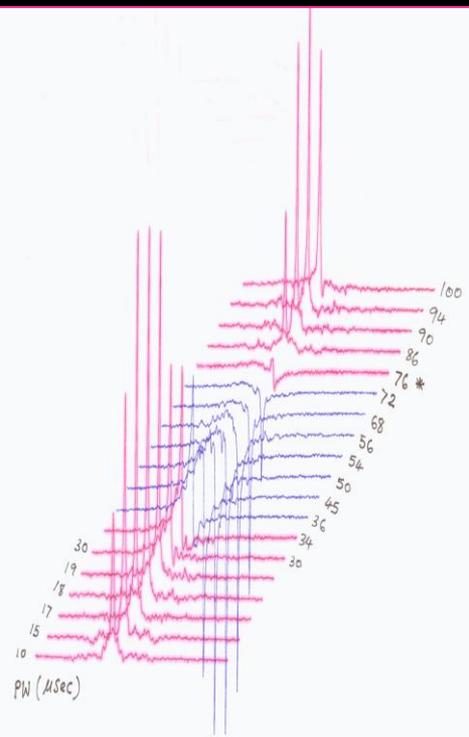


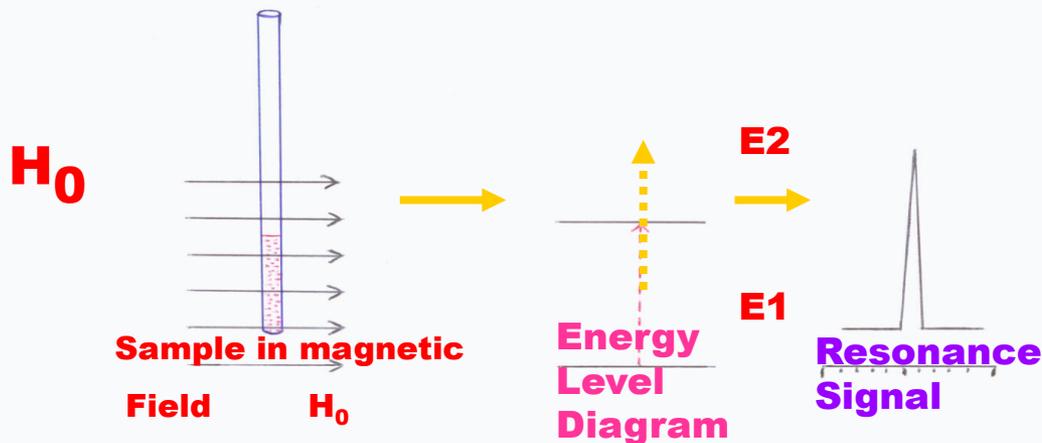
NMR SPECTROSCOPY



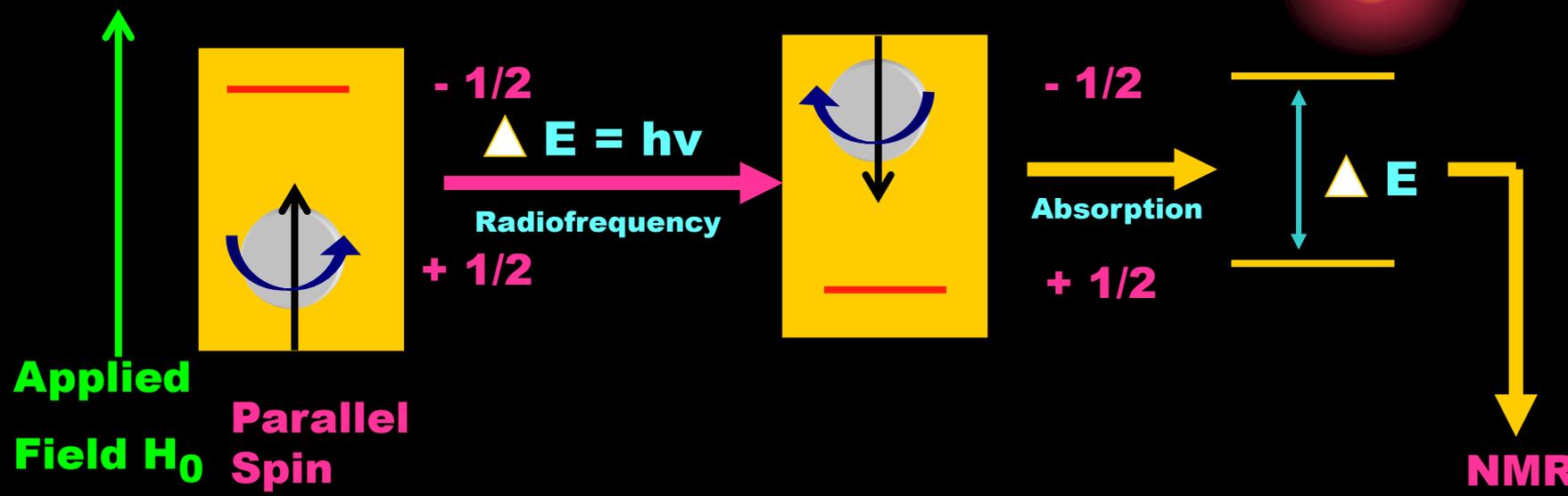
DR. M. KANJIA

When certain Nuclei are placed in a strong magnetic field, ^1H , ^{13}C , ^{19}F , ^{14}N , ^{15}N , ^{10}B , ^{11}B , & ^{31}P These nuclei can absorb electromagnetic radiation in the Radiofrequency (R.F.) range.

The absorption of energy can be detected, amplified and recorded as NMR signal. This phenomenon is known as NMR spectroscopy.



Absorption Of Energy



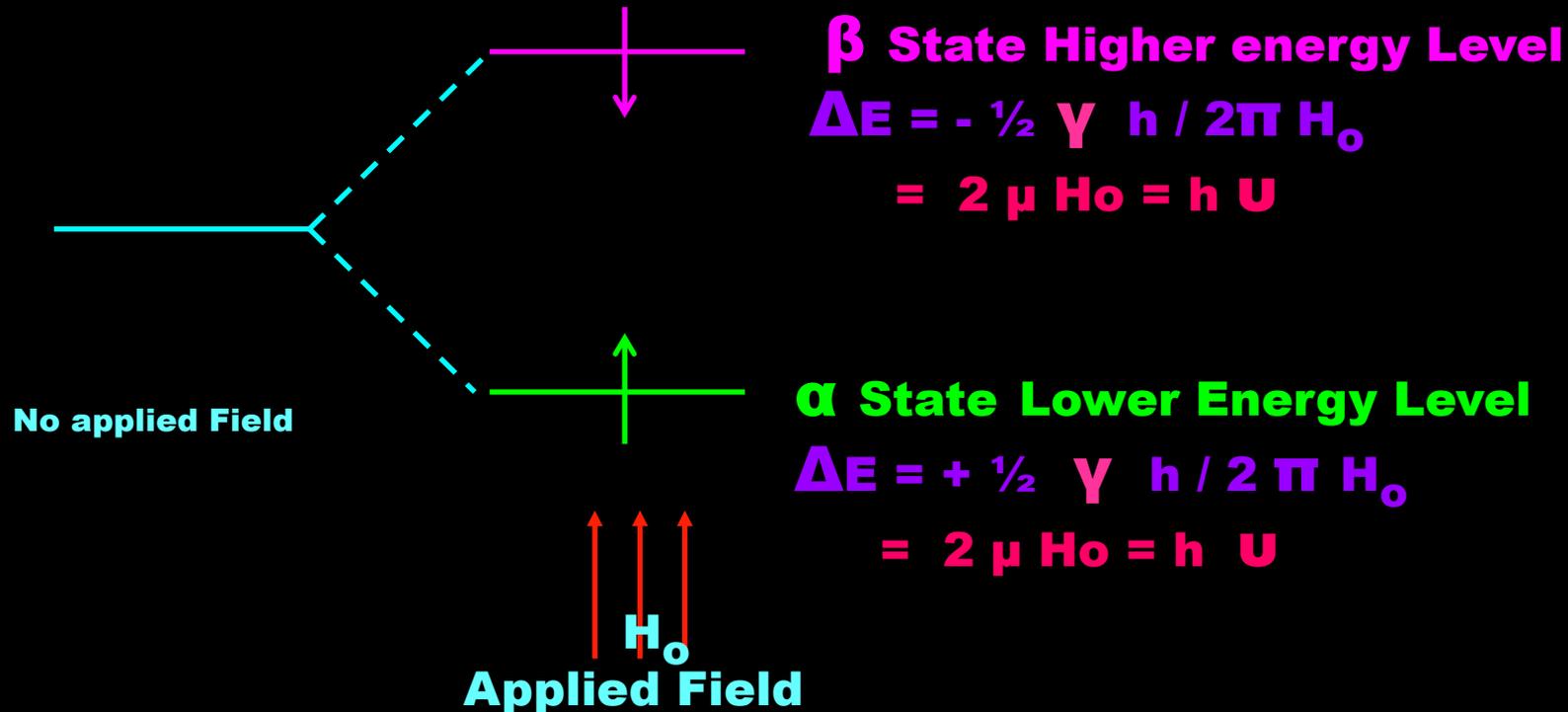
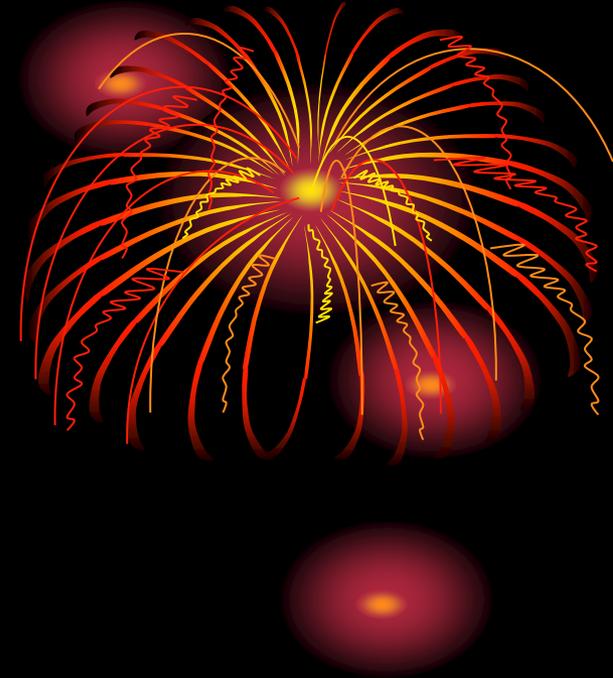
Energy Levels for Spin Active Nucleus ^1H , ^{13}C , ^{19}F Spin Number $I = \frac{1}{2}$

γ = Gyro magnetic ratio of spin active nucleus

ν = Radio frequency of electromagnetic radiation
 μ = Magnetic moment

H_0 = Applied Field

h = Planck 's Constant



Energy Levels for Spin Active Nucleus

^2H , ^7Li & ^{14}N Spin Number $I = 1$

γ = Gyro magnetic ratio of spin active nucleus

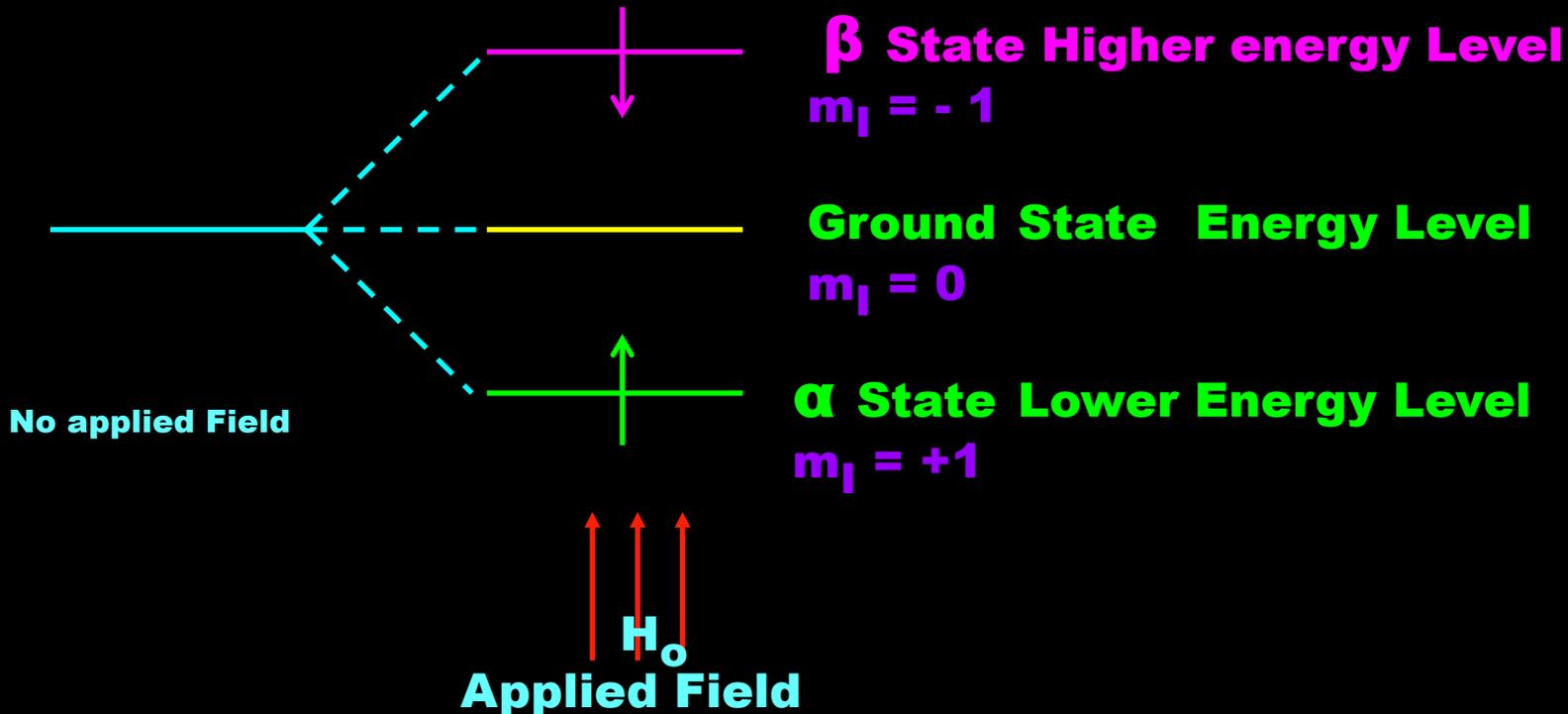
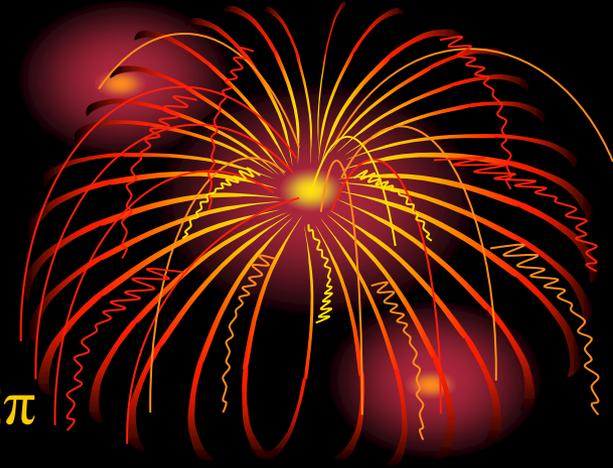
H_0 = Applied Field

h = Planck ' s Constant

J_z = Z component

$$J_z = m_I h/2\pi$$

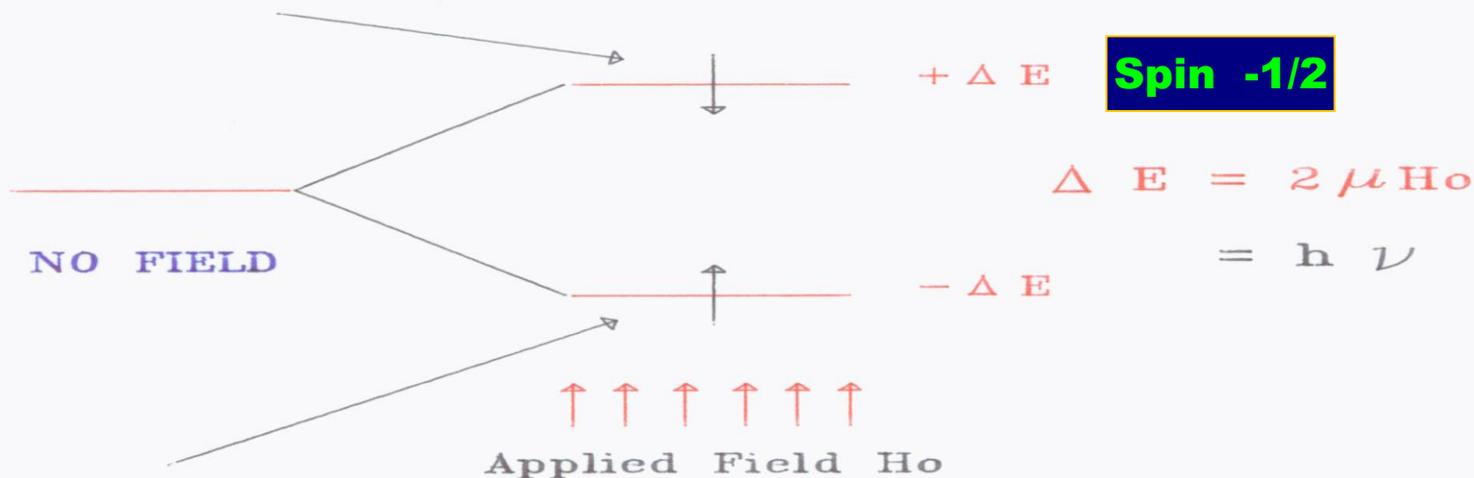
$$\Delta E = \gamma J_z H_0 = \gamma m_I h/2\pi H_0$$



Radio Frequency spectrum



Antiparallel Orientation (Higher Energy State)



Where :

- μ = Magnetic Moment
- H_o = Applied Magnetic Field
- h = Planck's Constant
- ν = Radiofrequency of Electromagnetic radiation

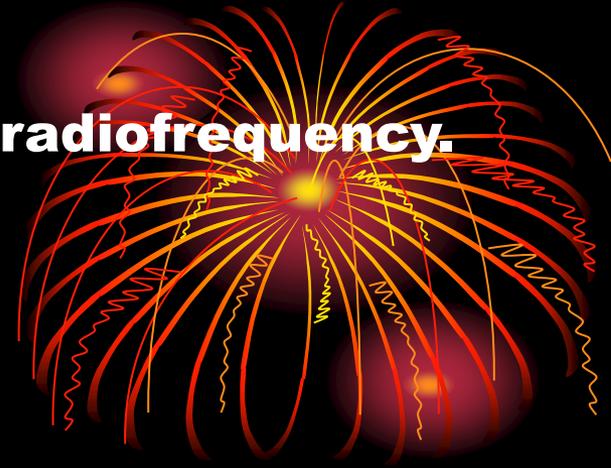
Applied field is directly proportional to radiofrequency.

H_0 = Magnetic Field

μ = Magnetic moment

ν = Radiofrequency

h = Planck's constant

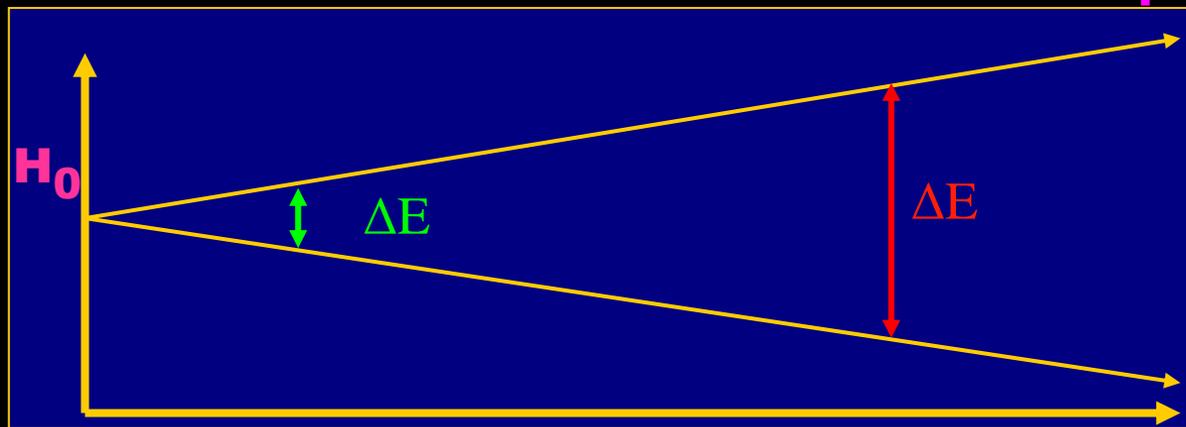


$$\Delta E = 2 \mu H_0 = h \nu$$

$$H_0 \propto \nu$$

For ^1H ^{13}C ^{19}F ^{15}N & ^{31}P nuclei only two orientations are allowed under applied magnetic field spins are aligned parallel (in line with applied field) and anti parallel (opposite with applied field)

- The energy difference ΔE between allowed spin states increases linearly with applied field (H_0) strength.
- ^1H @ 7.05 T the energy difference = 0.120 J/mol = 0.286 Cal/mol
- Which corresponds to electromagnetic radiation of 300 MHz
- (300 000 000 Hz = 300×10^6 Hz) .
- For ^{13}C = 0.030 J / mol = 0.00715 Cal / mol corresponds to RF of 75 MHz.



1.41 T

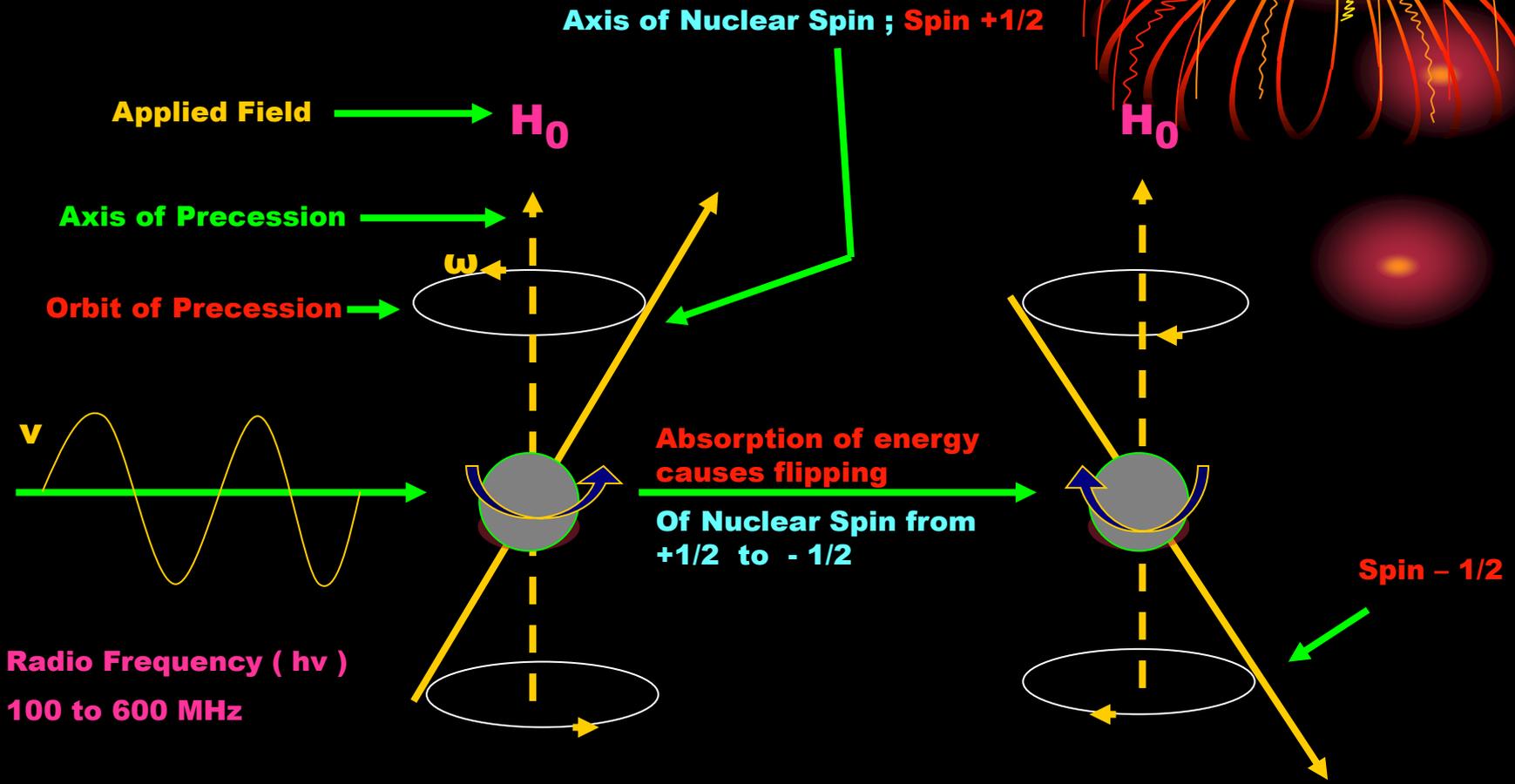
H_0 Tesla

7.05 T

$\Delta E = 0.0239$ J / mol

$\Delta E = 0.120$ J / mol

Nuclei precess at frequency ω when placed in a strong magnetic field.
If $\nu = \omega$ then energy will be absorbed and flipping of the spin will occur.
This process will give rise to NMR signal.



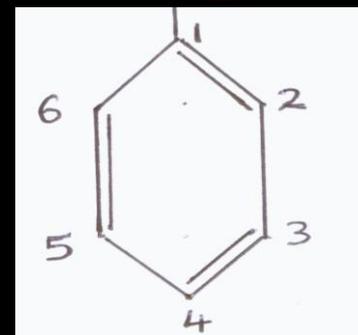
How NMR Signals are generated



- In Ethyl benzene different types of ^1H precess at different frequency at constant magnetic field H_0
- Radio frequency (R F) 250 MHz correspondence to 5.88 Tesla Field

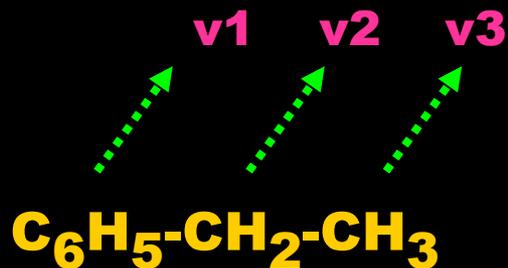
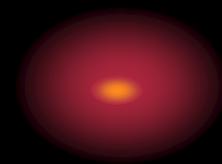


- C_6H_5 precess @ 249.998222 MHz (1778 Hz)
- CH_2 precess @ 249.999368 MHz (632 Hz)
- CH_3 precess @ 249.999721 MHz (279 Hz)



- The difference is very small in the parts per million range.
- C_6H_5 1778 / 250 = 7.11 PPM
- CH_2 632 / 250 = 2.53 PPM
- CH_3 279 / 250 = 1.12 PPM

Radio Frequency Pulsed NMR



Broad Band

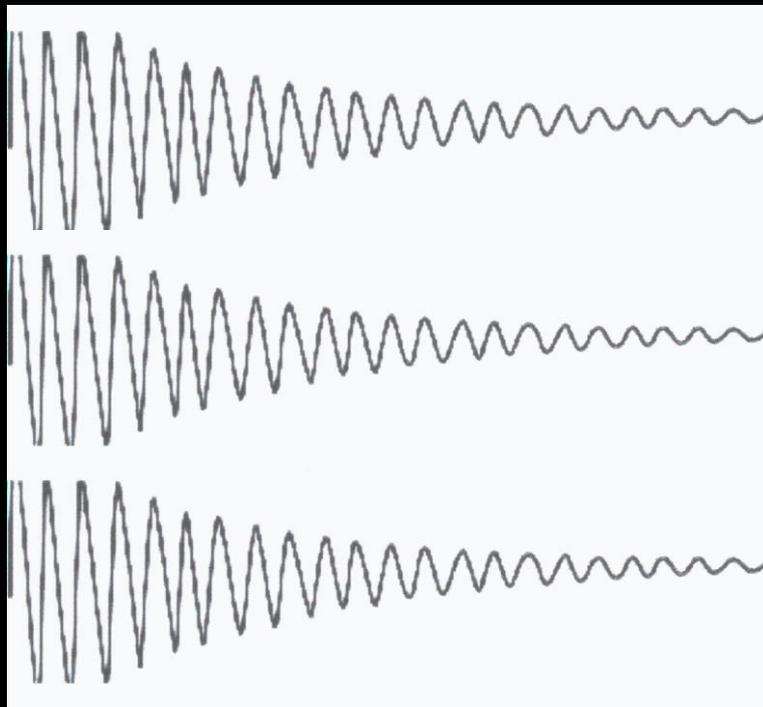


RF Pulse

Contains Range of
Frequencies v1, v2, v3

All kinds of ¹H are excited
simultaneously with the single
broad band RF pulse.

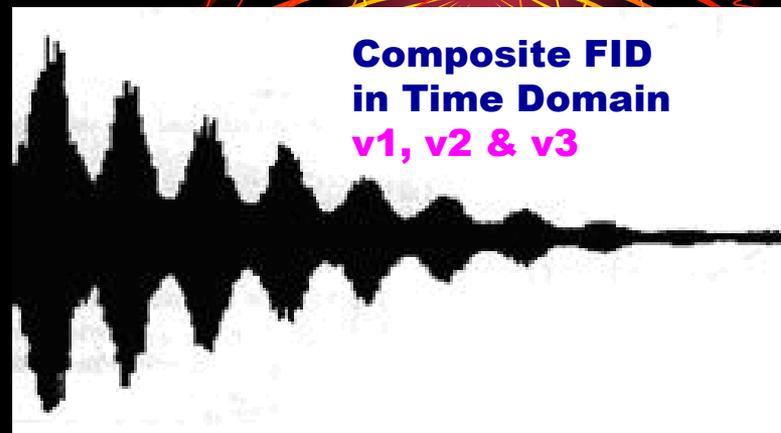
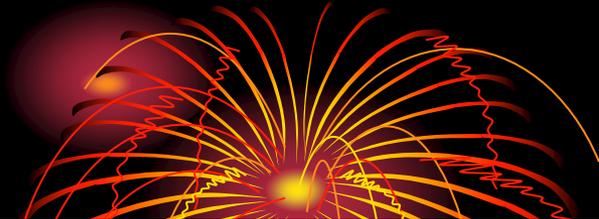
Free Induction Decay (FID)



v1

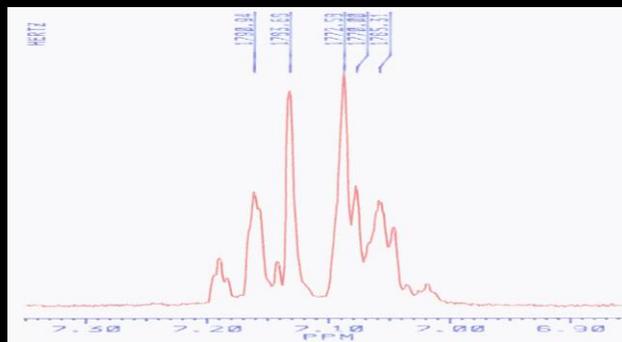
v2

v3

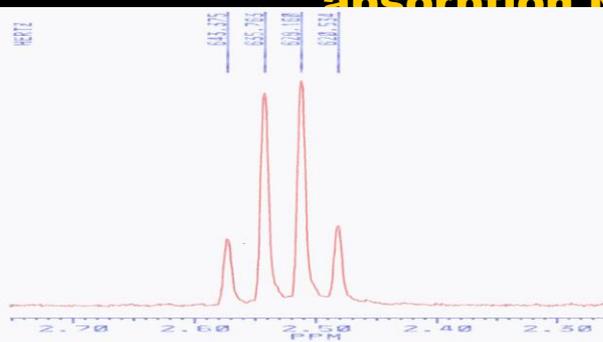


v1 , v2, & v3 have different half life.

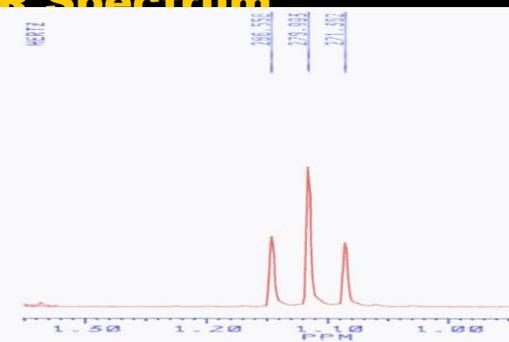
When these FID are Fourier Transformed (FT) gives normal absorption NMR Spectrum



v1 = C_6H_5



v2 = CH_2



v3 = CH_3

NMR SIGNAL STRENGTH

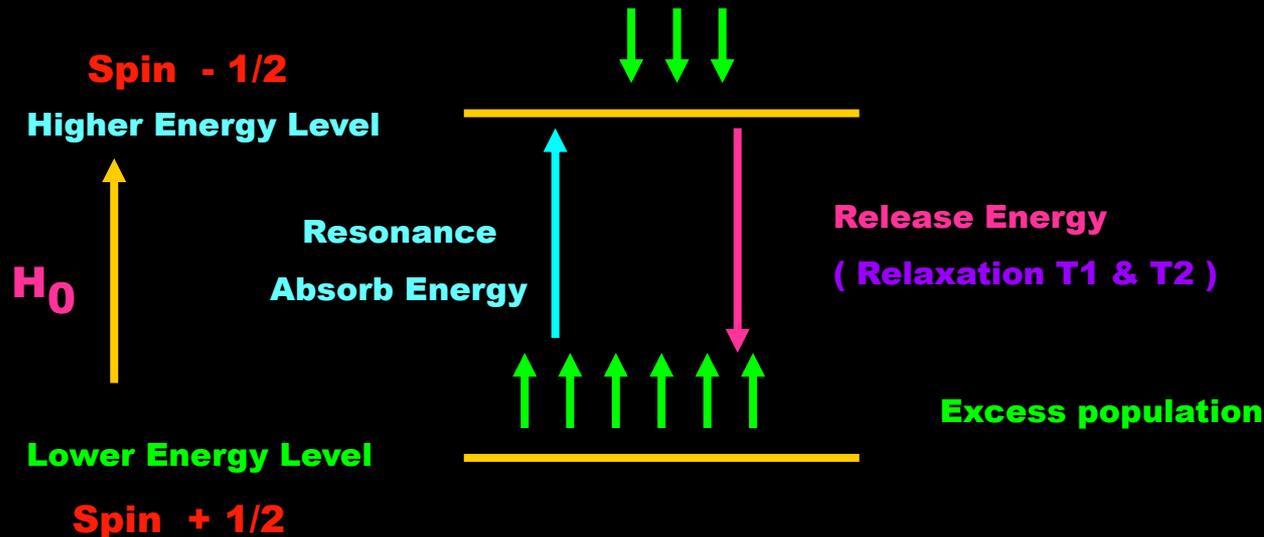
The strength of the NMR Signal depends on the Population Difference of the Parallel and Anti Parallel two spin states.

Applied Magnetic field induces both upward and downward transitions.

For NMR Signal there must be an excess of spins in the lower energy level.

Equal Populations = Saturation = No NMR Signal

Conditions for the detection of NMR Signal



Condition for NMR Signals

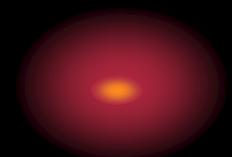


- **1. All the nuclei with odd mass number.**
 ^1H , ^{11}B , ^{13}C , ^{19}F , ^{29}Si & ^{31}P ($I = \text{Half Integer}$)
- **2. All the nuclei with even mass number**
• **and odd number of protons & neutrons.**
 ^2H , ^{10}B , & ^{14}N ($I = \text{whole integer}$)
- **3. Those nuclei which have a non zero**
• **magnetic moment (μ) and spin angular moment (I)**
• **produce NMR signals.**

Typical conditions which satisfy the relationship between radiofrequencies for different nuclei at fixed magnetic field strength are given in the below table.

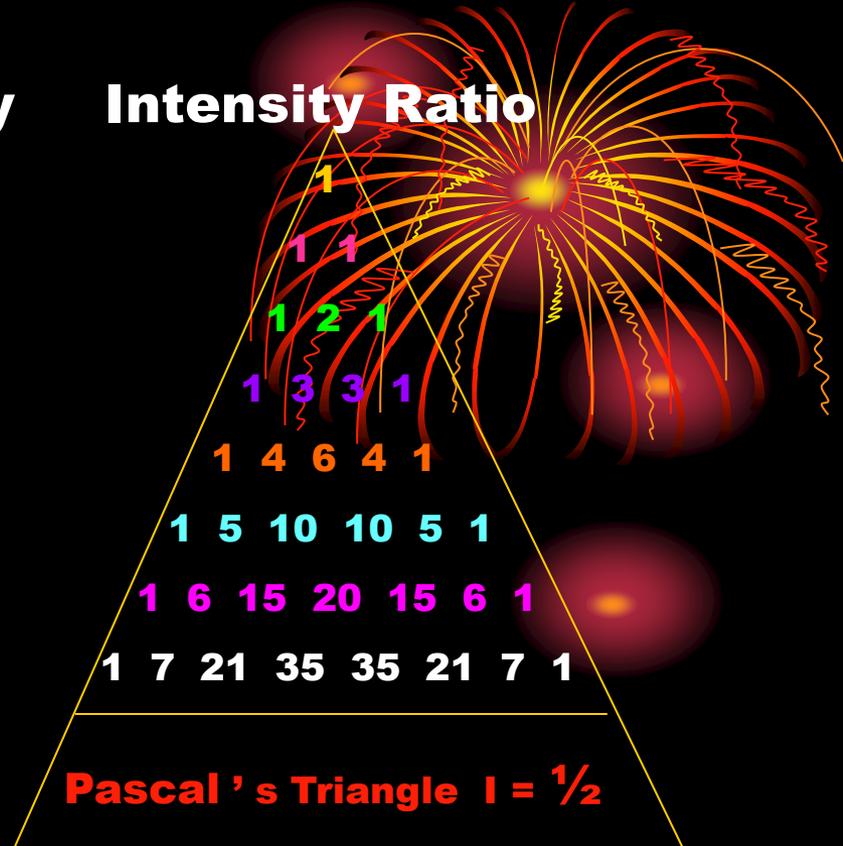


Nucleus	Spin No. I	% Natural Abundance	Frequency MHz	Field H0 Tesla
¹H	1/2	99.98	100.00	2.348
²H	1	0.0115	15.35	2.348
¹⁰B	3	19.00	10.74	2.348
¹¹B	3/2	81.00	32.07	2.348
¹³C	1/2	1.10	25.14	2.348
¹⁴N	1	99.60	7.22	2.348
¹⁵N	1/2	0.40	10.13	2.348
¹⁹F	1/2	100.00	94.05	2.348
²⁹Si	1/2	4.70	19.86	2.348
³¹P	1/2	100.00	40.45	2.348
¹²C	0 (zero)	98.80	NO NMR SIGNAL	
¹⁶O	0 (zero)	99.80	NO NMR SIGNAL	



- **No. of Peaks**
 - **n=0 One Peak**
 - **n=1 Two Peaks**
 - **n=2 Three Peaks**
 - **n=3 Four Peaks**
 - **n=4 Five Peaks**
 - **n=5 Six Peaks**
 - **n=6 Seven Peaks**
 - **n=7 Eight Peaks**
- Terminology**
- **Singlet**
 - **Doublet**
 - **Triplet**
 - **Quartet**
 - **Quintet**
 - **Sextet**
 - **Septet**
 - **Octet**

Intensity Ratio



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

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

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

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

Read the intensity ratio directly from Pascal Triangle.

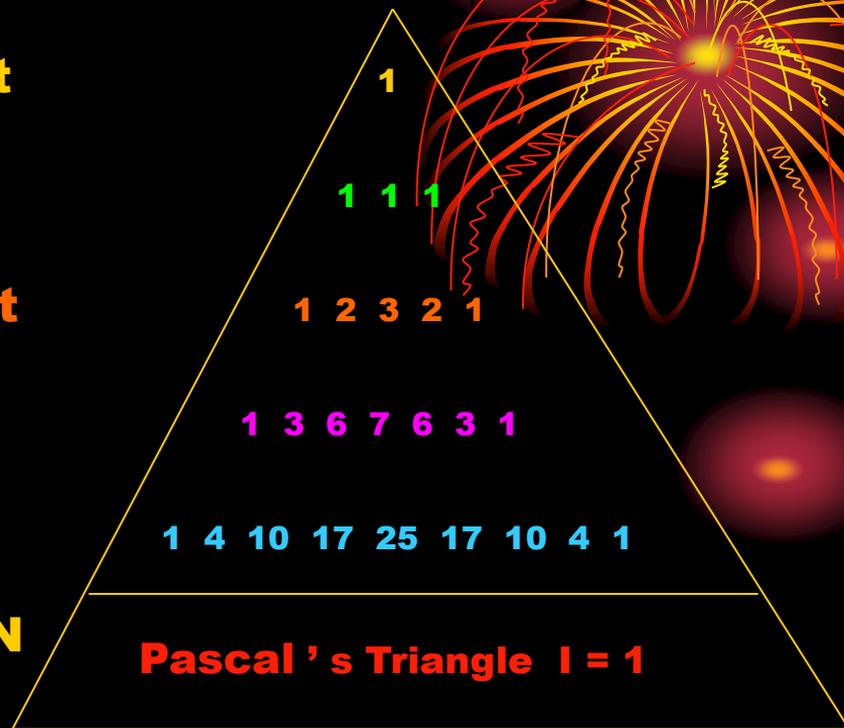
Pascal Triangle and Binomial Coefficient



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

- **No. of Peaks** **Terminology**
- **n=0** **One Peak** **Singlet**
- **n=1** **Three Peaks** **Triplet**
- **n=2** **Five Peaks** **Quintet**
- **n=3** **Seven Peaks** **Septet**
- **n=4** **Nine Peaks** **Nonet**

Intensity Ratio



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



^{13}C NMR of CDCl_3
I = 1 ^2H to ^{13}C
Intensity ratio 1 : 1 : 1

Read the intensity ratio directly from Pascal Triangle.

- **The most common Deuterated solvents used are**
- **1. Deuteriochloroform** CDCl_3
- **2. Deuteroacetone** CD_3COCD_3
- **3. Deuterobenzene** C_6D_6
- **4. Deuterodichloromethane** CD_2Cl_2
- **5. Deuterated water** D_2O
- **6. Deuterodimethylsulphoxide** CD_3SOCD_3

Note :- The hydrogen atoms are replaced with deuterium so that no signal from solvent and also used for locking the oscillating field by the lock frequency.

Referencing of NMR Spectra

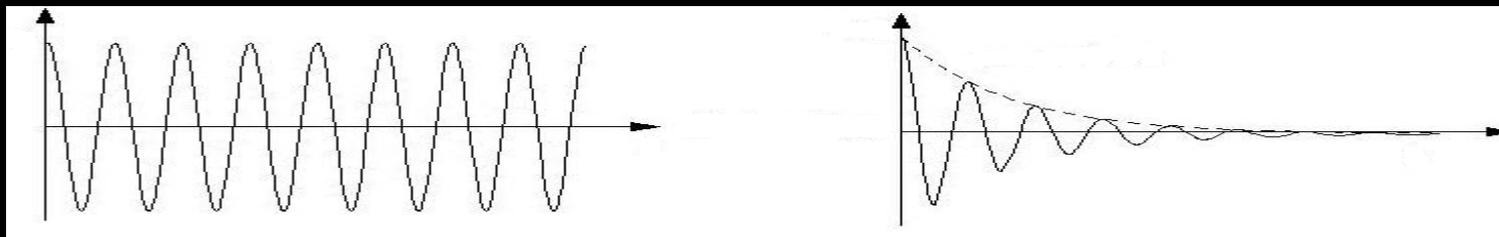
- The reference compound should have only one absorption peak for the interested compound.
- It should also be :-
 - 1. Chemically Stable.
 - 2. Chemically Inert.
 - 3. Soluble in most common solvents.



NMR OF	Reference Compounds
^1H	TMS (<u>T</u> etra <u>M</u> ethyl <u>S</u> ilane)
	TSP-D4 (<u>3</u> - <u>T</u> rimethyl <u>S</u> ilyl-2,2,3,3-tetra <u>D</u> eutero <u>P</u> ropionic acid Sodium salt.)
^{13}C	TMS, CDCl_3
^{14}N	NH_4NO_3 Acidified Saturated Solution
^{15}N	NH_2CHO 90% Formamide
	CD_3NO_2 Deuteronitromethane
^{19}F	TFA TriFluoroAcetic Acid
	CFCl_3 Freon 1,1
^{31}P	H_3PO_4 85% Phosphoric Acid

Relaxation Processes T1 & T2

- **T1 is called Longitudinal Relaxation Time**
- **T2 is called Transverse Relaxation Time**
- **The magnetization does not precess indefinitely in the transverse plane but goes back to the equilibrium state. This process is called Relaxation and can be describe by two time constants T1 and T2.**
- **T1 is the Re-establishment of the equilibrium of α (Alpha) And β (beta) States.**
- **T2 is the dephasing of the transverse component**
- **The destruction of the coherent state and it is the exponential decay of the NMR signal in the detector.**



No relaxation

With relaxation

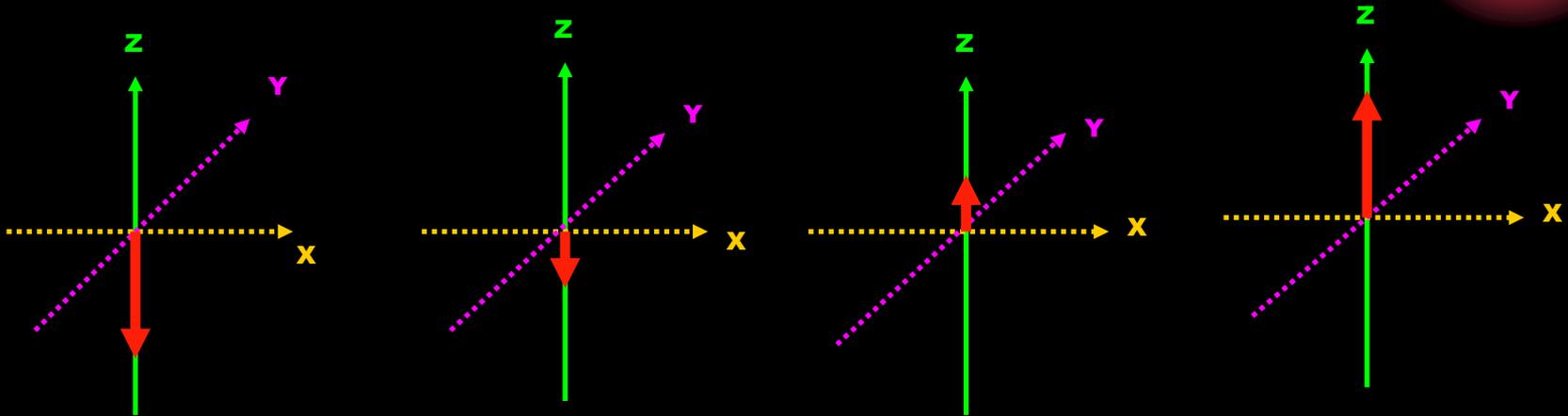
Relaxation Processes T1 & T2



- **T1 relaxation is an enthalpic process where the energy is taken from or transferred to neighbouring spins. The surrounding of the spins is called lattice hence T1 is also known as spin lattice relaxation. In this process the Z – Component of the magnetization is return back to its equilibrium state. T1 values are useful information for NMR experiment what to set up as repetition time between each NMR scan. For 1H T1 values are from 0.5 Seconds to few seconds.**
- **T2 relaxation is an entropic process and does not affect the population of spins hence there is no change in the energy. T2 is also known as spin spin relaxation. In this process the decay of the transverse (x , Y) components of the magnetization is described.**

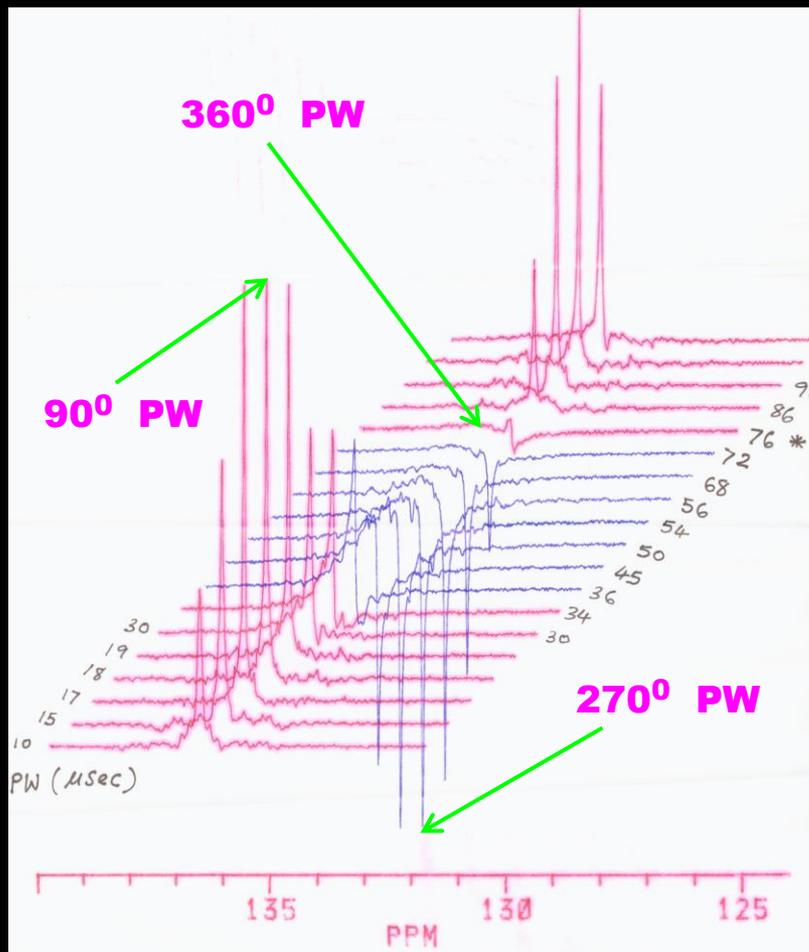
T1 Relaxation

- **T1 relaxation is an enthalpic process where the energy is taken from or transferred to neighbouring spins. The surrounding of the spins is called lattice hence T1 is also known as spin lattice relaxation. In this process the Z - Component of the magnetization is return back to its equilibrium state. T1 values are useful information for NMR experiment what to set up as repetition time between each NMR scan. For 1H T1 values are from 0.5 Seconds to few seconds.**



Return of the Z component of the magnetization to the equilibrium state

Spin Lattice or Longitudinal Relaxation Process T_1 And the Measurement of 90° & 180° Pulse width (PW) ^{13}C NMR Spectrum of Benzene in Acetone- D_6

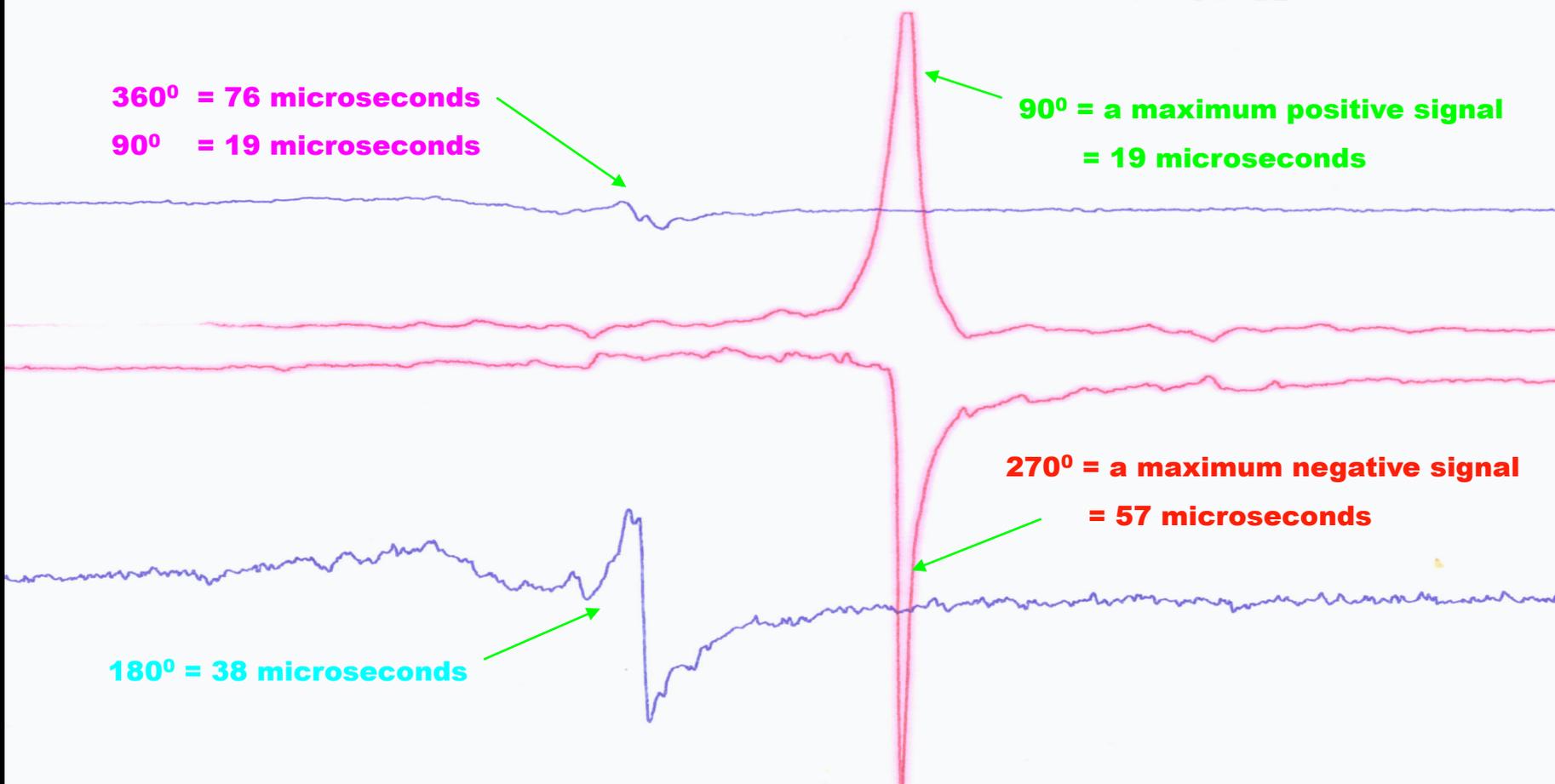


- when sample is placed in the magnetic field and radio frequency (RF) pulse is applied, the Boltzmann population of spins get upset and after a time delay T_1 the Boltzmann population of spins get re-established. This time delay T_1 is called the spin lattice or longitudinal relaxation time T_1
- Measurement of 90° and 180° pulses times
- for any spin active nucleus (^1H , ^{13}C , ^{19}F , ^{15}N) is required to set up all multipulses FT NMR experiments. An accurate value of 90° PW is crucial for T_1 value measurement. This is usually obtained using a concentrated sample to produce a strong signal after a single pulse. Record the signal intensity with various PW. All measurements must be made with the same intensity scaling and same phase corrections. The intensities should show a sinusoidal variation with pulse width PW
- 90° = A maximum positive signal
- 270° = A maximum negative signal
- 180° = A zero signal
- 360° = A zero signal
- It is easier to determine the position of null values at 180° and 360° PW The half of 180° or quarter of 360° values will be 90° PW

Measurement of 90° & 180° Pulse width (PW) ¹³C NMR Spectrum of Benzene in Acetone -D6



BENZENE TEST FOR 90 DEGREE PULSE FOR-BB

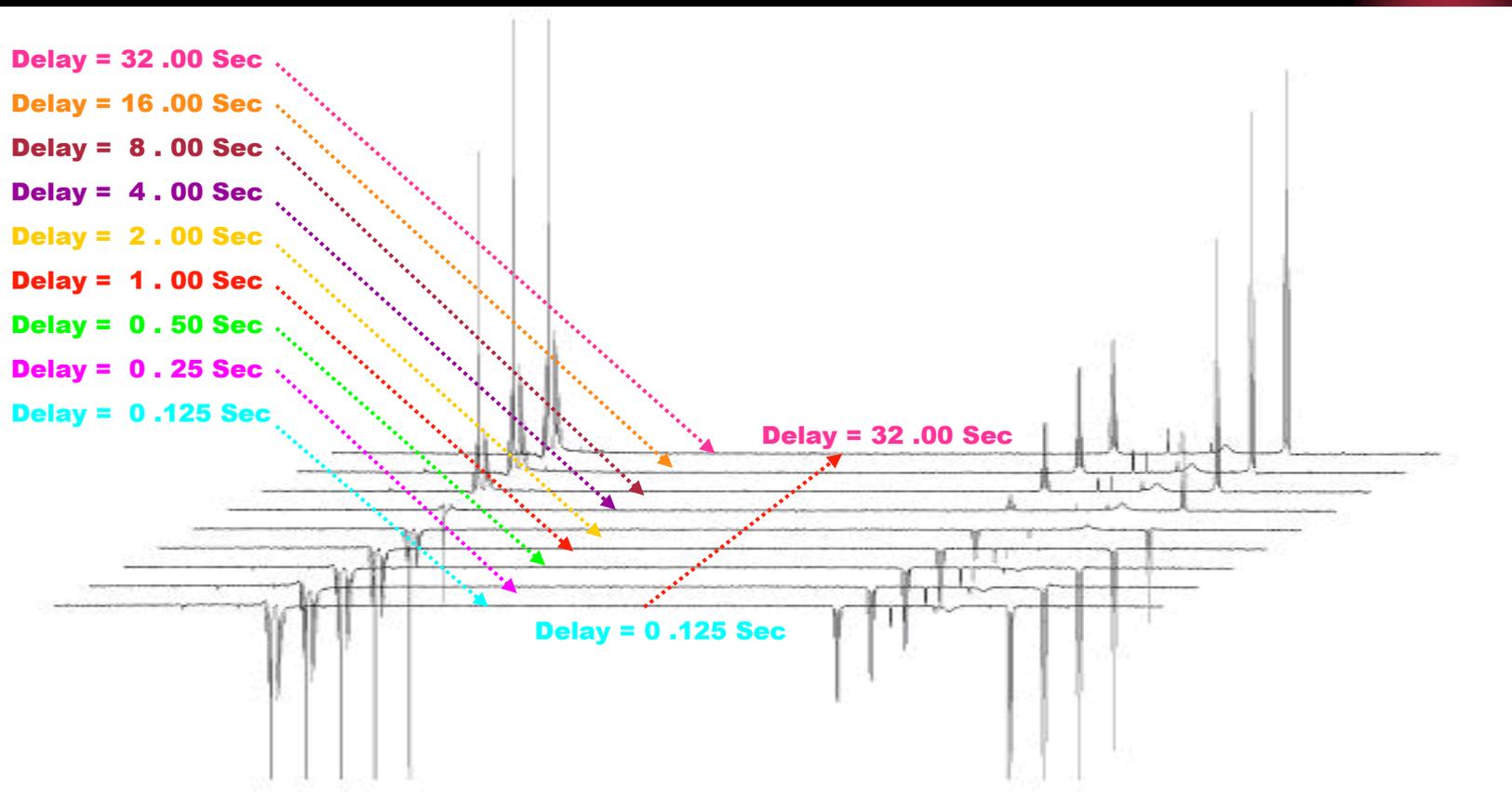


T1 Measurement using Inversion recovery method

^1H Spectrum of Ethyl Benzene

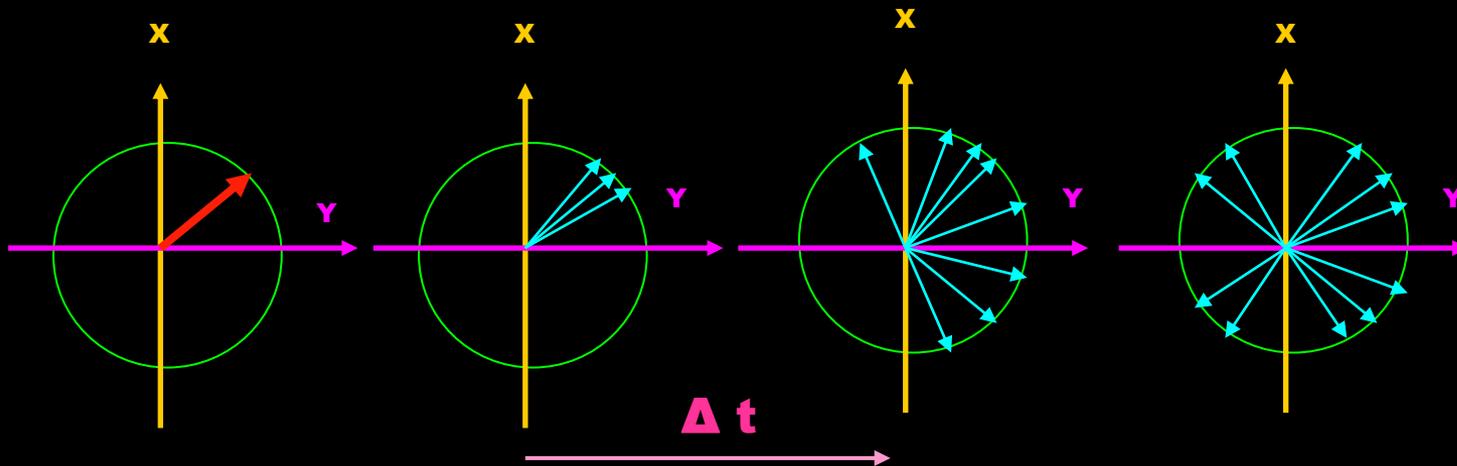
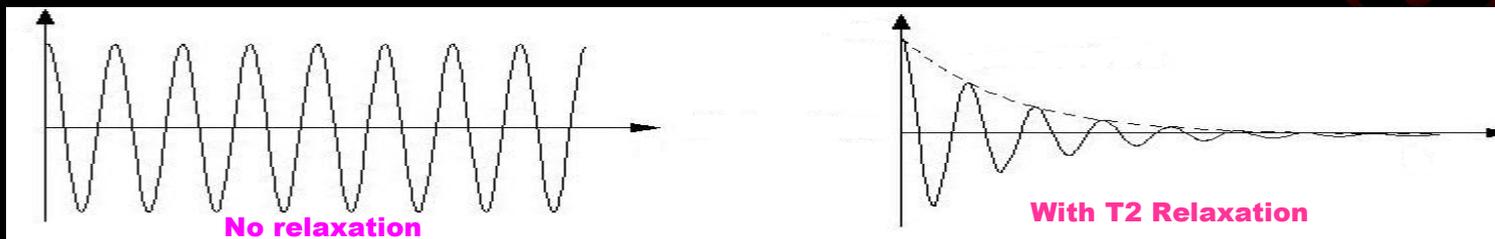


^1H NMR Spectrum of Ethyl Benzene



T2 Relaxation

- T2 relaxation is an entropic process and does not affect the population of spins hence there is no change in the energy. T2 is also known as spin spin relaxation. In this process the decay of the transverse (X , Y) components of the magnetization is described.

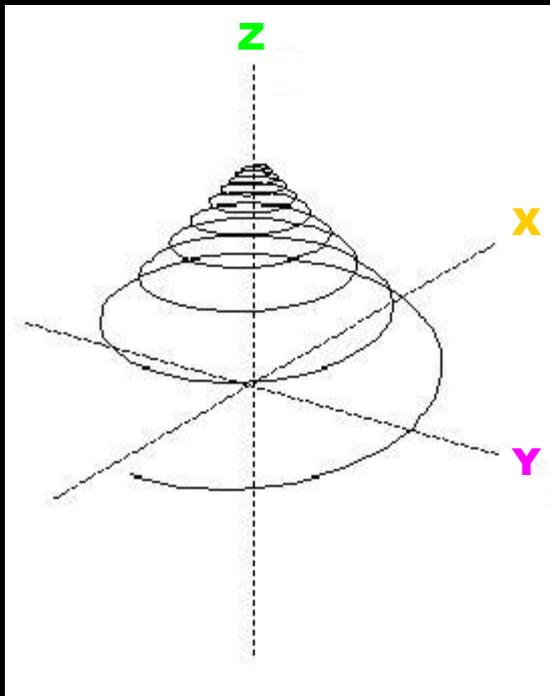


The Dephasing of the transverse coherence of (X , Y) magnetization leading to T2 relaxation

The effect of T2 on NMR signal (FID)

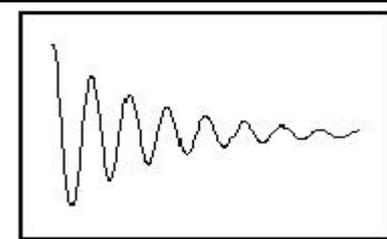
T2 Relaxation

- The precessing spins slowly return to the Z - axis. The movement is not circular in the transverse plane but spins follow a spiral trajectory until they have reached their initial position aligned with + / - Z - axis



Trajectory of the magnetization

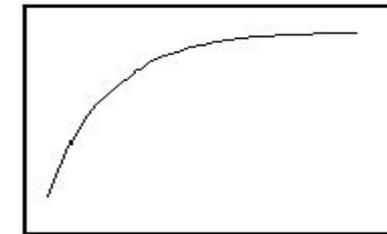
M_X



M_Y

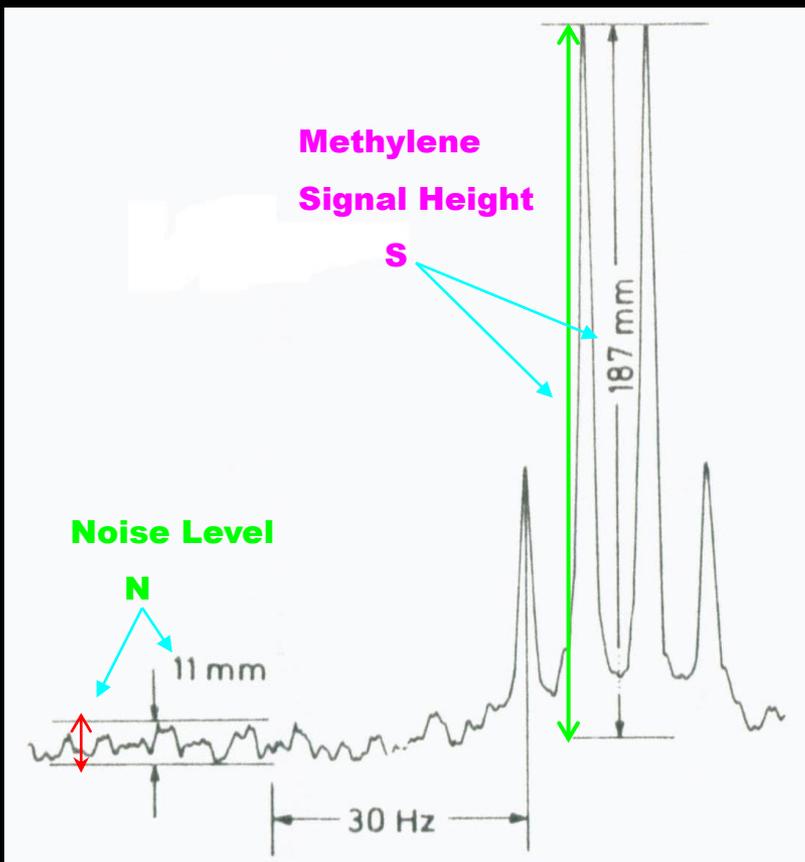
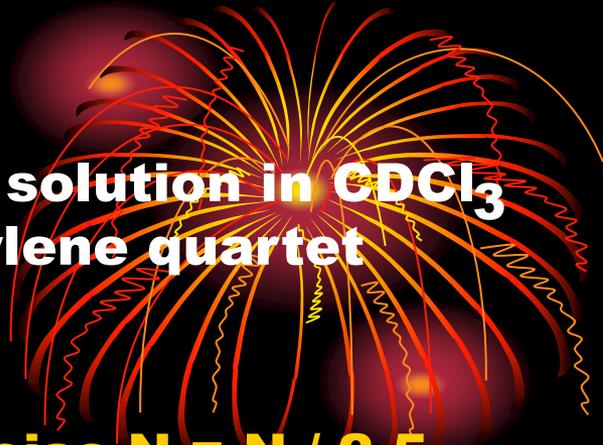


M_Z



X , Y , Z , Components

Sensitivity test with 1 % Ethyl Benzene solution in CDCl_3 Signal to noise ratio test S / N on methylene quartet



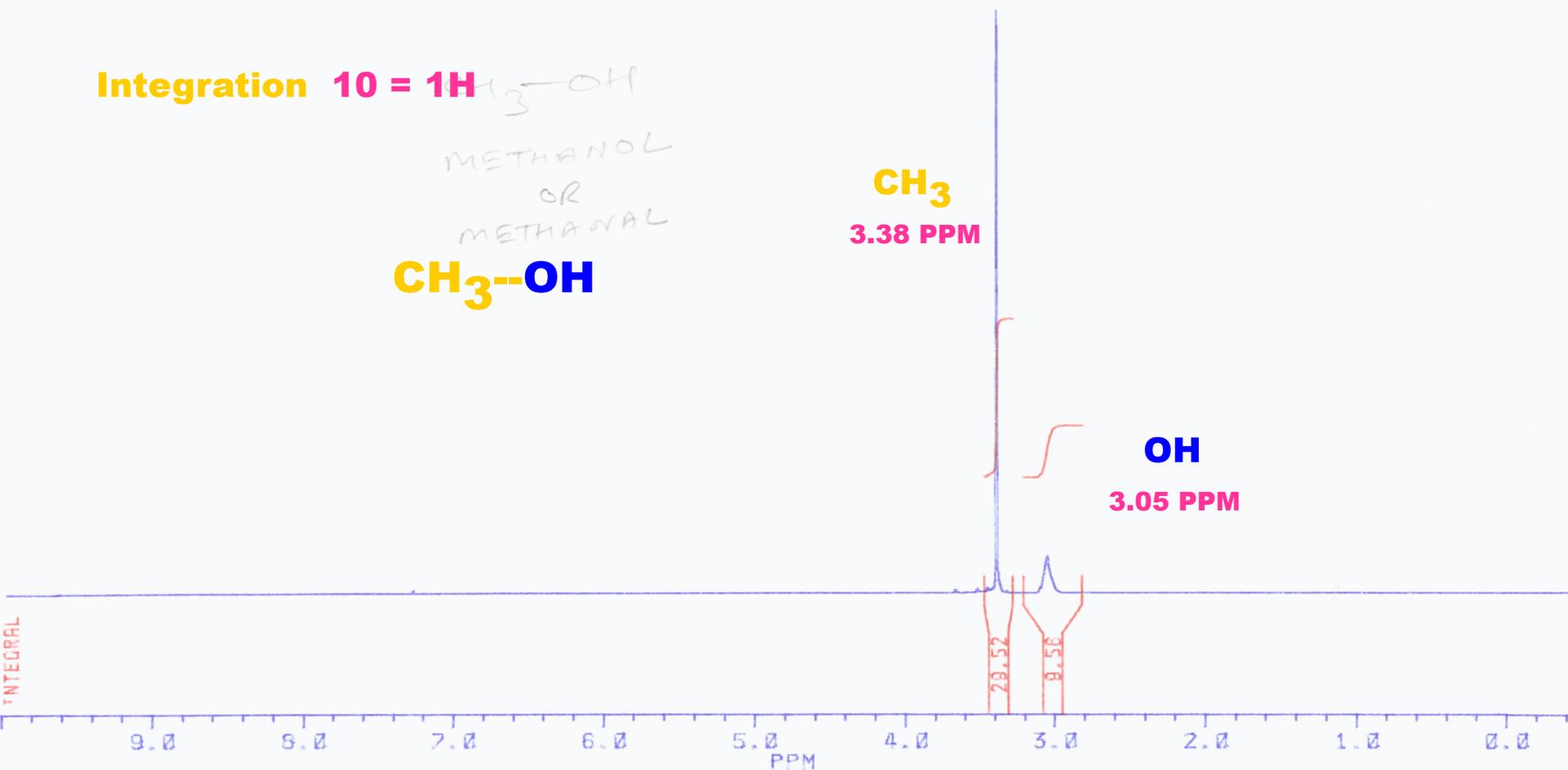
- **Average Noise $N = N / 2.5$**
- **$N = 11 / 2.5$**
- **$N = 4.4 \text{ mm}$**
- **The signal to noise ratio is defined as the quotient of the average signal height S and the average noise level N .**
- **$S = 187 \text{ mm}$**
- **$S / N = 187 / 4.4$**
- **$= 42.50$**
- **Before the sensitivity test tune the Spectrometer with D_2O sample.**

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

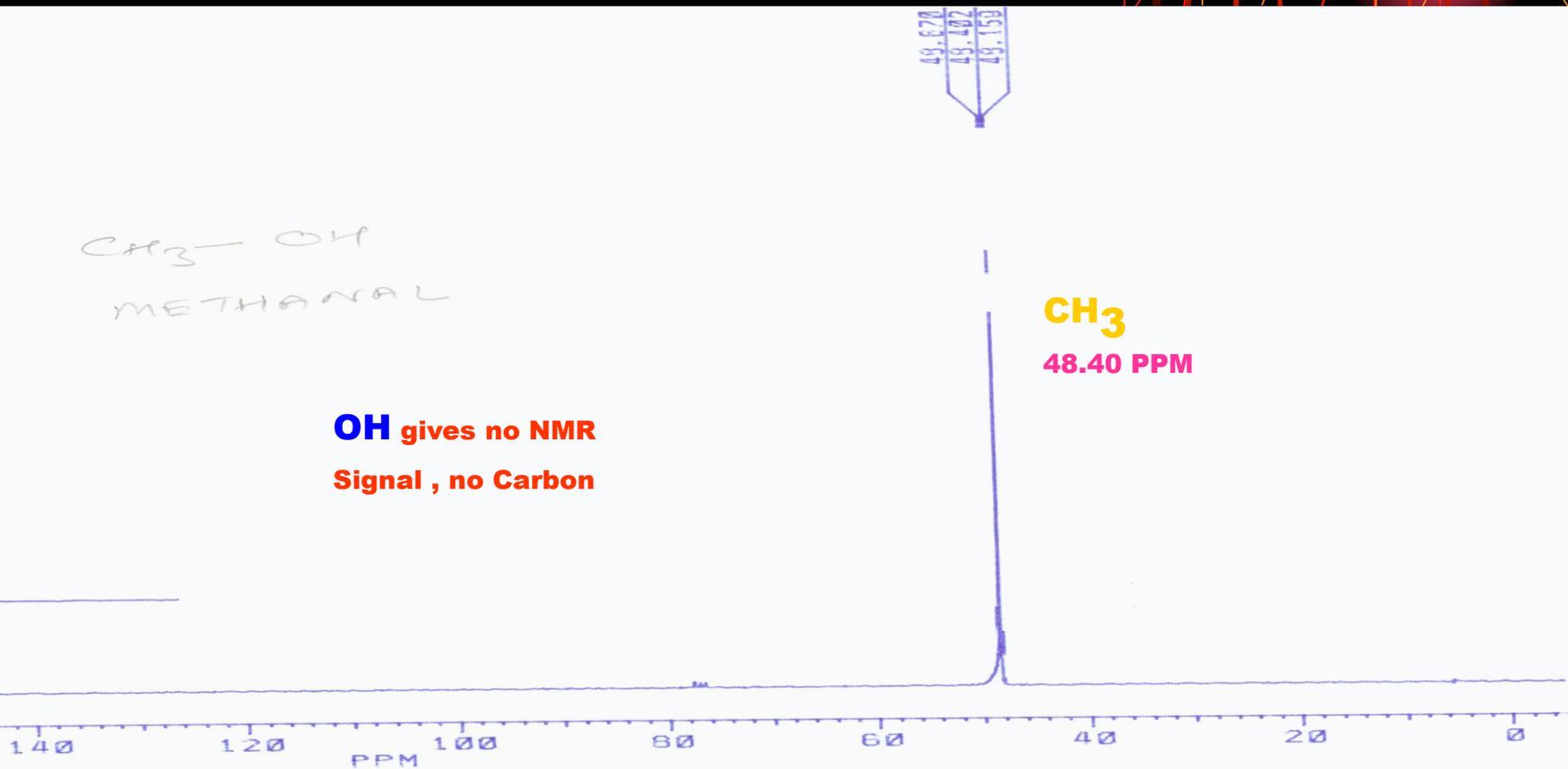
^1H NMR of $\text{CH}_3\text{-OH}$



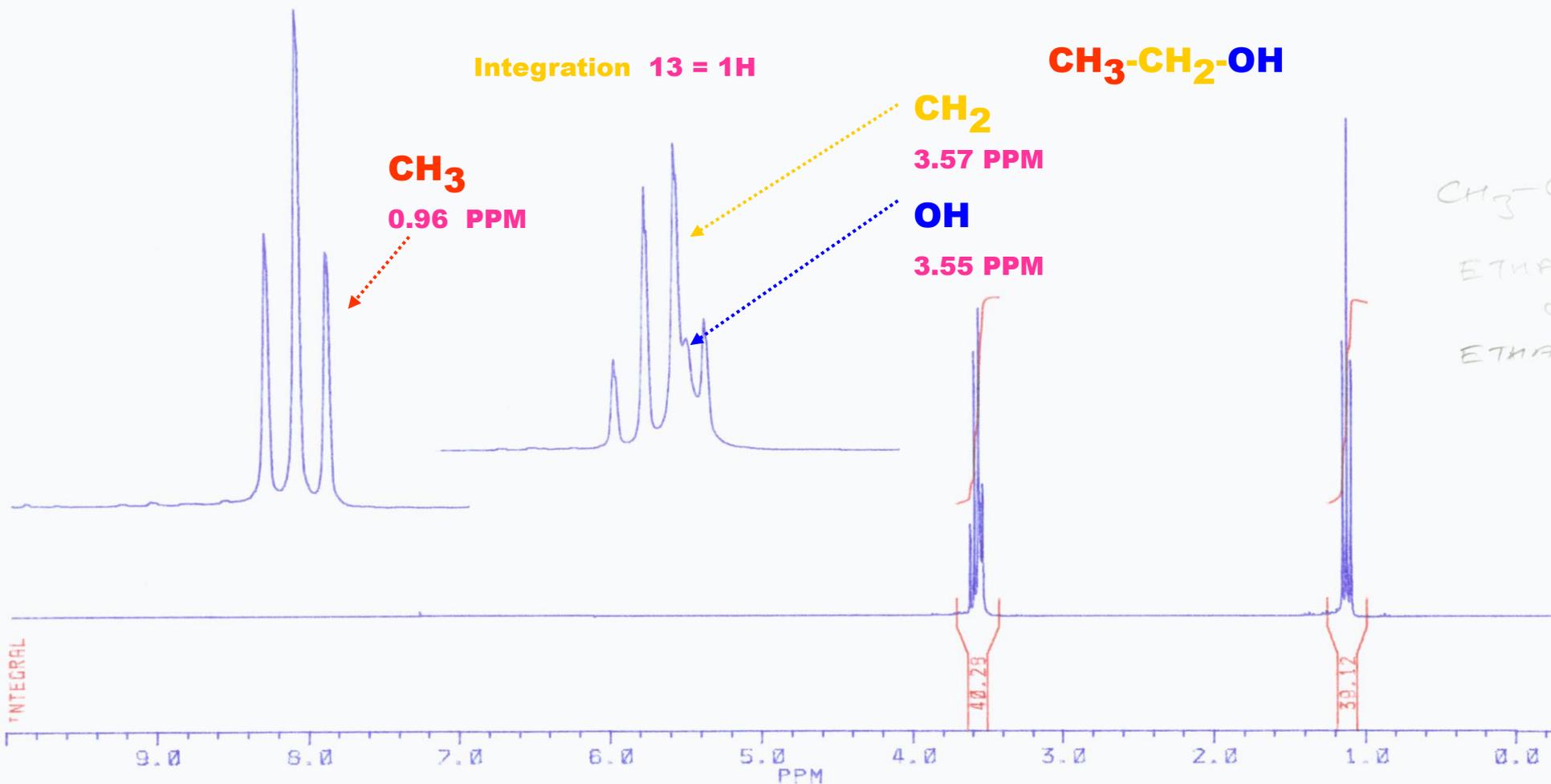
Integration 10 = 1H $\text{CH}_3\text{-OH}$
METHANOL
OR
METHANAL
 $\text{CH}_3\text{-OH}$



^{13}C NMR Spectrum of Methanol CH_3OH



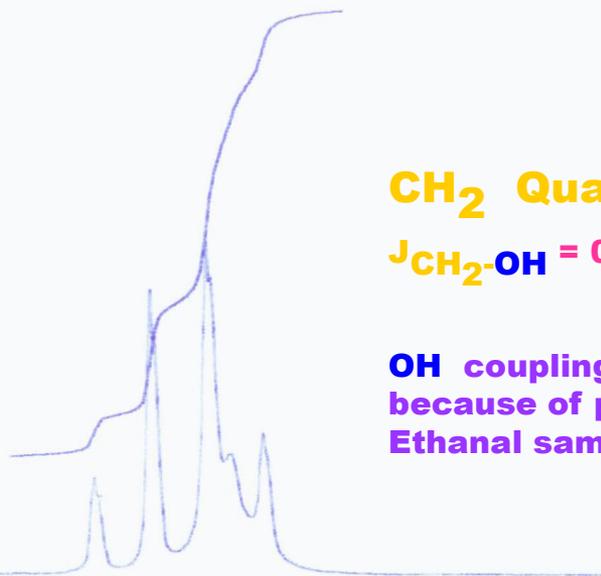
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Ethanal or Ethanol $\text{CH}_3\text{-CH}_2\text{-OH}$ ^1H NMR Spectrum



Expansion of ^1H NMR of Ethanal $\text{CH}_3\text{—CH}_2\text{—OH}$



HERTZ



CH_2 Quartet

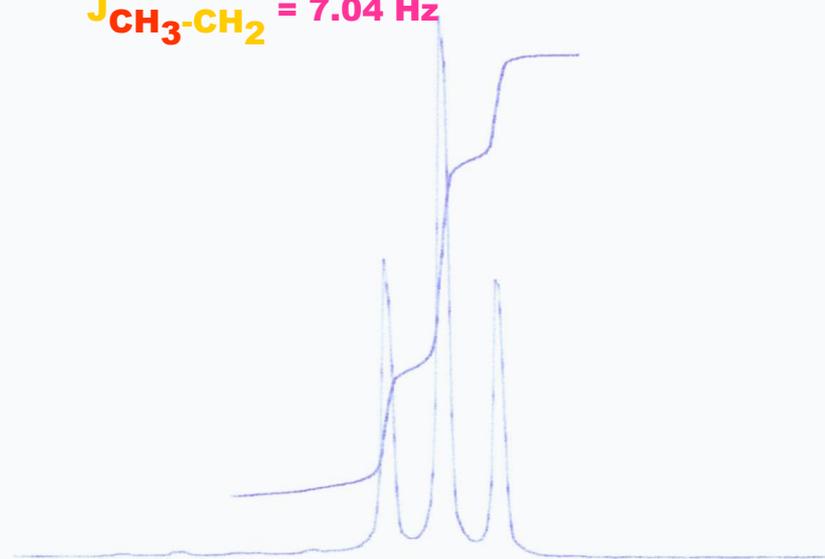
$J_{\text{CH}_2\text{—OH}} = 0.43 \text{ Hz}$

OH coupling is visible because of purity of Ethanal sample.

3.70 3.60 3.50 3.40
PPM

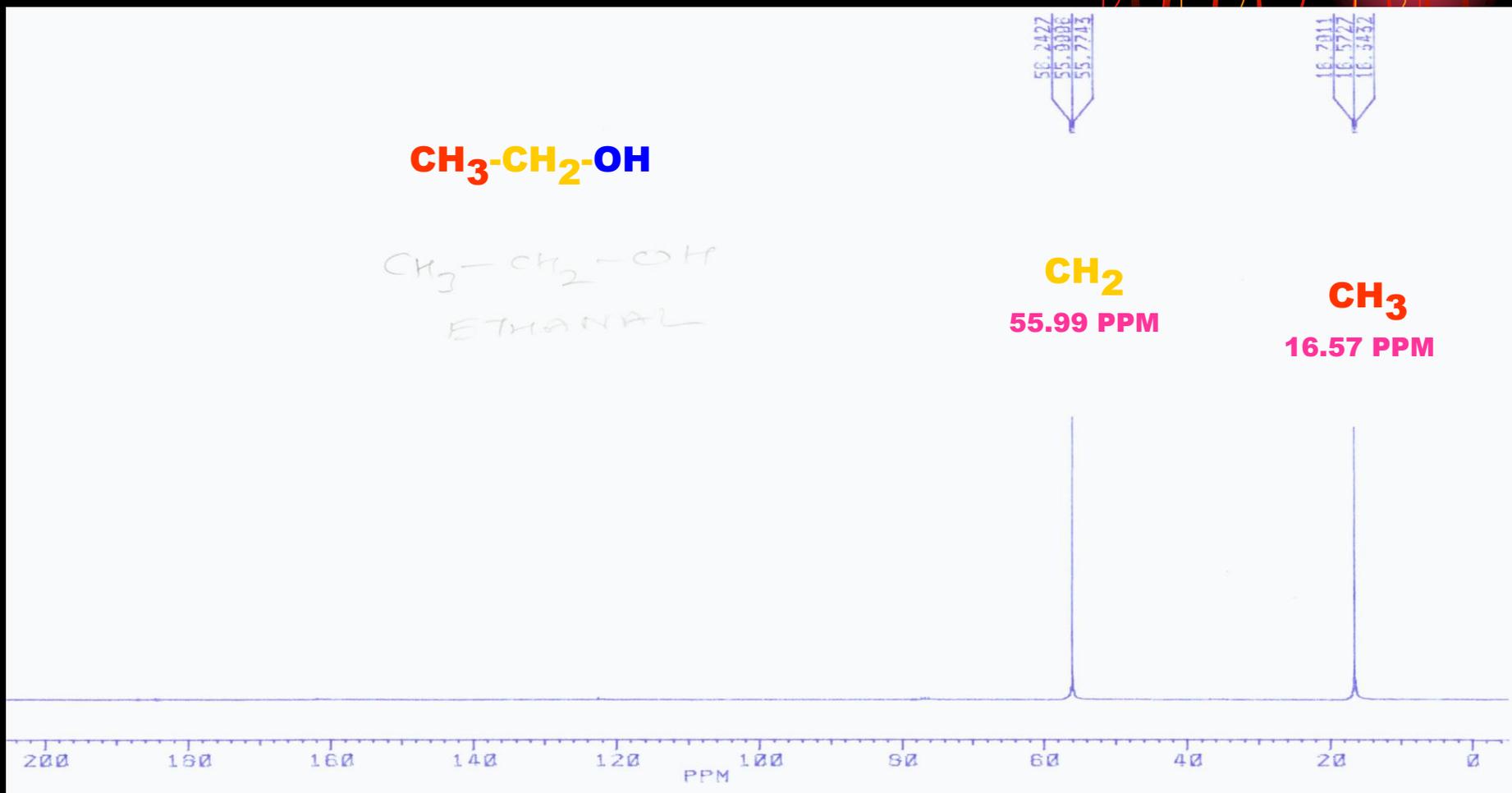
CH_3 Triplet

$J_{\text{CH}_3\text{—CH}_2} = 7.04 \text{ Hz}$

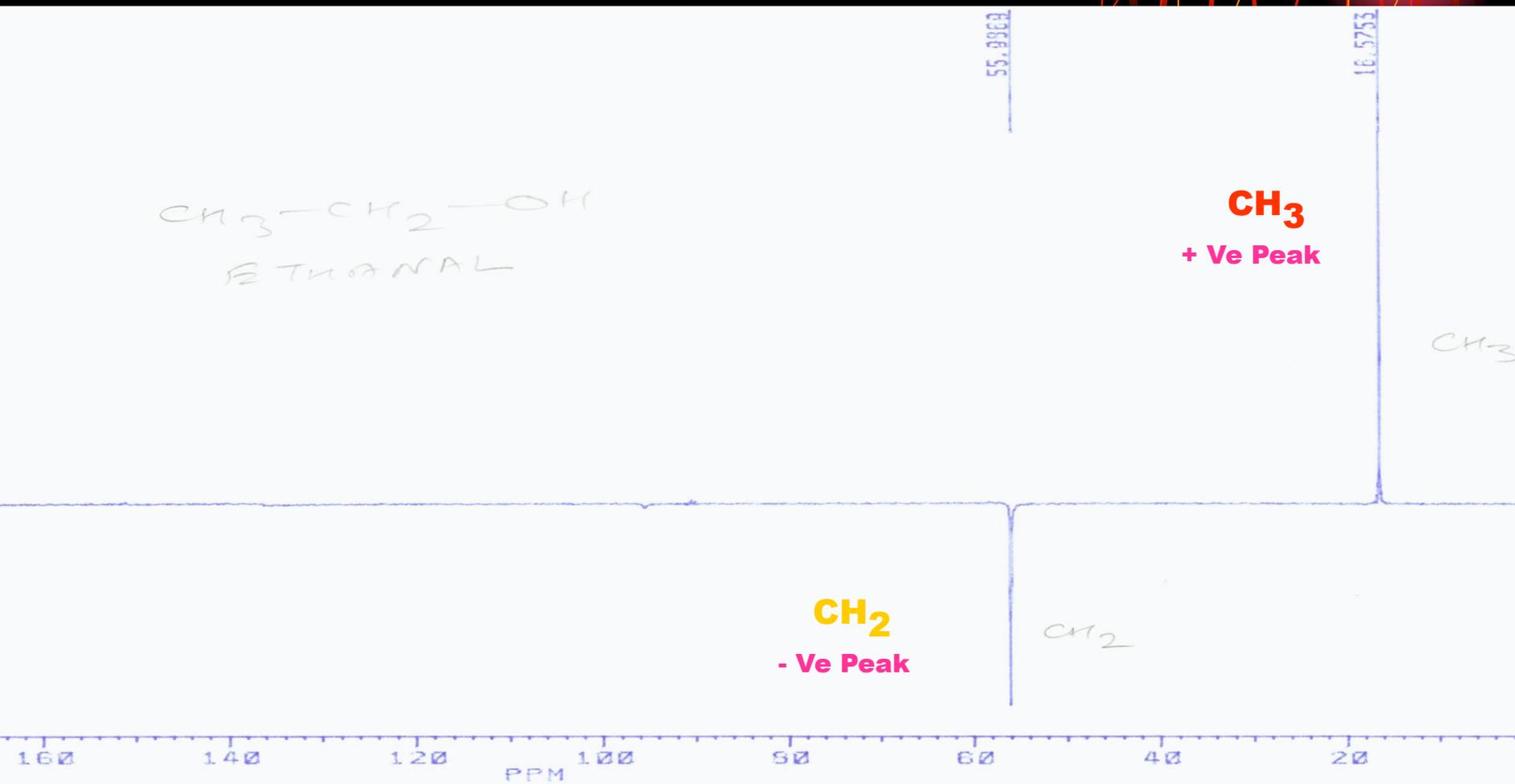


1.30 1.20 1.10 1.00
PPM

^{13}C NMR Spectrum of Ethanol $\text{CH}_3\text{—CH}_2\text{—OH}$



^{13}C Dept 135 NMR Spectrum of Ethanol



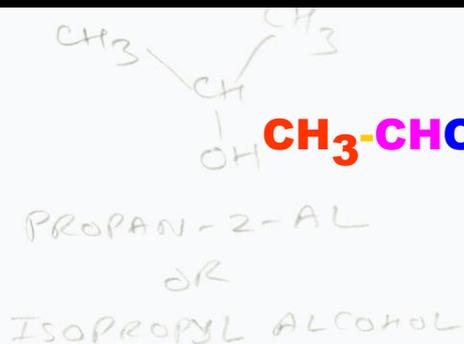
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Propan-2-ol



^1H NMR Spectrum



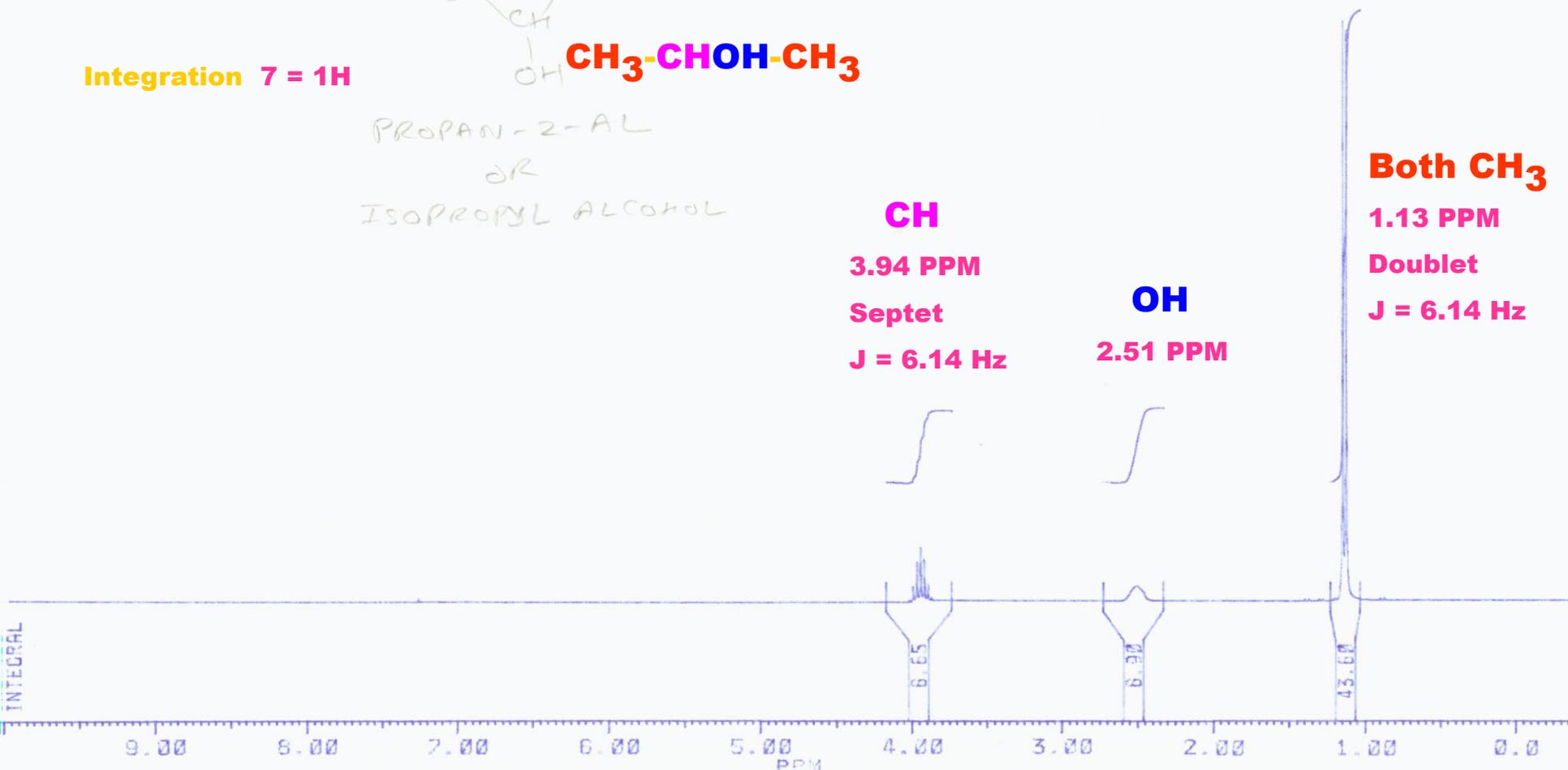
Integration 7 = 1H



CH
3.94 PPM
Septet
J = 6.14 Hz

OH
2.51 PPM

Both CH₃
1.13 PPM
Doublet
J = 6.14 Hz

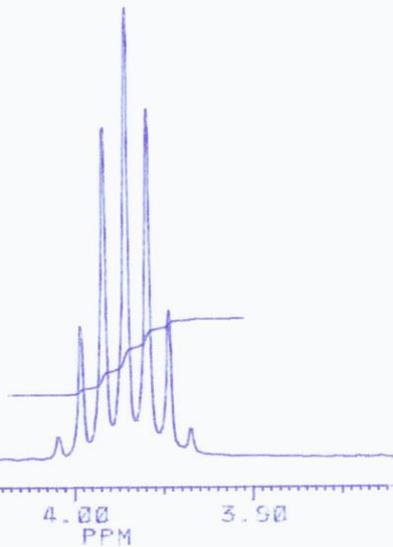


Expansion of ^1H NMR Spectrum of Propan-2-ol



1004.95
999.96
992.60
986.42
980.25
974.11
967.96

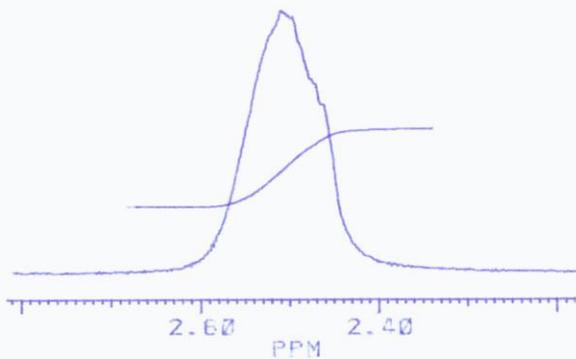
CH
3.94 PPM
Septet
 $J = 6.14$ Hz



HERTZ
627.531

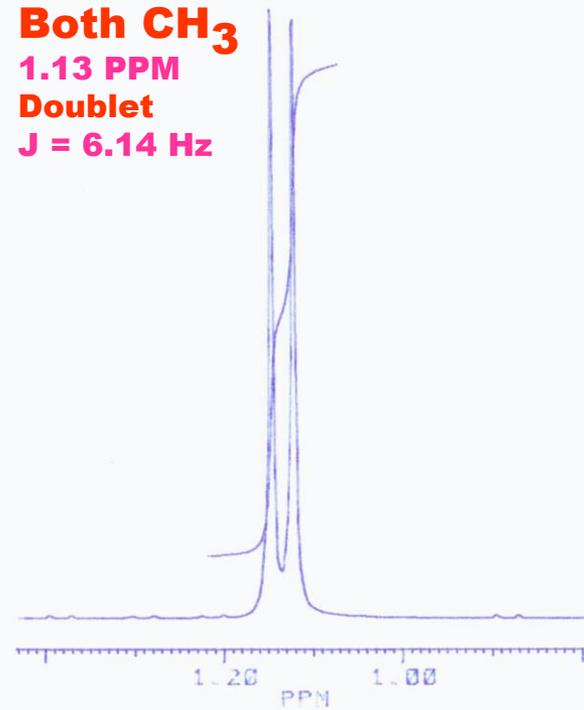
CH₃-CHOH-CH₃

OH
2.51 PPM
Broad complex

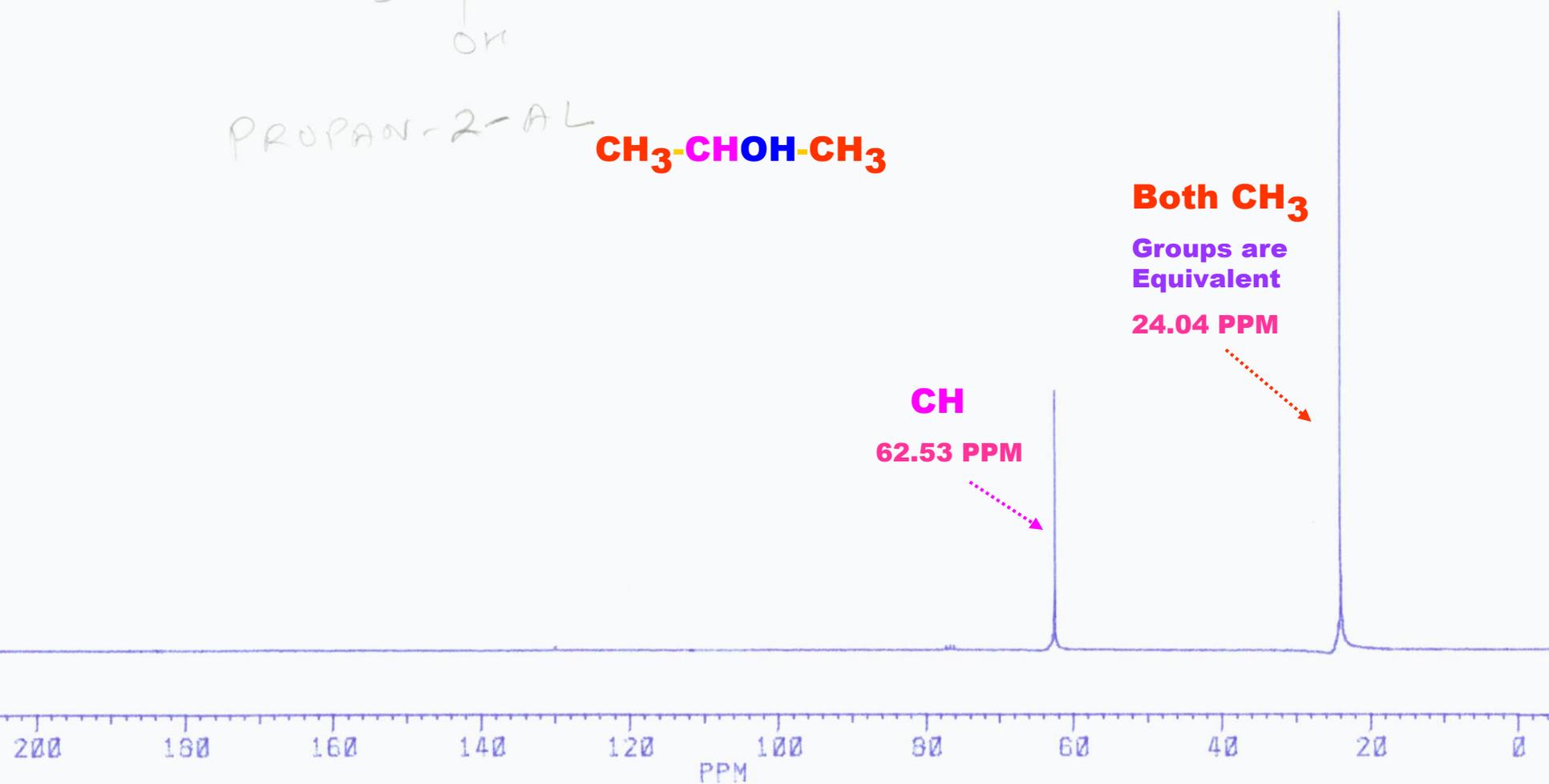
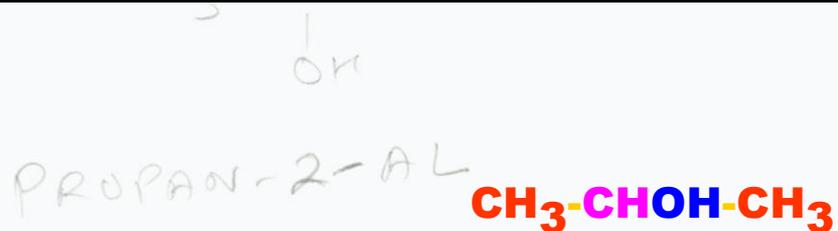


HERTZ
297.970
290.920

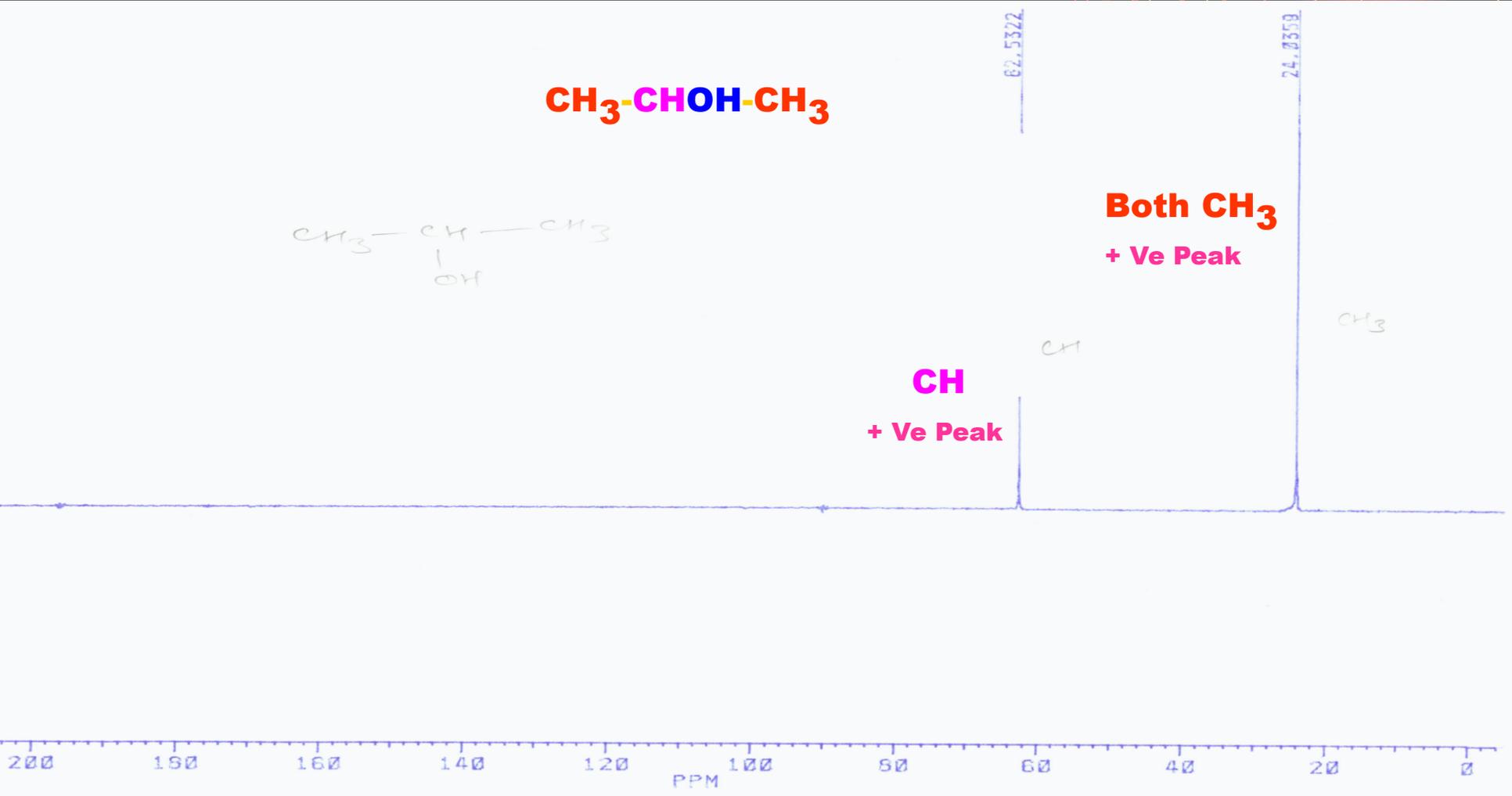
Both CH₃
1.13 PPM
Doublet
 $J = 6.14$ Hz



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



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



Analysis and interpretation of ^1H NMR Spectrum Of Butan-2-ol



Integration 12 = 1H

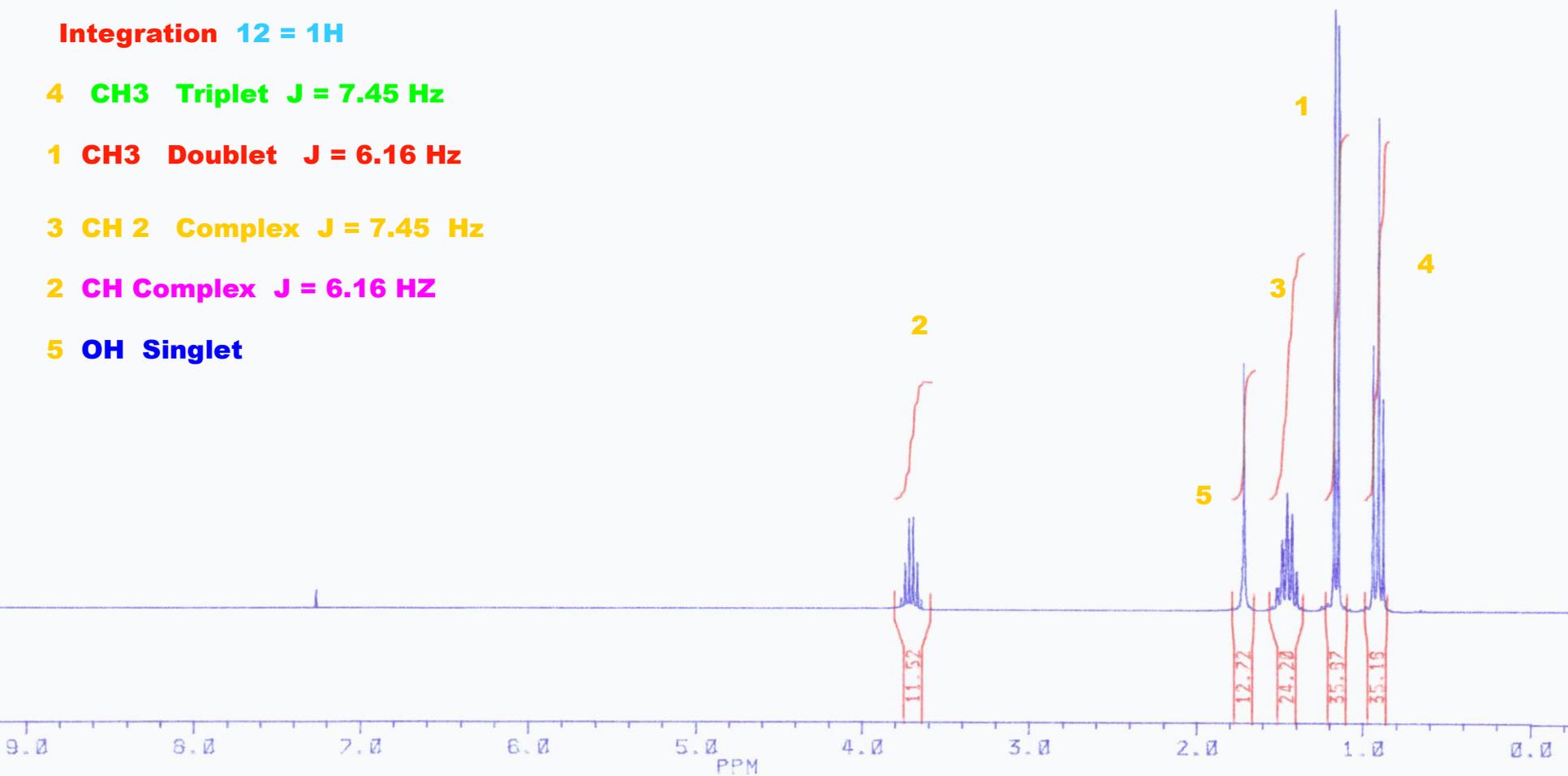
4 CH₃ Triplet J = 7.45 Hz

1 CH₃ Doublet J = 6.16 Hz

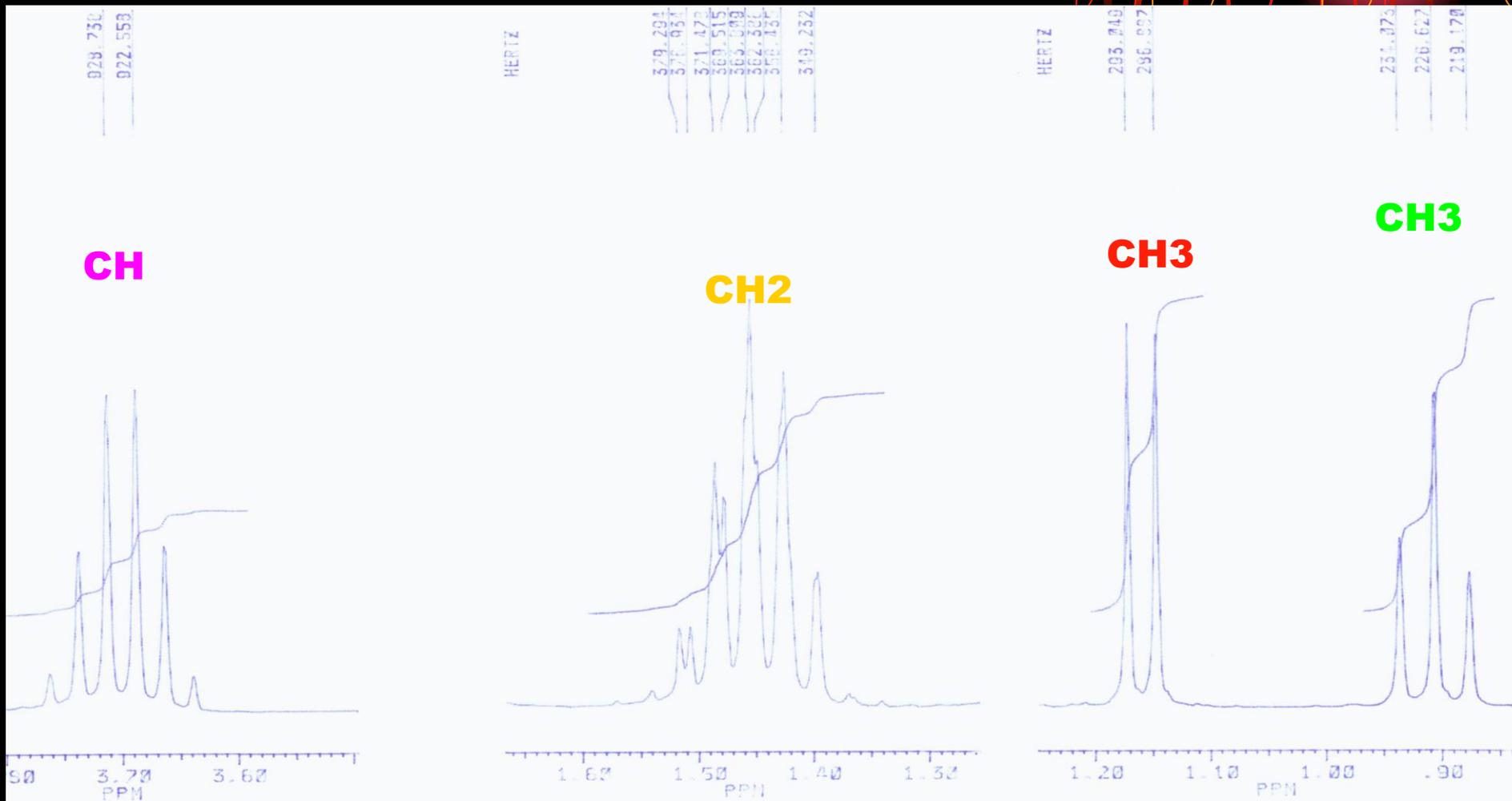
3 CH₂ Complex J = 7.45 Hz

2 CH Complex J = 6.16 Hz

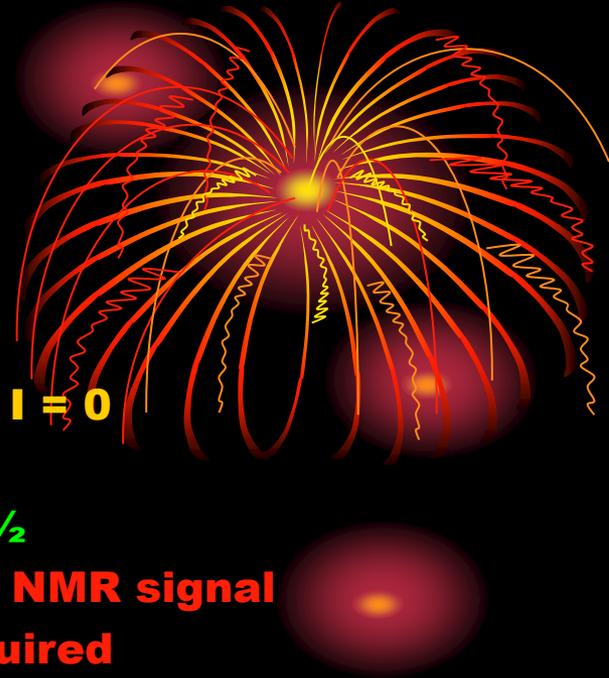
5 OH Singlet



Analysis and interpretation of ^1H NMR Spectrum Of Butan-2-ol



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 $I = \frac{1}{2}$
- ^{13}C NMR signal is 6000 times weaker than ^1H NMR signal
- To see ^{13}C NMR signals Pulsed FT NMR is required

- **Chemical Shift Range**

- ^1H 0 to 12.00 PPM
- ^{13}C 0 to 220.00 PPM

- **Resonance Frequency and Applied Field Strength**

Applied Field	^1H	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 — ^1H 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 ^2H (D), ^{19}F , ^{31}P then coupling are present from these nuclei. CDCl_3 solvent gives triplet in NMR spectrum due to ^2H coupling to ^{13}C . (^2H , $I = 1$)



^{13}C NMR
 CDCl_3

Distortion less Enhancement of Polarization Transfer

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

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

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

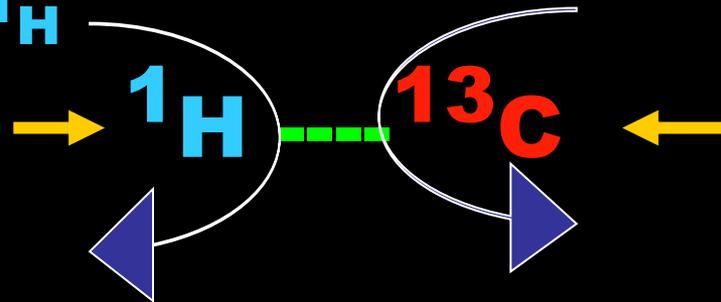


In this method all the ^1H are irradiated at certain RF and at the same time ^{13}C signals are measured at different RF.

Secondary RF source is required
To decouple ^1H

(Decoupler)

Continuously
Saturates ^1H



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 ^1H hence ^{13}C NMR signals are all singlet.

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



135 DEPT ^{13}C NMR

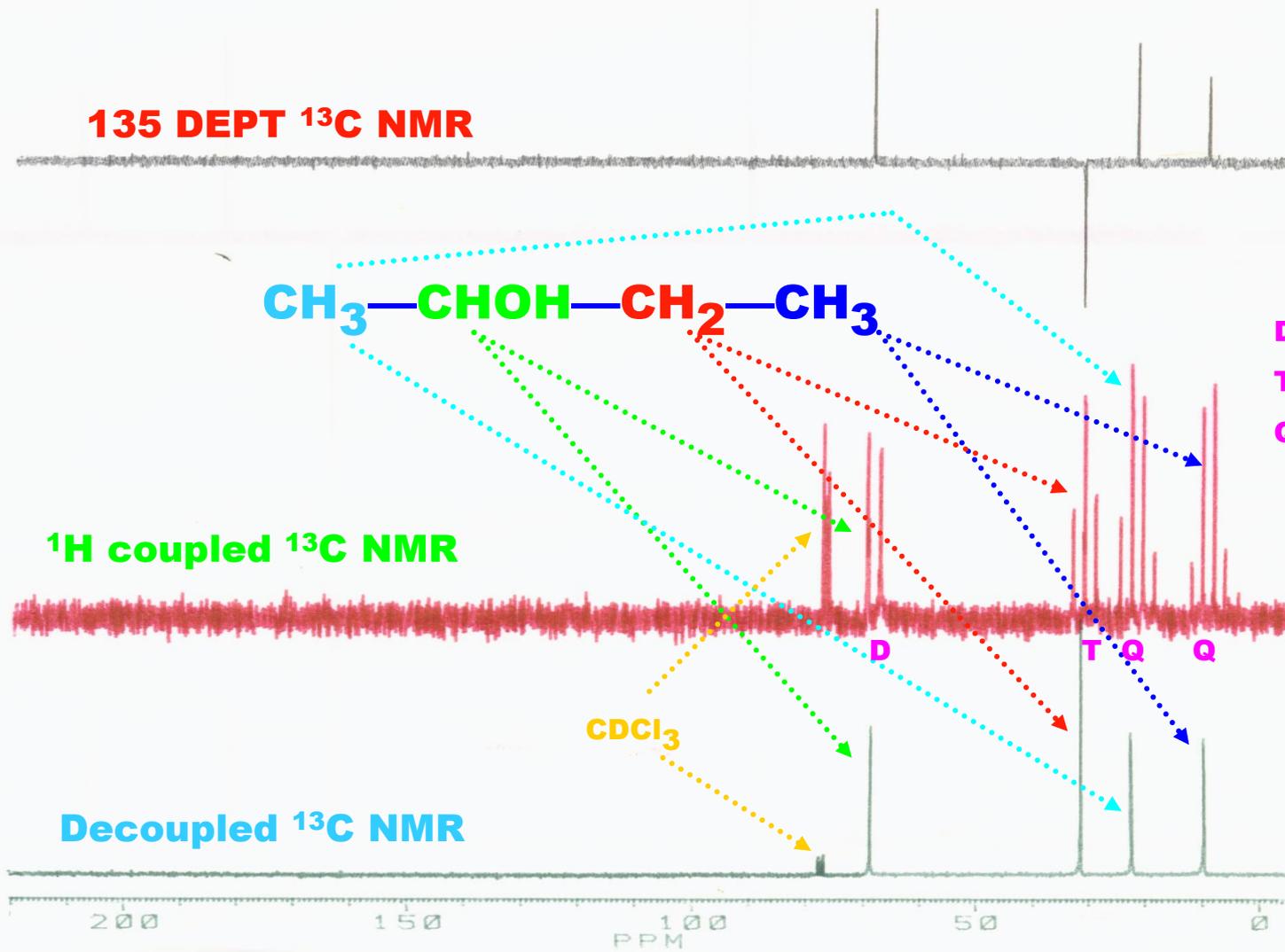


D = Doublet
T = Triplet
Q = Quartet

^1H coupled ^{13}C NMR

CDCl_3

Decoupled ^{13}C NMR

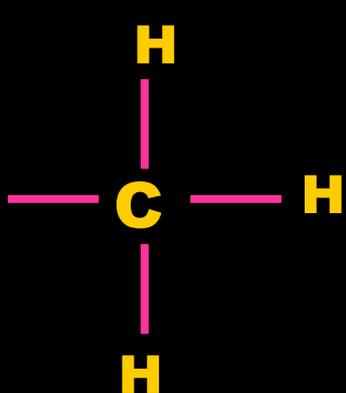


^1H coupling to ^{13}C in ^{13}C NMR Spectra

No. of peaks = $2nI + 1$

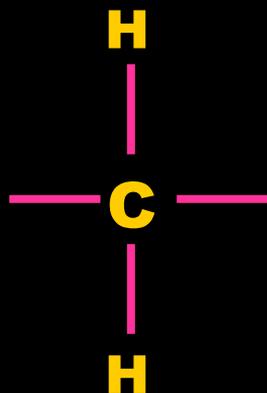
n is No of spin active nuclei (^1H) [Neighbours]

I is Spin number of the active nucleus ($^1\text{H} = 1/2$)



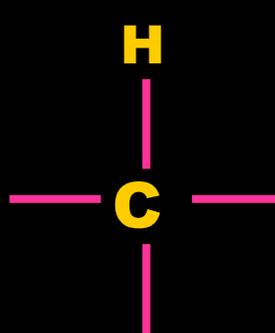
Methyl ^{13}C

Quartet



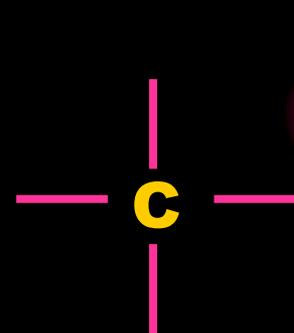
Methylene ^{13}C

Triplet



Methine ^{13}C

Doublet



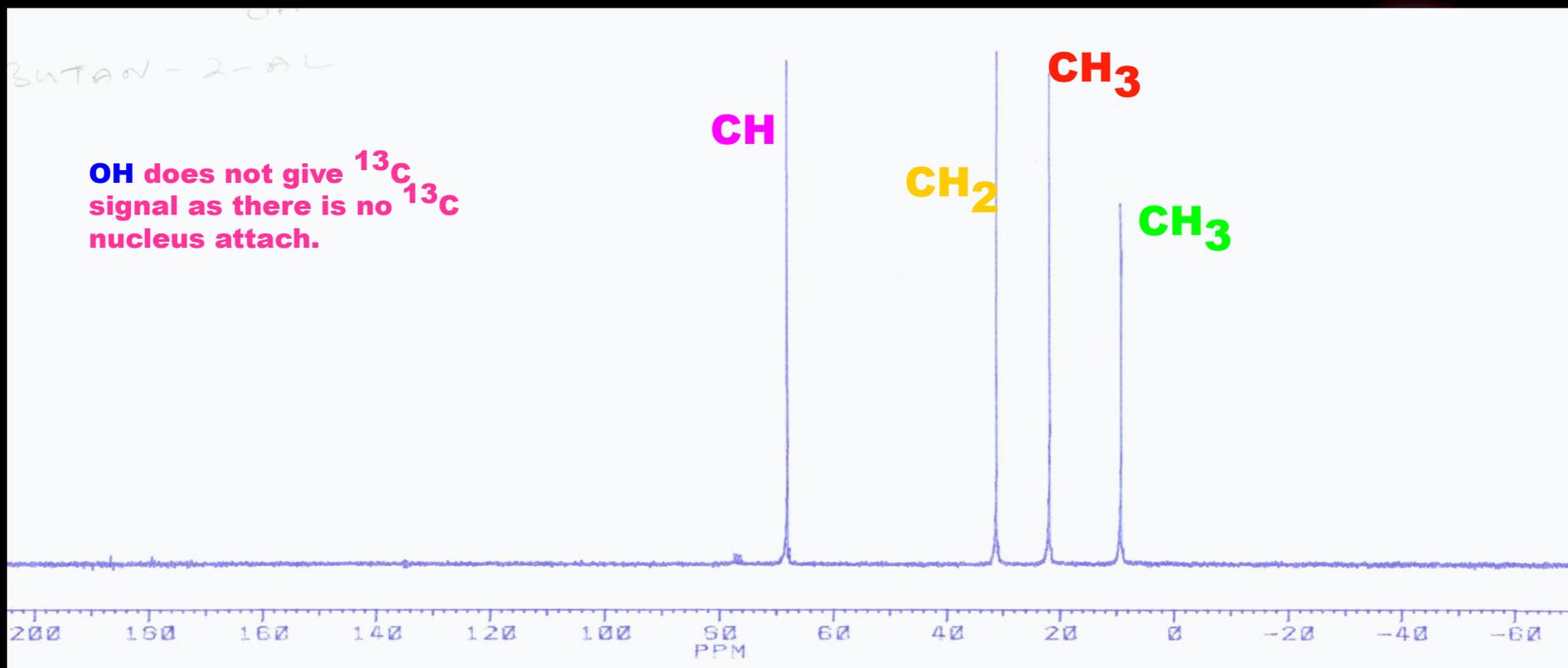
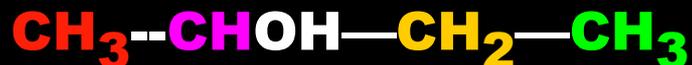
Quaternary ^{13}C

Singlet

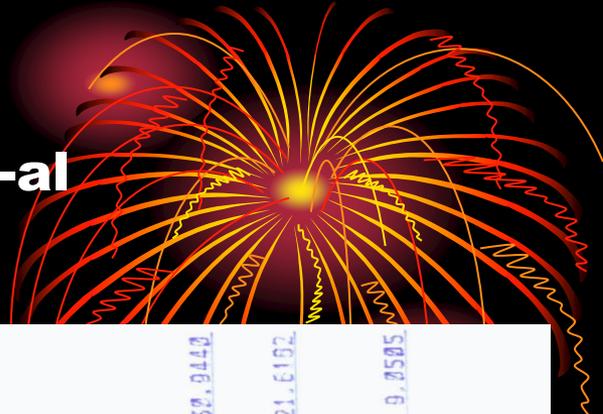


^{13}C NMR spectrum. Most of the ^{13}C NMR spectra are recorded as ^1H decoupled hence $\text{CH}/\text{CH}_2/\text{CH}_3$ give sharp singlet.

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



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

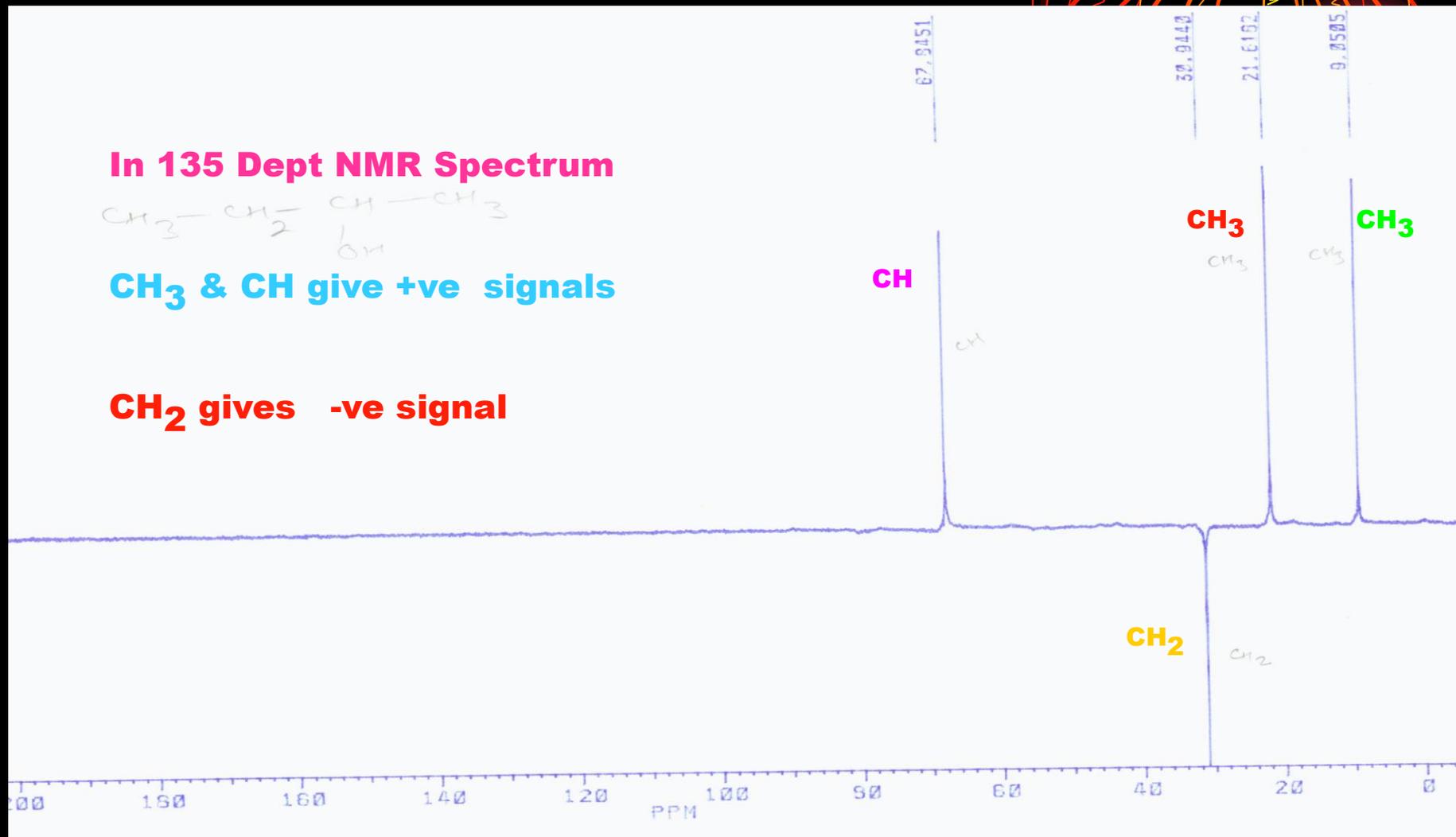


In 135 Dept NMR Spectrum

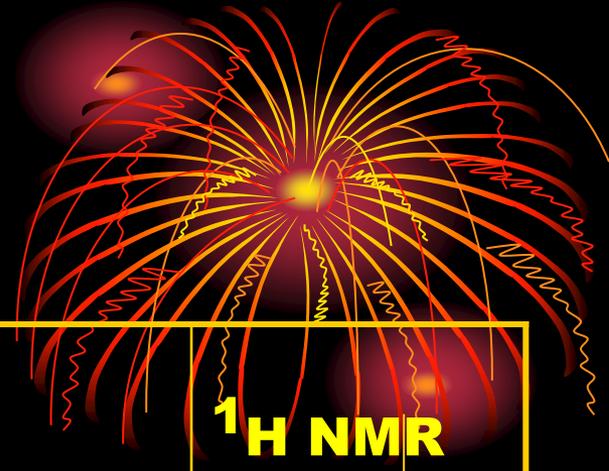


CH_3 & CH give +ve signals

CH_2 gives -ve signal

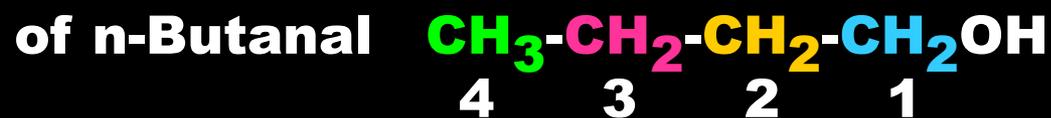


Analysis of ^1H and ^{13}C NMR Spectra Butan-2-ol



CH_3	CH_3	CH_2	OH	CH	$^1\text{H NMR}$
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	$^{13}\text{C NMR}$
9.03 PPM	21.63	30.96	No Signal	67.88	

Analysis and interpretation of ^1H NMR Spectrum



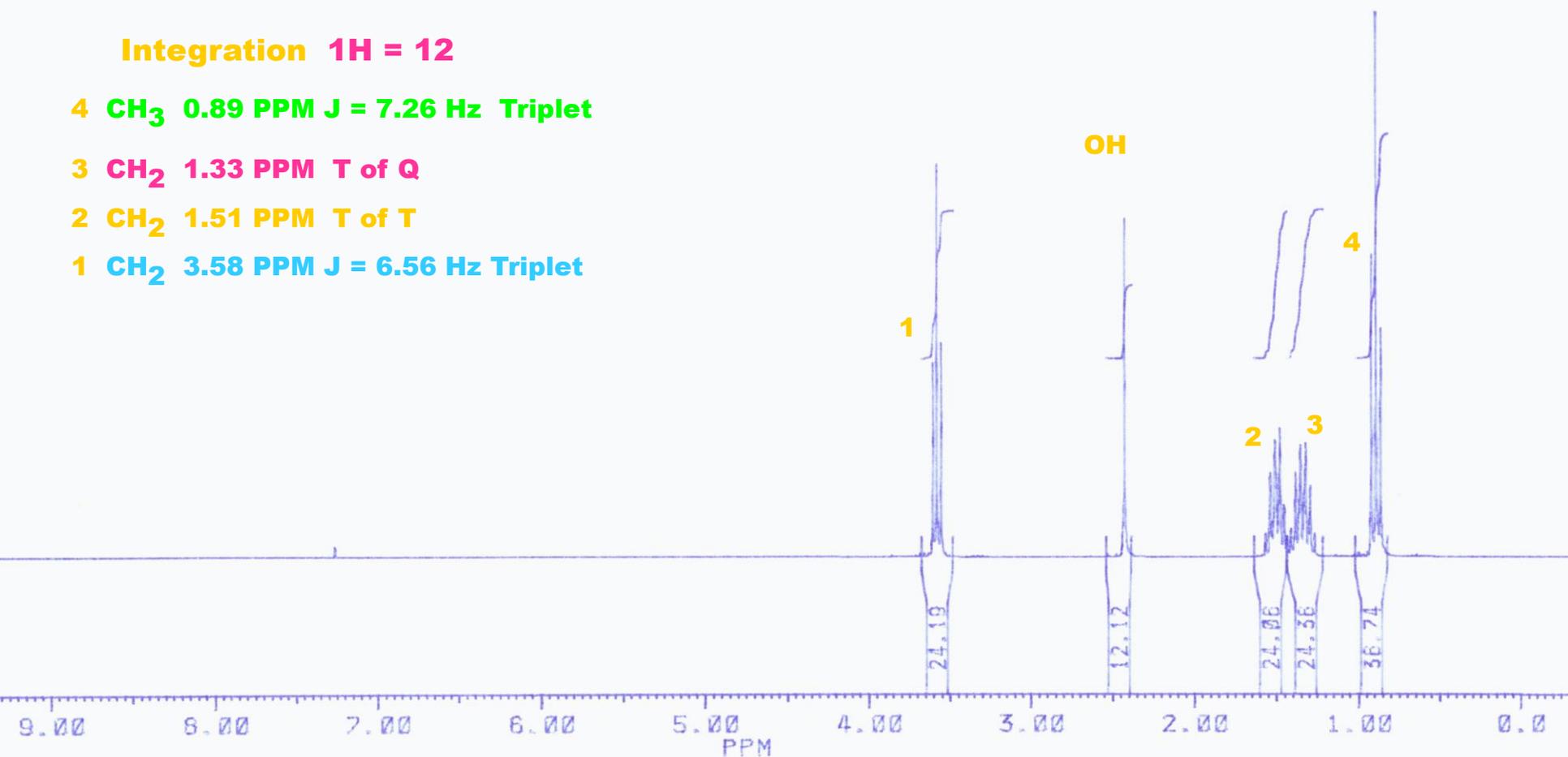
Integration 1H = 12

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

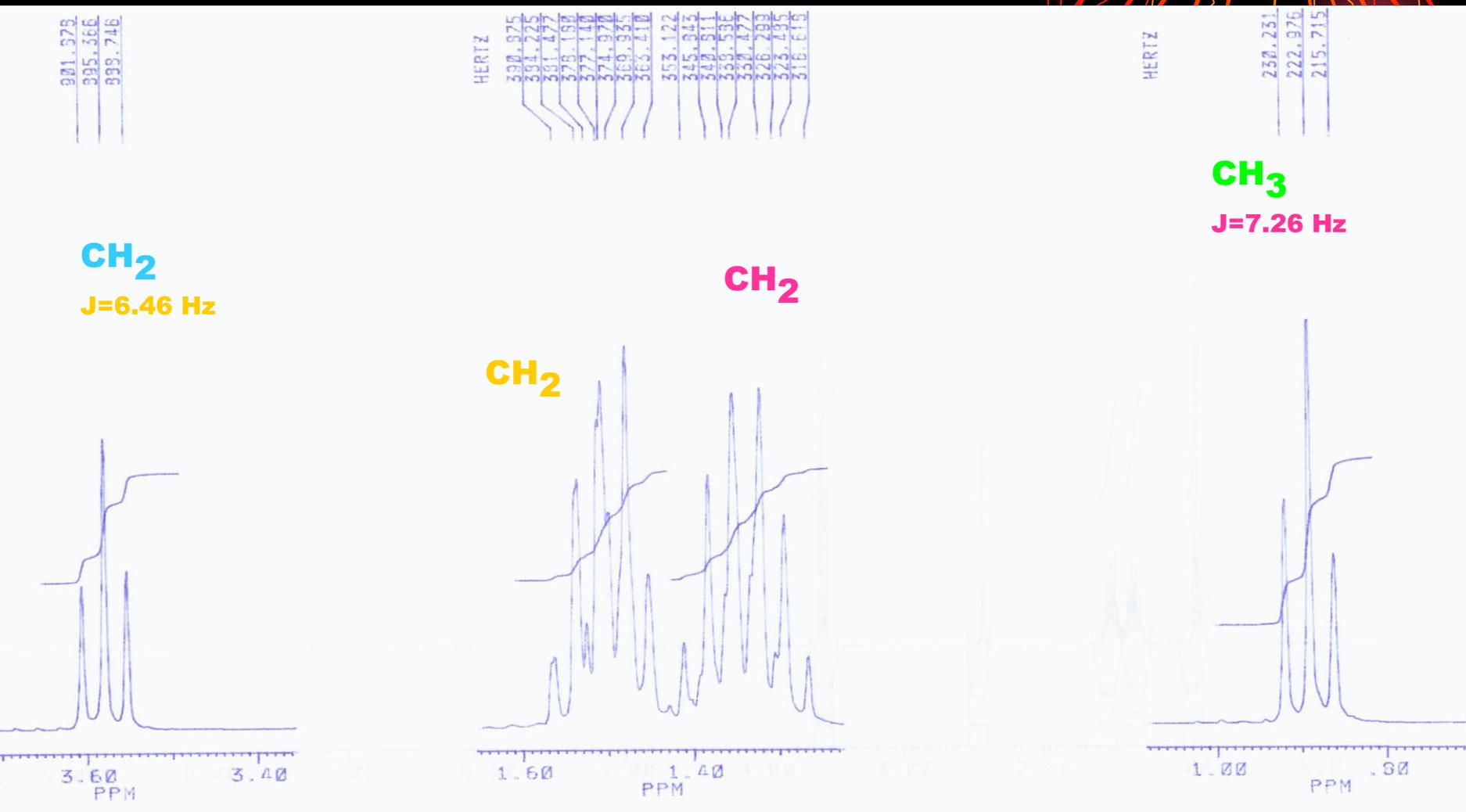
1 CH_2 3.58 PPM J = 6.56 Hz Triplet



Analysis and interpretation of ^1H NMR Spectrum

of n-Butanal $\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{OH}$

4 3 2 1



^{13}C NMR Spectrum of n-Butanol



4 3 2 1



Chemical Shifts

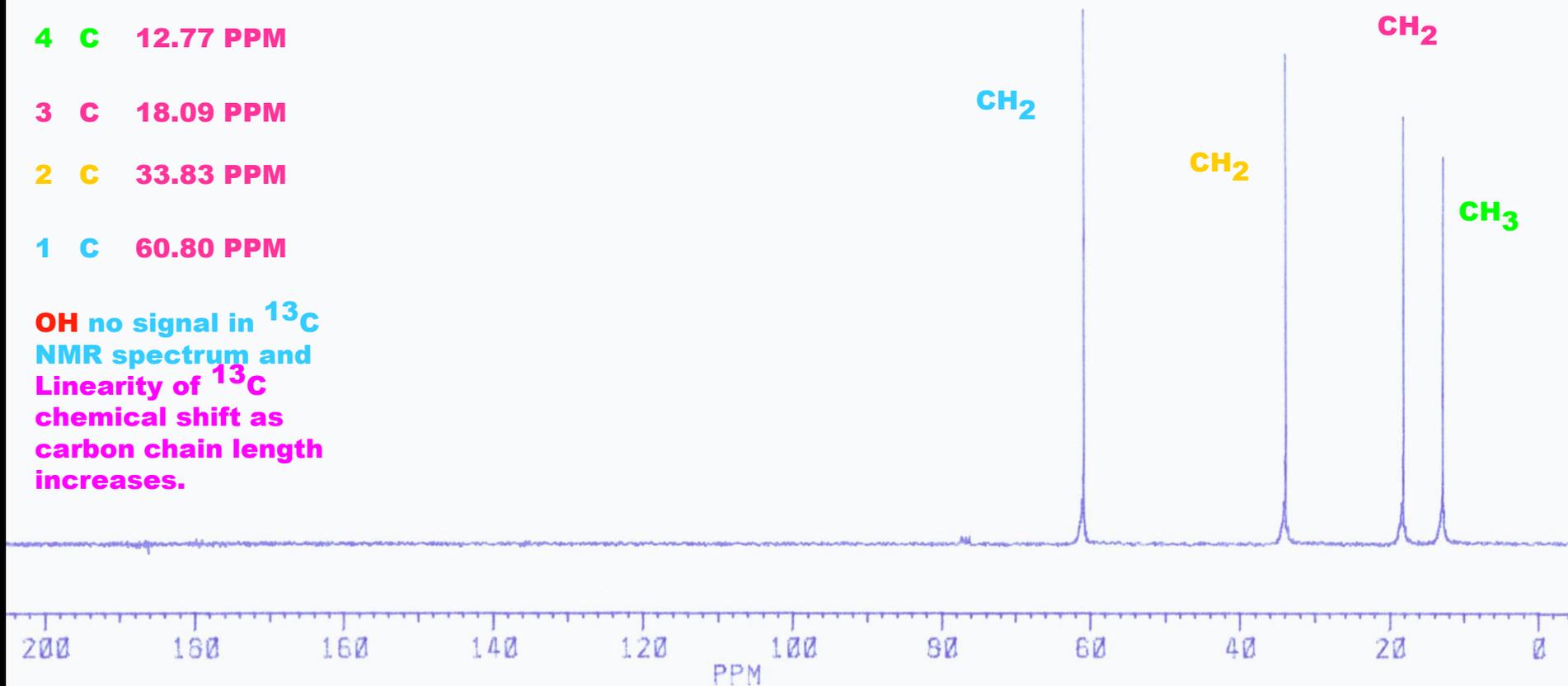
4 C 12.77 PPM

3 C 18.09 PPM

2 C 33.83 PPM

1 C 60.80 PPM

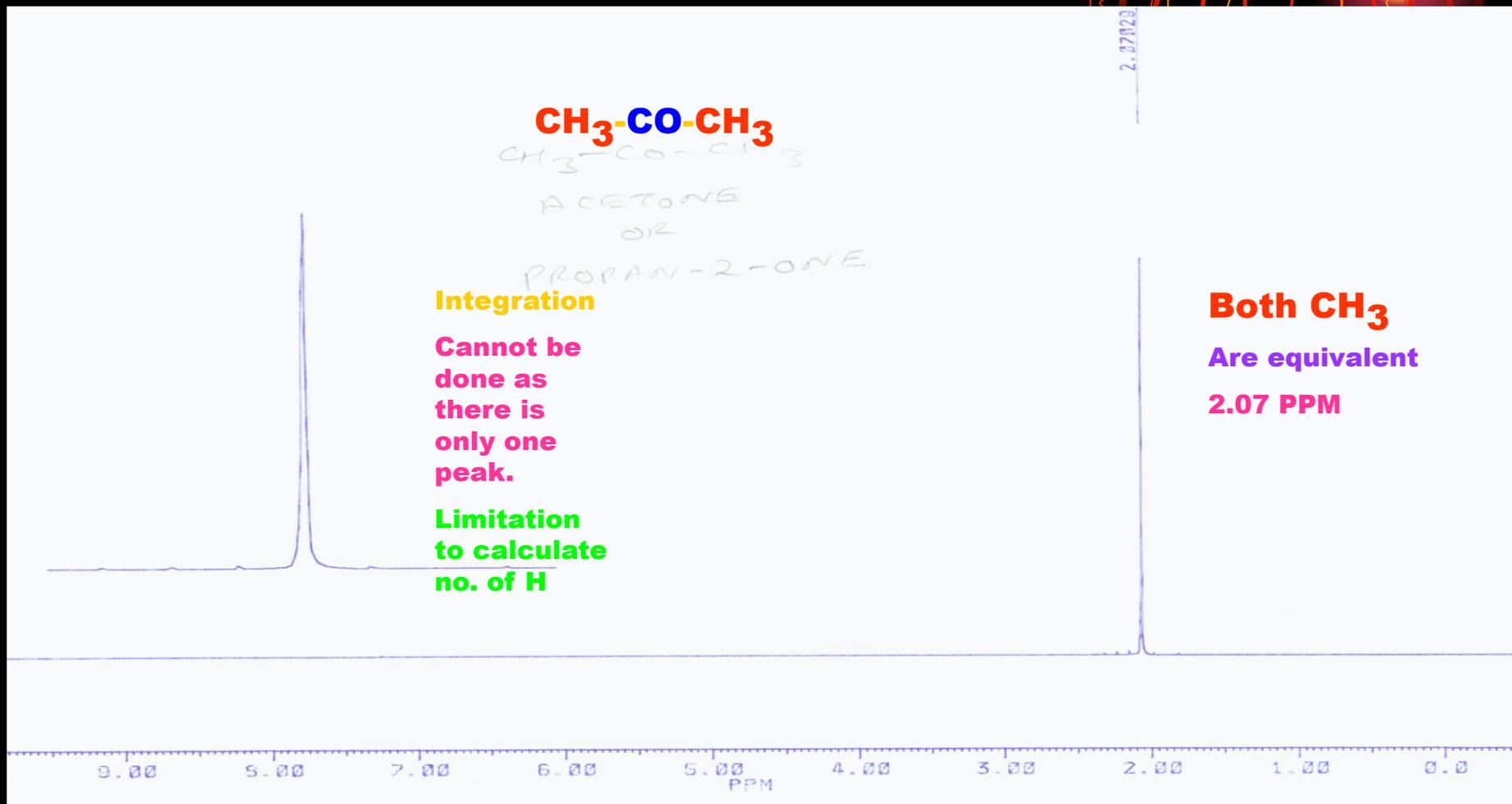
OH no signal in ^{13}C
NMR spectrum and
Linearity of ^{13}C
chemical shift as
carbon chain length
increases.



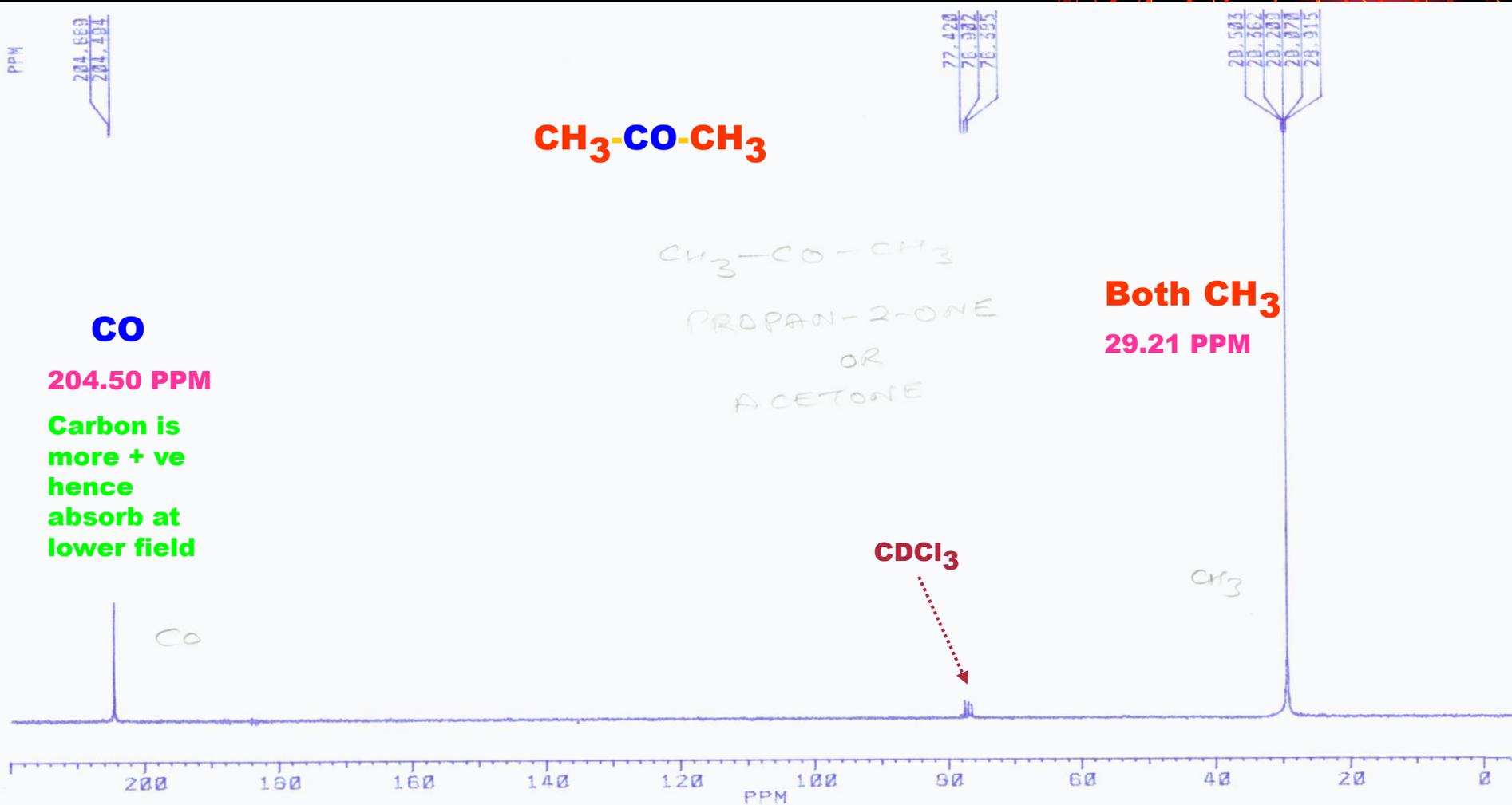
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Propan-2-one or Acetone



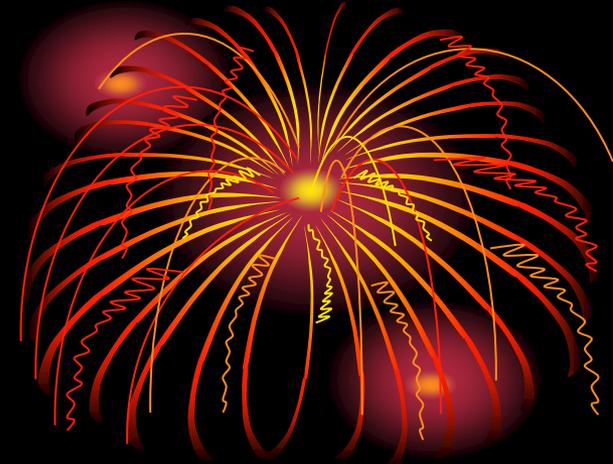
^1H NMR Spectrum



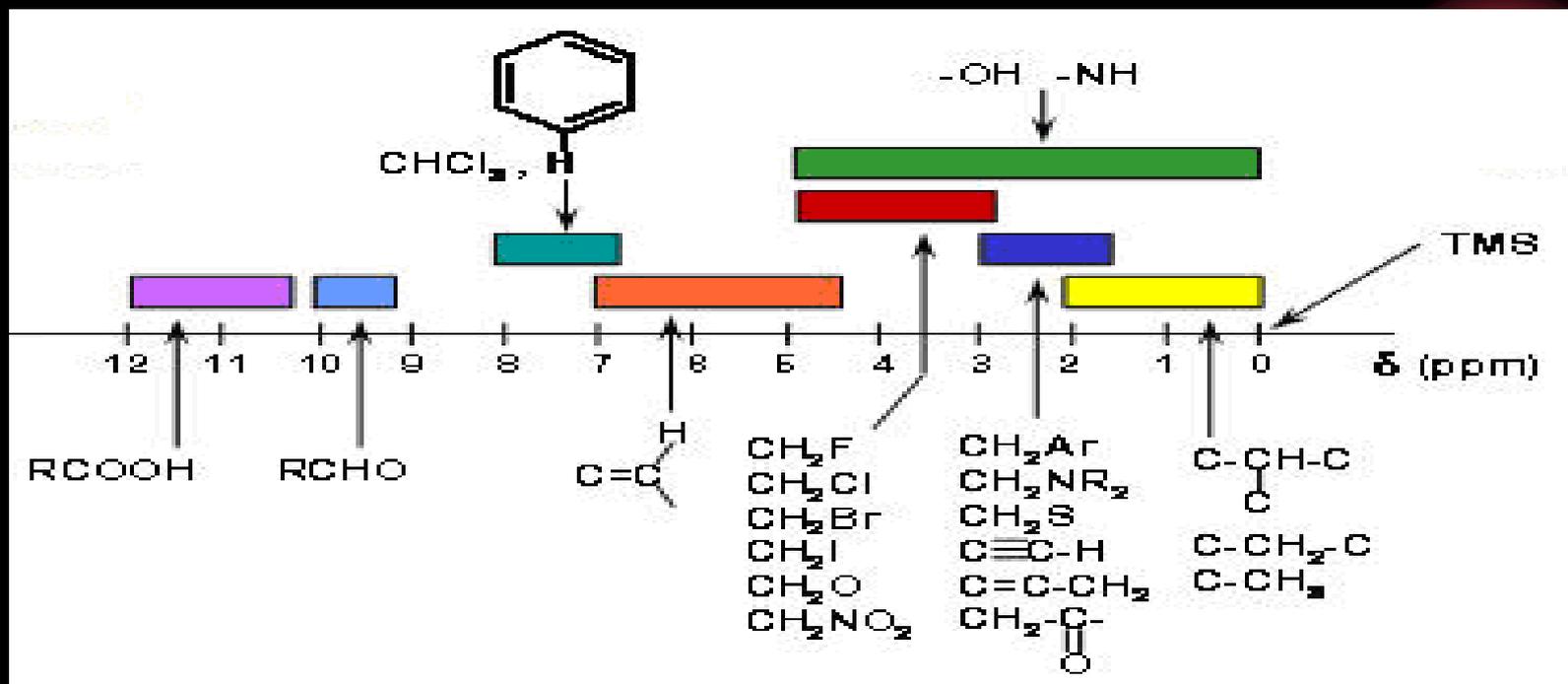
^{13}C NMR Spectrum of Propan-2-one (Acetone)



¹H Chemical Shift in PPM



- General Correlation Chart ¹H NMR Spectra**



Lower Field

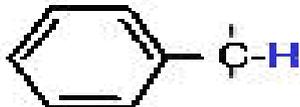


Higher Field

^1H Chemical Shift in more details



^1H Chemical Shift Range Table

R-CH_3	0.7 - 1.3	R-N-C-H	2.2 - 2.9	R-C=C-H	4.5 - 6.5
$\text{R-CH}_2\text{-R}$	1.2 - 1.4	R-S-C-H	2.0 - 3.0		6.5 - 8.0
R_3CH	1.4 - 1.7	I-C-H	2.0 - 4.0	R-C(=O)-N-H	5.0 - 9.0
R-C=C-C-H	1.6 - 2.6	Br-C-H	2.7 - 4.1	R-C(=O)-H	9.0 - 10.0
R-C(=O)-C-H	2.1 - 2.4	Cl-C-H	3.1 - 4.1	R-C(=O)-O-H	11.0 - 12.0
RO-C(=O)-C-H	2.1 - 2.5	RO-C-H	3.2 - 3.8		
HO-C(=O)-C-H	2.1 - 2.5	HO-C-H	3.2 - 3.8		
$\text{N}\equiv\text{C-C-H}$	2.1 - 3.0	R-C(=O)-O-C-H	3.5 - 4.8		
$\text{R-C}\equiv\text{C-C-H}$	2.1 - 3.0	$\text{O}_2\text{N-C-H}$	4.1 - 4.3		
	2.3 - 2.7	F-C-H	4.2 - 4.8		
$\text{R-C}\equiv\text{C-H}$	1.7 - 2.7				
		R-N-H	0.5 - 4.0	Ar-N-H	3.0 - 5.0
		R-O-H	0.5 - 5.0	Ar-O-H	4.0 - 7.0
				R-S-H	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.

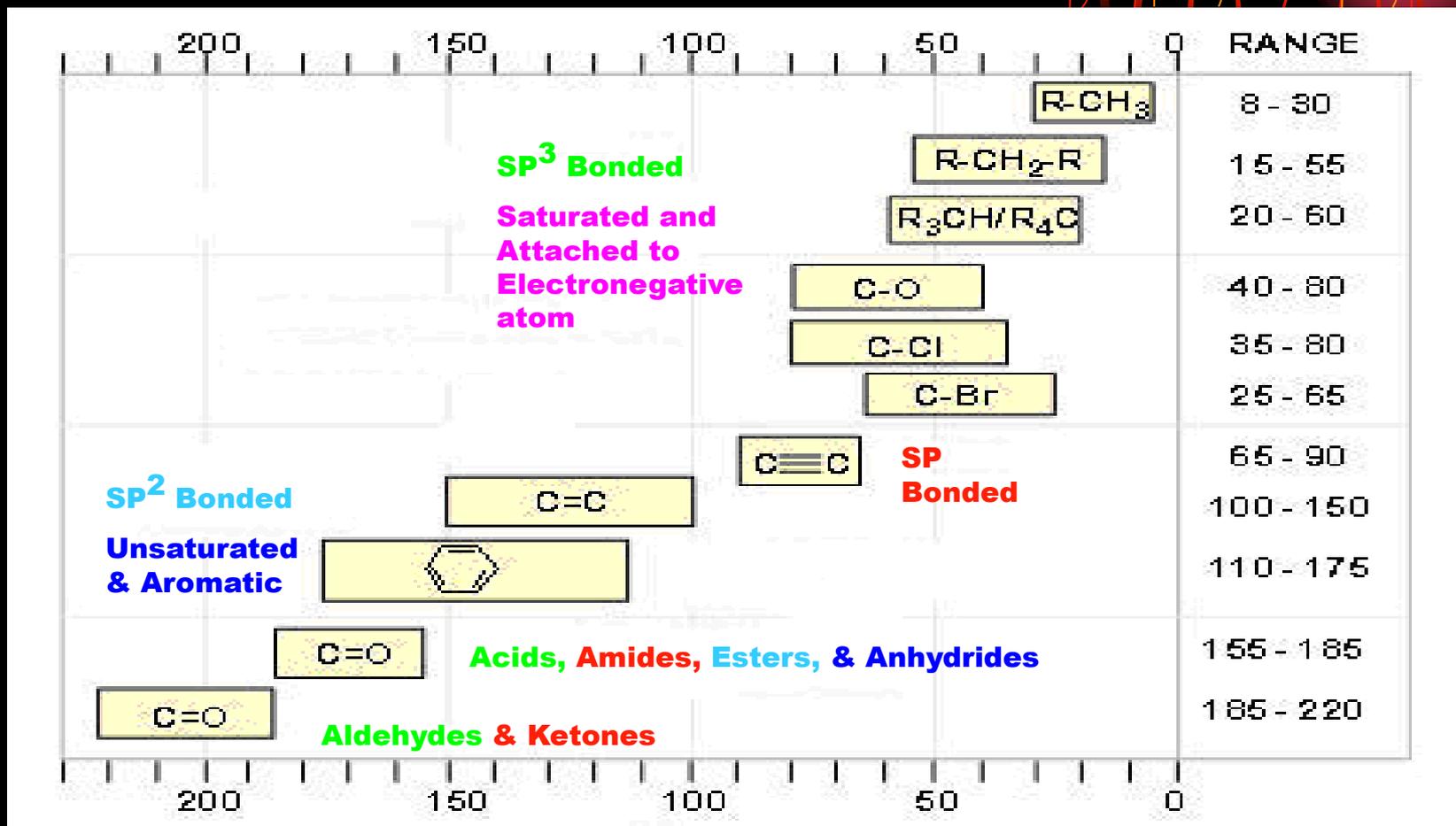


• RCH_3	0.0	to	35	PPM
• R_2CH_2	15	to	40	PPM
• R_3CH	25	to	50	PPM
• R_4C	30	to	40	PPM
• $\text{RC} = \text{CR}$	65	to	90	PPM
• $\text{R}_2\text{C} \equiv \text{CR}_2$	100	to	150	PPM
• C_6H_6 (Aromatic)	110	to	175	PPM
• R-CO-OR	160	to	185	PPM
• R-CO-R	190	to	220	PPM
• RCH_2Br	20	to	40	PPM
• RCH_2Cl	25	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

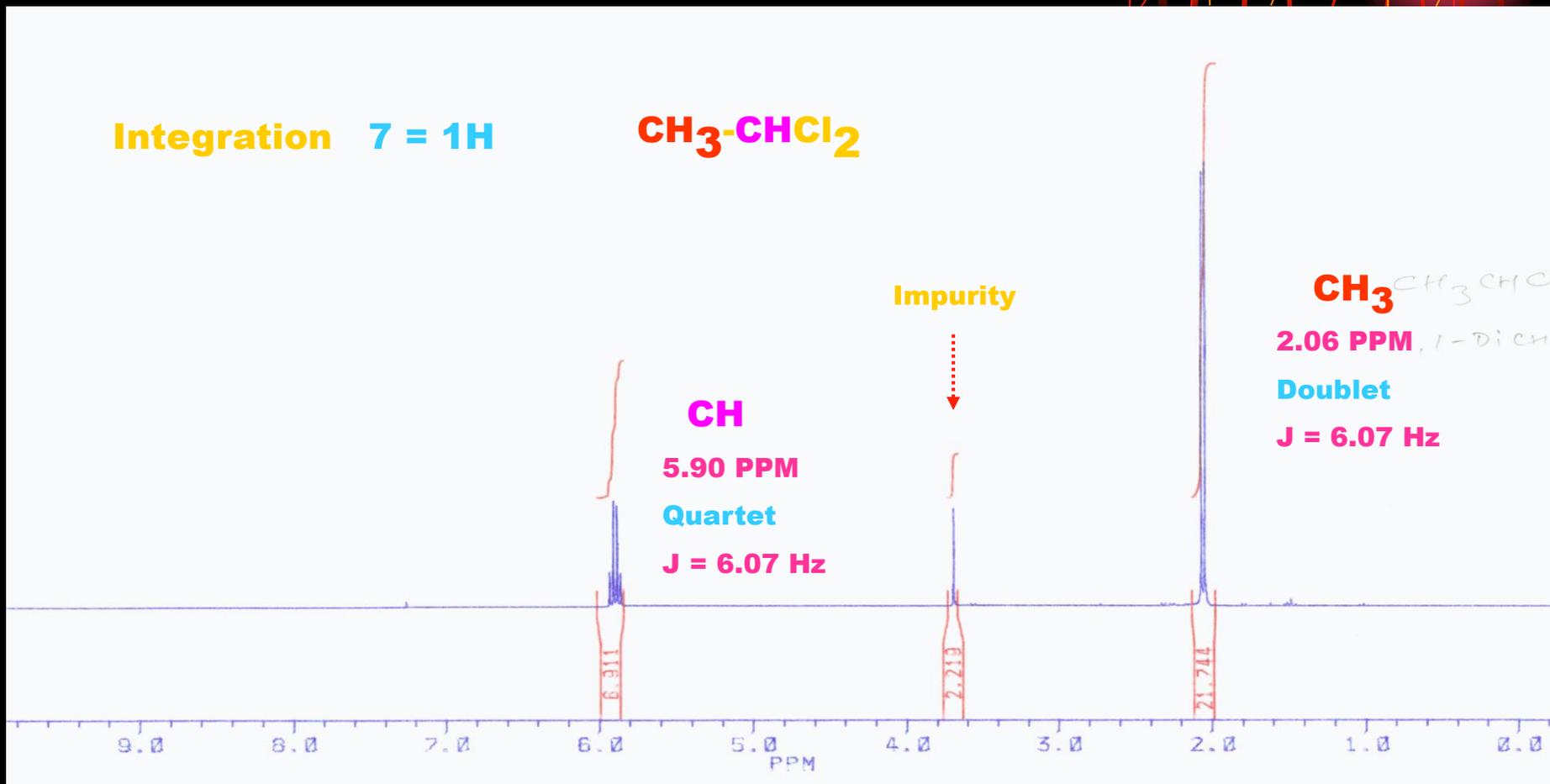
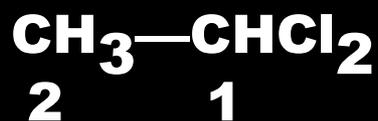


- ^{13}C Chemical Shift Range Table

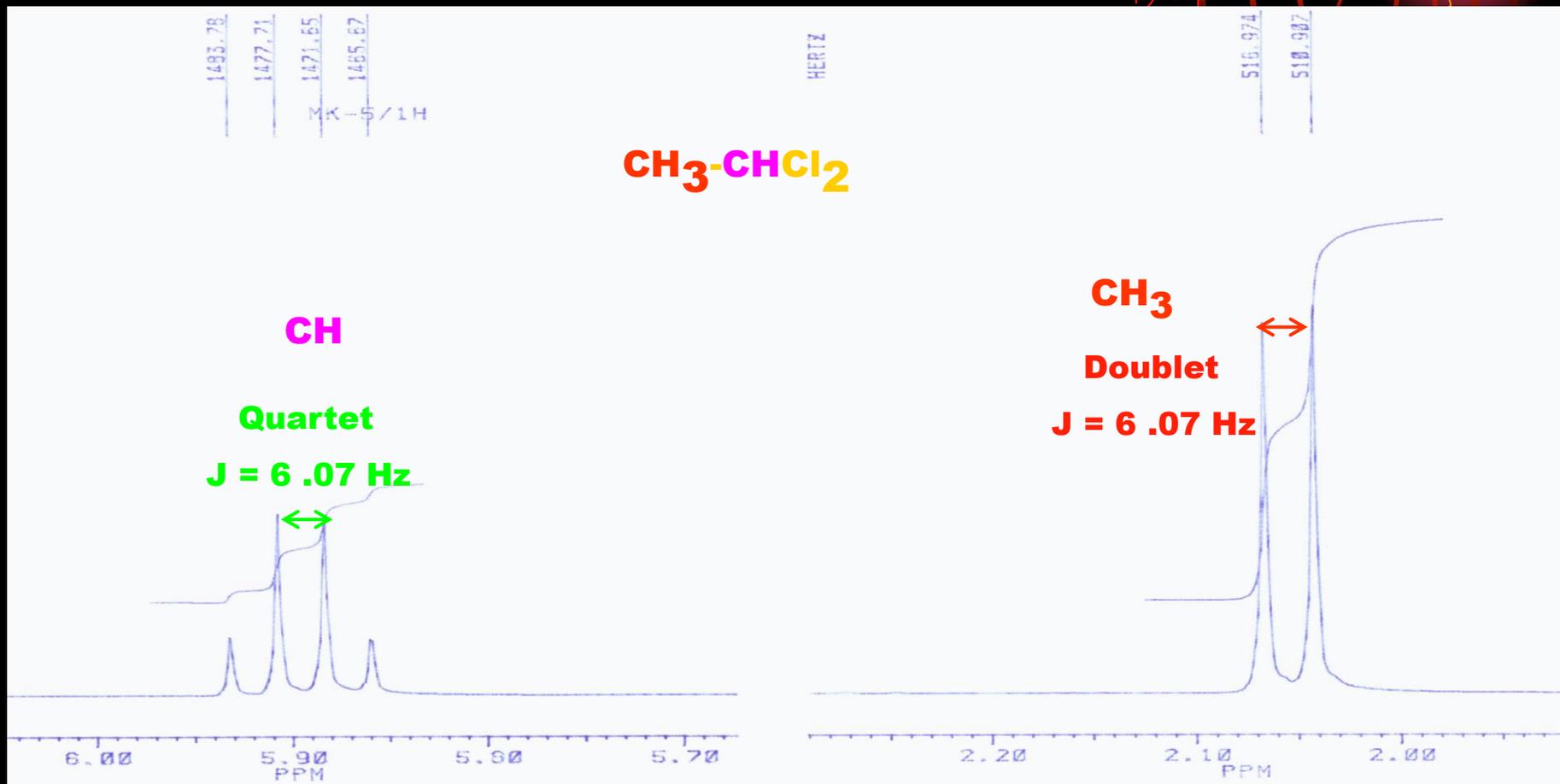


Analysis and interpretation of ^1H & ^{13}C NMR Spectra

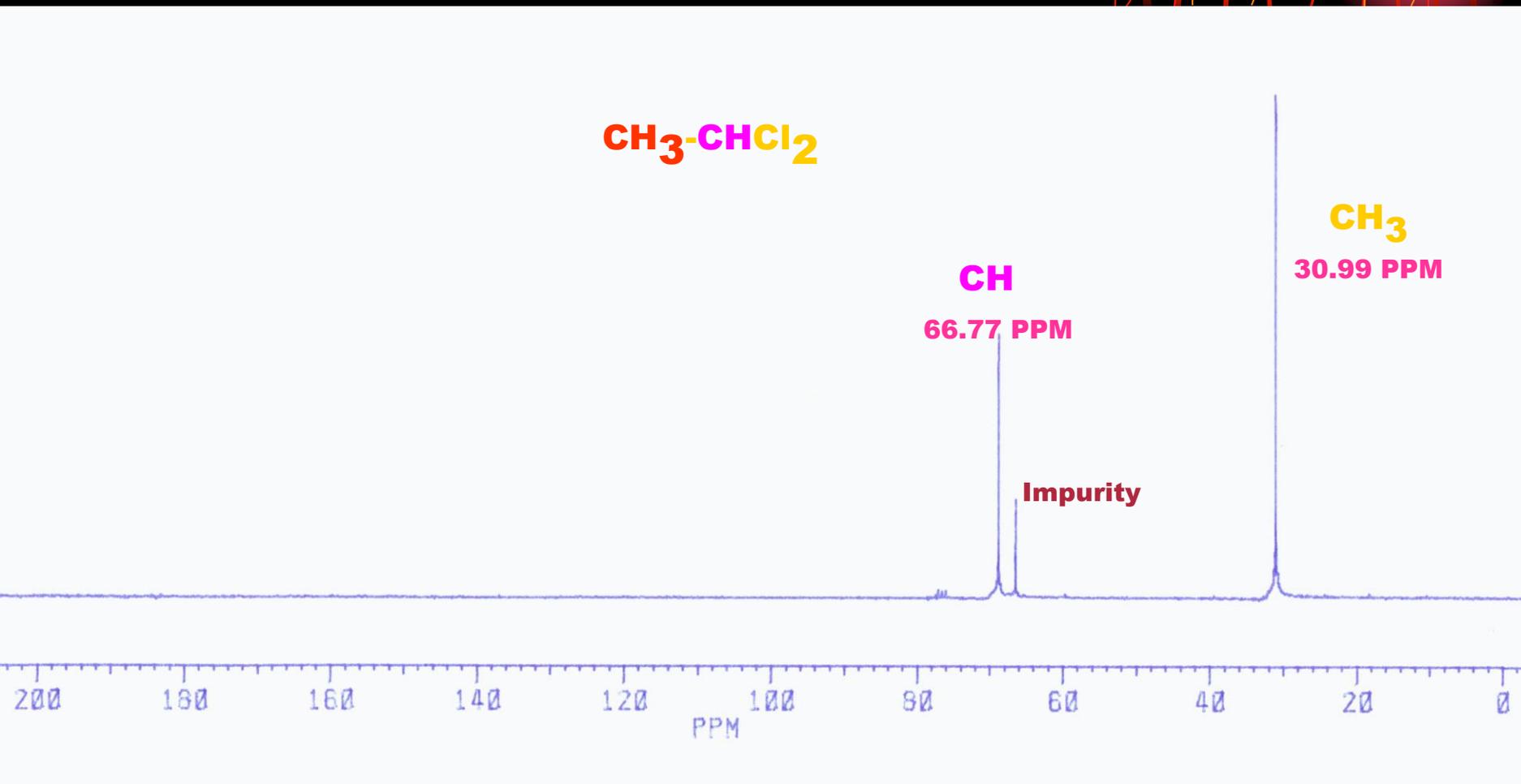
Of 1,1-Dichloroethane



Expansion of ^1H NMR of 1,1-Dichloroethane $\text{CH}_3\text{—CHCl}_2$

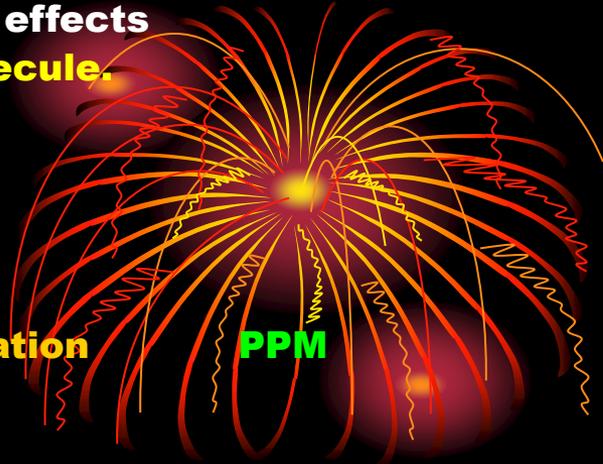


^{13}C NMR OF 1,1-Dichloroethane $\text{CH}_3\text{—CHCl}_2$



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.

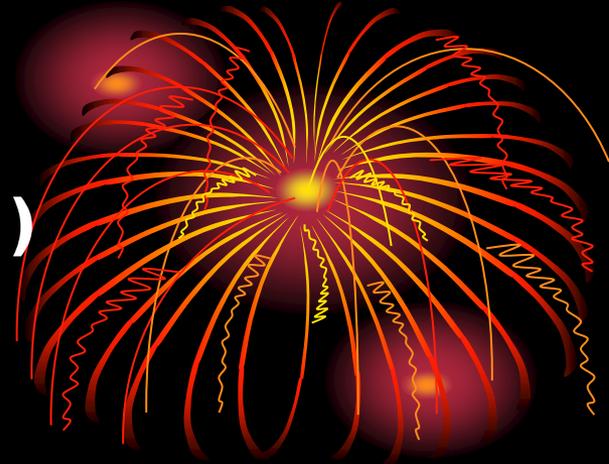


$\text{CH}_3\text{—X}$	Electro negativity of X	PPM	Type of ^1H R = Alkyl	Hybridization	PPM
$\text{CH}_3\text{—F}$	4 .00	4 .26	R-CH_3 , $\text{R}_2\text{-CH}_2$	Alkyl	0 .80 To 1 .70
$\text{CH}_3\text{—OH}$	3 .50	3 .57	$\text{R}_3\text{-CH}$		
$\text{CH}_3\text{—Cl}$	3 .10	3 .05	$\text{R}_2\text{C=C(R)CHR}_2$	Allylic	1 .60 To 2 .60
$\text{CH}_3\text{—Br}$	2 .80	2 .68	$\text{RC}\equiv\text{CH}$	Acetylenic	2 .00 To 3 .00
$\text{CH}_3\text{—I}$	2 .50	2 .16	$\text{R}_2\text{C=CHR}$	Vinylic	4 .60 To 5 .70
$(\text{CH}_3)_4\text{—C}$	2 .10	0 .86	$\text{R}_2\text{C=CH}_2$		
$(\text{CH}_3)_4\text{—Si}$	1 .80	0 .00	RCHO	Aldehydic	9 .50 To 10 .10

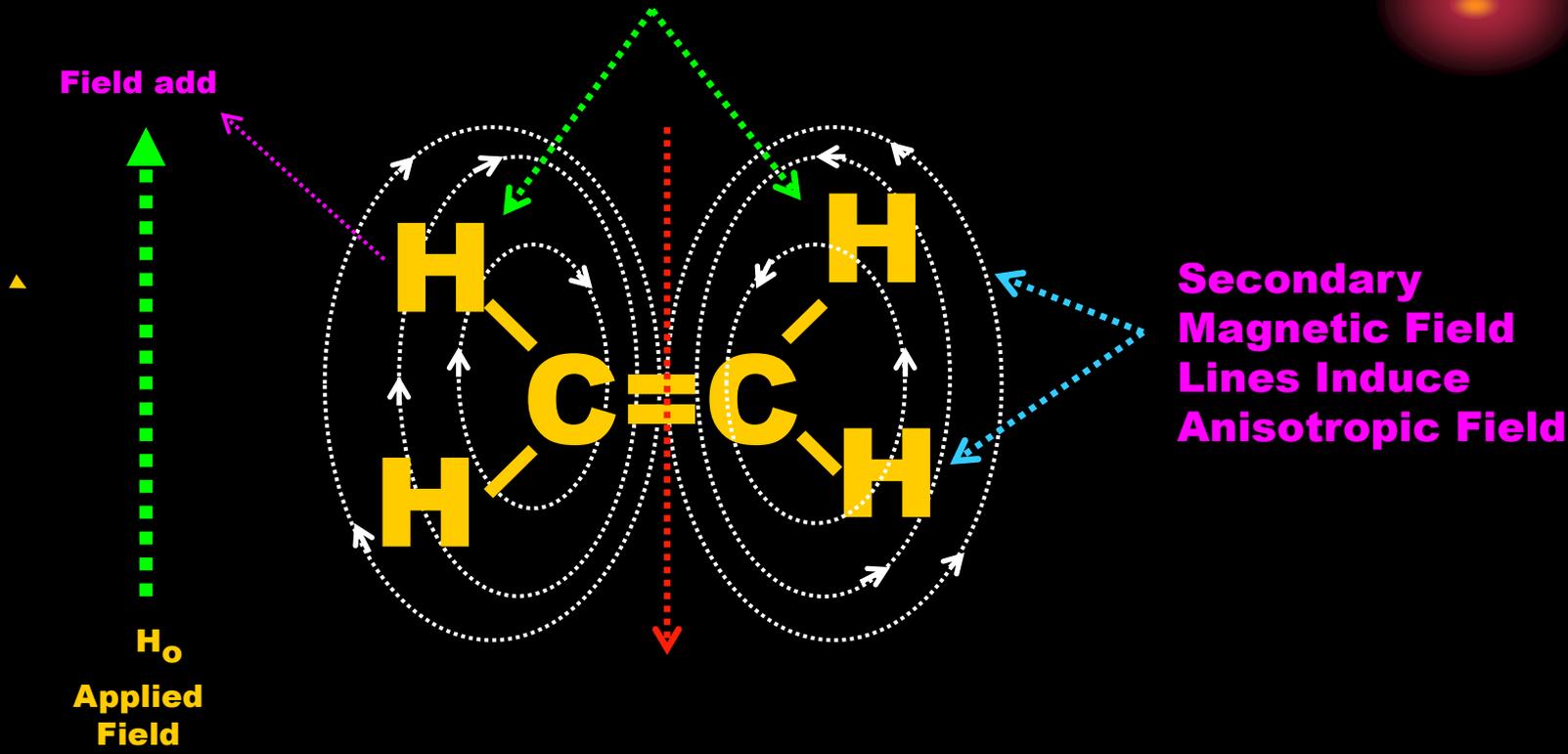
Type of ^1H	Name	PPM	Bonding (Diamagnetic effects)
RCH_3	Alkyl	0 .8 To 1 .0	SP^3
$\text{RC}\equiv\text{CH}$	Acetylenic	2 .0 To 3 .0	SP
$\text{R}_2\text{C=CH}_2$	Vinylic	4 .6 To 5 .7	SP^2

Anisotropic Field in an Alkenes (sp^2)

- Anisotropic Field Effect



Deshielded 1H Shift
To Lower Field
Away From TMS



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.

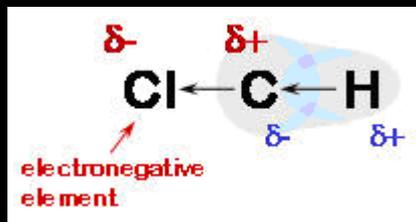
CH ₃ -X	Electronegativity of X	Chemical Shift (δ)
CH ₃ F	4.0	4.26
CH ₃ OH	3.5	3.47
CH ₃ Cl	3.1	3.05
CH ₃ Br	2.8	2.68
CH ₃ I	2.5	2.16
(CH ₃) ₄ C	2.1	0.86
(CH ₃) ₄ Si	1.8	0.00

Type of Hydrogen (R = alkyl)	Name of Hydrogen	Chemical Shift (δ)
RCH ₃ , R ₁ CH ₂ , R ₃ CH	Alkyl	0.8 - 1.7
R ₁ C=C(R ₂)CHR ₃	Allylic	1.6 - 2.6
RC≡CH	Acetylenic	2.0 - 3.0
R ₁ C=CHR ₂ , R ₂ C=CH ₂	Vinyllic	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 ₁ C=CH ₂	Vinyllic	4.6 - 5.7

Hybridization
SP³
SP
SP²

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

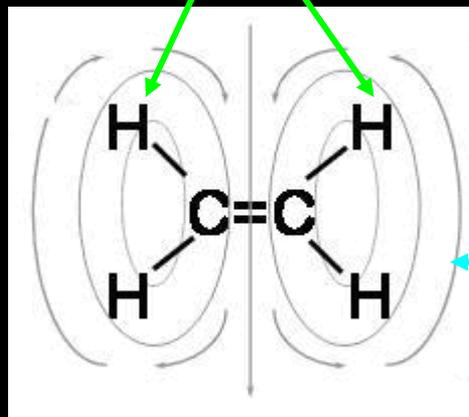
Deshielded 1H
Shift To Lower Field

Fields Add



H_0

Applied Field

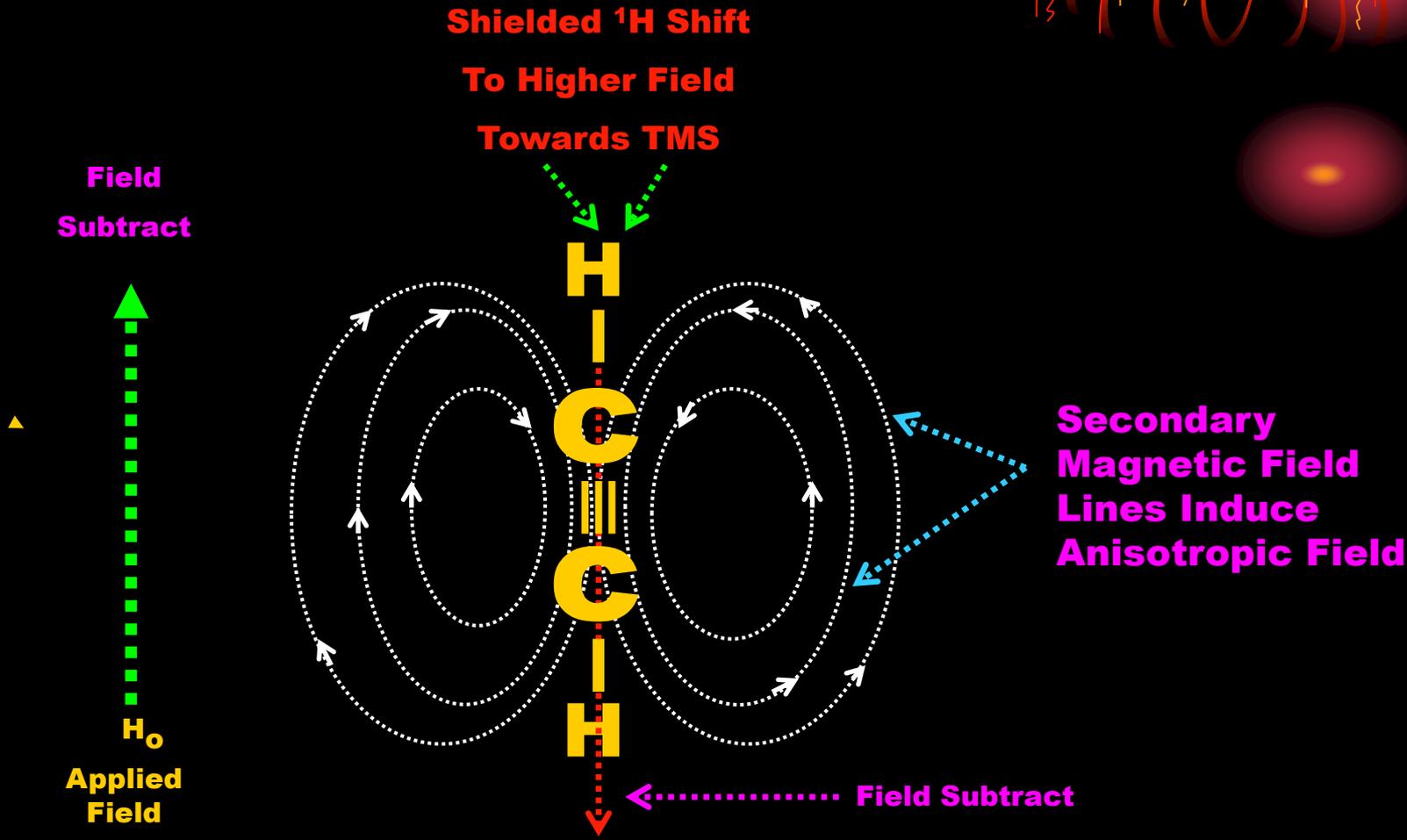


Secondary Magnetic
Field Lines Induce
Anisotropic Field



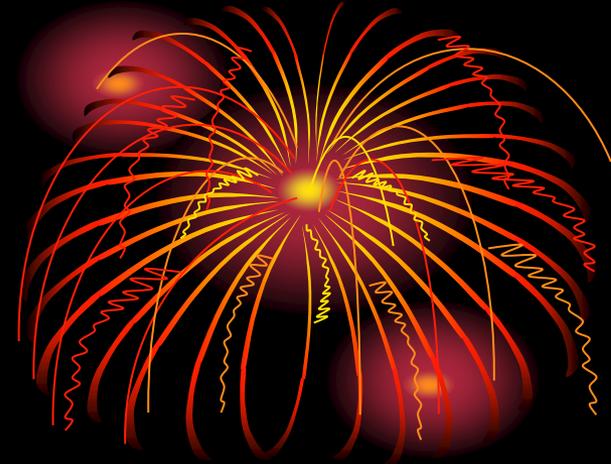
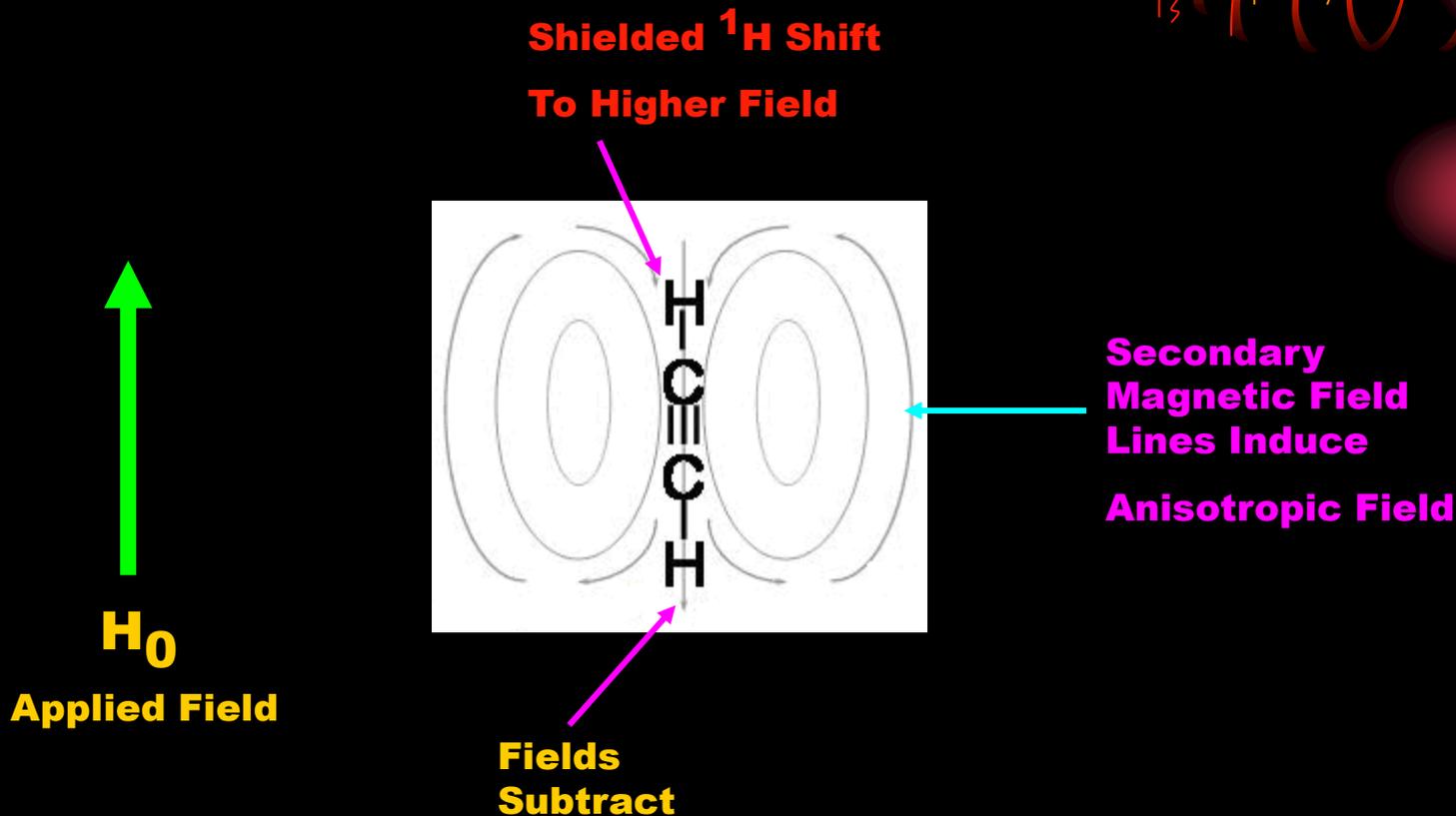
Anisotropic Field in an Alkynes (SP)

- **Anisotropic Field Effect**

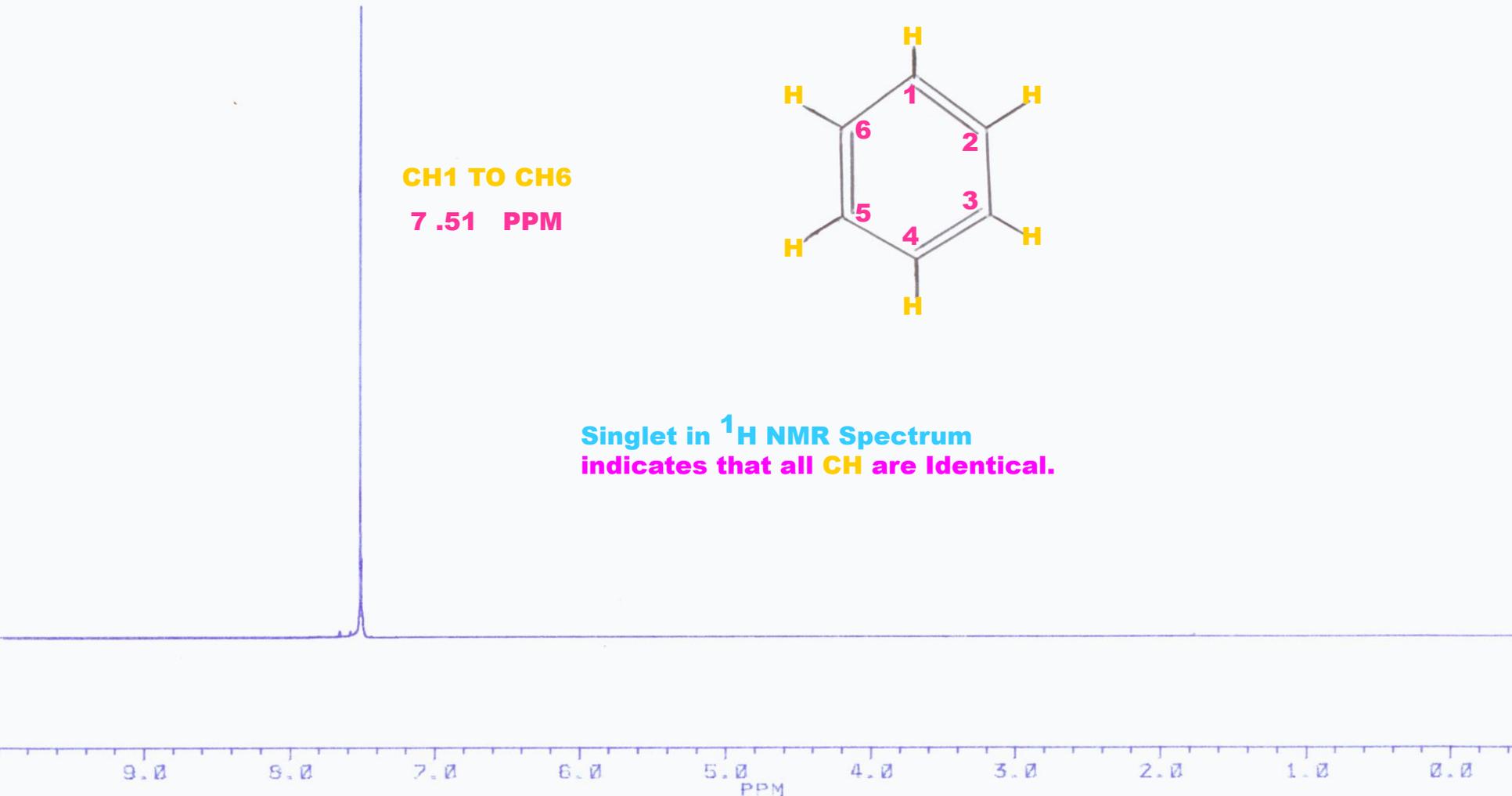


Anisotropic Field in an Alkynes (SP)

- Anisotropic Field Effect**



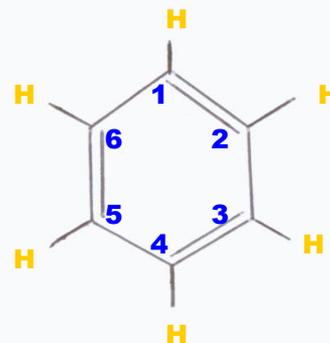
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Benzene C_6H_6 ^1H NMR Spectrum



^{13}C NMR Spectrum of Benzene C_6H_6



128.807



BENZENE

C1 to C6 128.81 PPM

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

200 180 160 140 120 100 90 80 60 40 20 0
PPM

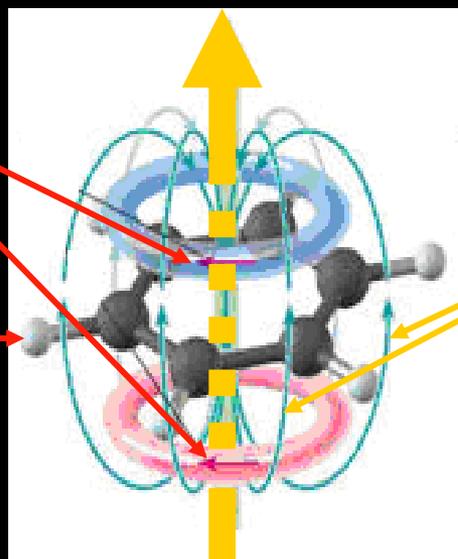
Magnetic Induction of the pi electrons in Aromatic Ring



- **Effect on Chemical Shift**

Induced circulation of pi electrons in the aromatic ring

^1H of Aromatic ring are Deshielded hence absorb at Lower Field.



Circulating pi electrons generate secondary field lines which reinforces the applied field (Adding Effect)

H_0
Applied Field

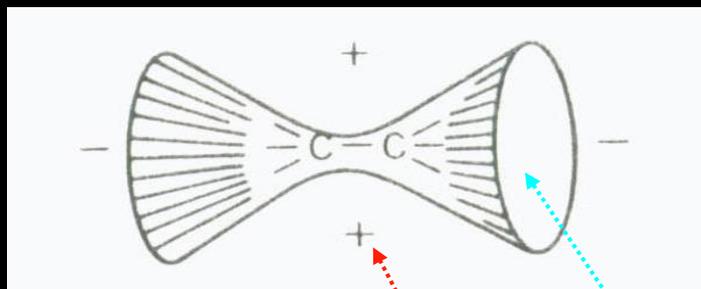
Anisotropic field effect of Various Bonds

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

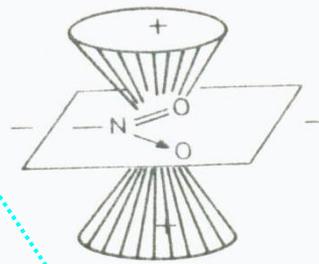
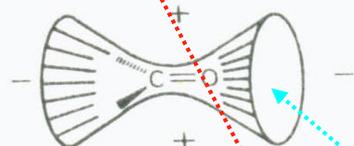
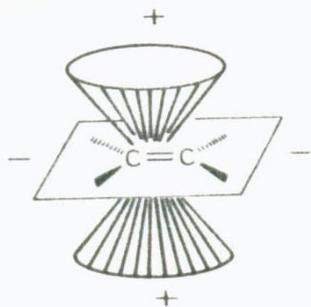
Deshielded ^1H Shift to Lower Field (Away from TMS)



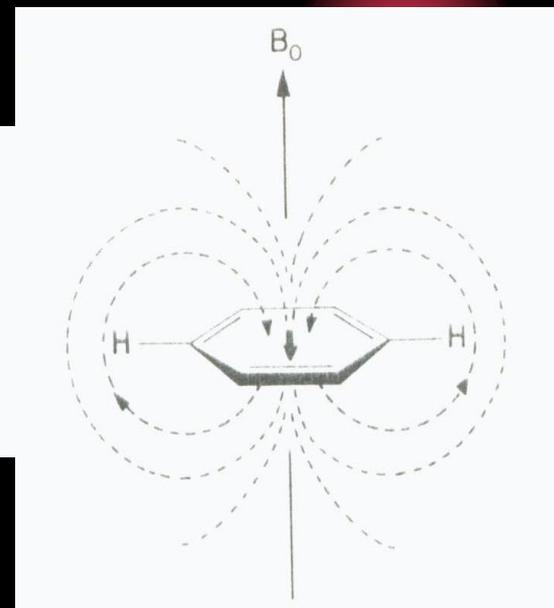
Single Bond



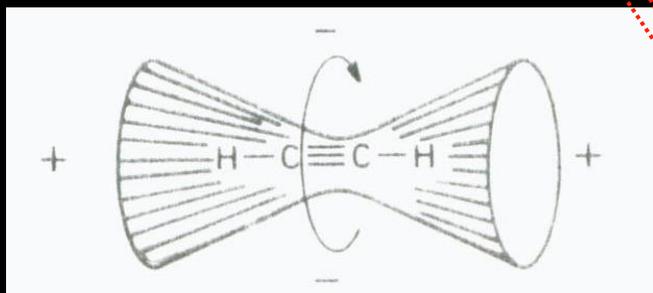
Double Bond



Aromatic
Double Bond



Triple Bond



Inside the cone = Deshielded

Out side the cone = Shielded

For triple bond this is reverse

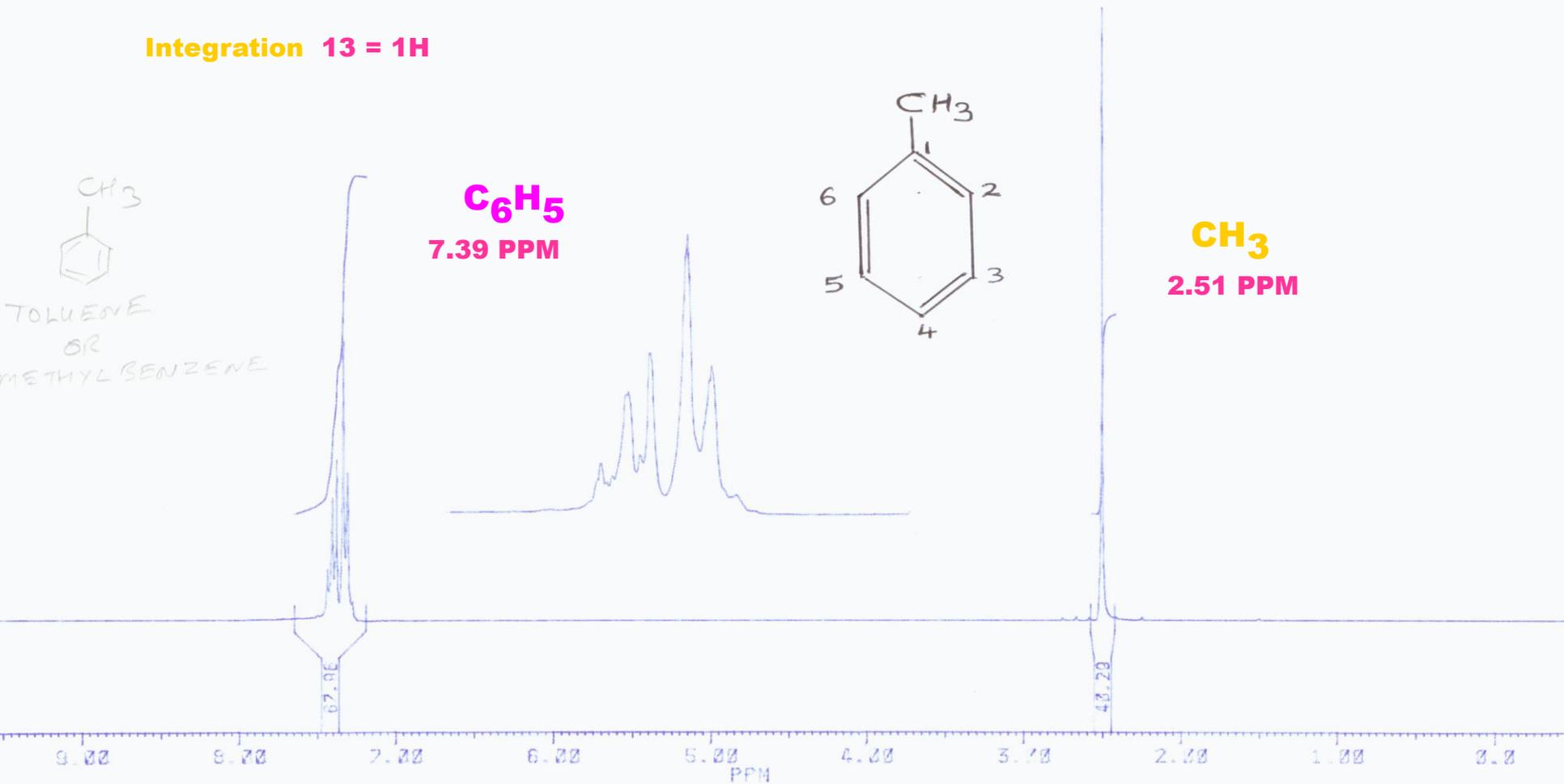
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Methyl Benzene or Toluene



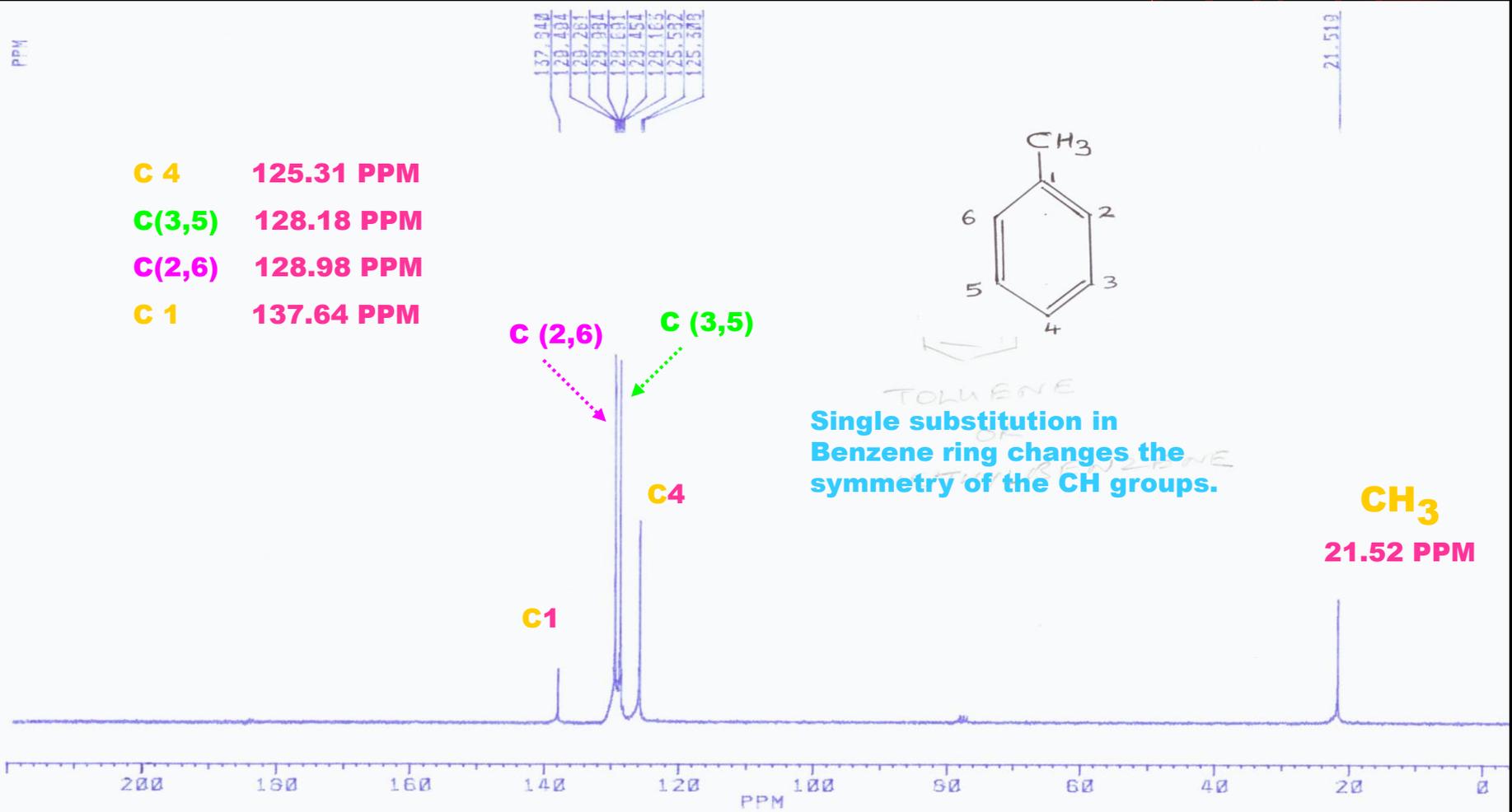
^1H NMR Spectrum



Integration 13 = 1H



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



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



^1H NMR

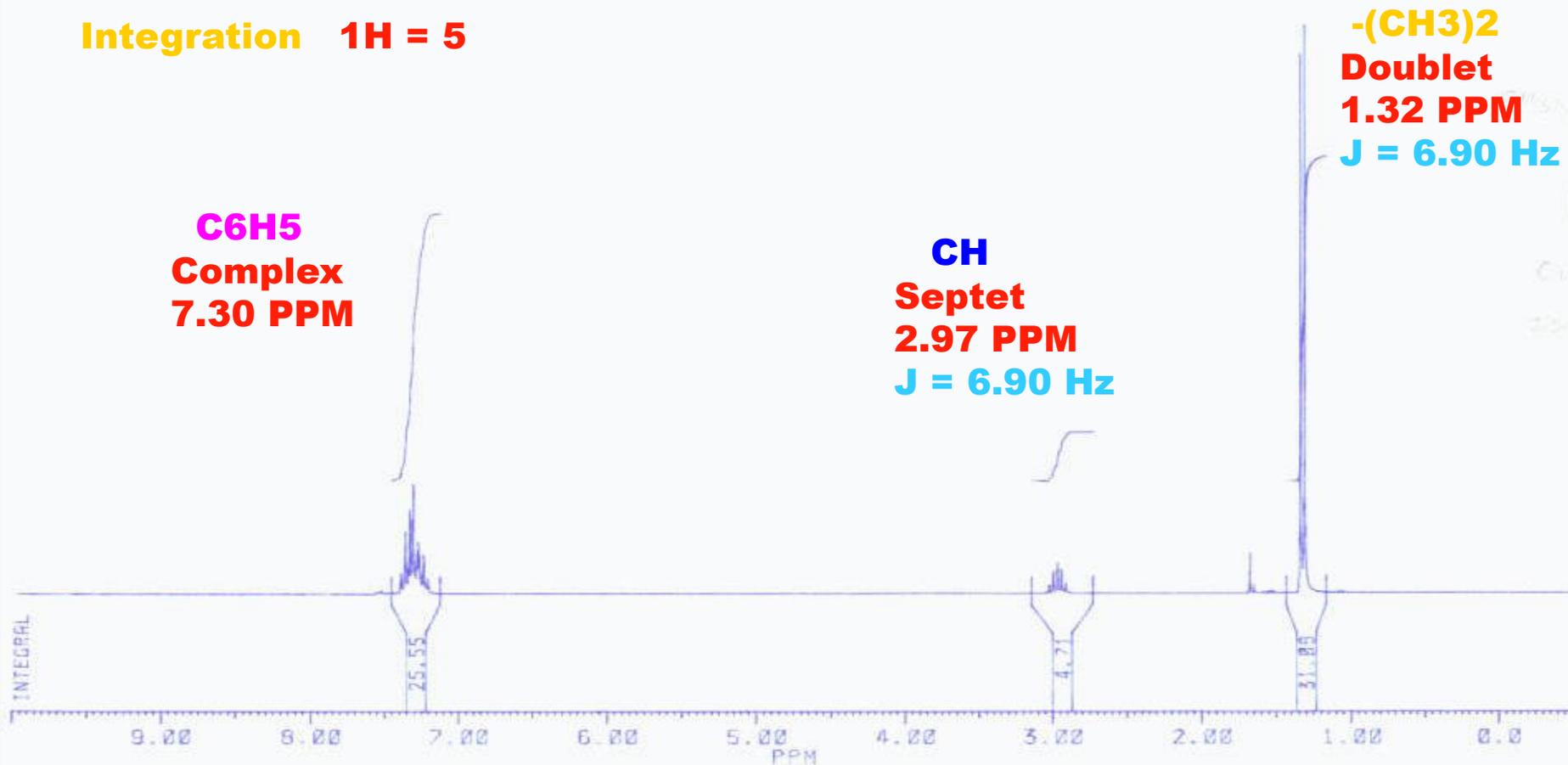


Integration $1\text{H} = 5$

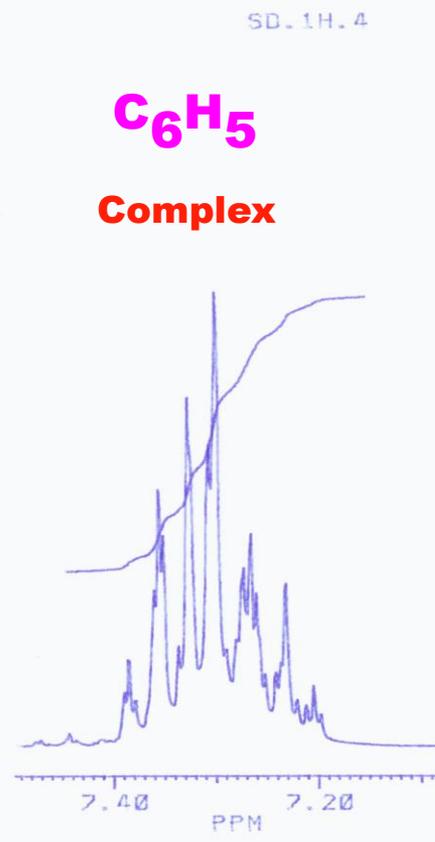
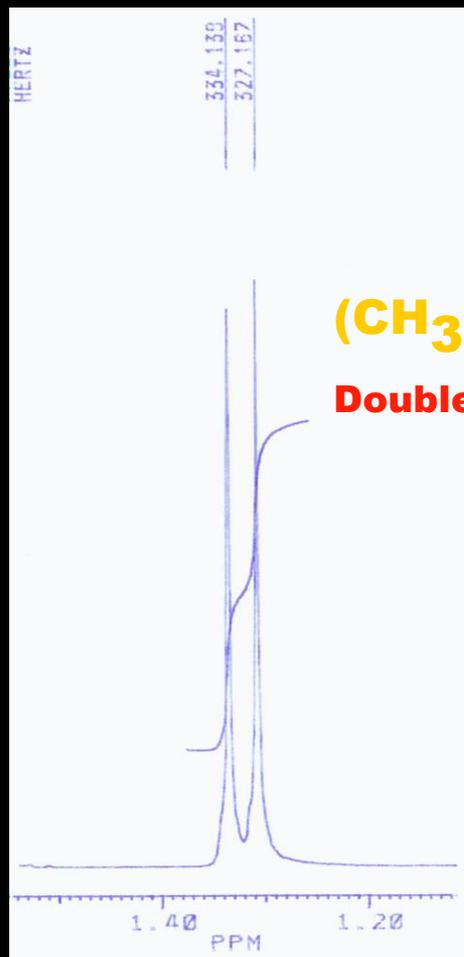
C6H5
Complex
7.30 PPM

CH
Septet
2.97 PPM
J = 6.90 Hz

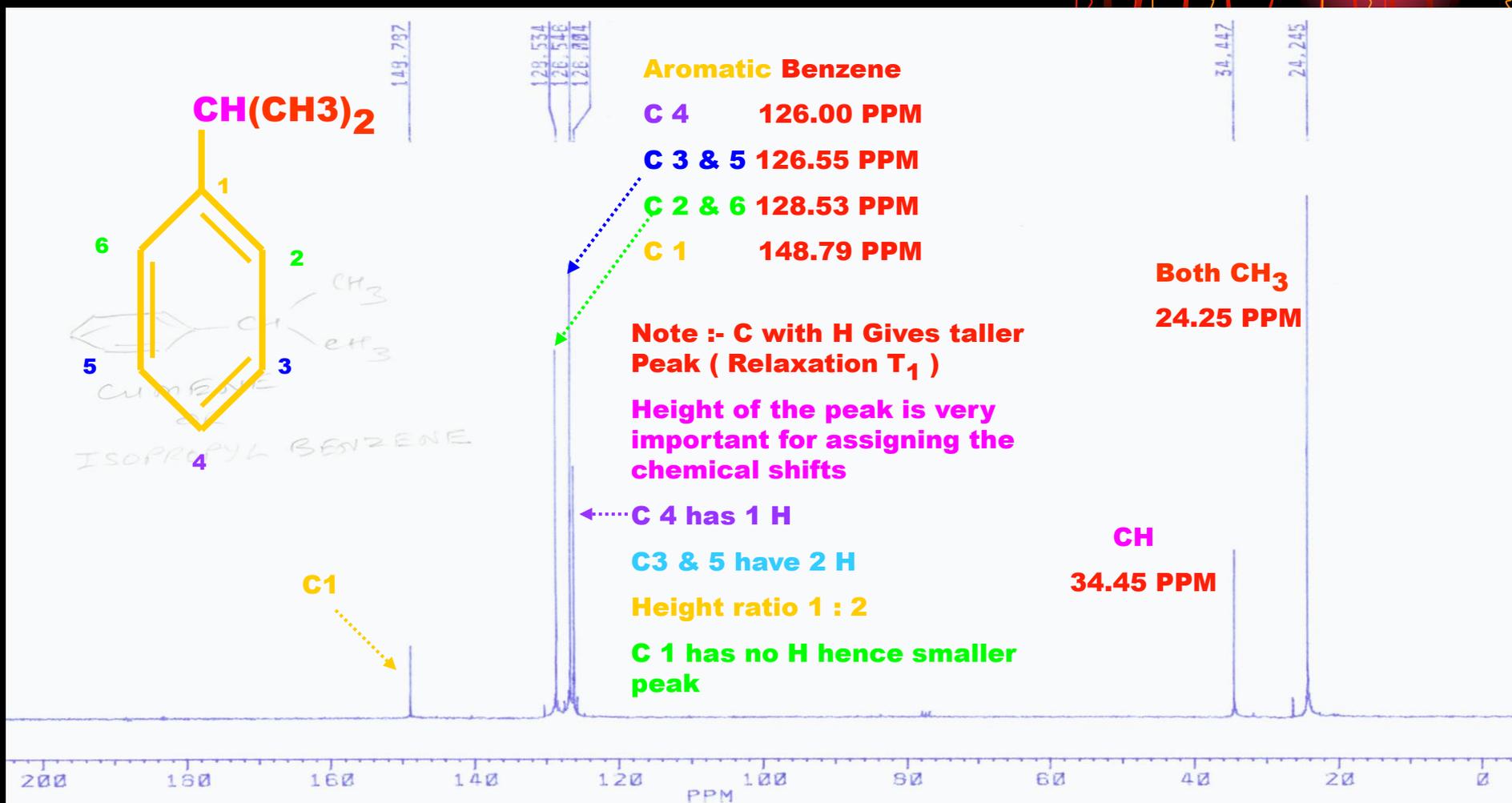
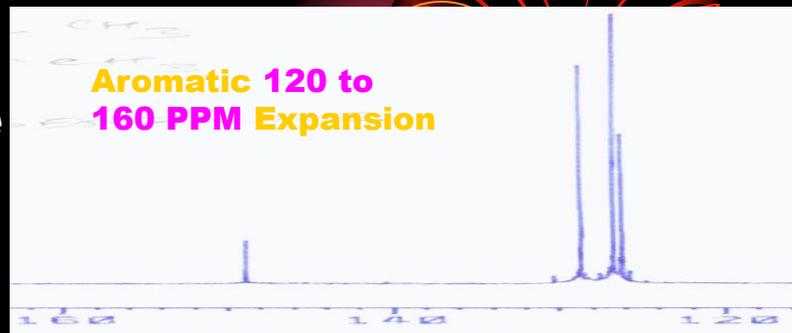
-(CH3)2
Doublet
1.32 PPM
J = 6.90 Hz



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



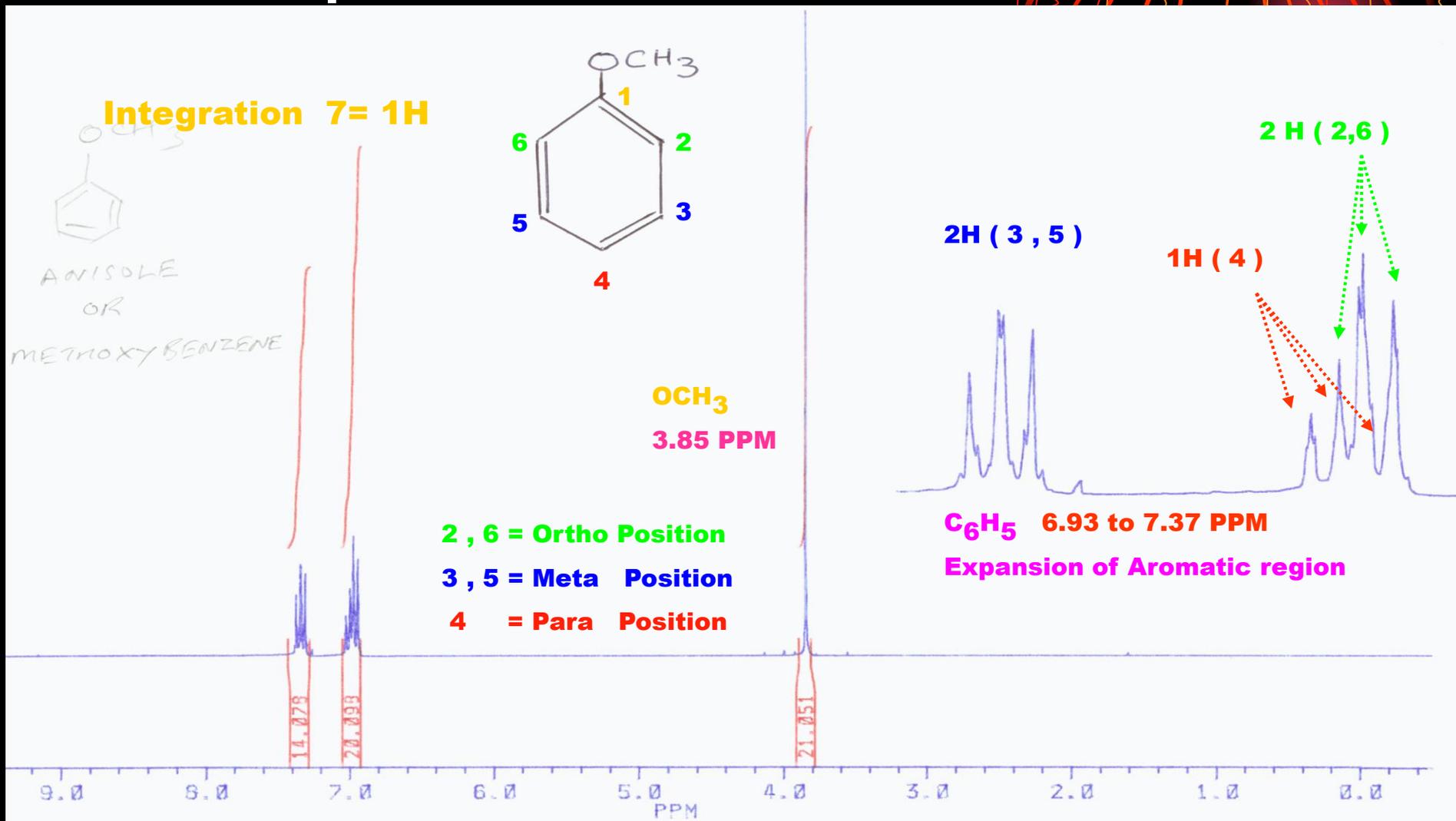
^{13}C NMR Spectrum of Cumene



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

of Anisole (Methoxy Benzene) $\text{C}_6\text{H}_5\text{—OCH}_3$

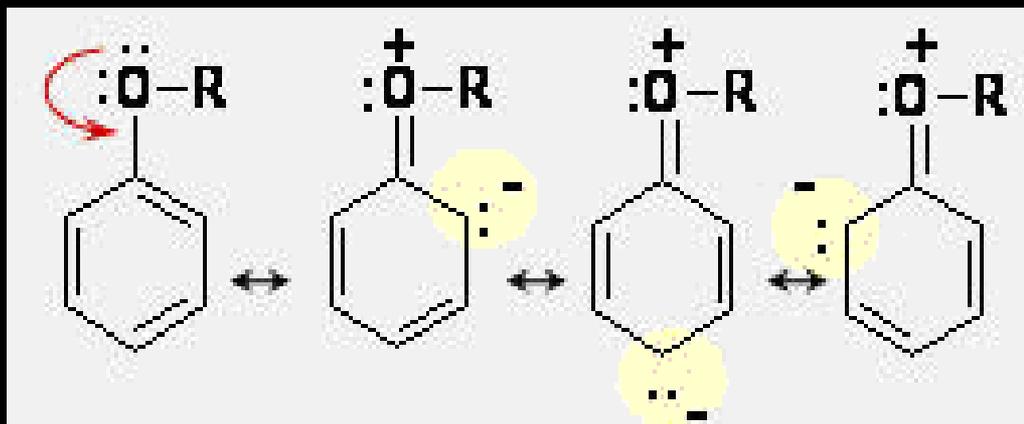
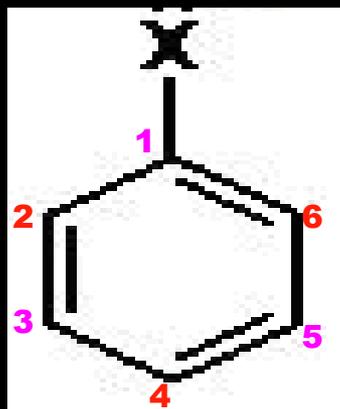
^1H NMR Spectrum



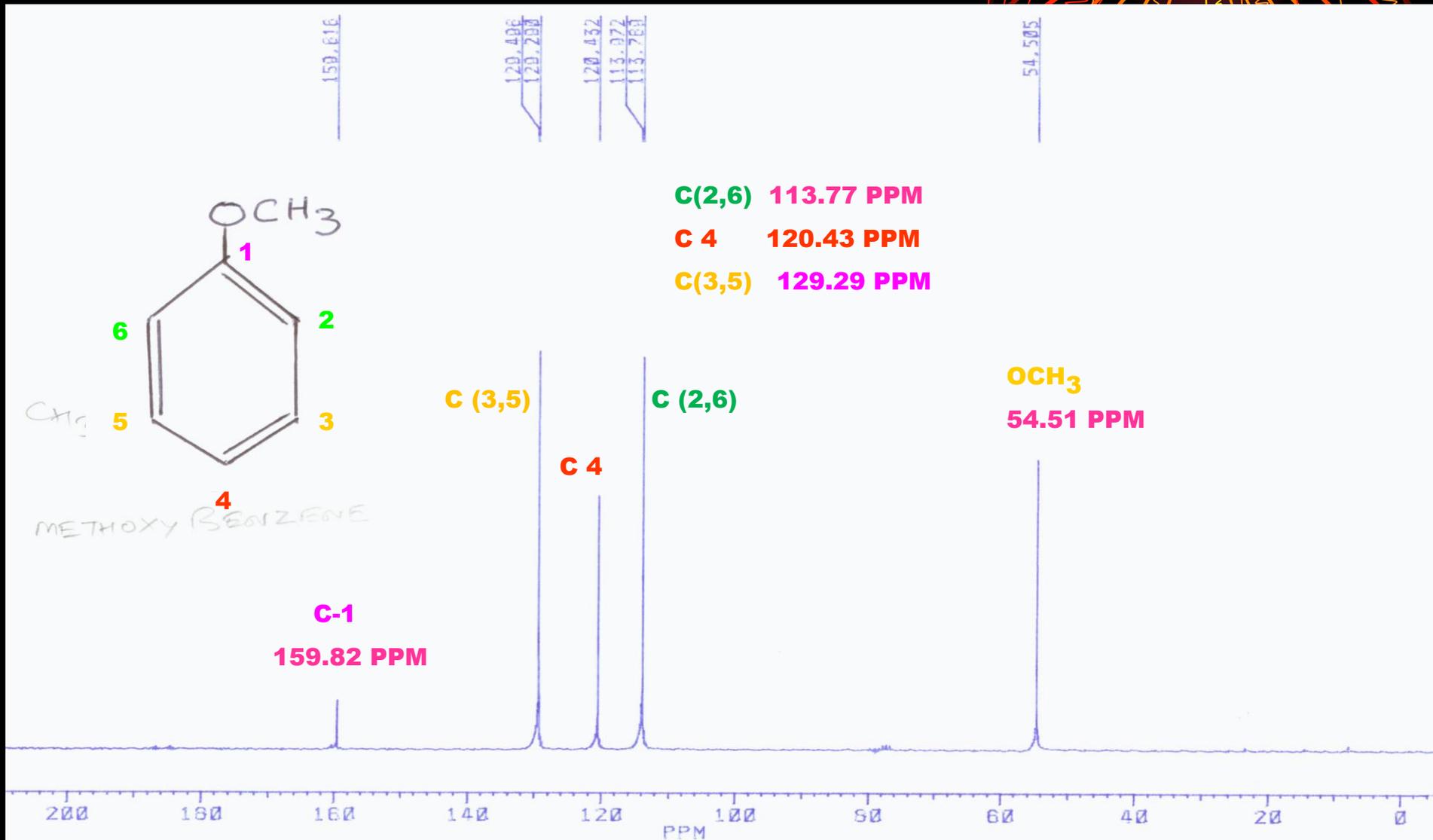
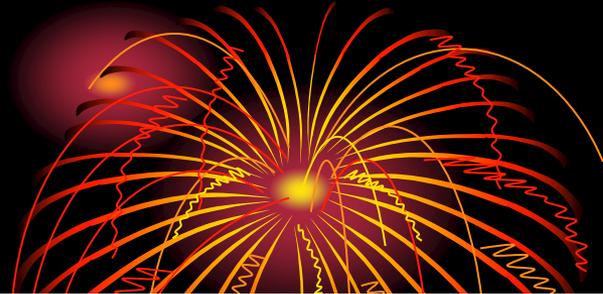
Shielding Effects on ^1H Ortho and Para Positions in Mono Substitution of Benzene.



- **Ortho and Para positions are shielded by mono substitution of electronegative group in benzene.**
- **X = OH, OR, NH₂, NR₂, O-CO-CH₃ Groups**
 ^1H attached to Positions 2, 4 and 6 are affected.
- **Shift towards to TMS (To Right or Higher Field)**



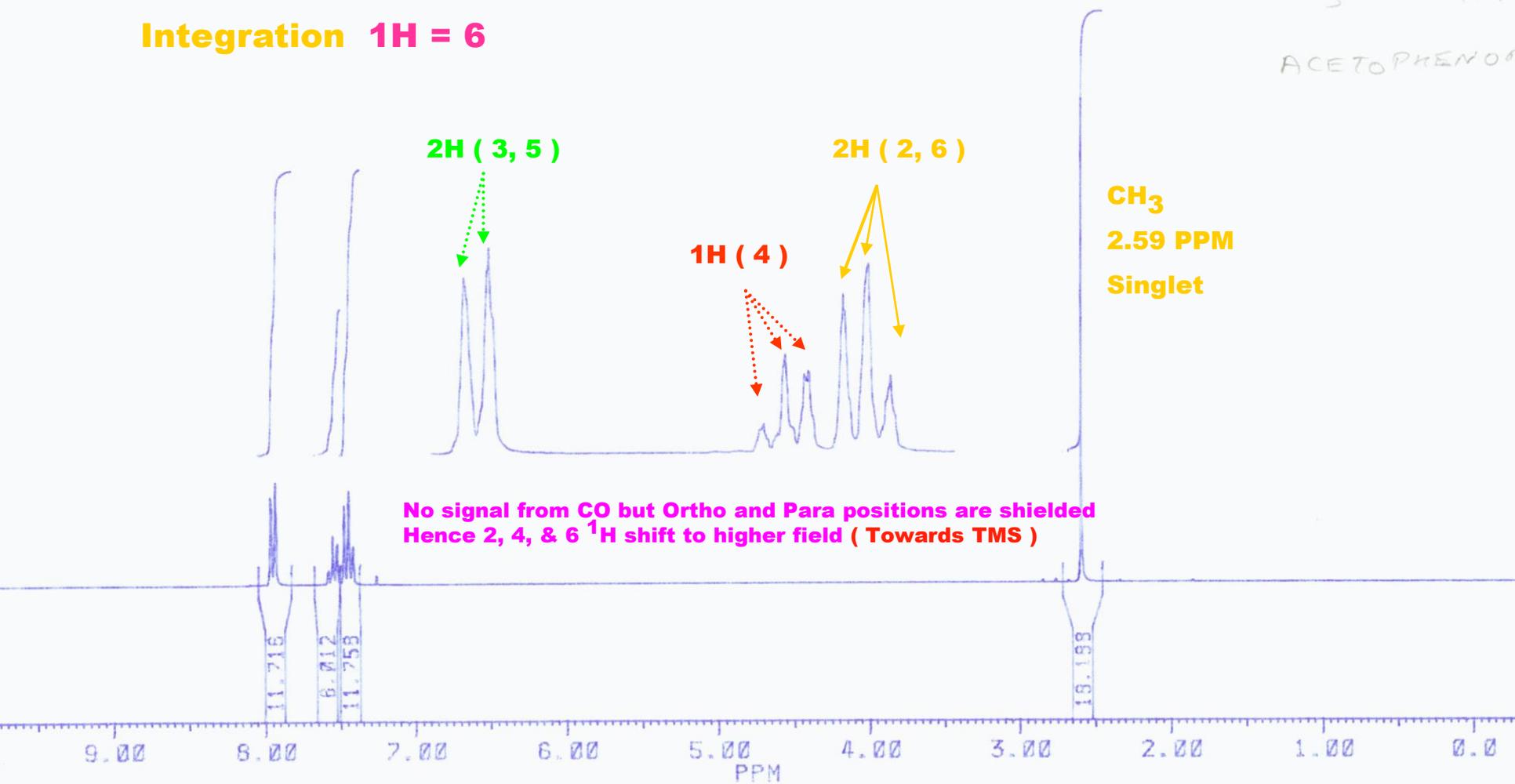
^{13}C NMR Spectrum of Anisole (Methoxy Benzene) $\text{C}_6\text{H}_5\text{—OCH}_3$



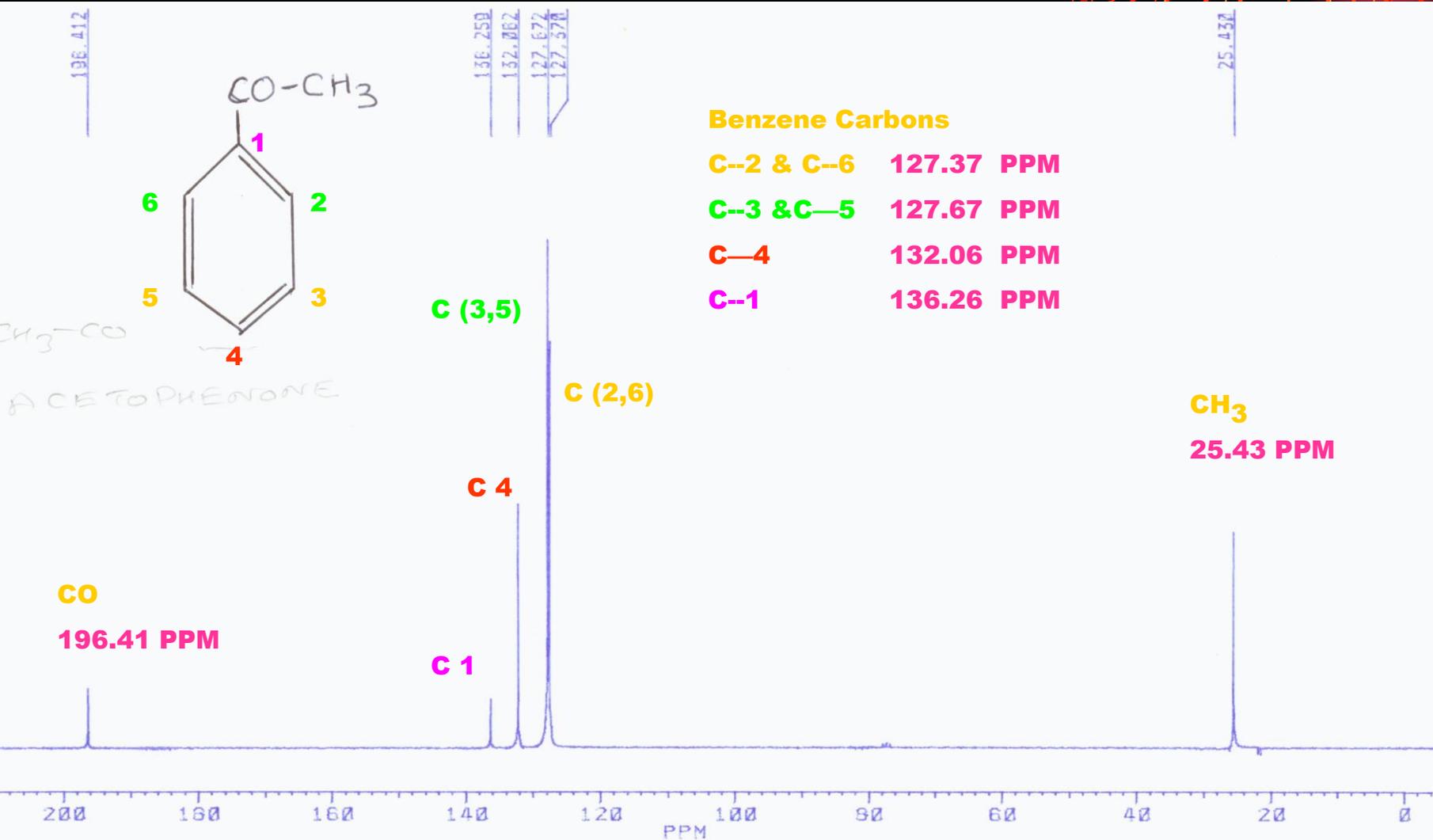
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Acetophenone $\text{C}_6\text{H}_5\text{—CO—CH}_3$



Integration $1\text{H} = 6$

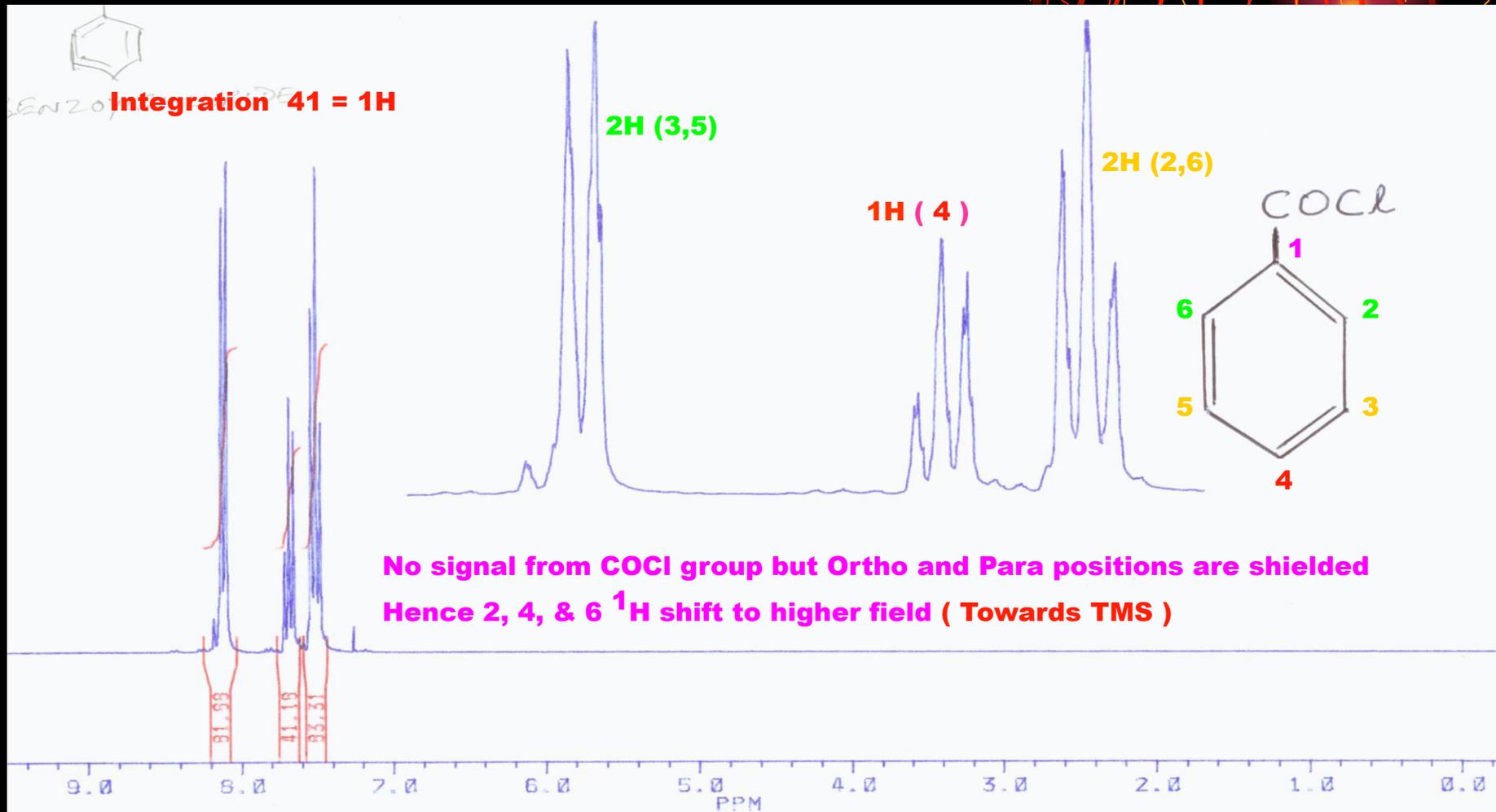


^{13}C NMR Spectrum of Acetophenone

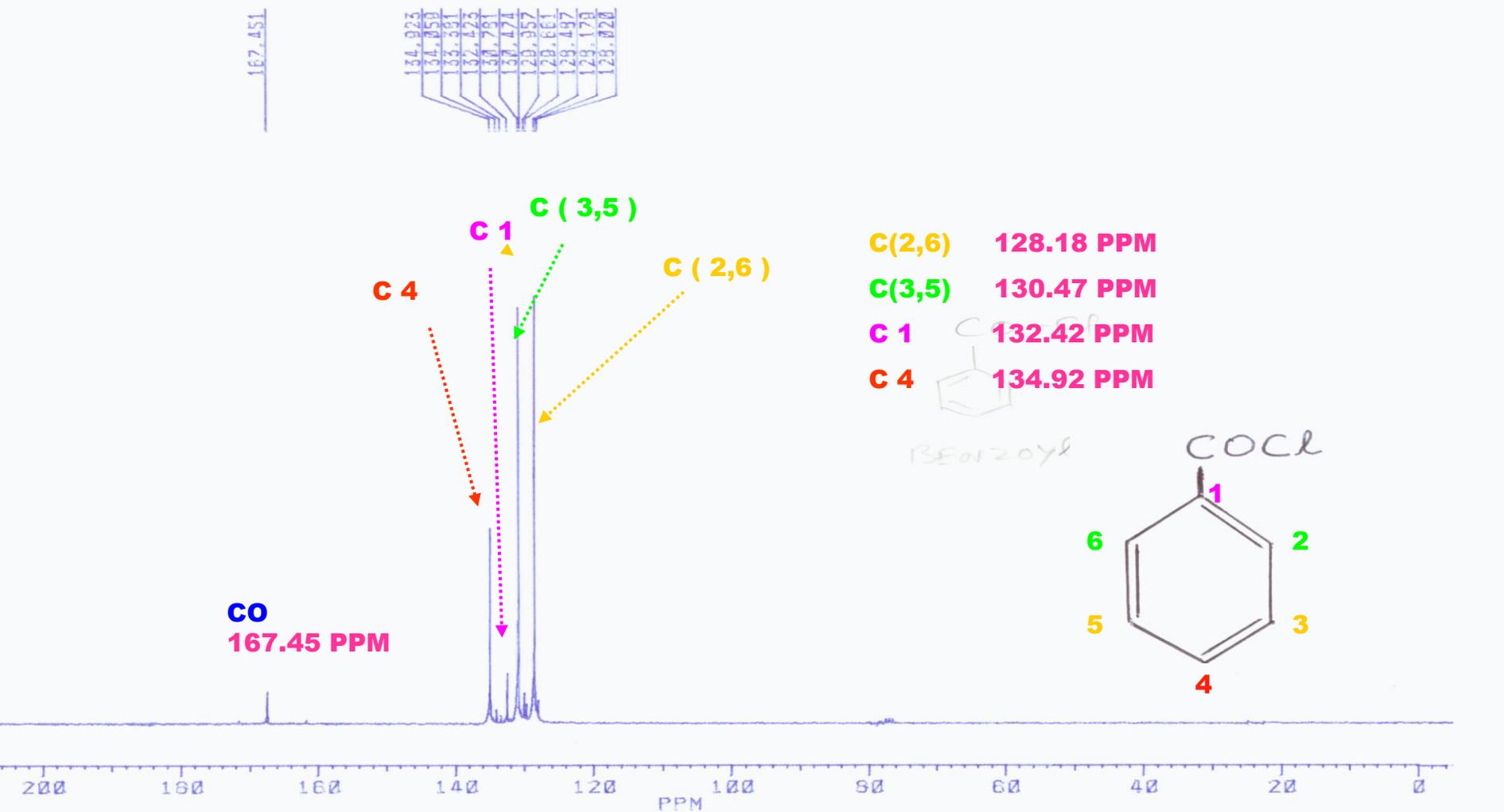


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Benzoylchloride $\text{C}_6\text{H}_5\text{—COCl}$

^1H NMR Spectrum



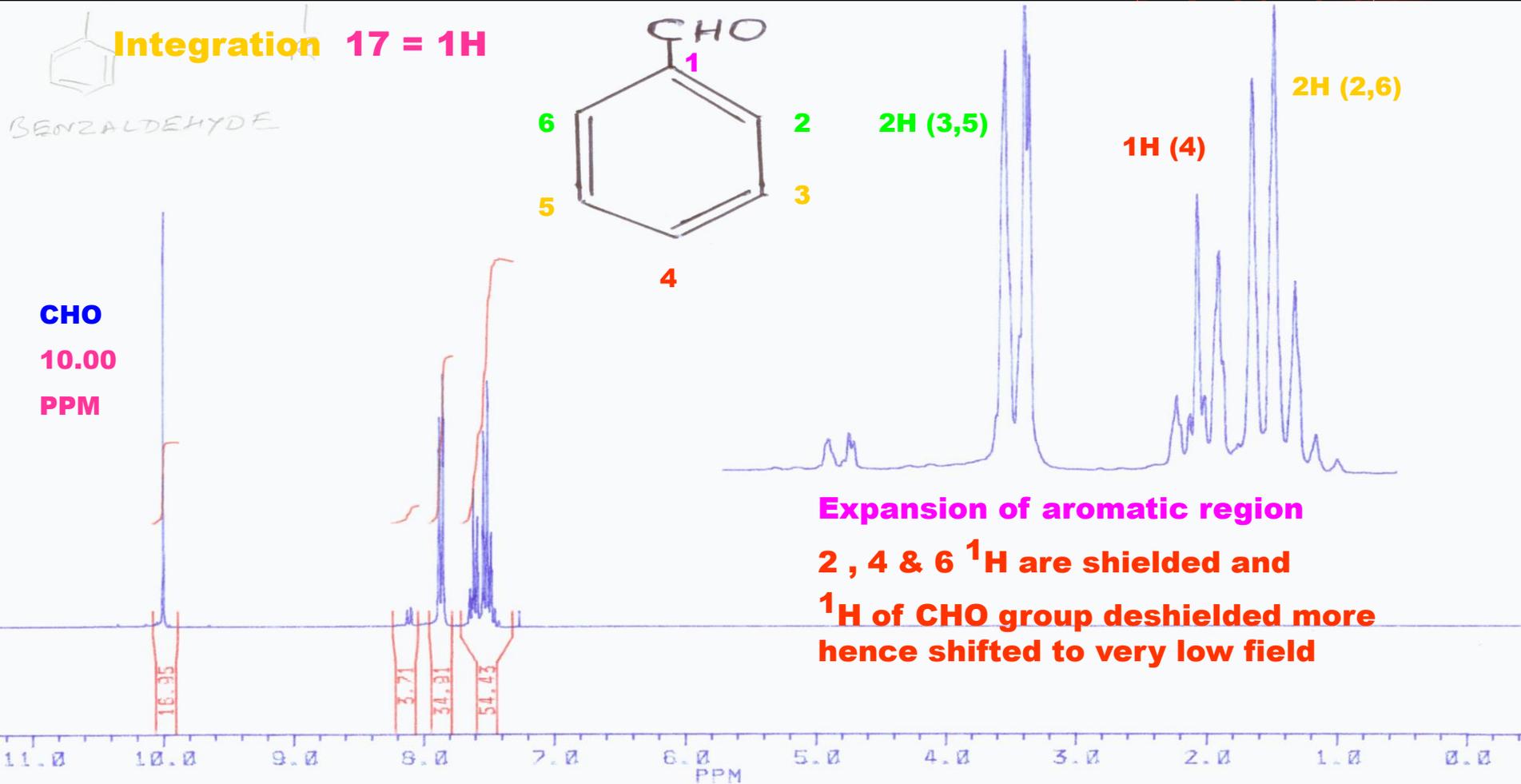
^{13}C NMR Spectrum of Benzoylchloride



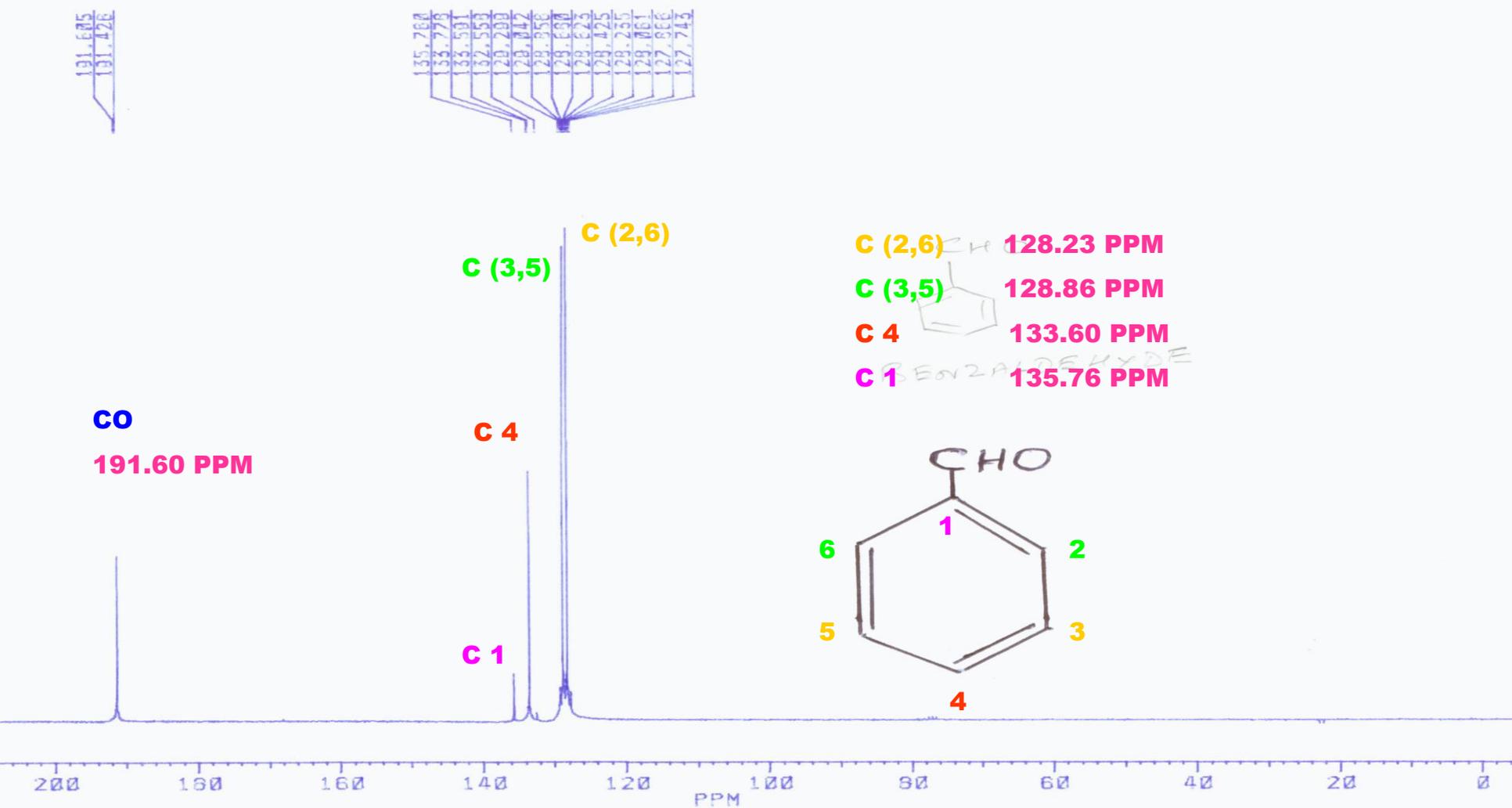
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Benzaldehyde $\text{C}_6\text{H}_5\text{—CHO}$



^1H NMR Spectrum



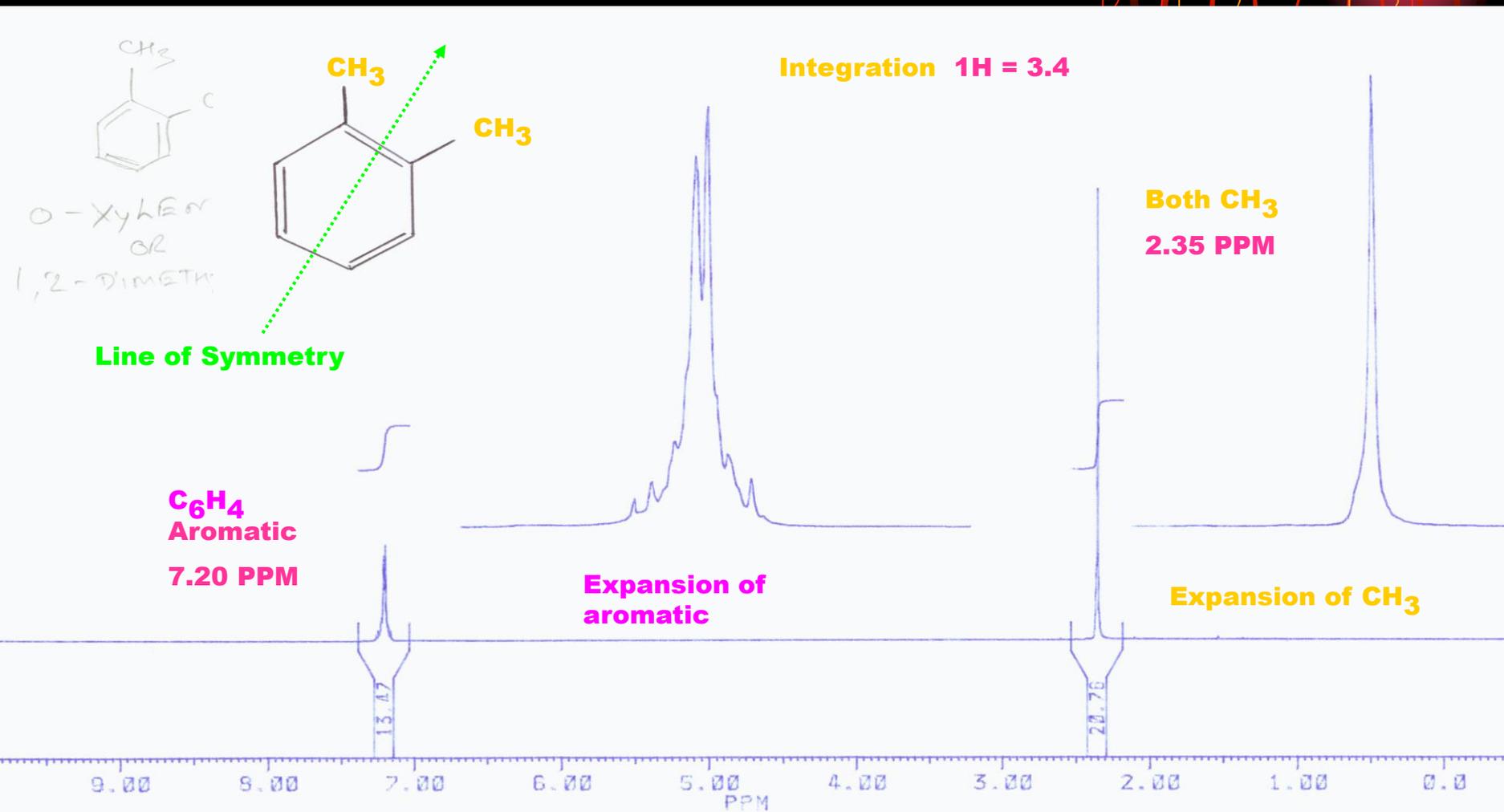
^{13}C NMR Spectrum of Benzaldehyde



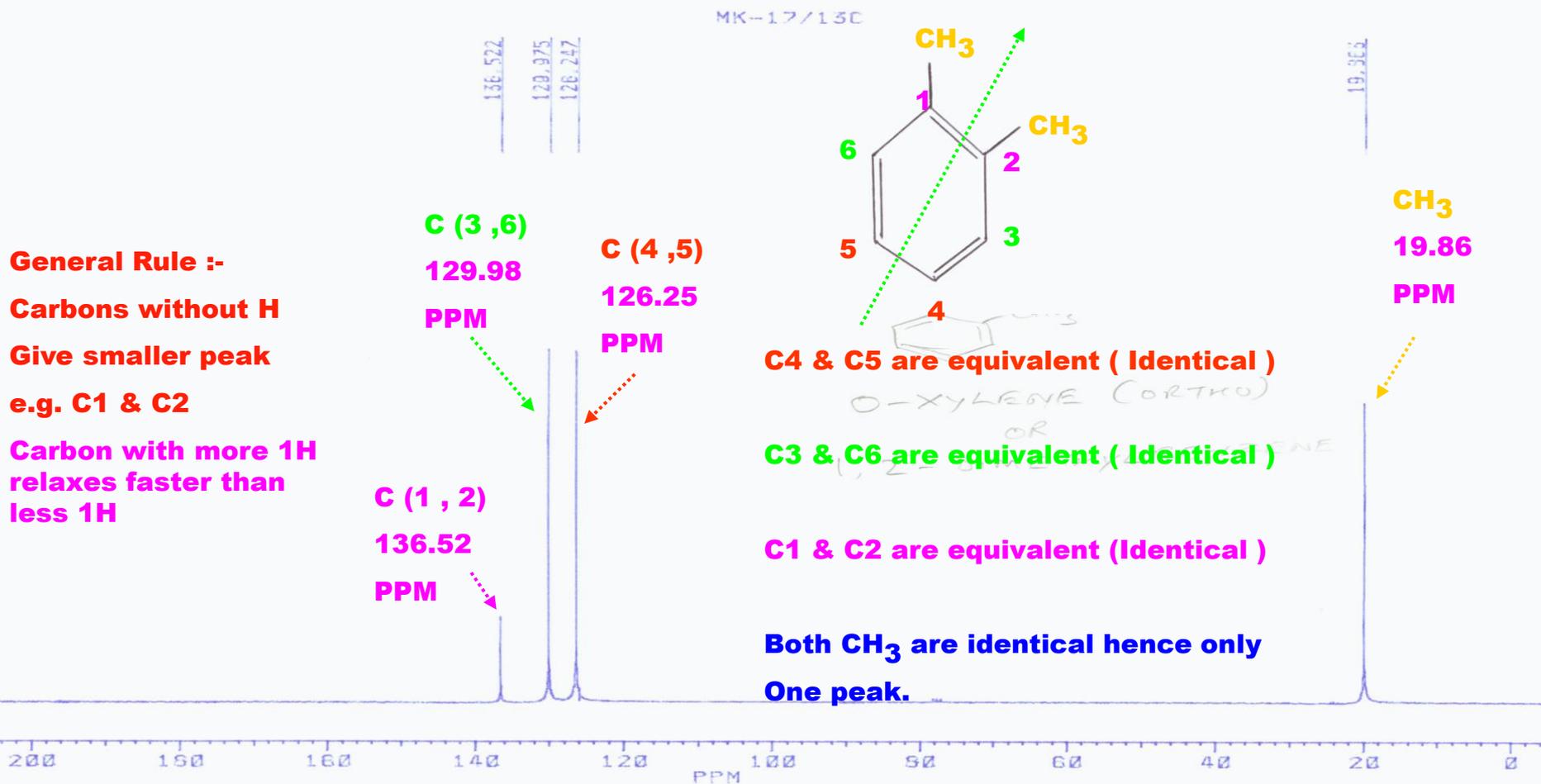
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,2-Dimethylbenzene (O-Xylene)



$\text{C}_6\text{H}_4(\text{CH}_3)_2$ ^1H NMR Spectrum



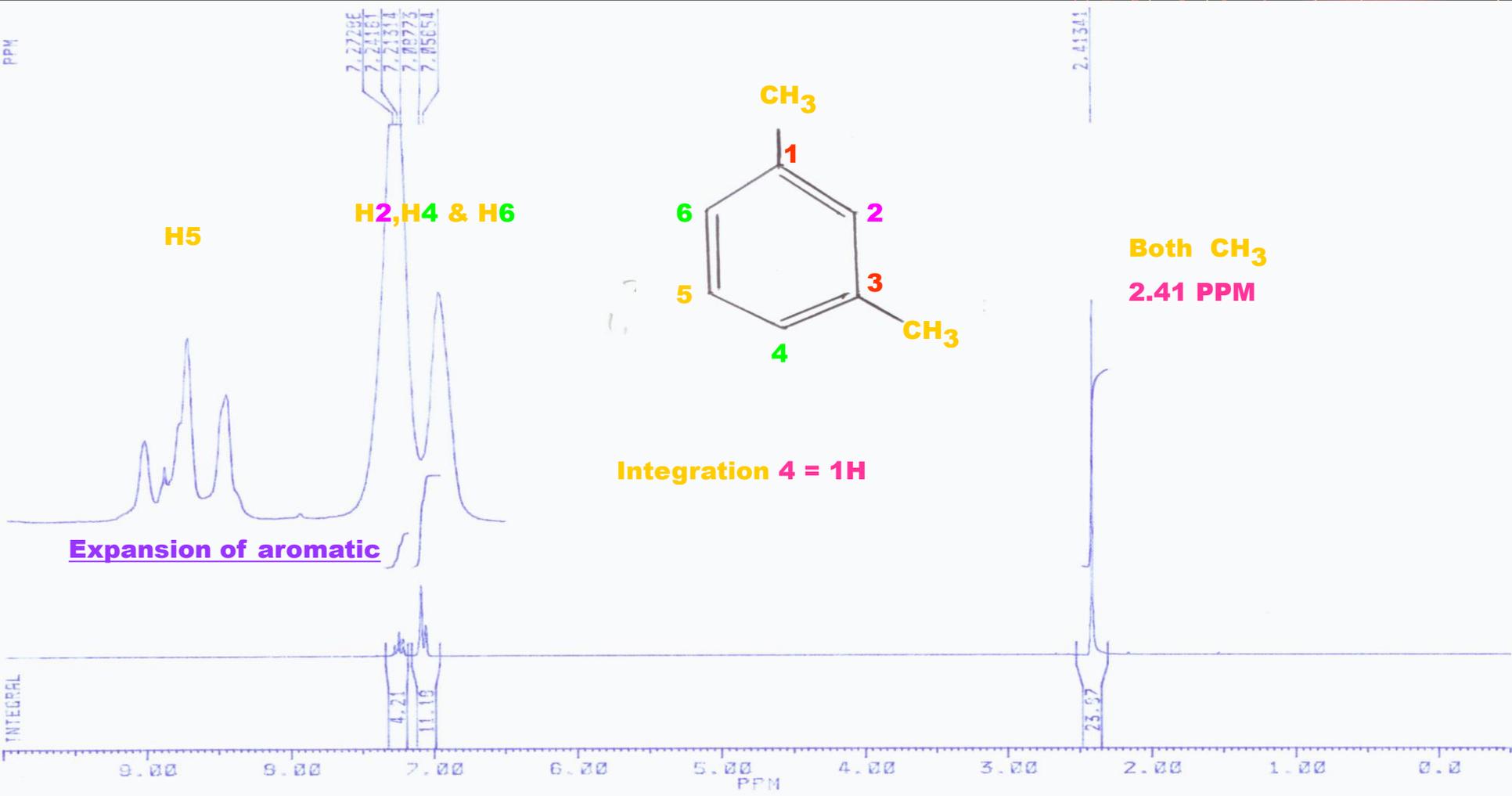
^{13}C NMR Spectrum of 1,2-Dimethylbenzene (O-Xylene)



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



$\text{C}_6\text{H}_4(\text{CH}_3)_2$ ^1H NMR Spectrum

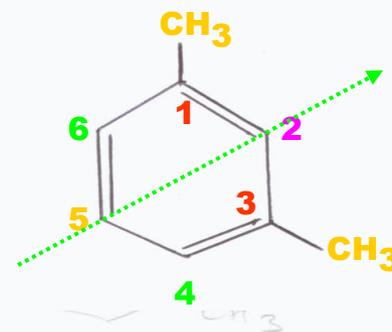


^{13}C NMR Spectrum of 1,3-Dimethylbenzene (m-Xylene)



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

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



m-XYLENE
1,3-DIMETHYLBENZENE

C4 & C6 126.50 PPM

C2 128.49 PPM

C5 130.24 PPM

C1 & C3 137.77 PPM

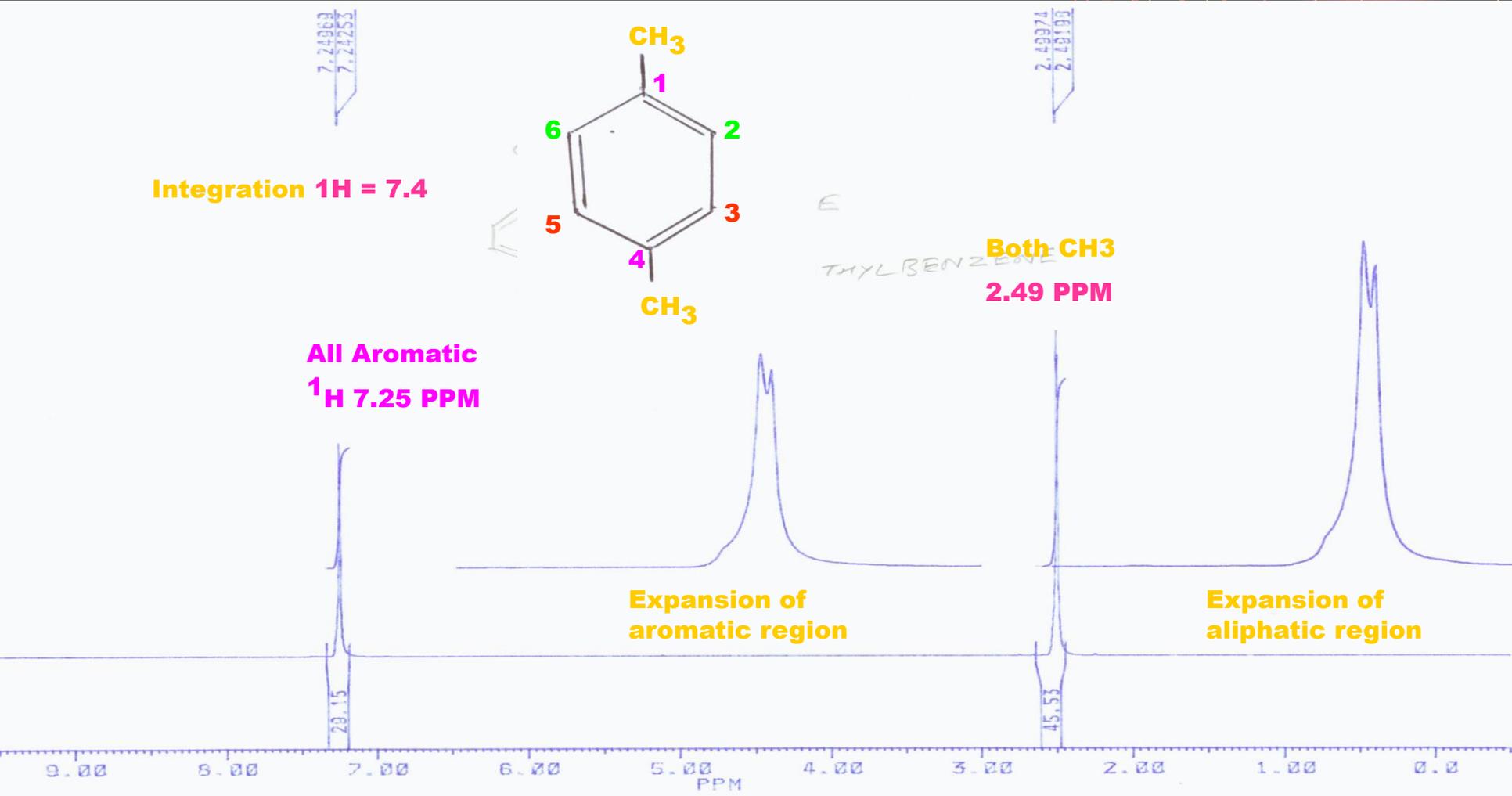
Both CH3
21.52 PPM



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

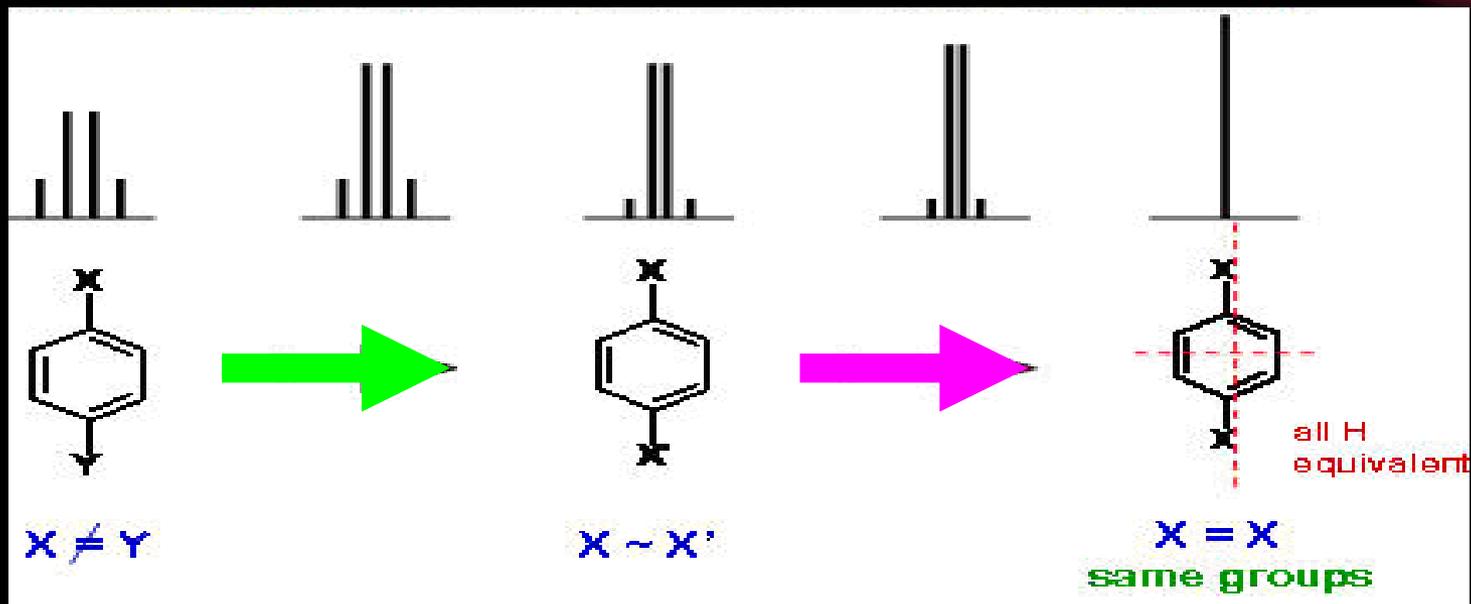


$\text{C}_6\text{H}_4(\text{CH}_3)_2$ ^1H NMR Spectrum

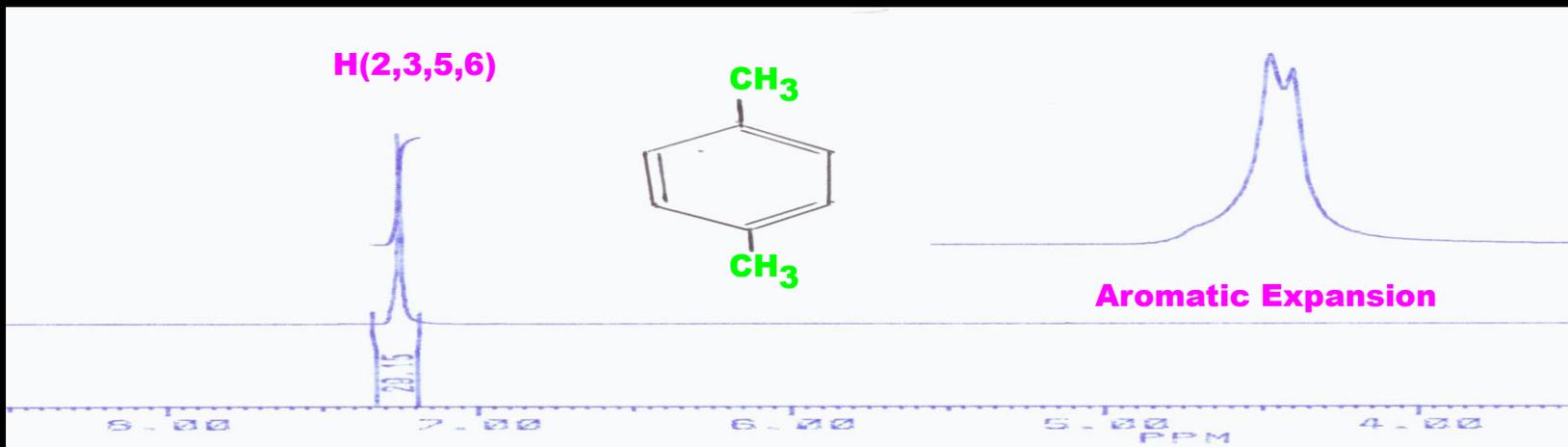
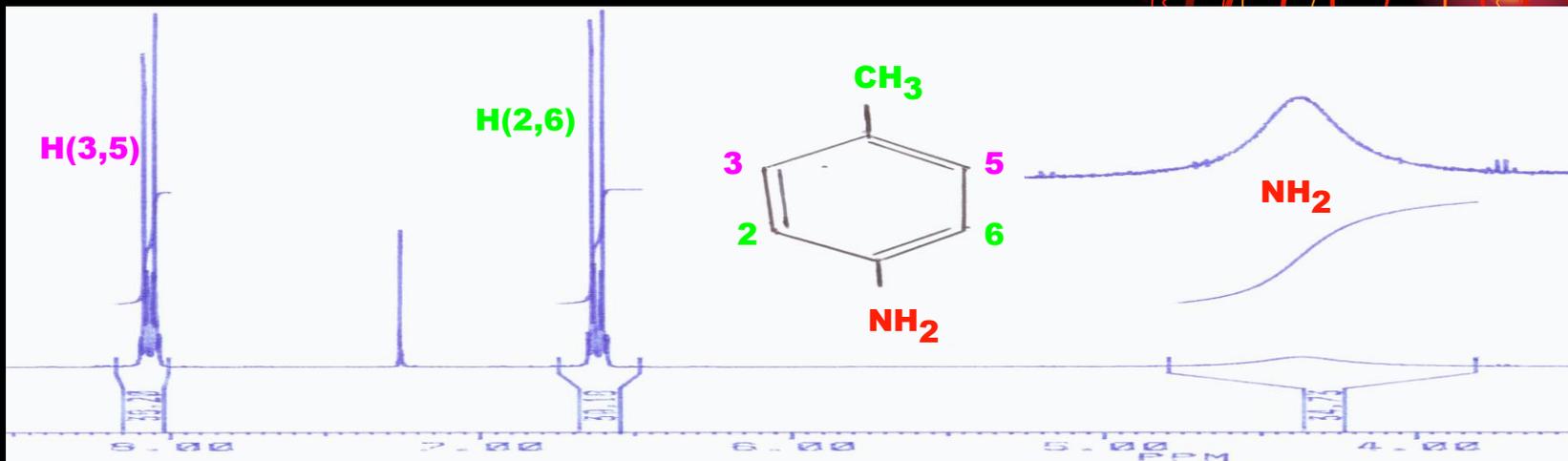


¹H NMR Patter of Para Disubstituted Benzene

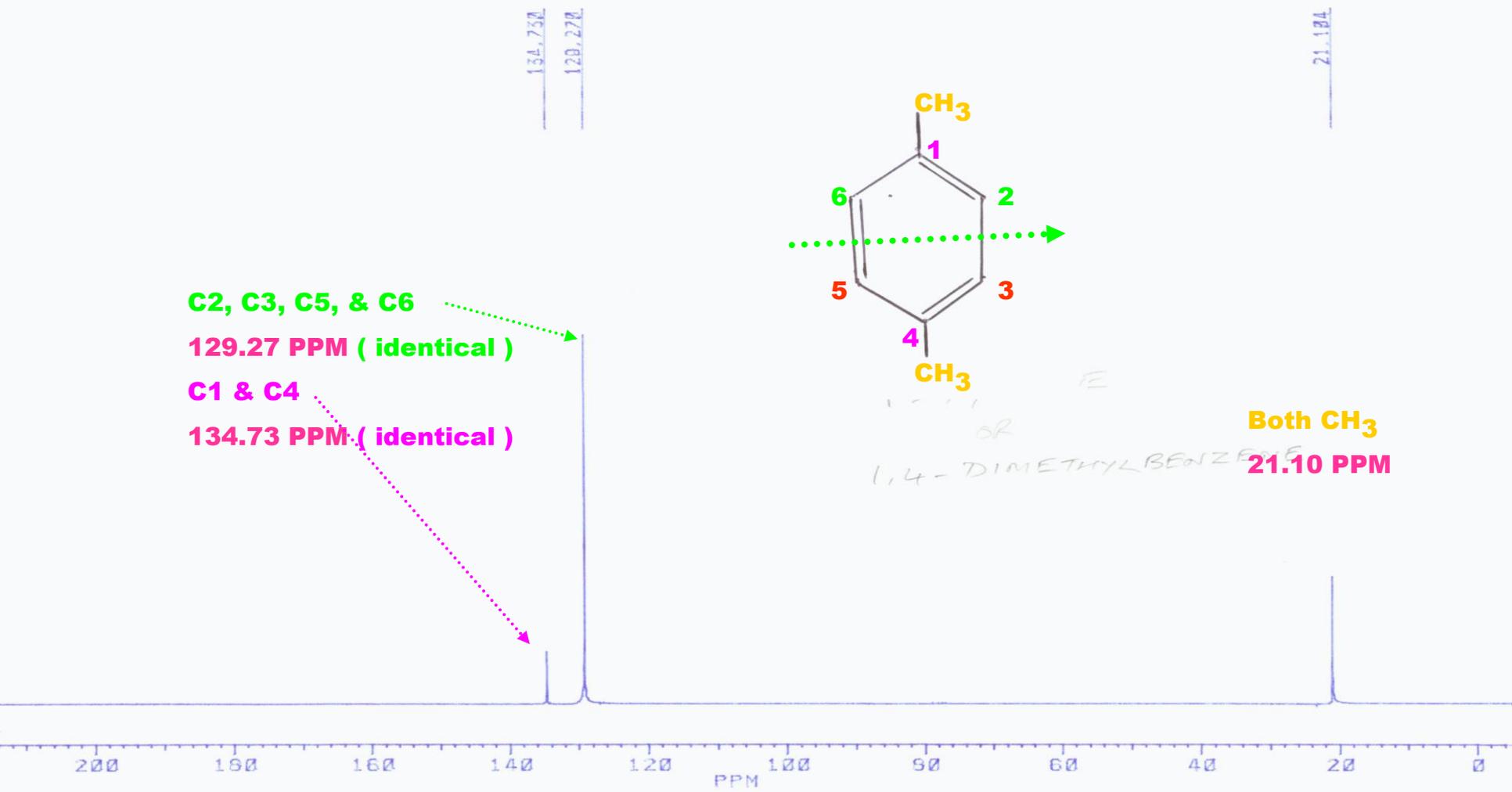
- When two groups X & Y become more similar then
- All NMR Peaks move closer hence
- Outer peaks get smaller and finally disappear but
- Inner peaks get taller and finally merge into single peak.



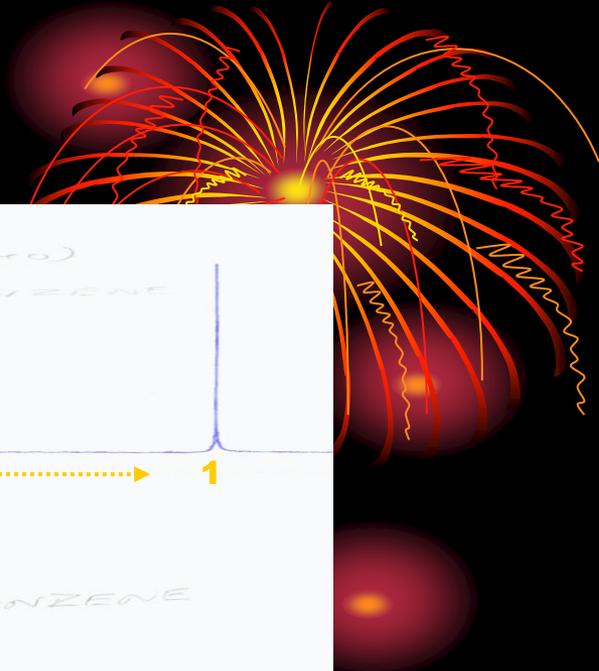
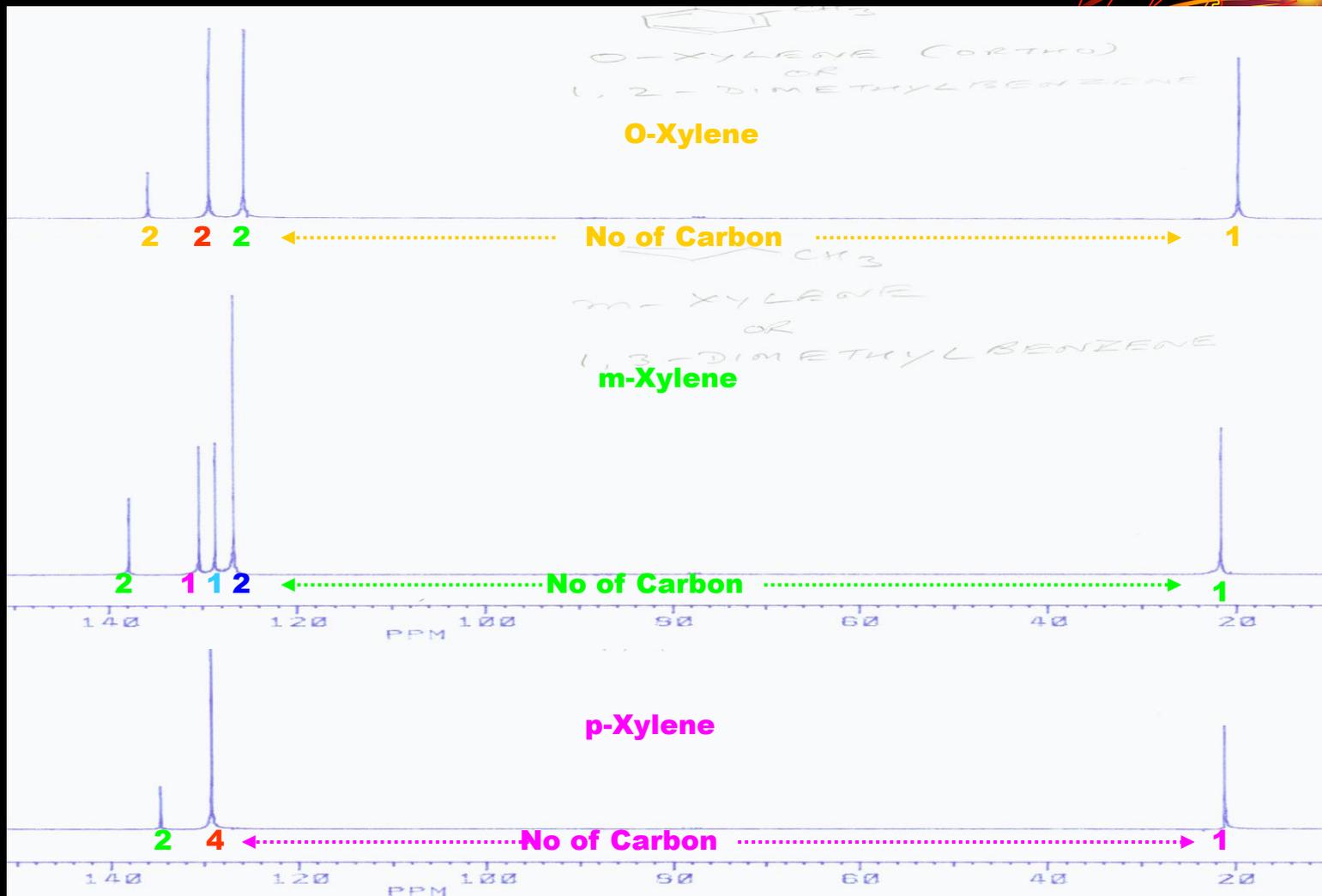
¹H NMR Spectra of 4-Methyl Aniline and p-Xylene only 8.5 to 4.5 PPM Region shown



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



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

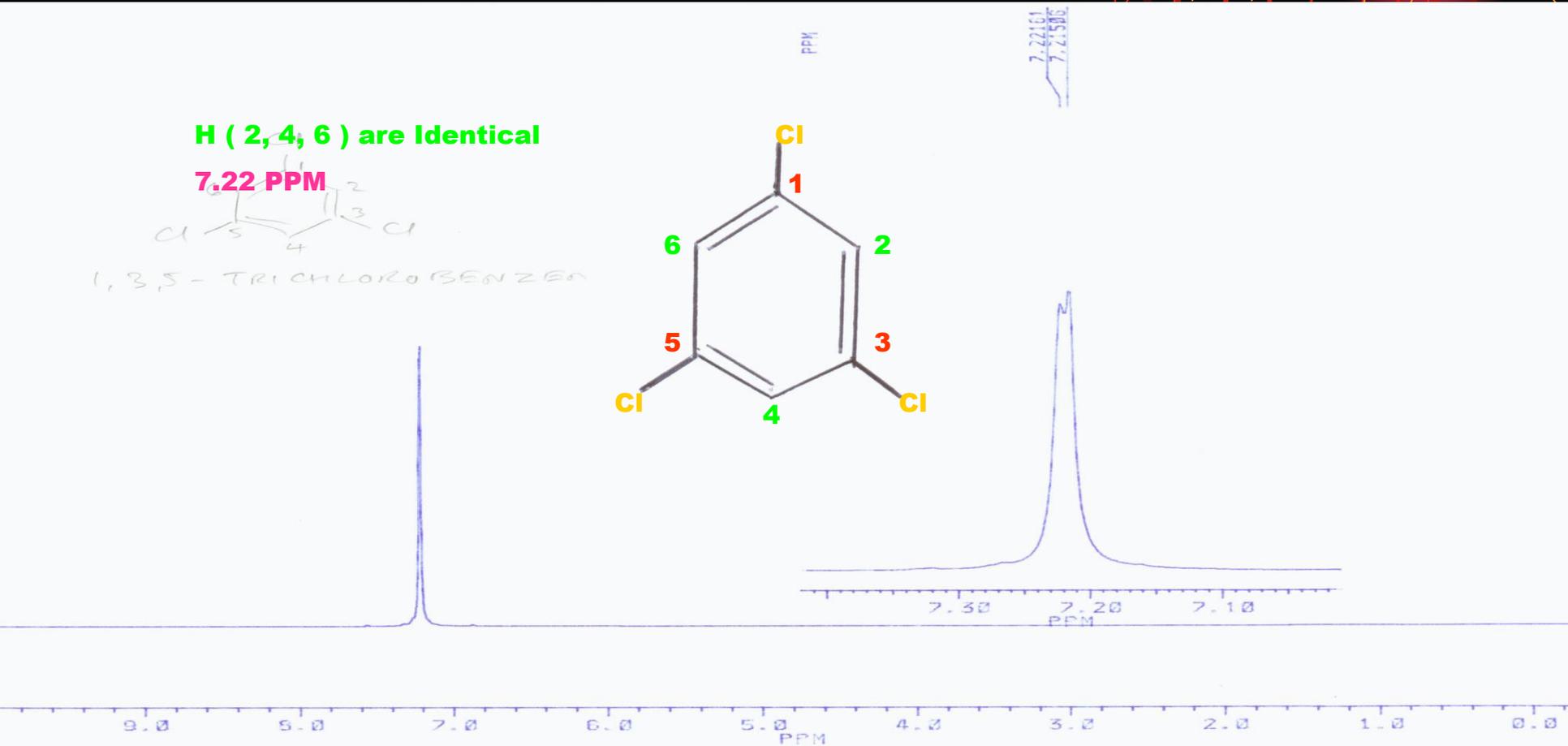
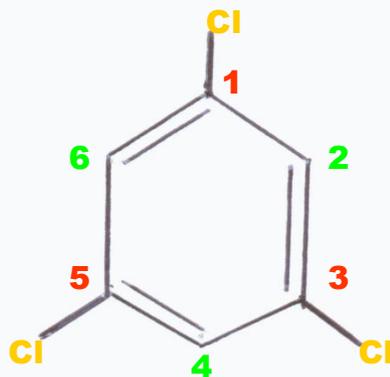


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,3,5-Trichlorobenzene

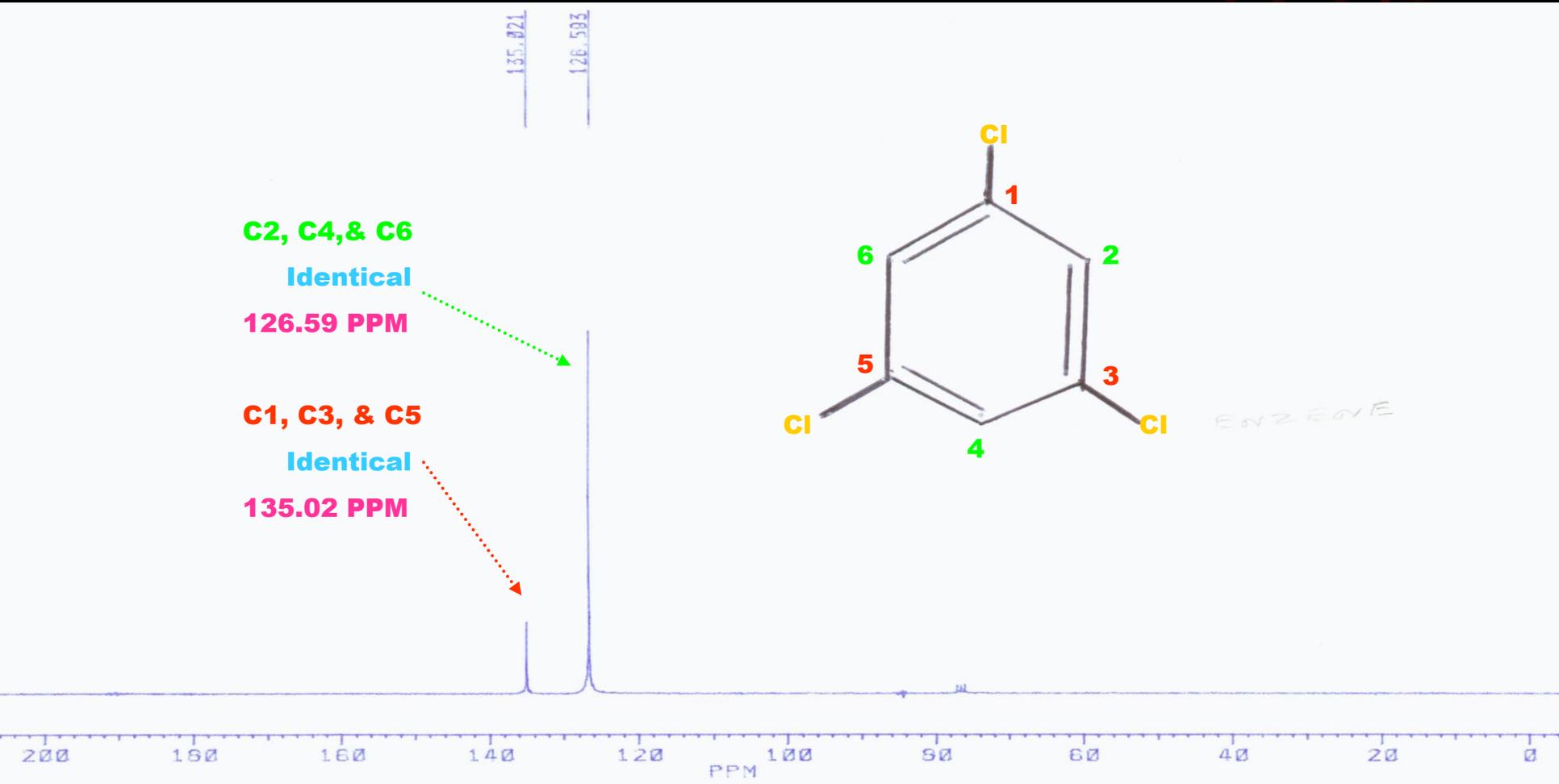
$\text{C}_6\text{H}_3\text{Cl}_3$ ^1H NMR Spectrum



H (2, 4, 6) are Identical
7.22 PPM
1, 3, 5 - TRICHLORO BENZENE



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

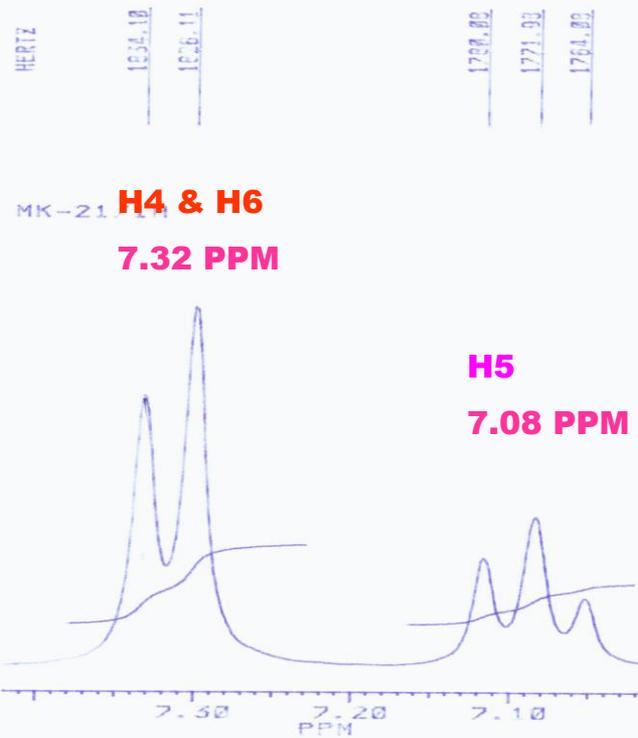
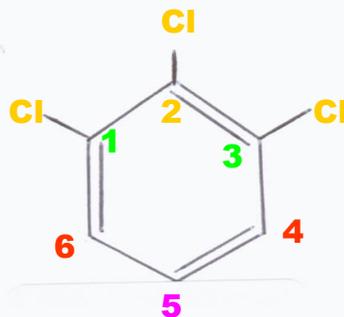


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,2,3-Trichlorobenzene



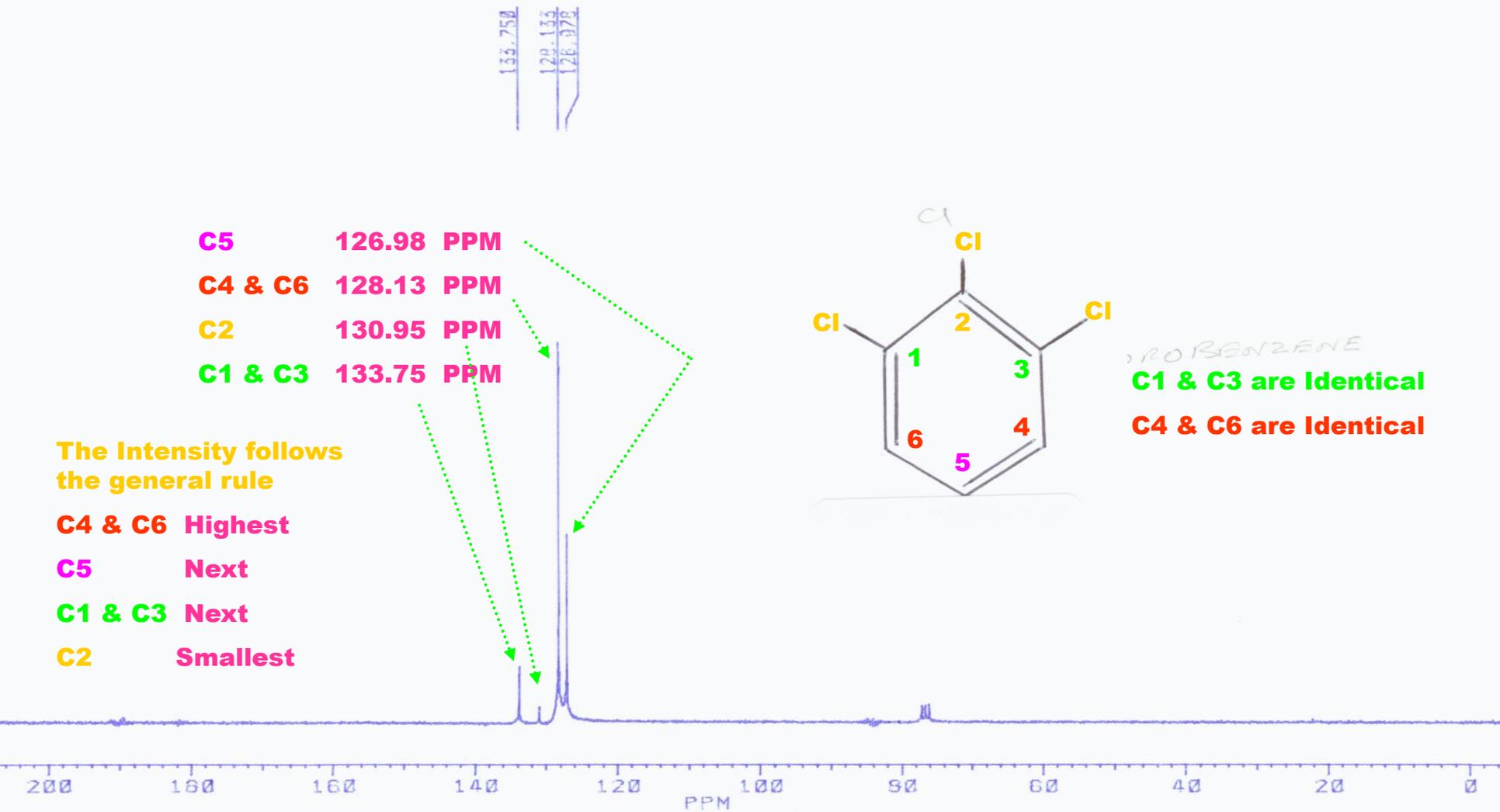
$\text{C}_6\text{H}_3\text{Cl}_3$ ^1H NMR Spectrum

Integration 1H = 61



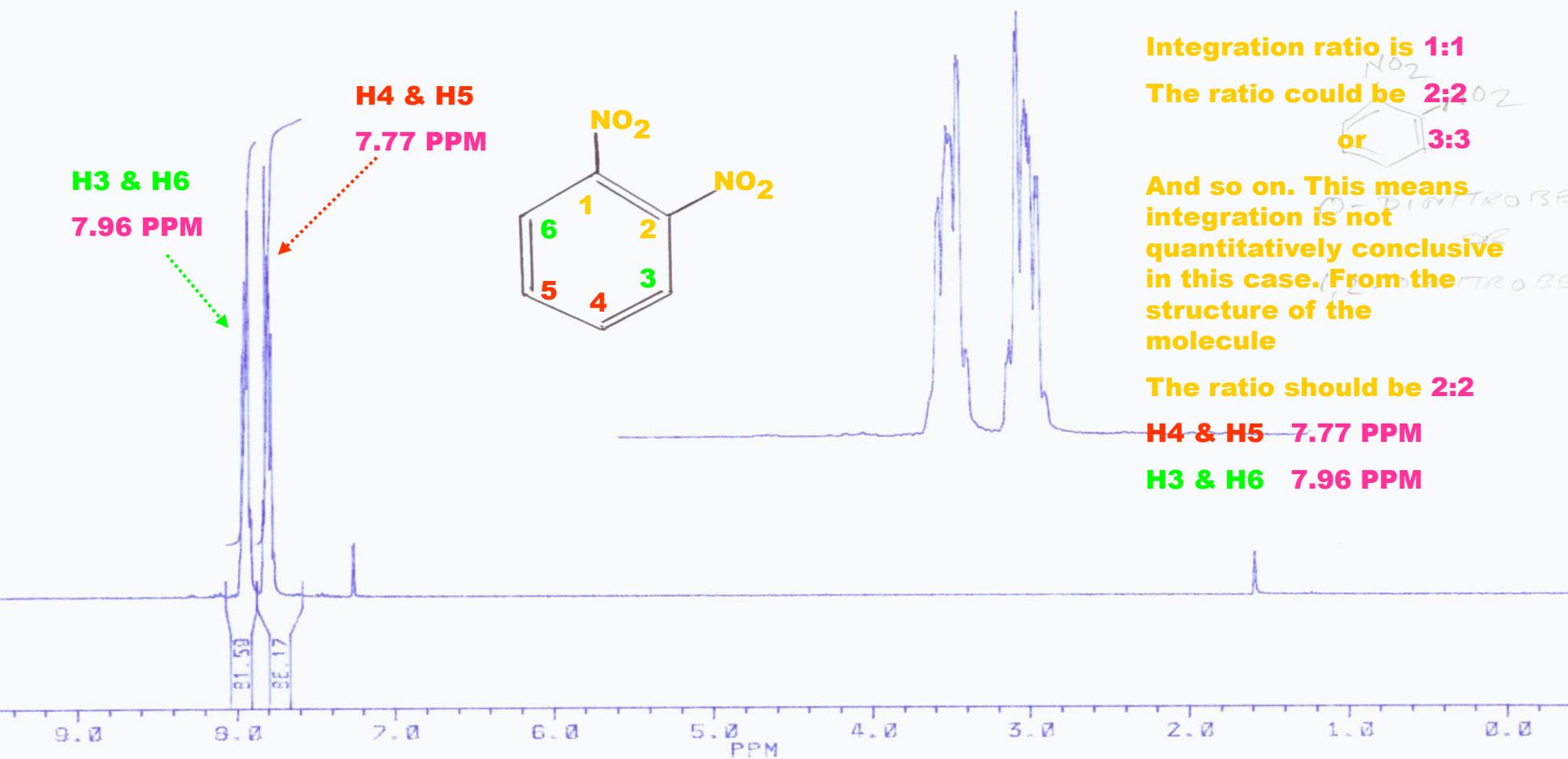
Expansion of Aromatic Region

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

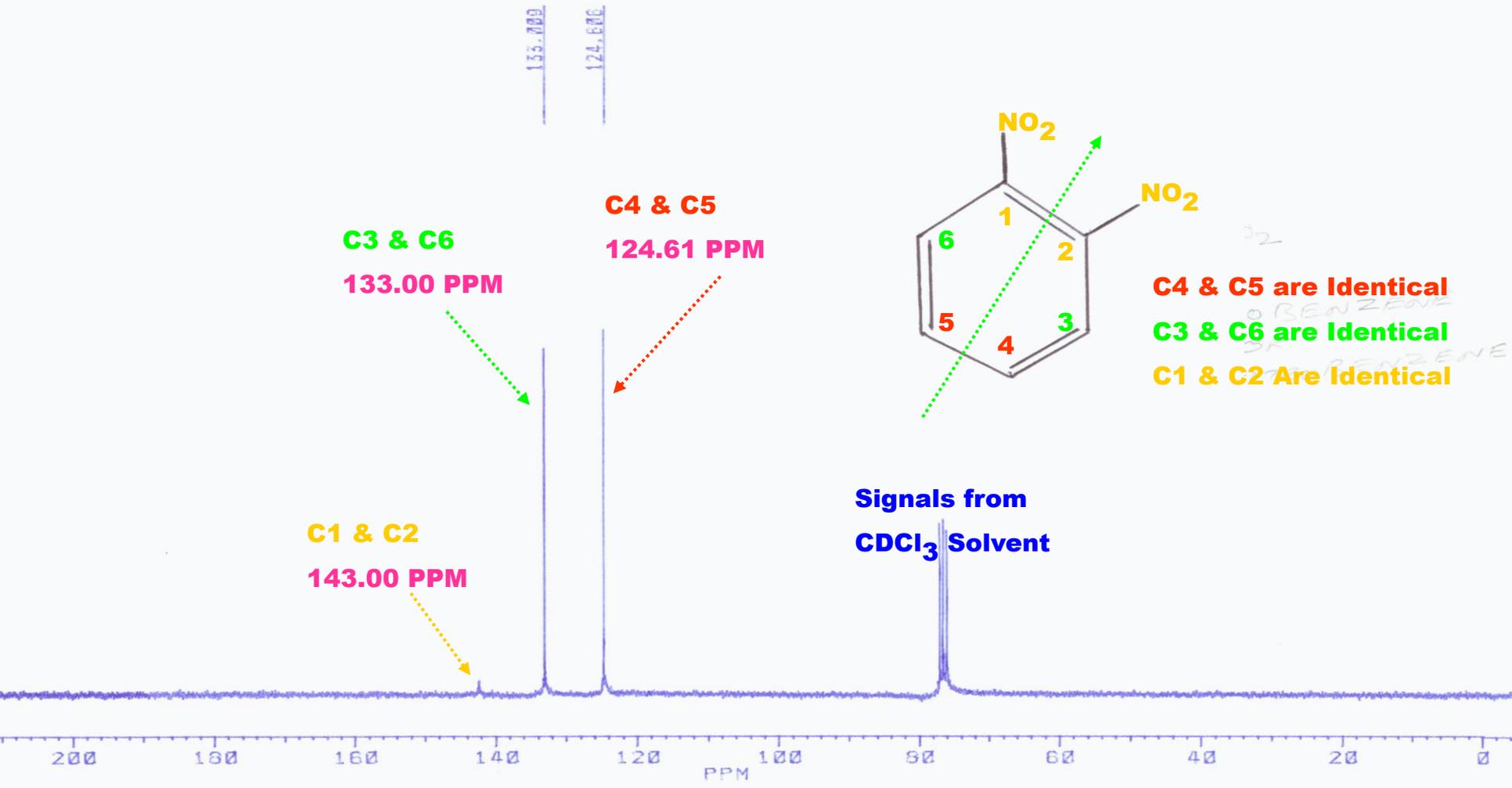


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,2-Dinitrobenzene

$\text{C}_6\text{H}_4(\text{NO}_2)_2$ ^1H NMR Spectrum



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

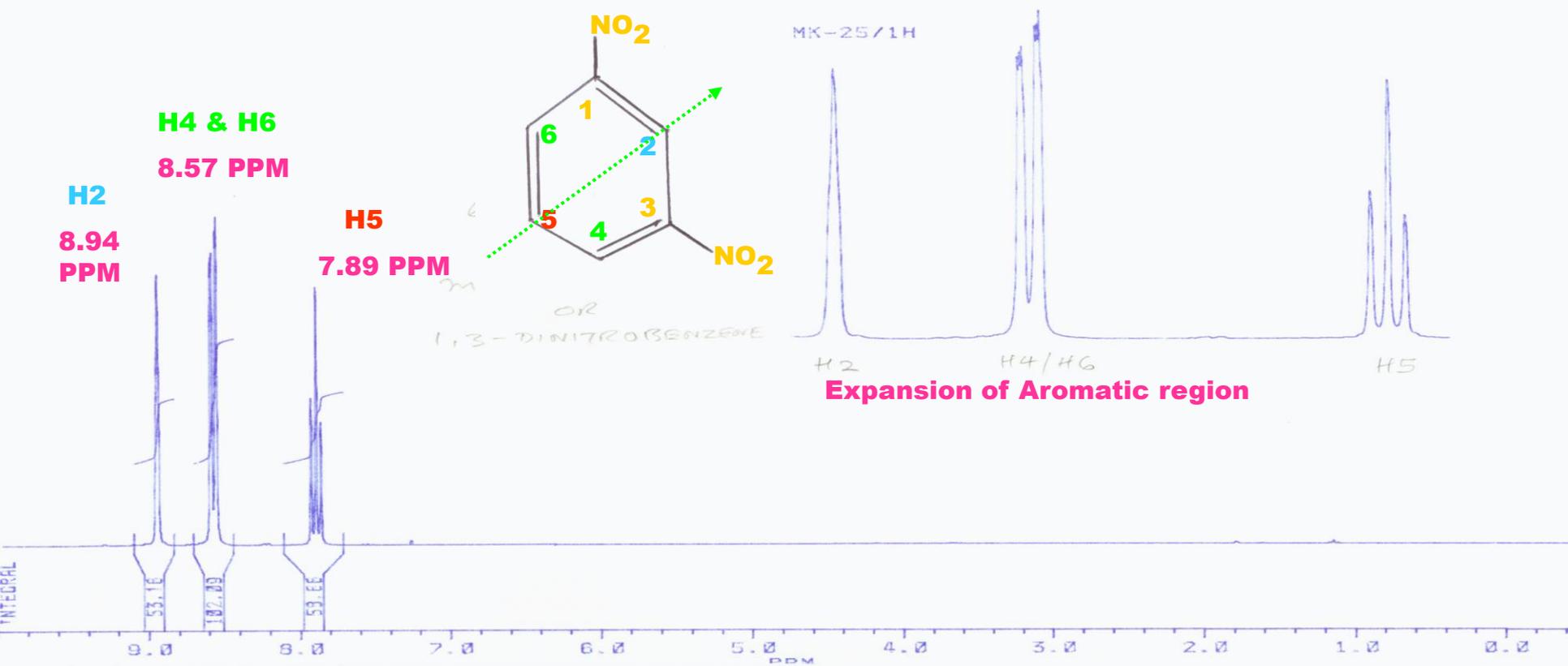


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,3-Dinitrobenzene

$\text{C}_6\text{H}_4(\text{NO}_2)_2$ ^1H NMR Spectrum

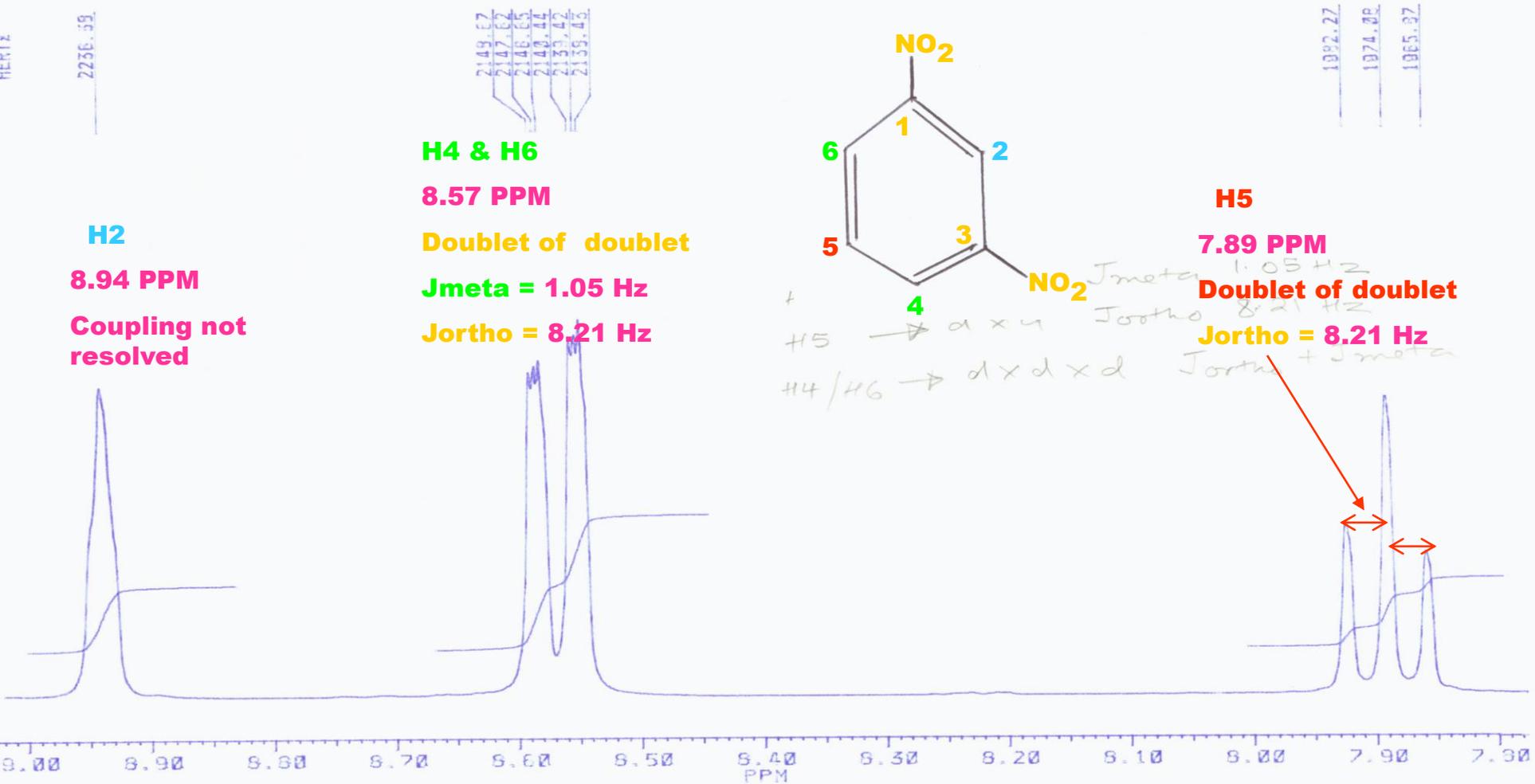


Integration 1H = 54

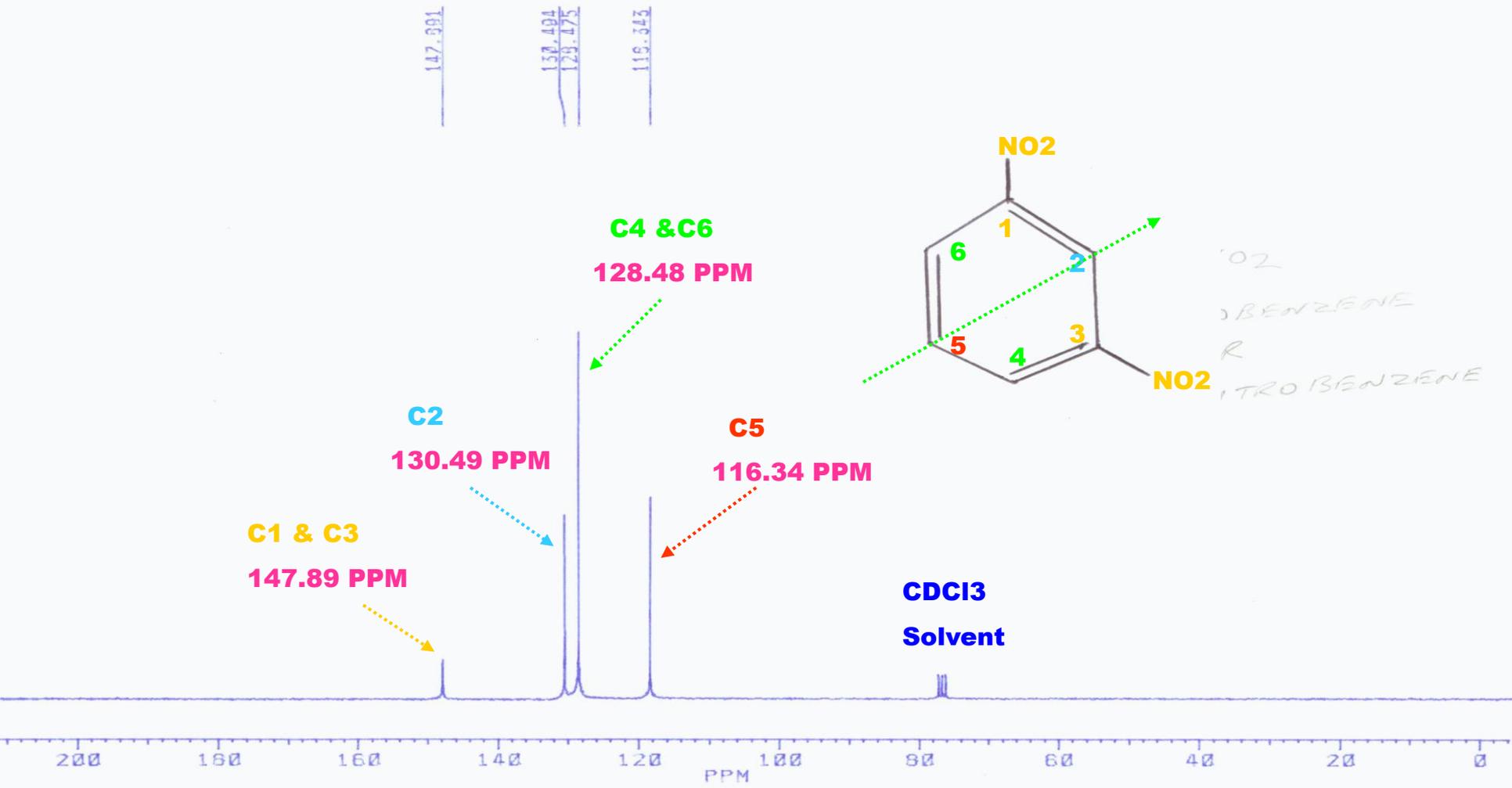


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 1,2,3-Trichlorobenzene

$\text{C}_6\text{H}_3\text{Cl}_3$ ^1H NMR Spectrum



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



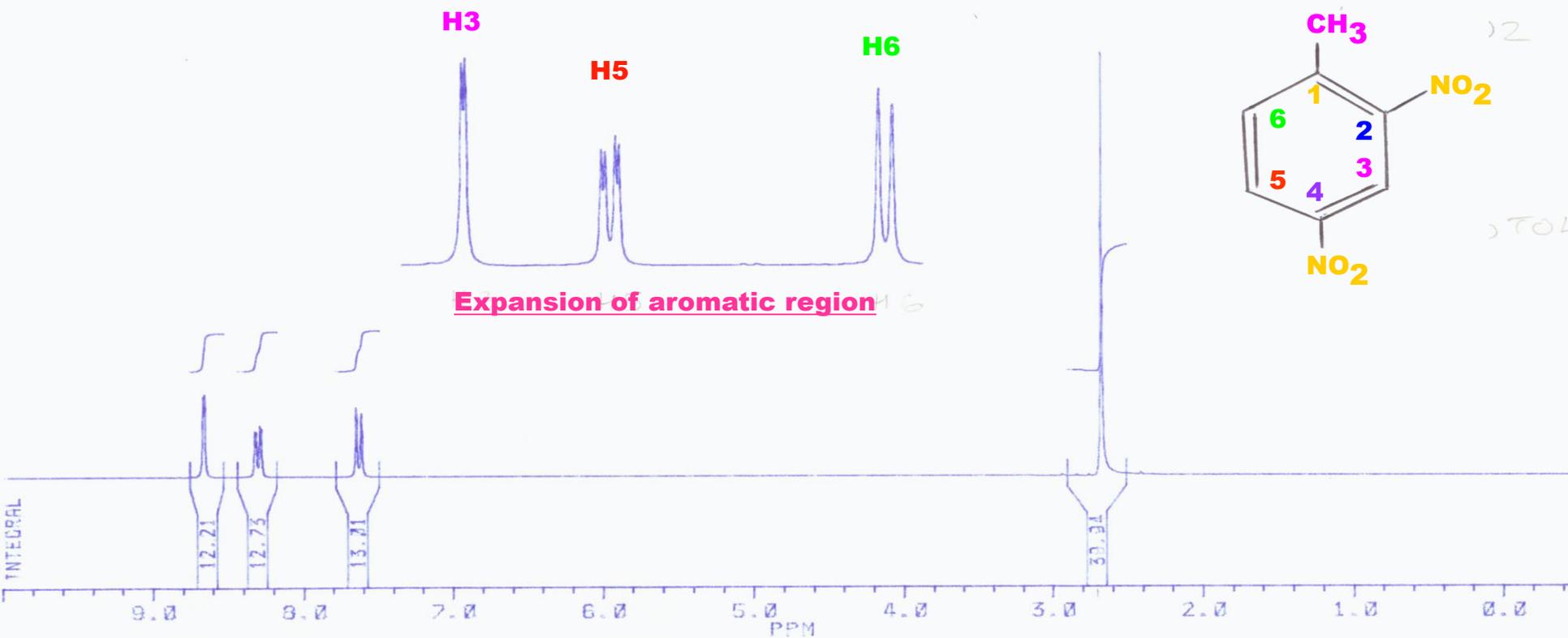
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

$\text{C}_6\text{H}_3\text{CH}_3(\text{NO}_2)_2$ ^1H NMR Spectrum



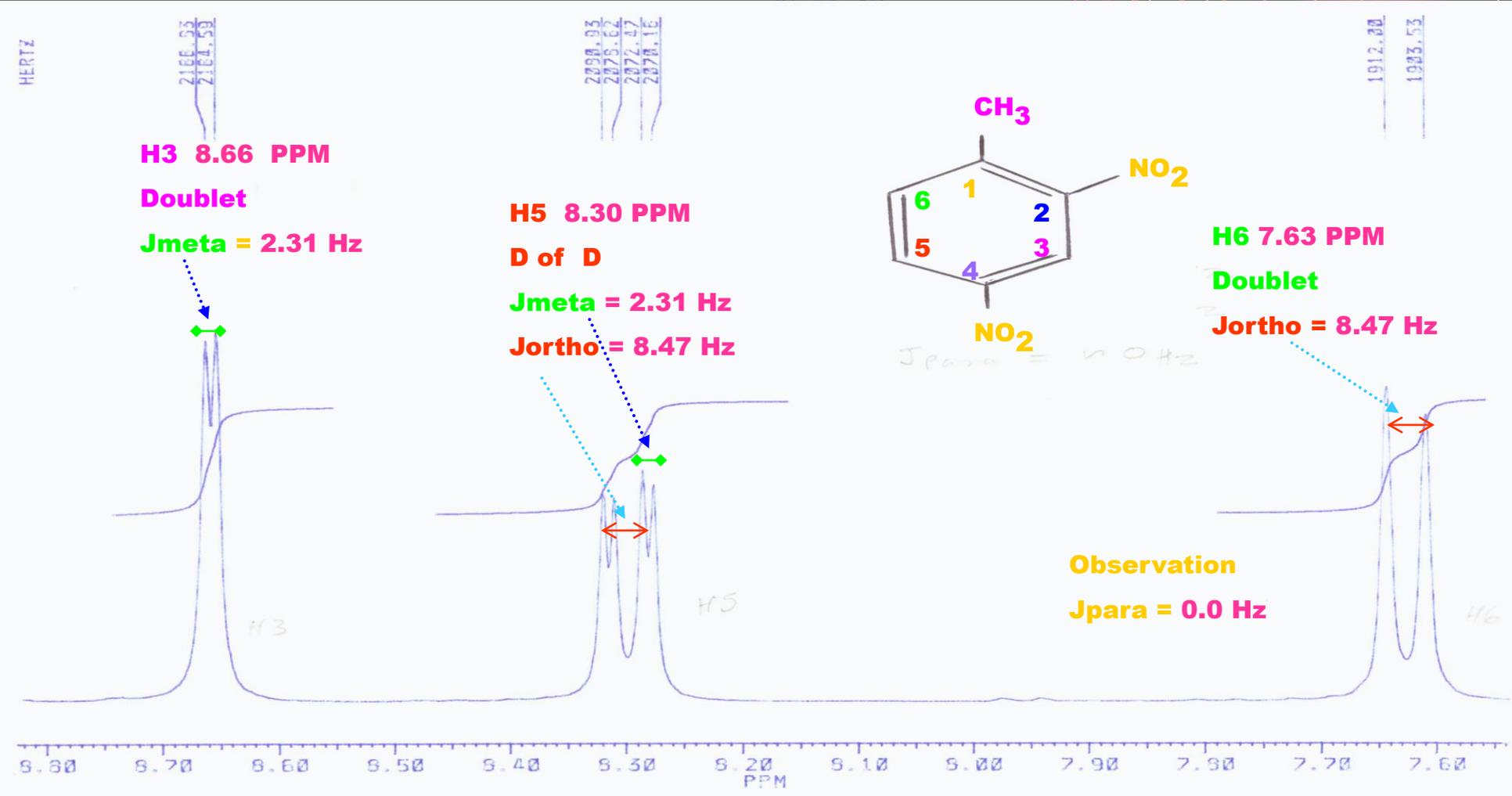
Integration 12.5 = 1H

CH_3
2.73 PPM

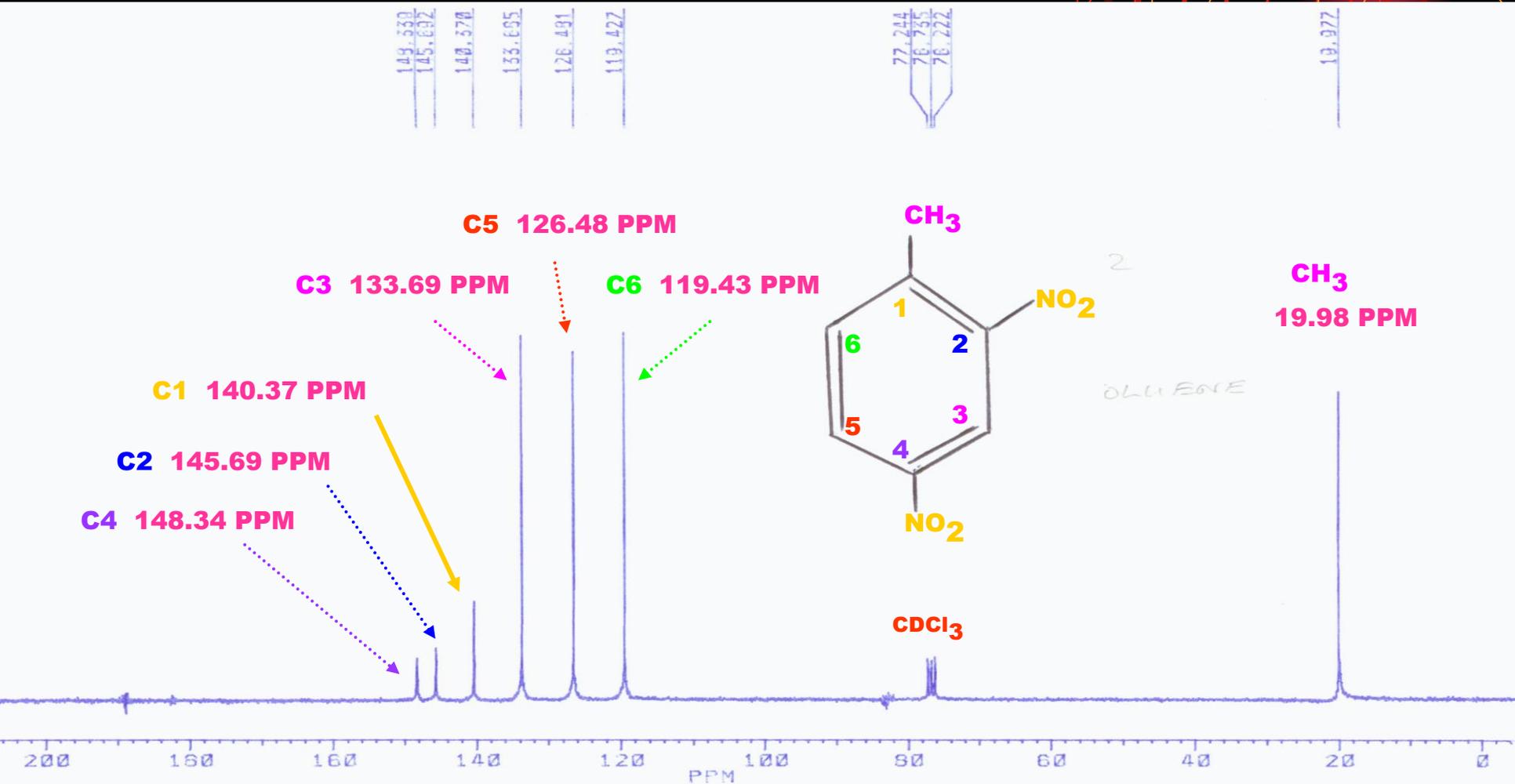


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

$\text{C}_6\text{H}_3\text{CH}_3(\text{NO}_2)_2$ ^1H NMR Spectrum

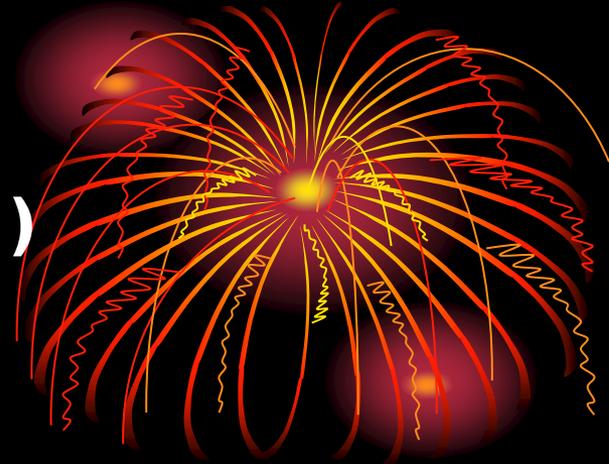


^{13}C NMR Spectra of 2,4-Dinitromethylbenzene

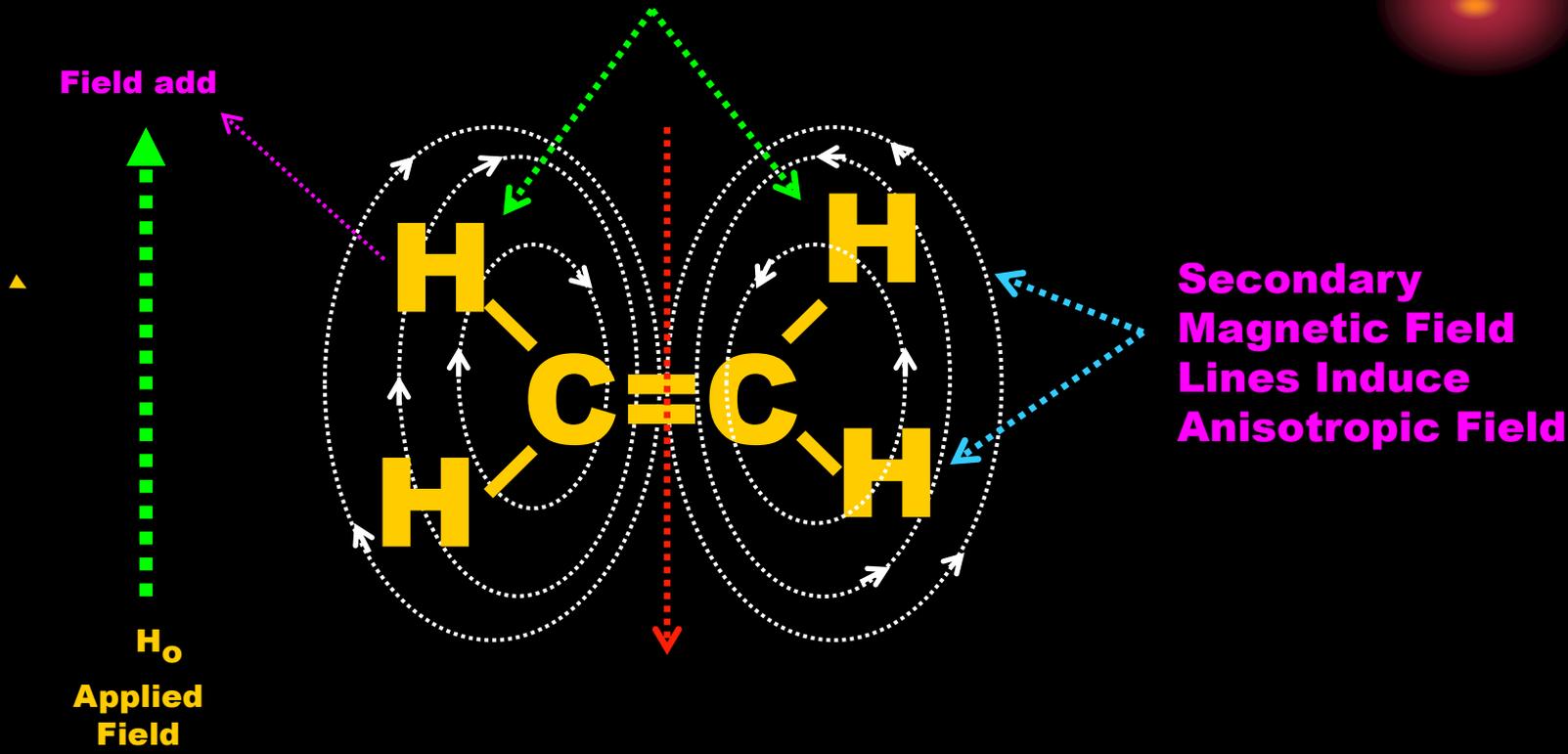


Anisotropic Field in an Alkenes (sp^2)

- **Anisotropic Field Effect**



Deshielded 1H Shift
To Lower Field
Away From TMS



Secondary
Magnetic Field
Lines Induce
Anisotropic Field

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

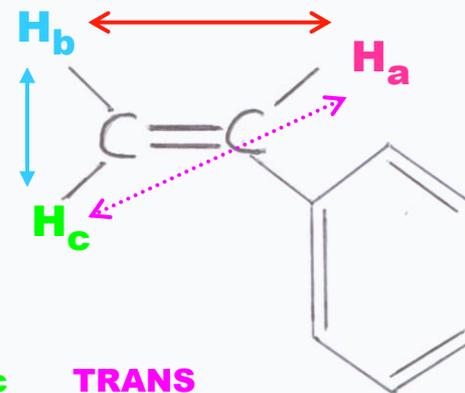


$\text{C}_6\text{H}_5\text{-CH=CH}_2$ ^1H NMR Spectrum

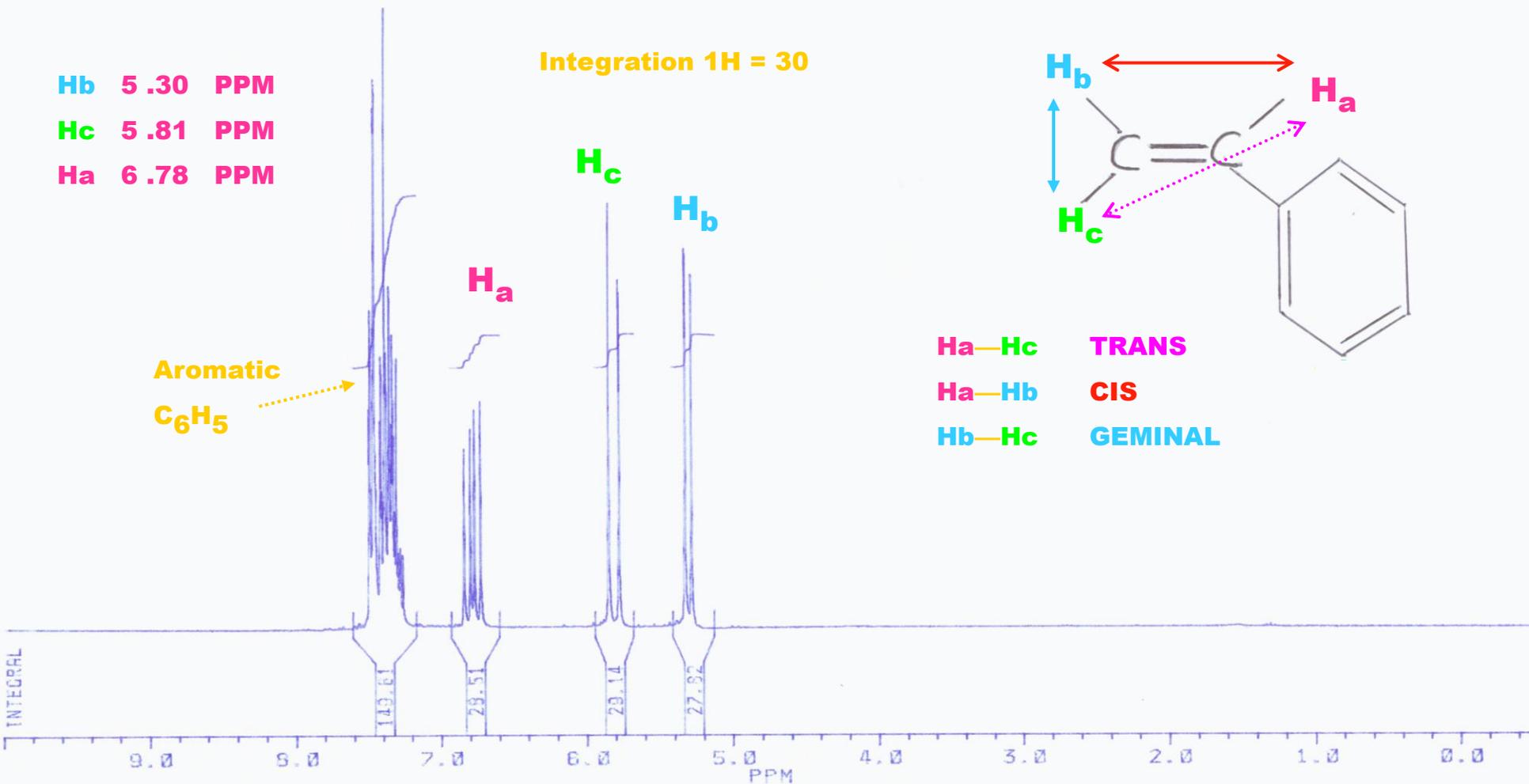
H_b 5.30 PPM
H_c 5.81 PPM
H_a 6.78 PPM

Integration 1H = 30

Aromatic
 C_6H_5

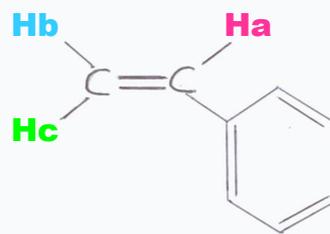
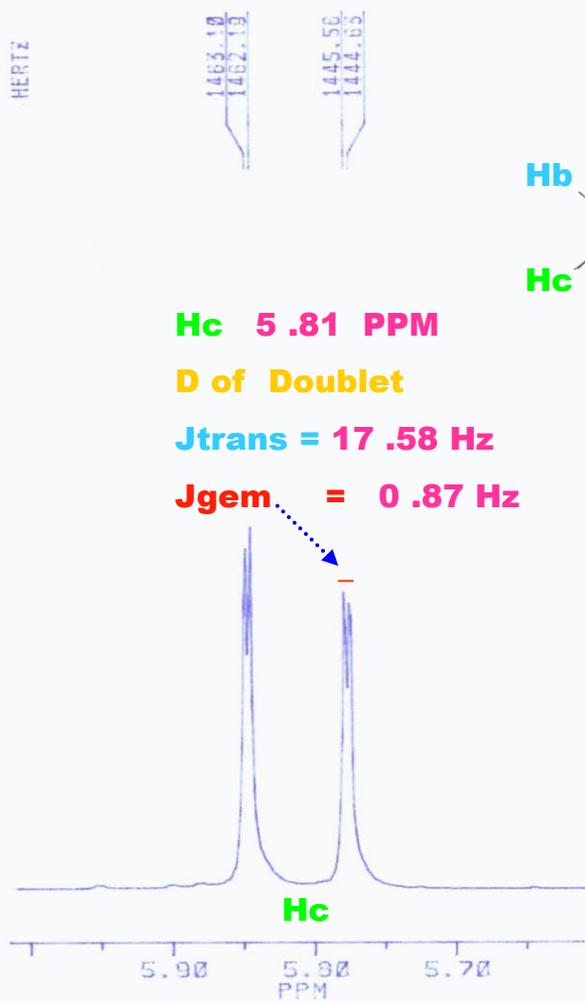
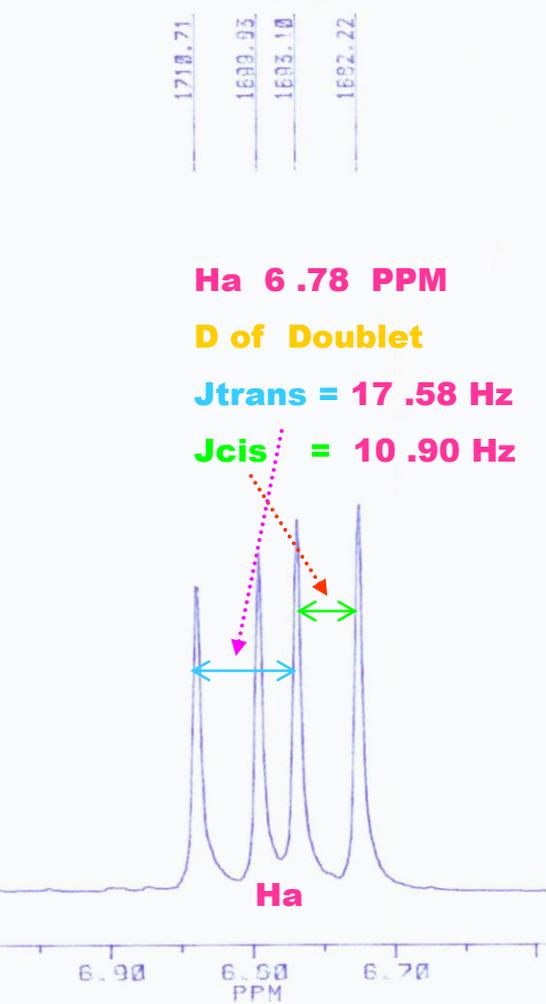


H_a—H_c TRANS
H_a—H_b CIS
H_b—H_c GEMINAL



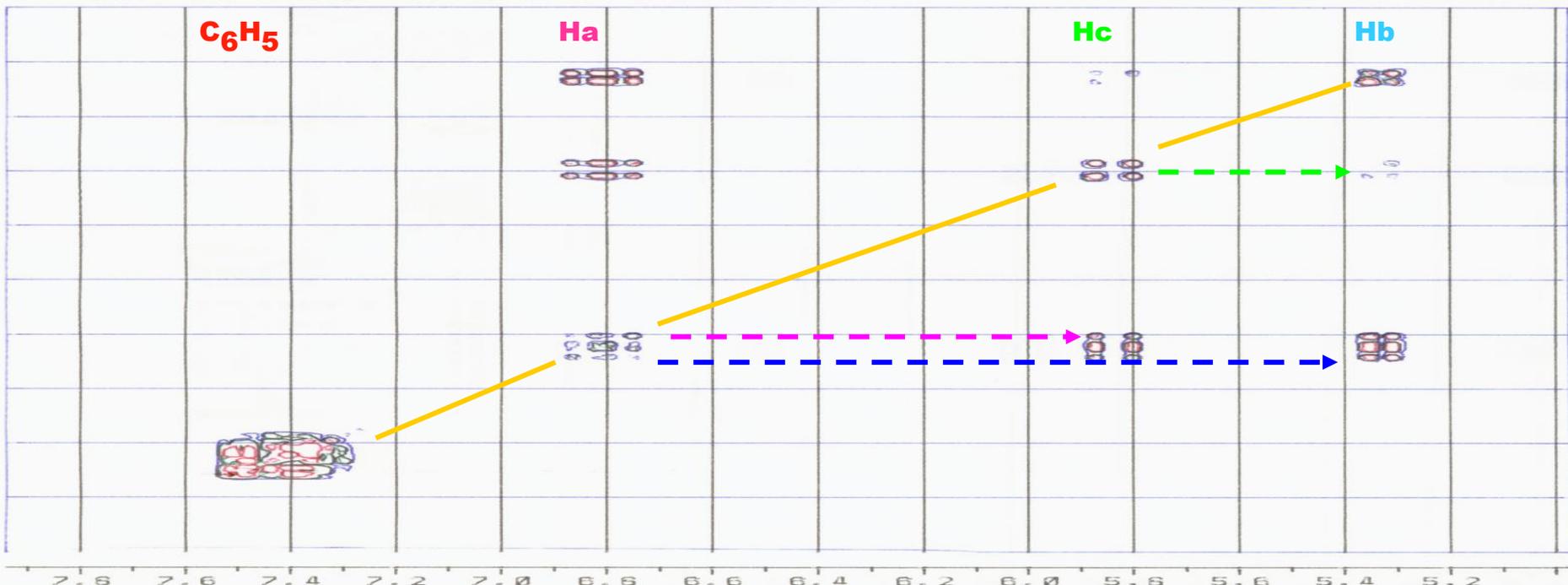
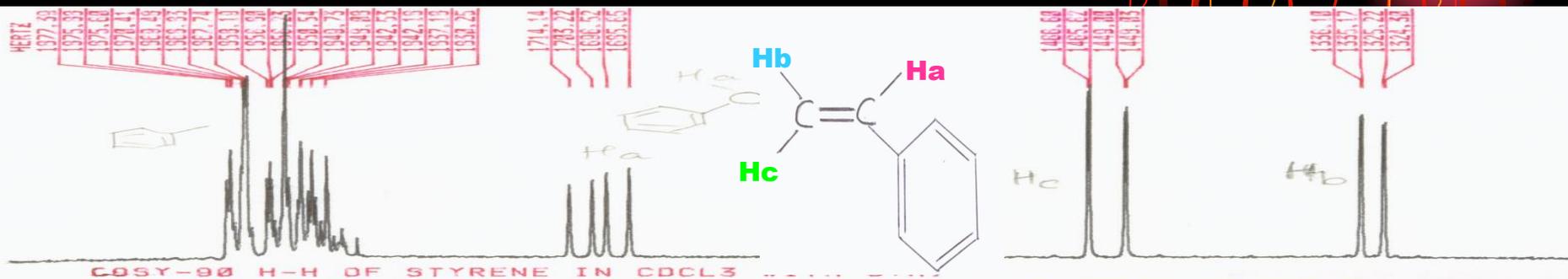
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Styrene

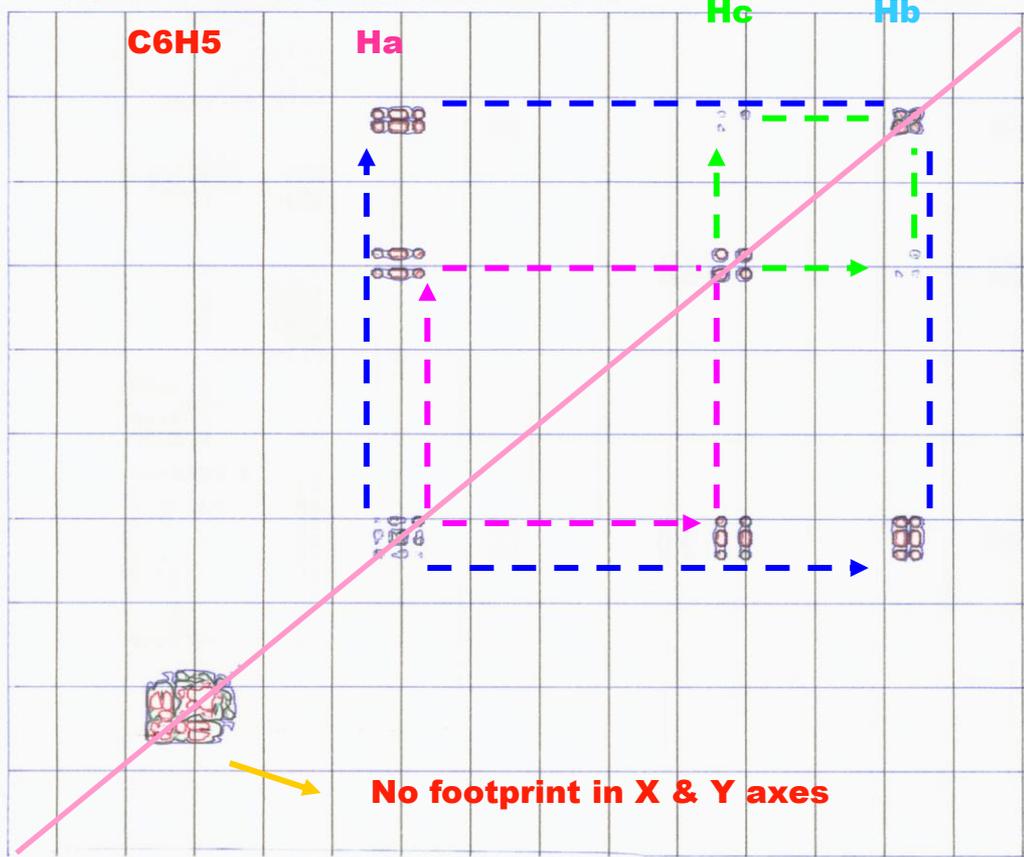
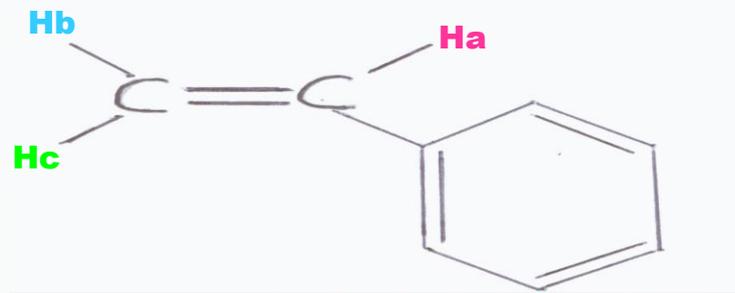
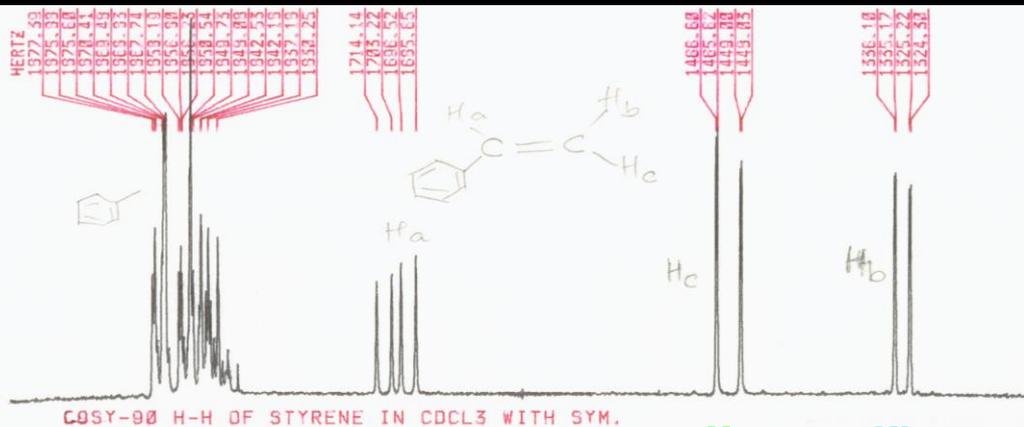
$\text{C}_6\text{H}_5\text{-CH=CH}_2$ ^1H NMR Spectrum



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

$\text{C}_6\text{H}_5\text{-CH=CH}_2$ 2D COSY ^1H NMR Spectrum



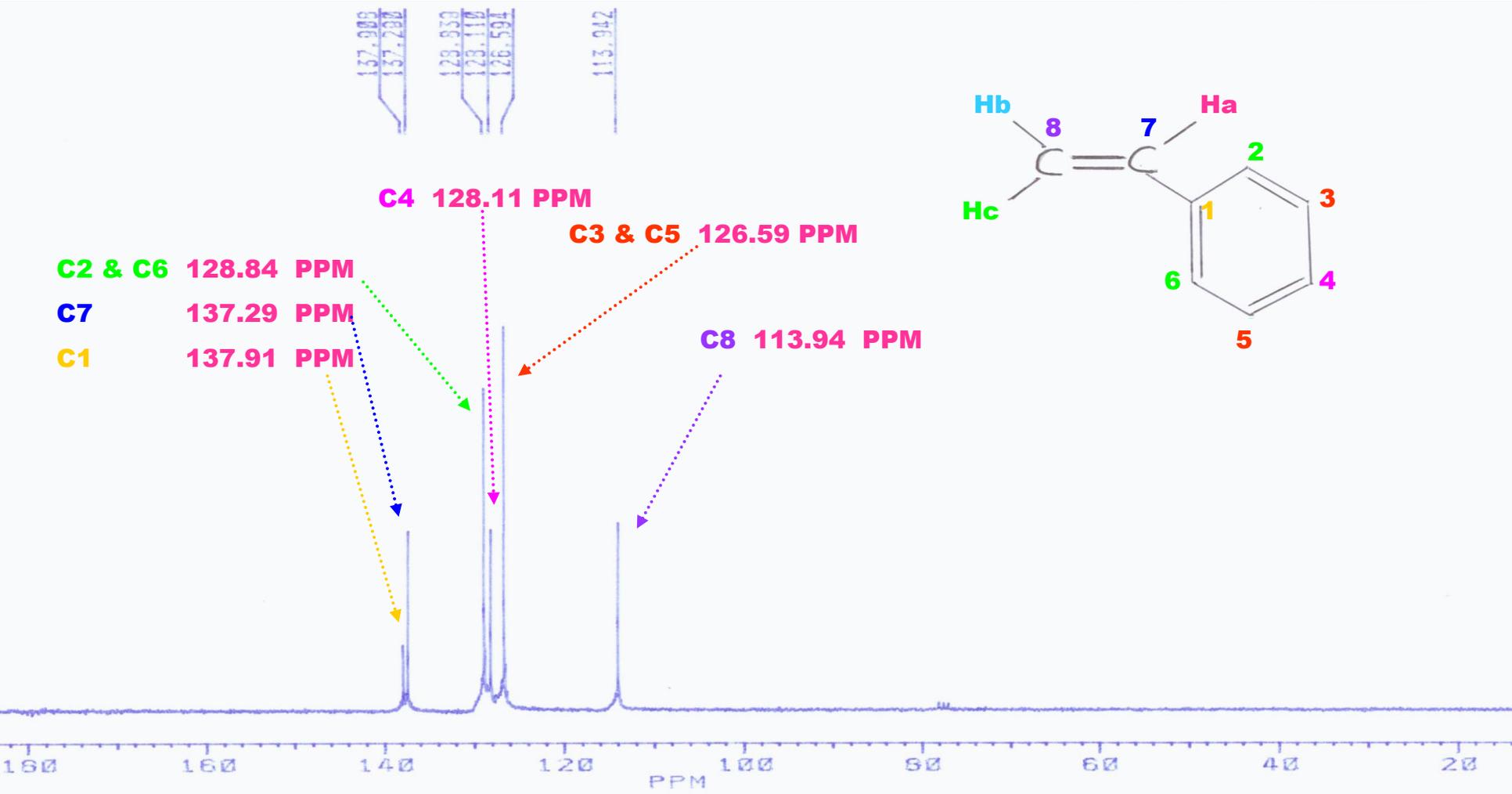


Analysis and interpretation of 2D COSY 90 1H NMR Spectrum of Styrene

$C_6H_5-CH=CH_2$

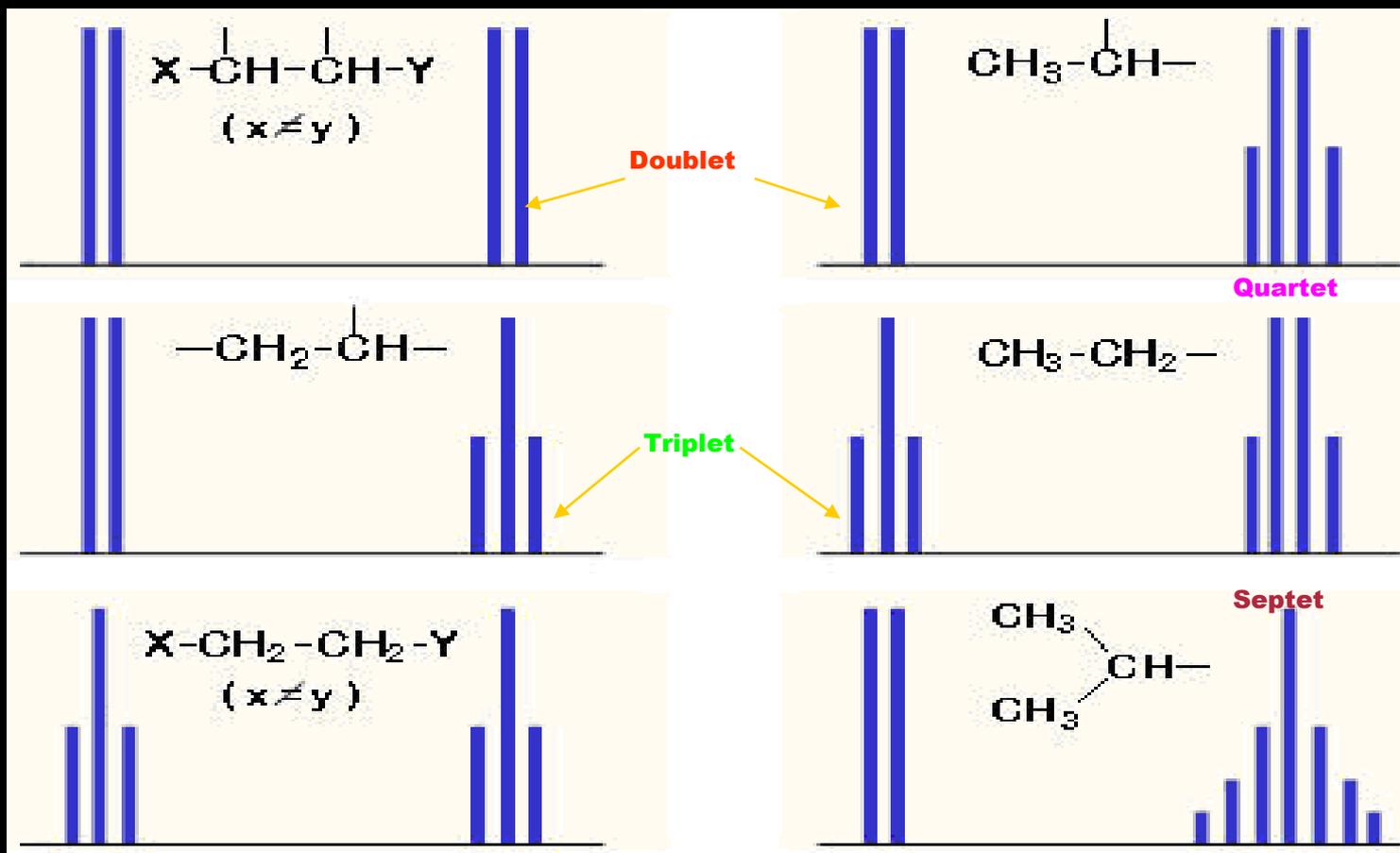
1. Every peak in spectrum gives the diagonal footprint in cosy spectrum.
2. Non coupled 1H gives only diagonal footprint and no footprint in X & Y axes.
3. Coupled 1H will give footprint in X & Y axes.
4. Number of coupling can be seen easily just by counting the number of footprints along either X or 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 $\text{C}_6\text{H}_5\text{-CH=CH}_2$



Splitting Patterns for Aliphatic ^1H

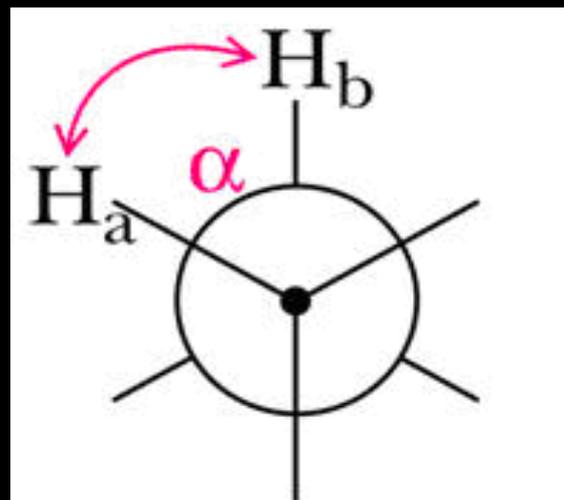
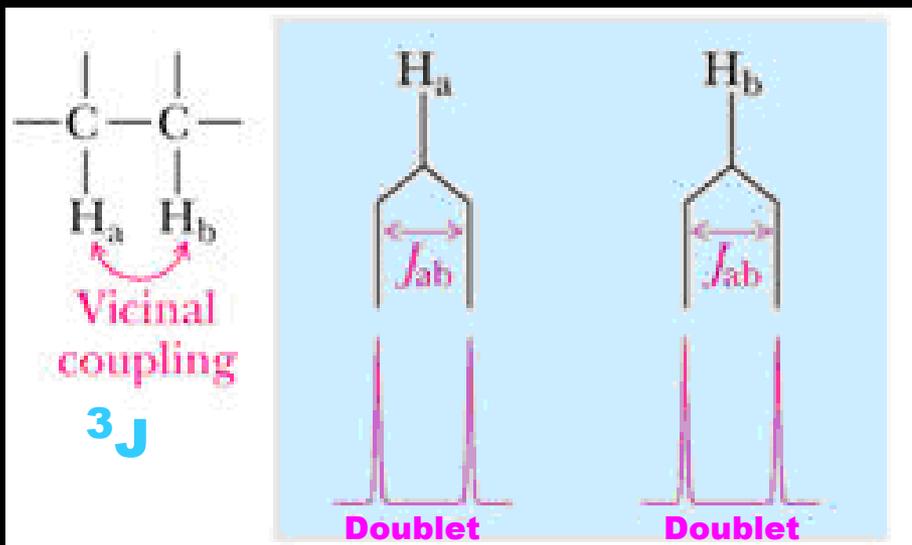
Common Patterns in ^1H NMR Spectra



Notation For Coupling Constant (1J , 2J , 3J , 4J & so on)

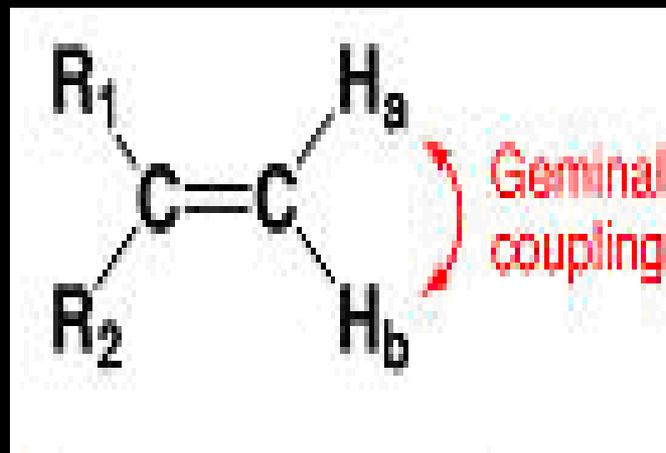
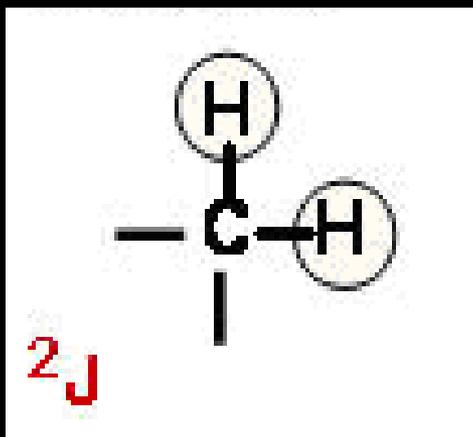


- In ^1H NMR spectra, the most common coupling constant is encountered ^1H three bonds apart 3J . This is also called as Vicinal Coupling.
- The angle alpha factor in vicinal coupling.
- When angle alpha = 0° and 180° The coupling constant is maximum
- = 90° The coupling constant is minimum



2J coupling constant

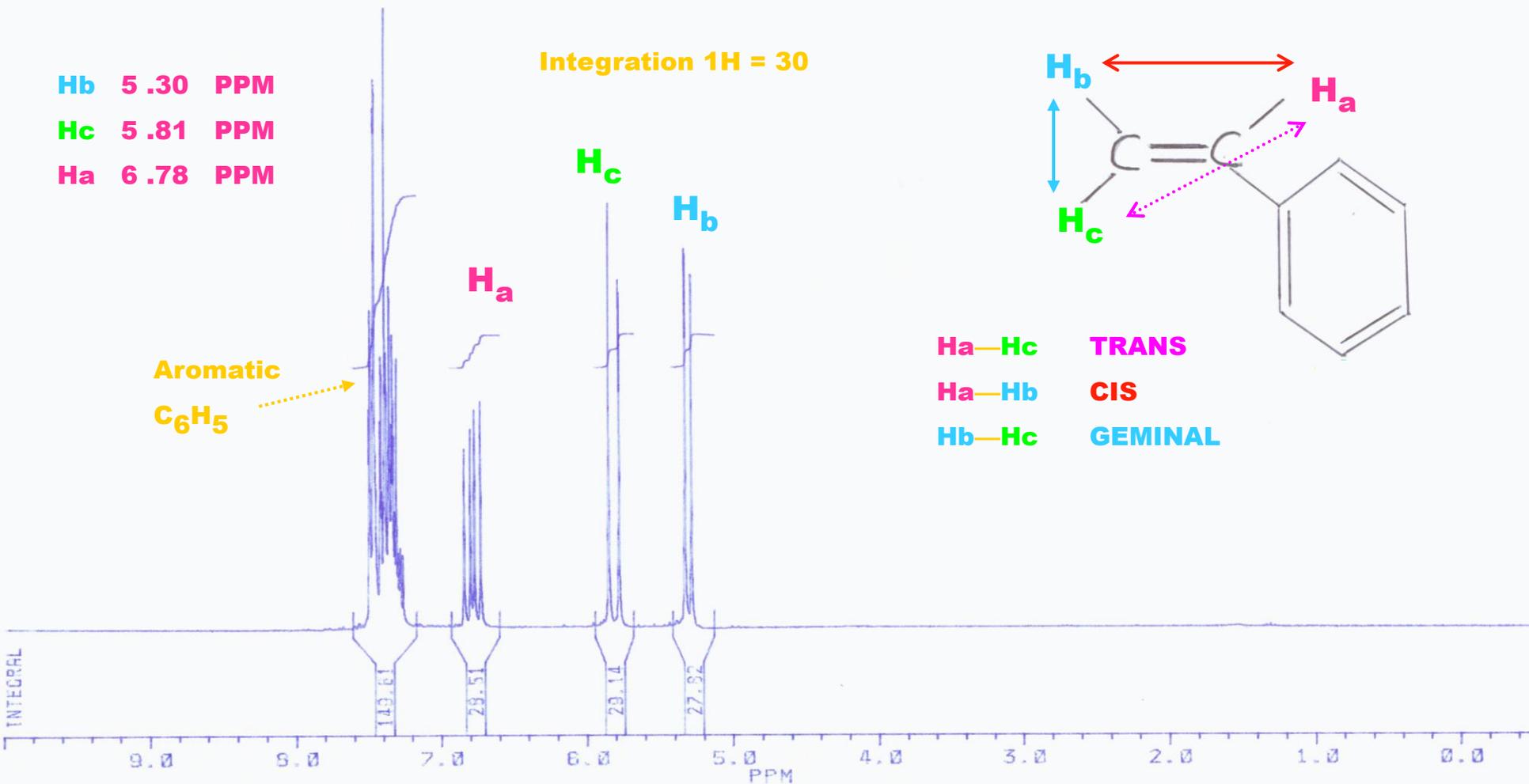
- The alpha angle $H-C-C-H$ and the rotation round $--C-C--$ sigma bonds is also a key parameter for 1H coupling constant.
- In Ethyl CH_3-CH_2- Group the free rotation make 1H attached to the same carbon equivalent hence do not show coupling $^2J = 00$ Hz
- In alkenes and cyclic compounds the sigma 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



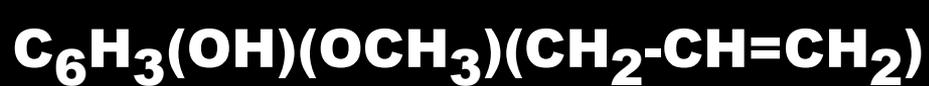
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Styrene



$\text{C}_6\text{H}_5\text{-CH=CH}_2$ ^1H NMR Spectrum



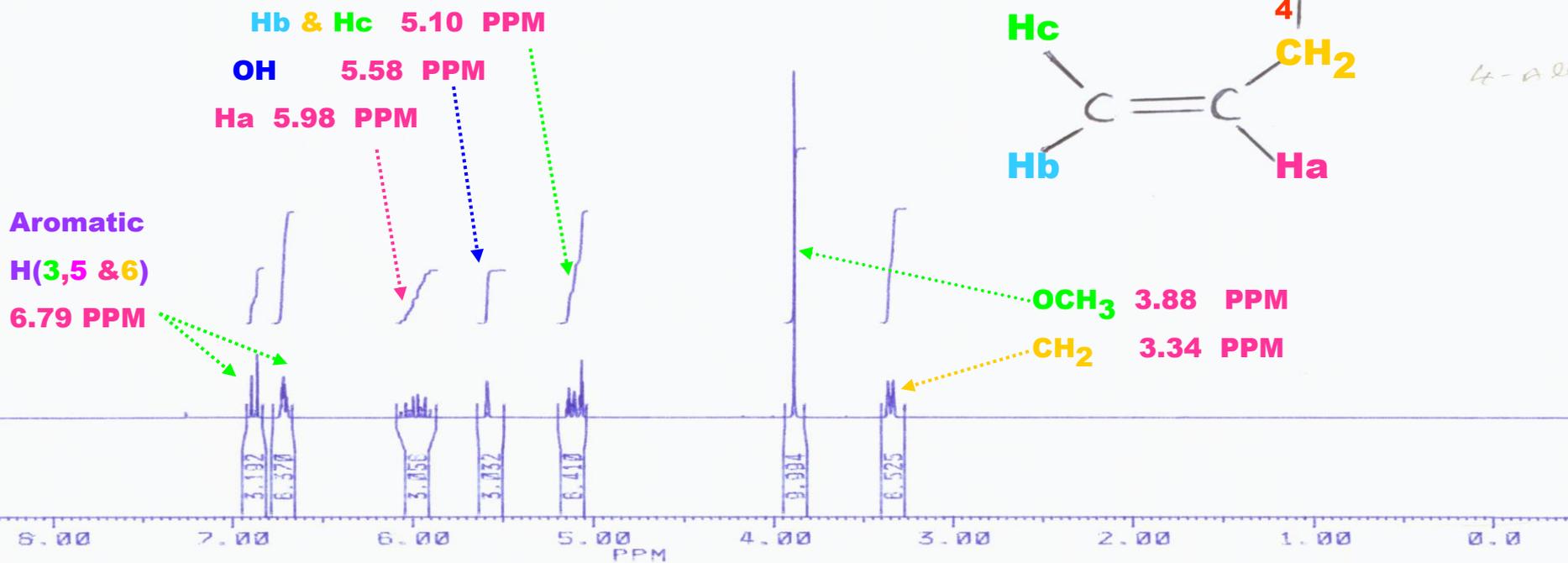
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol



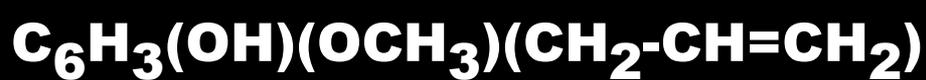
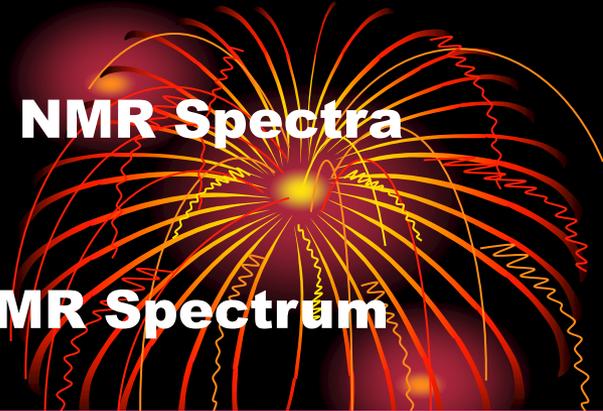
^1H NMR Spectrum



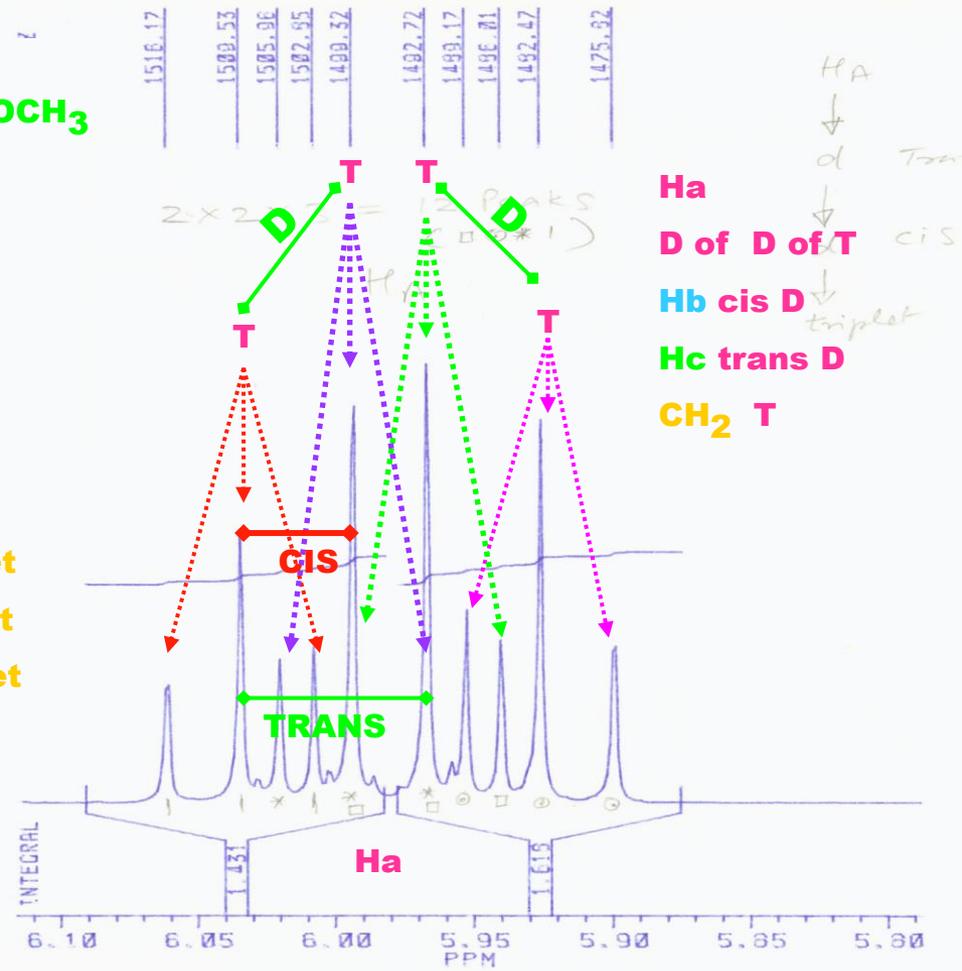
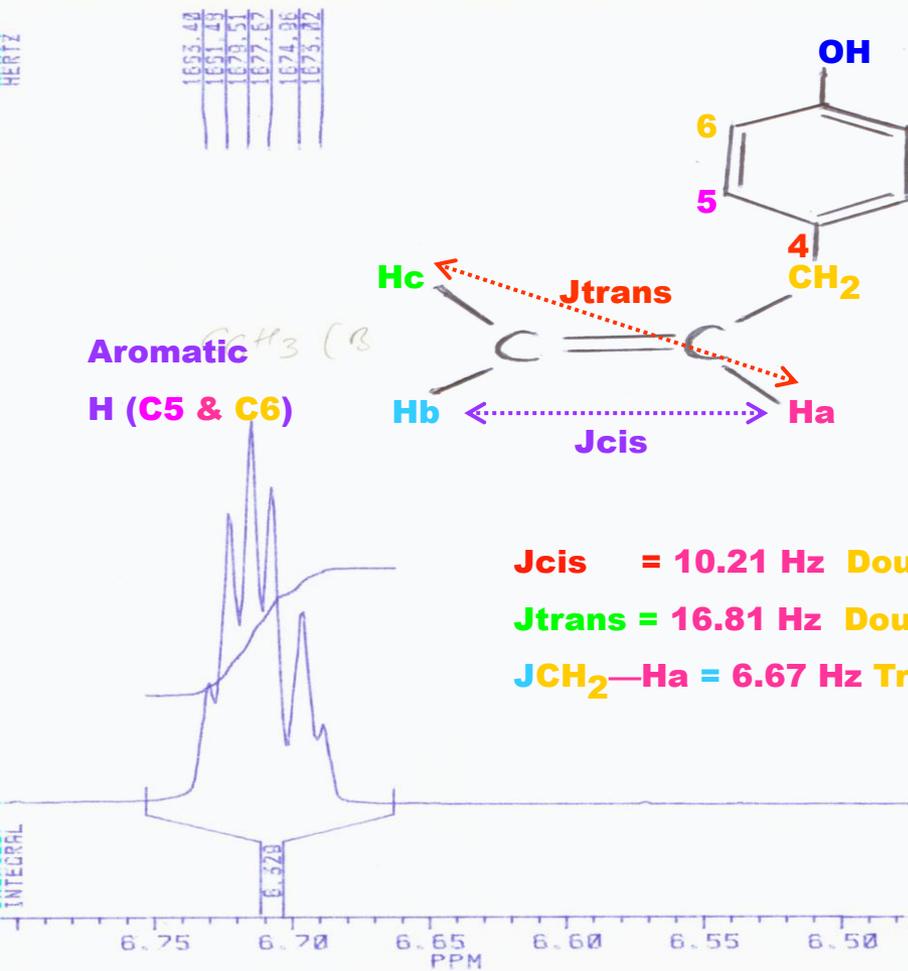
Integration 1H = 3



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

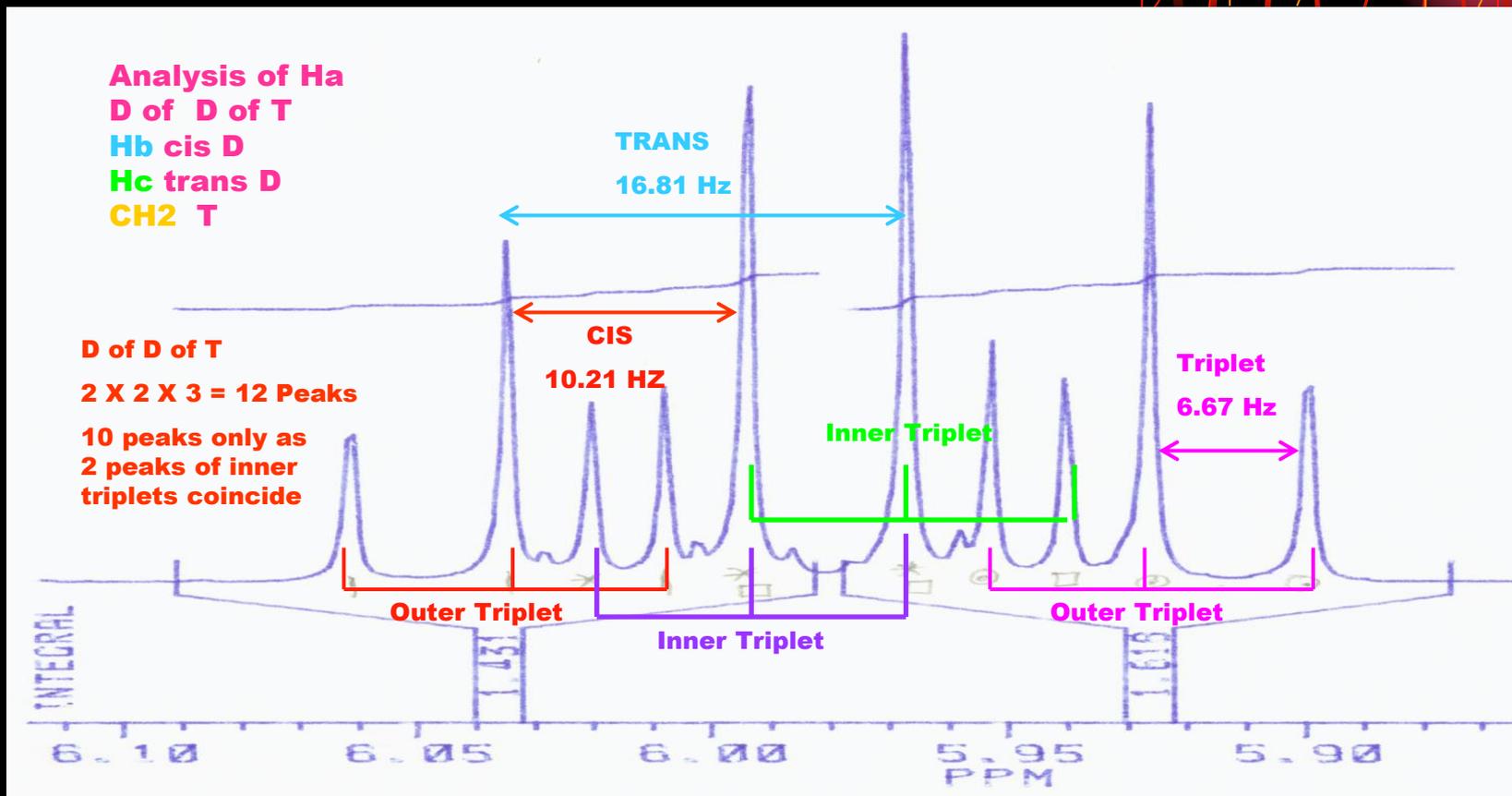


^1H NMR Spectrum



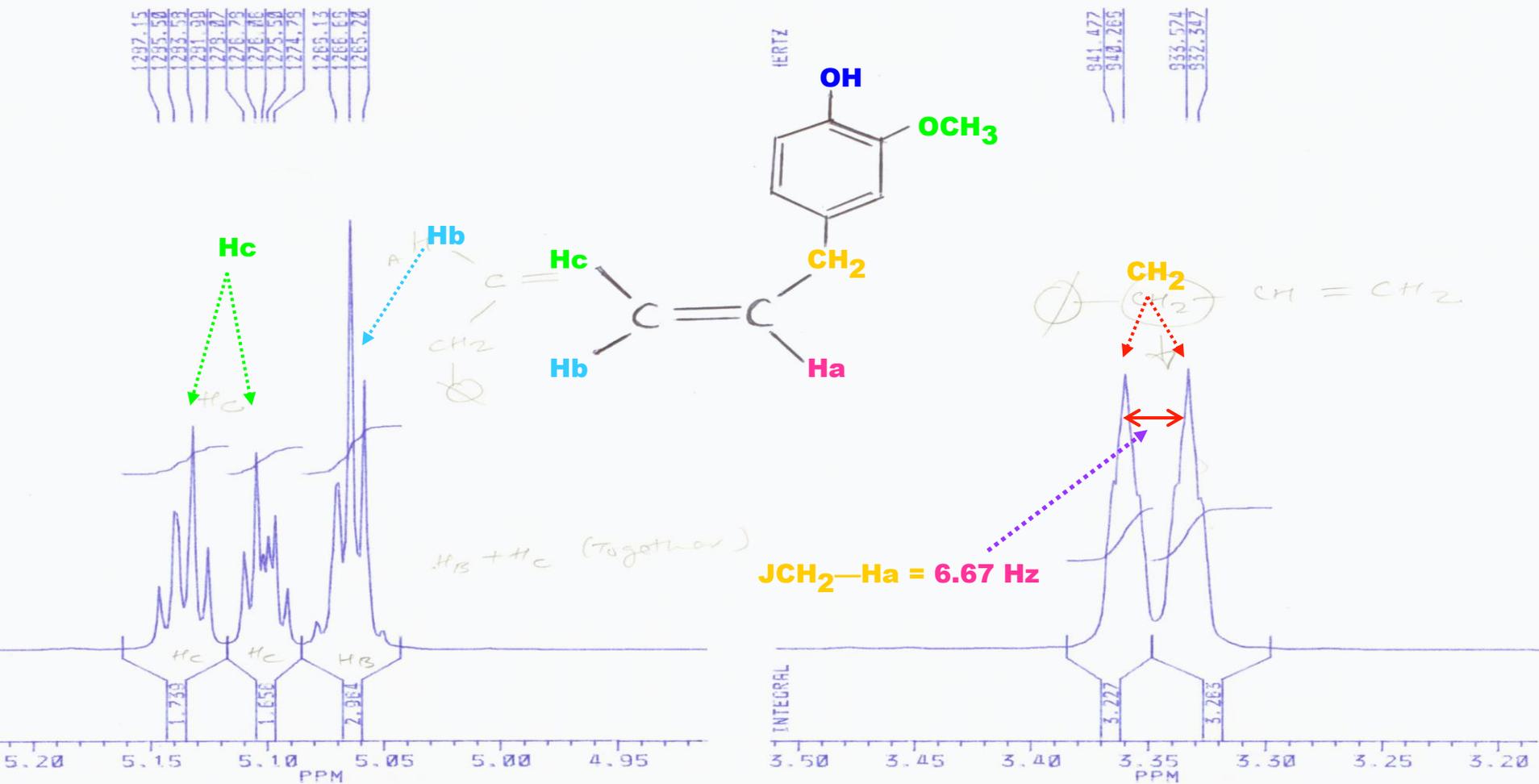
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 4-Allyl-2-MethoxyPhenol

$\text{C}_6\text{H}_3(\text{OH})(\text{OCH}_3)(\text{CH}_2\text{-CH=CH}_2)$ ^1H NMR Spectrum



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

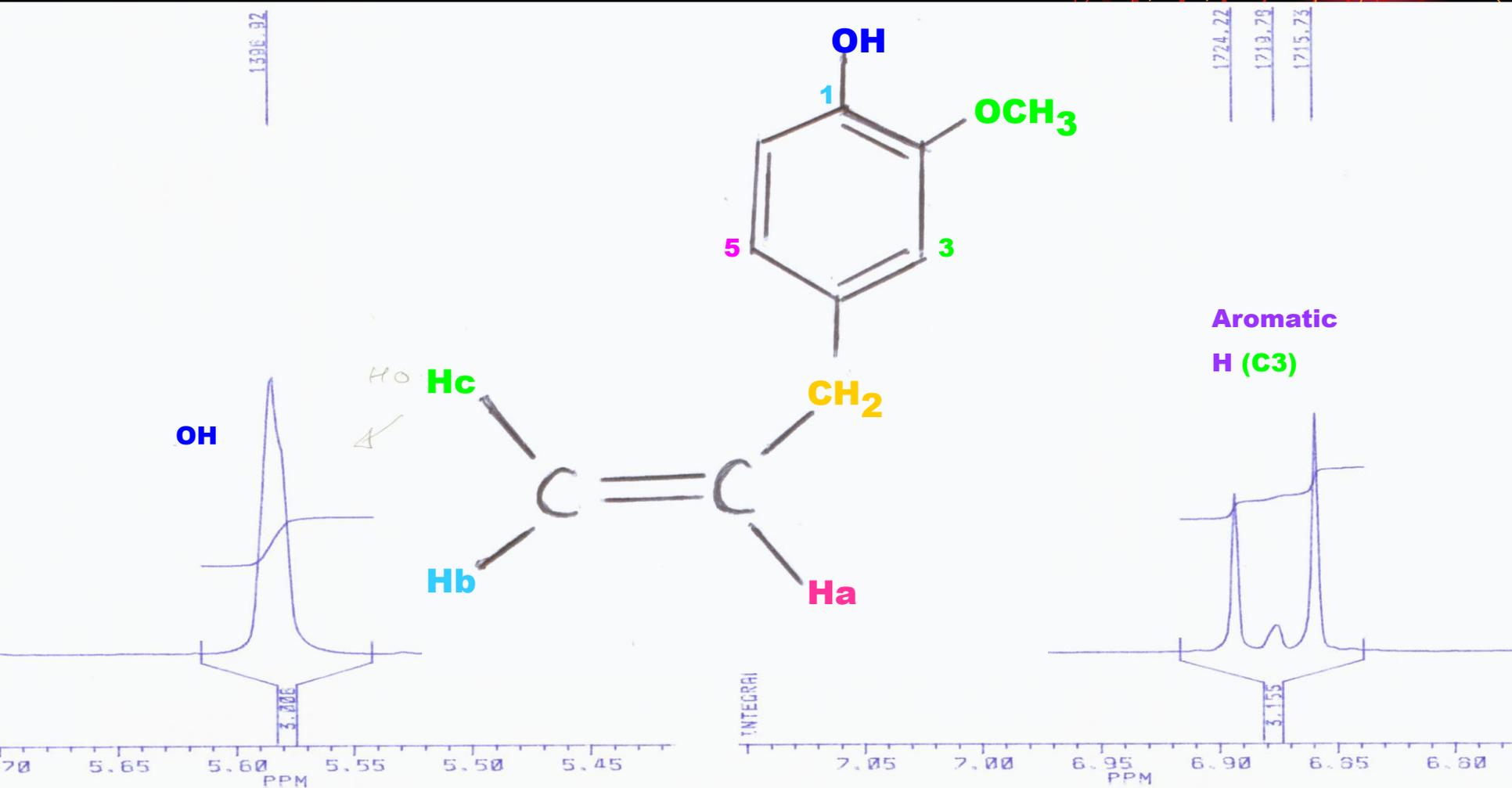
$\text{C}_6\text{H}_3(\text{OH})(\text{OCH}_3)(\text{CH}_2\text{-CH=CH}_2)$ ^1H NMR Spectrum



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

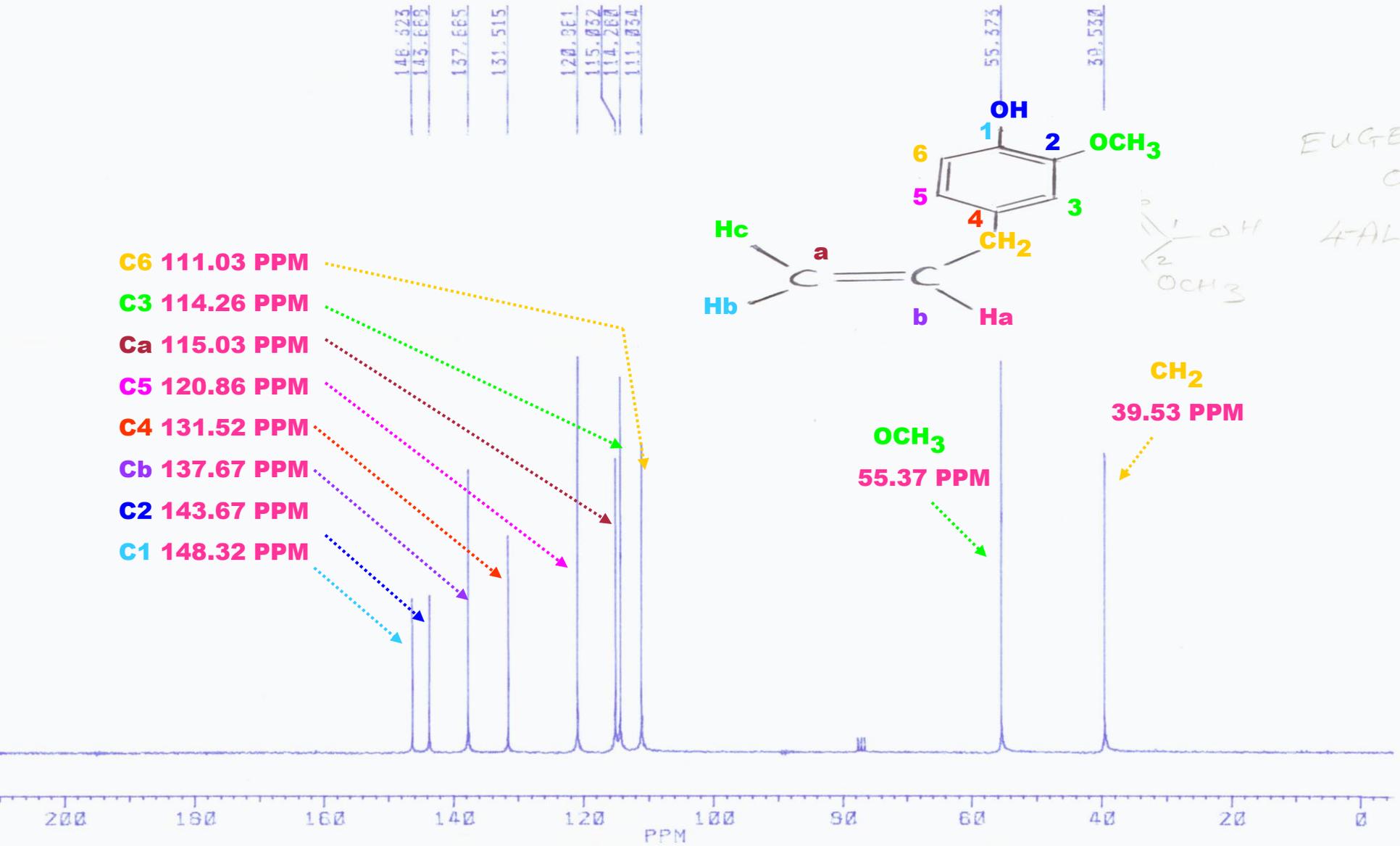
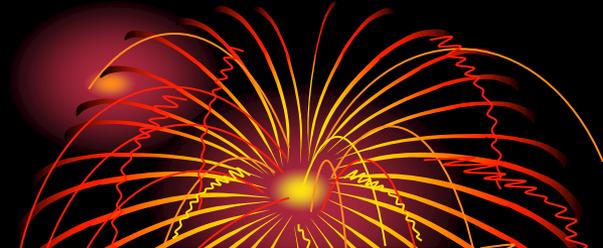


^1H NMR Spectrum

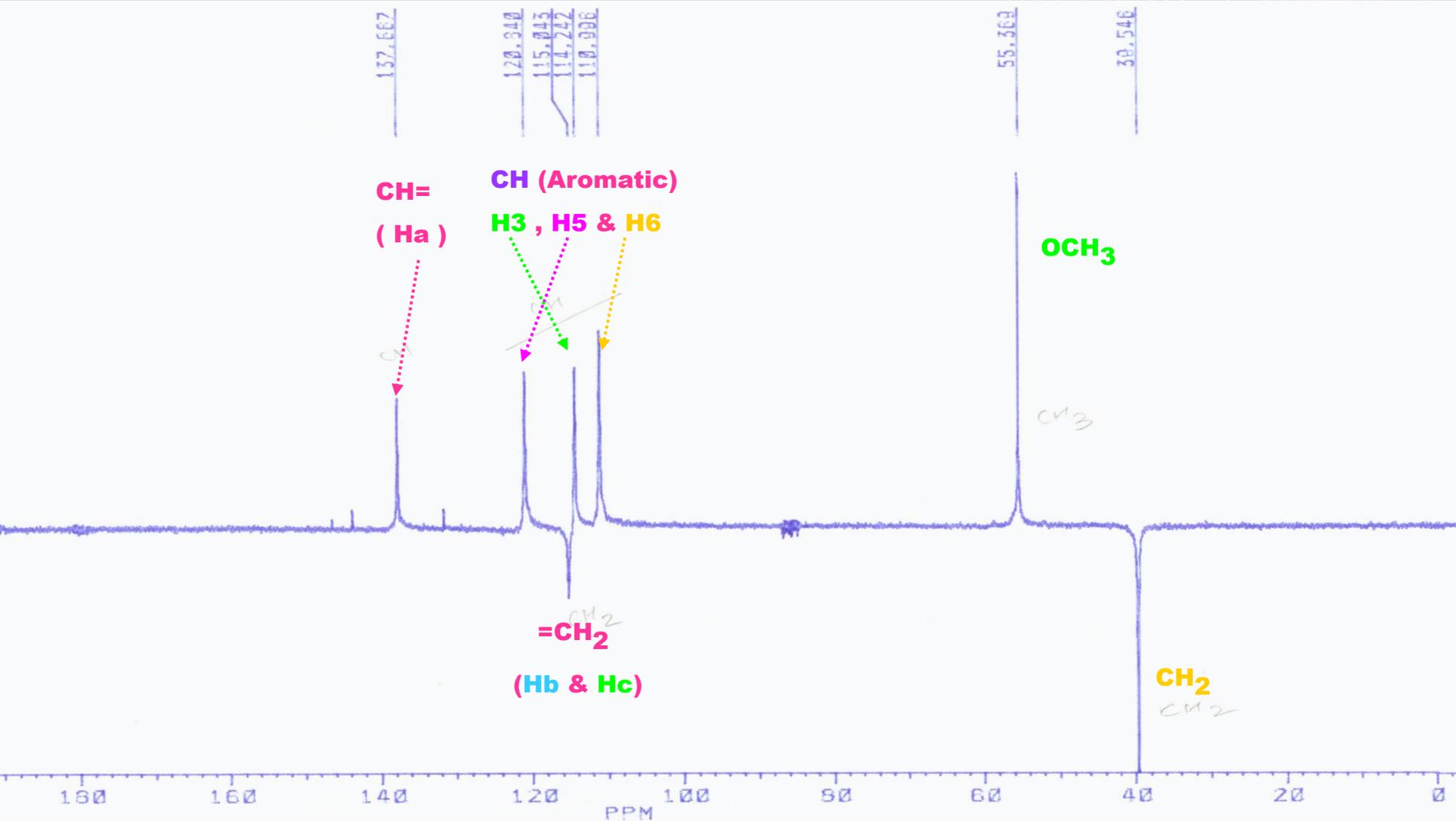
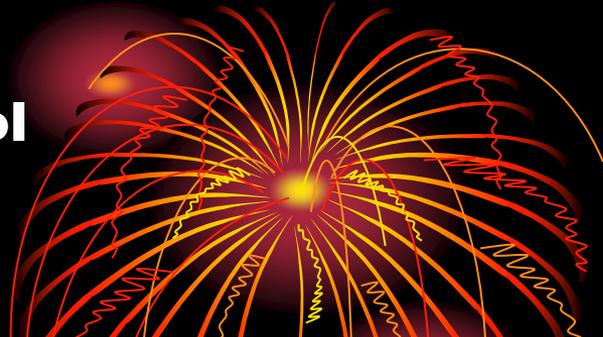
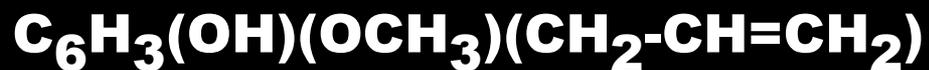


^{13}C NMR Spectrum of Eugenol.

4-Allyl-2-MethoxyPhenol



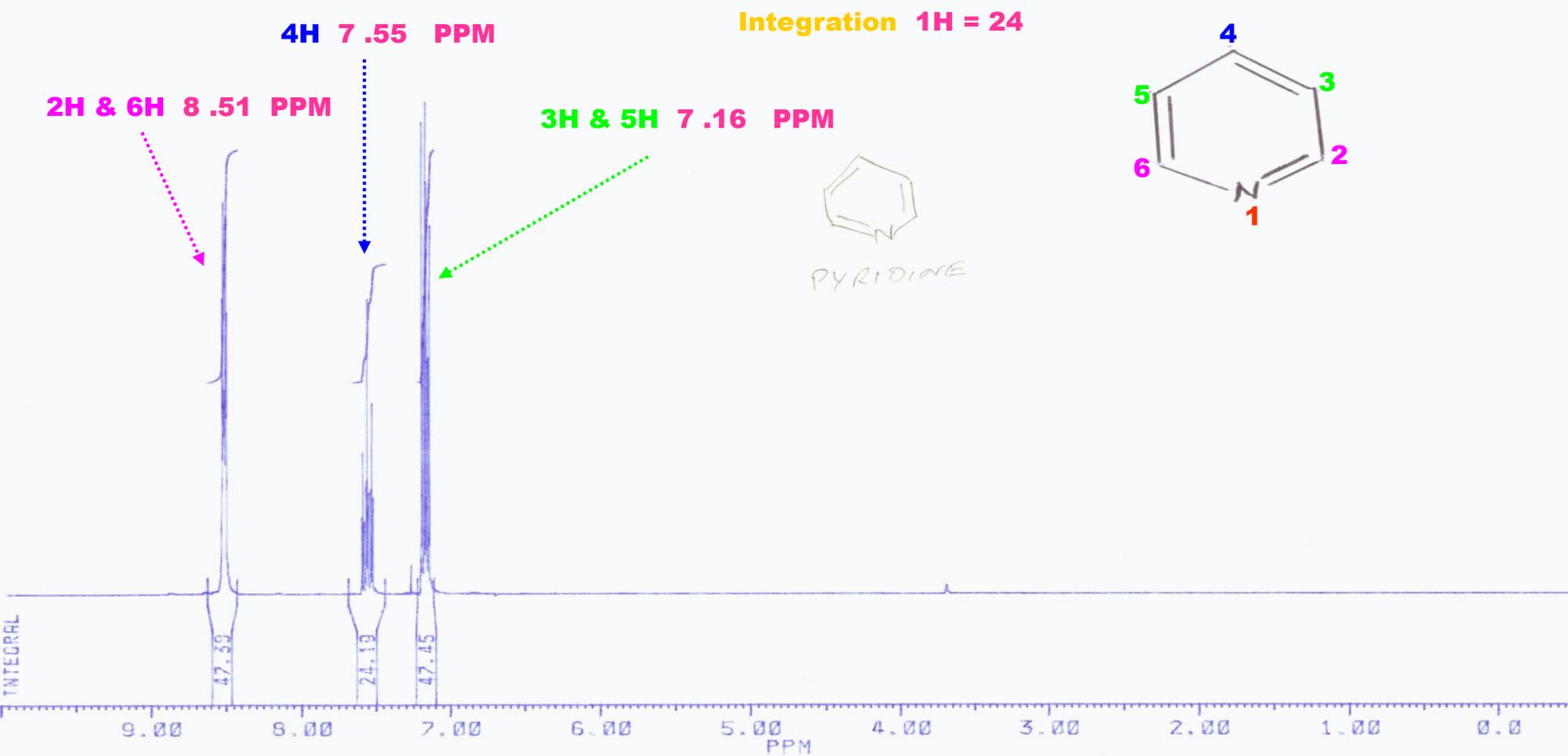
^{13}C Dept 135 of 4-Allyl-2-MethoxyPhenol



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



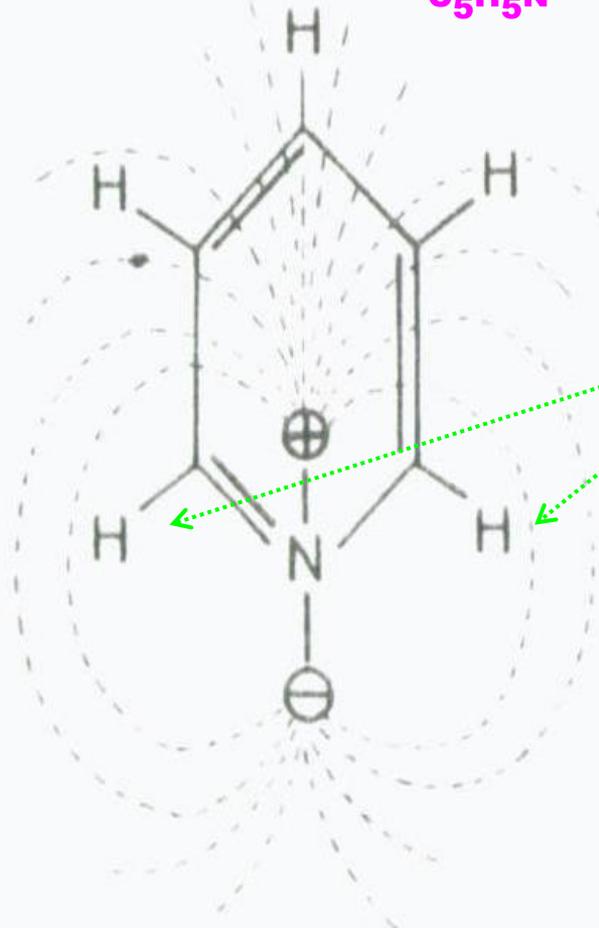
$\text{C}_5\text{H}_5\text{N}$ ^1H NMR Spectrum



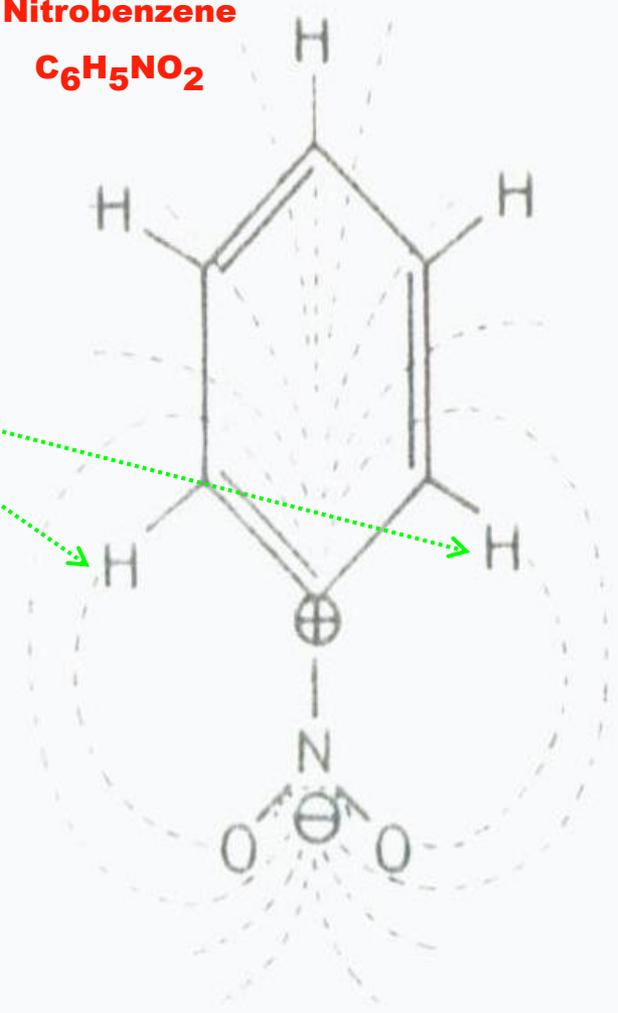
The Electric Field Effect on Pyridine & Nitrobenzene



Pyridine
 C_5H_5N



Nitrobenzene
 $C_6H_5NO_2$



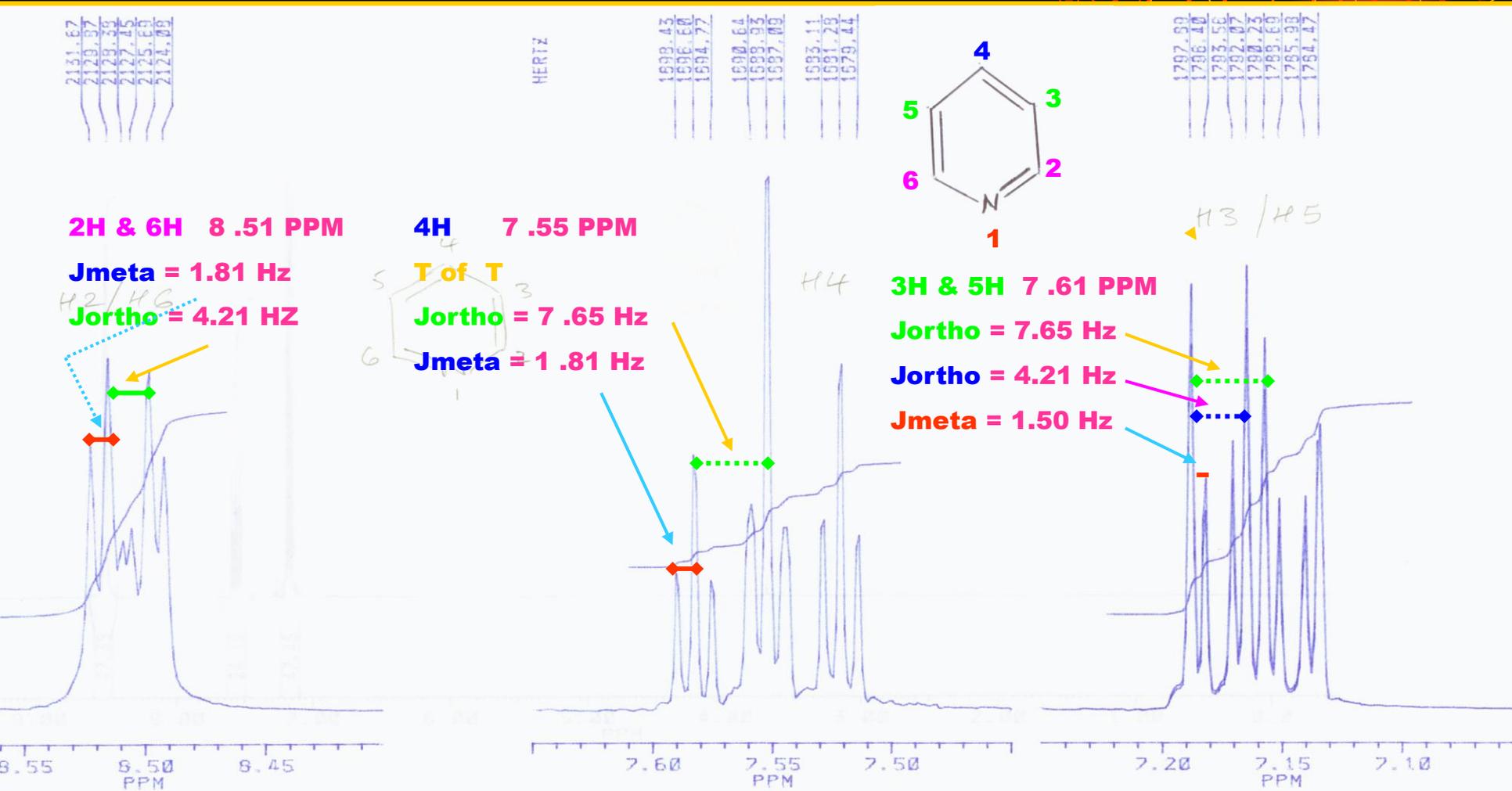
Deshielded 1H



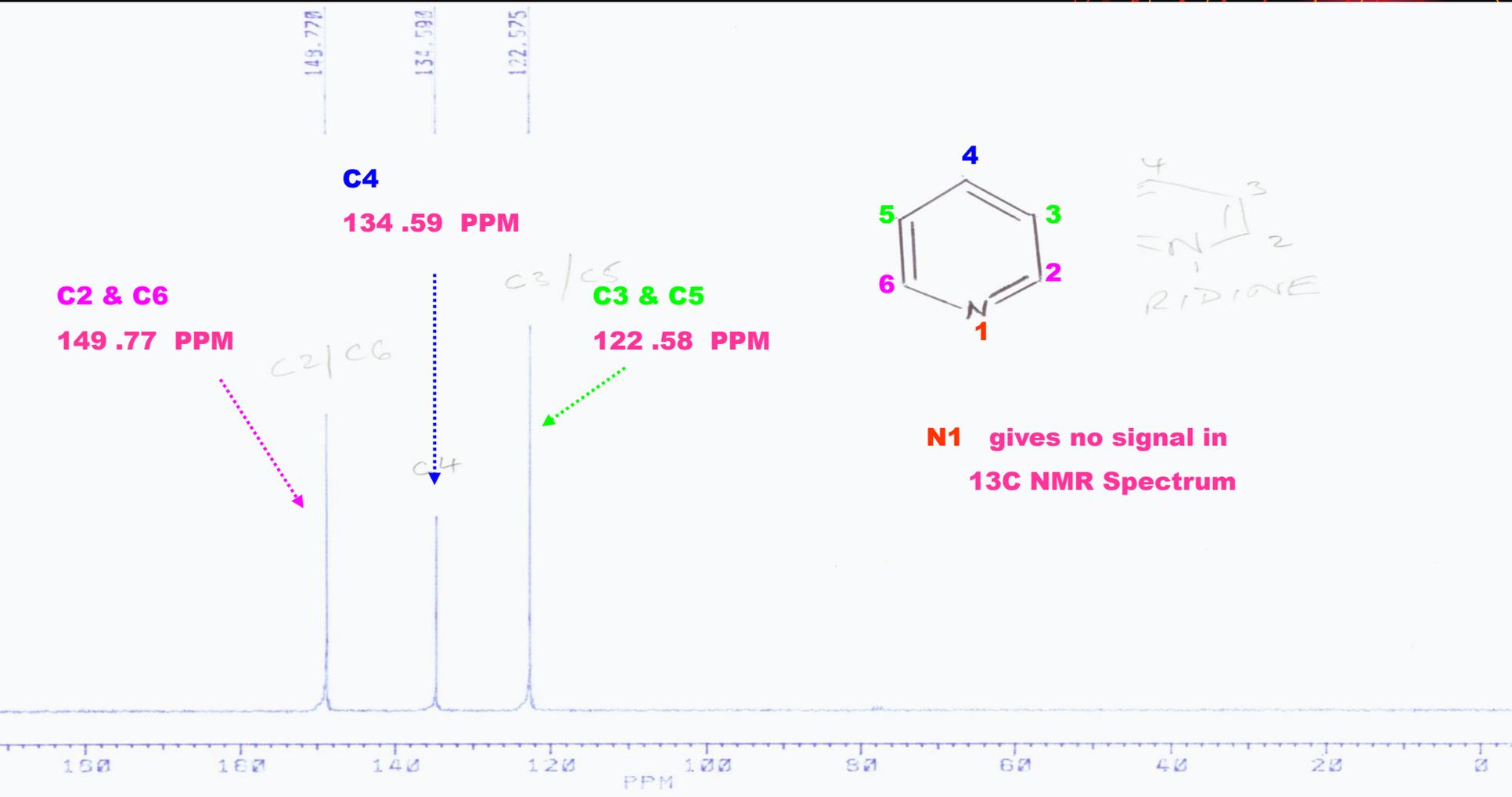
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Pyridine



$\text{C}_5\text{H}_5\text{N}$ ^1H NMR Spectrum Expansion



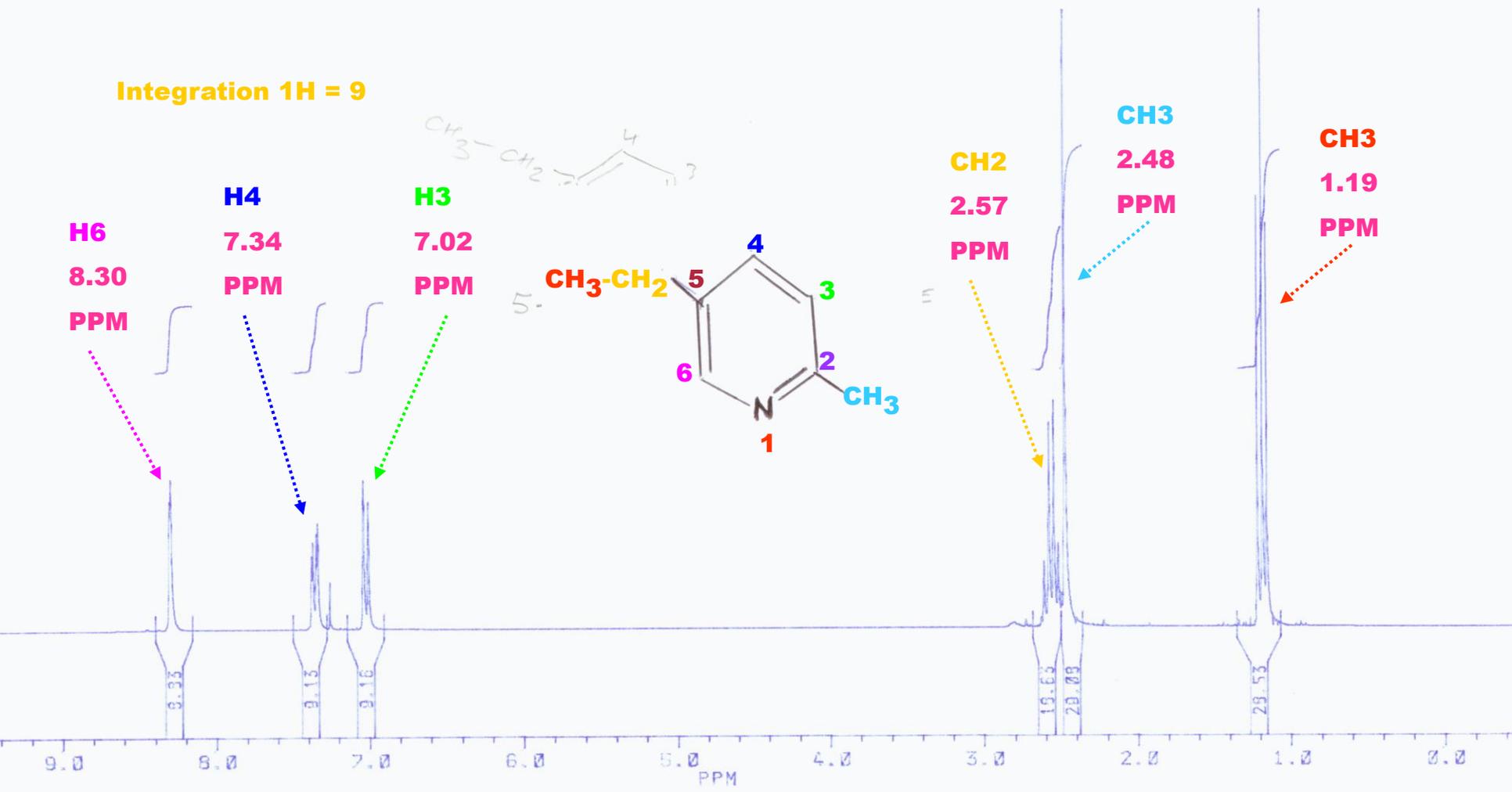
Analysis and interpretation of ^{13}C NMR Spectrum of Pyridine $\text{C}_5\text{H}_5\text{N}$



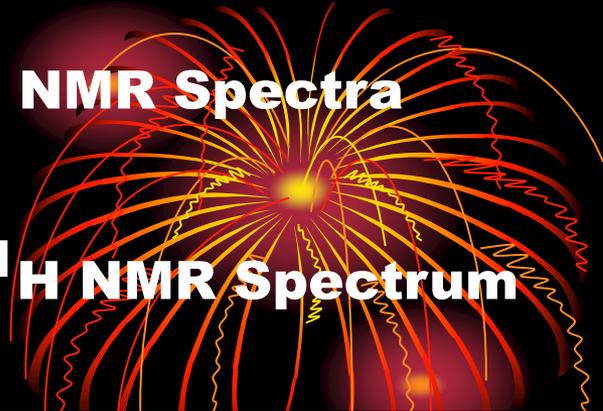
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 5-Ethyl-2-Methylpyridine



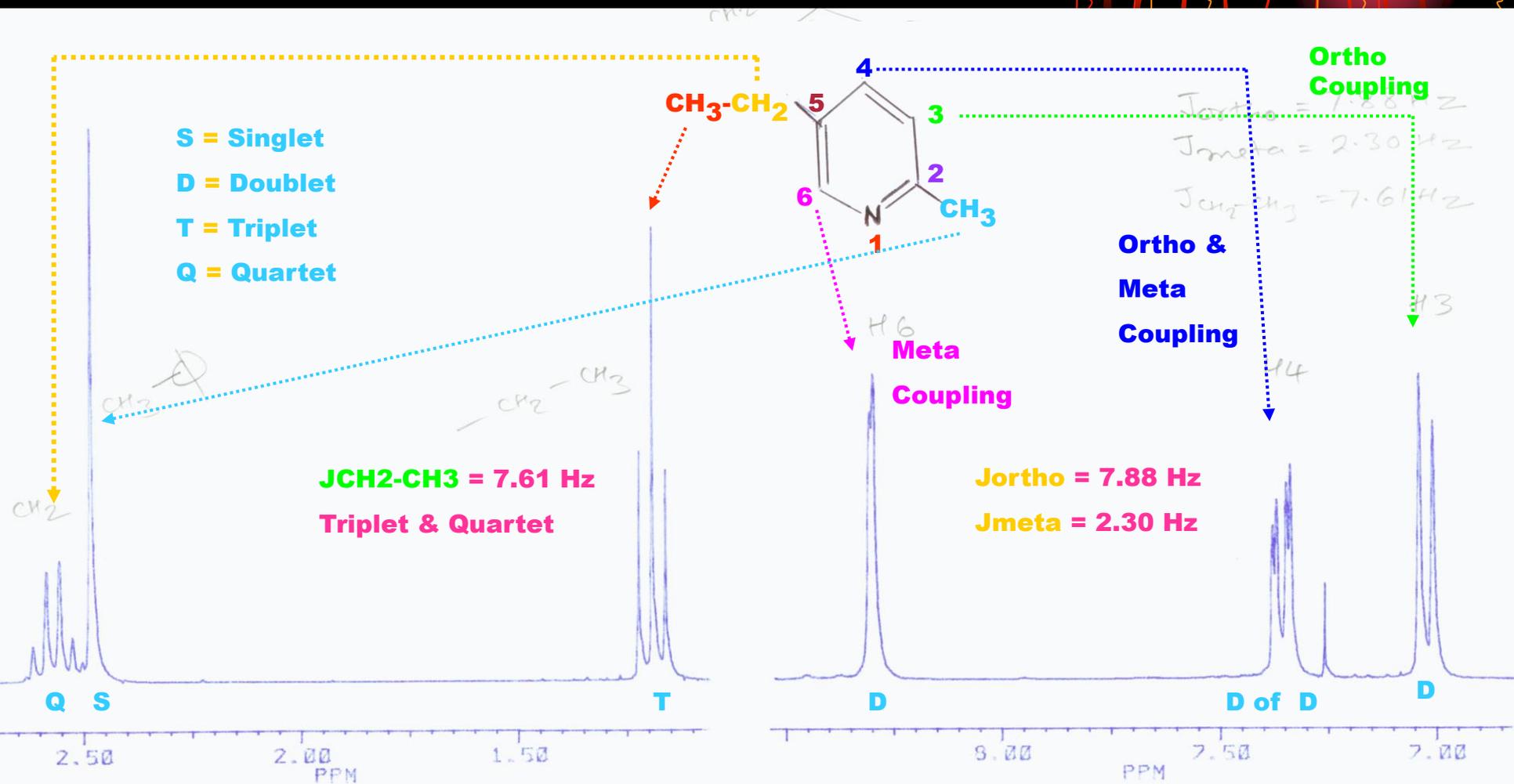
^1H NMR Spectrum



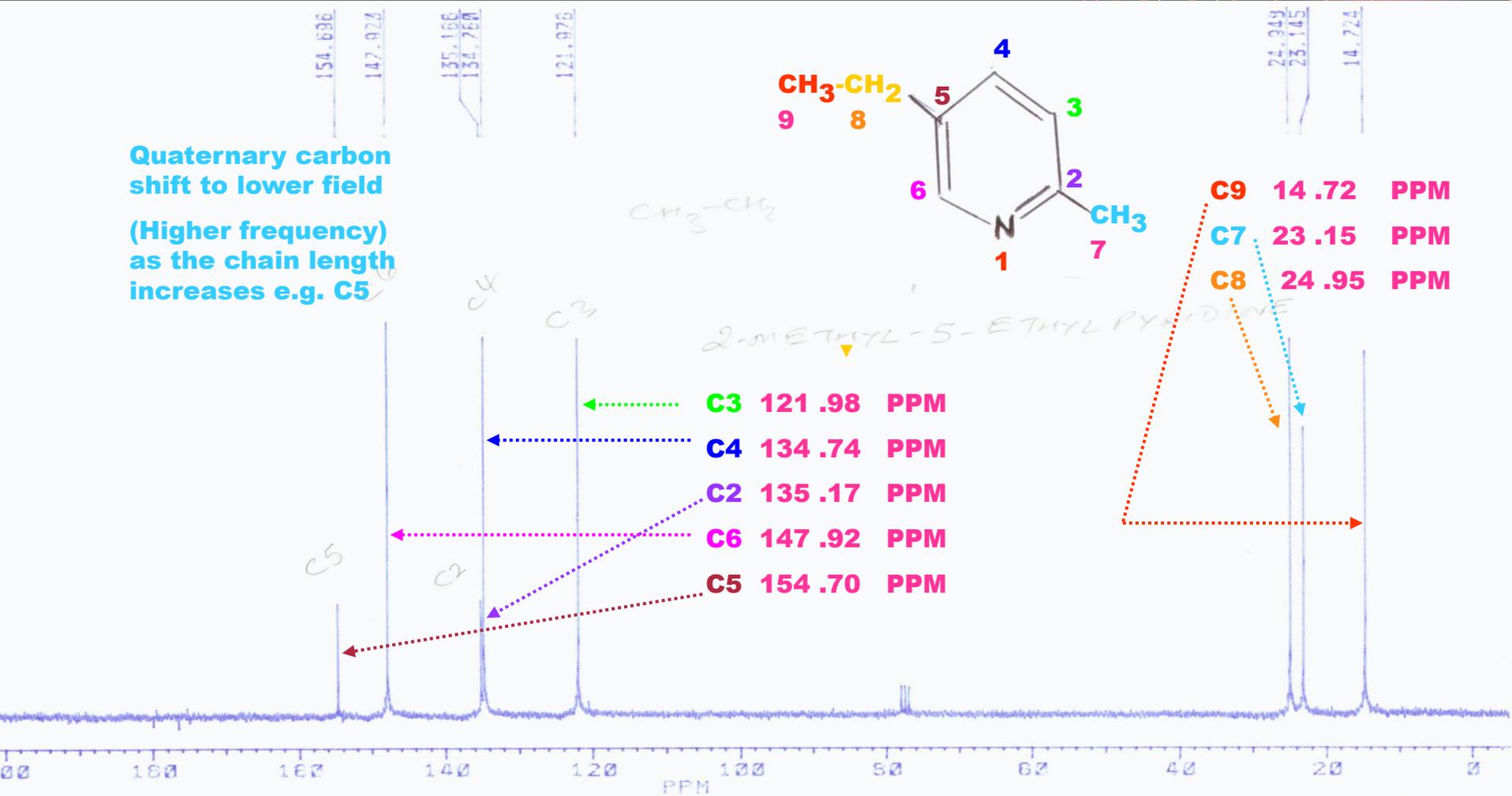
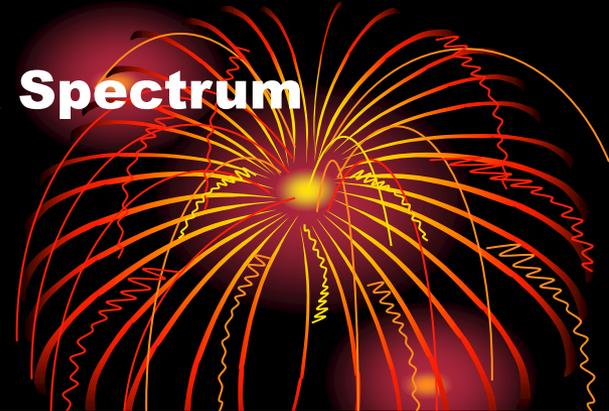
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 5-Ethyl-2-Methylpyridine



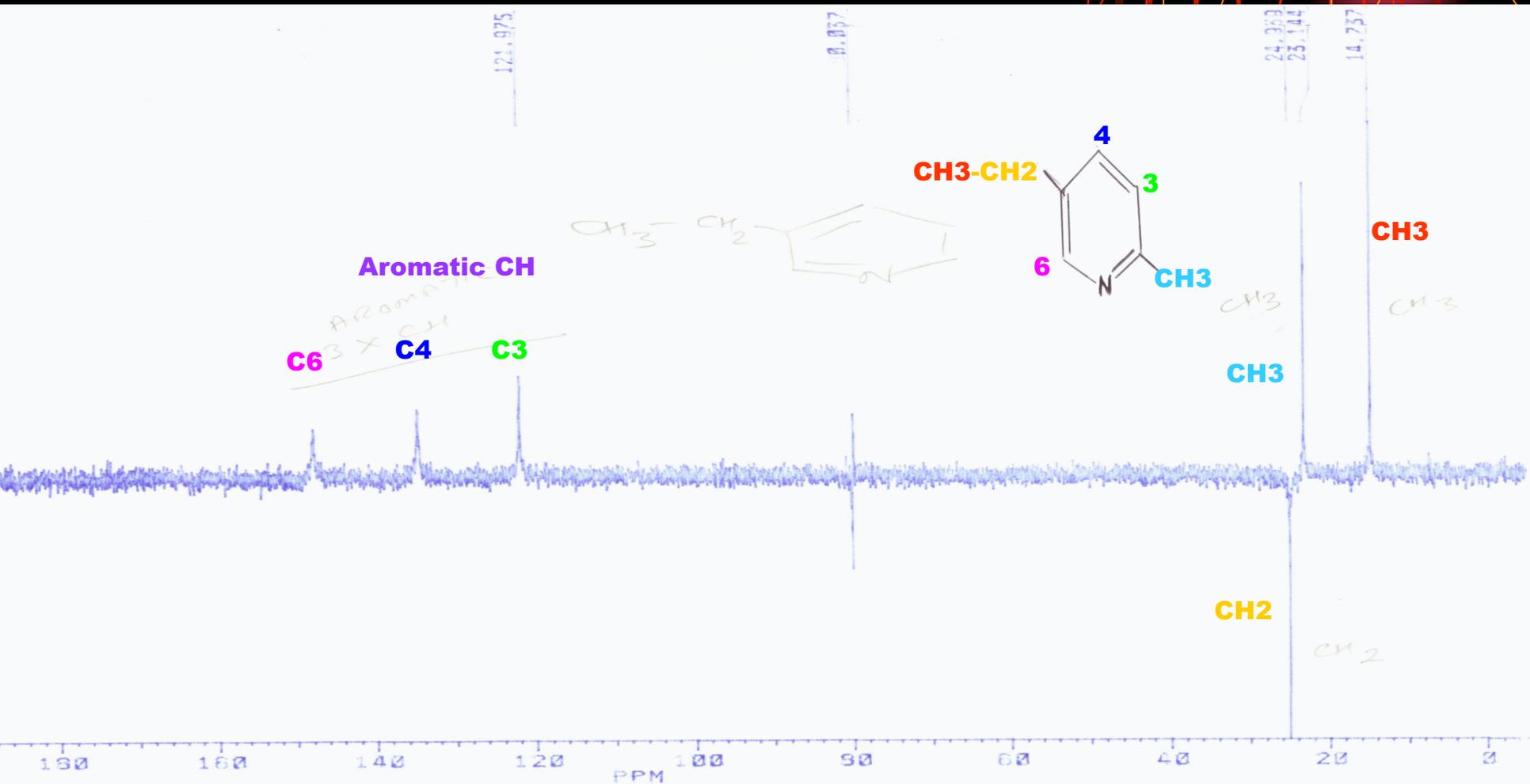
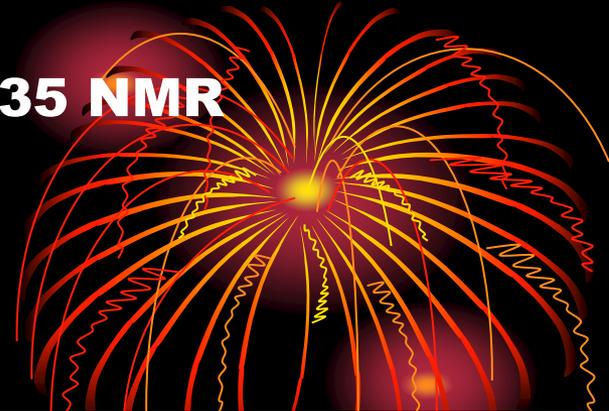
$\text{C}_5\text{H}_7\text{N}(\text{CH}_3)(\text{CH}_2\text{-CH}_3)$ Expansion of ^1H NMR Spectrum



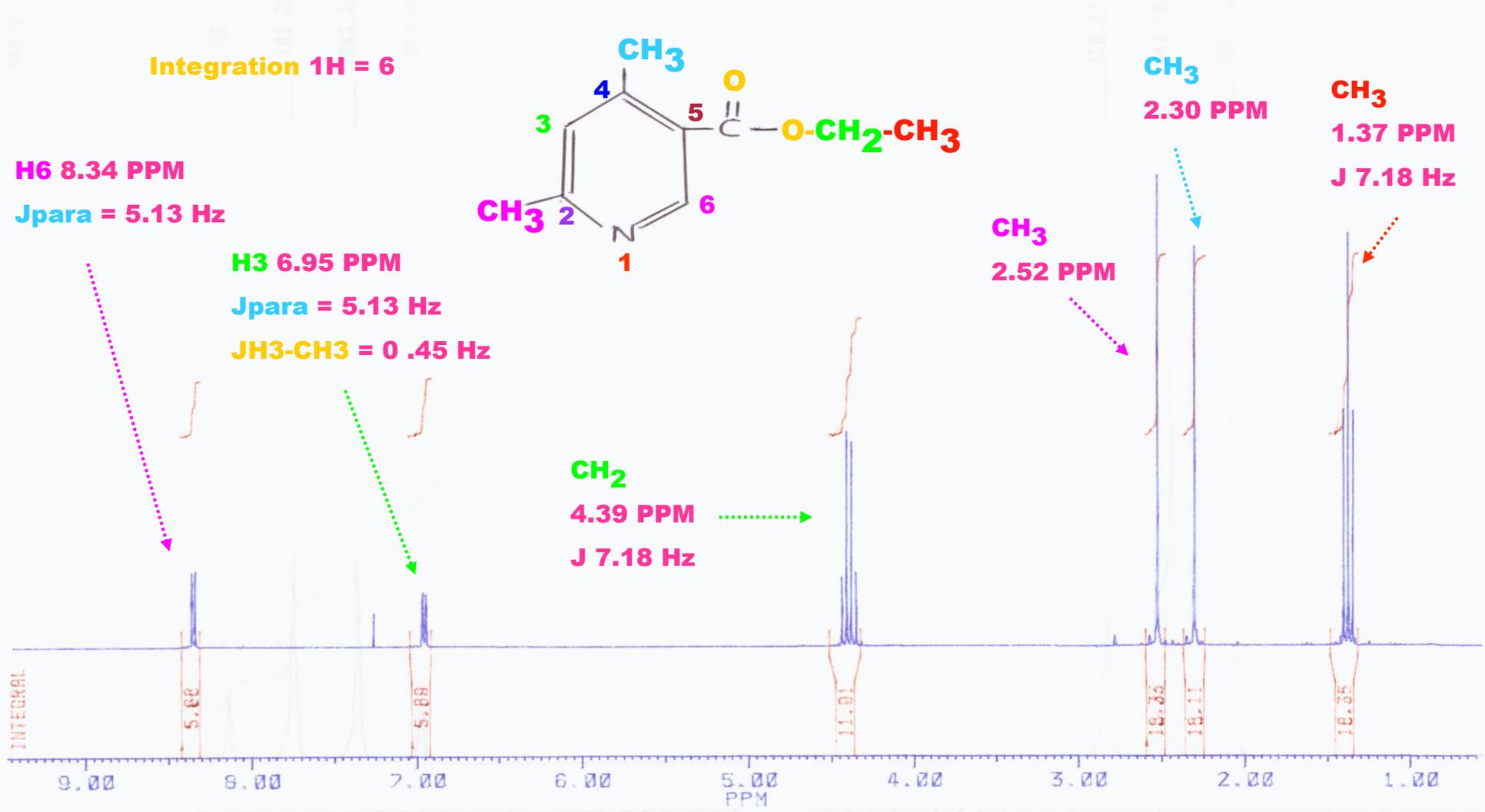
Analysis and interpretation of ^{13}C NMR Spectrum of 5-Ethyl-2-Methylpyridine



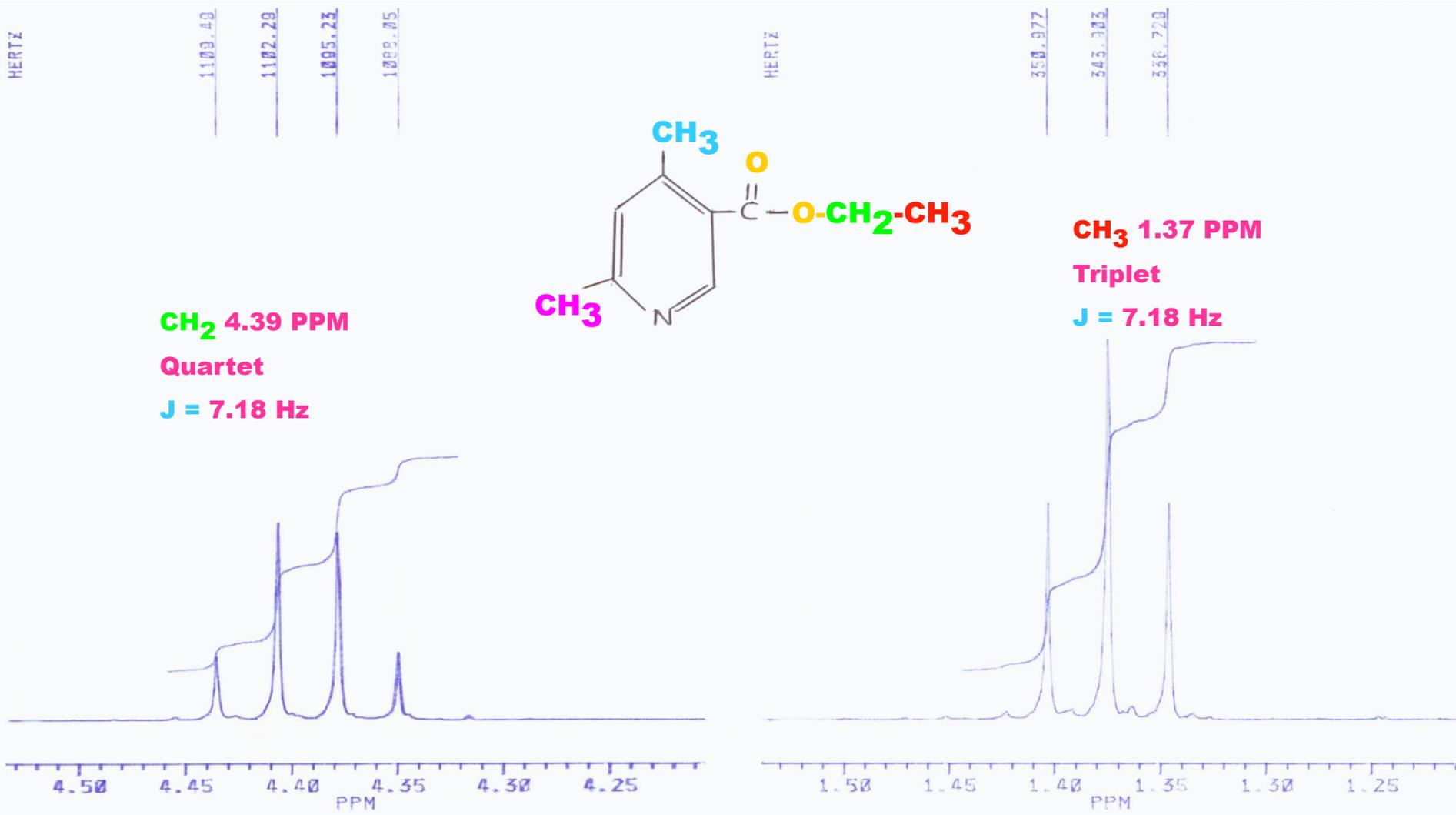
Analysis and interpretation ^{13}C DEPT 135 NMR Spectrum of 5-Ethyl-2-Methylpyridine



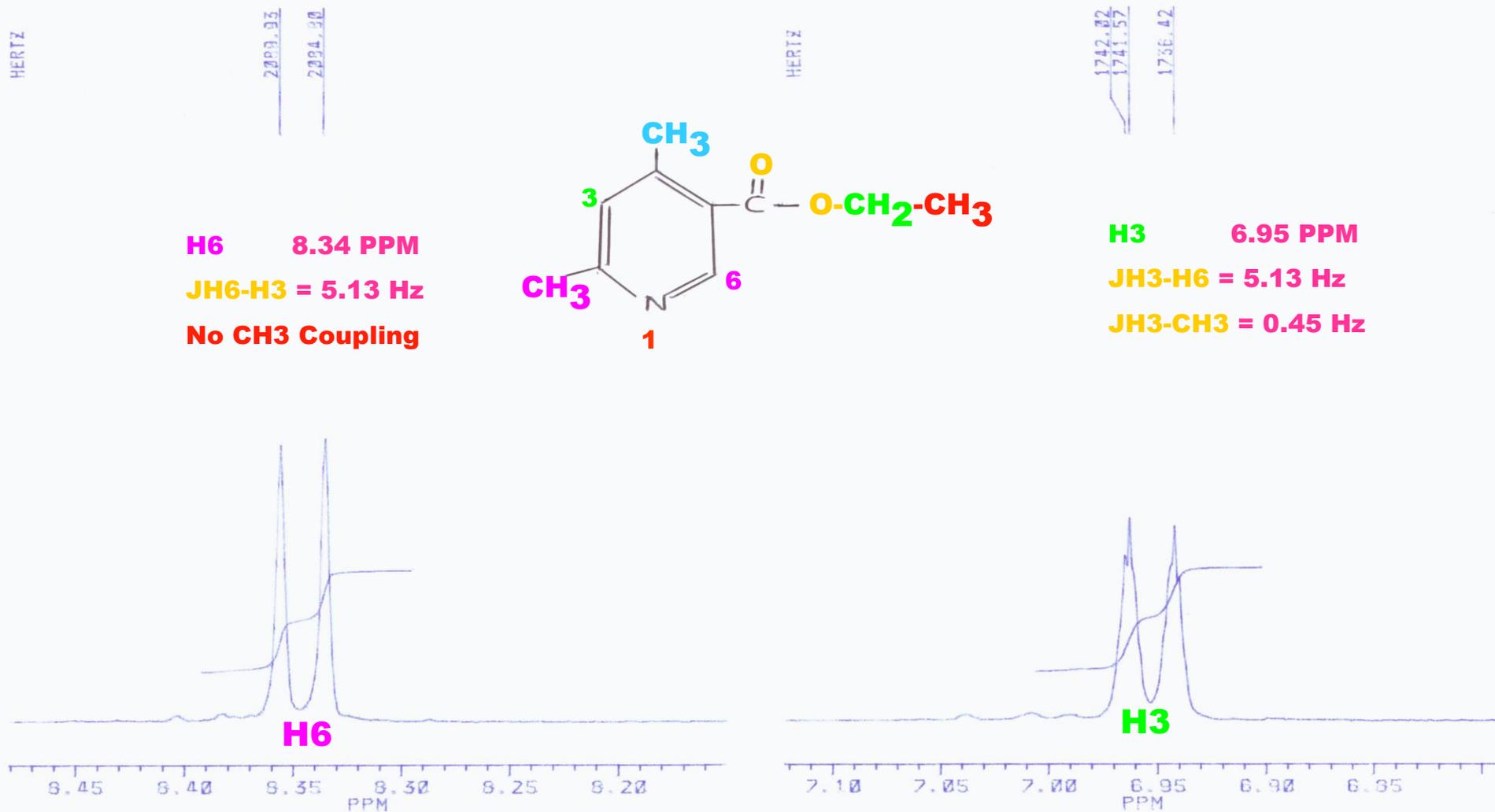
Analysis and Interpretation of ^1H NMR Spectrum of Ethyl-2,4-Dimethylnicotinate



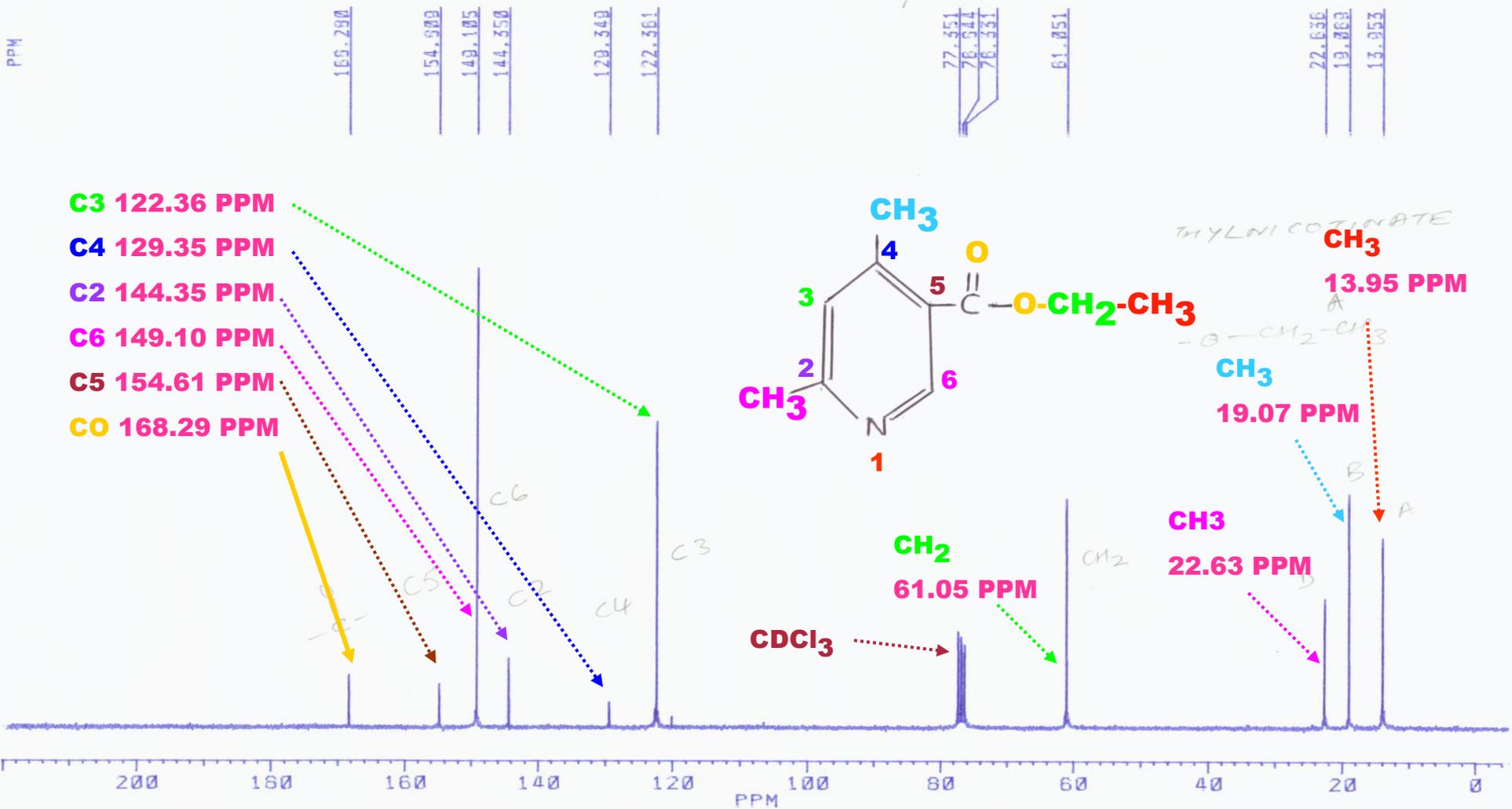
Analysis and Interpretation of ^1H NMR Spectrum of Ethyl-2,4-Dimethylnicotinate



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



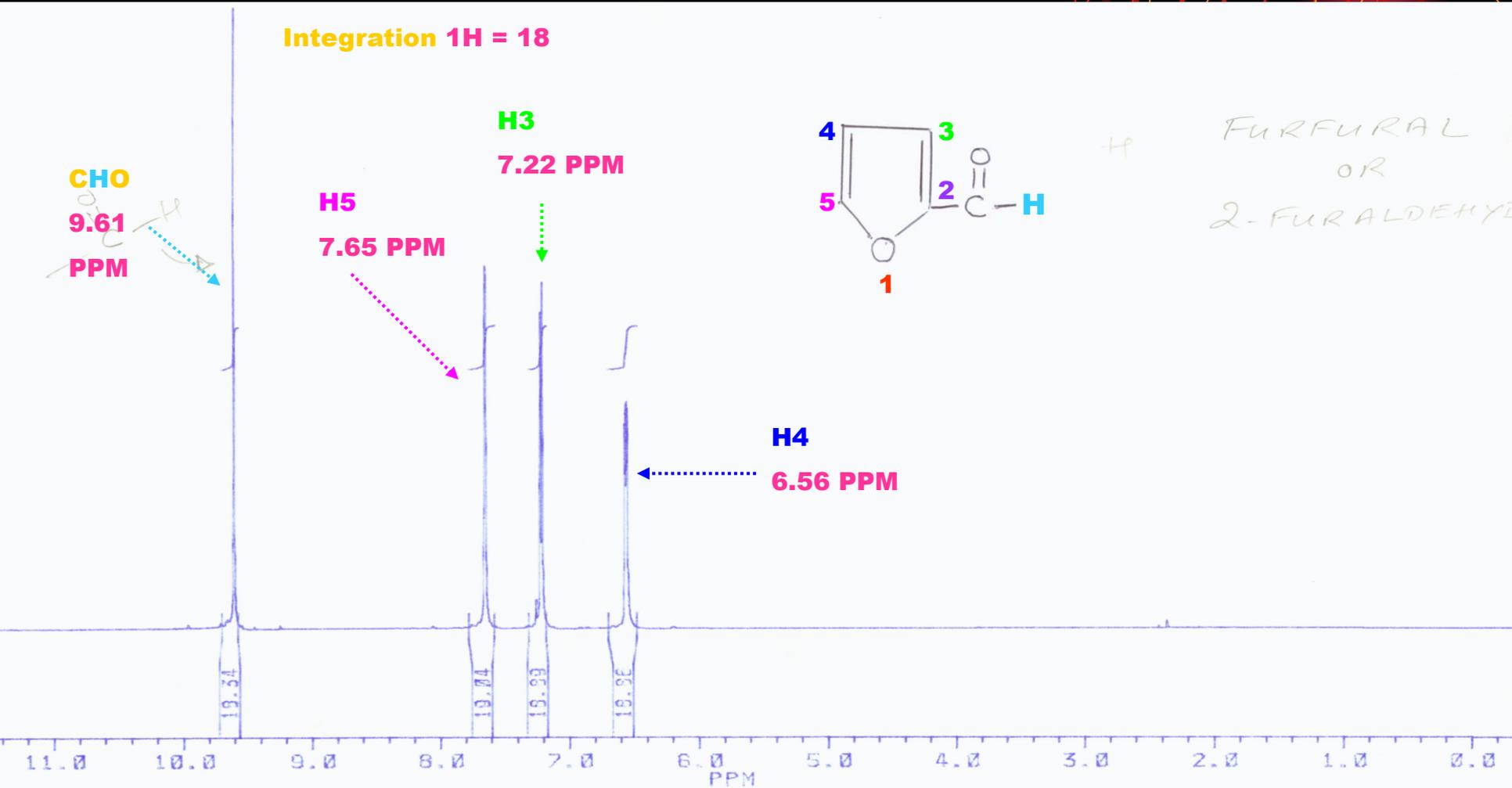
Analysis and Interpretation of ^{13}C NMR Spectrum of Ethyl-2,4-Dimethylnicotinate



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



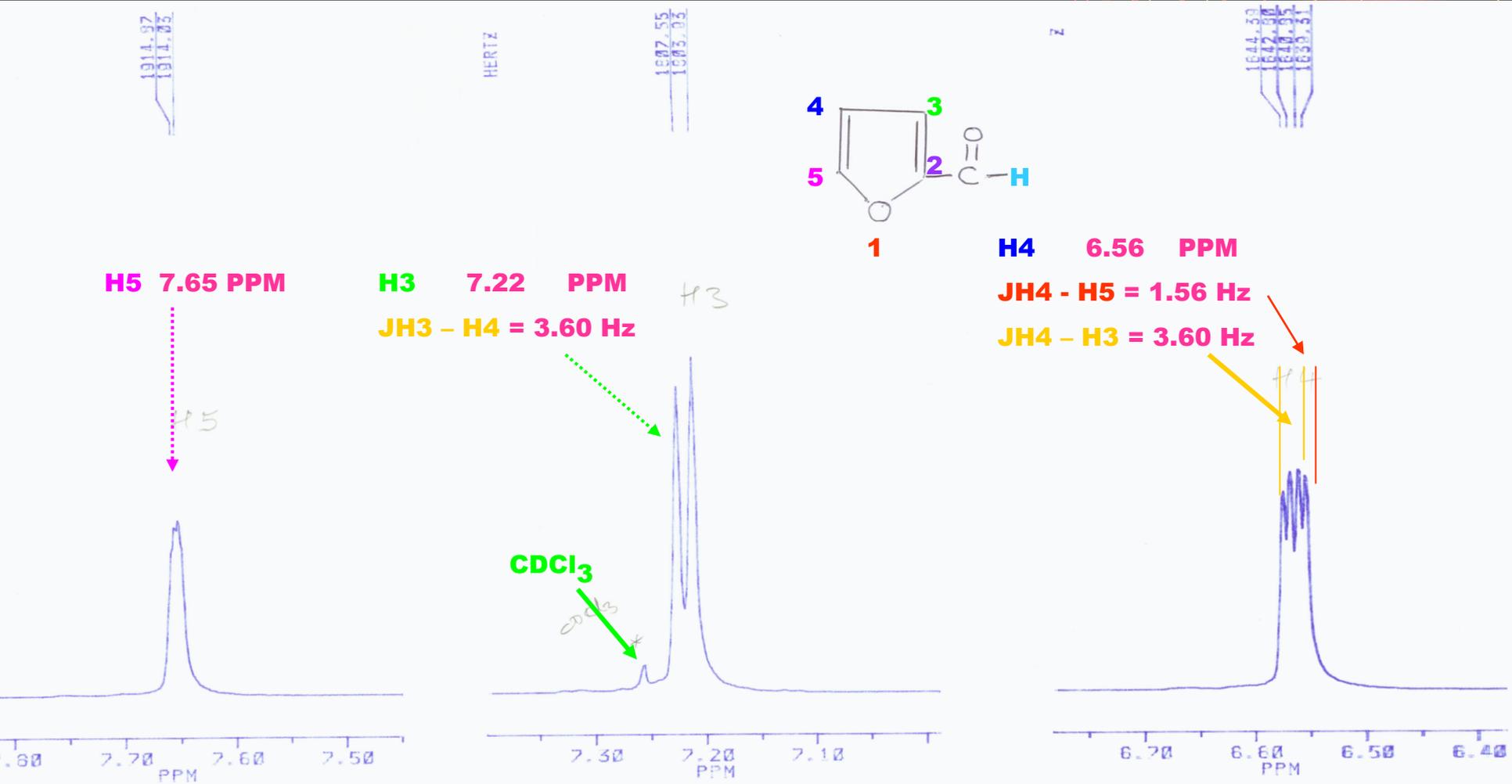
$\text{C}_4\text{H}_3\text{O}-\text{CHO}$ ^1H NMR Spectrum



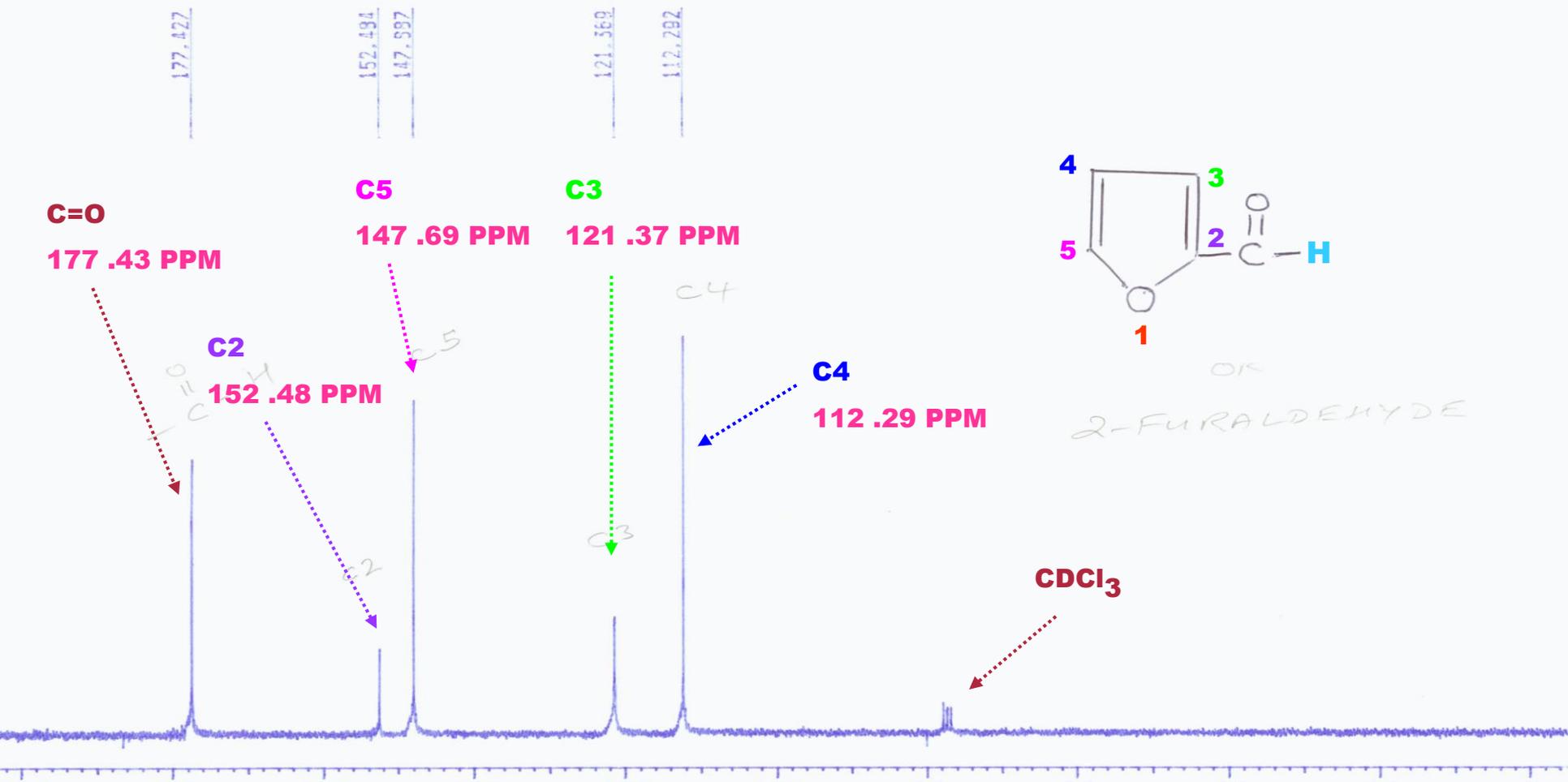
Analysis and interpretation of ^1H & ^{13}C NMR Spectra of Furfural (2-Furaldehyde)



$\text{C}_4\text{H}_3\text{O}-\text{CHO}$ Expansion of ^1H NMR Spectrum



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

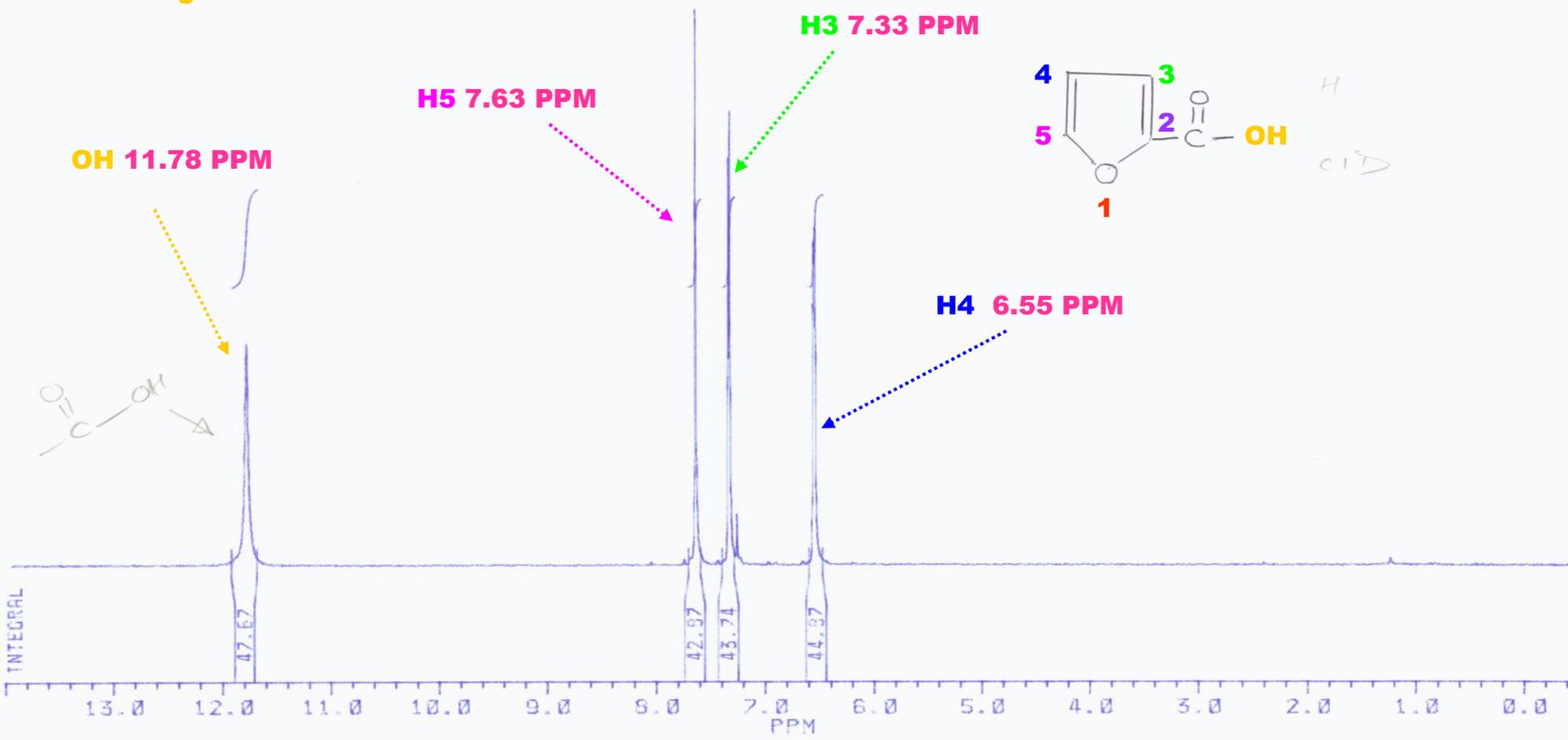


Analysis and interpretation of ^1H & ^{13}C NMR Spectra of 2-Furoic Acid



$\text{C}_4\text{H}_3\text{O}(\text{CO-OH})$ ^1H NMR Spectrum

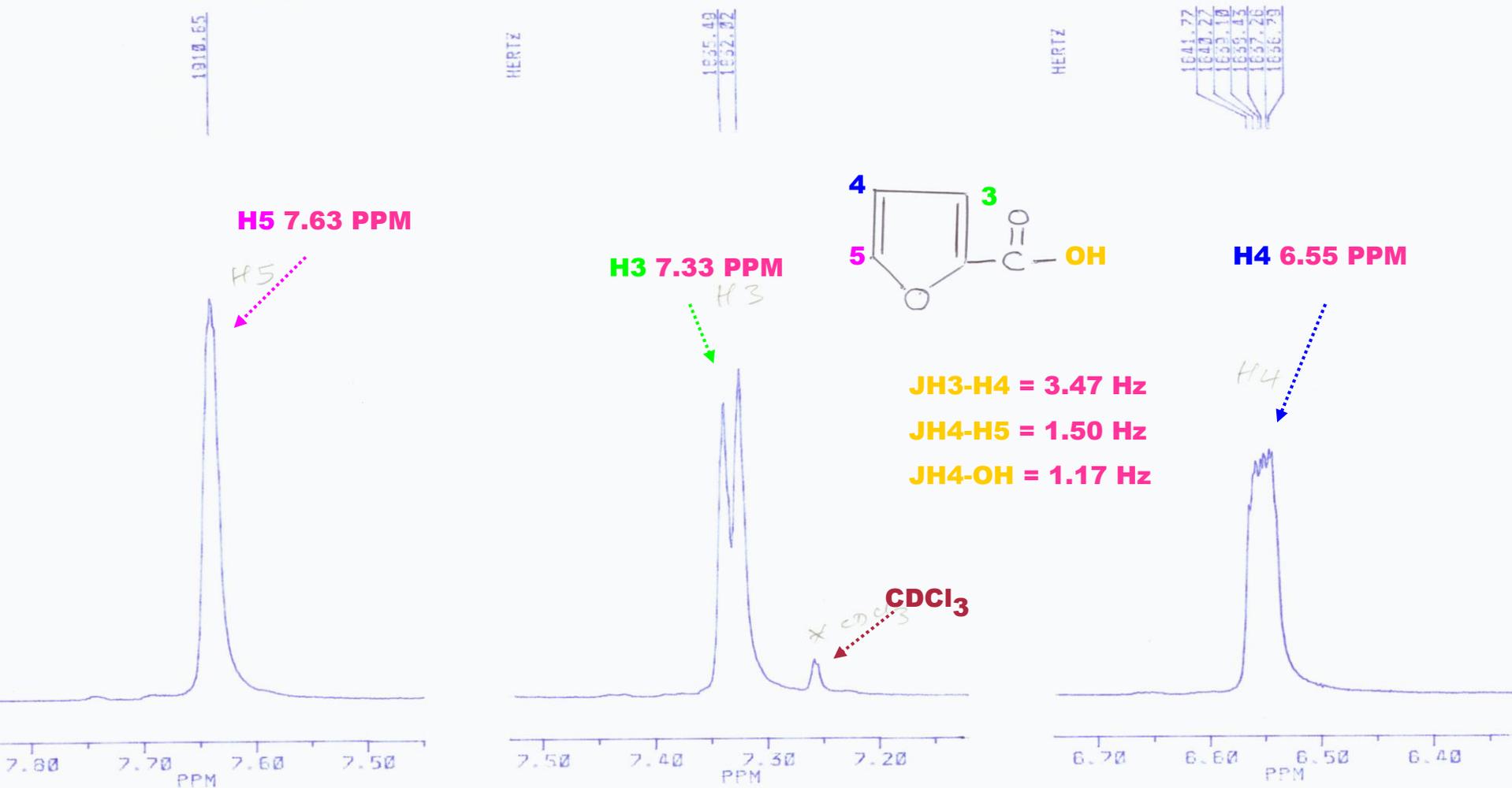
Integration $1\text{H} = 44$



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

$\text{C}_4\text{H}_3\text{O}(\text{CO-OH})$

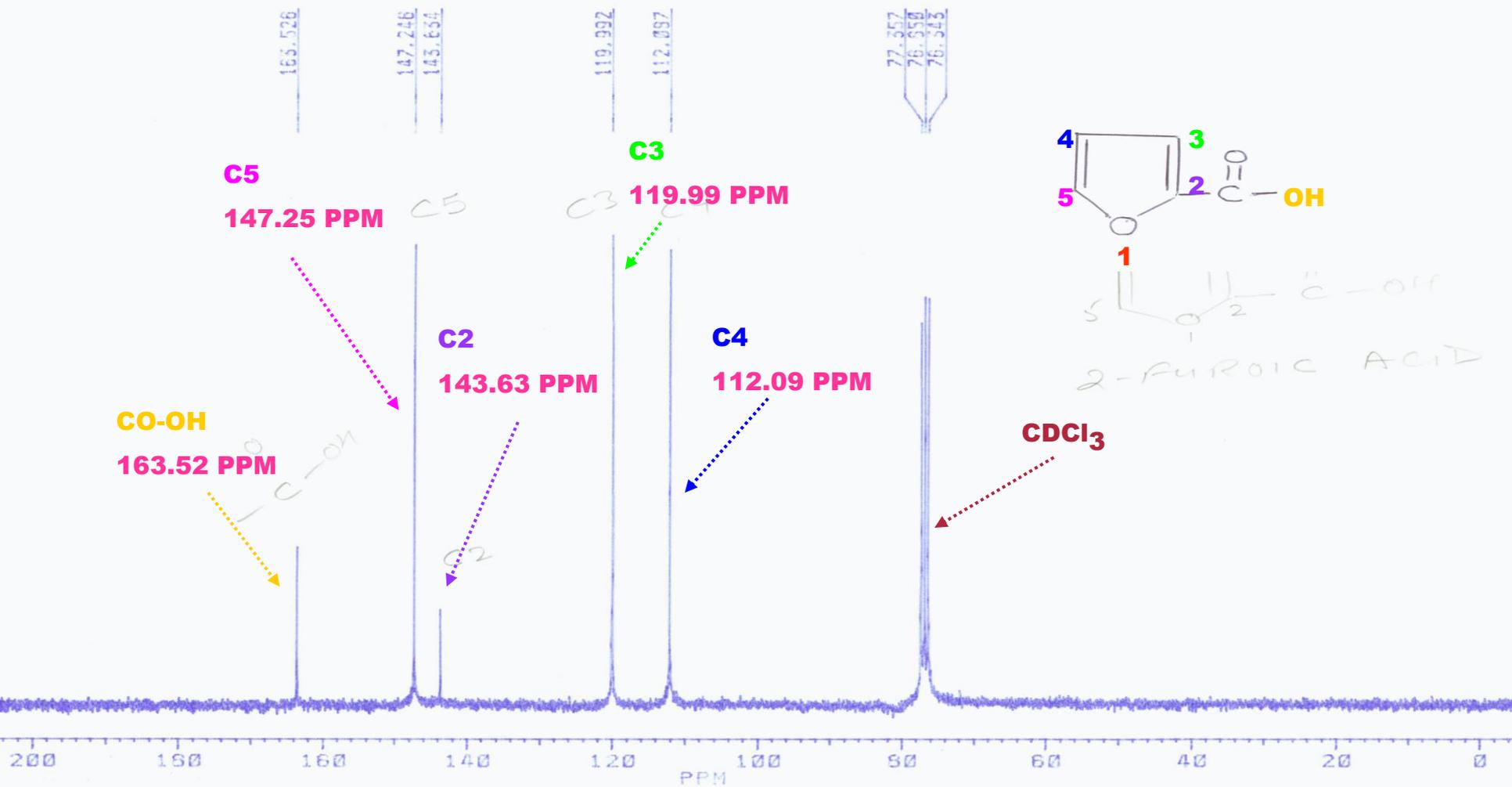
Expansion of ^1H NMR Spectrum



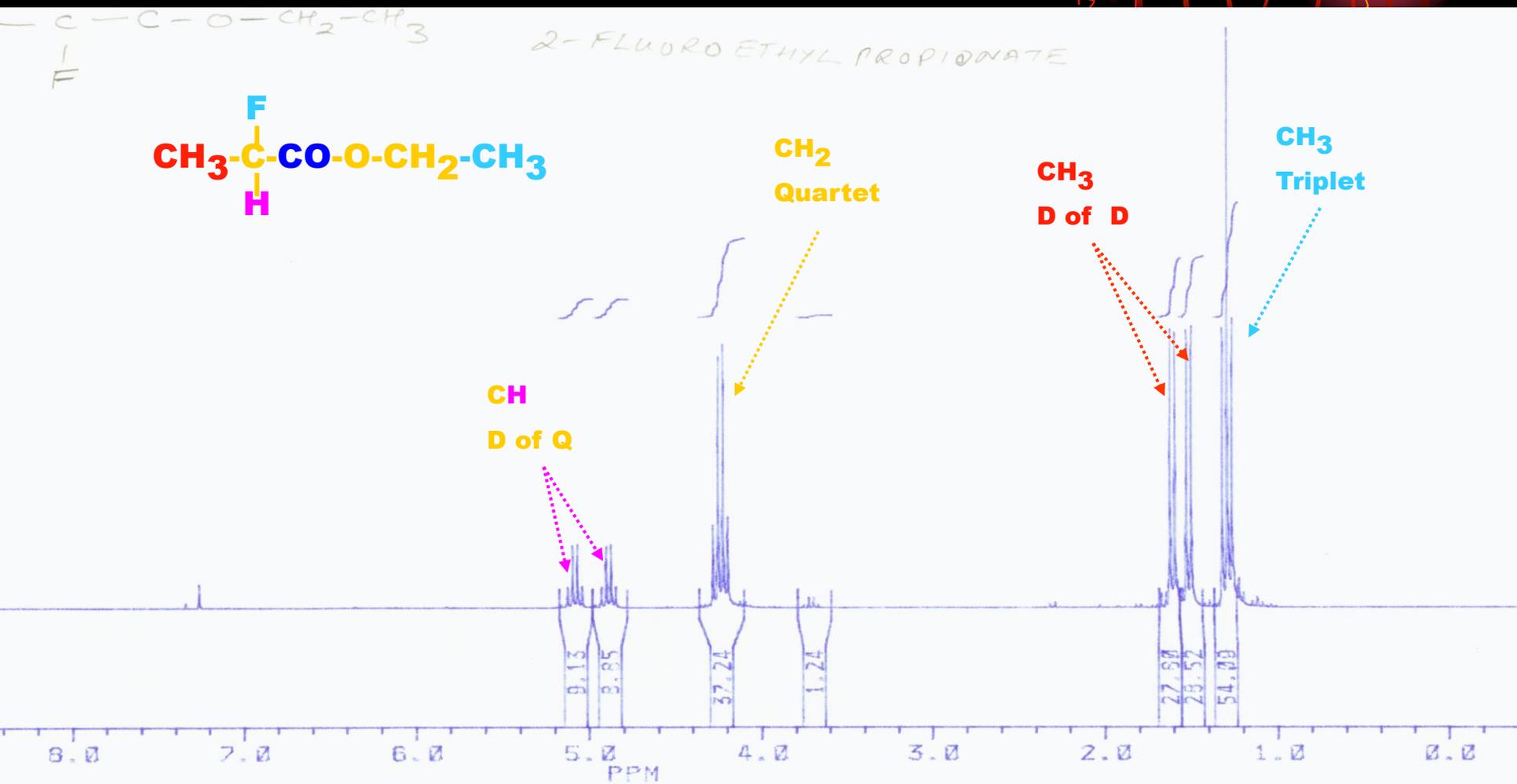
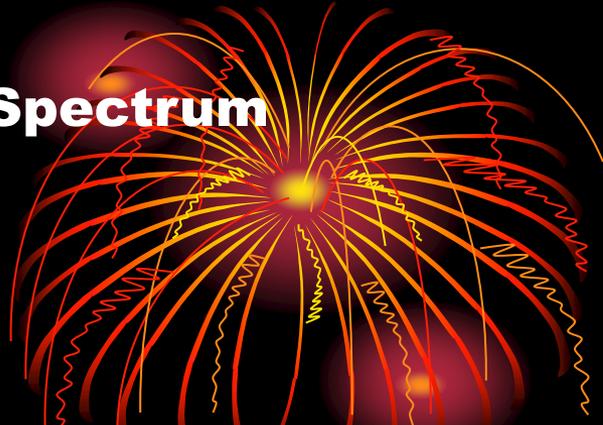
Analysis and interpretation of ^{13}C NMR Spectra of 2-Furoic Acid



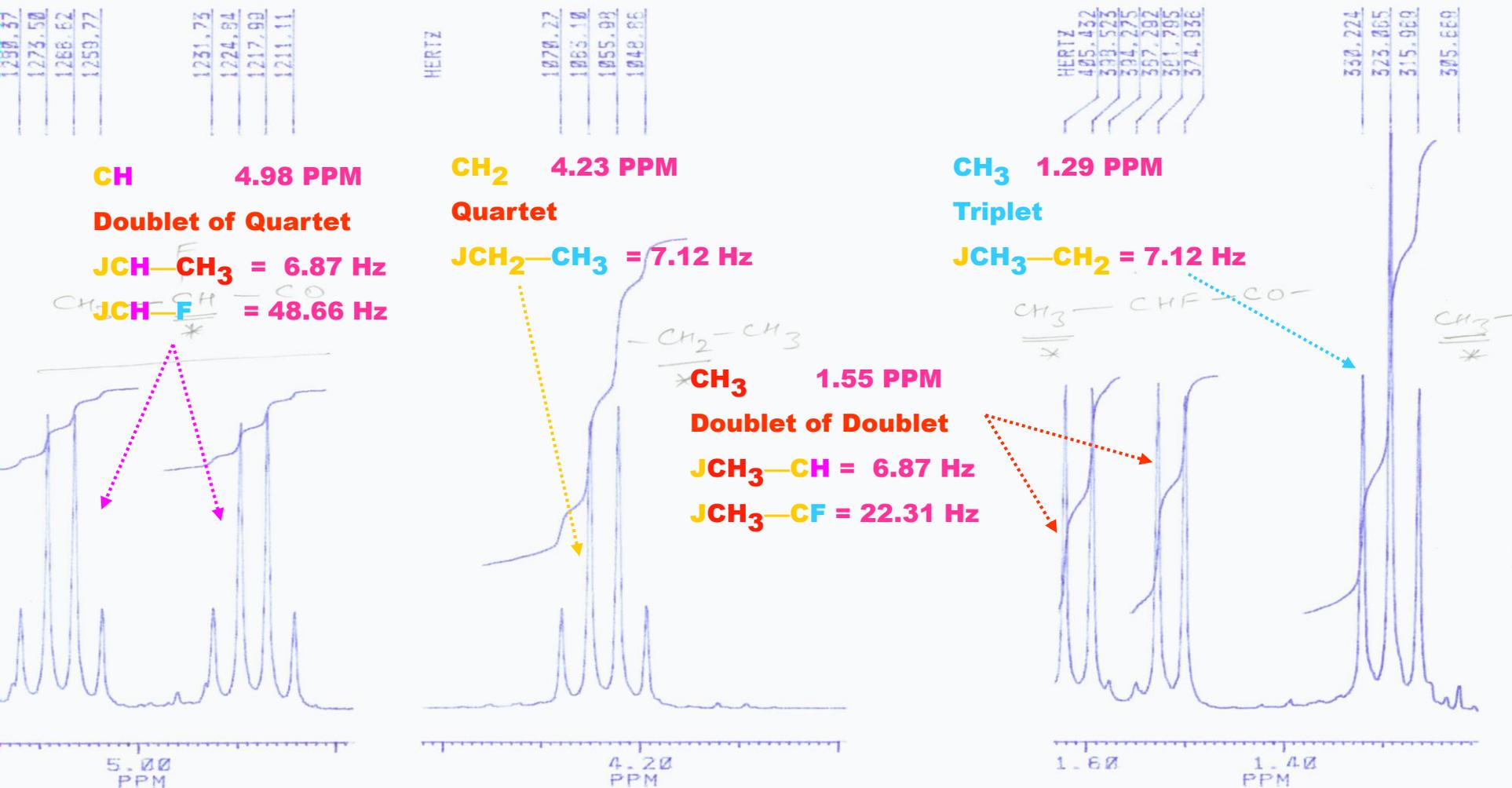
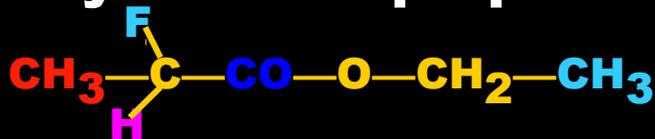
^{13}C NMR Spectrum



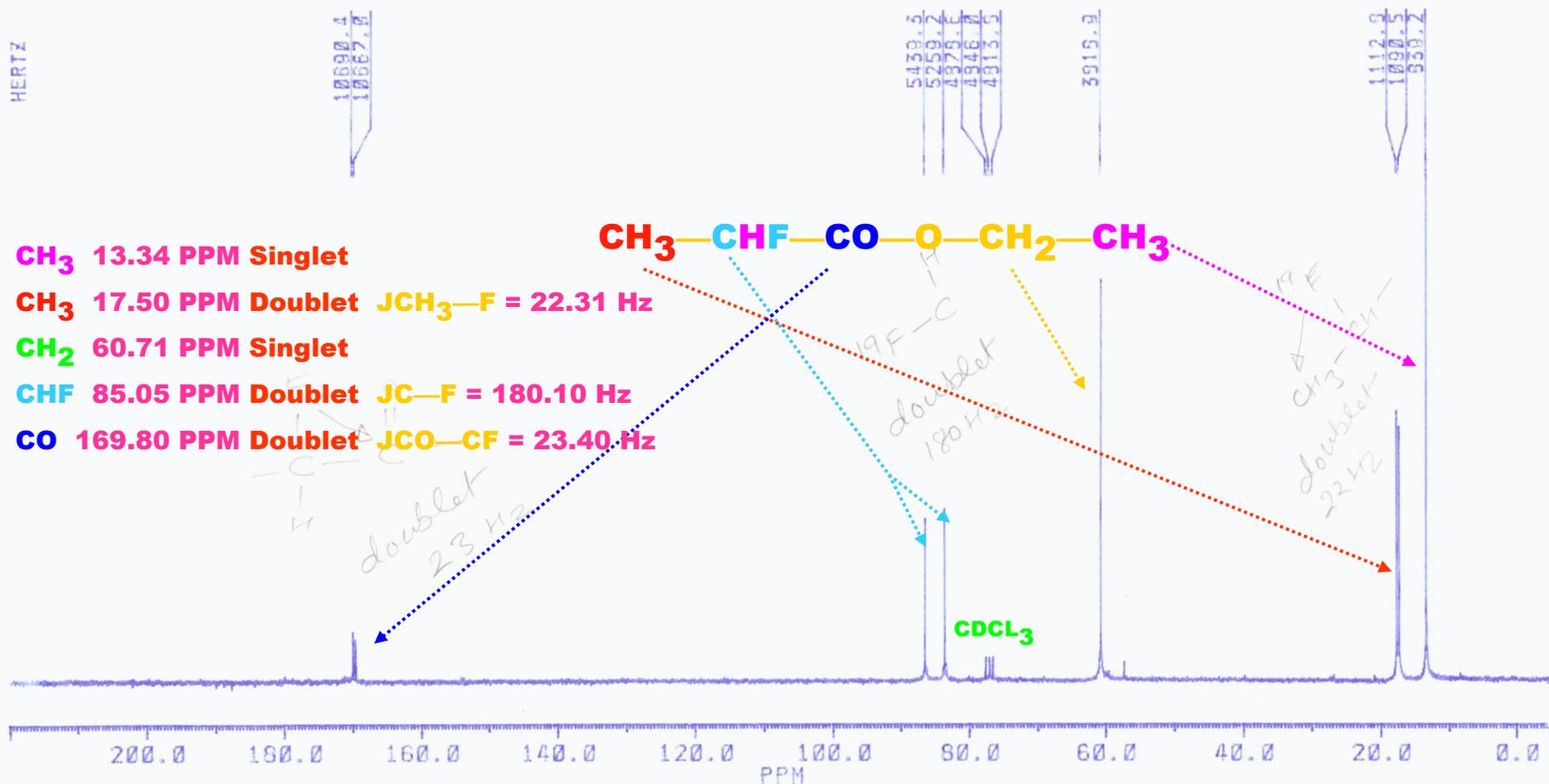
Analysis and Interpretation of ^1H NMR Spectrum of Ethyl-2-Fluoropropionate



Analysis and Interpretation of ^1H NMR Spectrum of Ethyl-2-Fluoropropionate $\text{CH}_3\text{-CHF-CO-O-CH}_2\text{CH}_3$



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



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

$\text{CH}_3\text{-CHF-CO-O-CH}_2\text{CH}_3$



10590.4
10567.0

^{19}F spin $I = \frac{1}{2}$

No. Peak = $2nI + 1$

= $n + 1$

= $1 + 1$

= 2 (Doublet)

Here $n=1$ F nucleus

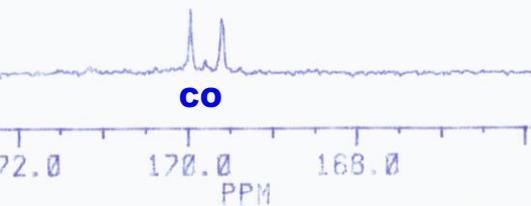
Hence all are doublets

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

CO—CF Doublet

169.80 PPM

$^2J = 23.40$ Hz



HERTZ

5439.34

5259.19

HERTZ

1112.79

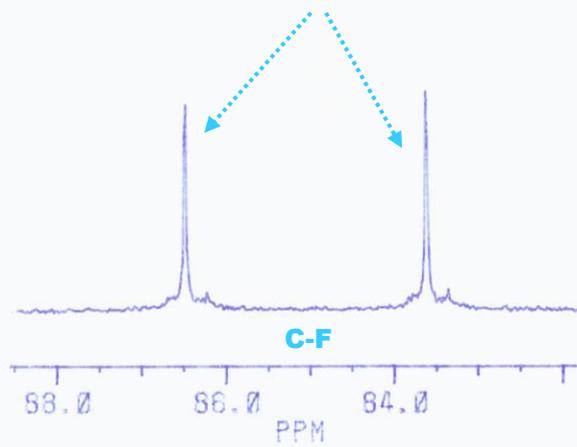
1092.47



C—F Doublet

85.05 PPM

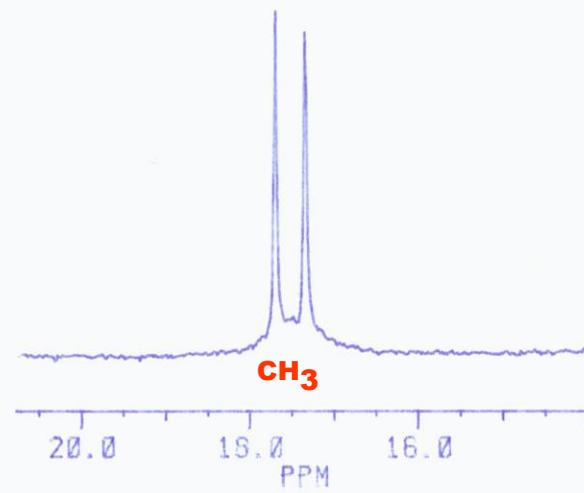
$^1J = 180.10$ Hz



CH₃—CF doublet

17.50 PPM

$^2J = 22.31$ Hz



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

$\text{CH}_3\text{-CHF-CO-O-CH}_2\text{CH}_3$



Quaternary
Carbon gives
no peak hence
CO no signal



CHF

CH₃

CH₃

CH₂

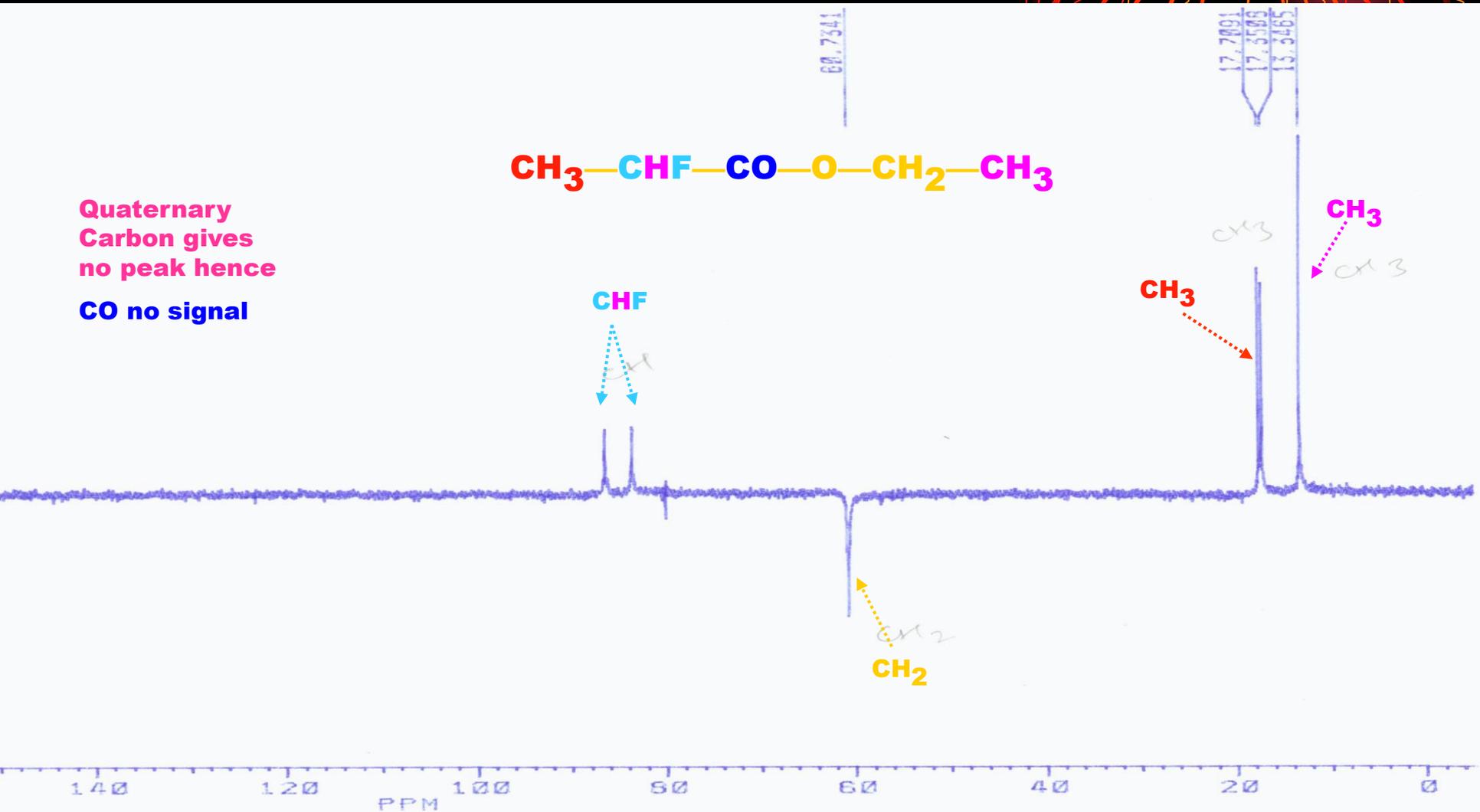
140 120 100 80 60 40 20 0 PPM

69.7341

17.7091

17.5569

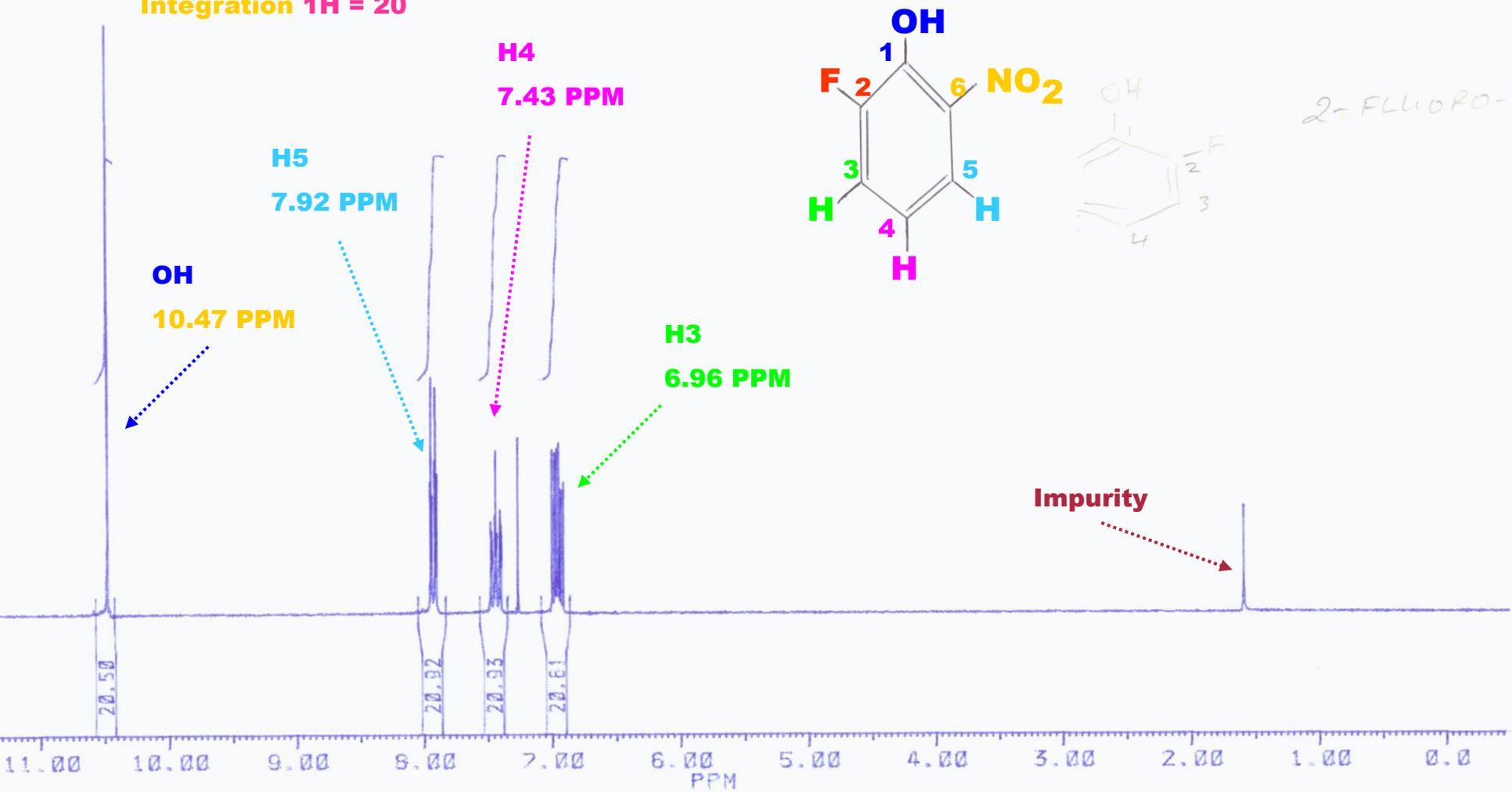
13.3465



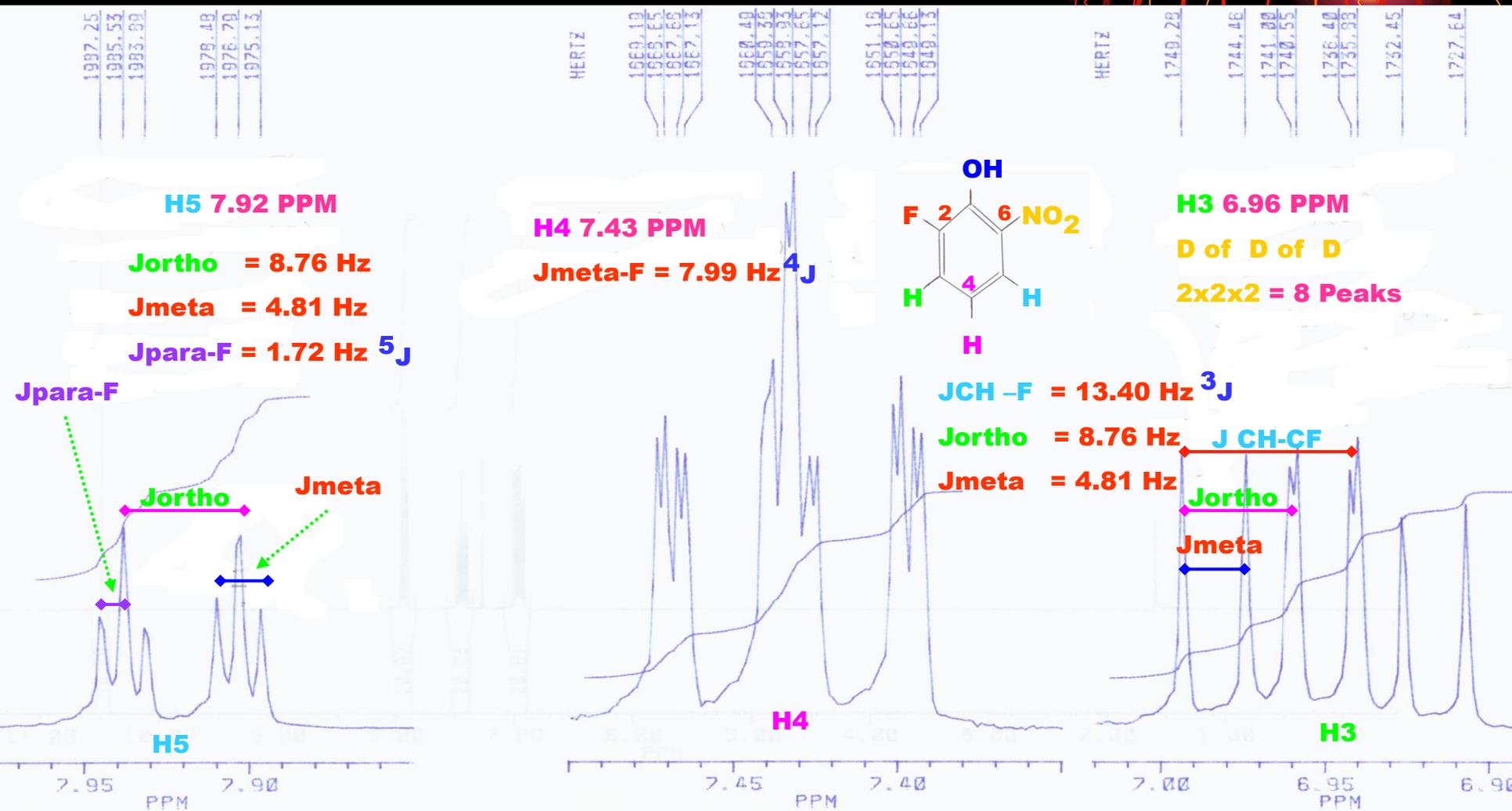
^1H NMR spectrum of 2-Fluoro-6-Nitrophenol



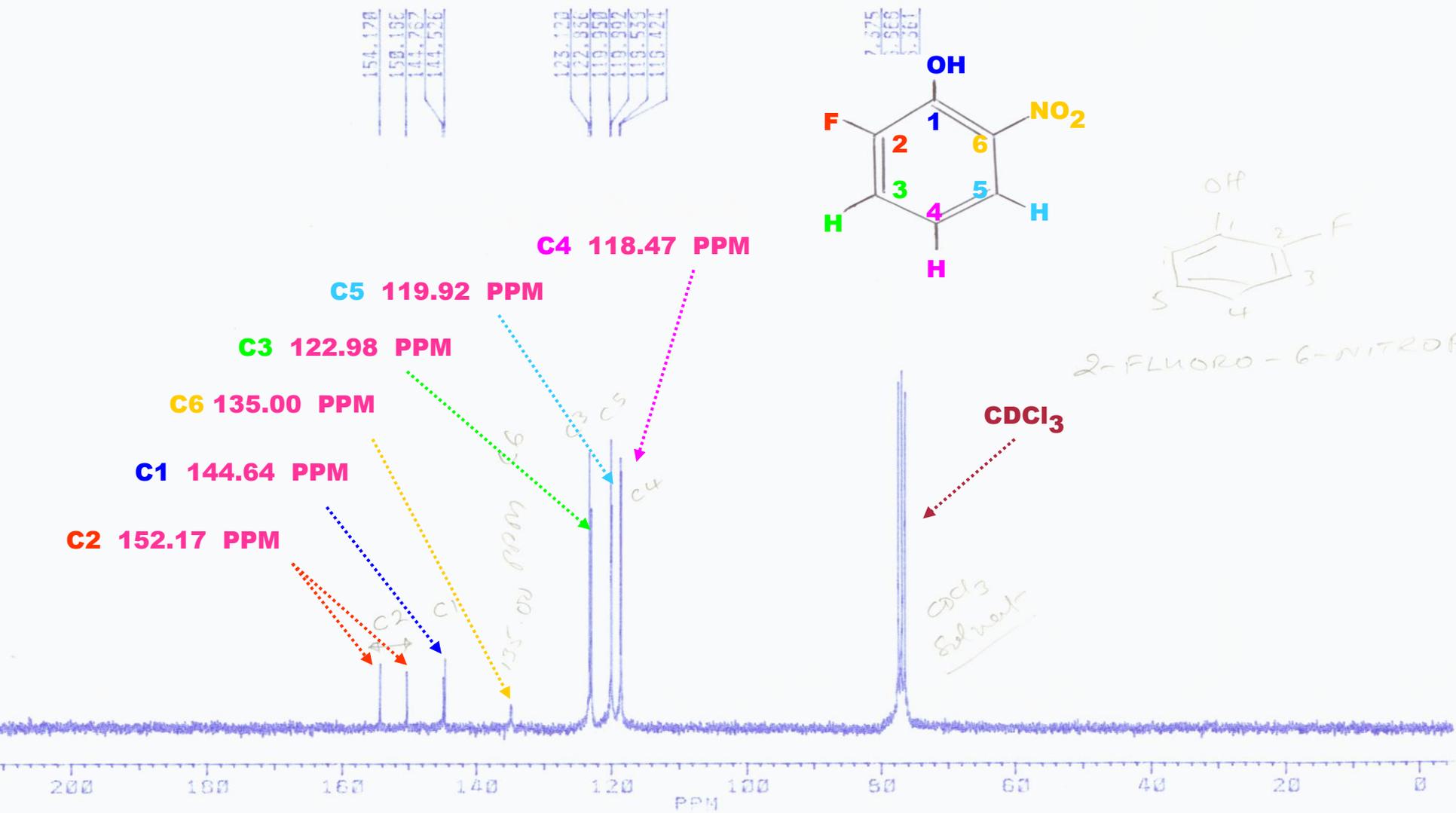
Integration 1H = 20



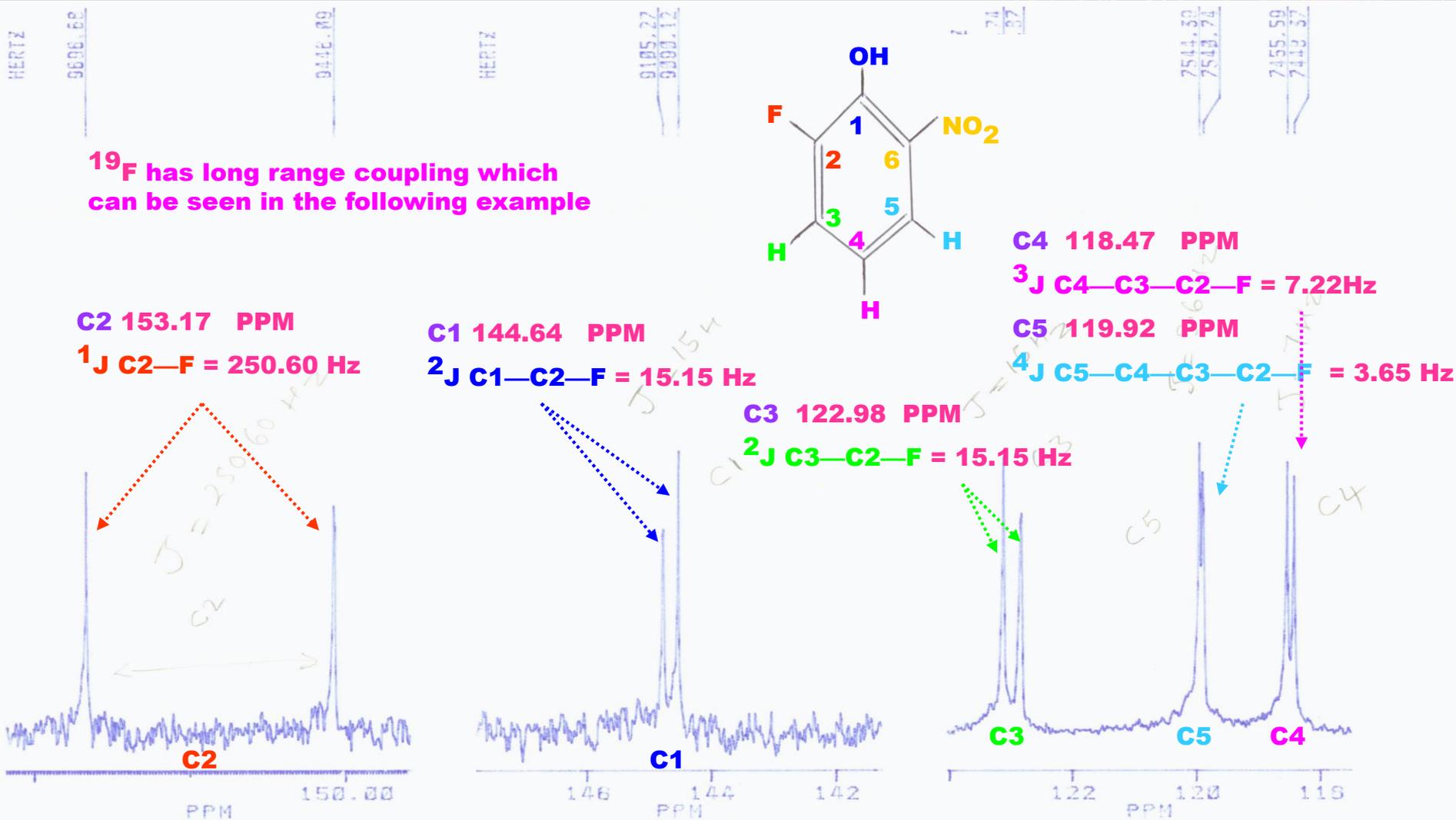
¹H NMR spectrum of 2-Fluoro-6-Nitrophenol



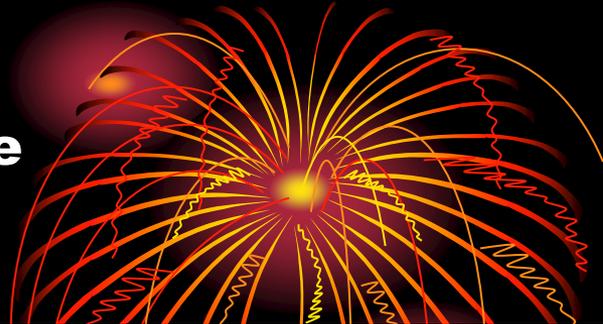
^{13}C NMR spectrum of 2-Fluoro-6-Nitrophenol



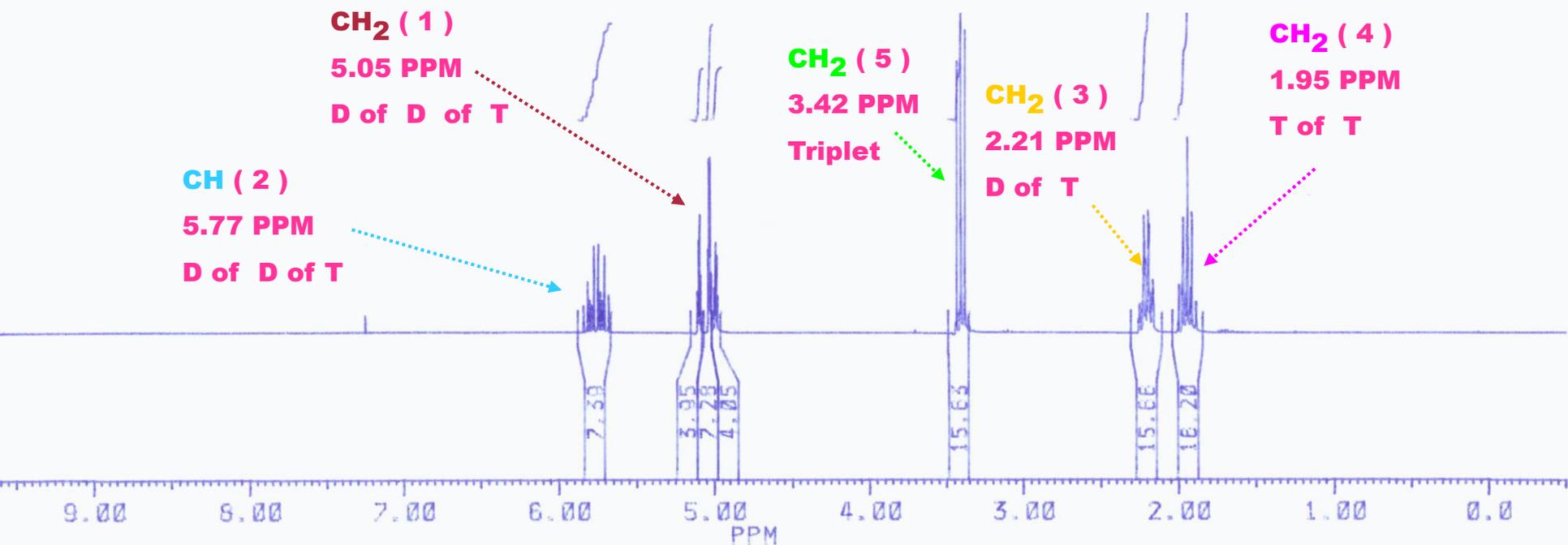
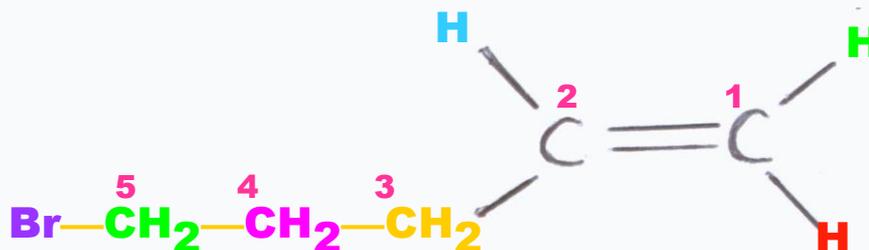
Expansion of ^{13}C NMR spectrum of 2-Fluoro-6-Nitrophenol



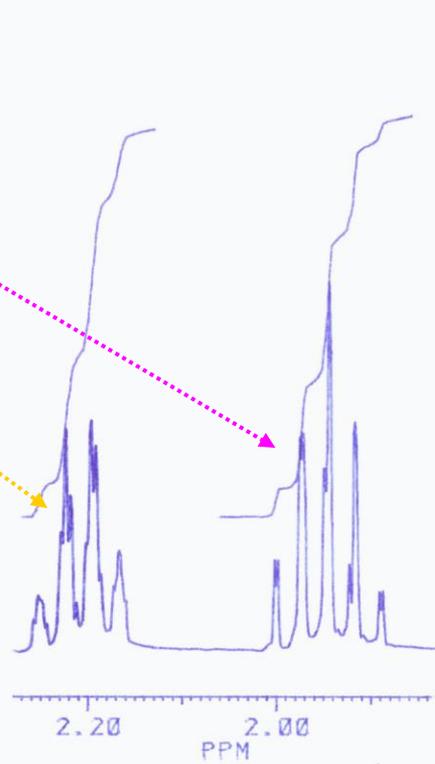
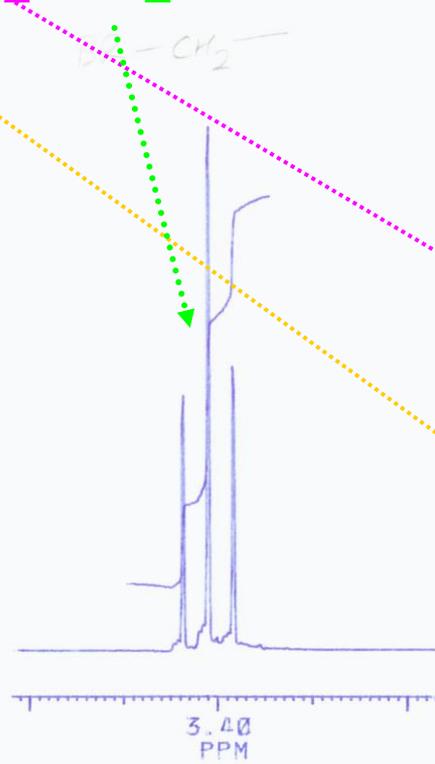
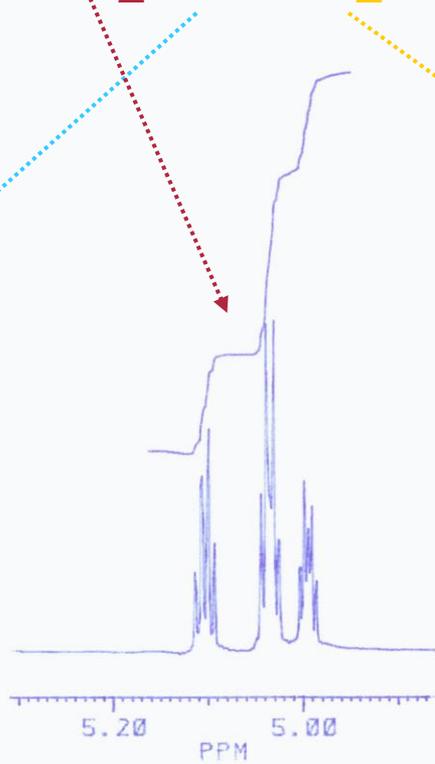
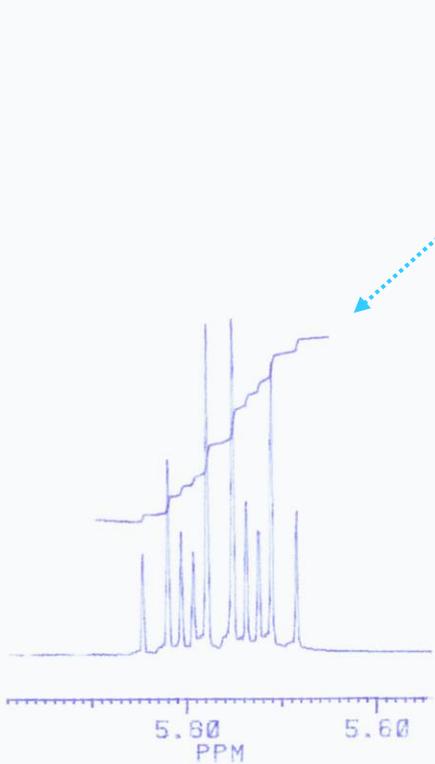
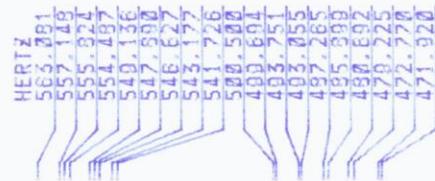
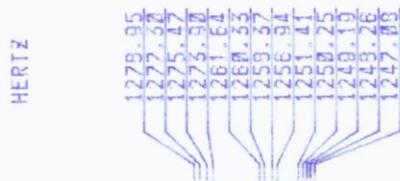
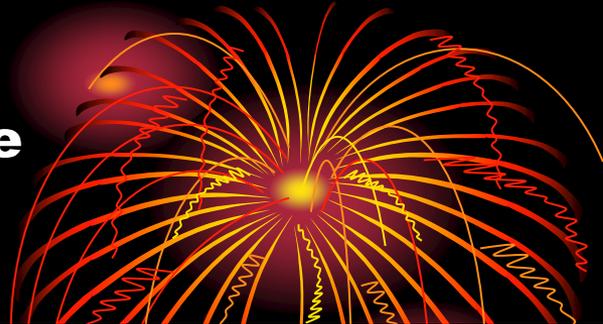
^1H NMR Spectrum of 5-Bromopent-1-ene $\text{Br-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH=CH}_2$



Integration 1H = 7.5

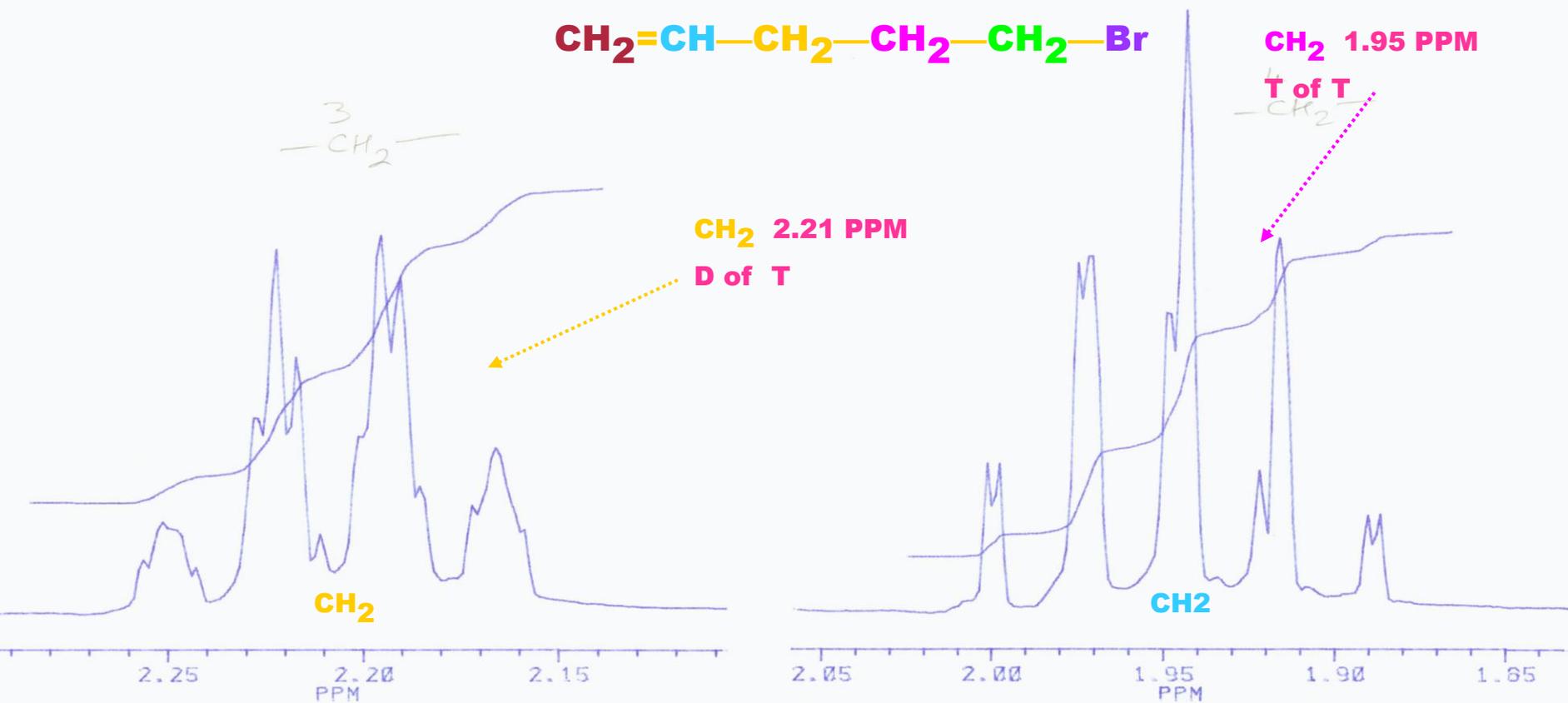
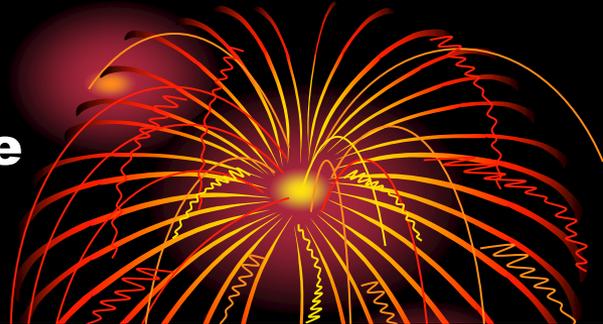


¹H NMR Spectrum of 5-Bromopent-1-ene Br-CH₂-CH₂-CH₂-CH=CH₂

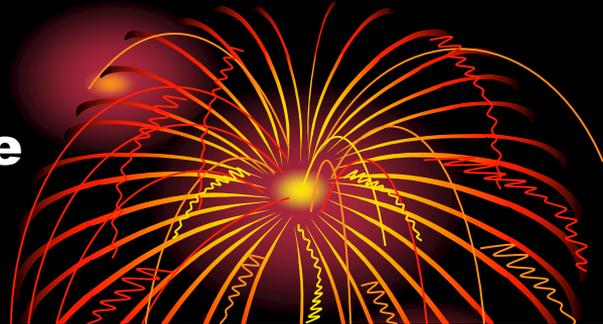


^1H NMR Spectrum of 5-Bromopent-1-ene

Br-CH2-CH2-CH2-CH=CH2



¹H NMR Spectrum of 5-Bromopent-1-ene Br-CH₂-CH₂-CH₂-CH=CH₂



HERTZ

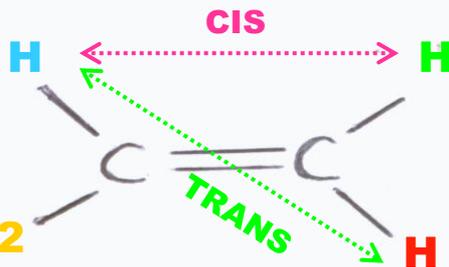


CH 5.77 PPM

D of D Of T

2 x 2 x 3 = 12

Handwritten: $2 \times 2 \times 3 = 12$
d x d x t

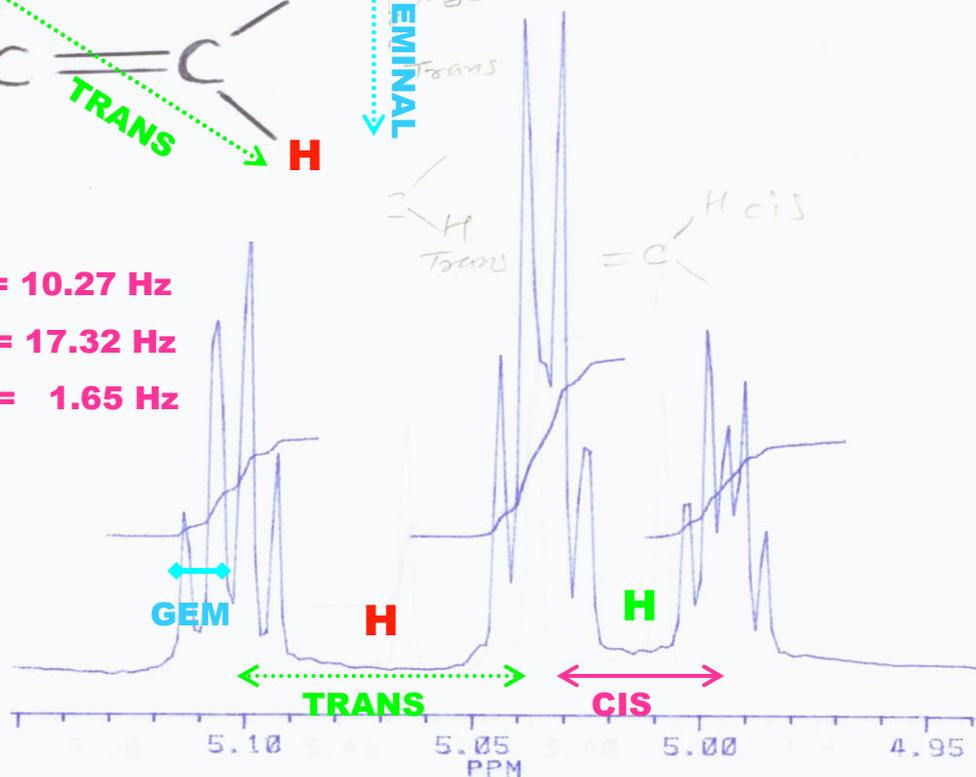
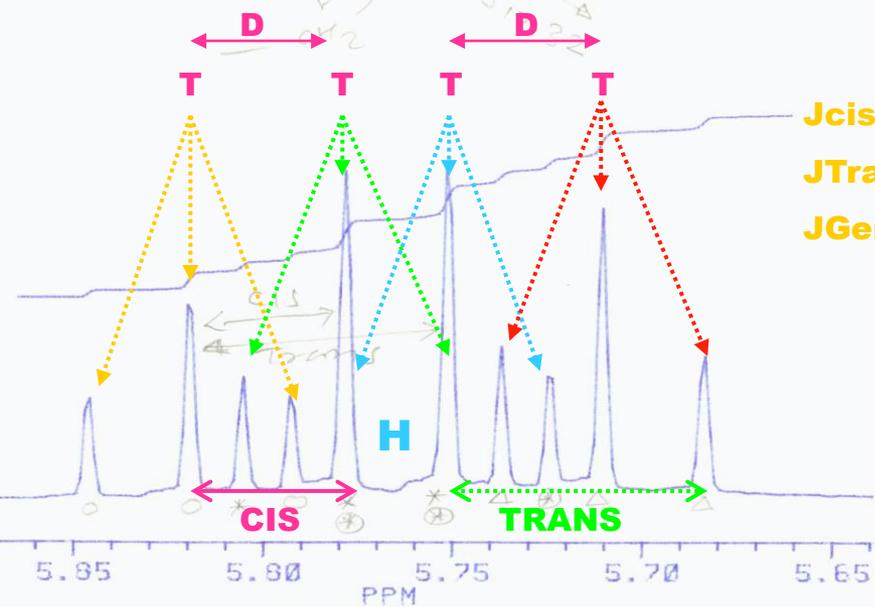


Handwritten: H cis
GEMINAL
Trans

J_{cis} = 10.27 Hz

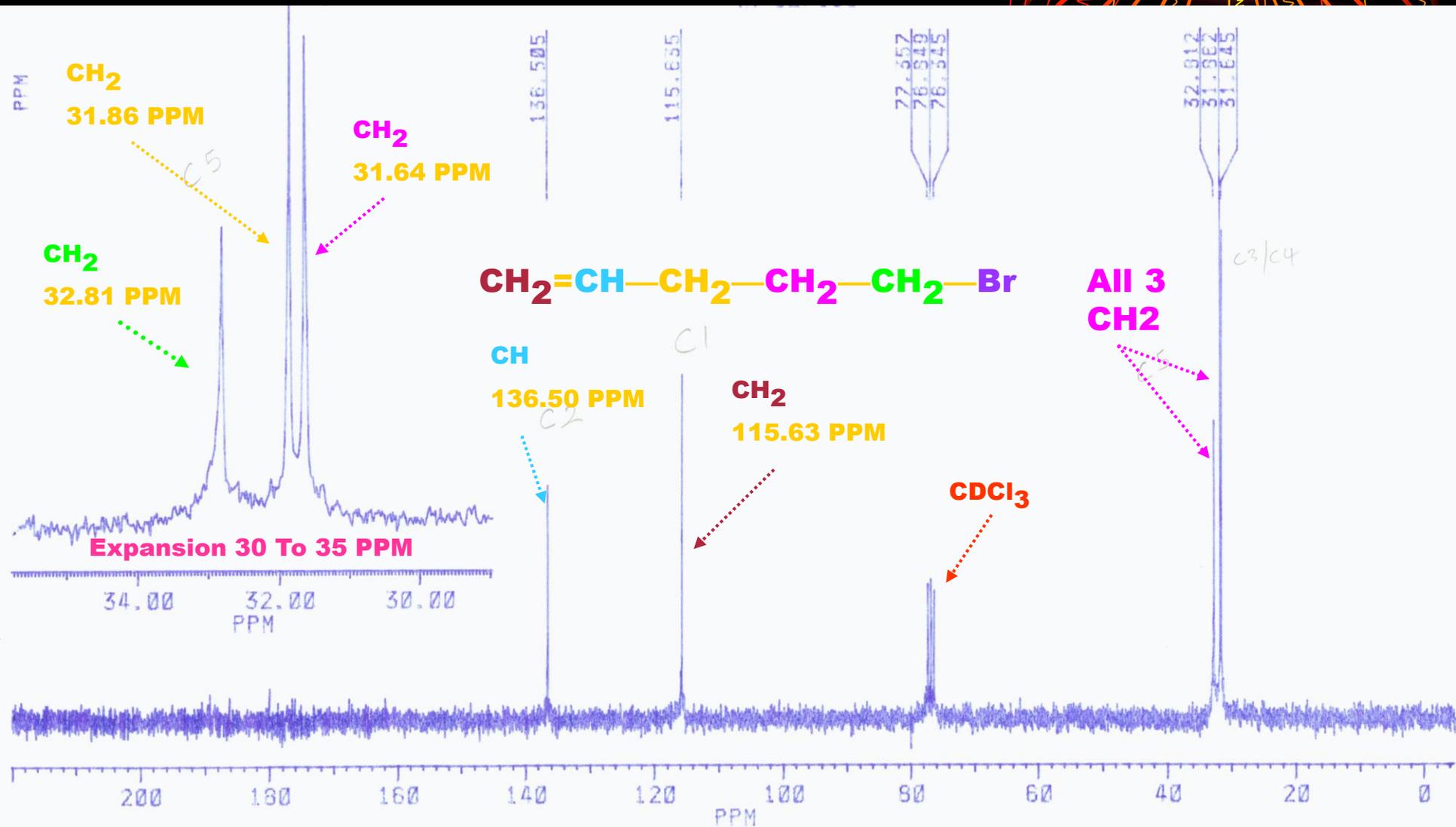
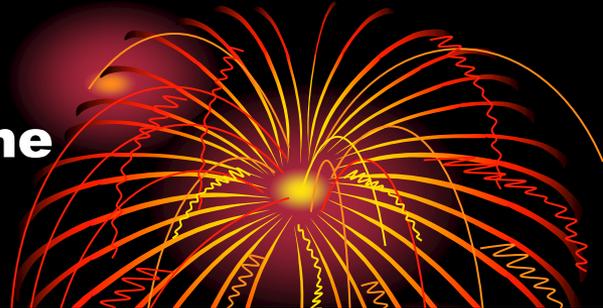
J_{Trans} = 17.32 Hz

J_{Gem} = 1.65 Hz



¹³C NMR Spectrum of 5-Bromopent-1-ene

Br-CH2-CH2-CH2-CH=CH2



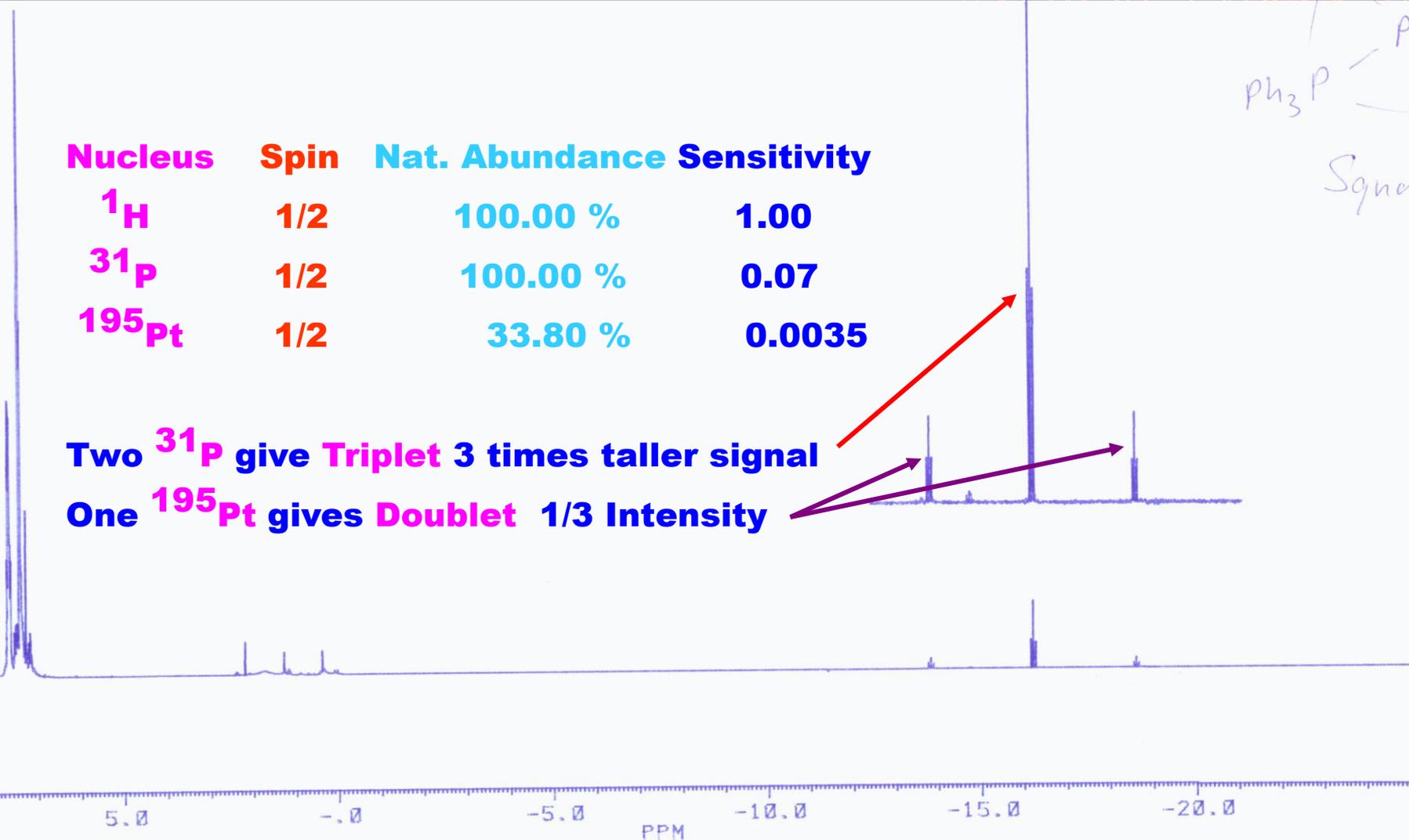
^1H NMR Spectrum of $[(\text{C}_6\text{H}_5)_3\text{P}]_2\text{PtHCl}$ in CDCl_3 DiPhosphine Platinum Hydrochloride Complex + 10.00 to -25.00 PPM Range



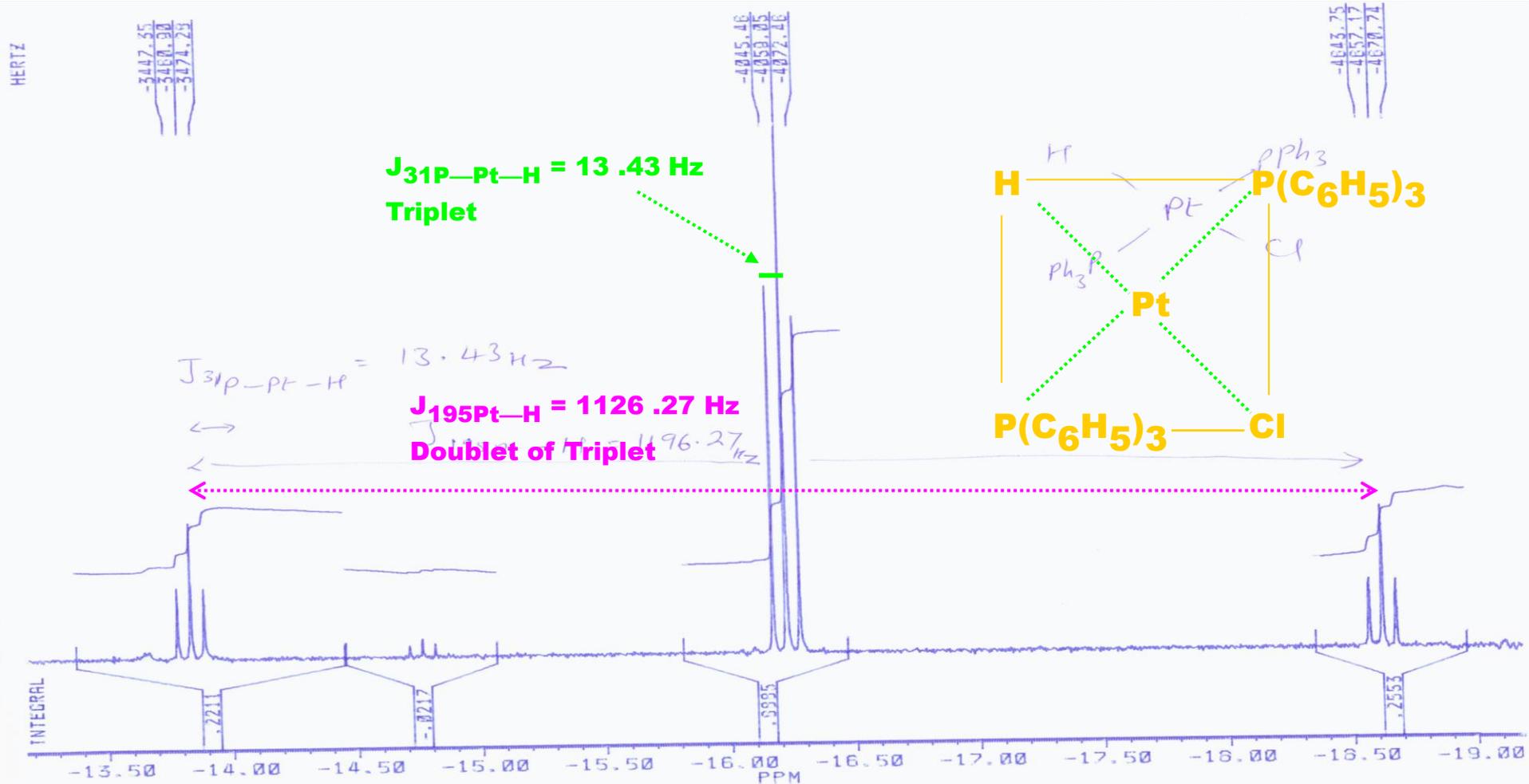
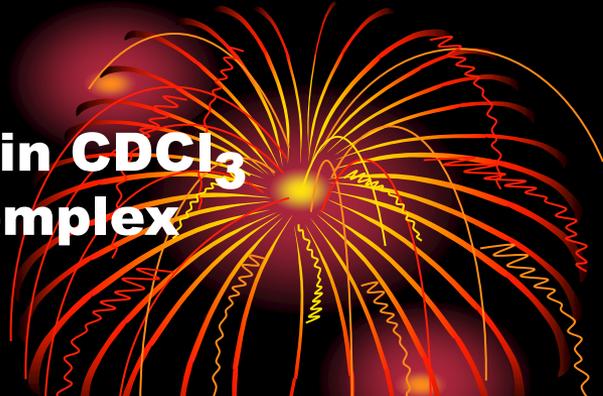
Nucleus	Spin	Nat. Abundance	Sensitivity
^1H	1/2	100.00 %	1.00
^{31}P	1/2	100.00 %	0.07
^{195}Pt	1/2	33.80 %	0.0035

Two ^{31}P give Triplet 3 times taller signal

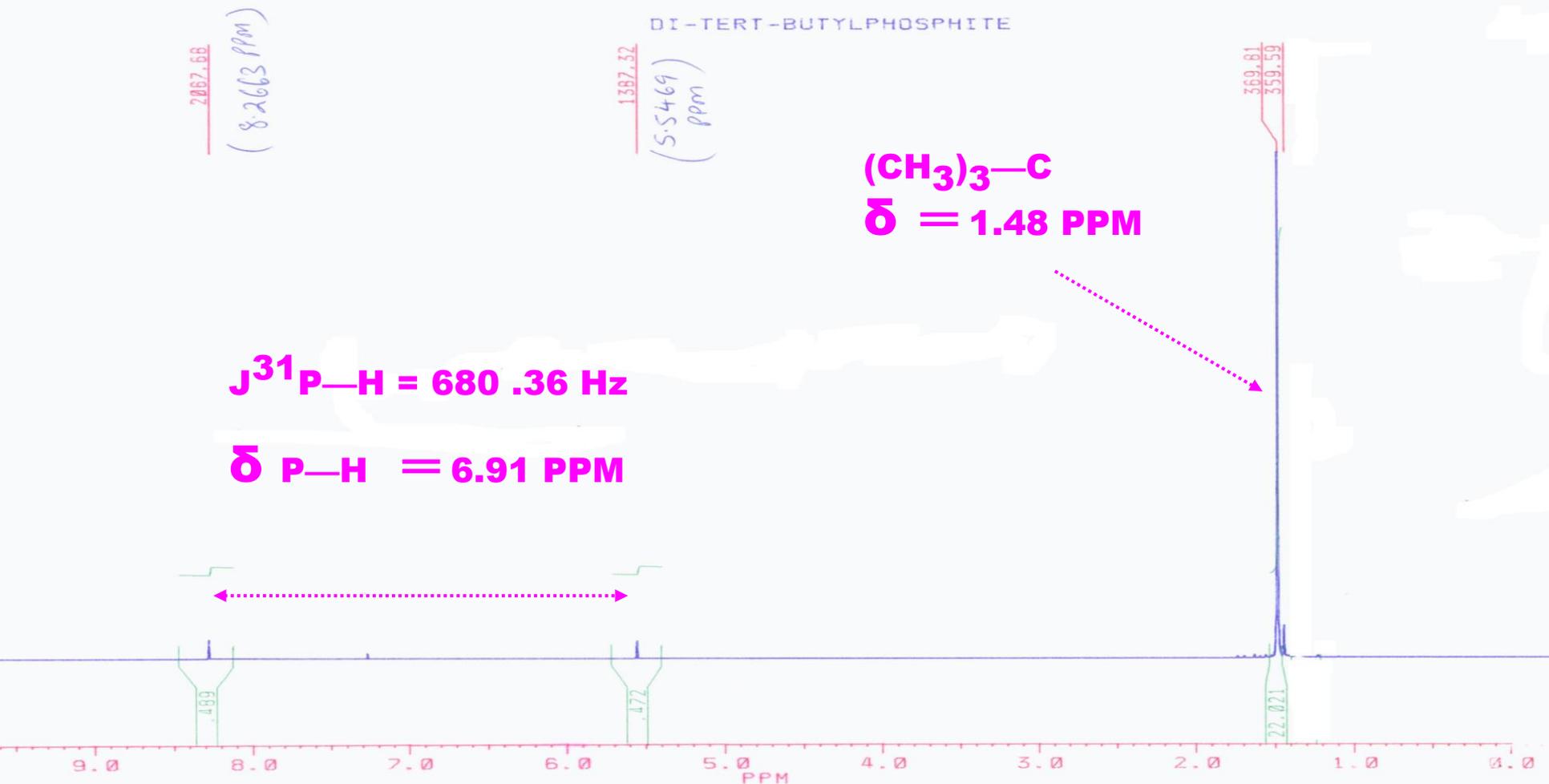
One ^{195}Pt gives Doublet 1/3 Intensity



¹H NMR Spectrum of [(C₆H₅)₃P]₂PtHCl in CDCl₃ DiPhosphine Platinum Hydrochloride Complex expansion of 13.00 PPM to 19.00PPM

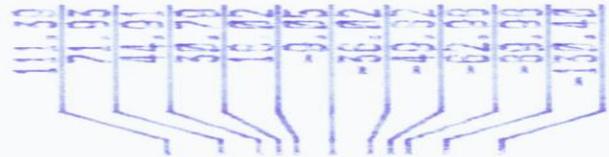
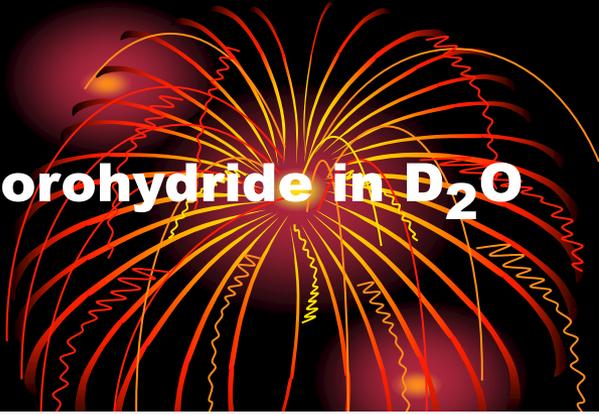


^1H NMR Spectrum of Ditertiary Butylphosphite [(CH₃)₃C-O]₂P(O)H



Expansion of ^1H NMR Spectrum Of Sodium Borohydride in D_2O

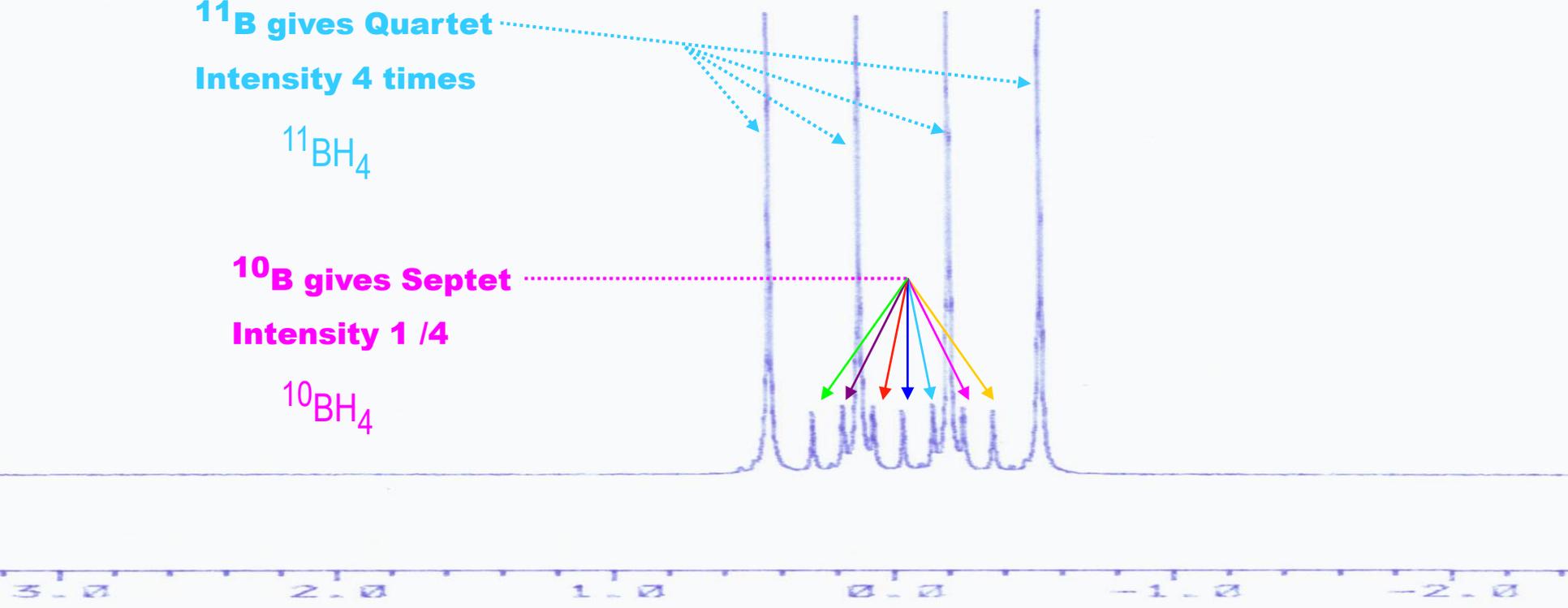
NaBH_4



^{11}B gives Quartet
Intensity 4 times

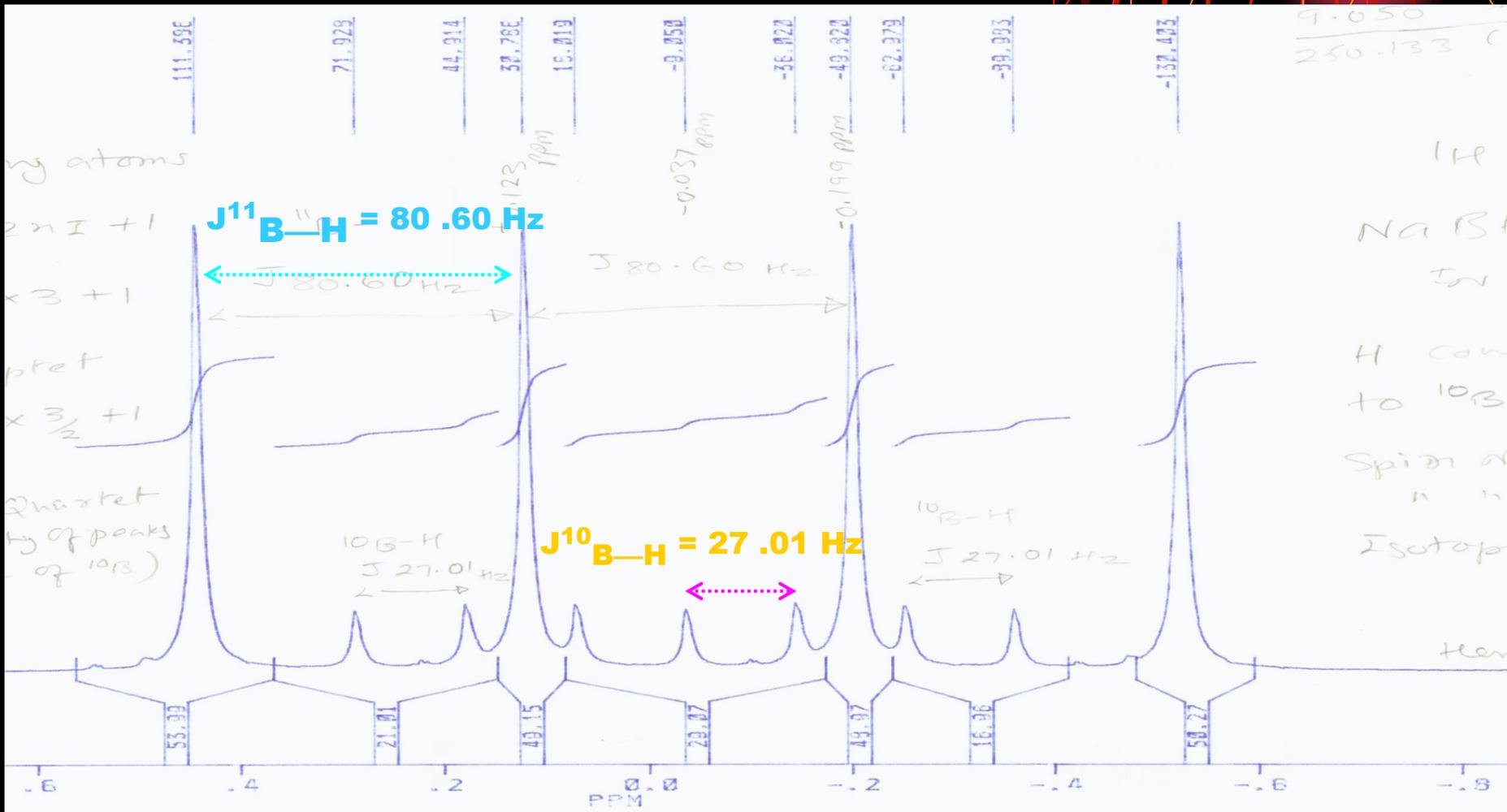
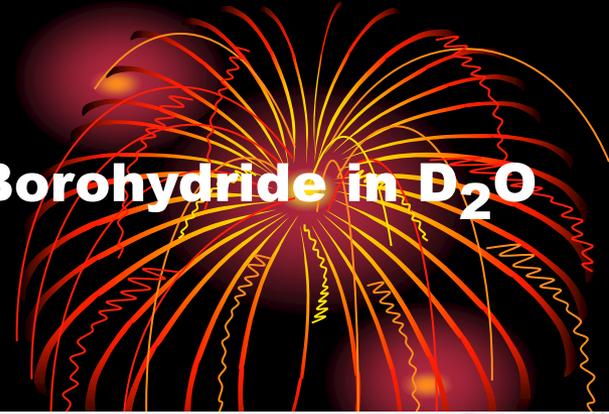


^{10}B gives Septet
Intensity 1 / 4

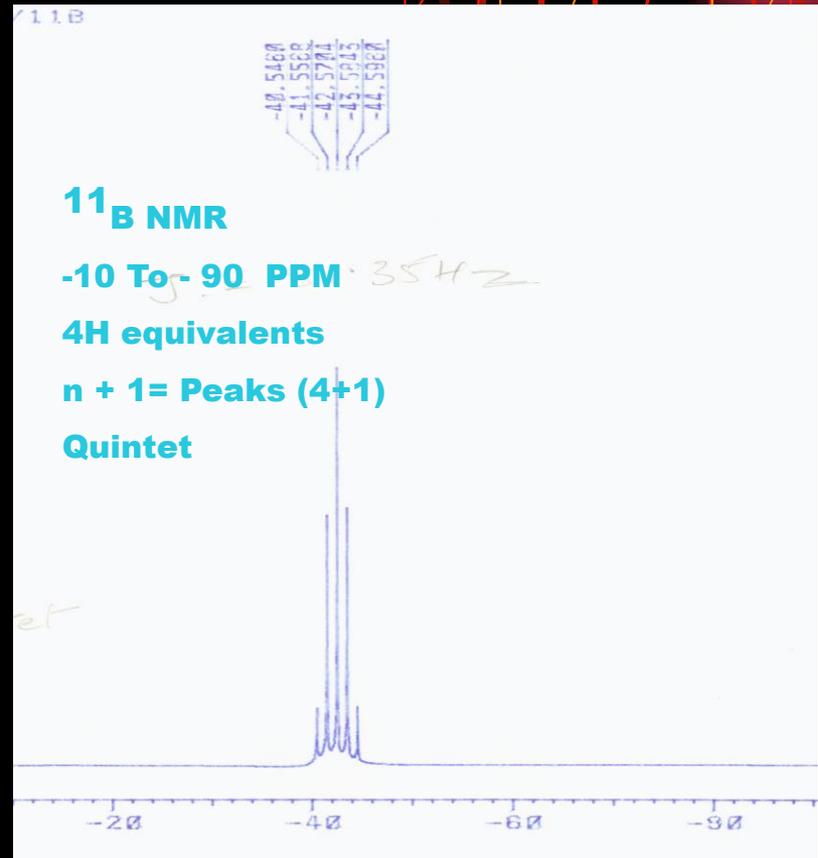
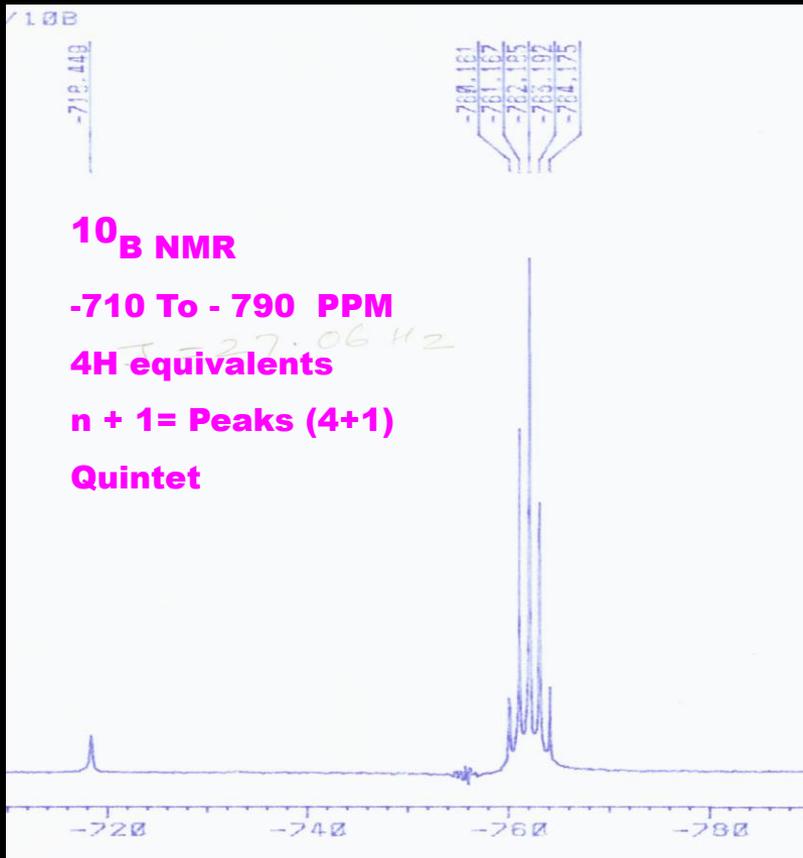


Expansion of ^1H NMR Spectrum Of Sodium Borohydride in D_2O

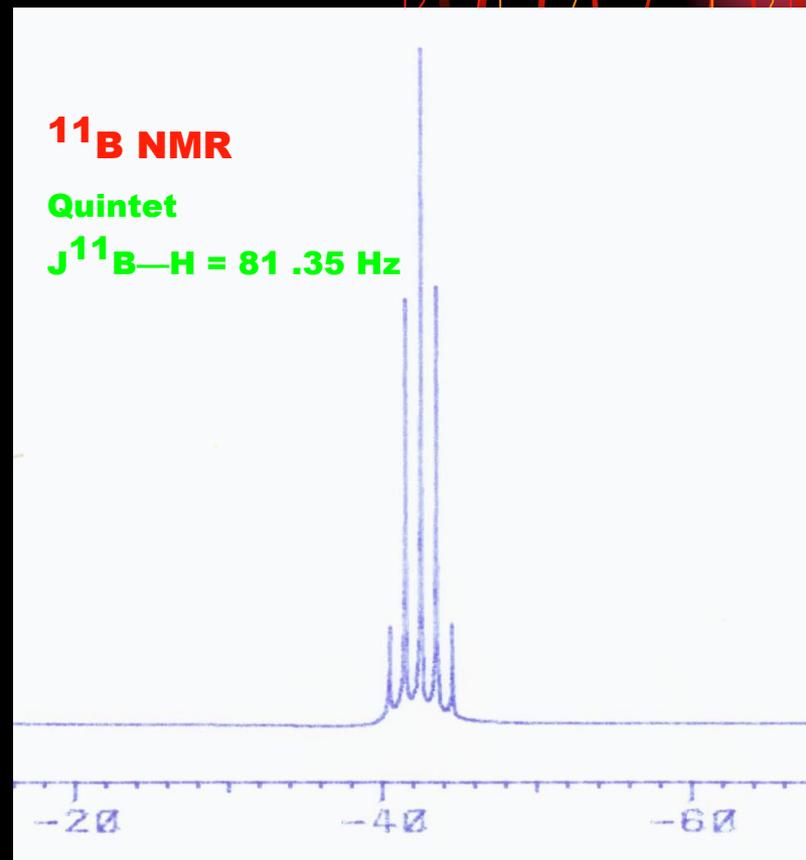
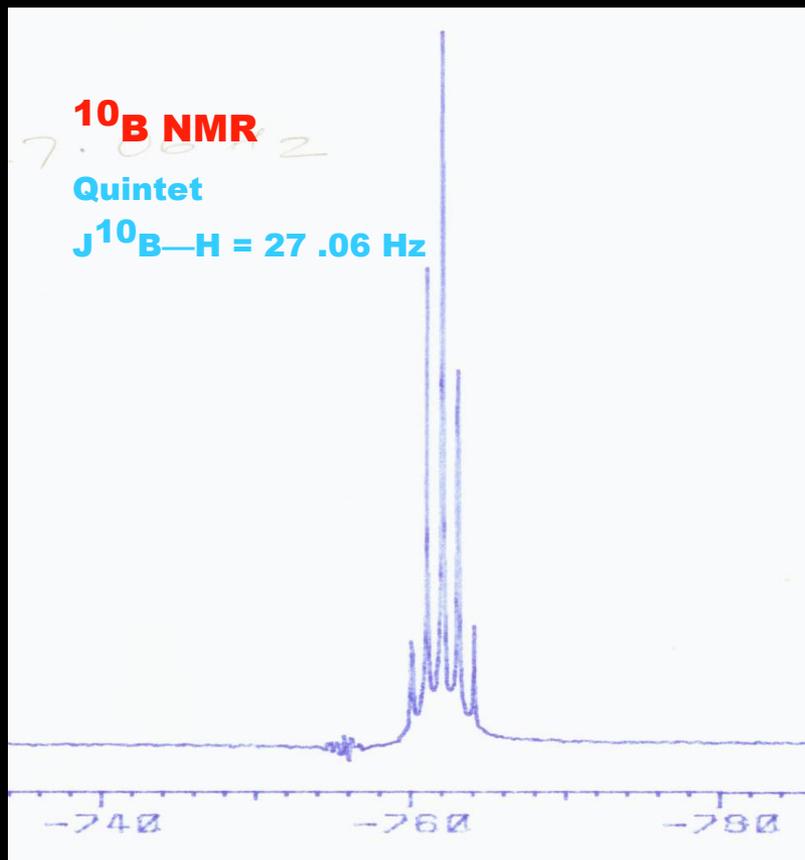
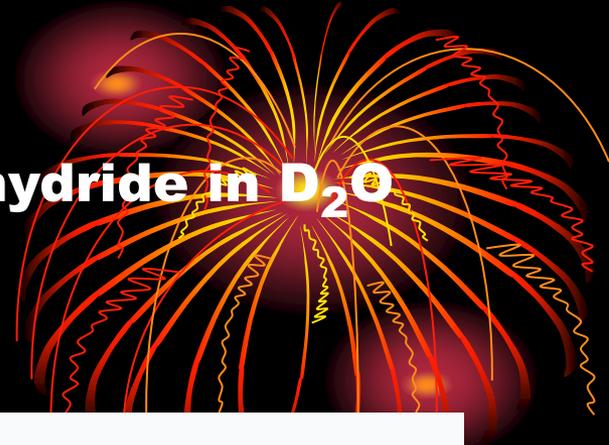
NaBH_4



^{10}B & ^{11}B NMR Spectra Of Sodium Borohydride in D_2O NaBH_4

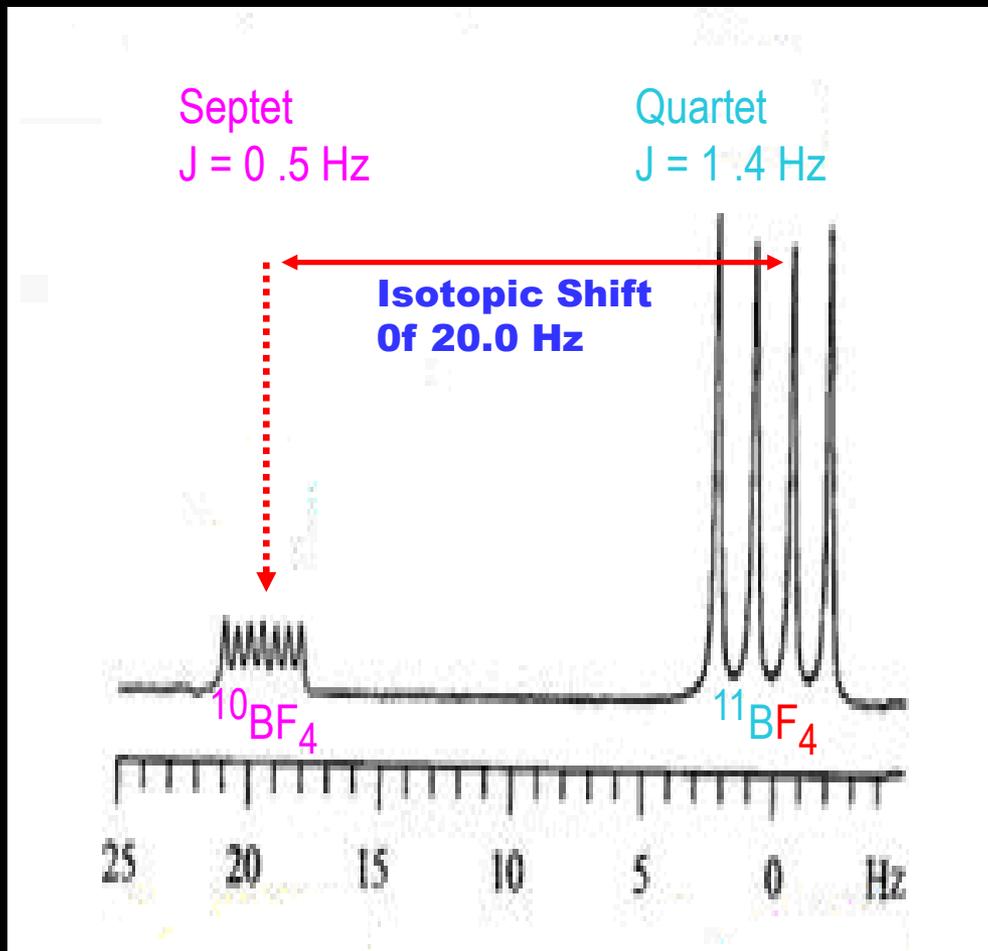


^{10}B & ^{11}B NMR Spectra Of Sodium Borohydride in D_2O NaBH_4



^{19}F NMR of Sodium tetrafluoroborate In D_2O

NaBF_4



Coupling from the same atom of different spin

Isotope	%	Spin No.	SF MHz
^{10}B	19.90	3	26.875
^{11}B	80.10	3/2	80.243

For ^{19}F No. of peaks = $2 \times n \times I + 1$
 ($n = 1$) Spin active nucleus neighbour
 (Boron)

^{10}B interaction to ^{19}F

No. of Peaks = $2 \times 1 \times 3 + 1 = 7$ septet

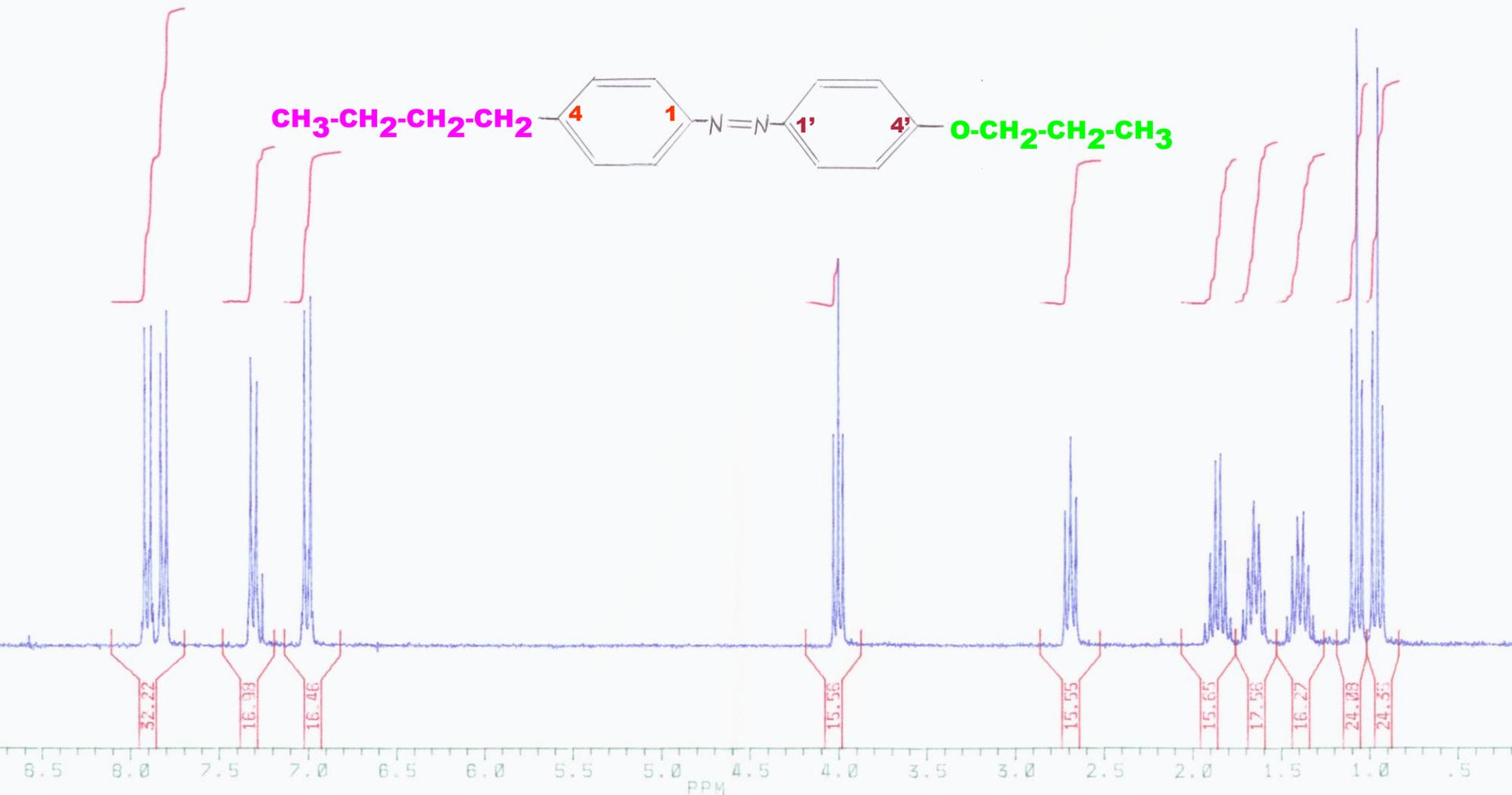
^{11}B interaction to ^{19}F

No. of Peaks = $2 \times 1 \times 3/2 + 1$
 $= 3 + 1 = 4$ Quartet

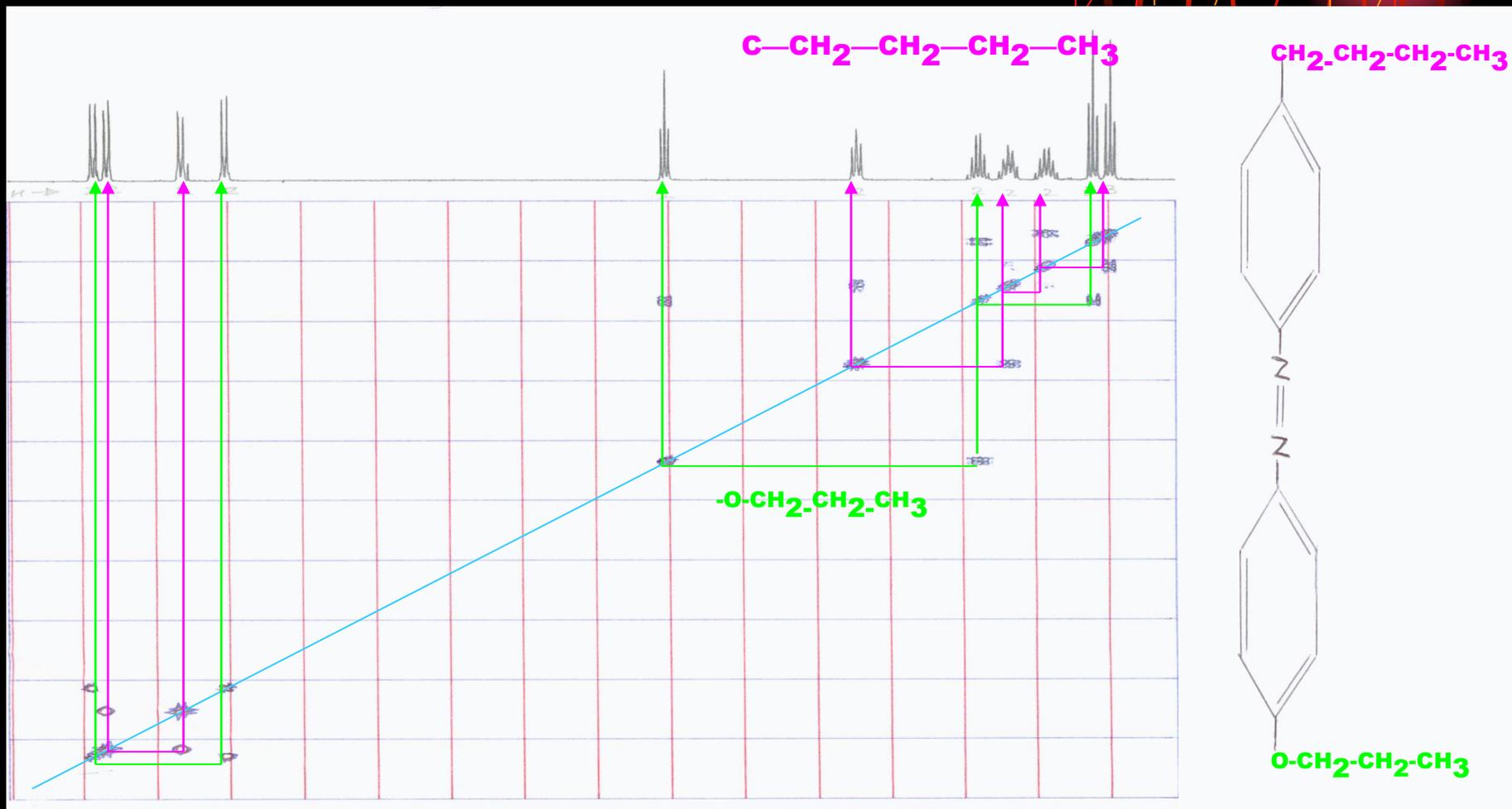
Intensity Ratio of NMR Signal from
 ^{10}B & ^{11}B will be 1 : 4 reflecting its
 isotopic concentration in the atom.

Hence Quartet is four times taller than
 Septet.

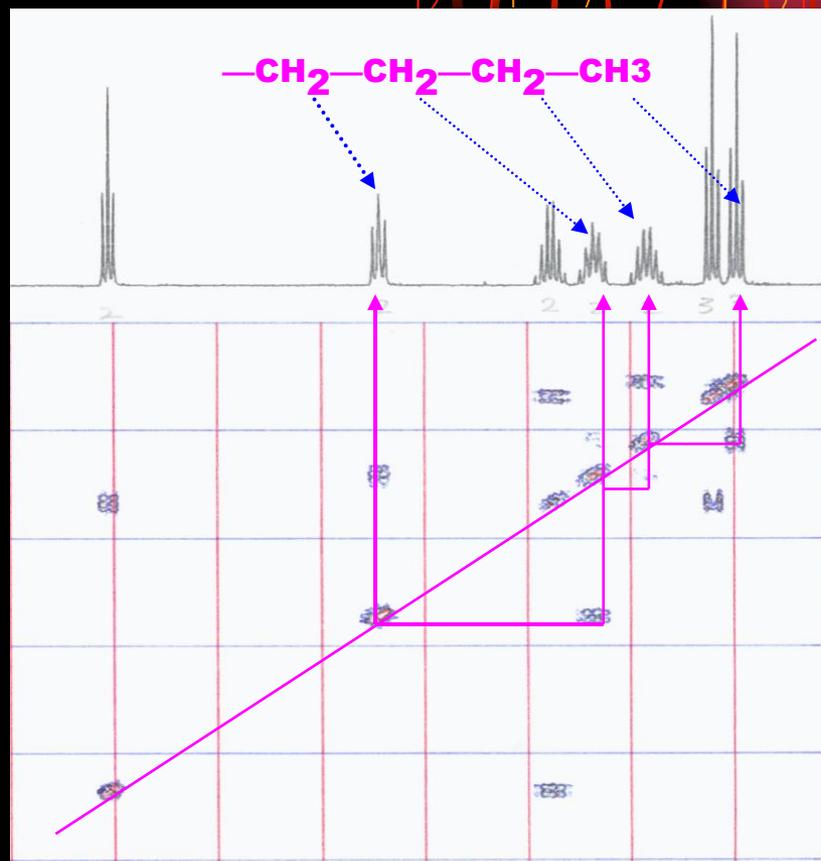
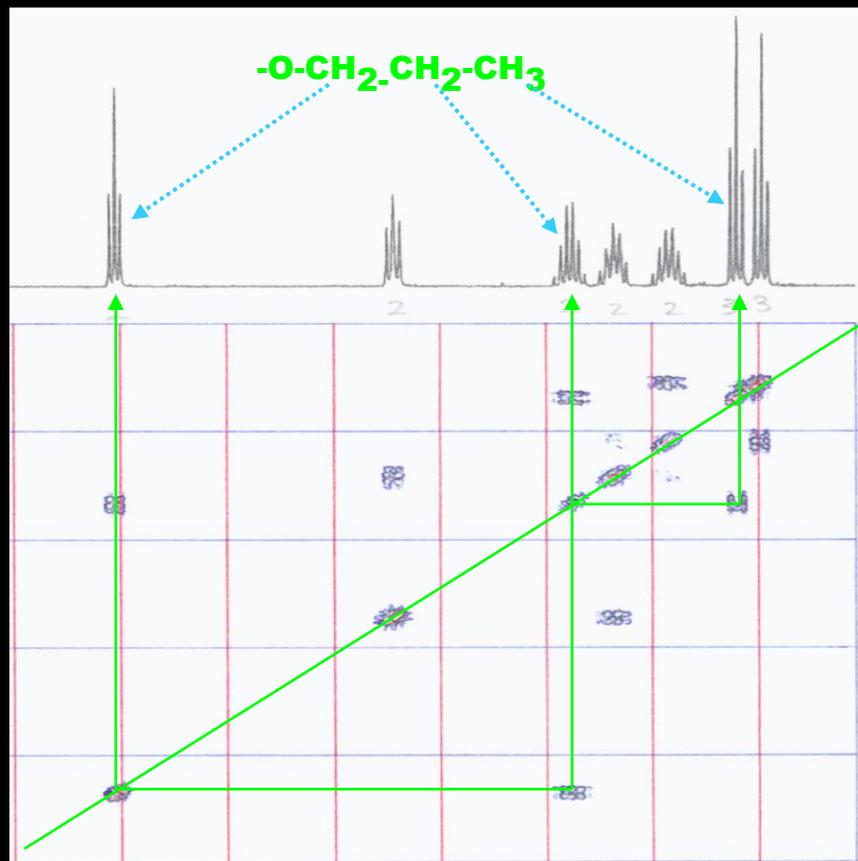
^1H NMR Spectrum of $\text{CH}_3(\text{CH}_2)_3\text{-C}_6\text{H}_4\text{-N=N-C}_6\text{H}_4\text{-O-(CH}_2)_2\text{CH}_3$ 4-n-Butyl, 4'-Propoxy Diazobenzene



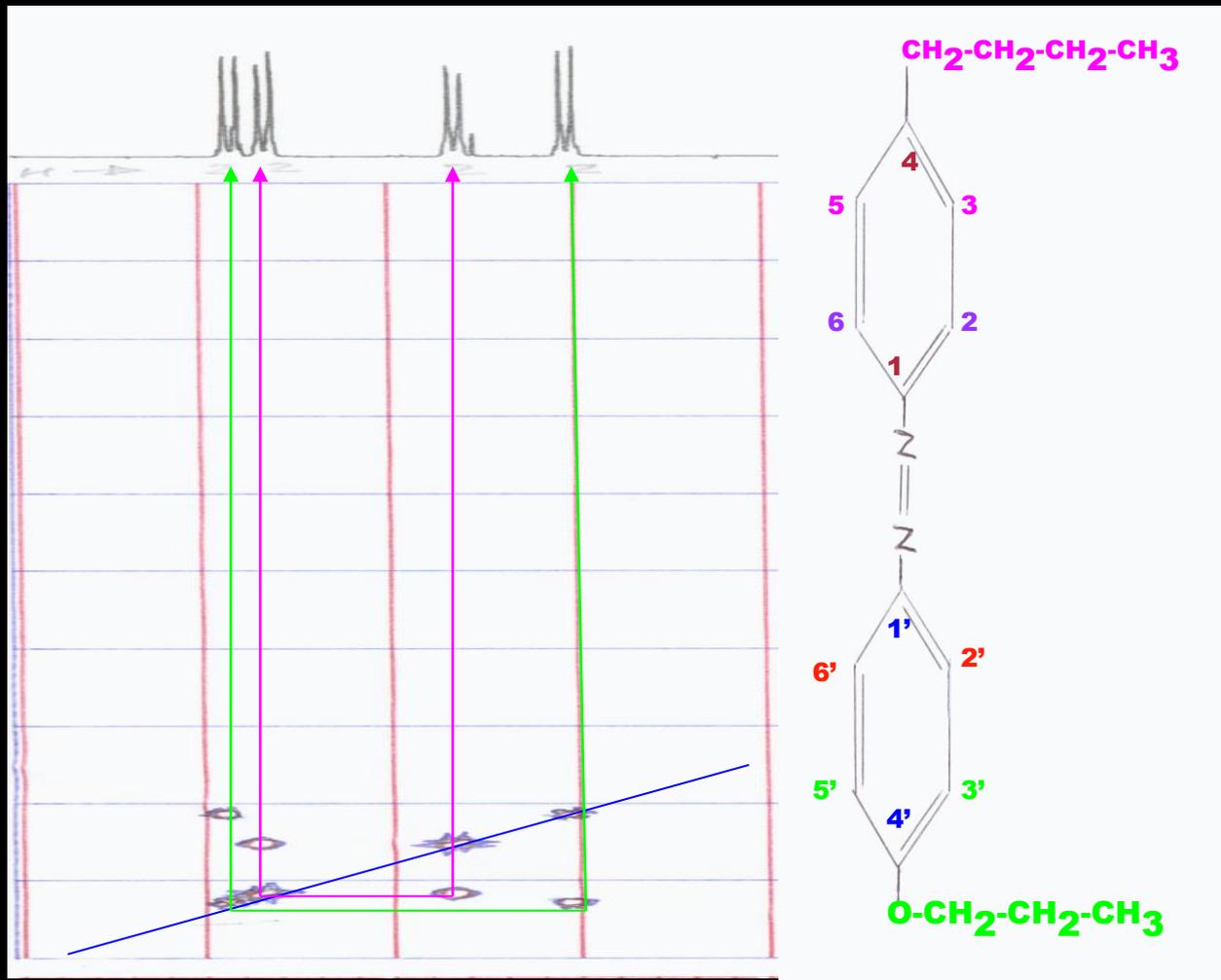
^1H COSY 2D NMR Spectrum of $\text{CH}_3(\text{CH}_2)_3\text{-C}_6\text{H}_4\text{-N=N-C}_6\text{H}_4\text{-O-(CH}_2)_2\text{CH}_3$ 4-n-Butyl, 4'-n-Propoxy Diazobenzene



^1H COSY 2D NMR Spectrum of $\text{CH}_3(\text{CH}_2)_3\text{-C}_6\text{H}_4\text{-N=N-C}_6\text{H}_4\text{-O-(CH}_2)_2\text{CH}_3$ 4-n-Butyl, 4'-n-Propoxy Diazobenzene



¹H COSY 2D NMR Spectrum of CH₃(CH₂)₃-C₆H₄-N=N-C₆H₄-O-(CH₂)₂CH₃ 4-n-Butyl, 4'-n-Propoxy Diazobenzene



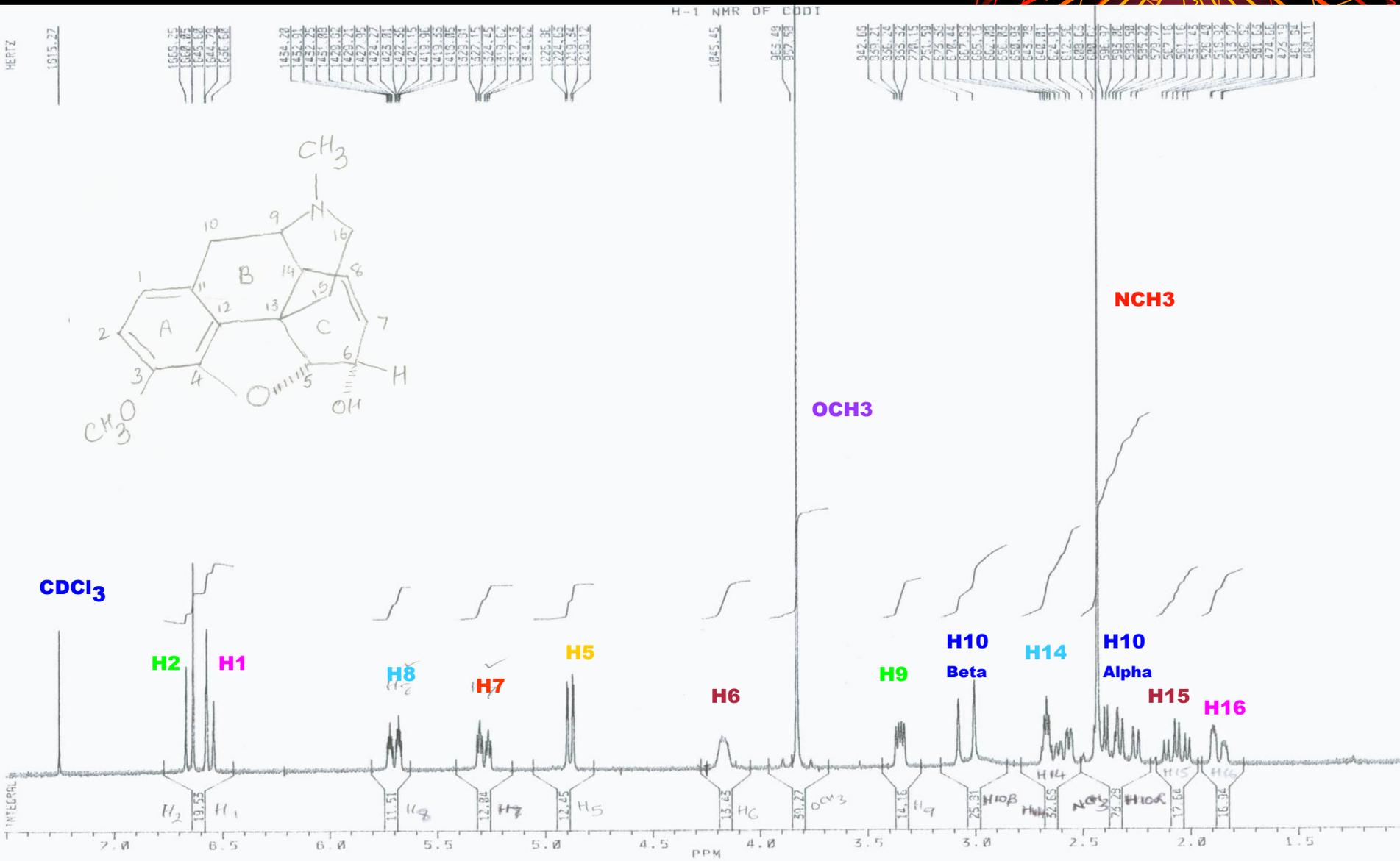
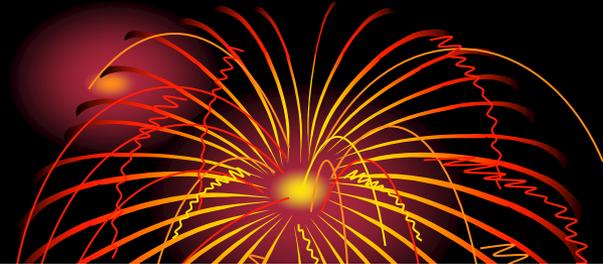
3, 5 1H 7.35 PPM &
2, 6 1H 7.85 PPM
Inner Doublets

Due to Shielding effects of
n-Propoxy group

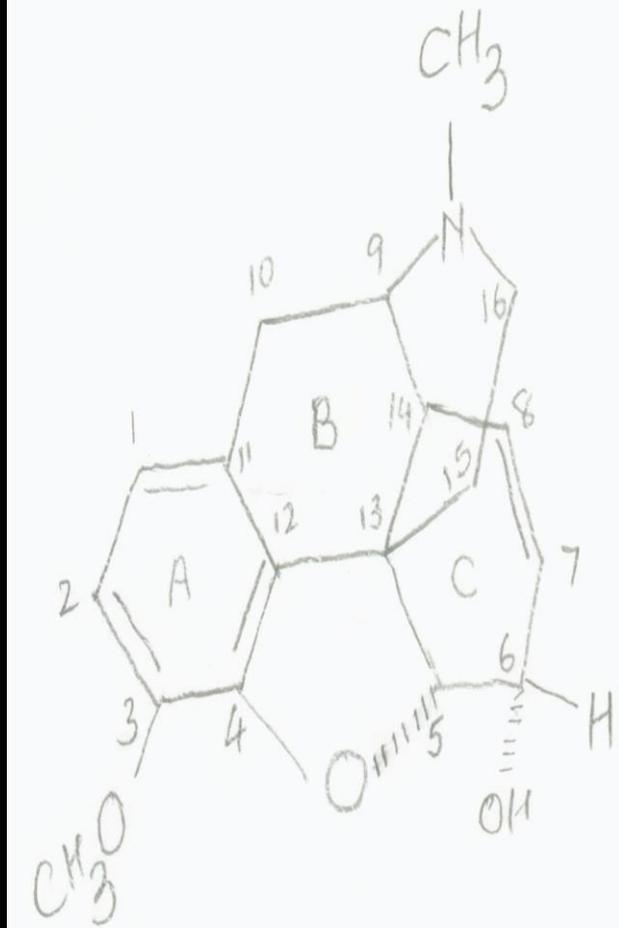
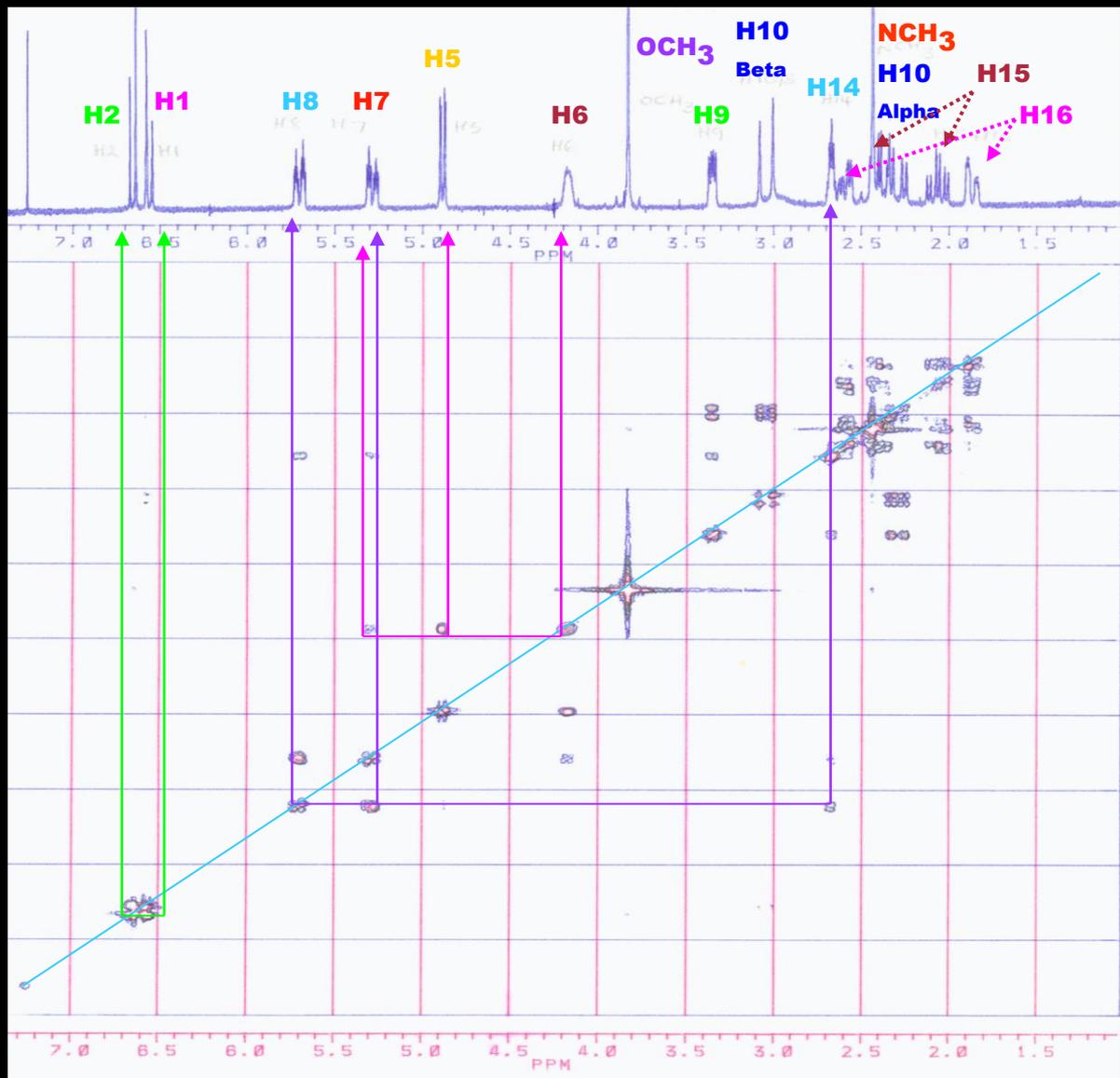
3', 5' ortho 1H 7.00 PPM &
2', 6' meta 1H 7.90 PPM
Outer Doublets Green Trace

In the above example
2D COSY NMR spectrum
is very useful to sort out the
Complexity of peaks.

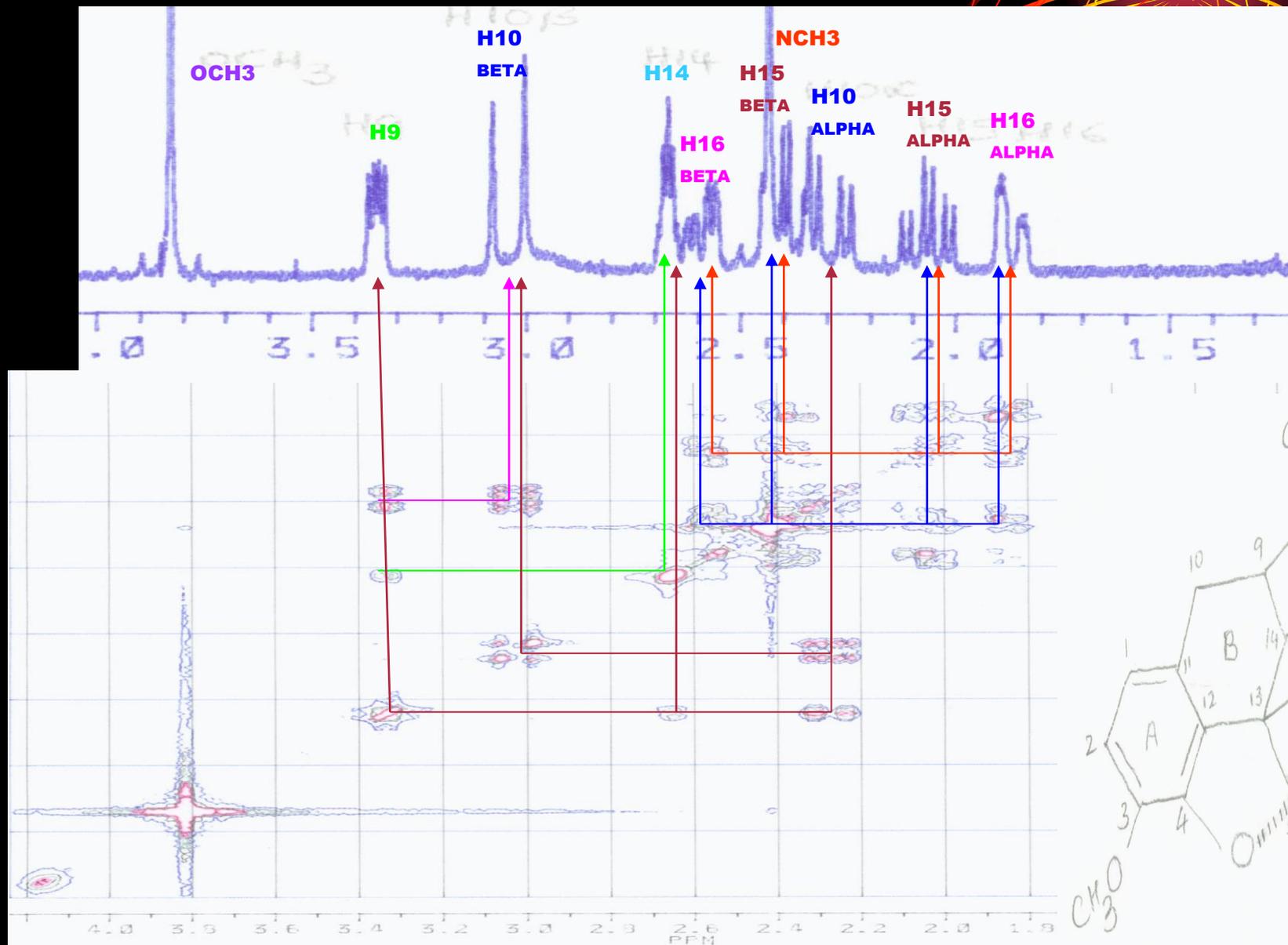
¹H NMR of Codeine In CDCl₃



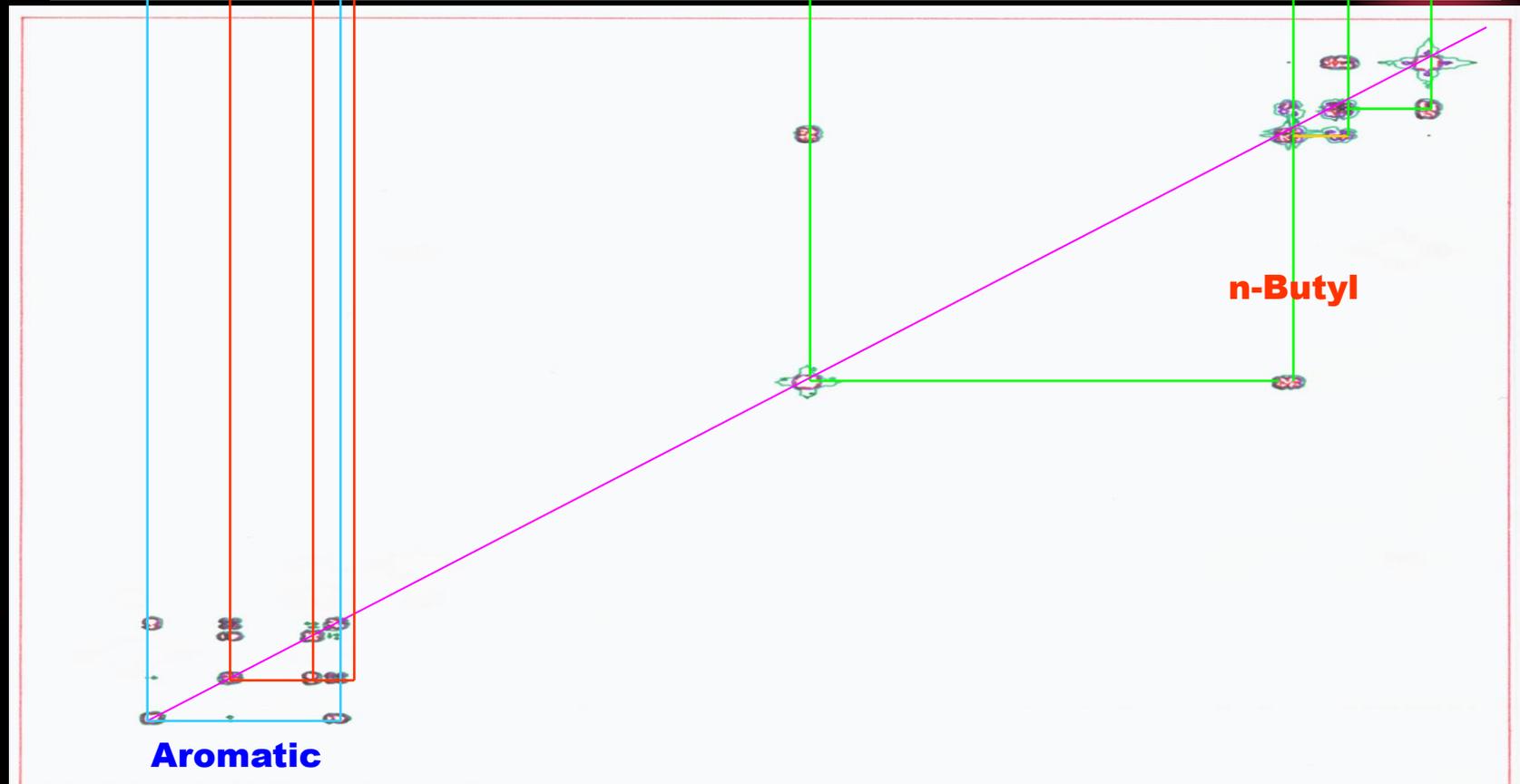
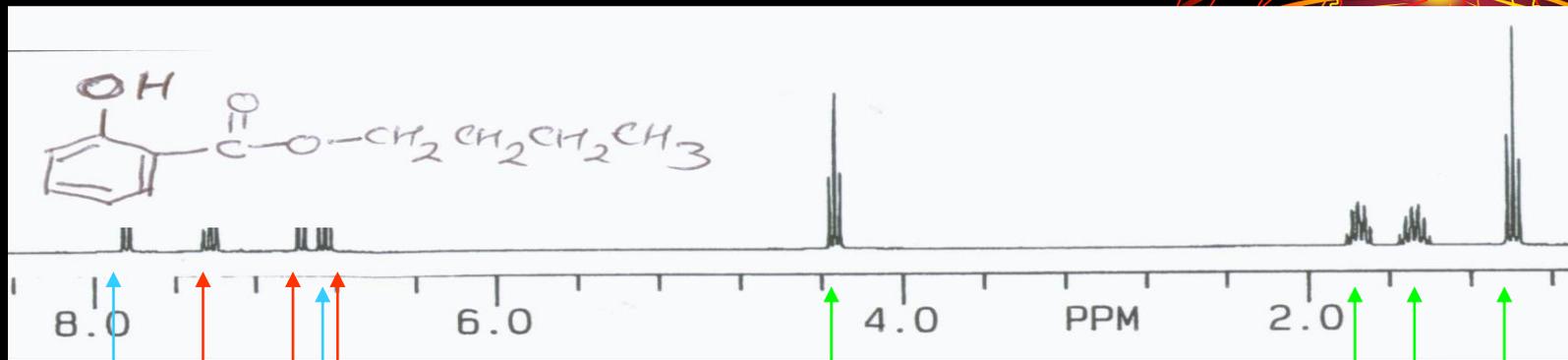
2D COSY NMR Spectrum of Codeine In CDCl₃



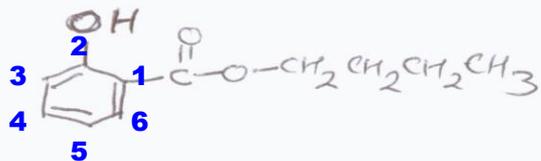
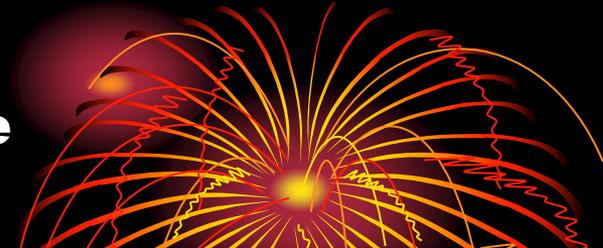
2D COSY NMR Spectrum of Codeine In CDCl₃ Expansion from 4.00 To 1.40 PPM Range



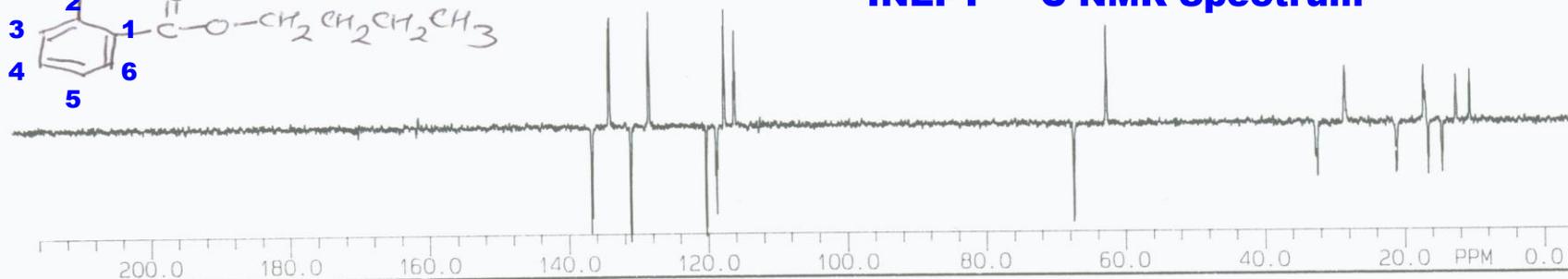
2D COSY ^1H NMR Spectrum of n-Butyl salicylate



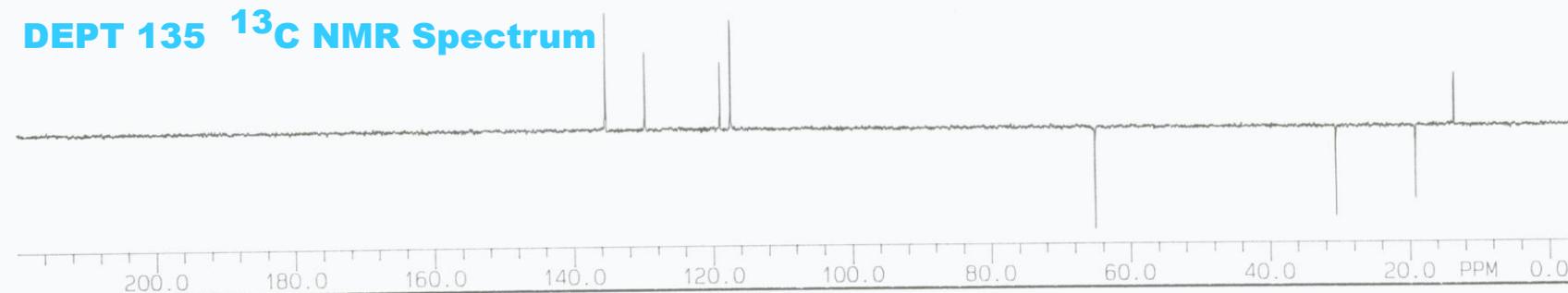
^{13}C NMR Spectrum of n-Butyl Salicylate



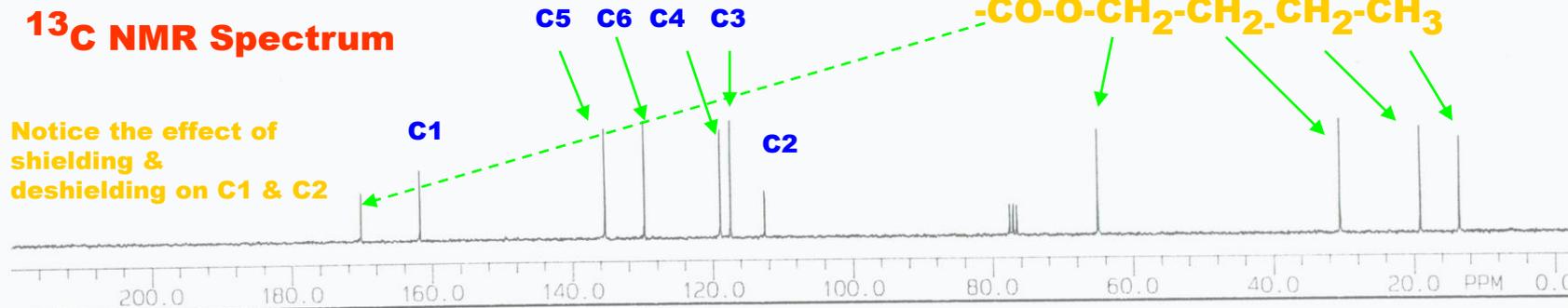
INEPT ^{13}C NMR Spectrum



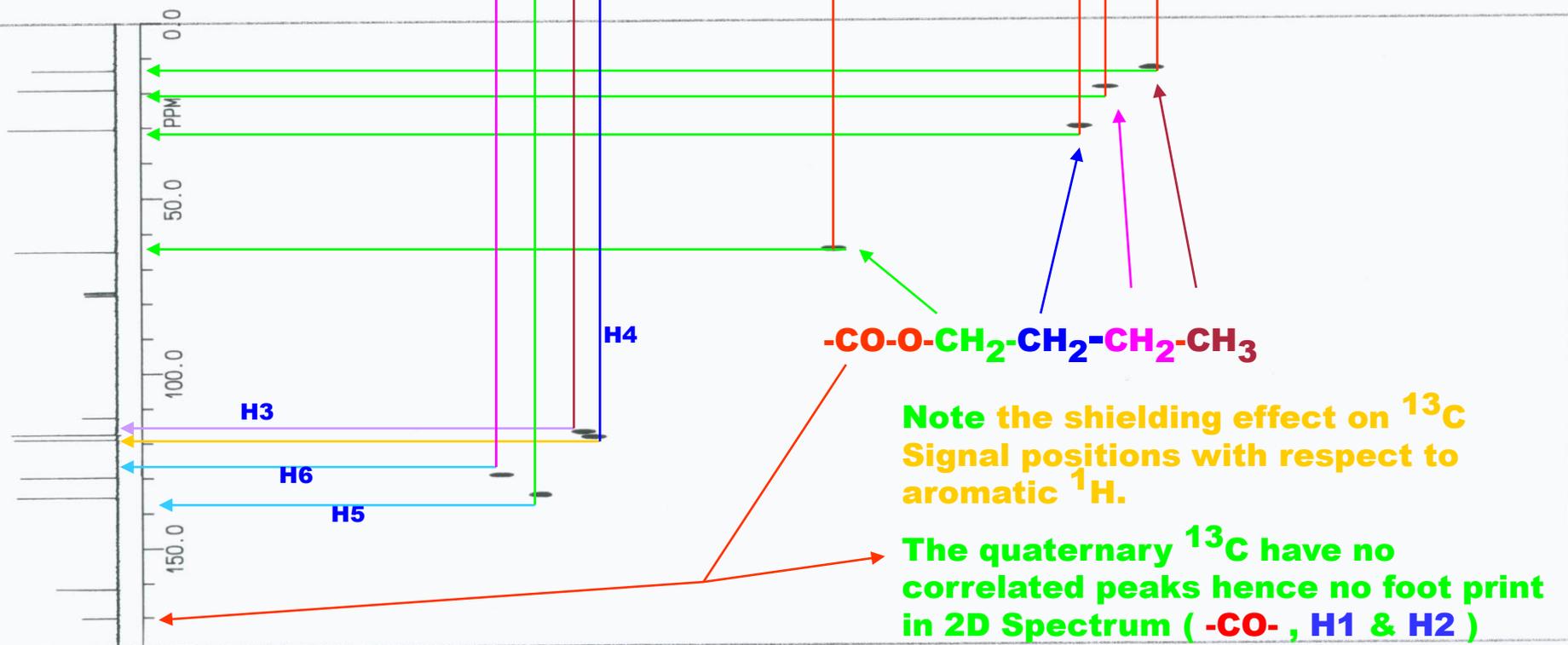
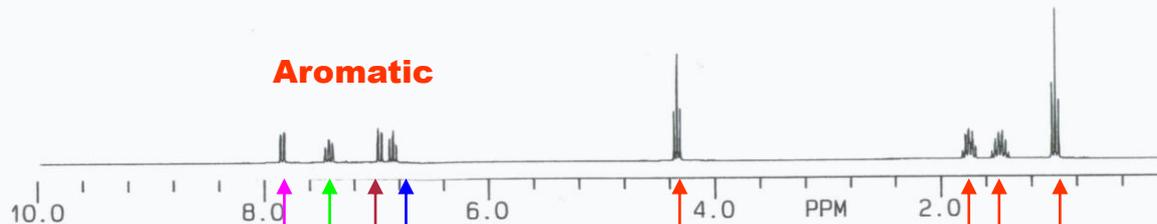
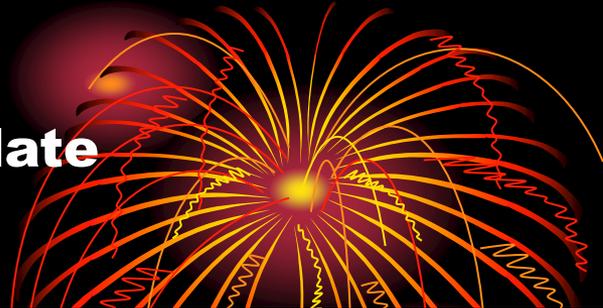
DEPT 135 ^{13}C NMR Spectrum



^{13}C NMR Spectrum



$^1\text{H}-^{13}\text{C}$ CORR Spectrum n-Butyl Salicylate



^1H NMR of Trans FARNESOL $\text{C}_{15}\text{H}_{26}\text{O}$



^1H NMR SPECTRUM OF TRANS-TRANS-FARNESOL

7.25165

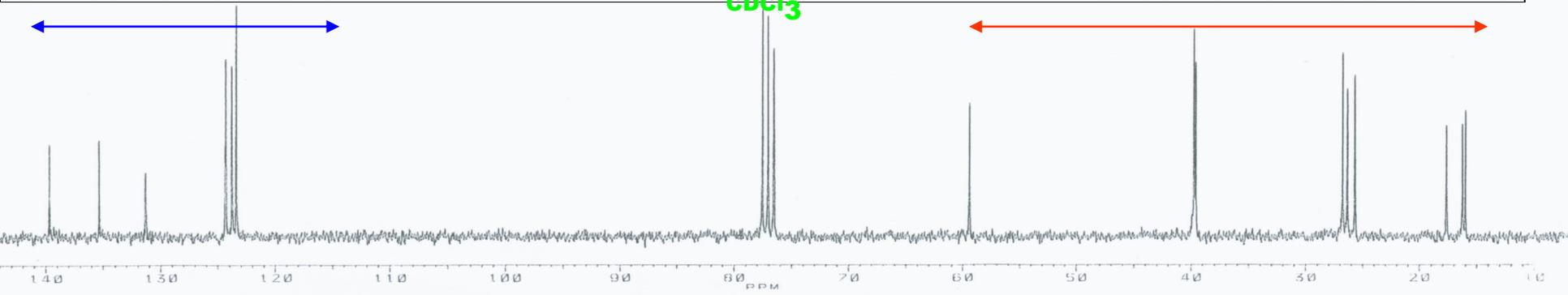
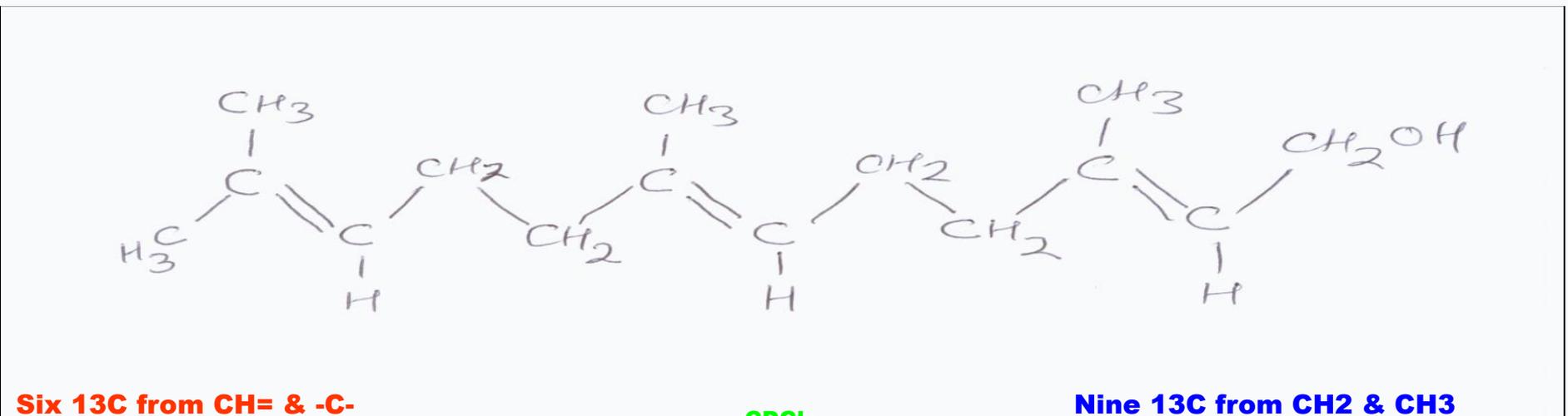
5.44221
5.45720
5.47435
5.49045
5.50655
5.52265
5.53875
5.55485
5.57095
5.58705
5.60315
5.61925
5.63535
5.65145
5.66755

4.15015
4.15745

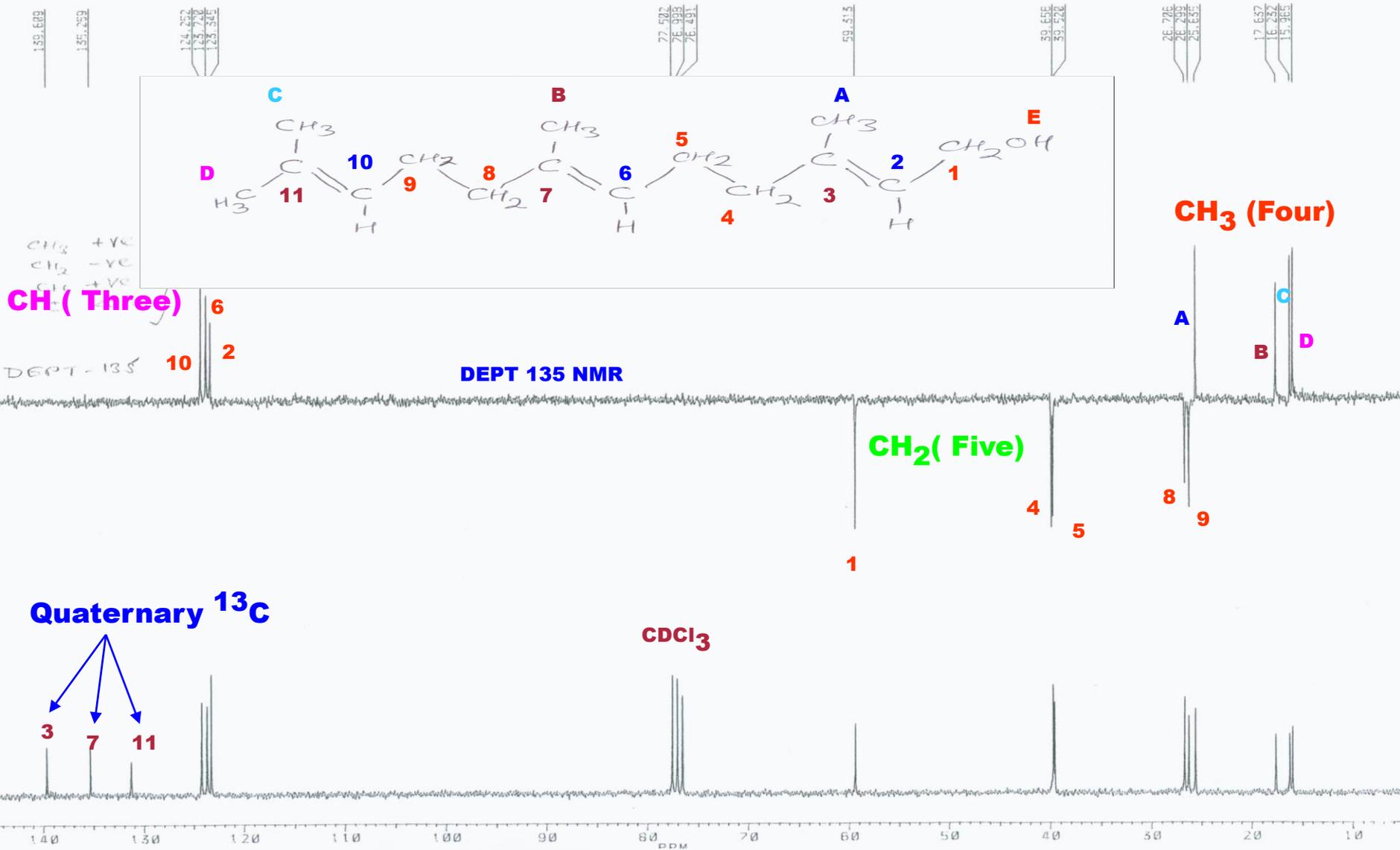
2.12022
2.09650
2.07278
2.04906
2.02534
2.00162
1.97790
1.95418
1.93046
1.90674
1.88302
1.85930
1.83558
1.81186
1.78814
1.76442
1.74070
1.71698
1.69326
1.66954
1.64582
1.62210
1.59838
1.57466
1.55094
1.52722
1.50350
1.47978
1.45606
1.43234
1.40862
1.38490
1.36118
1.33746
1.31374
1.29002
1.26630
1.24258
1.21886
1.19514
1.17142
1.14770
1.12398
1.10026
1.07654
1.05282
1.02910
1.00538
0.98166
0.95794
0.93422
0.91050
0.88678
0.86306
0.83934
0.81562
0.79190
0.76818
0.74446
0.72074
0.69702
0.67330
0.64958
0.62586
0.60214
0.57842
0.55470
0.53098
0.50726
0.48354
0.45982
0.43610
0.41238
0.38866
0.36494
0.34122
0.31750
0.29378
0.27006
0.24634
0.22262
0.19890
0.17518
0.15146
0.12774
0.10402
0.08030
0.05658
0.03286
0.00914
-0.01458
-0.03830
-0.06202
-0.08574
-0.10946
-0.13318
-0.15690
-0.18062
-0.20434
-0.22806
-0.25178
-0.27550
-0.29922
-0.32294
-0.34666
-0.37038
-0.39410
-0.41782
-0.44154
-0.46526
-0.48898
-0.51270
-0.53642
-0.56014
-0.58386
-0.60758
-0.63130
-0.65502
-0.67874
-0.70246
-0.72618
-0.74990
-0.77362
-0.79734
-0.82106
-0.84478
-0.86850
-0.89222
-0.91594
-0.93966
-0.96338
-0.98710
-1.01082
-1.03454
-1.05826
-1.08198
-1.10570
-1.12942
-1.15314
-1.17686
-1.20058
-1.22430
-1.24802
-1.27174
-1.29546
-1.31918
-1.34290
-1.36662
-1.39034
-1.41406
-1.43778
-1.46150
-1.48522
-1.50894
-1.53266
-1.55638
-1.58010
-1.60382
-1.62754
-1.65126
-1.67498
-1.69870
-1.72242
-1.74614
-1.76986
-1.79358
-1.81730
-1.84102
-1.86474
-1.88846
-1.91218
-1.93590
-1.95962
-1.98334
-2.00706
-2.03078
-2.05450
-2.07822
-2.10194
-2.12566
-2.14938
-2.17310
-2.19682
-2.22054
-2.24426
-2.26798
-2.29170
-2.31542
-2.33914
-2.36286
-2.38658
-2.41030
-2.43402
-2.45774
-2.48146
-2.50518
-2.52890
-2.55262
-2.57634
-2.60006
-2.62378
-2.64750
-2.67122
-2.69494
-2.71866
-2.74238
-2.76610
-2.78982
-2.81354
-2.83726
-2.86098
-2.88470
-2.90842
-2.93214
-2.95586
-2.97958
-3.00330
-3.02702
-3.05074
-3.07446
-3.09818
-3.12190
-3.14562
-3.16934
-3.19306
-3.21678
-3.24050
-3.26422
-3.28794
-3.31166
-3.33538
-3.35910
-3.38282
-3.40654
-3.43026
-3.45398
-3.47770
-3.50142
-3.52514
-3.54886
-3.57258
-3.59630
-3.62002
-3.64374
-3.66746
-3.69118
-3.71490
-3.73862
-3.76234
-3.78606
-3.80978
-3.83350
-3.85722
-3.88094
-3.90466
-3.92838
-3.95210
-3.97582
-3.99954
-4.02326
-4.04698
-4.07070
-4.09442
-4.11814
-4.14186
-4.16558
-4.18930
-4.21302
-4.23674
-4.26046
-4.28418
-4.30790
-4.33162
-4.35534
-4.37906
-4.40278
-4.42650
-4.45022
-4.47394
-4.49766
-4.52138
-4.54510
-4.56882
-4.59254
-4.61626
-4.63998
-4.66370
-4.68742
-4.71114
-4.73486
-4.75858
-4.78230
-4.80602
-4.82974
-4.85346
-4.87718
-4.90090
-4.92462
-4.94834
-4.97206
-4.99578
-5.01950
-5.04322
-5.06694
-5.09066
-5.11438
-5.13810
-5.16182
-5.18554
-5.20926
-5.23298
-5.25670
-5.28042
-5.30414
-5.32786
-5.35158
-5.37530
-5.39902
-5.42274
-5.44646
-5.47018
-5.49390
-5.51762
-5.54134
-5.56506
-5.58878
-5.61250
-5.63622
-5.65994
-5.68366
-5.70738
-5.73110
-5.75482
-5.77854
-5.80226
-5.82598
-5.84970
-5.87342
-5.89714
-5.92086
-5.94458
-5.96830
-5.99202
-6.01574
-6.03946
-6.06318
-6.08690
-6.11062
-6.13434
-6.15806
-6.18178
-6.20550
-6.22922
-6.25294
-6.27666
-6.30038
-6.32410
-6.34782
-6.37154
-6.39526
-6.41898
-6.44270
-6.46642
-6.49014
-6.51386
-6.53758
-6.56130
-6.58502
-6.60874
-6.63246
-6.65618
-6.67990
-6.70362
-6.72734
-6.75106
-6.77478
-6.79850
-6.82222
-6.84594
-6.86966
-6.89338
-6.91710
-6.94082
-6.96454
-6.98826
-7.01198
-7.03570
-7.05942
-7.08314
-7.10686
-7.13058
-7.15430
-7.17802
-7.20174
-7.22546
-7.24918
-7.27290
-7.29662
-7.32034
-7.34406
-7.36778
-7.39150
-7.41522
-7.43894
-7.46266
-7.48638
-7.51010
-7.53382
-7.55754
-7.58126
-7.60498
-7.62870
-7.65242
-7.67614
-7.70086
-7.72458
-7.74830
-7.77202
-7.79574
-7.81946
-7.84318
-7.86690
-7.89062
-7.91434
-7.93806
-7.96178
-7.98550
-8.00922
-8.03294
-8.05666
-8.08038
-8.10410
-8.12782
-8.15154
-8.17526
-8.19898
-8.22270
-8.24642
-8.27014
-8.29386
-8.31758
-8.34130
-8.36502
-8.38874
-8.41246
-8.43618
-8.45990
-8.48362
-8.50734
-8.53106
-8.55478
-8.57850
-8.60222
-8.62594
-8.64966
-8.67338
-8.69710
-8.72082
-8.74454
-8.76826
-8.79198
-8.81570
-8.83942
-8.86314
-8.88686
-8.91058
-8.93430
-8.95802
-8.98174
-9.00546
-9.02918
-9.05290
-9.07662
-9.10034
-9.12406
-9.14778
-9.17150
-9.19522
-9.21894
-9.24266
-9.26638
-9.29010
-9.31382
-9.33754
-9.36126
-9.38498
-9.40870
-9.43242
-9.45614
-9.47986
-9.50358
-9.52730
-9.55102
-9.57474
-9.59846
-9.62218
-9.64590
-9.66962
-9.69334
-9.71706
-9.74078
-9.76450
-9.78822
-9.81194
-9.83566
-9.85938
-9.88310
-9.90682
-9.93054
-9.95426
-9.97798
-10.00170
-10.02542
-10.04914
-10.07286
-10.09658
-10.12030
-10.14402
-10.16774
-10.19146
-10.21518
-10.23890
-10.26262
-10.28634
-10.31006
-10.33378
-10.35750
-10.38122
-10.40494
-10.42866
-10.45238
-10.47610
-10.49982
-10.52354
-10.54726
-10.57098
-10.59470
-10.61842
-10.64214
-10.66586
-10.68958
-10.71330
-10.73702
-10.76074
-10.78446
-10.80818
-10.83190
-10.85562
-10.87934
-10.90306
-10.92678
-10.95050
-10.97422
-10.99794
-11.02166
-11.04538
-11.06910
-11.09282
-11.11654
-11.14026
-11.16398
-11.18770
-11.21142
-11.23514
-11.25886
-11.28258
-11.30630
-11.33002
-11.35374
-11.37746
-11.40118
-11.42490
-11.44862
-11.47234
-11.49606
-11.51978
-11.54350
-11.56722
-11.59094
-11.61466
-11.63838
-11.66210
-11.68582
-11.70954
-11.73326
-11.75698
-11.78070
-11.80442
-11.82814
-11.85186
-11.87558
-11.89930
-11.92302
-11.94674
-11.97046
-11.99418
-12.01790
-12.04162
-12.06534
-12.08906
-12.11278
-12.13650
-12.16022
-12.18394
-12.20766
-12.23138
-12.25510
-12.27882
-12.30254
-12.32626
-12.34998
-12.37370
-12.39742
-12.42114
-12.44486
-12.46858
-12.49230
-12.51602
-12.53974
-12.56346
-12.58718
-12.61090
-12.63462
-12.65834
-12.68206
-12.70578
-12.72950
-12.75322
-12.77694
-12.80066
-12.82438
-12.84810
-12.87182
-12.89554
-12.91926
-12.94298
-12.96670
-12.99042
-13.01414
-13.03786
-13.06158
-13.08530
-13.10902
-13.13274
-13.15646
-13.18018
-13.20390
-13.22762
-13.25134
-13.27506
-13.29878
-13.32250
-13.34622
-13.36994
-13.39366
-13.41738
-13.44110
-13.46482
-13.48854
-13.51226
-13.53598
-13.55970
-13.58342
-13.60714
-13.63086
-13.65458
-13.67830
-13.70202
-13.72574
-13.74946
-13.77318
-13.79690
-13.82062
-13.84434
-13.86806
-13.89178
-13.91550
-13.93922
-13.96294
-13.98666
-14.01038
-14.03410
-14.05782
-14.08154
-14.10526
-14.12898
-14.15270
-14.17642
-14.20014
-14.22386
-14.24758
-14.27130
-14.29502
-14.31874
-14.34246
-14.36618
-14.38990
-14.41362
-14.43734
-14.46106
-14.48478
-14.50850
-14.53222
-14.55594
-14.57966
-14.60338
-14.62710
-14.65082
-14.67454
-14.69826
-14.72198
-14.74570
-14.76942
-14.79314
-14.81686
-14.84058
-14.86430
-14.88802
-14.91174
-14.93546
-14.95918
-14.98290
-15.00662
-15.03034
-15.05406
-15.07778
-15.10150
-15.12522
-15.14894
-15.17266
-15.19638
-15.22010
-15.24382
-15.26754
-15.29126
-15.31498
-15.33870
-15.36242
-15.38614
-15.40986
-15.43358
-15.45730
-15.48102
-15.50474
-15.52846
-15.55218
-15.57590
-15.60062
-15.62434
-15.64806
-15.67178
-15.69550
-15.71922
-15.74294
-15.76666
-15.79038
-15.81410
-15.83782
-15.86154
-15.88526
-15.90898
-15.93270
-15.95642
-15.98014
-16.00386
-16.02758
-16.05130
-16.07502
-16.09874
-16.12246
-16.14618
-16.16990
-16.19362
-16.21734
-16.24106
-16.26478
-16.28850
-16.31222
-16.33594
-16.35966
-16.38338
-16.40710
-16.43082
-16.45454
-16.47826
-16.50198
-16.52570
-16.54942
-16.57314
-16.59686
-16.62058
-16.64430
-16.66802
-16.69174
-16.71546
-16.73918
-16.76290
-16.78662
-16.81034
-16.83406
-16.85778
-16.88150
-16.90522
-16.92894
-16.95266
-16.97638
-17.00010
-17.02382
-17.04754
-17.07126
-17.09498
-17.11870
-17.14242
-17.16614
-17.18986
-17.21358
-17.23730
-17.26102
-17.28474
-17.30846
-17.33218
-17.35590
-17.37962
-17.40334
-17.42706
-17.45078
-17.47450
-17.49822
-17.52194
-17.54566
-17.56938
-17.59310
-17.61682
-17.64054
-17.66426
-17.68798
-17.71170
-17.73542
-17.75914
-17.78286
-17.80658
-17.83030
-17.85402
-17.87774
-17.90146
-17.92518
-17.94890
-17.97262
-17.99634
-18.02006
-18.04378
-18.06750
-18.09122
-18.11494
-18.13866
-18.16238
-18.18610
-18.20982
-18.23354
-18.25726
-18.28098
-18.30470
-18.32842
-18.35214
-18.37586
-18.39958
-18.42330
-18.44702
-18.47074
-18.49446
-18.51818
-18.54190
-18.56562
-18.58934
-18.61306
-18.63678
-18.66050
-18.68422
-18.70794
-18.73166
-18.75538
-18.77910
-18.80282
-18.82654
-18.85026
-18.87398
-18.89770
-18.92142
-18.94514
-18.96886
-18.99258
-19.01630
-19.04002
-19.06374
-19.08746
-19.11118
-19.13490
-19.15862
-19.18234
-19.20606
-19.22978
-19.25350
-19.27722
-19.30094
-19.32466
-19.34838
-19.37210
-19.39582
-19.41954
-19.44326
-19.46698
-19.49070
-19.51442
-19.53814
-19.56186
-19.58558
-19.60930
-19.63302
-19.65674
-19.68046
-19.70418
-19.72790
-19.75162
-19.77534
-19.79906
-19.82278
-19.84650
-19.87022
-19.89394
-19.91766
-19.94138
-19.96510
-19.98882
-20.01254
-20.03626
-20.05998
-20.08370
-20.10742
-20.13114
-20.15486
-20.17858
-20.20230
-20.22602
-20.24974
-20.27346
-20.29718
-20.32090
-20.34462
-20.36834
-20.39206
-20.41578
-20.43950
-20.46322
-20.48694
-20.51066
-20.53438
-20.55810
-20.58182
-20.60554
-20.62926
-20.65298
-20.67670
-20.70042
-20.72414
-20.74786
-20.77158
-20.79530
-20.81902
-20.84274
-20.86646
-20.89018
-20.91390
-20.93762
-20.96134
-20.98506
-21.00878
-21.03250
-21.05622
-21.07994
-21.10366
-21.12738
-21.15110
-21.17482
-21.19854
-21.22226
-21.24598
-21.26970
-21.29342
-21.31714
-21.34086
-21.36458
-21.38830
-21.41202
-21.43574
-21.45946
-21.48318
-21.50690
-21.53062
-21.55434
-21.57806
-21.60178
-21.62550
-21.64922
-21.67294
-21.69666
-21.72038
-21.74410
-21.76782
-21.79154
-21.81526
-21.83898
-21.86270
-21.88642
-21.91014
-21.93386
-21.95758
-21.98130
-22.00502
-22.02874
-22.05246
-22.07618
-22.10090
-22.12462
-22.14834
-22.17206
-22.19578
-22.21950
-22.24322
-22.26694
-22.29066
-22.31438
-22.33810
-22.36182
-22.38554
-22.40926
-22.43298
-22.45670
-22.48042
-22.50414
-22.52786
-22.55158
-22.57530
-22.59902
-22.62274
-22.64646
-22.67018
-22.69390
-22.71762
-22.74134
-22.76506
-22.78878
-22.81250
-22.83622
-22.85994
-22.88366
-22.90738
-22.93110
-22.95482
-22.97854
-23.00226
-23.02598
-23.04970
-23.07342
-23.09714
-23.12086
-23.14458
-23.16830
-23.19202
-23.21574
-23.23946
-23.26318
-23.28690
-23.31062
-23.33434
-23.35806
-23.38178
-23.40550
-23.42922
-23.45294
-23.47666
-23.50038
-23.52410
-23.54782
-23.57154
-23.59526
-23.61898
-23.64270
-23.66642
-23.69014
-23.71386
-23.73758
-23.76130
-23.78502
-23.80874
-23.83246
-23.85618
-23.87990
-23.90362
-23.92734
-23.95106
-23.97478
-23.99850
-24.02222
-24.04594
-24.06966
-24.09338
-24.11710
-24.14082
-24.16454
-24.18826
-24.21198
-24.23570
-24.25942
-24.28314
-24.30686
-24.33058
-24.35430
-24.37802
-24.40174
-24.42546
-24.44918
-24.47290
-24.49662
-24.52034
-24.54406
-24.56778
-24.59150
-24.61522
-24.63894
-24.66266
-24.68638
-24.71010
-24.73382
-24.75754
-24.7812

^{13}C NMR Spectrum of Trans FARNESOL In CDCl_3

$\text{C}_{15}\text{H}_{26}\text{O}$

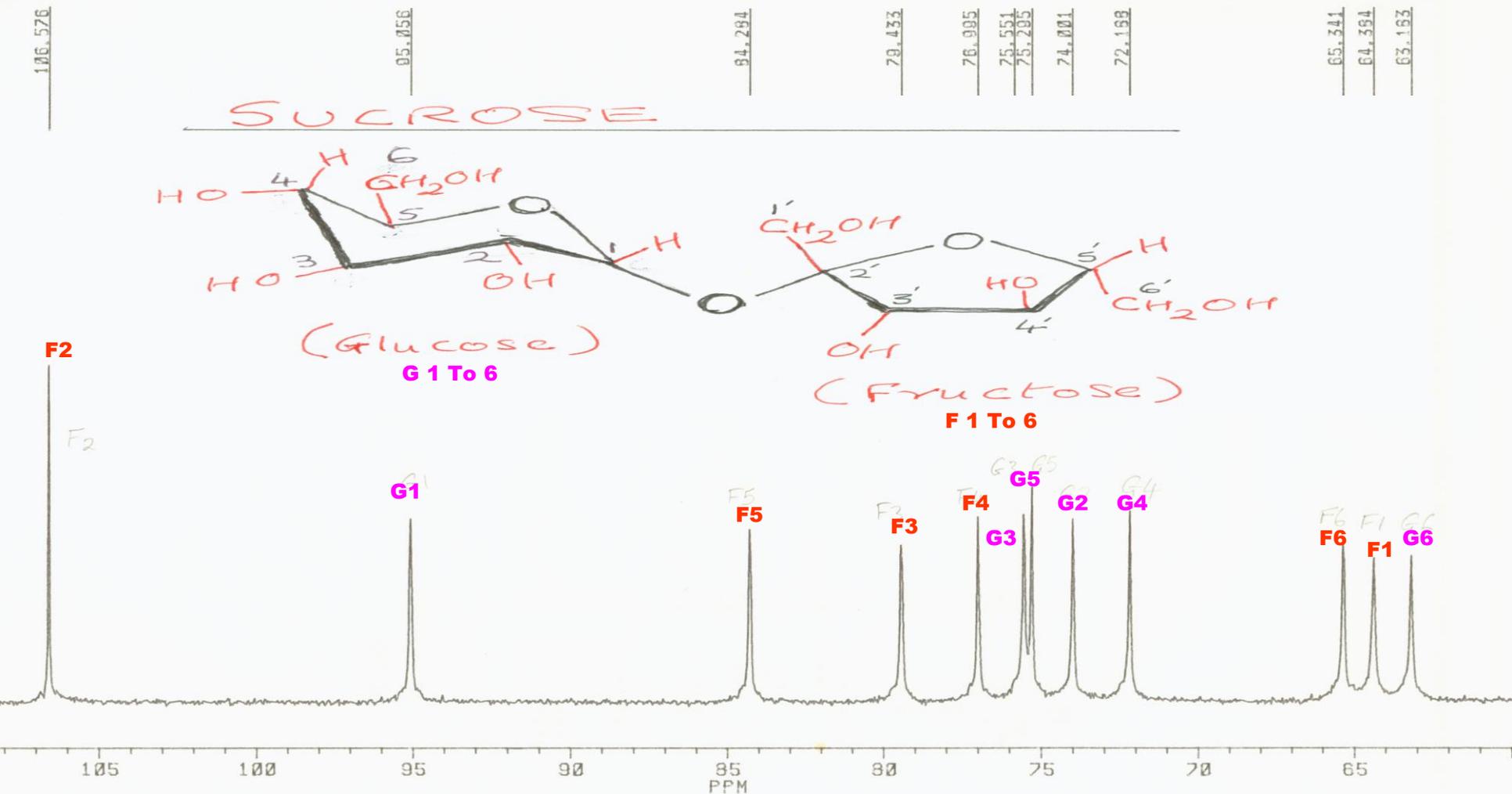


^{13}C & DEPT 135 NMR Spectra of Trans Farnesol In CDCl_3 $\text{C}_{15}\text{H}_{26}\text{O}$



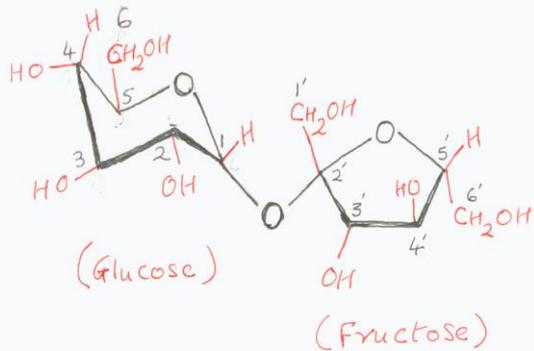
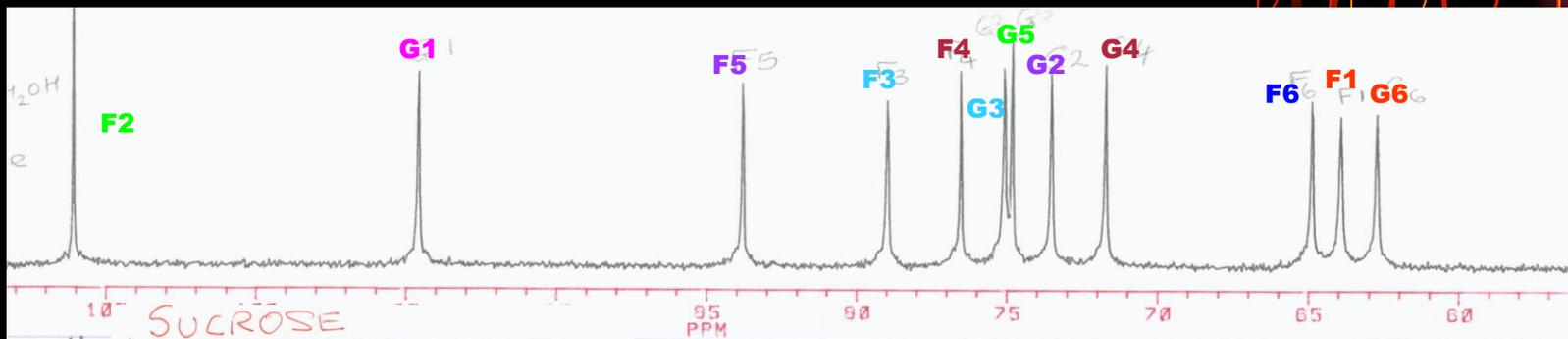
^{13}C NMR Spectrum of sucrose In D_2O

$\text{C}_{12}\text{H}_{22}\text{O}_{11}$

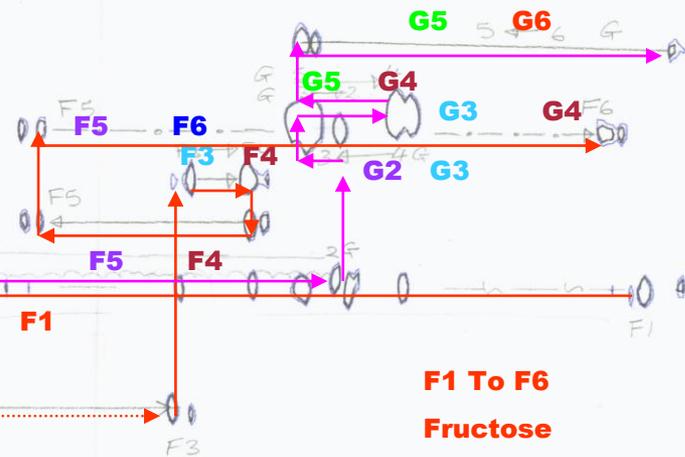


2D ^{13}C Connectivity NMR Spectrum of sucrose In D_2O

$\text{C}_{12}\text{H}_{22}\text{O}_{11}$

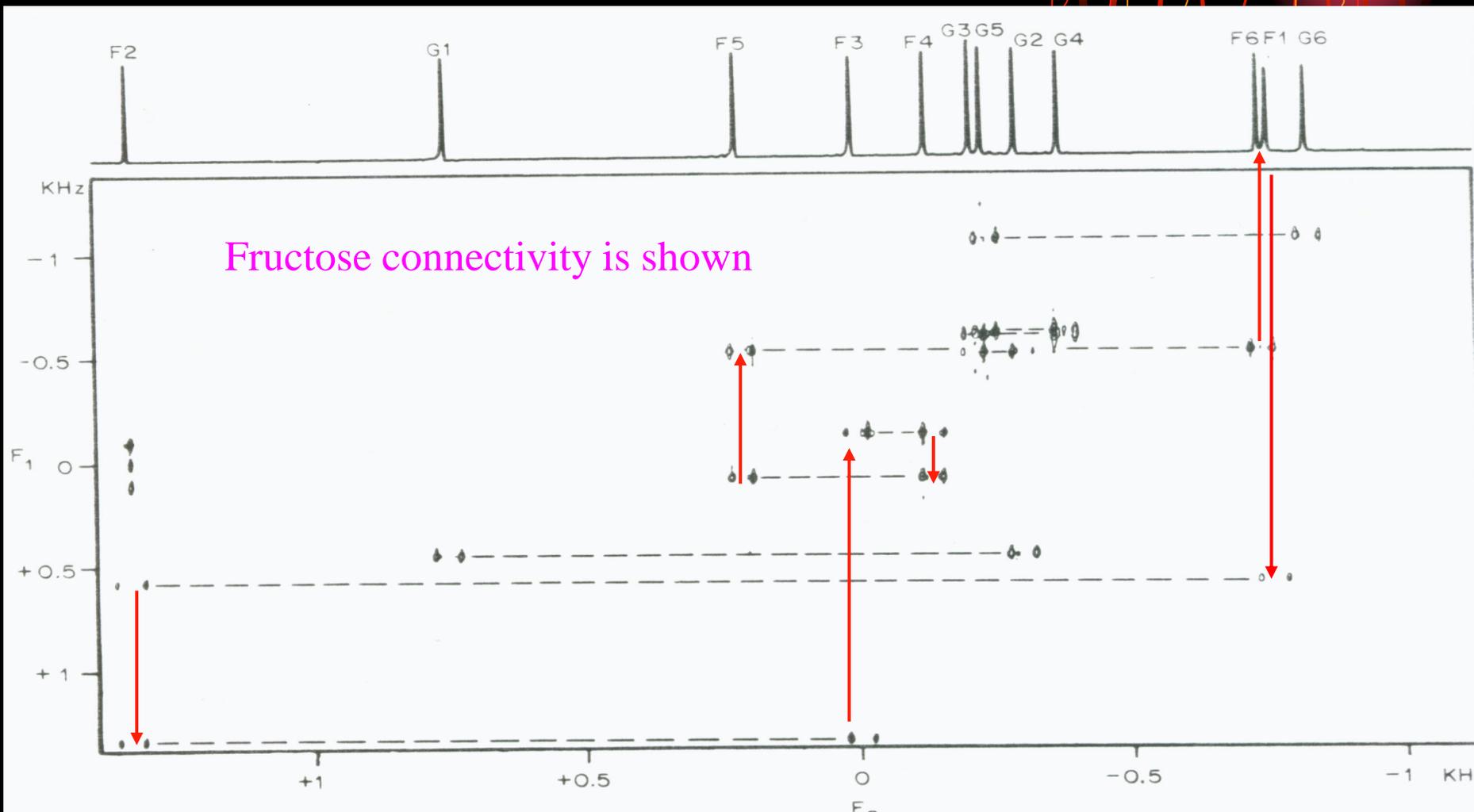


**G1 To G6
Glucose**

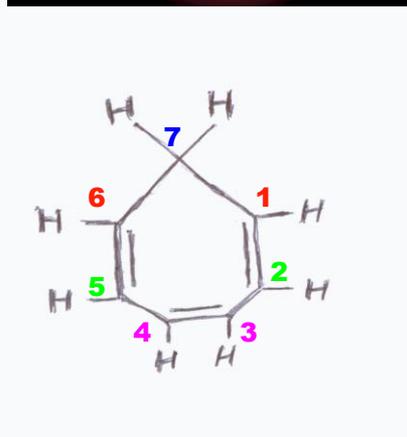
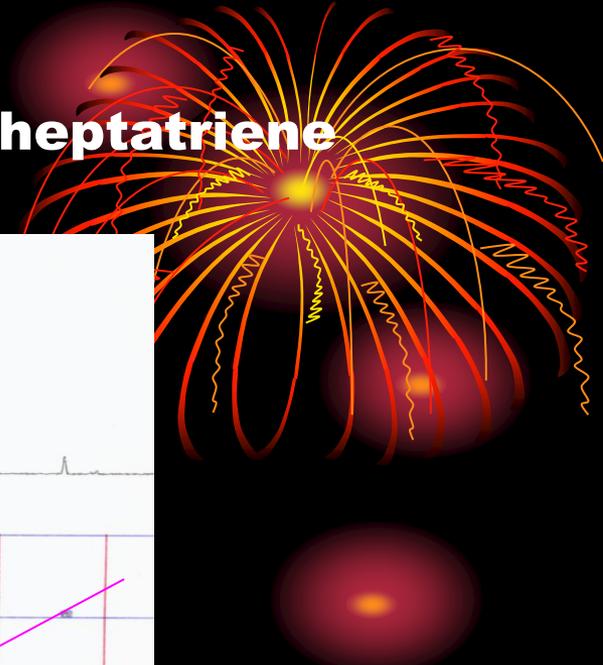
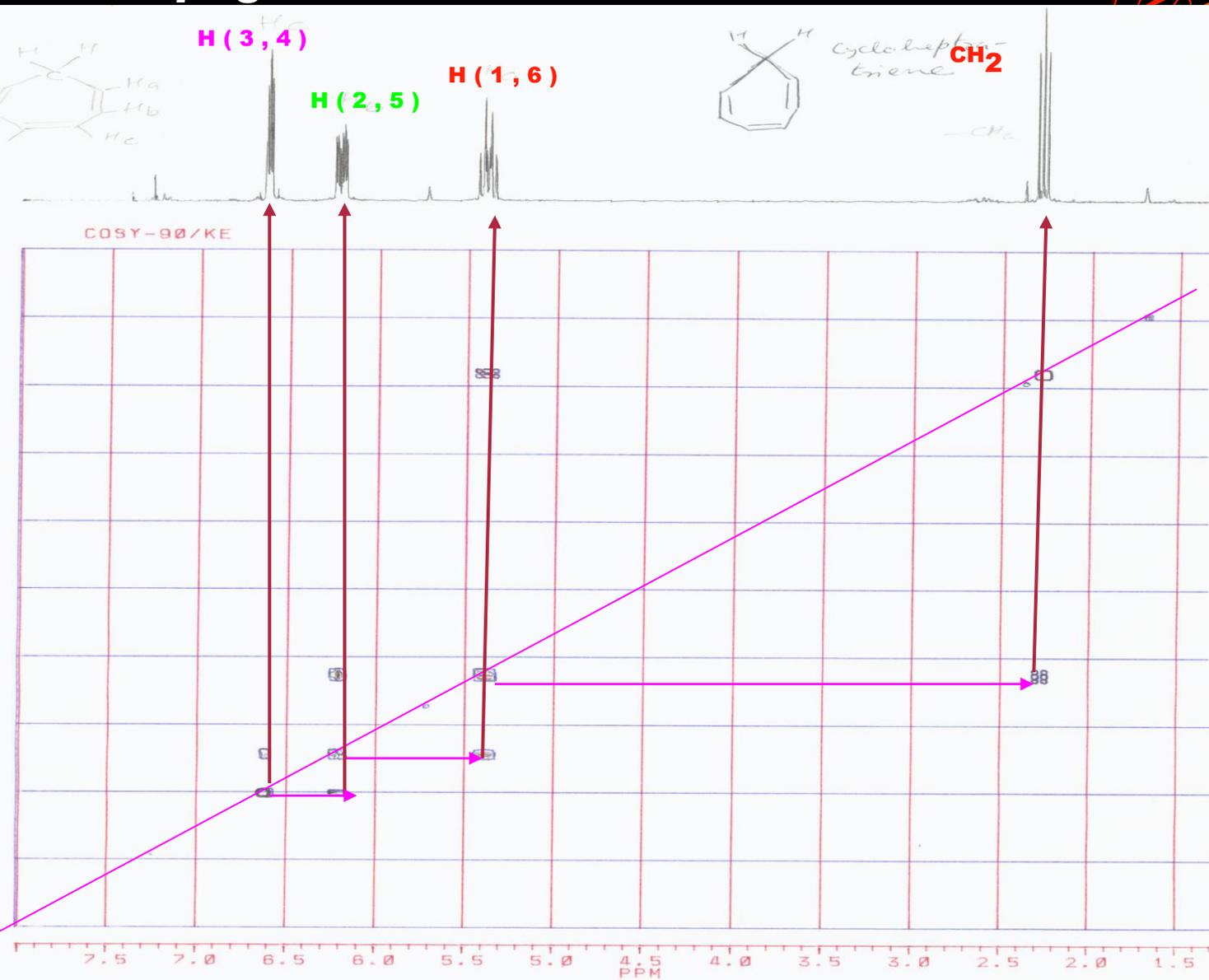


**F1 To F6
Fructose**

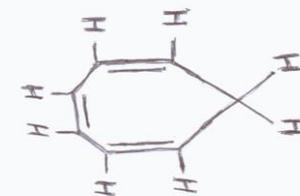
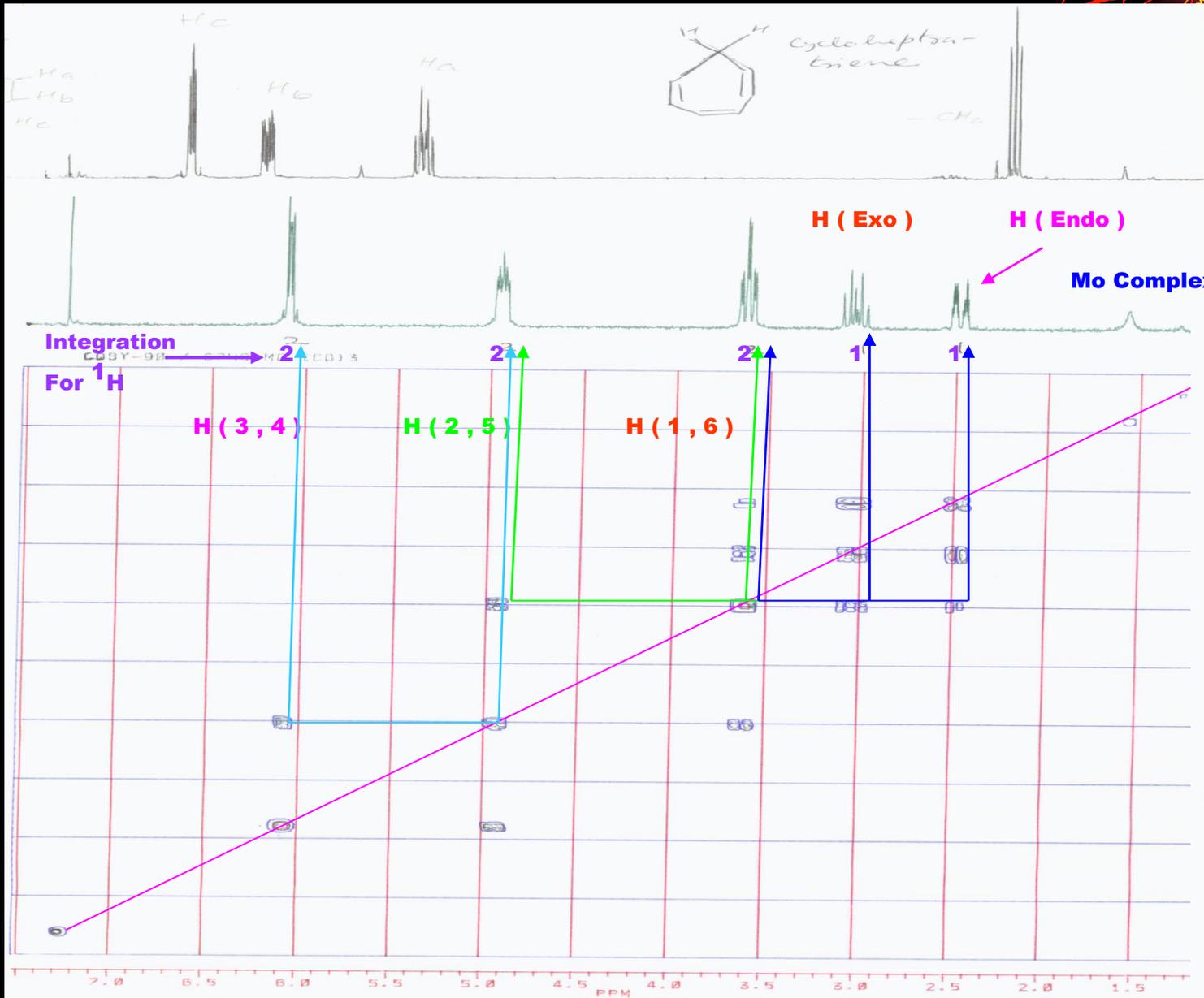
2D¹³C Connectivity NMR Spectrum of sucrose In D₂O



^1H 2D COSY 90 NMR Spectrum of Cycloheptatriene C_7H_8

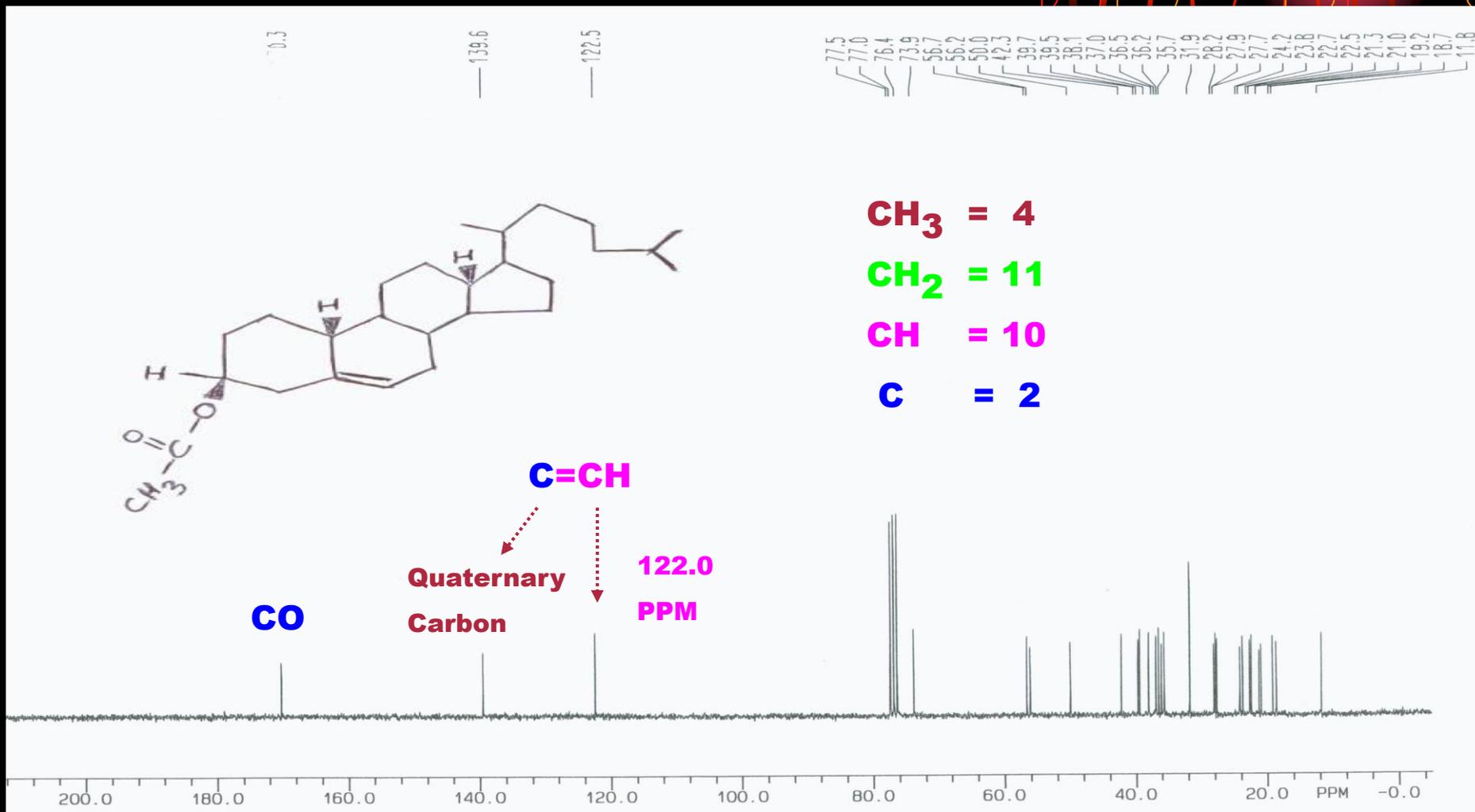


^1H 2D COSY 90 NMR Spectrum of Cycloheptatriene Molybdenum Tricarbonyl Complex $\text{C}_7\text{H}_8 \text{Mo} (\text{CO})_3$

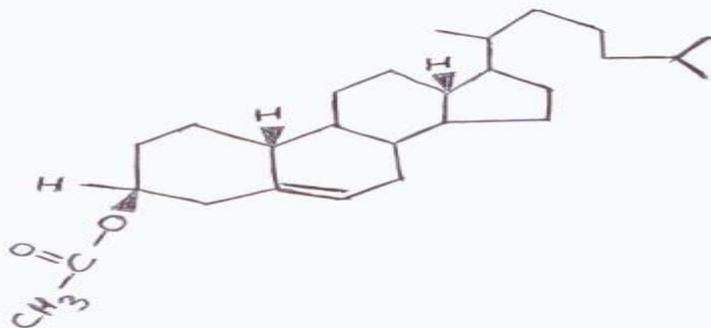


^{13}C NMR Spectrum of Cholesteryl Acetate

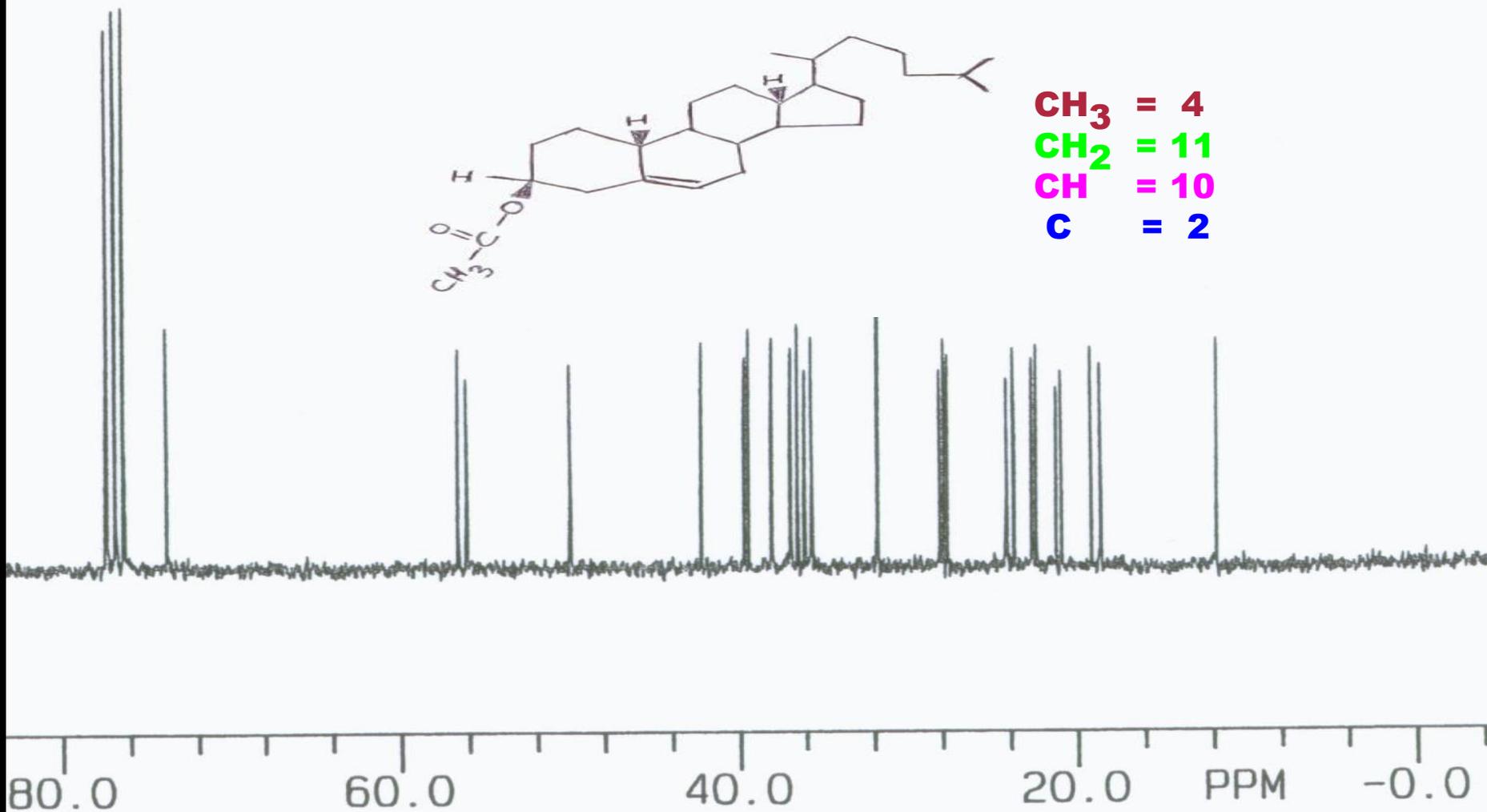
$\text{C}_{25}\text{H}_{45}\text{-OCOCH}_3$



Expansion of ^{13}C NMR Spectrum of Cholesteryl Acetate 0.0 To 80.0 PPM $\text{C}_{25}\text{H}_{45}\text{-OCOCH}_3$

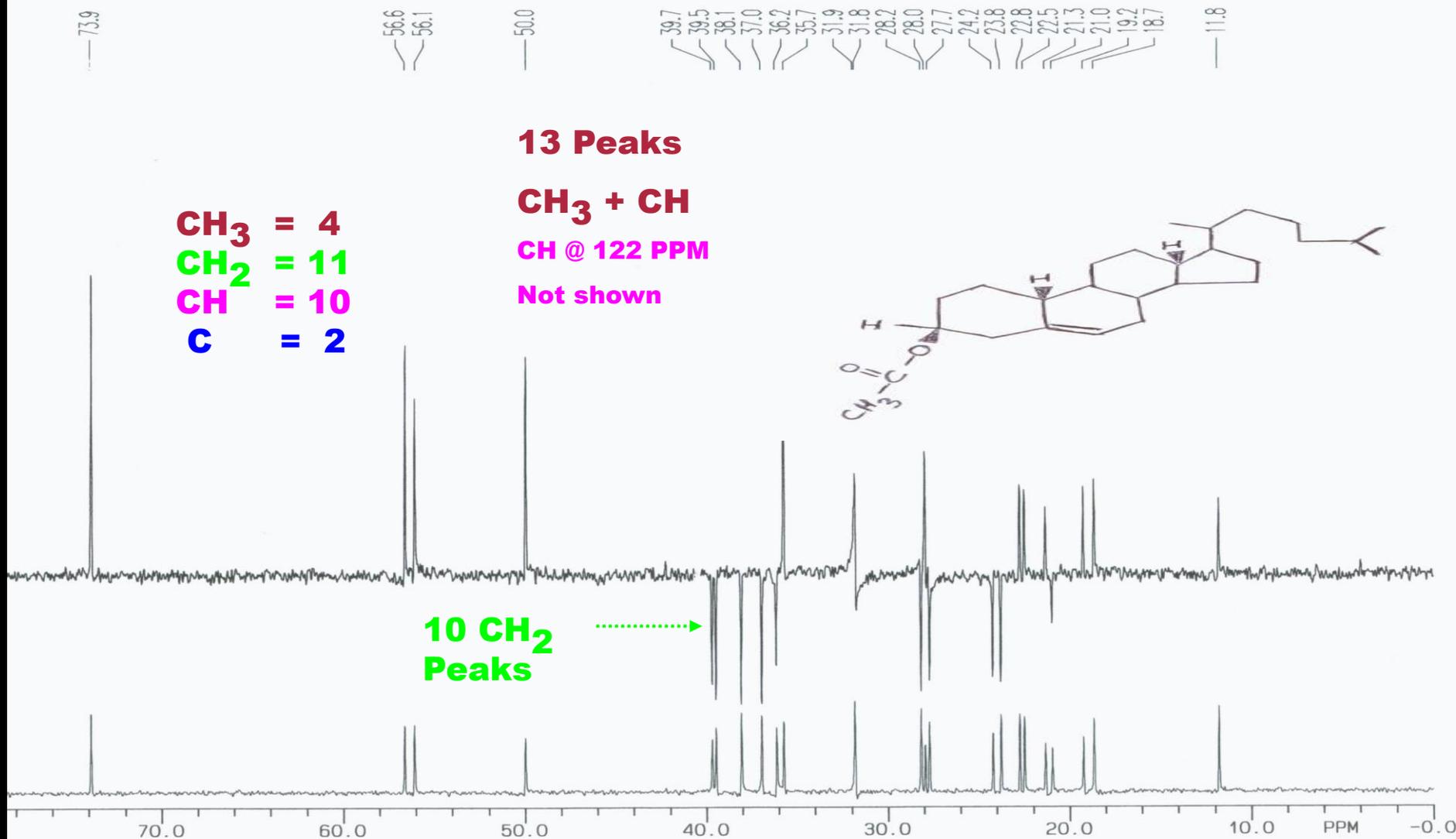


CH₃ = 4
CH₂ = 11
CH = 10
C = 2

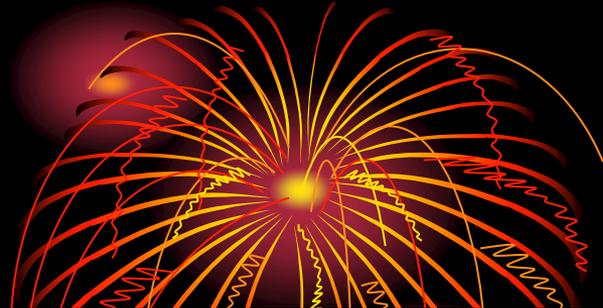


¹³C DEPT 135 NMR Spectrum of Cholesteryl Acetate

C₂₅H₄₅-OCOCH₃ 80.0 to 0.0 PPM



^{31}P NMR Spectrum of $\text{PF}_2\text{H}(\text{NH}_2)_2$ With Labelled ^{15}N



P-H Doublets **P-F2** Triplets **P-N** Triplets **P-H** Quintets

2 x 3 x 3 x 5 = 90 Lines NMR Spectrum

