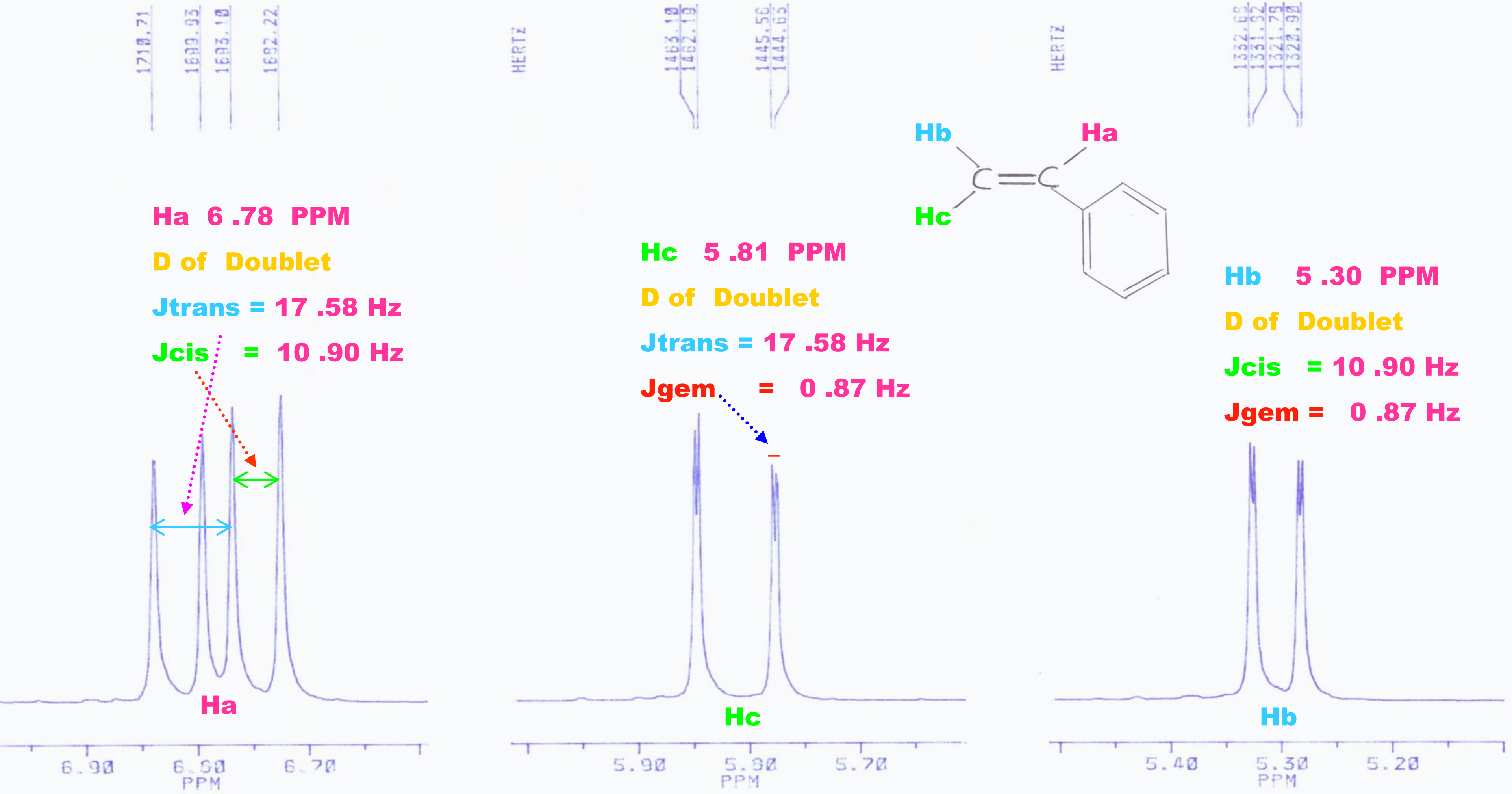
Hb	5 .30	PPM
Hc	5 .81	PPM
Ha	6 .78	PPM

Aromatic C_6H_5

Ha—Hc	TRANS
Ha—Hb	CIS
Hb—Hc	GEMINAL

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Styrene

C_6H_5-CH=CH_2 ^{1}H NMR Spectrum



Ha 6.78 PPM

D of Doublet

Jtrans = 17.58 Hz

Jcis = 10.90 Hz

Hc 5.81 PPM

D of Doublet

Jtrans = 17.58 Hz

Jgem = 0.87 Hz

Hb 5.30 PPM

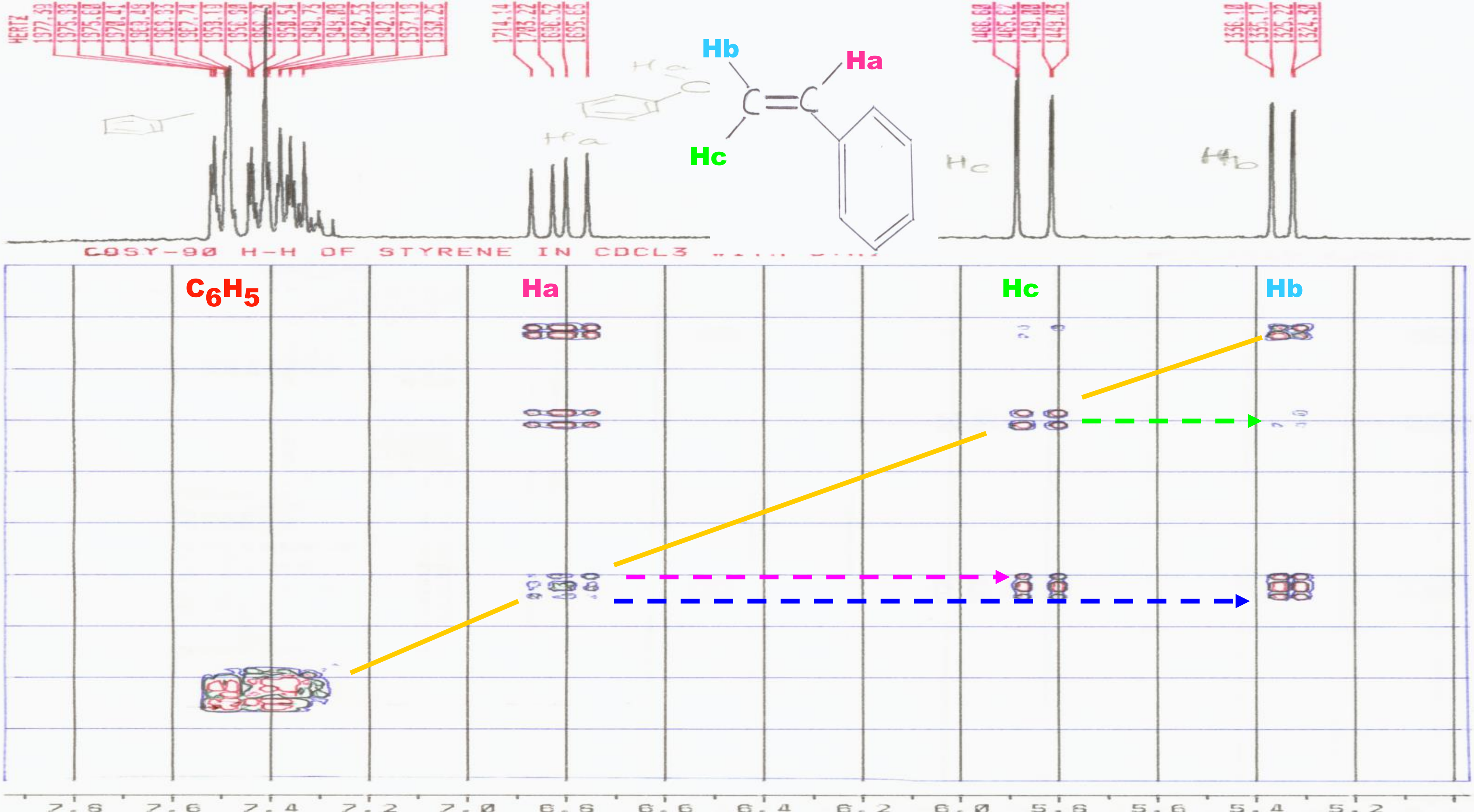
D of Doublet

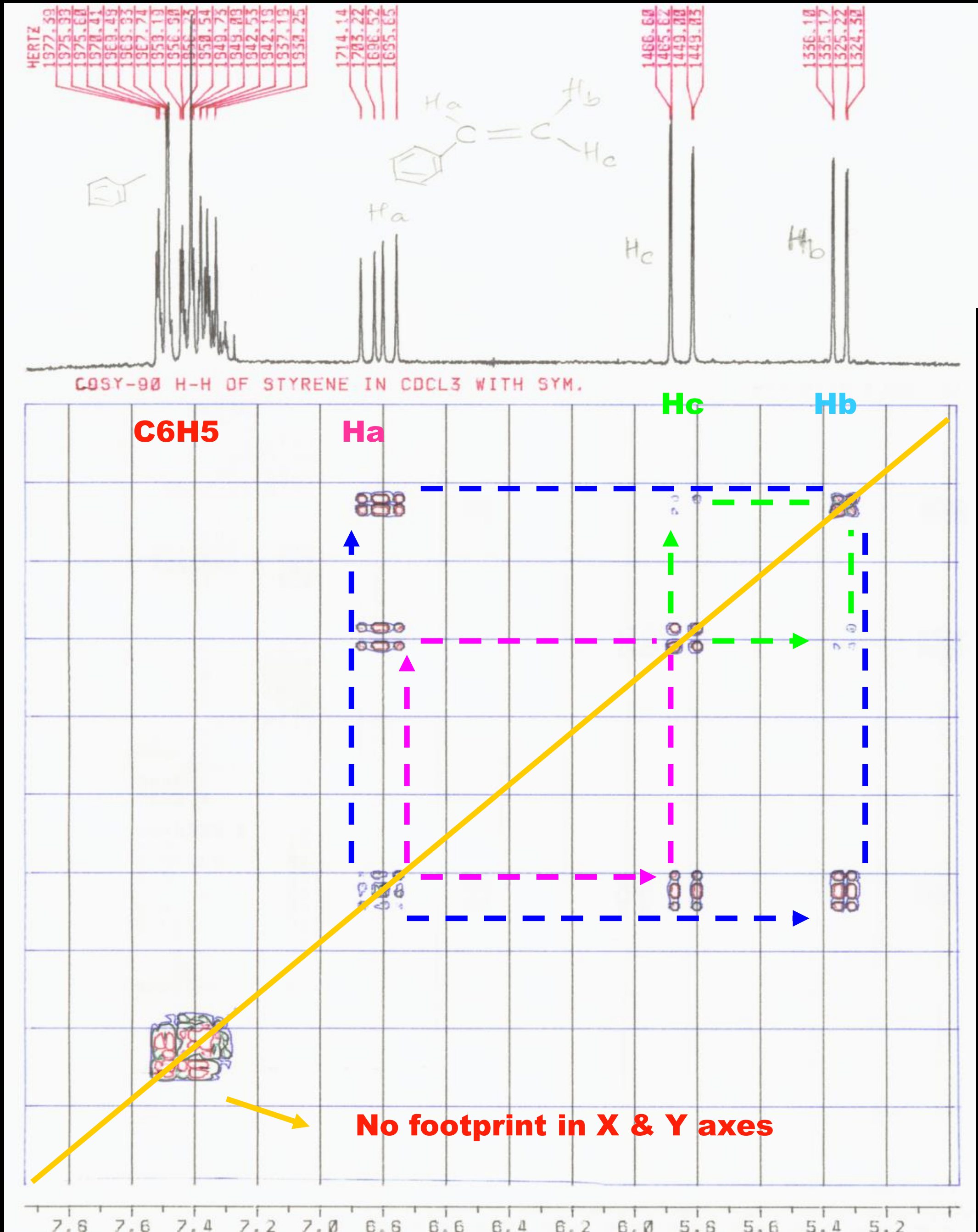
Jcis = 10.90 Hz

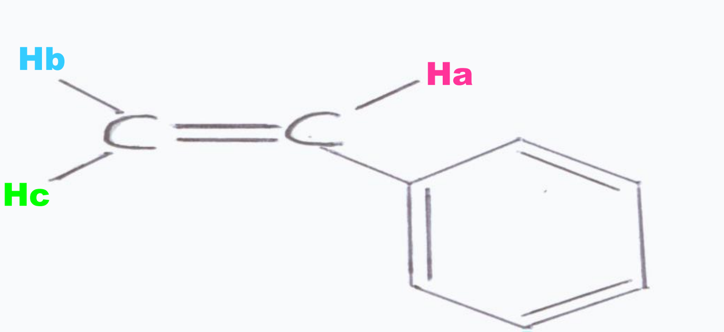
Jgem = 0.87 Hz

Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Styrene

C_6H_5-CH=CH_2 2D COSY ^1H NMR Spectrum





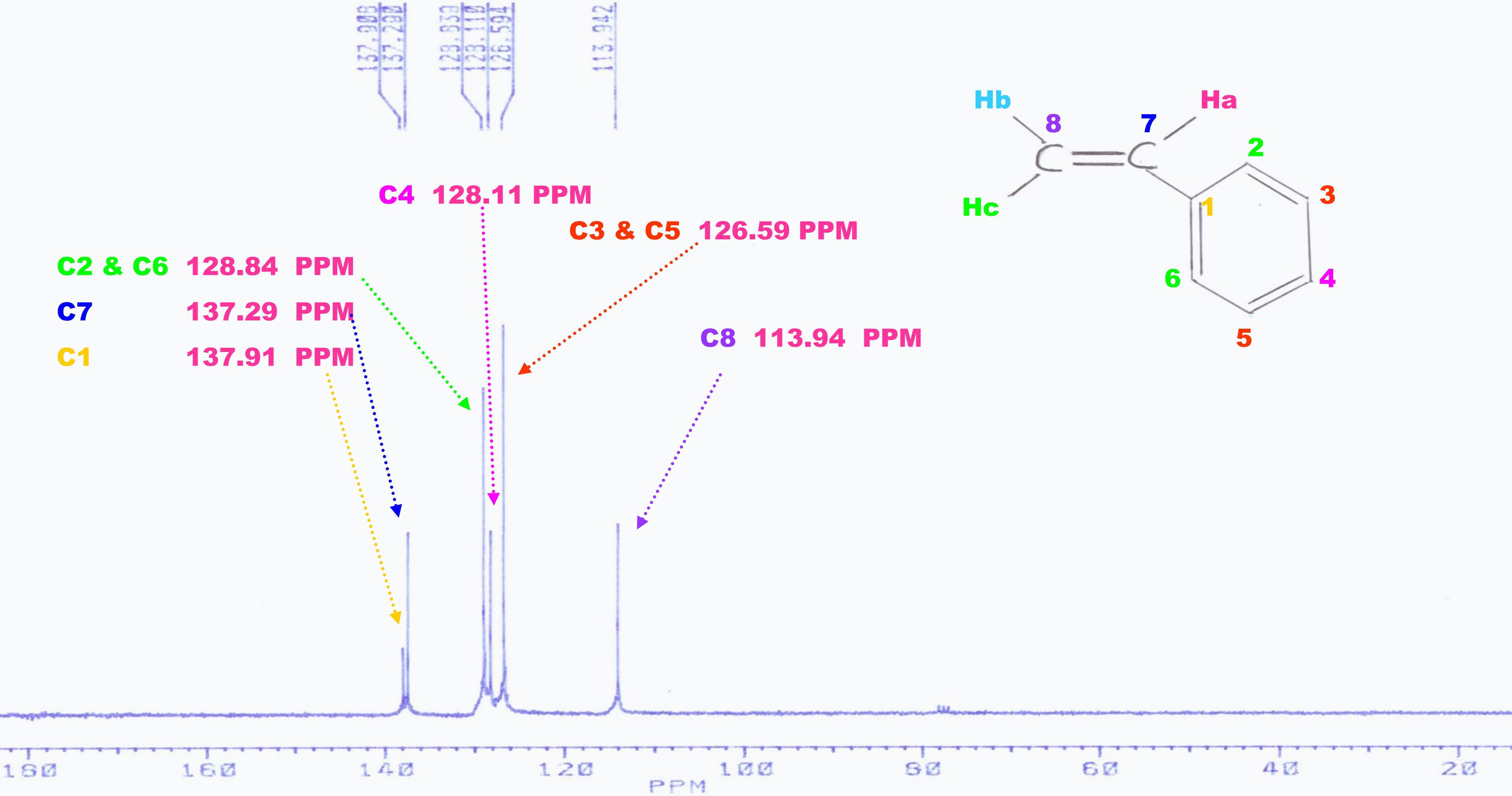


Analysis and interpretation of 2D COSY 90 1H NMR Spectrum of Styrene

$C_6H_5\text{-}CH{=}CH_2$

1. Every peak in spectrum gives the diagonal footprint in cosy spectrum.
2. Non coupled 1H gives only diagonal footprint and no footprint in X & Y axes.
3. Coupled 1H will give footprint in X & Y axes.
4. Number of coupling can be seen easily just by counting the number of footprints along either X or Y axis.
   In the Styrene Ha gives two footprints as shown by dashed arrows hence it is coupled to two 1H (Hb & Hc).
   Where as C6H5 give s no footprint in X & Y axes hence they are not coupled to any other 1H (Ha, Hb or Hc).
5. Aromatic region is complex to analyse.

Analysis and interpretation of ^{13}C NMR Spectrum of Styrene $C_6H_5\text{-}CH{=}CH_2$



C4 128.11 PPM

C3 & C5 126.59 PPM

C2 & C6 128.84 PPM

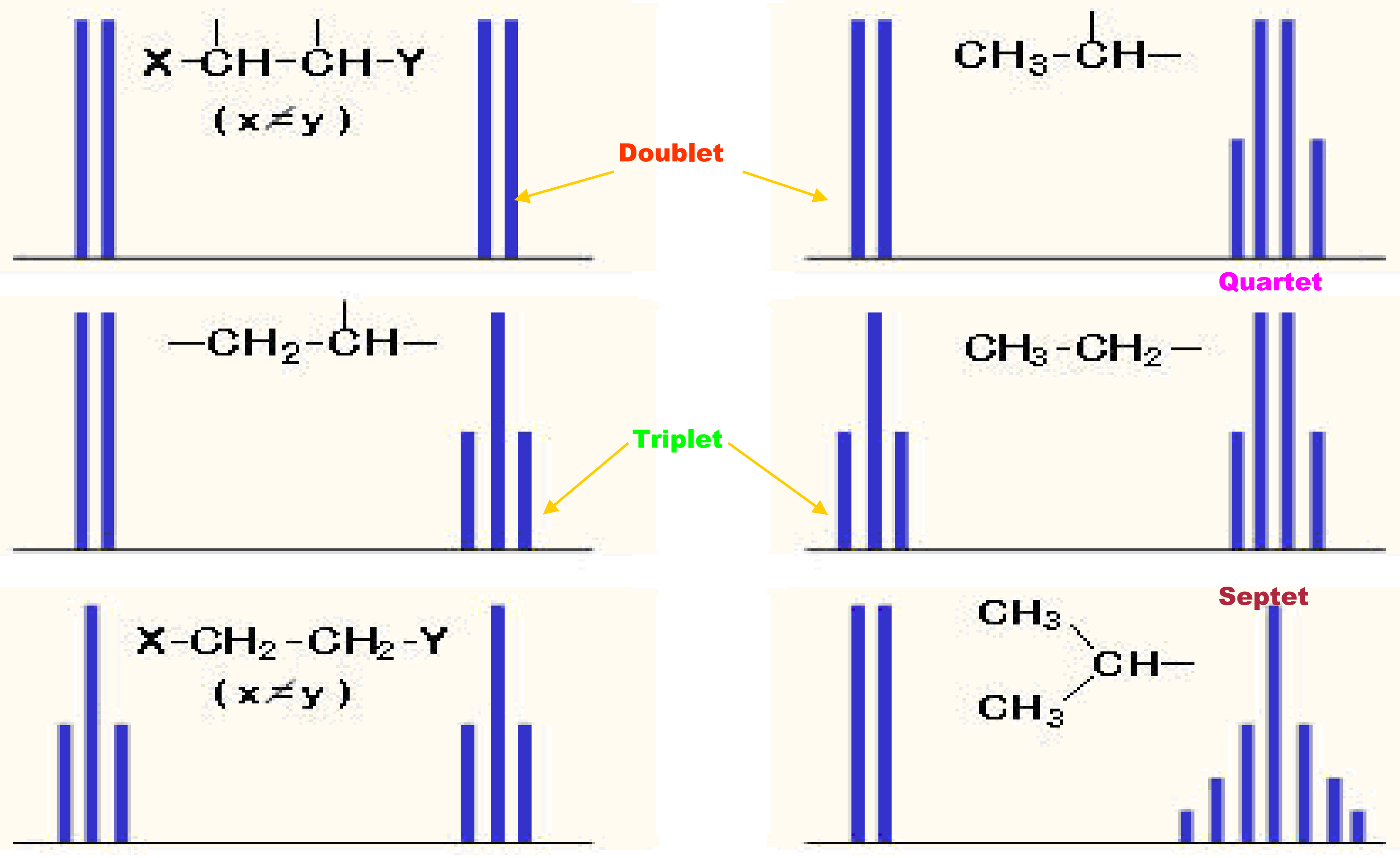
C7 137.29 PPM

C1 137.91 PPM

C8 113.94 PPM

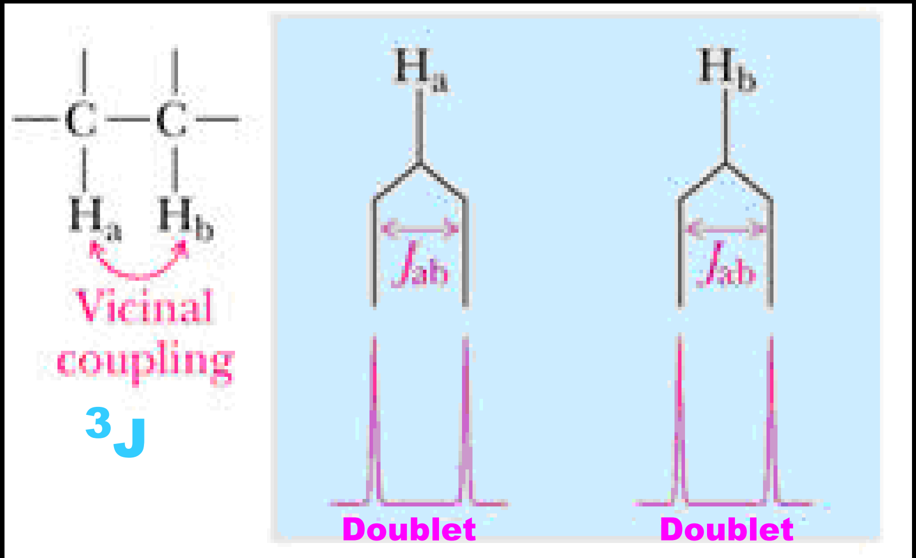
Splitting Patterns for Aliphatic ^1H

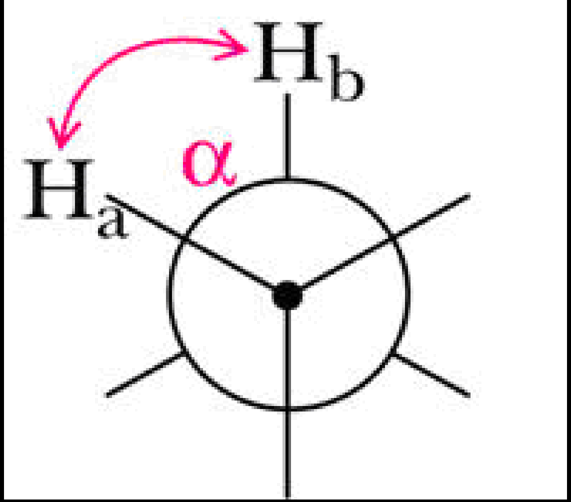
Common Patterns in ^1H NMR Spectra



Notation For Coupling Constant (^2J, ^3J, ^4J & so on)

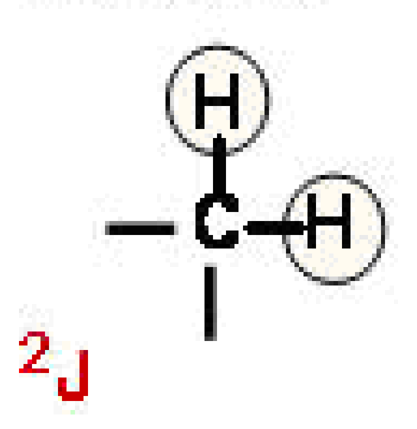
- In ^{1}H NMR spectra, the most common coupling constant is encountered ^{1}H three bonds apart ^3J. This is also called as Vicinal Coupling.
- The angle alpha factor in vicinal coupling.
- When angle alpha = 0^0 and 180^0 The coupling constant is maximum
- = 90^0 The coupling constant is minimum

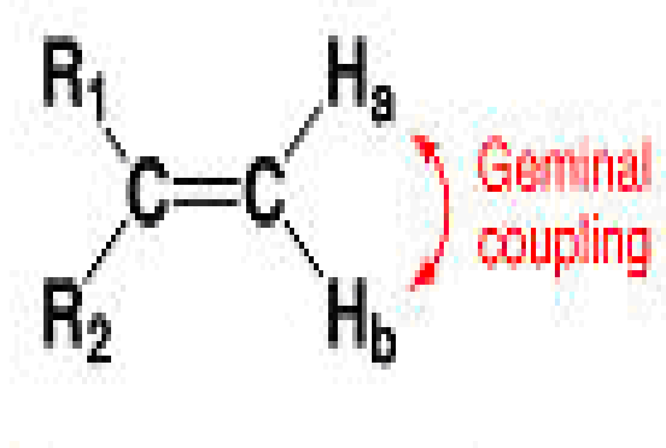




^2J coupling constant

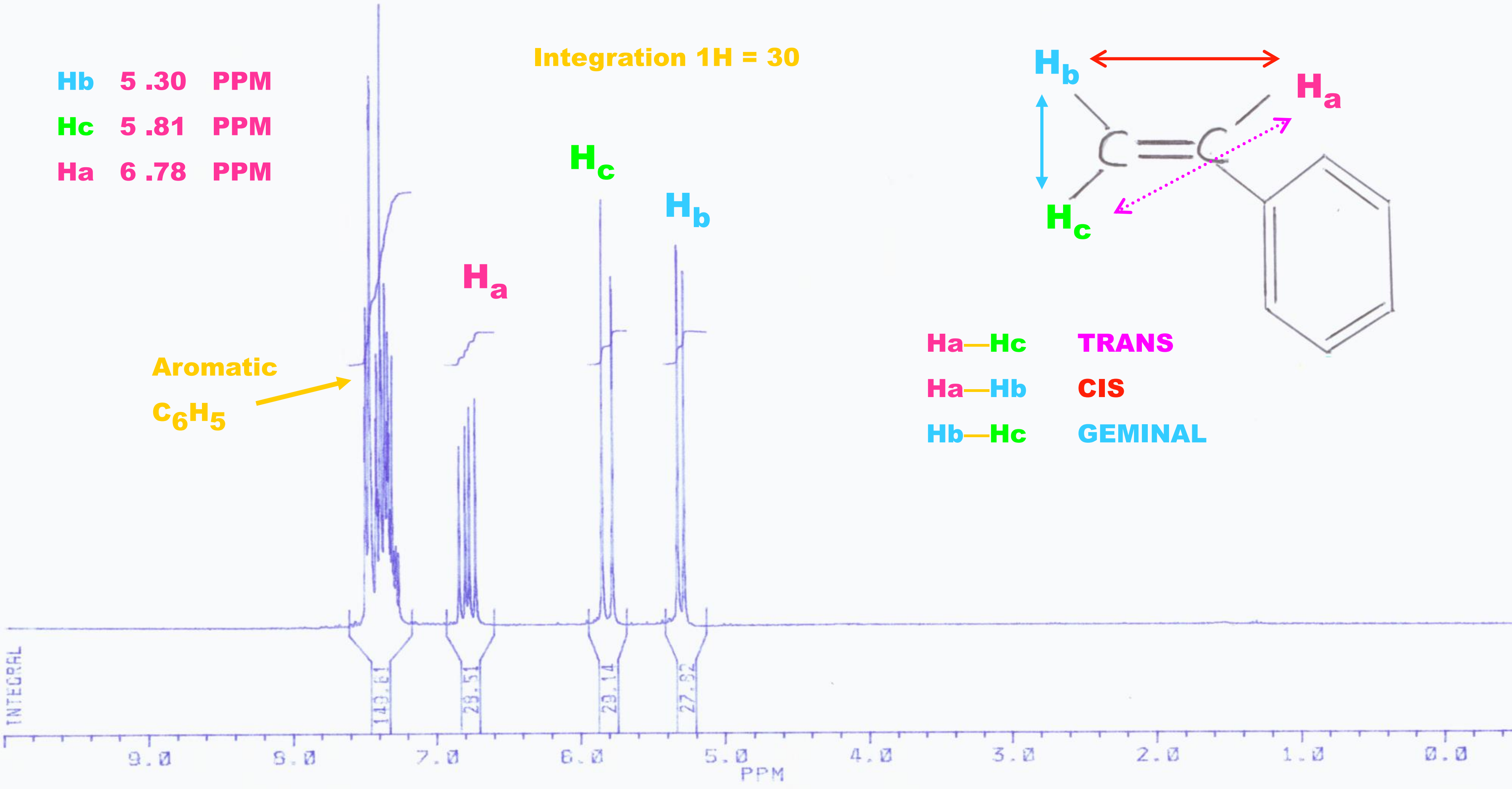
- The alpha angle H—C—C—H and the rotation round
- --C—C-- sigma bonds is also a key parameter for ^1H coupling constant.
- In Ethyl CH_3—CH_2— Group the free rotation make ^1H attached to the same carbon equivalent hence do not show coupling ^2J = 00 Hz
- In alkenes and cyclic compounds the sigma bonds rotation restricted, this may give rise the ^1H attached to the same carbon becomes non-equivalent hence couples to each other.
- This coupling is called Geminal Coupling and denoted by ^2J
- On the next slide shows the Vinylic ^1H interactions in Styrene





Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Styrene

C_6H_5-CH=CH$_2$ ^{1}H NMR Spectrum



Hb	5 .30	PPM
Hc	5 .81	PPM
Ha	6 .78	PPM

Integration 1H = 30

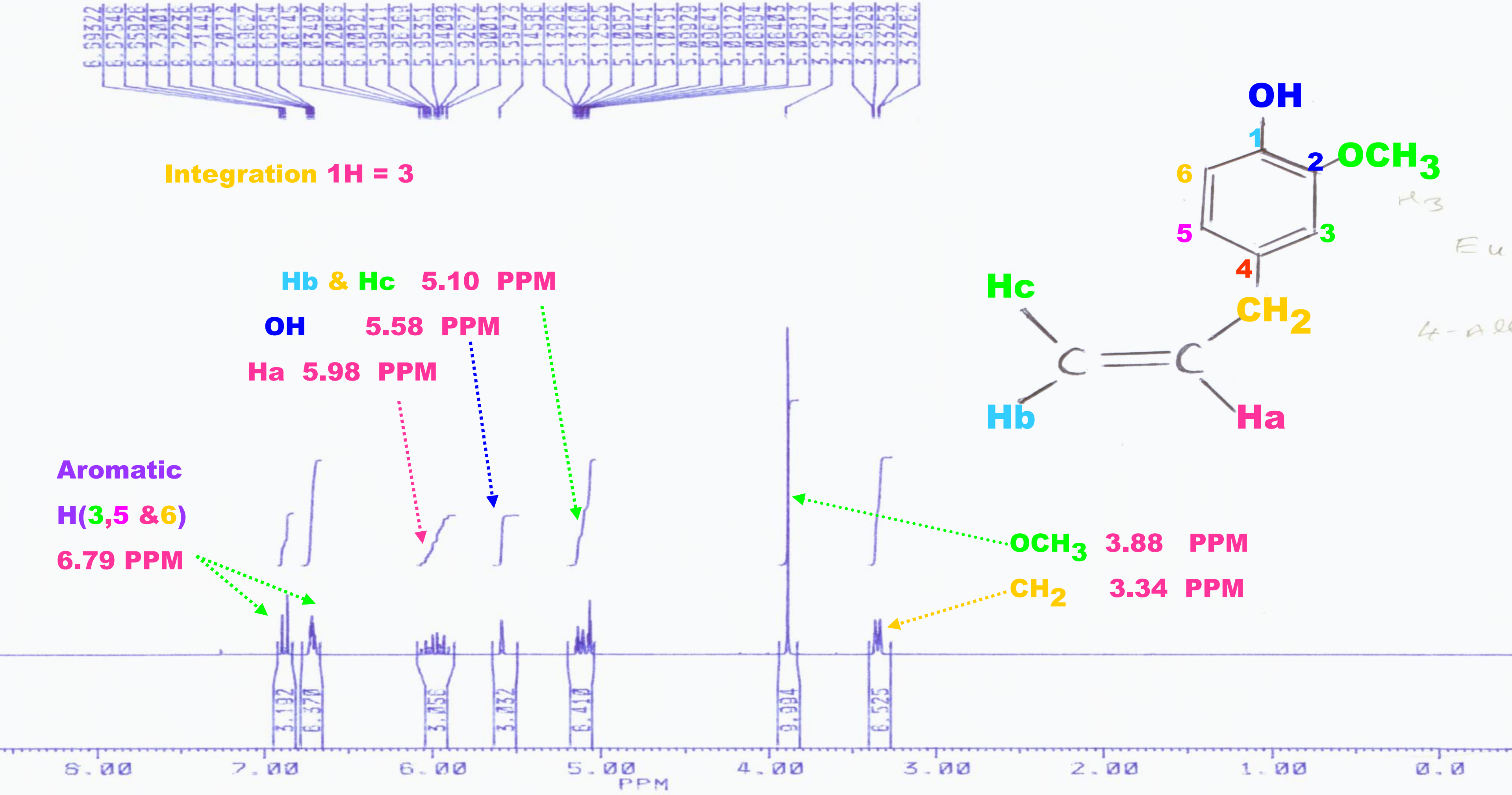
Aromatic C_6H_5

Ha—Hc	TRANS
Ha—Hb	CIS
Hb—Hc	GEMINAL

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol

$C_6H_3(OH)(OCH_3)(CH_2\text{-}CH{=}CH_2)$

^{1}H NMR Spectrum



Integration 1H = 3

Hb & Hc 5.10 PPM

OH 5.58 PPM

Ha 5.98 PPM

Aromatic

H(3,5 &6)

6.79 PPM

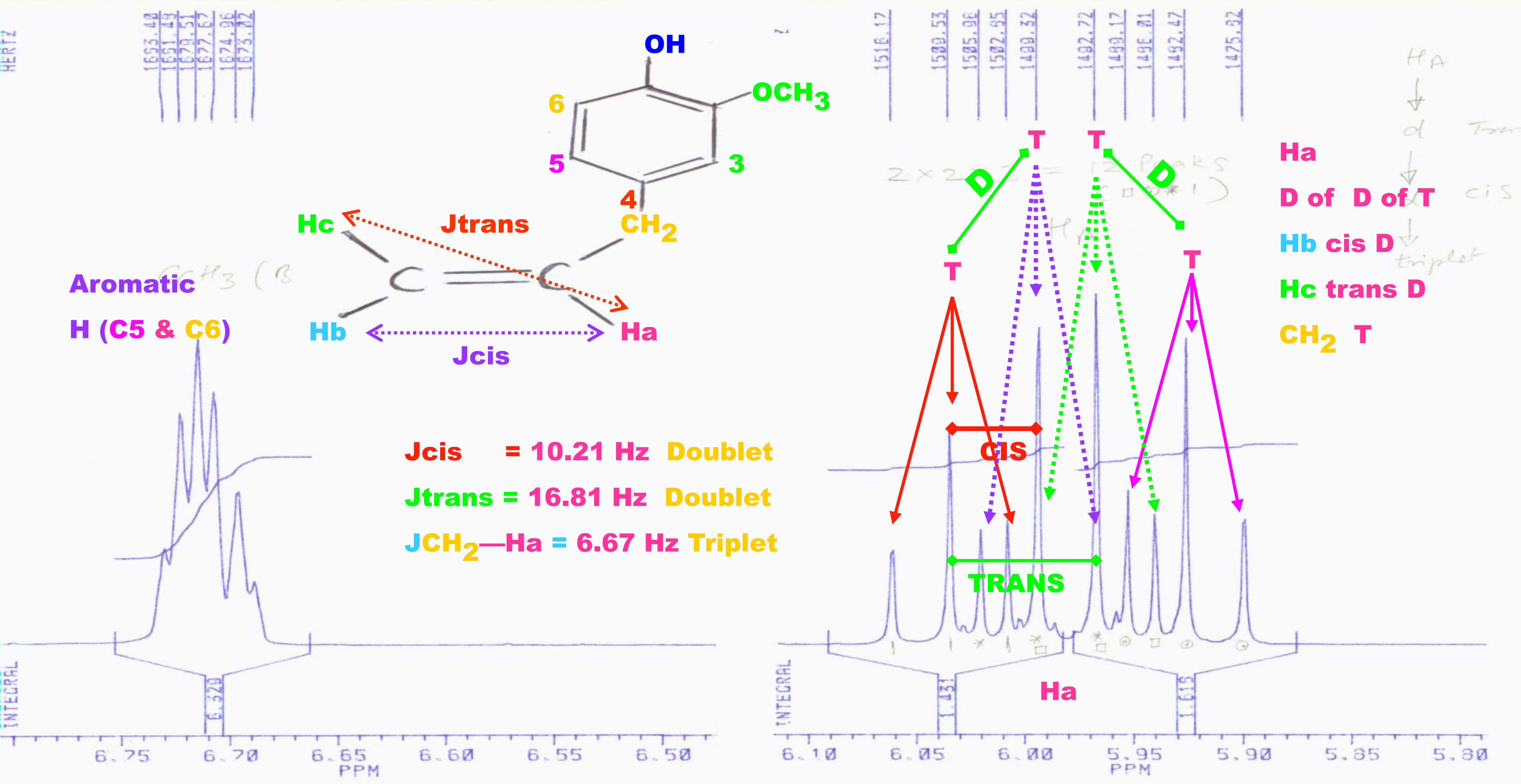
OCH_3 3.88 PPM

CH_2 3.34 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol

$C_6H_3(OH)(OCH_3)(CH_2\text{-}CH{=}CH_2)$

^{1}H NMR Spectrum



Jcis = 10.21 Hz Doublet

Jtrans = 16.81 Hz Doublet

JCH_2—Ha = 6.67 Hz Triplet

Ha

D of D of T

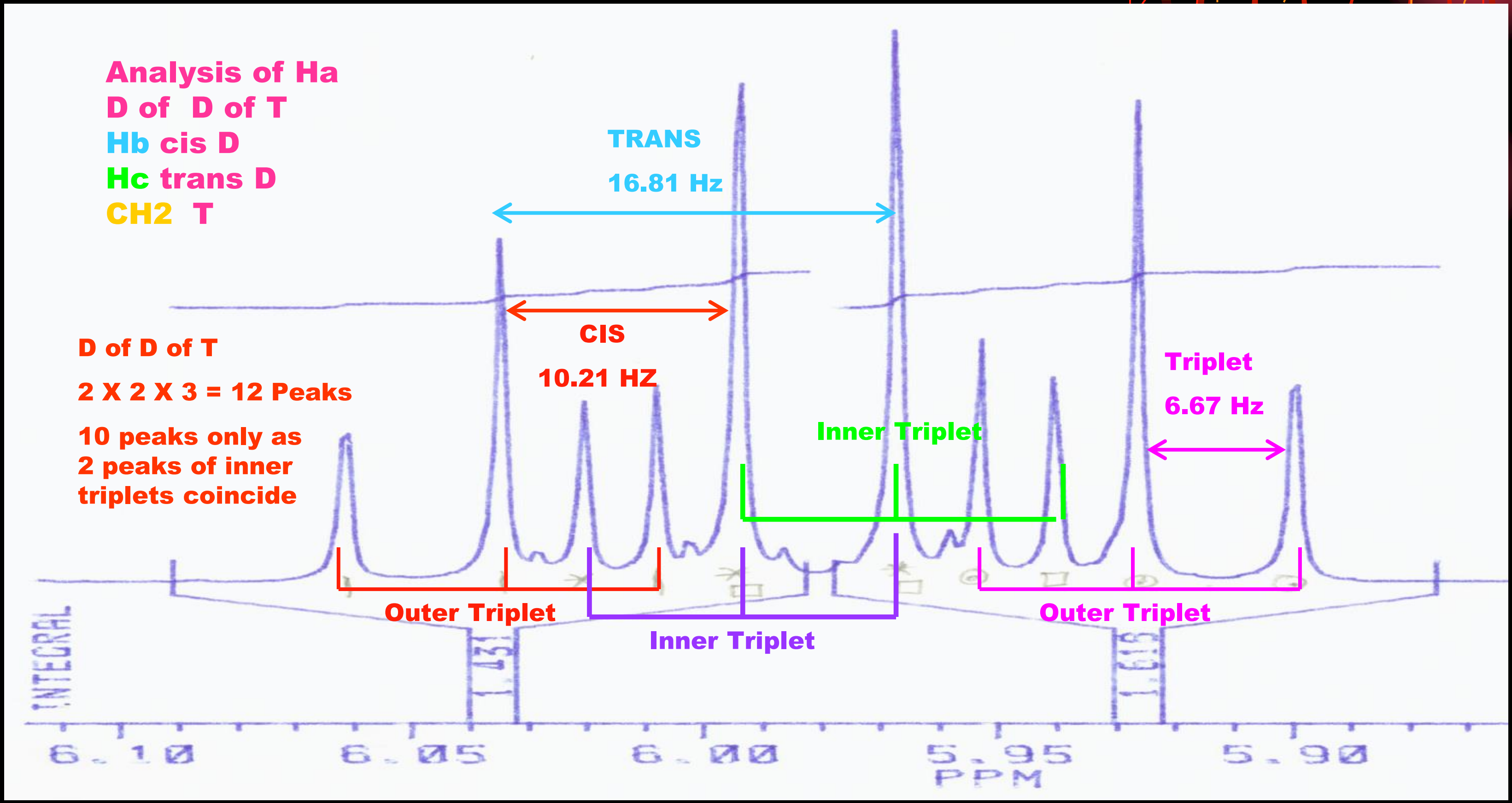
Hb cis D

Hc trans D

CH_2 T

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol

$C_6H_3(OH)(OCH_3)(CH_2\text{-}CH=CH_2)$ ^{1}H NMR Spectrum

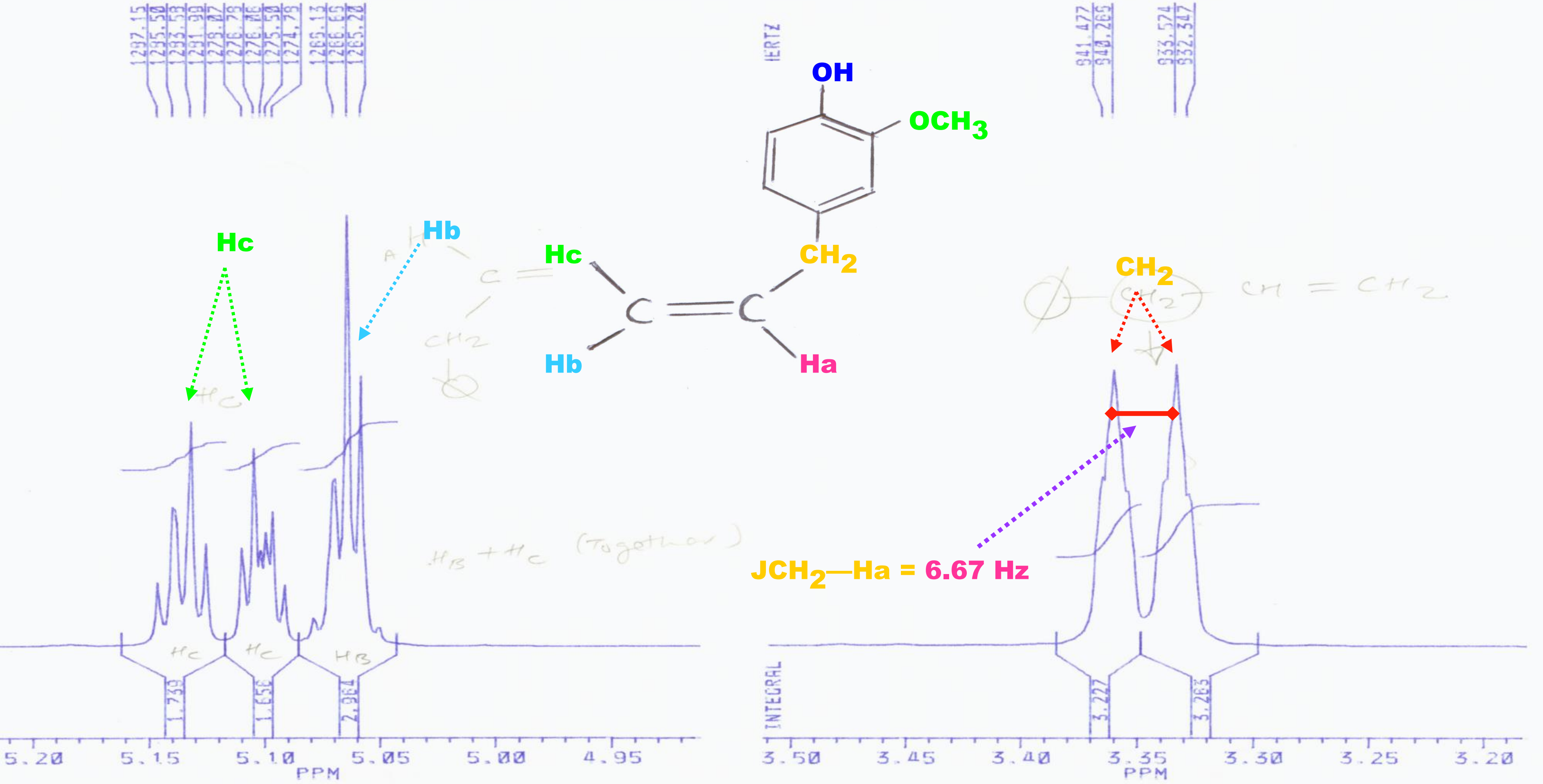


Analysis of Ha
D of D of T
Hb cis D
Hc trans D
CH2 T

D of D of T
2 X 2 X 3 = 12 Peaks
10 peaks only as 2 peaks of inner triplets coincide

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol

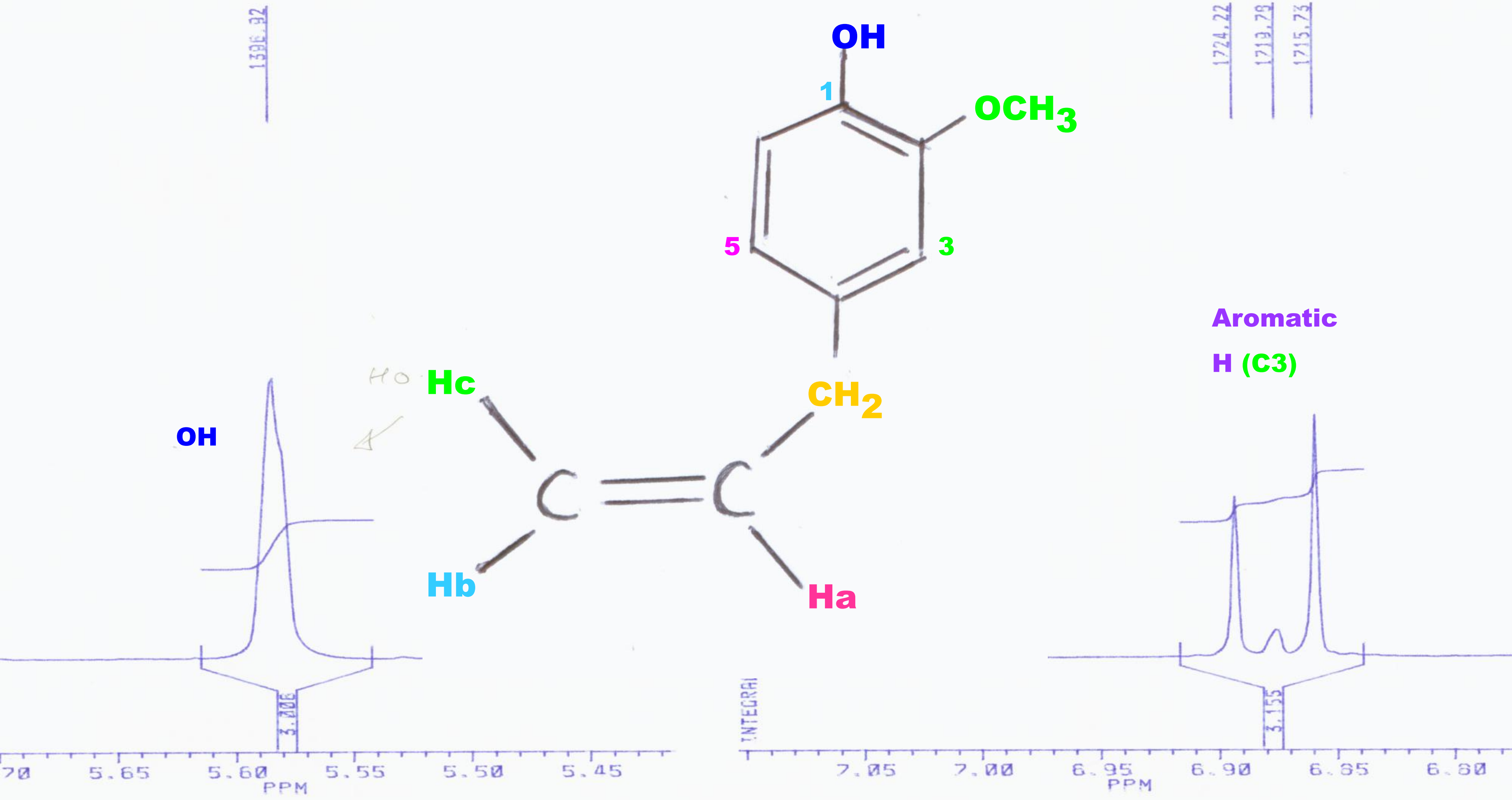
$C_6H_3(OH)(OCH_3)(CH_2\text{-}CH{=}CH_2)$ ^{1}H NMR Spectrum



J_{CH_2}—Ha = 6.67 Hz

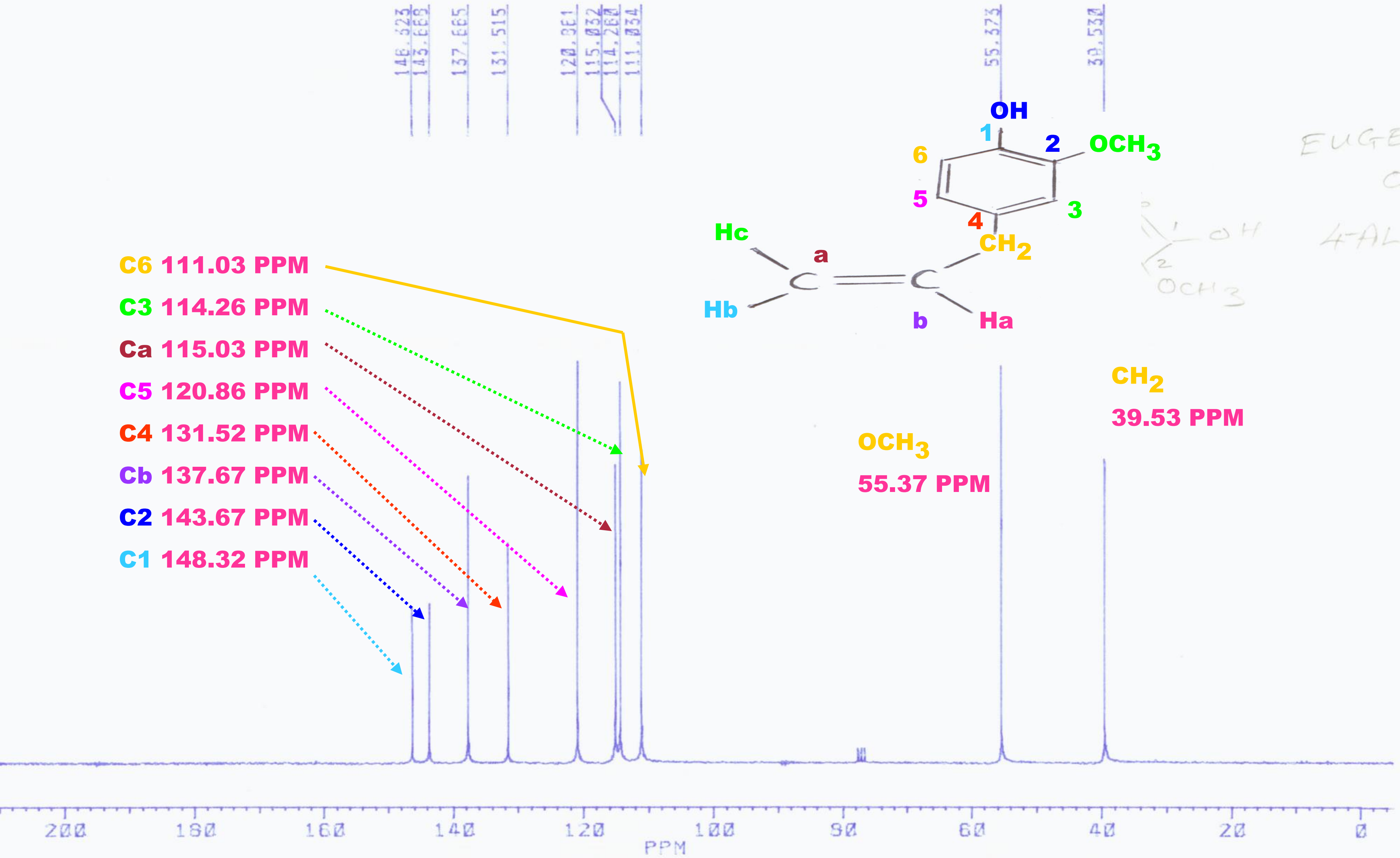
Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Eugenol

^{1}H NMR Spectrum



^{13}C NMR Spectrum of Eugenol.

4-Allyl-2-MethoxyPhenol



C6 111.03 PPM

C3 114.26 PPM

Ca 115.03 PPM

C5 120.86 PPM

C4 131.52 PPM

Cb 137.67 PPM

C2 143.67 PPM

C1 148.32 PPM

OCH_3

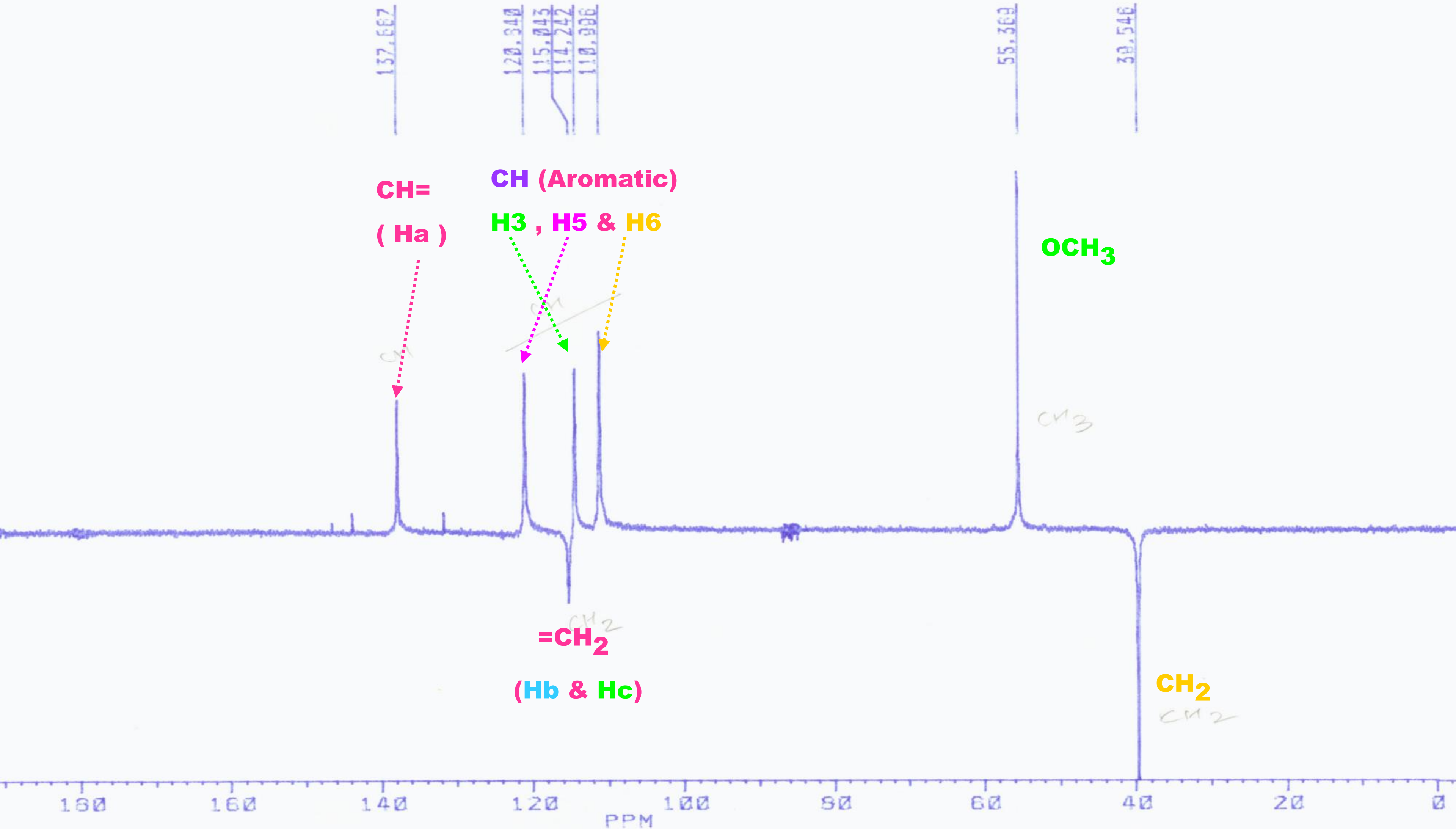
55.37 PPM

CH_2

39.53 PPM

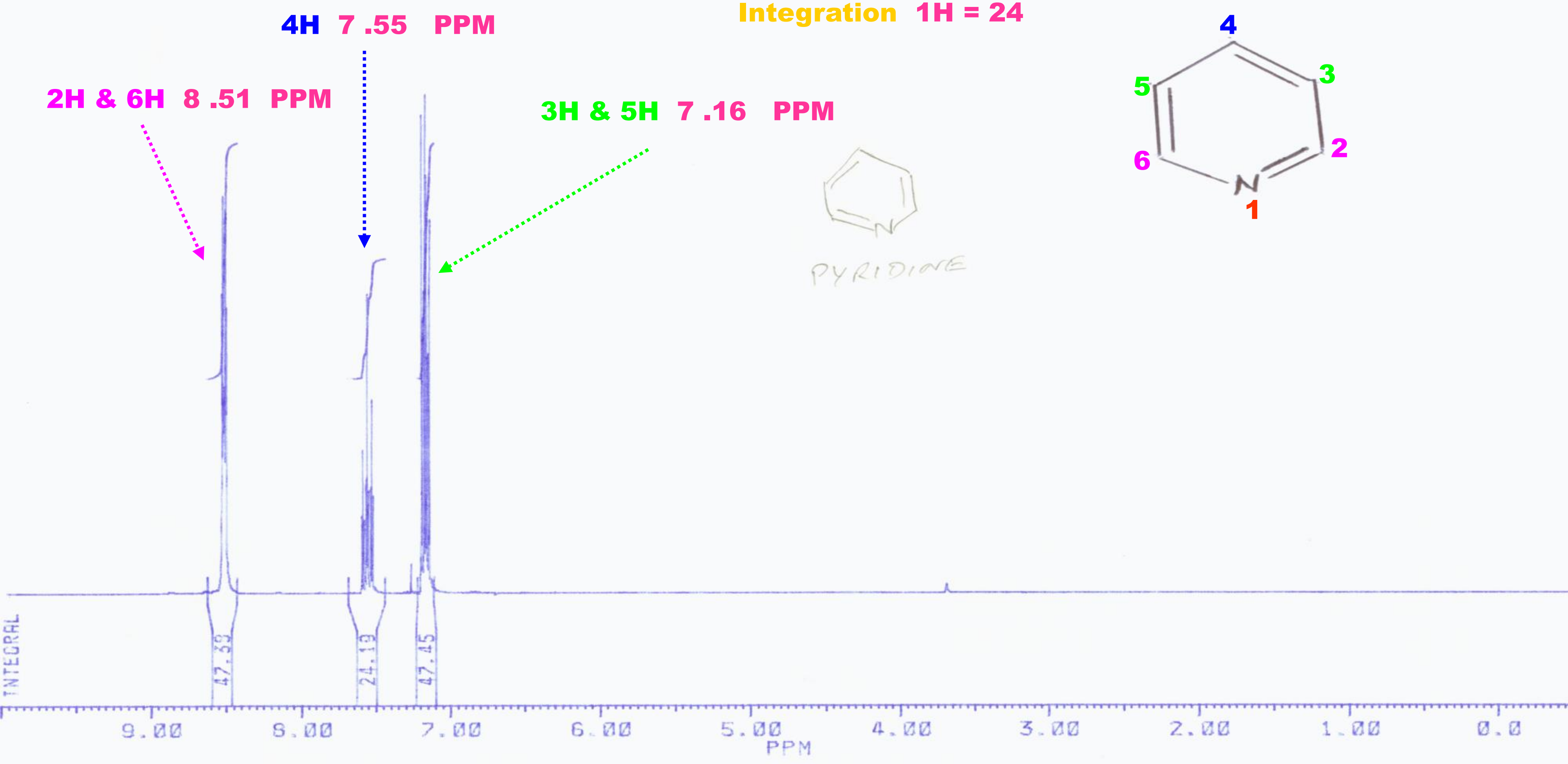
13C Dept 135 of 4-Allyl-2-MethoxyPhenol

$C_6H_3(OH)(OCH_3)(CH_2\text{-}CH{=}CH_2)$



Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Pyridine

C_5H_5N ^{1}H NMR Spectrum



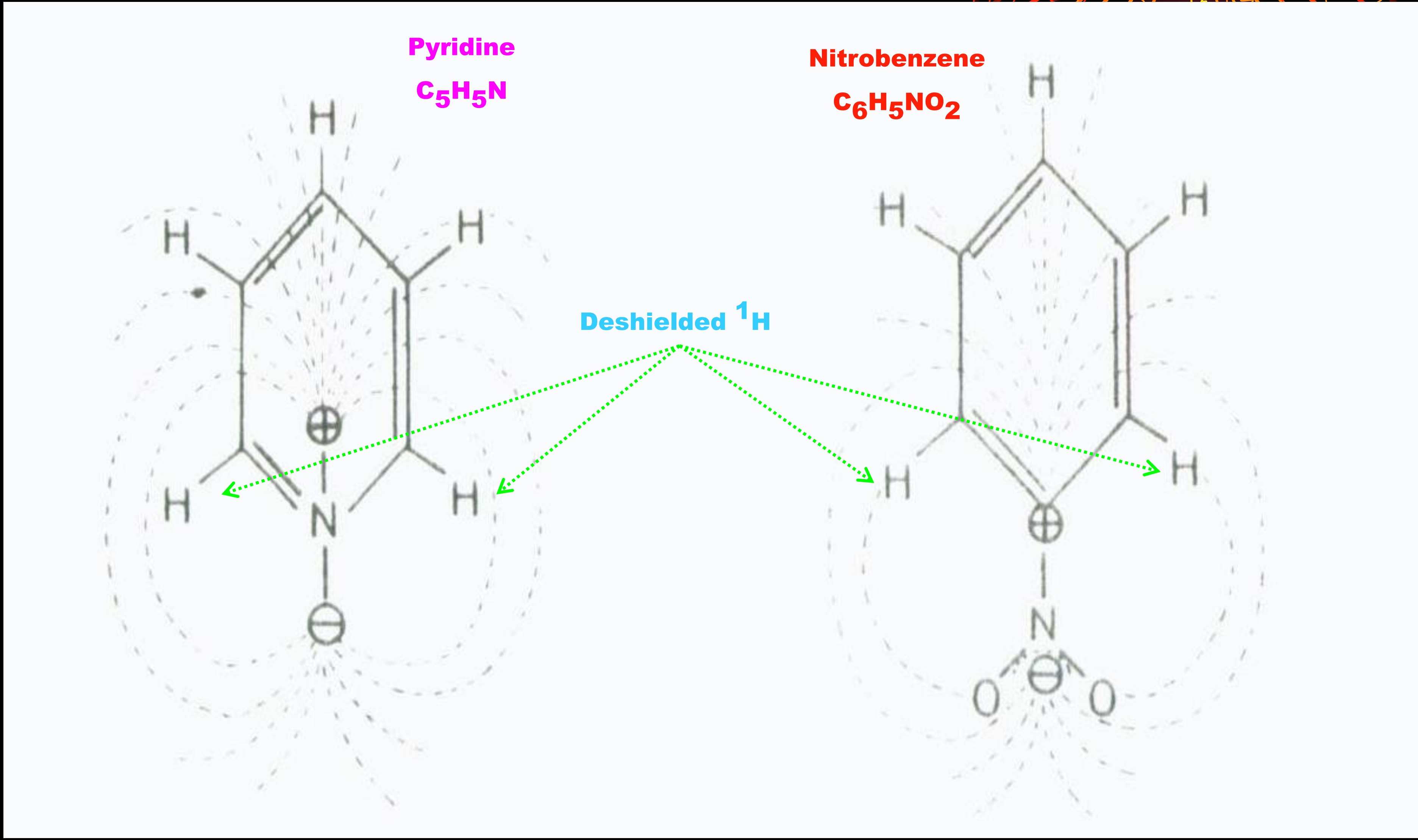
4H 7 .55 PPM

Integration 1H = 24

2H & 6H 8 .51 PPM

3H & 5H 7 .16 PPM

The Electric Field Effect on Pyridine & Nitrobenzene



Pyridine

C_5H_5N

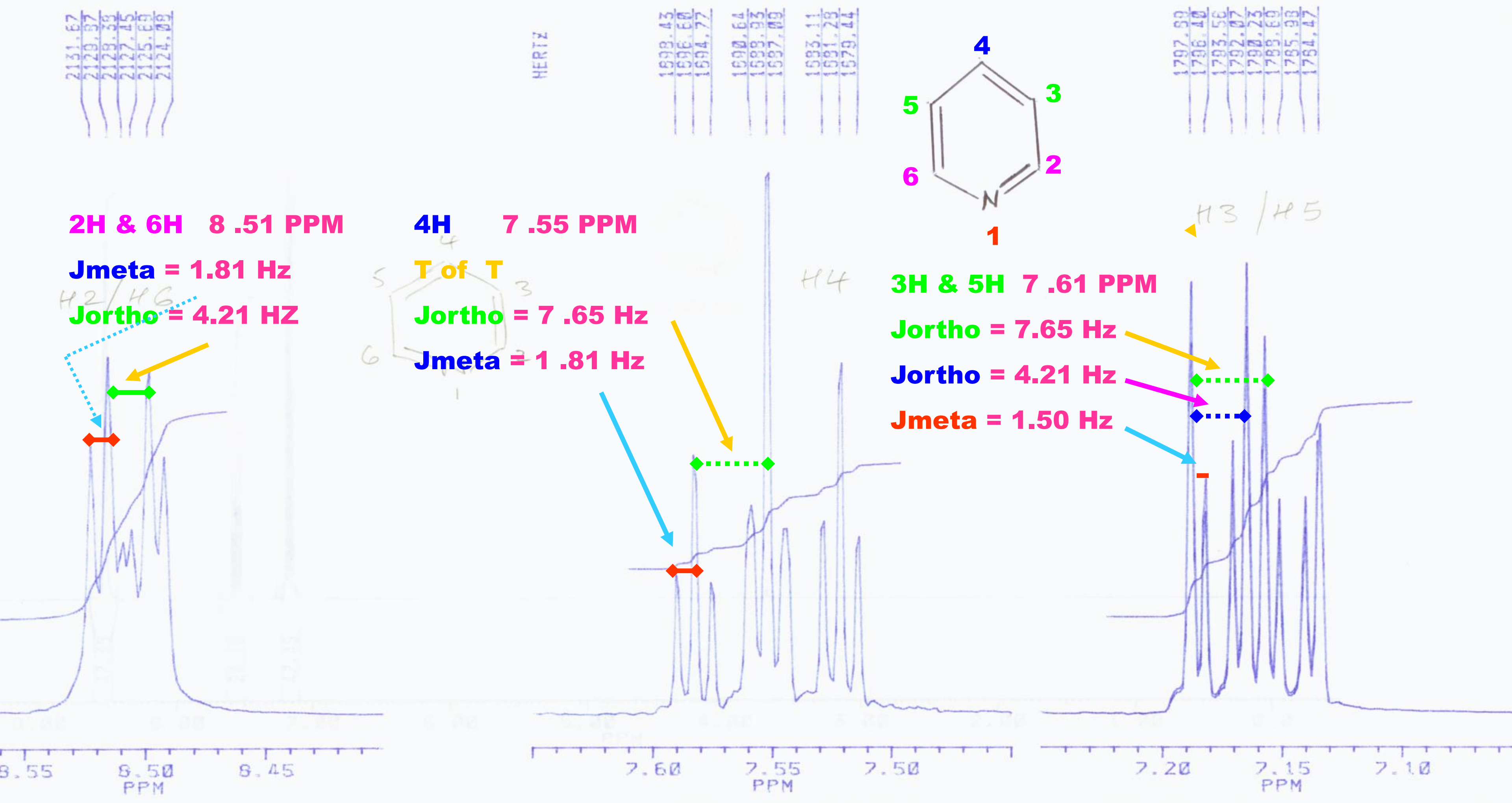
Nitrobenzene

$C_6H_5NO_2$

Deshielded ^1H

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Pyridine

C_5H_5N ^{1}H NMR Spectrum Expansion



2H & 6H 8 .51 PPM

Jmeta = 1.81 Hz

Jortho = 4.21 HZ

4H 7 .55 PPM

T of T

Jortho = 7 .65 Hz

Jmeta = 1 .81 Hz

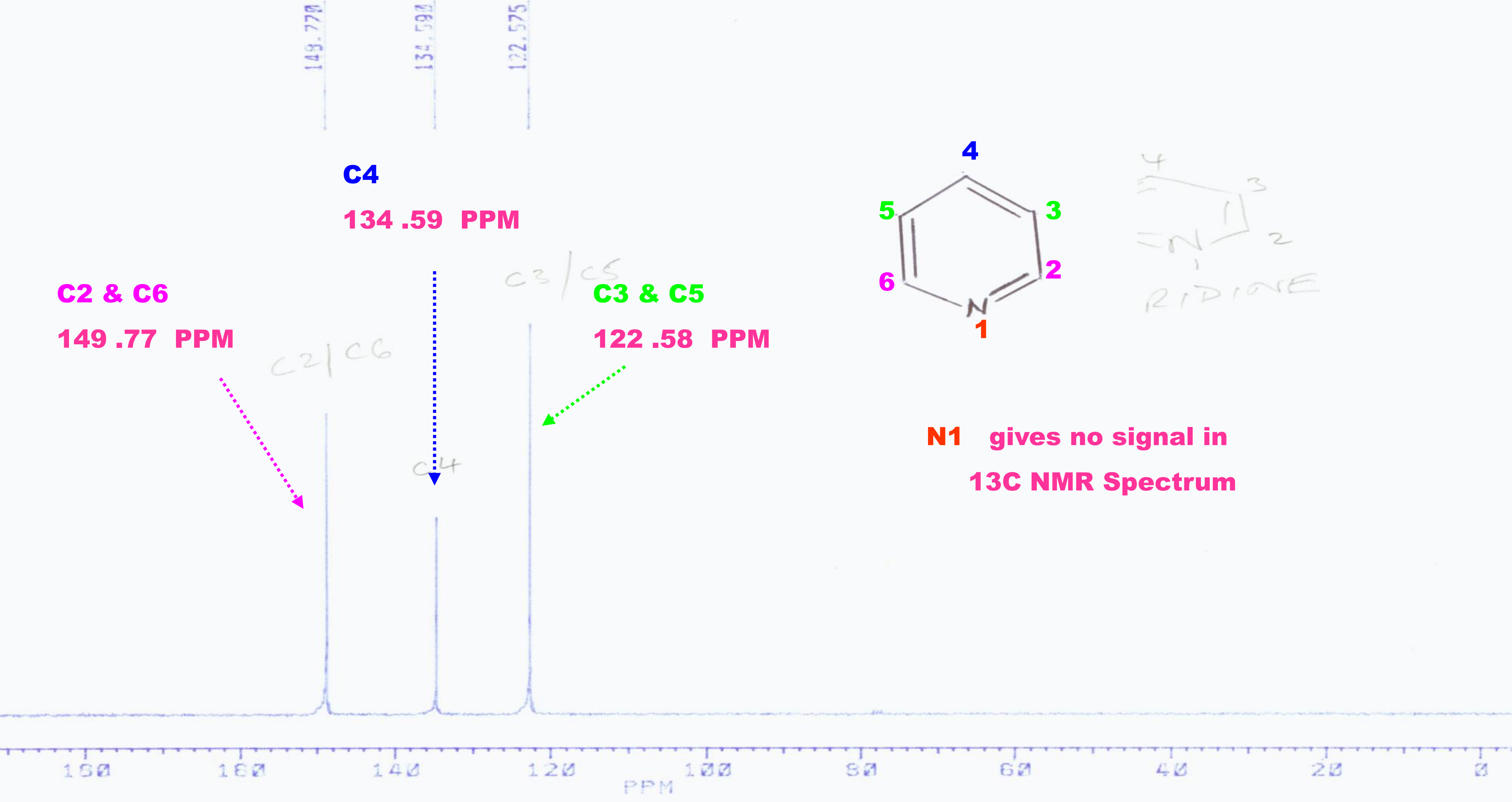
3H & 5H 7 .61 PPM

Jortho = 7.65 Hz

Jortho = 4.21 Hz

Jmeta = 1.50 Hz

Analysis and interpretation of ^{13}C NMR Spectrum of Pyridine C_5H_5N



C4

134 .59 PPM

C2 & C6

149 .77 PPM

C3 & C5

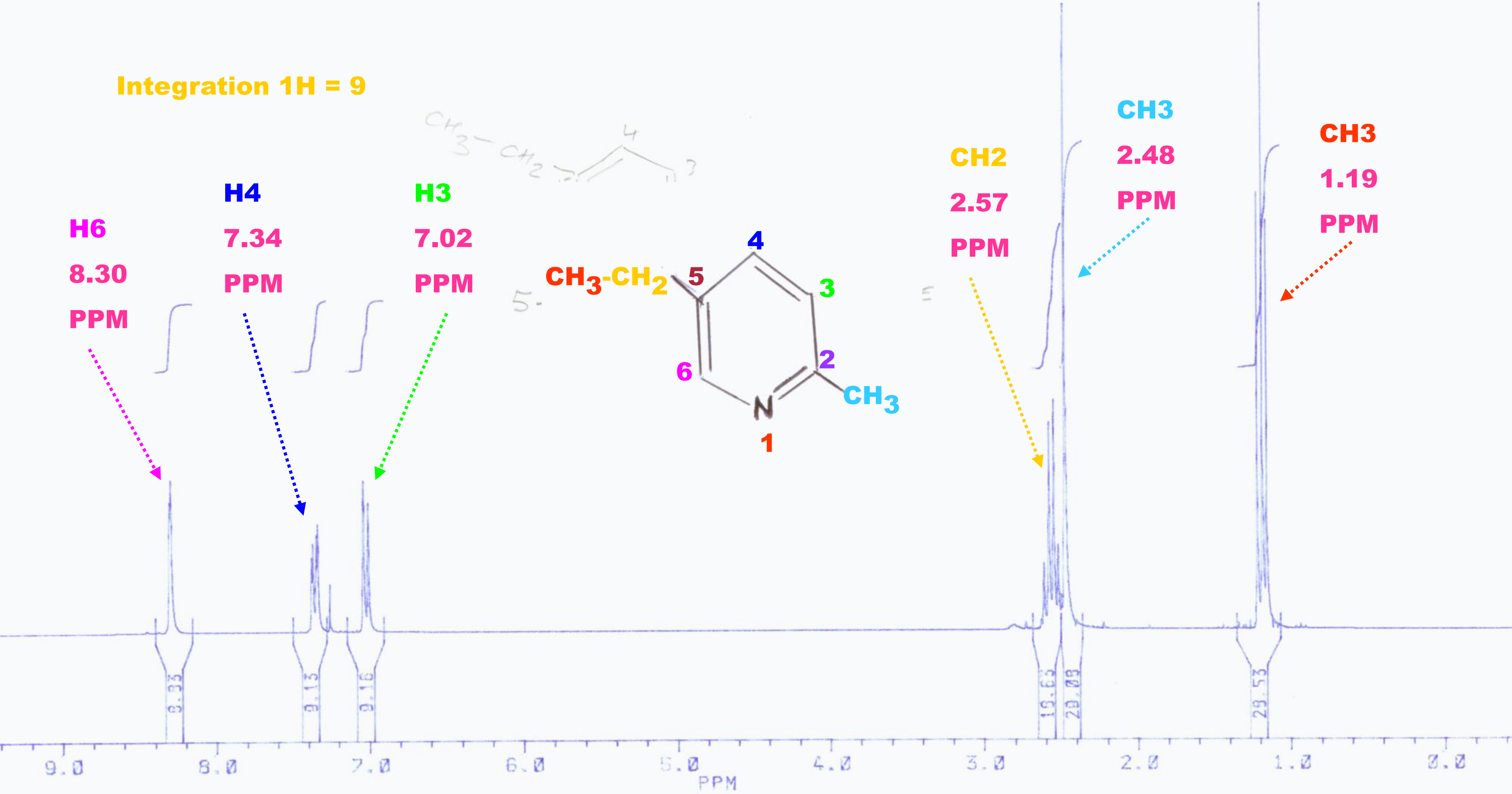
122 .58 PPM

N1 gives no signal in 13C NMR Spectrum

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 5-Ethyl-2-MethylPyridine

$C_5H_3N(CH_3)(CH_2\text{-}CH_3)$

^{1}H NMR Spectrum



Integration 1H = 9

H6 8.30 PPM

H4 7.34 PPM

H3 7.02 PPM

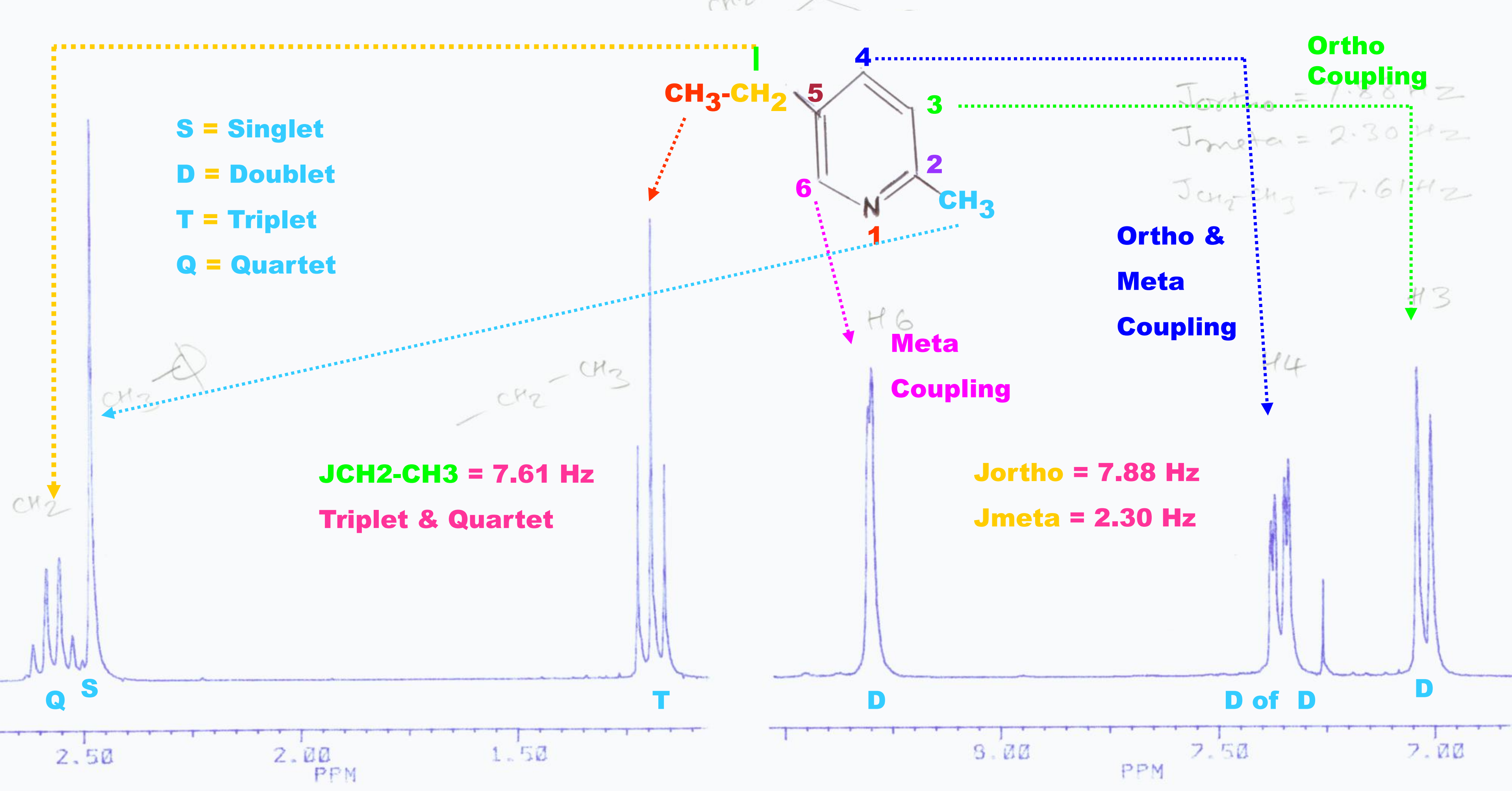
CH2 2.57 PPM

CH3 2.48 PPM

CH3 1.19 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 5-Ethyl-2-MethylPyridine

$C_5H_3N(CH_3)(CH_2\text{-}CH_3)$ Expansion of ^{1}H NMR Spectrum



S = Singlet

D = Doublet

T = Triplet

Q = Quartet

Ortho Coupling

Ortho & Meta Coupling

Meta Coupling

JCH2-CH3 = 7.61 Hz

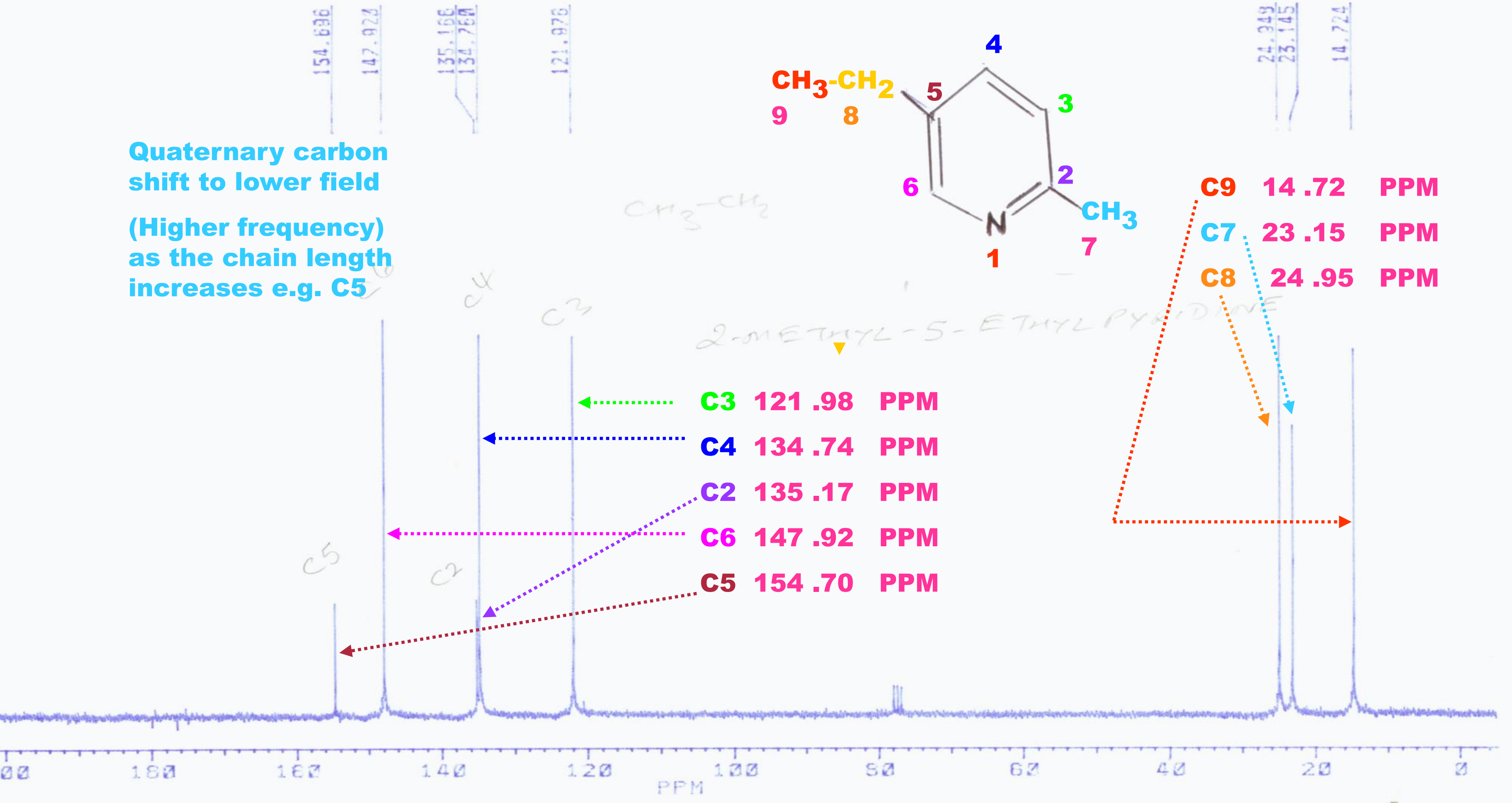
Triplet & Quartet

Jortho = 7.88 Hz

Jmeta = 2.30 Hz

Analysis and interpretation of ^{13}C NMR Spectrum of 5-Ethyl-2-MethylPyridine

$C_5H_3N(CH_3)(CH_2\text{-}CH_3)$



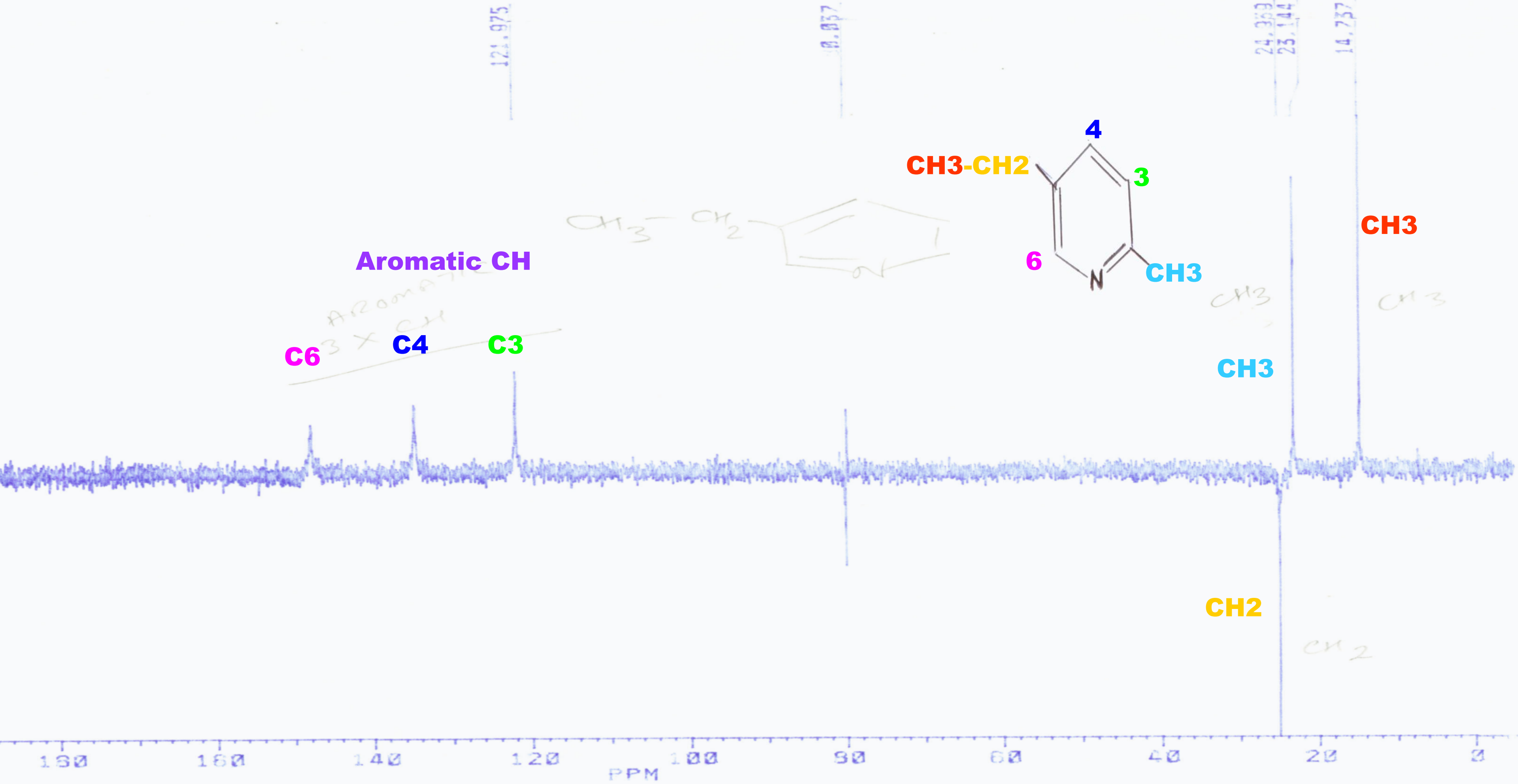
Quaternary carbon shift to lower field

(Higher frequency) as the chain length increases e.g. C5

C3	**121 .98**	**PPM**
C4	**134 .74**	**PPM**
C2	**135 .17**	**PPM**
C6	**147 .92**	**PPM**
C5	**154 .70**	**PPM**
C9	**14 .72**	**PPM**
C7	**23 .15**	**PPM**
C8	**24 .95**	**PPM**

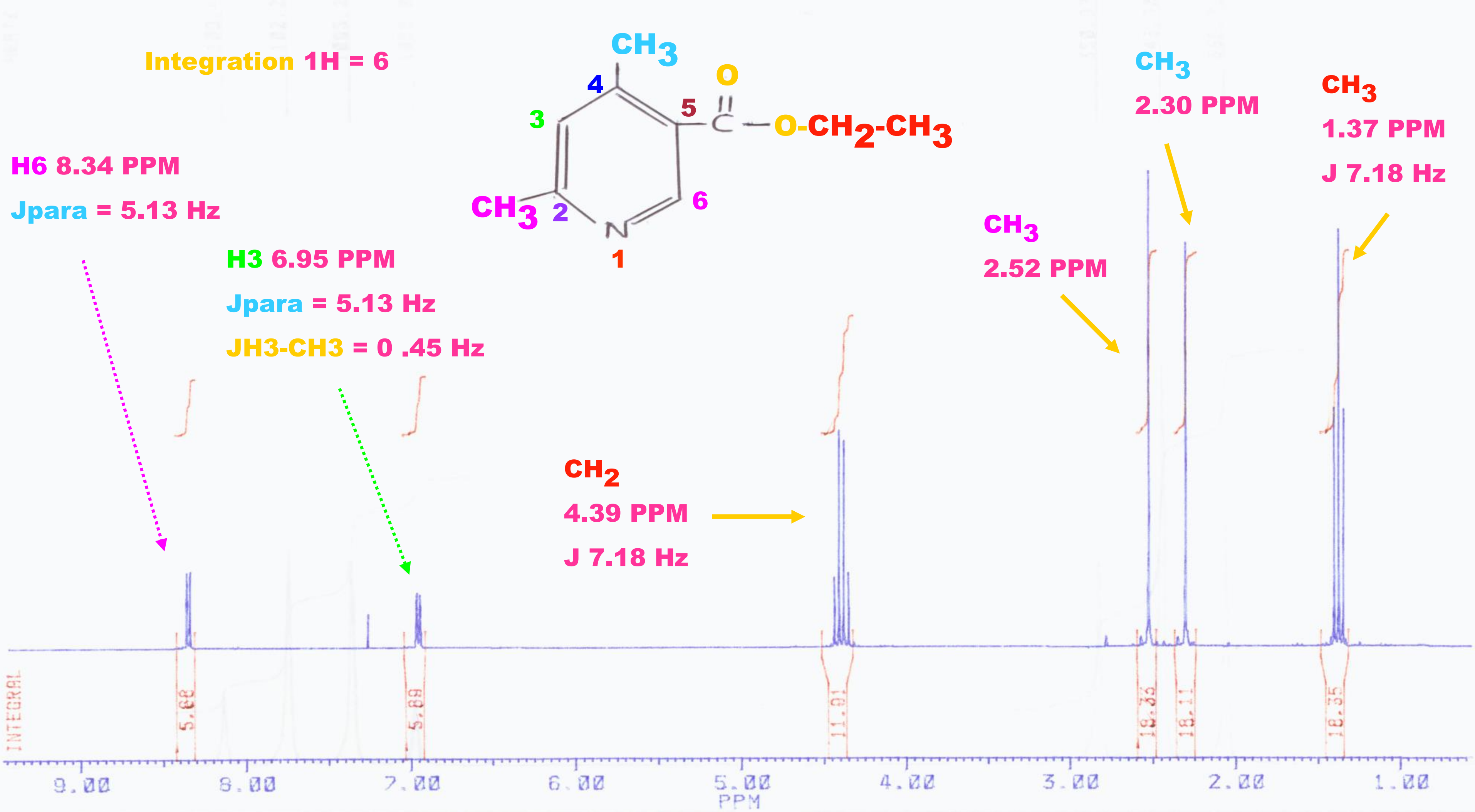
Analysis and interpretation ^{13}C DEPT 135 NMR Spectrum of 5-Ethyl-2-MethylPyridine

$C_5H_3N(CH_3)(CH_2\text{-}CH_3)$



Analysis and Interpretation of ^{1}H NMR Spectrum of Ethyl-2,4-Dimethylnicotinate

$C_5H_2N(CH_3)(CH_3)(CO\text{-}O\text{-}CH_2CH_3)$



Integration 1H = 6

H6 8.34 PPM
Jpara = 5.13 Hz

H3 6.95 PPM
Jpara = 5.13 Hz
JH3-CH3 = 0 .45 Hz

CH_2
4.39 PPM
J 7.18 Hz

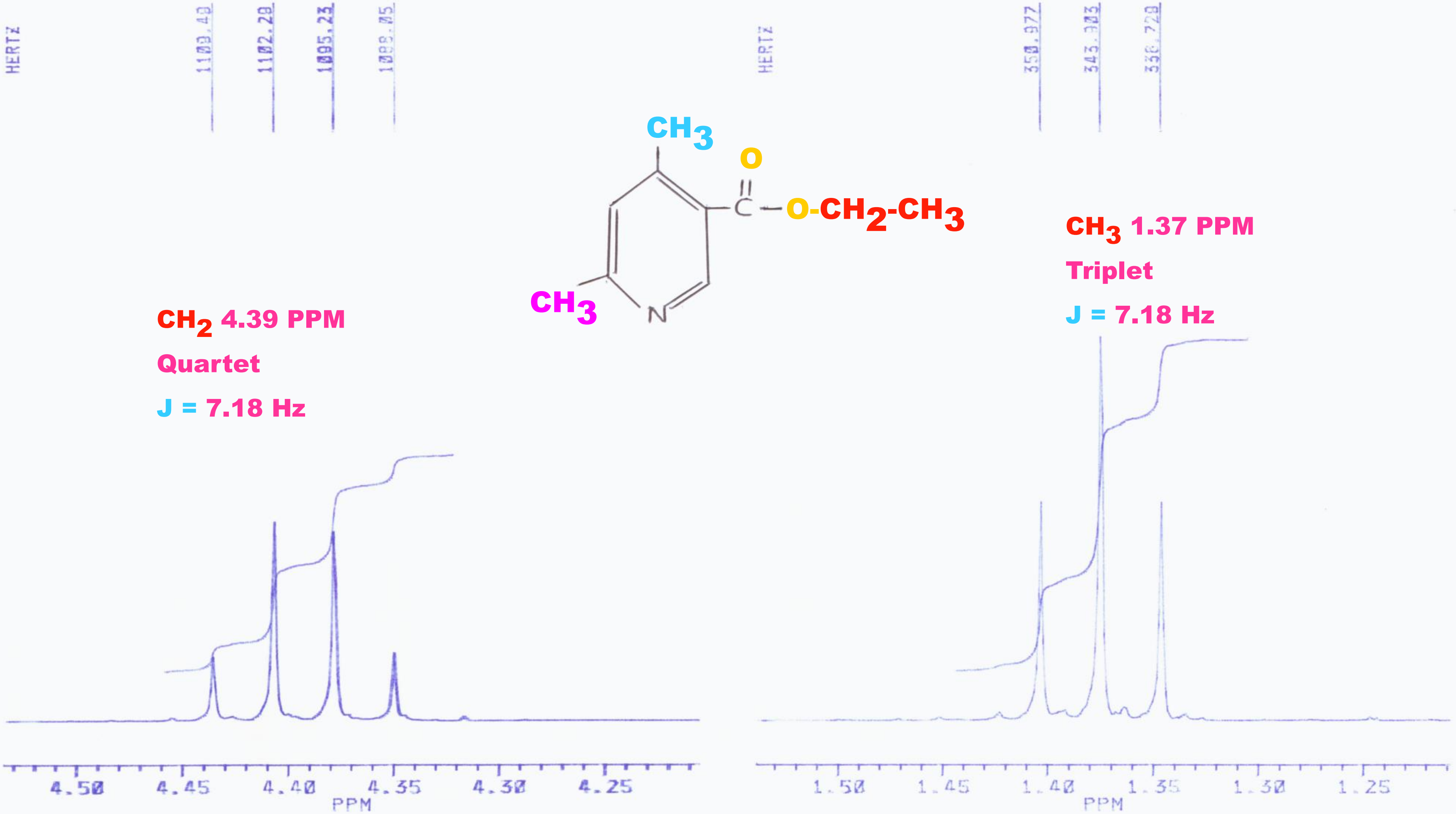
CH_3
2.52 PPM

CH_3
2.30 PPM

CH_3
1.37 PPM
J 7.18 Hz

Analysis and Interpretation of ^{1}H NMR Spectrum of Ethyl-2,4-Dimethylnicotinate

$C_5H_2N(CH_3)(CH_3)(CO\text{-}O\text{-}CH_2CH_3)$



CH_2 4.39 PPM

Quartet

J = 7.18 Hz

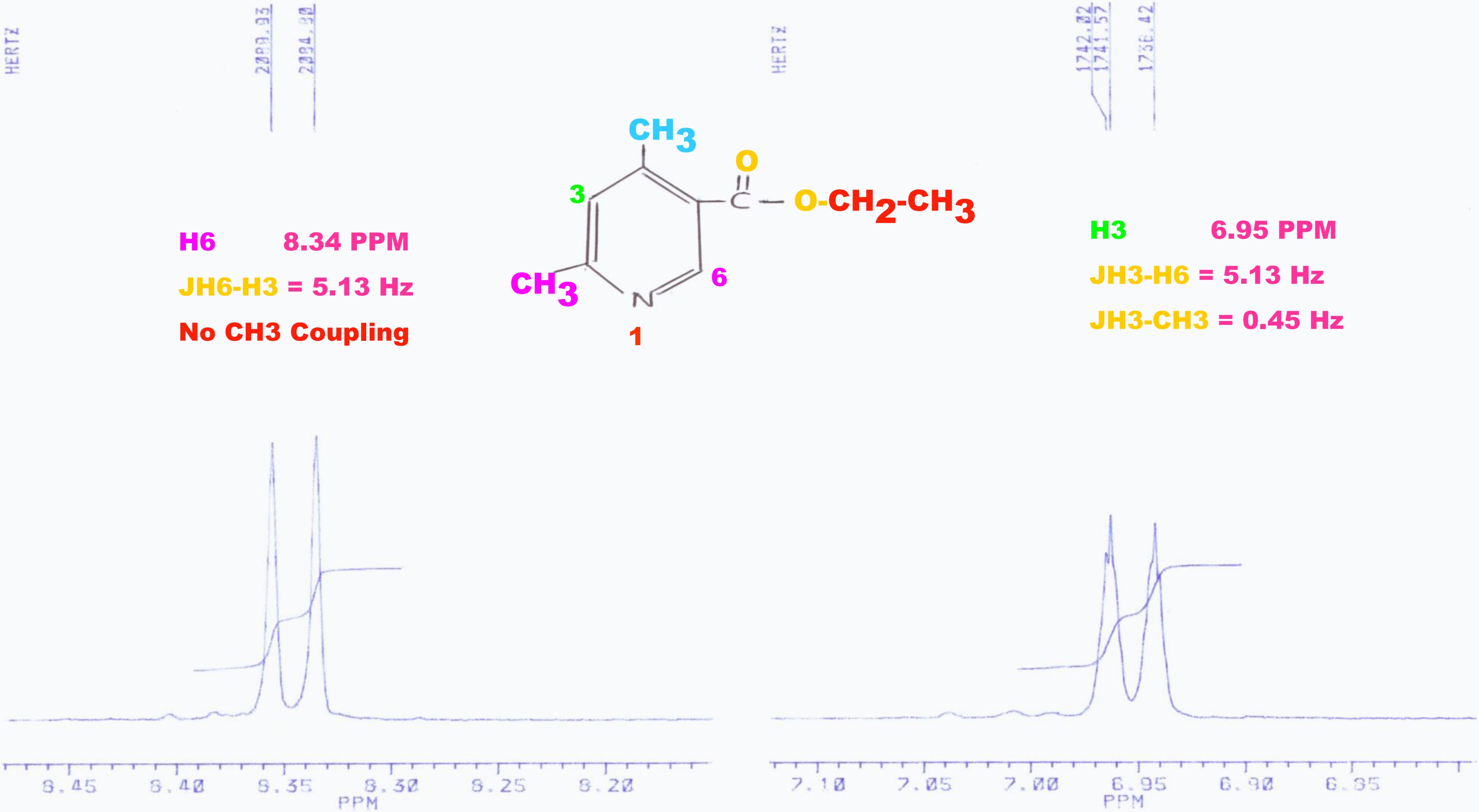
CH_3 1.37 PPM

Triplet

J = 7.18 Hz

Analysis and Interpretation of ^{1}H NMR Spectrum of Ethyl-2,4-Dimethylnicotinate

$C_5H_2N(CH_3)(CH_3)(CO\text{-}O\text{-}CH_2CH_3)$



H6 **8.34 PPM**

JH6-H3 = 5.13 Hz

No CH3 Coupling

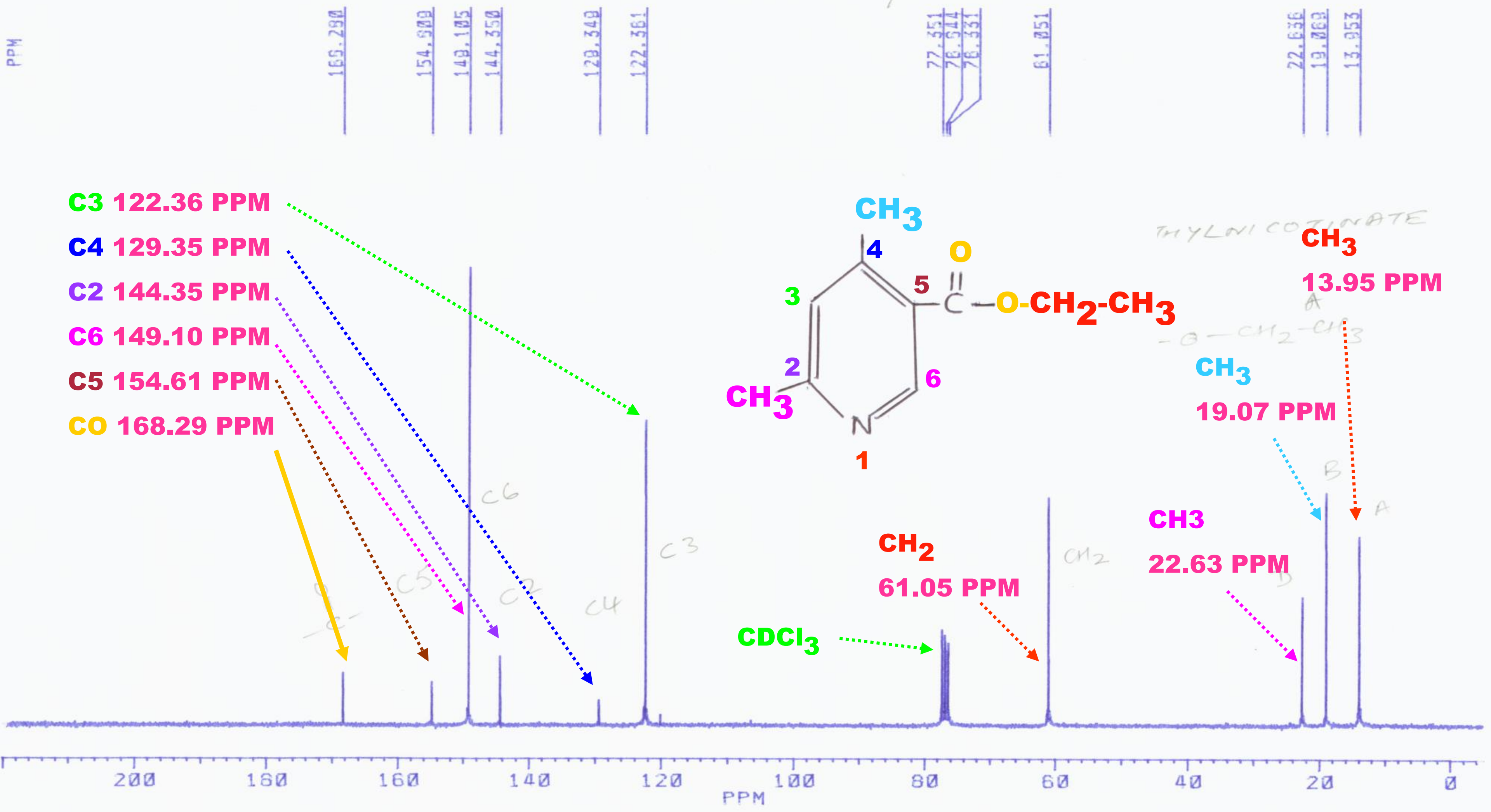
H3 **6.95 PPM**

JH3-H6 = 5.13 Hz

JH3-CH3 = 0.45 Hz

Analysis and Interpretation of ^{13}C NMR Spectrum of Ethyl-2,4-Dimethylnicotinate

$C_5H_2N(CH_3)(CH_3)(CO\text{-}O\text{-}CH_2CH_3)$



C3 122.36 PPM

C4 129.35 PPM

C2 144.35 PPM

C6 149.10 PPM

C5 154.61 PPM

CO 168.29 PPM

CH_3 13.95 PPM

CH_3 19.07 PPM

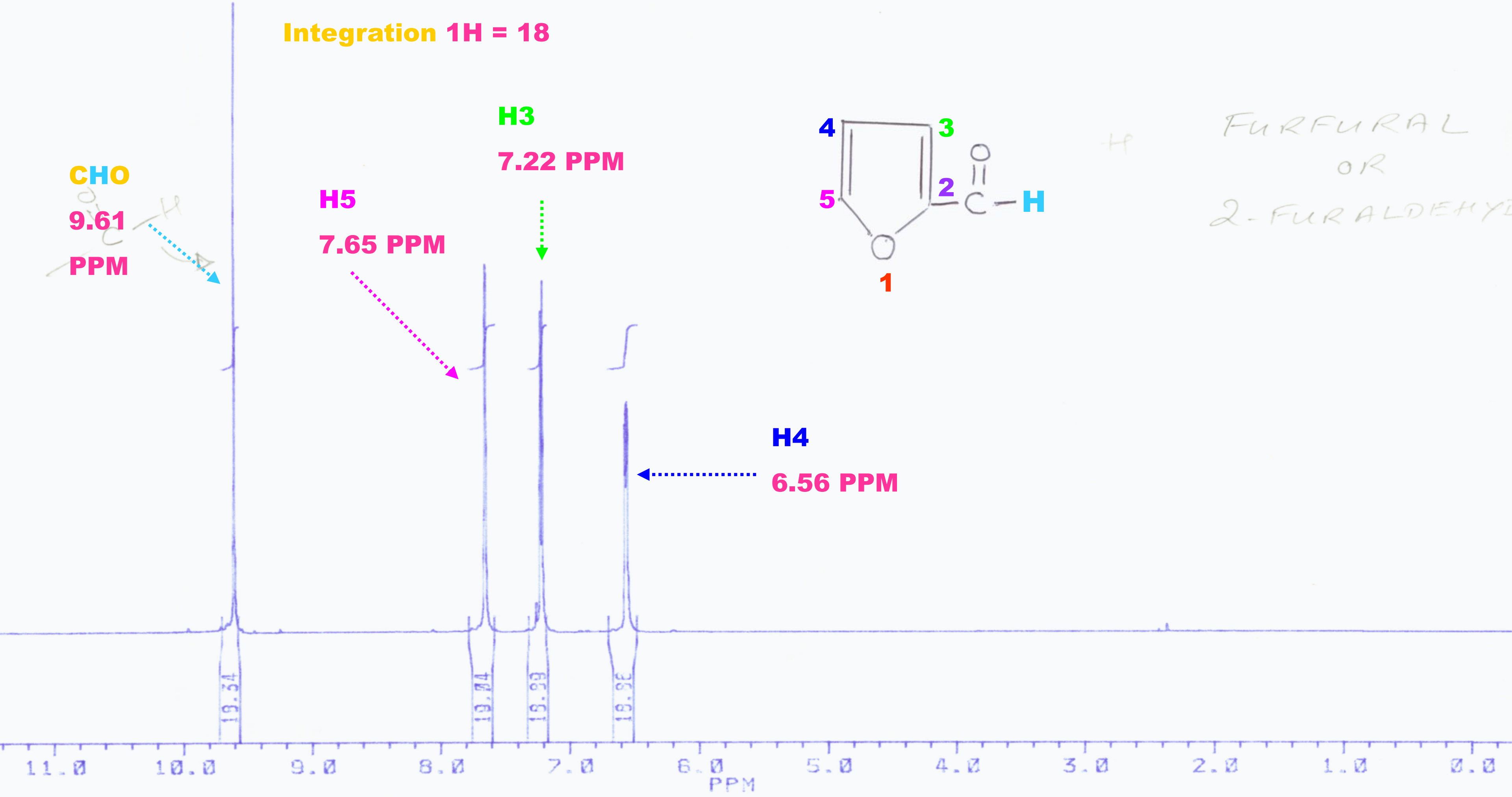
CH3 22.63 PPM

CH_2 61.05 PPM

$CDCl_3$

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Furfural (2-Furaldehyde)

$C_4H_3O\text{-}CHO$ ^{1}H NMR Spectrum



Integration 1H = 18

CHO

9.61

PPM

H5

7.65 PPM

H3

7.22 PPM

H4

6.56 PPM

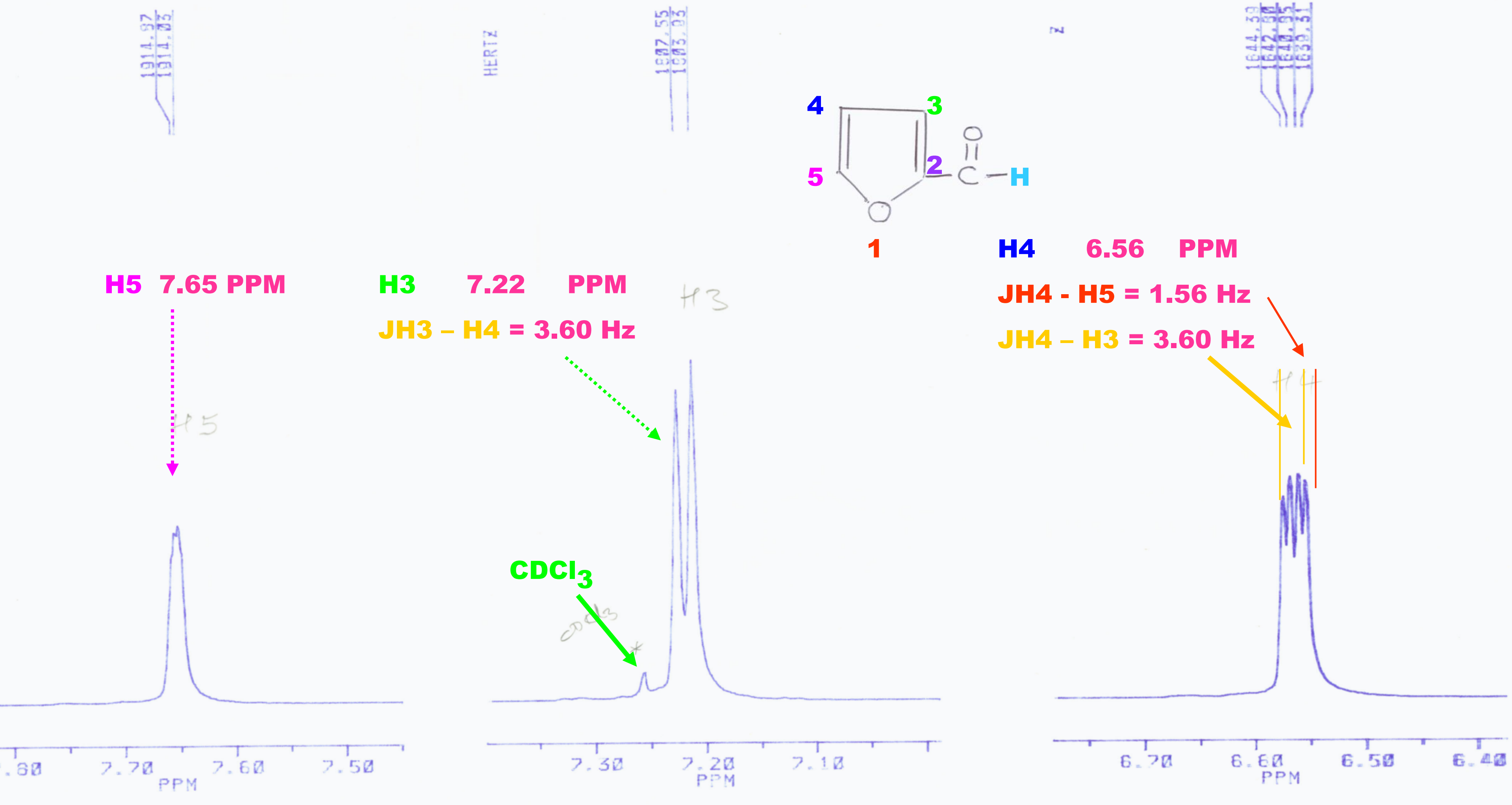
FURFURAL

OR

2-FURALDEHYDE

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of Furfural (2-Furaldehyde)

C_4H_3O-CHO   Expansion of ^{1}H NMR Spectrum



H4 6.56 PPM

JH4 - H5 = 1.56 Hz

JH4 – H3 = 3.60 Hz

H5 7.65 PPM

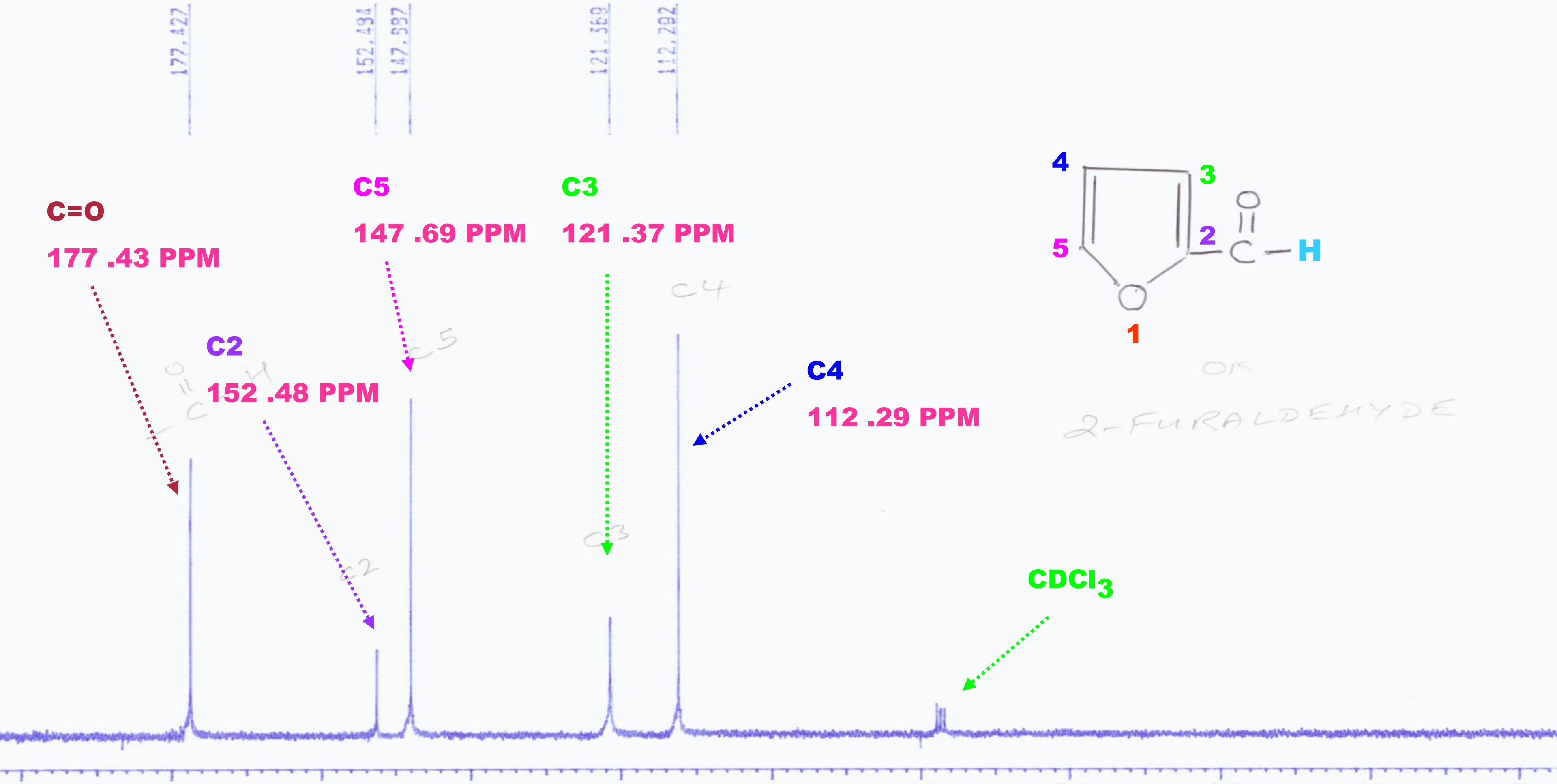
H3 7.22 PPM

JH3 – H4 = 3.60 Hz

$CDCl_3$

Analysis and interpretation of ^{13}C NMR Spectrum of Furfural (2-Furaldehyde)

C_4H_3O-CHO



C=O

177 .43 PPM

C5

147 .69 PPM

C3

121 .37 PPM

C2

152 .48 PPM

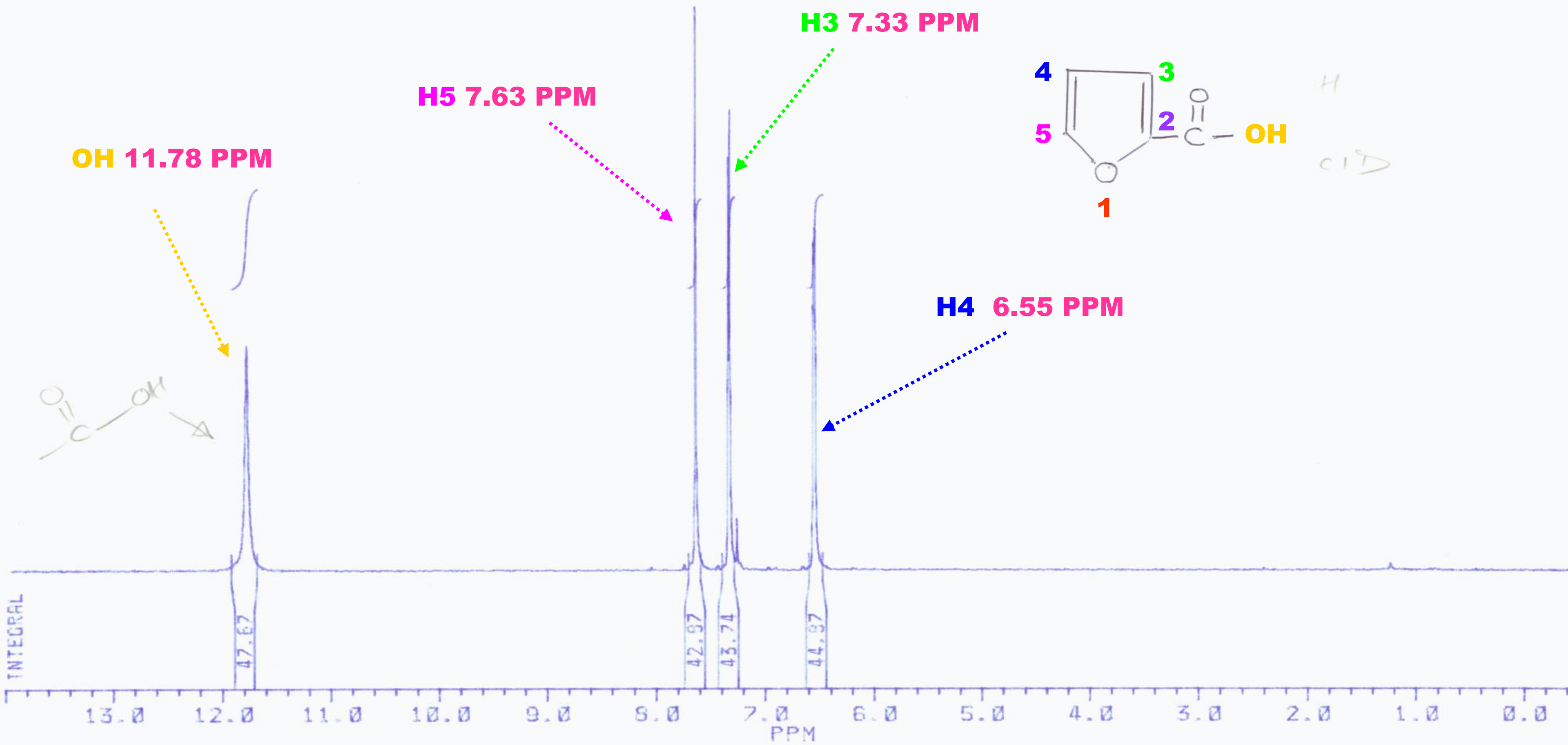
C4

112 .29 PPM

$CDCl_3$

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 2-Furoic Acid

C_4H_3O-(CO-OH) ^{1}H NMR Spectrum



Integration 1H = 44

OH 11.78 PPM

H5 7.63 PPM

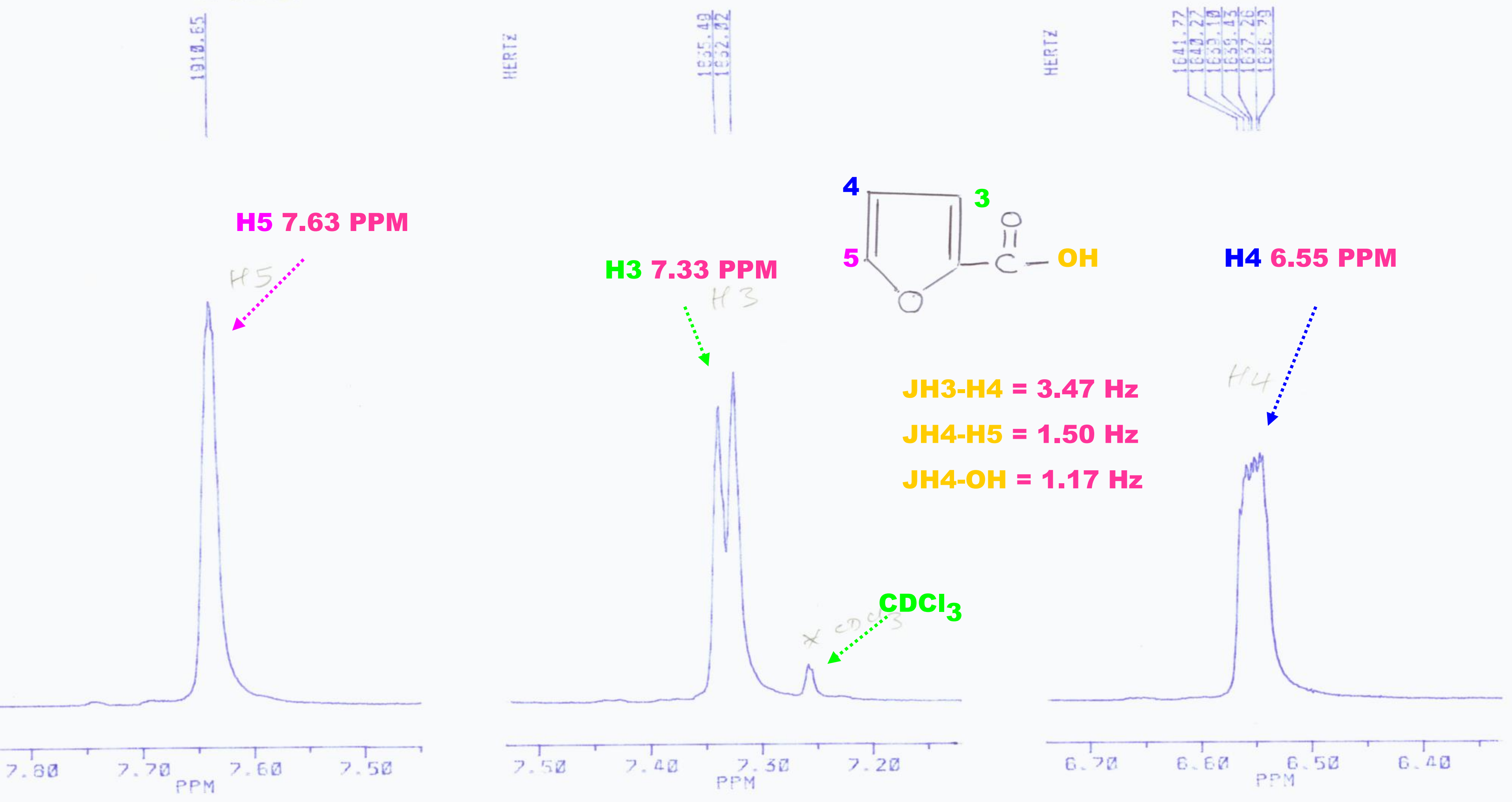
H3 7.33 PPM

H4 6.55 PPM

Analysis and interpretation of ^{1}H & ^{13}C NMR Spectra of 2-Furoic Acid

C_4H_3O-(CO-OH)

Expansion of ^{1}H NMR Spectrum



H5 7.63 PPM

H3 7.33 PPM

H4 6.55 PPM

$CDCl_3$

JH3-H4 = 3.47 Hz

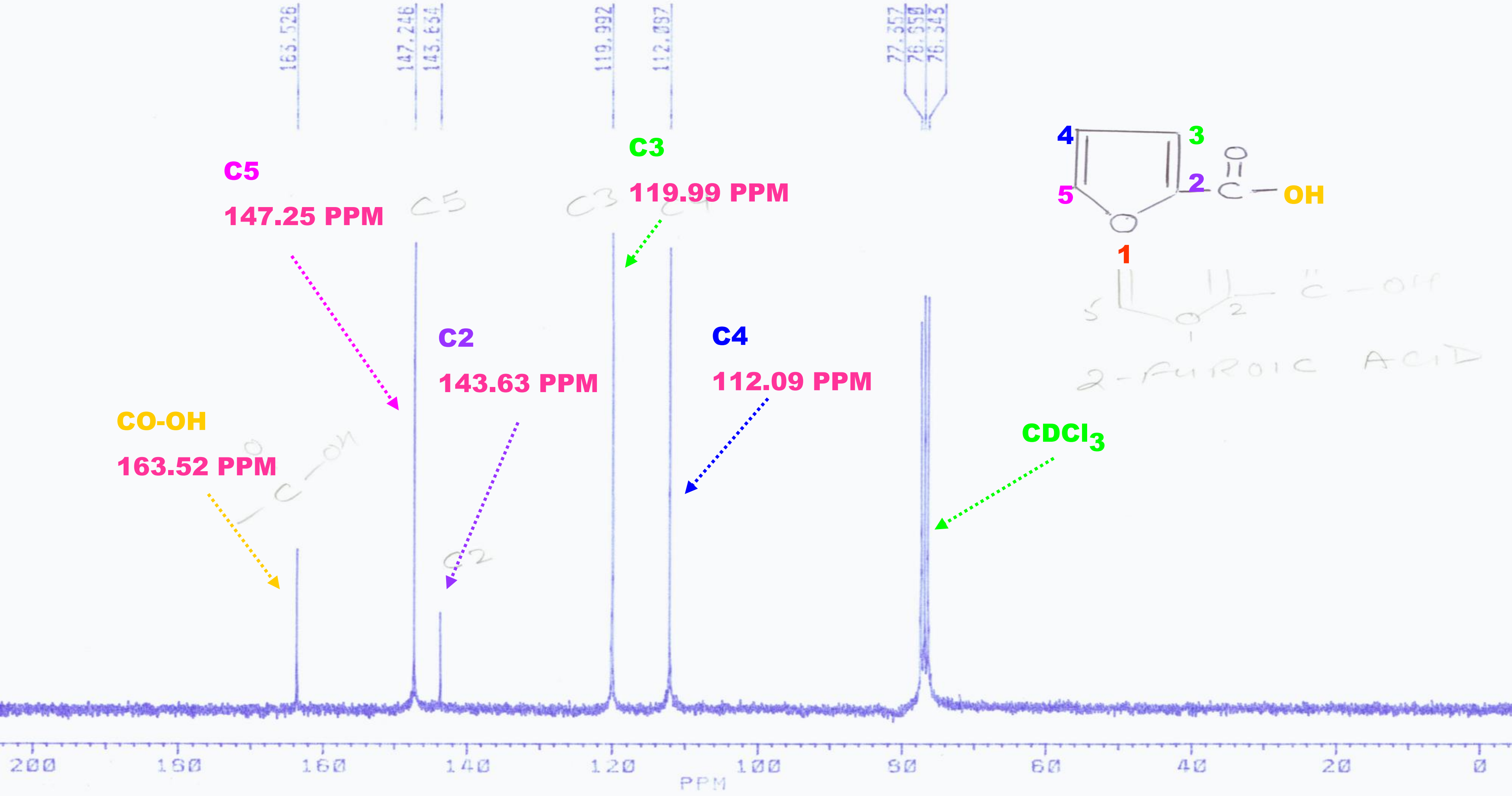
JH4-H5 = 1.50 Hz

JH4-OH = 1.17 Hz

Analysis and interpretation of ^{13}C NMR Spectra of 2-Furoic Acid

$C_4H_3O\text{-}(CO\text{-}OH)$

^{13}C NMR Spectrum



C5

147.25 PPM

C3

119.99 PPM

C2

143.63 PPM

C4

112.09 PPM

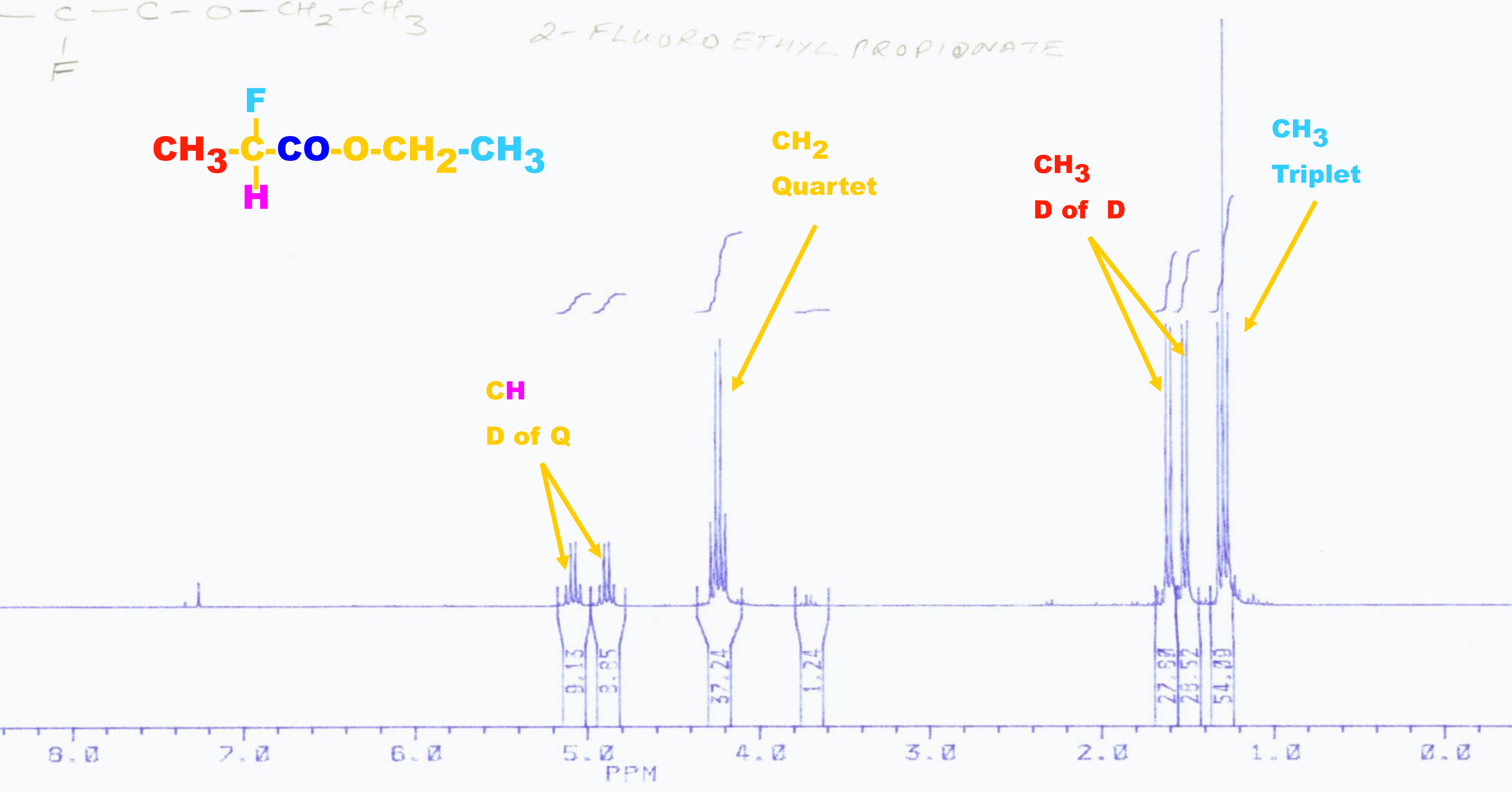
CO-OH

163.52 PPM

$CDCl_3$

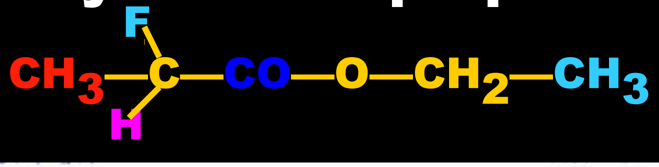
Analysis and Interpretation of ^{1}H NMR Spectrum of Ethyl-2-Fluoropropionate

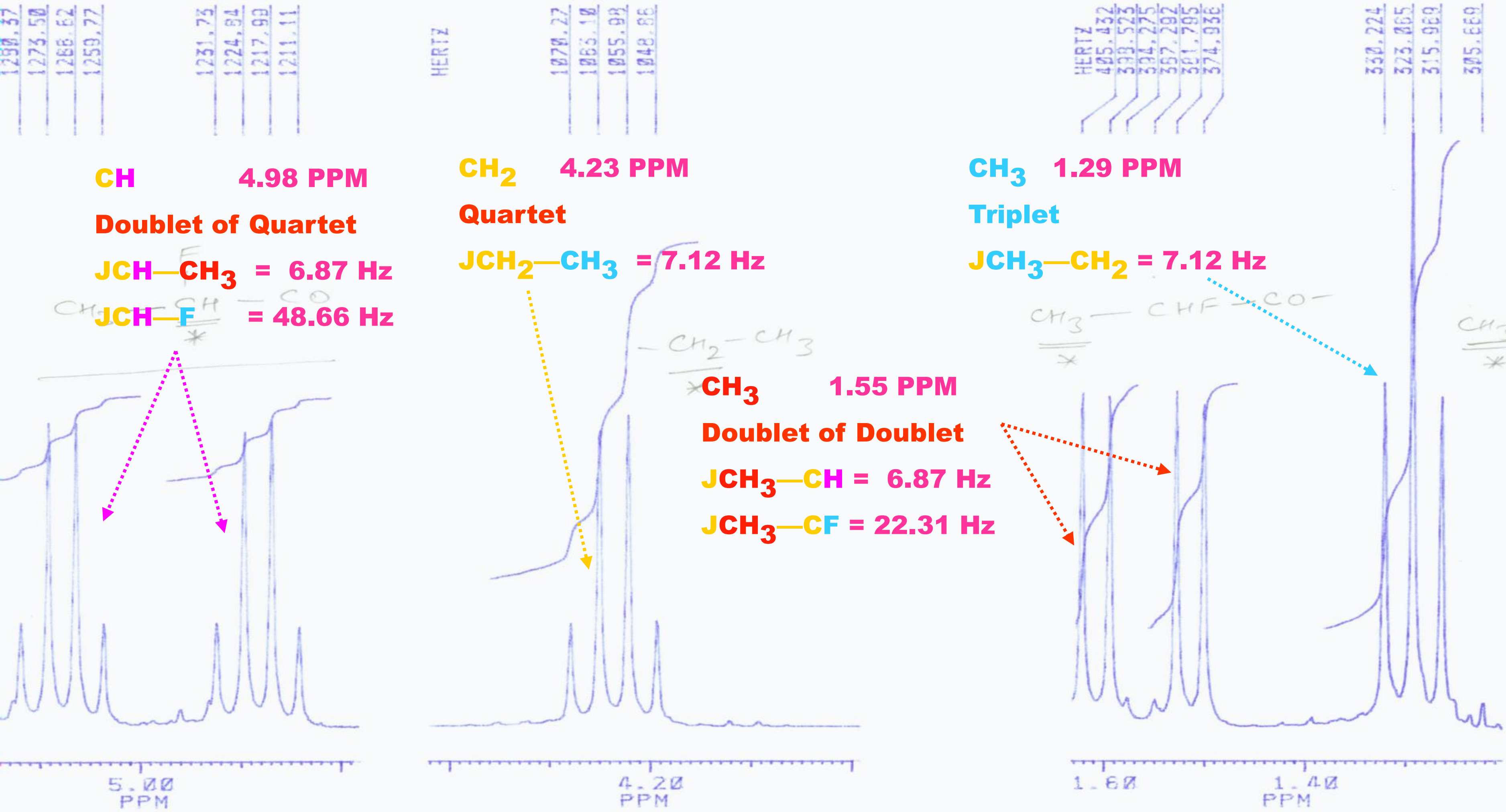
CH_3-CHF-CO-O-CH_2CH_3



$$CH_3\text{-}\overset{F}{\underset{H}{C}}\text{-CO-O-}CH_2\text{-}CH_3$$

Analysis and Interpretation of ^{1}H NMR Spectrum of Ethyl-2-Fluoropropionate CH_3-CHF-CO-O-CH_2CH_3





CH 4.98 PPM

Doublet of Quartet

JCH—CH_3 = 6.87 Hz

JCH—F = 48.66 Hz

CH_2 4.23 PPM

Quartet

JCH_2—CH_3 = 7.12 Hz

CH_3 1.29 PPM

Triplet

JCH_3—CH_2 = 7.12 Hz

CH_3 1.55 PPM

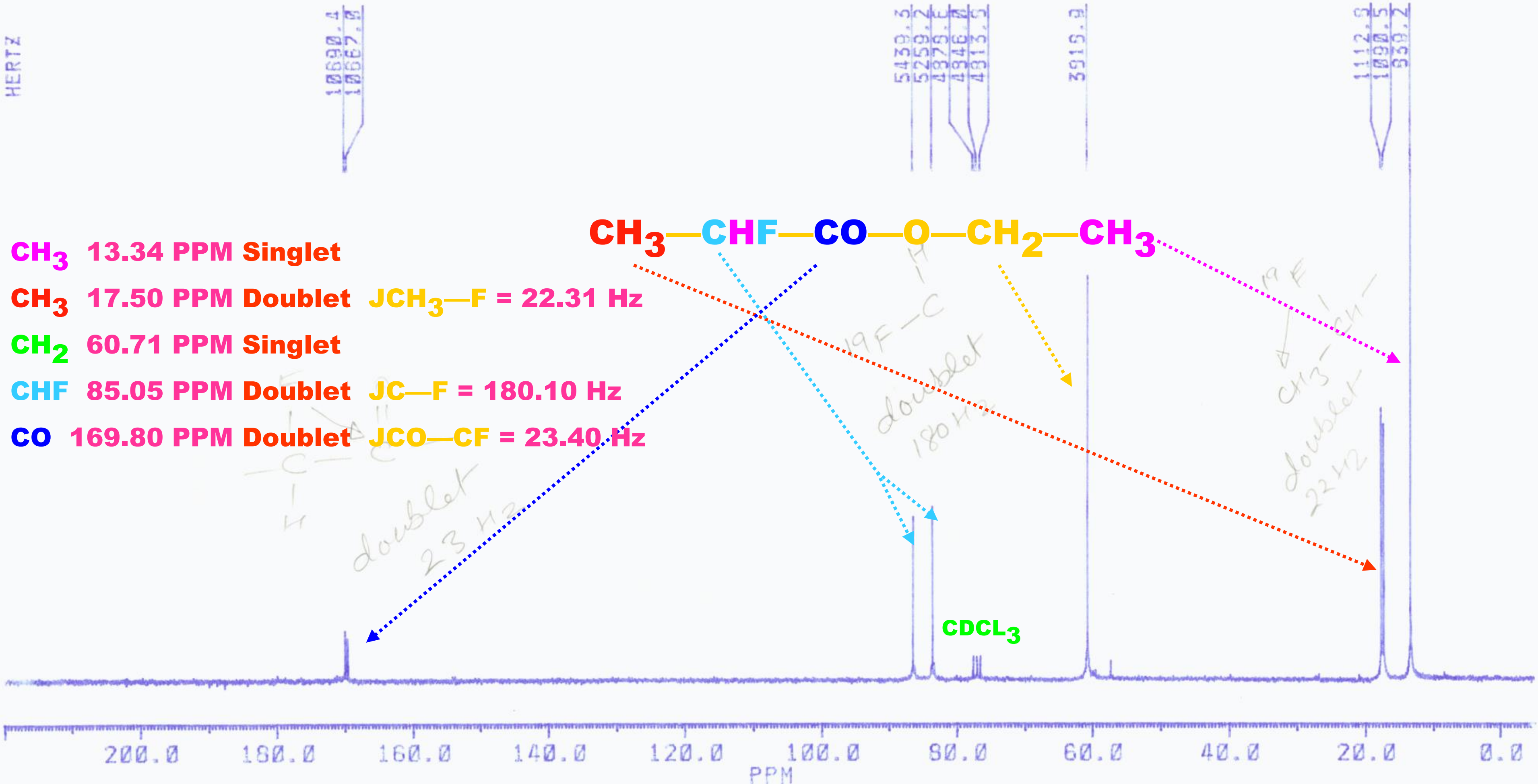
Doublet of Doublet

JCH_3—CH = 6.87 Hz

JCH_3—CF = 22.31 Hz

Analysis and Interpretation of ^{13}C NMR Spectrum of Ethyl-2-Fluoropropionate

CH_3-CHF-CO-O-CH_2CH_3



CH_3—CHF—CO—O—CH_2—CH_3

CH_3 13.34 PPM Singlet

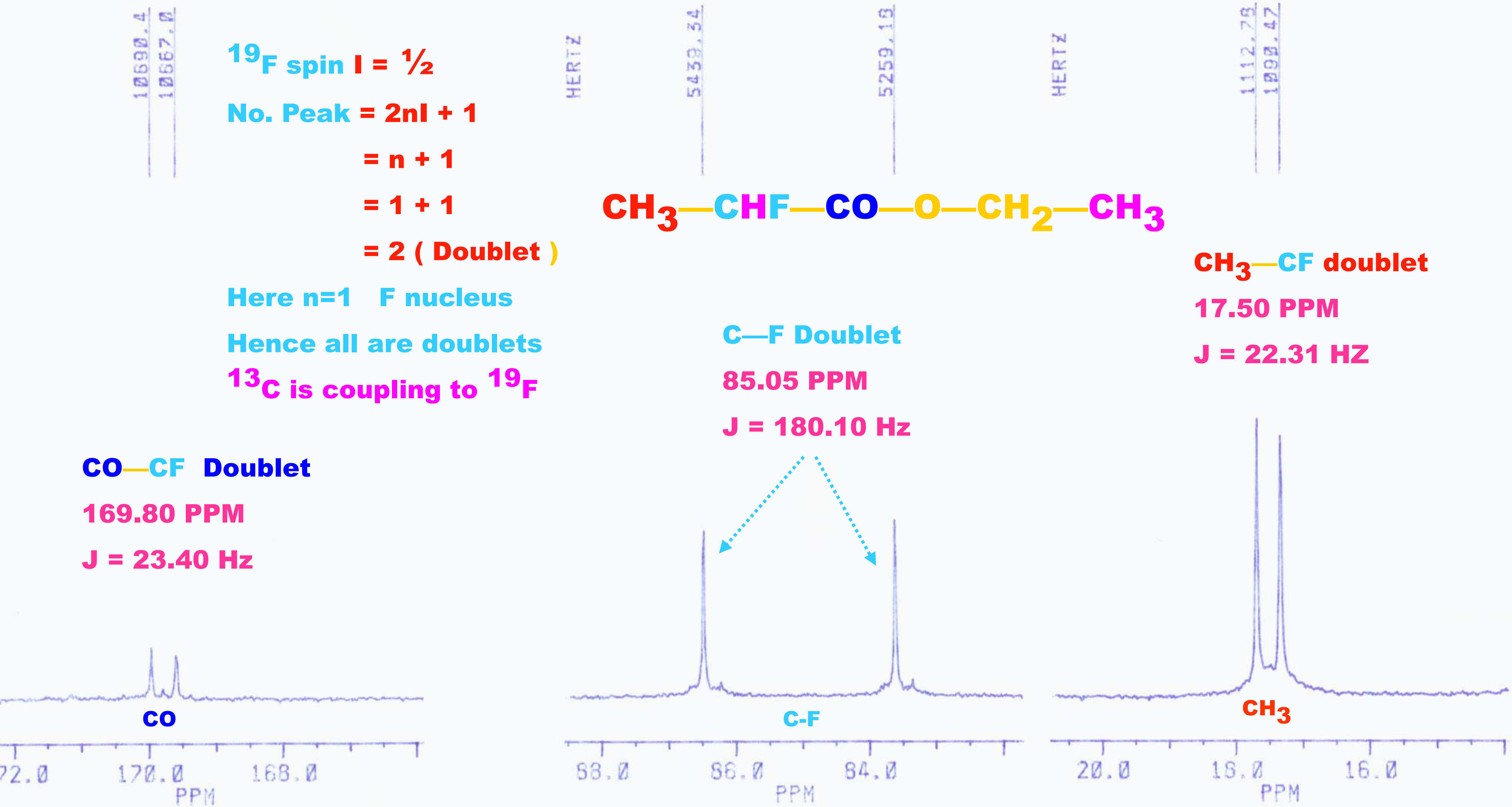
CH_3 17.50 PPM Doublet JCH_3—F = 22.31 Hz

CH_2 60.71 PPM Singlet

CHF 85.05 PPM Doublet JC—F = 180.10 Hz

CO 169.80 PPM Doublet JCO—CF = 23.40 Hz

Analysis and Interpretation of ^{13}C NMR Spectrum of Ethyl-2-Fluoropropionate (Expansion) CH_3-CHF-CO-O-CH_2CH_3



^{19}F spin I = ½

No. Peak = 2nI + 1

= n + 1

= 1 + 1

= 2 (Doublet)

Here n=1 F nucleus

Hence all are doublets

^{13}C is coupling to ^{19}F

CH_3—CHF—CO—O—CH_2—CH_3

CH_3—CF doublet

17.50 PPM

J = 22.31 HZ

C—F Doublet

85.05 PPM

J = 180.10 Hz

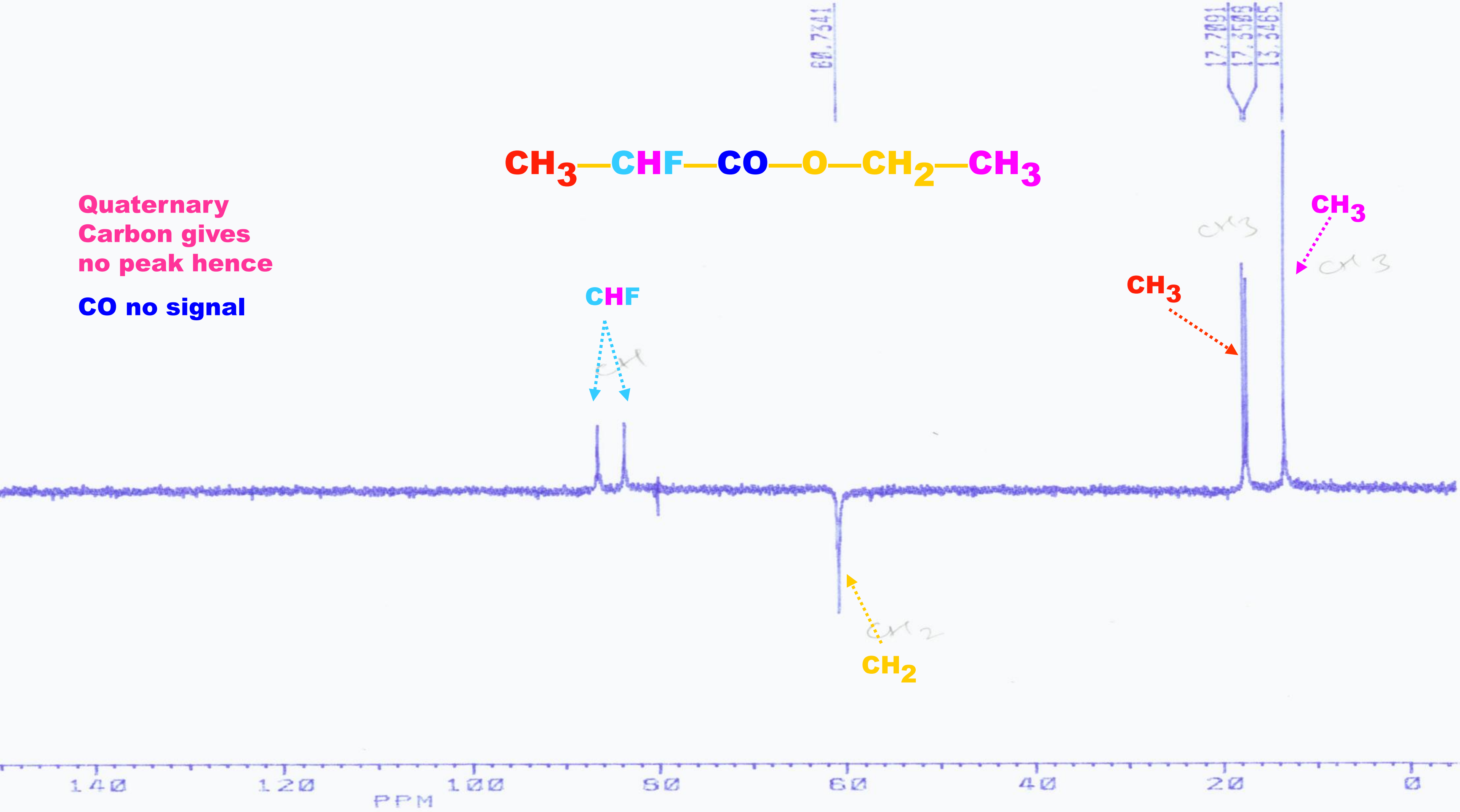
CO—CF Doublet

169.80 PPM

J = 23.40 Hz

Analysis and Interpretation of ^{13}C NMR Spectrum of Ethyl-2-Fluoropropionate (Dept 135)

CH_3-CHF-CO-O-CH_2CH_3



CH_3—CHF—CO—O—CH_2—CH_3

Quaternary Carbon gives no peak hence

CO no signal

CHF

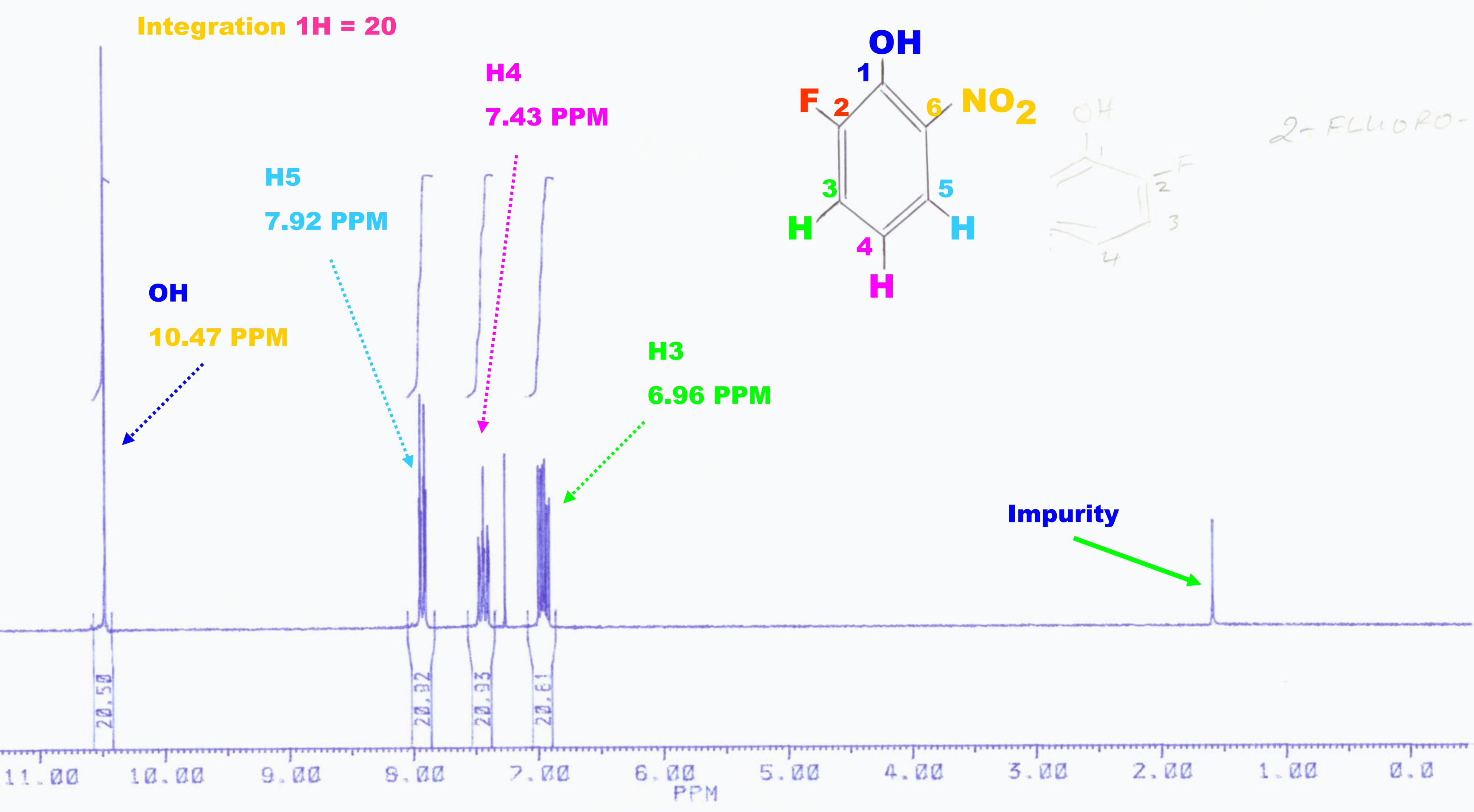
CH_3

CH_3

CH_2

^1H NMR spectrum of 2-Fluoro-6-Nitrophenol

$C_6H_3(F)(NO_2)(OH)$



Integration 1H = 20

OH

10.47 PPM

H5

7.92 PPM

H4

7.43 PPM

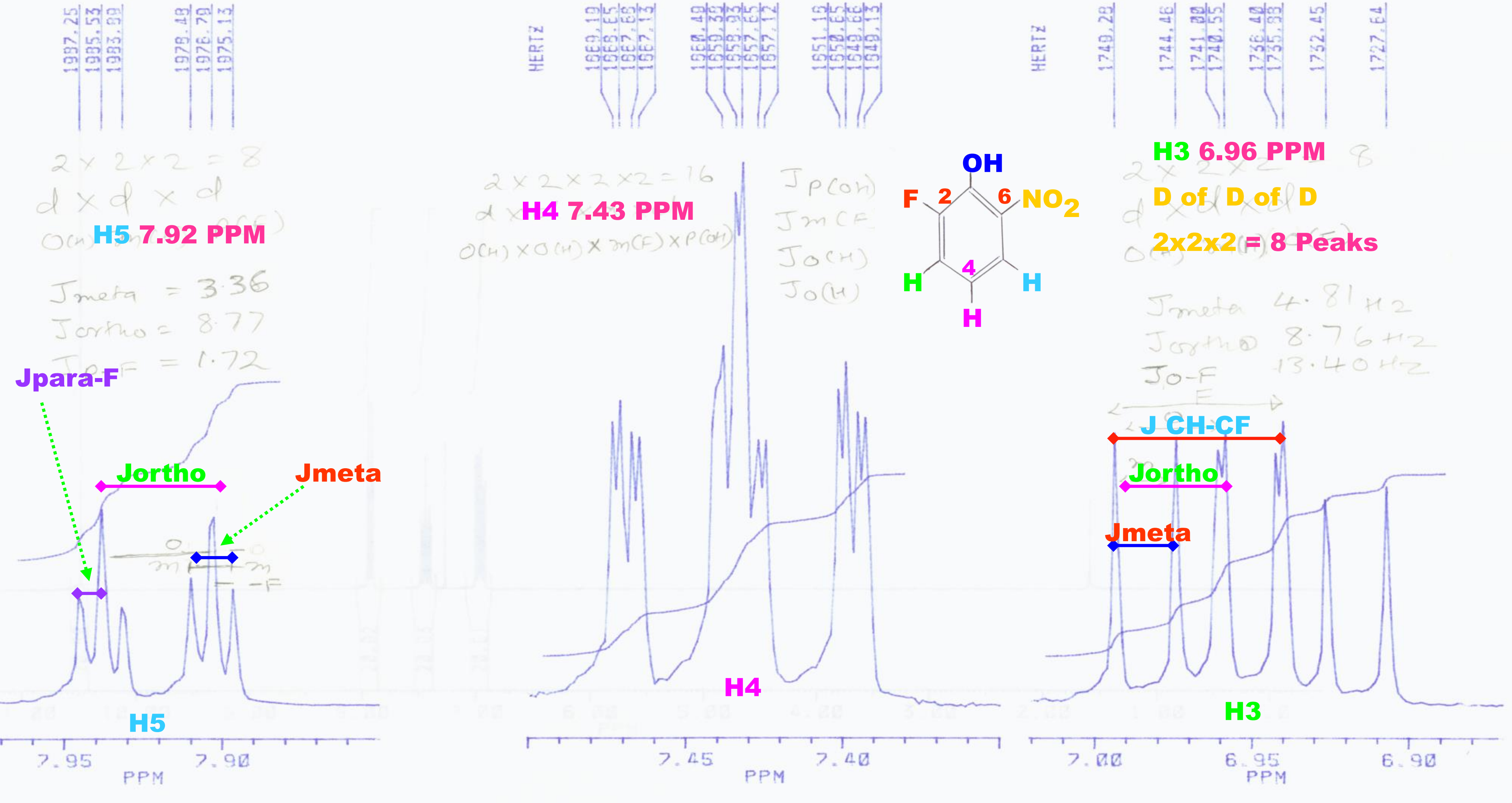
H3

6.96 PPM

Impurity

^{1}H NMR spectrum of 2-Fluoro-6-Nitrophenol

$C_6H_3(F)(NO_2)(OH)$



H5 7.92 PPM

H4 7.43 PPM

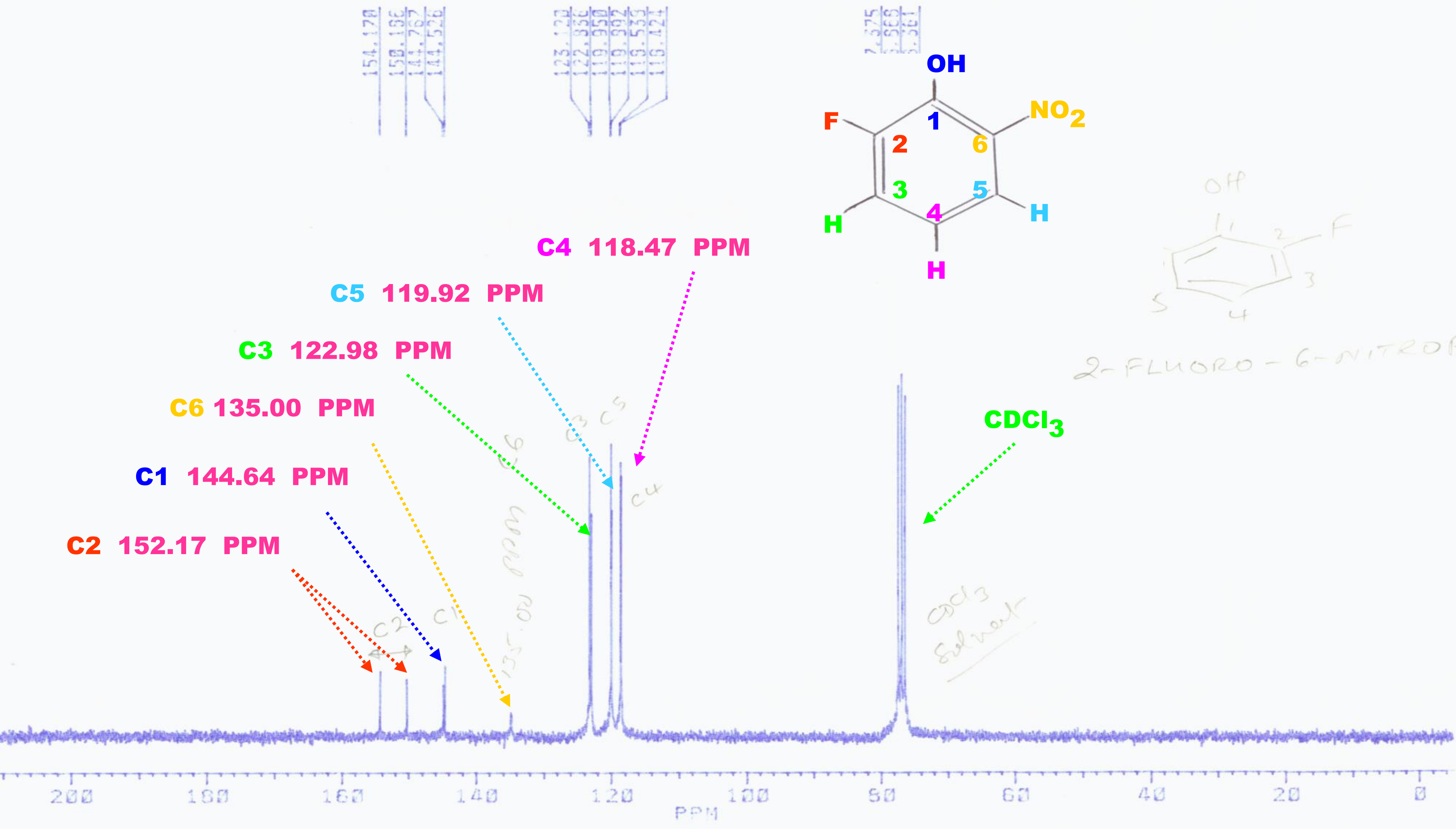
H3 6.96 PPM

D of D of D

2x2x2 = 8 Peaks

^{13}C NMR spectrum of 2-Fluoro-6-Nitrophenol

$C_6H_3(F)(NO_2)(OH)$



C4 118.47 PPM

C5 119.92 PPM

C3 122.98 PPM

C6 135.00 PPM

C1 144.64 PPM

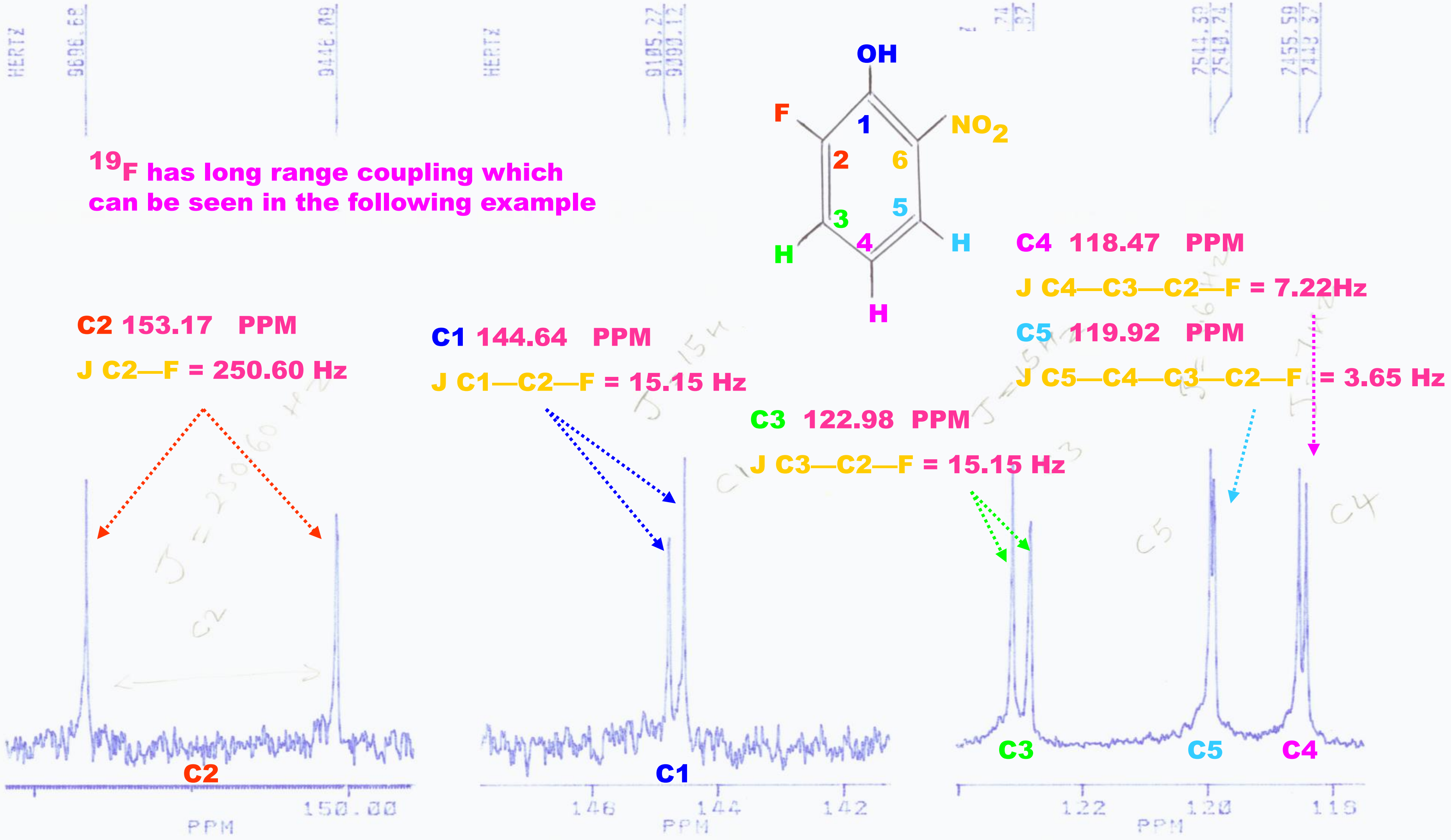
C2 152.17 PPM

CDCl$_3$

Expansion of ^{13}C NMR spectrum of 2-Fluoro-6-Nitrophenol

$C_6H_3(F)(NO_2)(OH)$

^{19}F has long range coupling which can be seen in the following example



C2 153.17 PPM

J C2—F = 250.60 Hz

C1 144.64 PPM

J C1—C2—F = 15.15 Hz

C3 122.98 PPM

J C3—C2—F = 15.15 Hz

C4 118.47 PPM

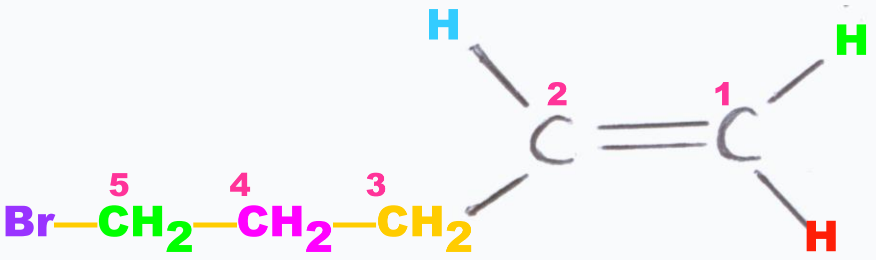
J C4—C3—C2—F = 7.22Hz

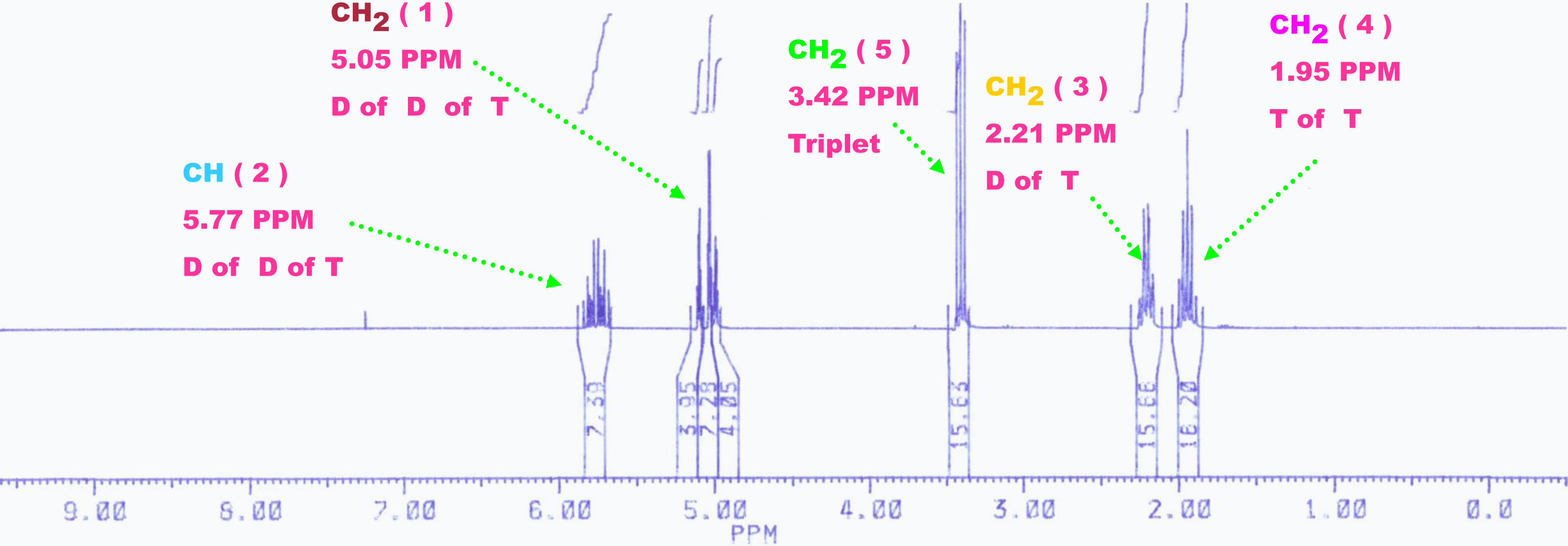
C5 119.92 PPM

J C5—C4—C3—C2—F = 3.65 Hz

^{1}H NMR Spectrum of 5-Bromopent-1-ene
Br-CH$_2$-CH$_2$-CH$_2$-CH=CH$_2$

Integration 1H = 7.5





CH$_2$ (1)
5.05 PPM
D of D of T

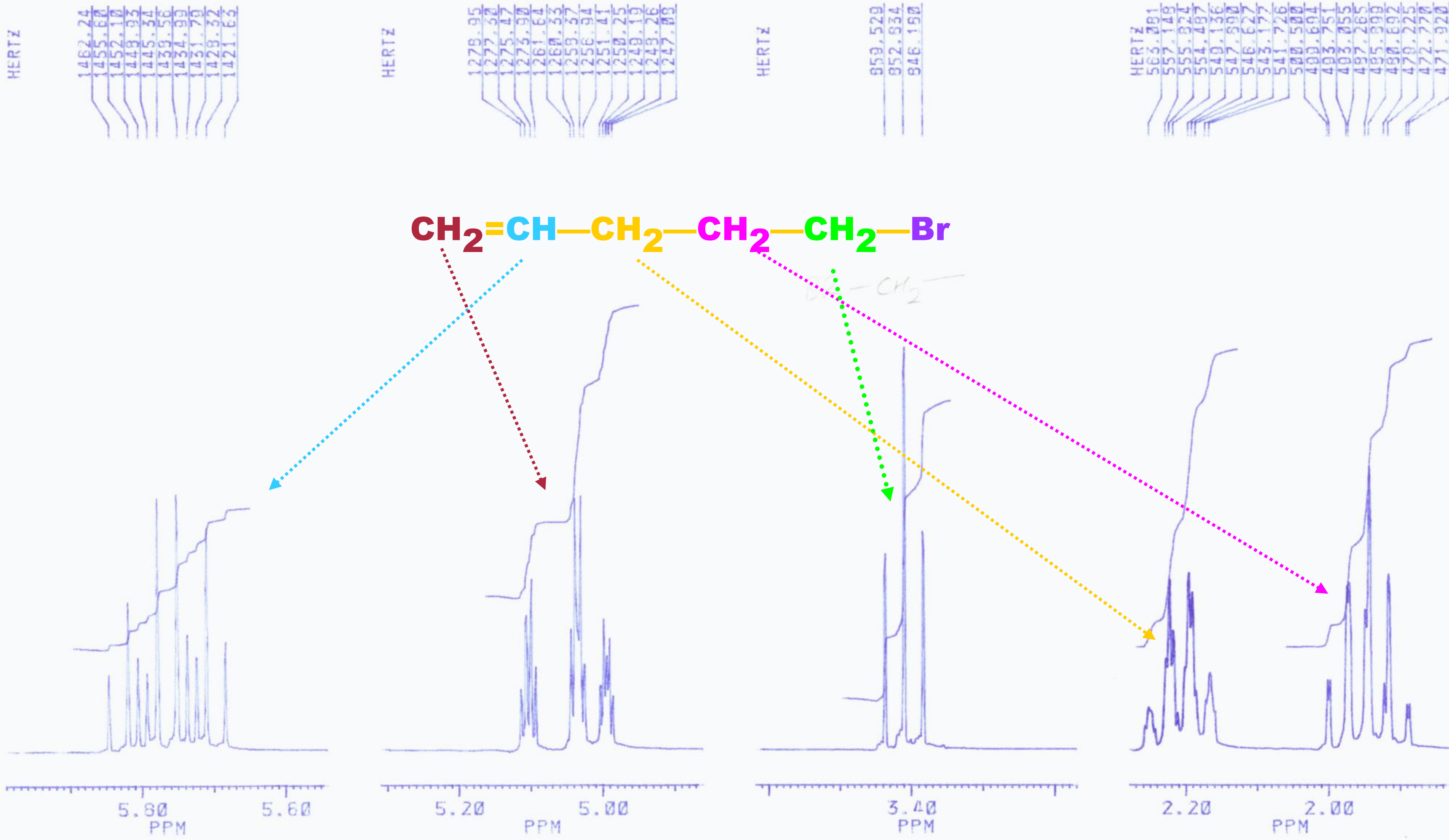
CH (2)
5.77 PPM
D of D of T

CH$_2$ (5)
3.42 PPM
Triplet

CH$_2$ (3)
2.21 PPM
D of T

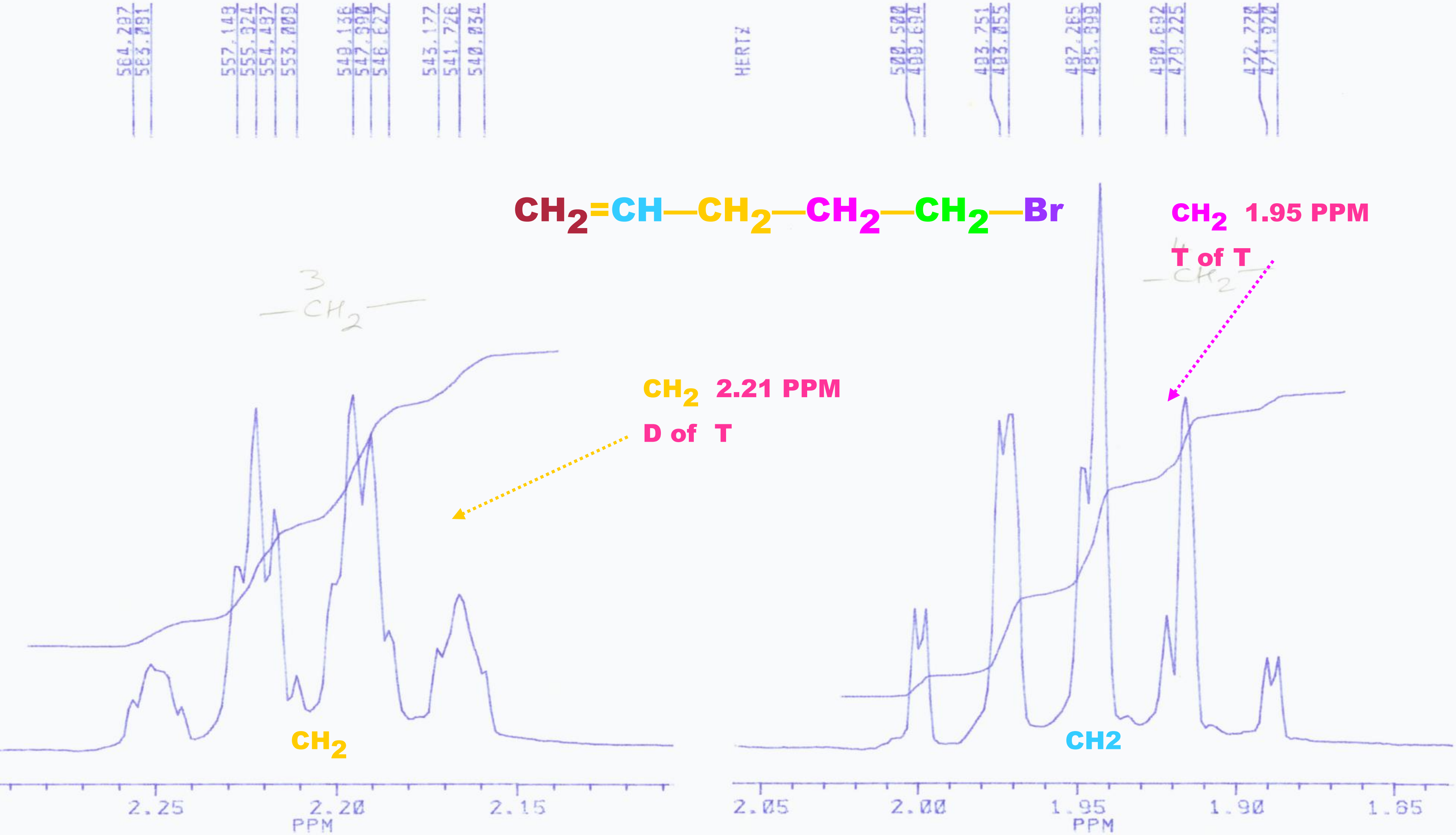
CH$_2$ (4)
1.95 PPM
T of T

^{1}H NMR Spectrum of 5-Bromopent-1-ene
$Br{-}CH_2{-}CH_2{-}CH_2{-}CH{=}CH_2$



$CH_2{=}CH{-}CH_2{-}CH_2{-}CH_2{-}Br$

^{1}H NMR Spectrum of 5-Bromopent-1-ene
$Br{-}CH_2{-}CH_2{-}CH_2{-}CH{=}CH_2$



$CH_2{=}CH{-}CH_2{-}CH_2{-}CH_2{-}Br$

CH_2 1.95 PPM

T of T

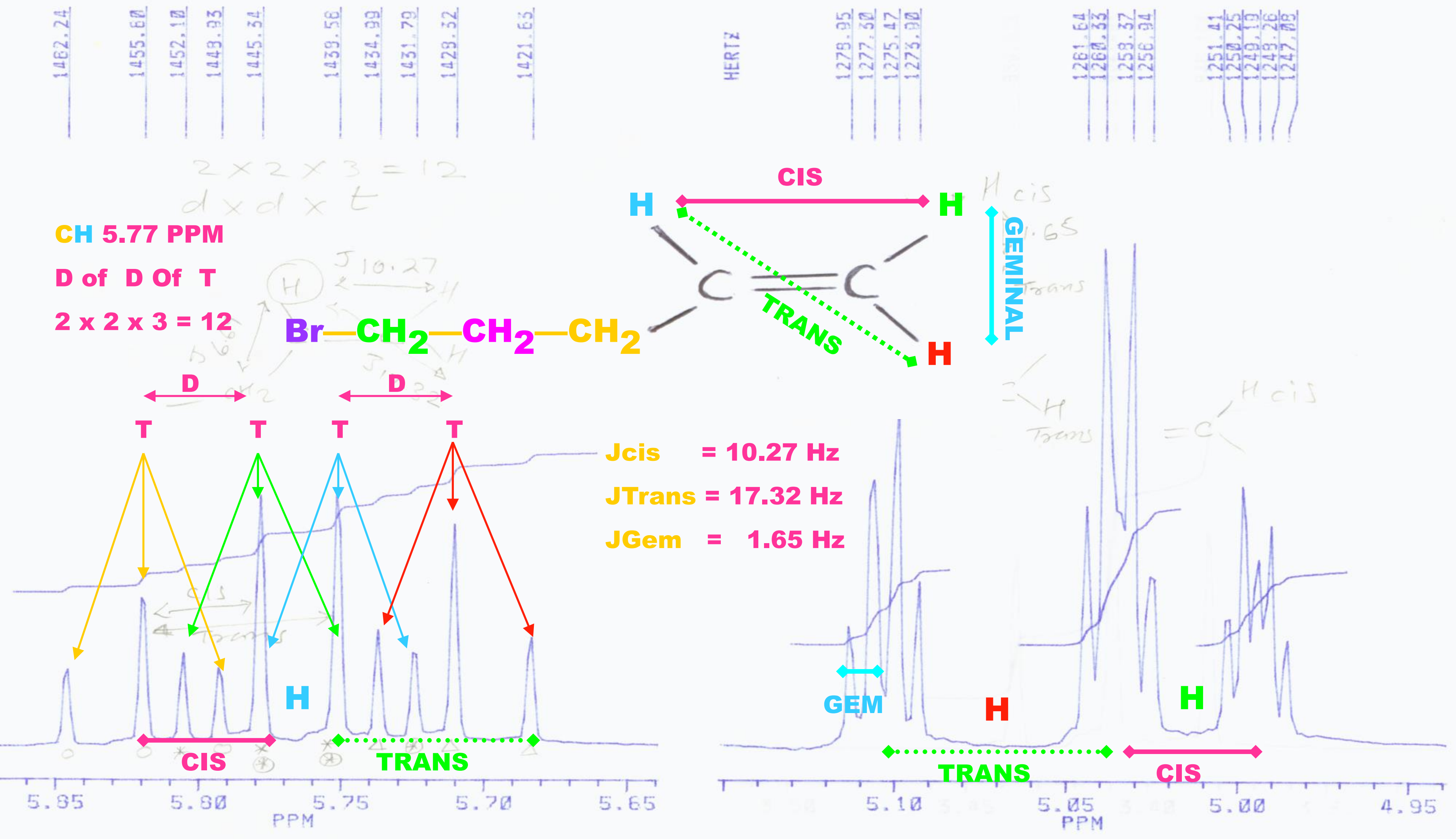
CH_2 2.21 PPM

D of T

CH_2

CH2

^{1}H NMR Spectrum of 5-Bromopent-1-ene
$Br\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH{=}CH_2$



CH 5.77 PPM

D of D Of T

2 x 2 x 3 = 12

Jcis = 10.27 Hz

JTrans = 17.32 Hz

JGem = 1.65 Hz

^{13}C NMR Spectrum of 5-Bromopent-1-ene

Br-CH_2-CH_2-CH_2-CH=CH_2