B.Sc (Hons. VIth Semester)

Paper: CHB 605 B (Application of Spectroscopy)

Topic: NMR Spectroscopy

by

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NMR spectroscopy is one of the most powerful tools or structural elucidation. Various applications, that is the various aspects such as such as classification of chemical shifts into different region, effect of structure on spin-spin coupling, hydrogen bonding and different types of π electron circulation with several example have been already discussed. Nuclear magnetic resonance (NMR) spectroscopy, as is implied in the name, involved the change of the spin state of a nuclear magnetic moment when the nucleus absorbs electromagnetic radiation in a strong magnetic field. Two types of NMR spectroscopy in common use today are notably ^{1}H (proton, i.e. PMR) and ^{13}C (carbon, i.e. CMR). To study the radio-frequency radiation of nuclei is called nuclear magnetic resonance. The method was first discovered by E.M. Purchell and Felix Bloch in 1946. Three broad principles for the nuclear spins:

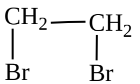
1) If the sum of protons and neutrons is odd, then I is half integral (1/2, 3/2, 5/2, …). For example: ^{1}H, ^{13}C => I = 1/2; ^{11}B, ^{35}Cl => I = 3/2. (I = spin quantum number)
2) If the sum of protons and neutrons is even, then I is zero or integral (0, 1, 2, 3 …).
3) If both protons and neutrons are even in numbered, then I is zero. ^{12}C and ^{16}O fall this category and give No NMR signal

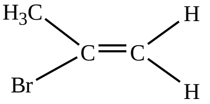
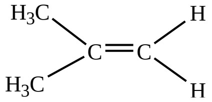
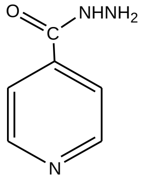
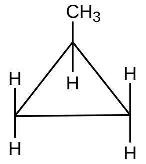
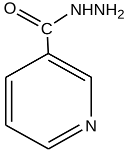
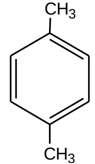
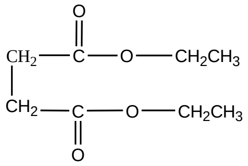
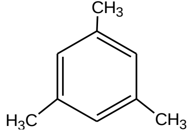
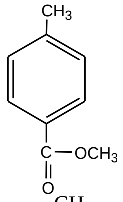
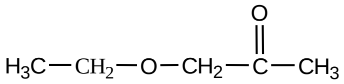
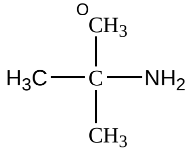
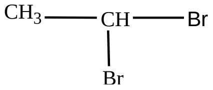
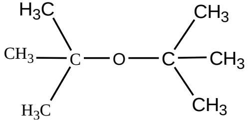
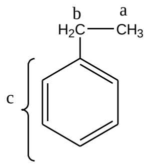
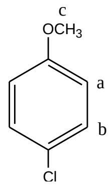
In fact magnetic properties occur with those nuclei which have…

a) Odd atomic number and odd mass number, e.g. $^{1}H_{1}$, $^{15}N_{7}$, etc.
b) Odd atomic number and even mass number, e.g. $^{2}H_{1}$, $^{14}N_{7}$, etc.
c) Even atomic number and odd mass number, e.g. $^{13}C_{6}$, etc.

The NMR spectroscopy is most often concerned with I = 1/2, the best example of which is proton $^{1}H_{1}$ with a spin of ½, so, the NMR spectroscopy sometimes also known as proton magnetic resonance (PMR) spectroscopy.

Number of Signals:- (Depends upon equivalent and non-equivalent protons).

Compounds	No of ^{1}H signals	Compounds	No of ^{1}H signals
 $BrCH_2-CH_2Br$ 1,2-dibromoethane	One	$CH_3-CH_2-CH_3$	Two

 2-Bromopropane	Three		Two
CH_3-$CH_2OCH_2CH_3$ Diethyl ether	Two	 Isonicotinic acid hydrazide	Four
 Methyl Cyclopropane	Four	 Nicotinic acid hydrazide	Six
	Two		Three
 Mesitylene	Two		Four
 $H_3C-CH_2-O-CH_2-\overset{\overset{O}{\|}}{C}-CH_3$ Ethoxy acetic acid	Four	 $H_3C-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-NH_2$ t-Butylamine	Two
 $CH_3-\underset{\underset{Br}{|}}{CH}-Br$ 1,2-dibromoethane	Two	 2-*tert*-Butoxy-2-ethyl-propane	One
	Three		Three

Environmental effects on NMR spectra:

1- **Chemical Shift:** The observed NMR frequency of nuclei in atoms or molecules is slightly differ from the theoretical value. This is chemical shift or shielding effects. It arises from the magnetic field generated due to the movement of electron around a nucleus when it is placed in magnetic field, opposes the applied field. Thus the effective field observed by a nucleus is not equal to the external magnetic field but less by a factor equal to induced magnetic field.

$$H_{eff} = H_{applied} - H_{induced}$$

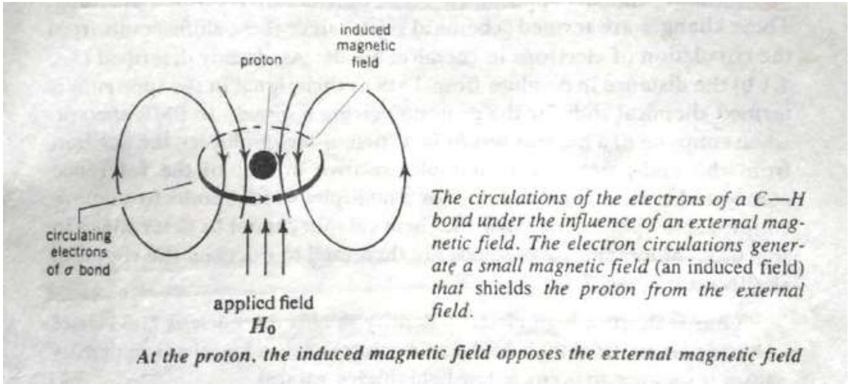
Chemical shift described the dependence of nuclear magnetic energy levels on the electronic environment in a molecule.

$$\delta = \frac{\text{Differnce in expression frequency between two nucleus}}{\text{Operating frequecy of the magnet}} = \frac{300\ \text{Hz}}{1\times10^{6}\text{Hz}} = 1 \times 10^{-6}\ \text{PPM}$$

The separation in the position of the spectral signal of hydrogen atom in different chemical environment from that of some arbitrarily chosen standard is called the chemical shift. The difference is usually reported as the chemical shift δ, described as

$$\delta = \frac{H_{sample} - H_{ref}}{H_{ref}} \times 10^{-6}$$

It is also reported as τ value.



The circulations of the electrons of a C—H bond under the influence of an external magnetic field. The electron circulations generate a small magnetic field (an induced field) *that* shields *the proton from the external field.*

At the proton, the induced magnetic field opposes the external magnetic field

Electron surrounding a nucleus, under the influence of magnetic field will circulate and in doing so they generate their own magnetic field. This is opposed to be applied field at the nucleus as shown for a proton of a C-H bond (see above figure).

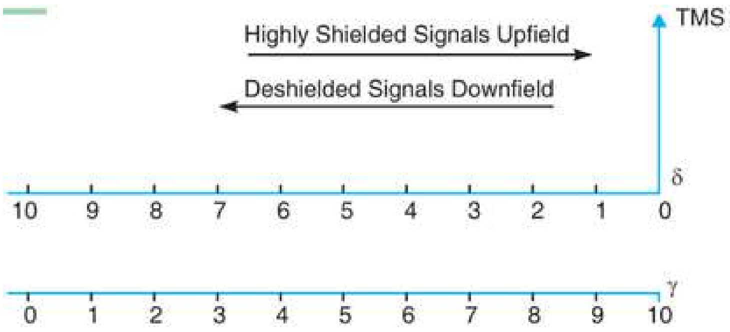
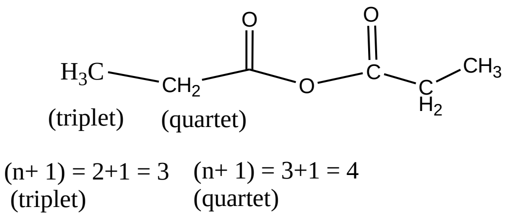
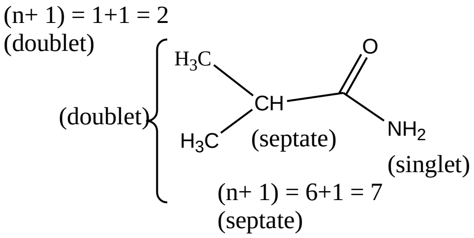


Fig.: Chemical shift.

Spin-spin coupling: The actual field observed by a proton (or nucleus) not only depends on the surrounding electrons but also on the influence made by neighboring magnetically active nuclei. This is due to spin-spin interaction. A proton can have either α spin (MI = +1/2) or β spin (MI = -1/2). Now let us consider the proton A is present in the neighboring of the other proton B. The field observed by proton A will be dependent on spin of proton B. Example:



(i)



(ii)

n= number of neighboring protons (neighboring magneticalyy active nucli)

In real protons are surrounded by a cloud of charge due to adjacent bonds and atoms. In an applied magnetic field (B_o) electron circulate and produce an induced field (B_i).

In all the PMR spectra presented so far, one has seen almost undistorted multiplets, with the multiplicity obeying the (n+1) rule. The splitting patterns are rather easy to recognize, since in each case, one has only two sets of non-equivalent protons. A modification of the n+1 rule. Generally, when a proton has neighboring sets n_a, n_b, n_c and so on of chemically equivalent protons, then its signal is split into (n_a+1) (n_b+1) (n_c+1) and so on. This leads to complex multiplet patterns, and their analysis is of great help in structure determination.

Factors influencing chemical shift:

1: Inductive effect (Electronegativity): In an organic compound a proton is covalently bonded to carbon, nitrogen, oxygen or other atoms by sigma bond. When placed in a strong magnetic field the electrons of the sigma bond circulate to generate a small magnetic field which opposes the applied field. The chemical shift for the protons of halomethane is directly related to the electronegativity of the halogen atom. F is most effective at drawing electron density from the methyl group. Therefore it will be more deshielded than other halogen.

CH_3F	CH_3Cl	CH_3Br	CH_3I	CH_4
4.26	3.0	2.80	2.16	0.9 (ppm)

downfield ⟷ upfield

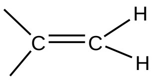
2: Hydrogen Bonding: If a proton is hydrogen bonded, it causes downfield shift relative to the unbounded state. For example, the paramagnetic shifts associated with hydrogen bonding in hydrogen bonded protons of phenol and carboxylic acids appear at δ values greater than 10 (negative τ values). Other factors which affect chemical shifts are the deshielding effect caused by anisotropy of carbonyl group and van der Waals deshielding effect

Approximate chemical shift δ (ppm) for certain protons:

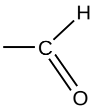
Group	**δ (ppm)**	**Group**	**δ (ppm)**
R-CHO	9.0-10.0	>C-H	1.5
Carboxylic acid	10.0-12.0	$>CH=CH_2$	4.5-5.0
Acid H-C-COOH	2.0-2.6	-CH=CH=	5.0-5.5
Enolic C=C-OH	15.0-17.0	-CH=CH-(cyclic)	5.5-6.0
Ar-OH	4.0-7.0	-C≡CH-	2.0-3.0
Aliphatic OH	2.0-5.0	Aromatic CH=CH	6.5-9.0
Aromatic C-H	6.0-8.5	$CHCl_3$	7.25
Benzylic Ar-CH	2.2-3.0	CH_2Cl_2	5.28
R-SH	1.0-2.0	CH_3Cl	3.0
CH_3-C=O	2.0-3.0	CH_4	0.9
$-CH_3$	0.8-0.9	H-C-F	4.0-4.5
$-CH_2$	1.2-1.5	H-C-Cl	3.0-4.0
H-C-OR	3.3-4.0	Cyclopropane	0.2-0.3
H-C-COOR	2.0-2.2		

Magnetic Anisotropy:

It means different magnetic properties at different points in space due to the application of magnetic field. It is observed that proton attached to C=C in alkene is more deshielded than alkane and their peaks at higher δ value.

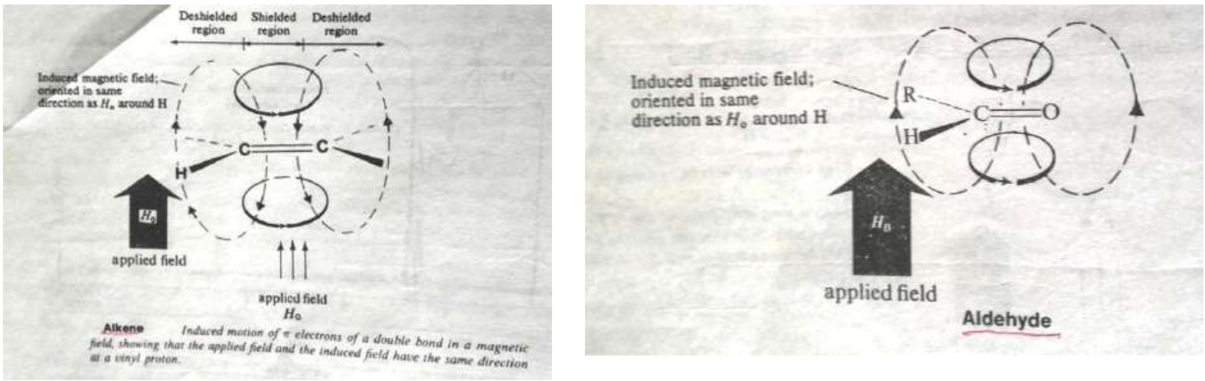


(4-8 ppm) Ar-H (6-9 ppm)



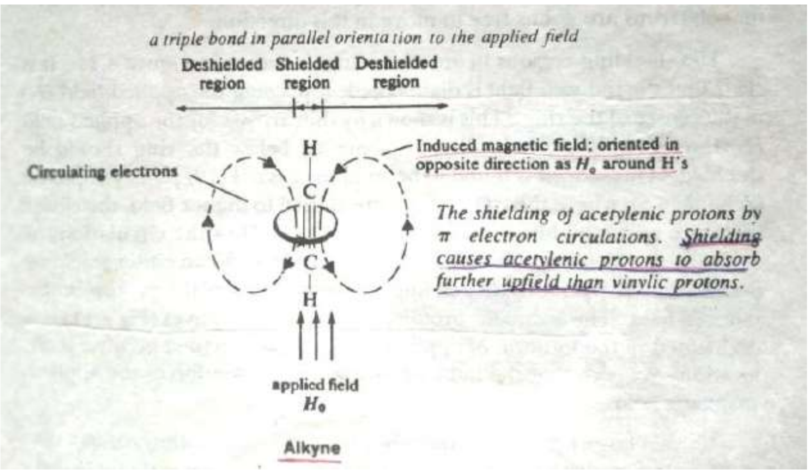
(9.5-10.0 ppm)

But for alkyne (C≡C-H) it is very low (1.5-3.5) but it is expected to come at larger δ value. This is because of the induced magnetic field generated due to the movement of π electrons in >C≡C< is parallel to the applied field. Alkyne molecule is linear and symmetrical distribution of π electrons that's why the alkyne protons are shielded.



Induced motion of π electrons of a double bond in a magnetic field, showing that the applied field and the induced field have the same direction at a vinyl proton.

Fig.: Deshielding of alkene and aldehydic protons.



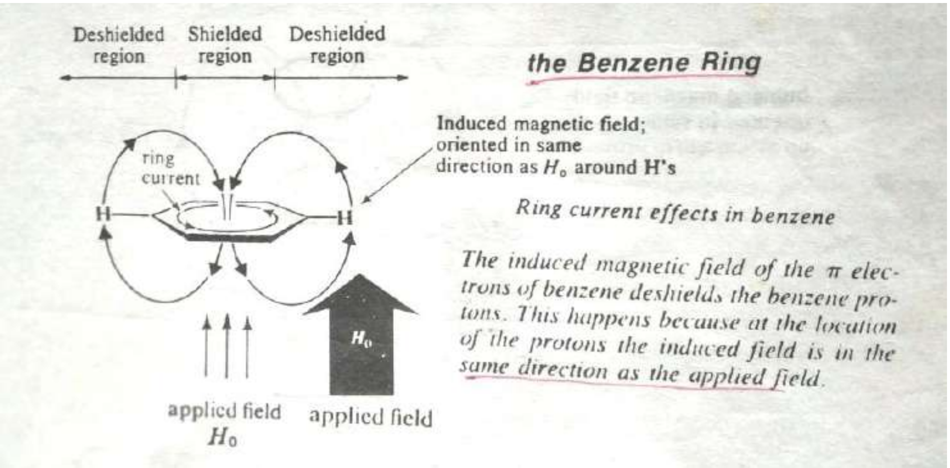
a triple bond in parallel orientation to the applied field

The shielding of acetylenic protons by π electron circulations. Shielding causes acetylenic protons to absorb further upfield than vinylic protons.

Fig.: Shielding of acetylene protons.

A proton may experience shielding effects caused by electronic circulations that originate in other parts of the molecule. Effects resulting from electronic currents in other parts of the molecule will not contribute to the shielding of a proton because such effects will be averaged to zero by rapid thermal motions. But in a relatively rigid molecule such currents can affect either shielding or deshielding of a proton. These effects depend on the orientation of the proton relative to the induced magnetic currents and are called anisotropy effects.

A ring current is similar to current in a wire loop that is a secondary induced field that acts in opposition the applied field. This induced field however exerts a magnetic effect on the protons attached to the ring in the direction of the field as shown in below figure.



the Benzene Ring

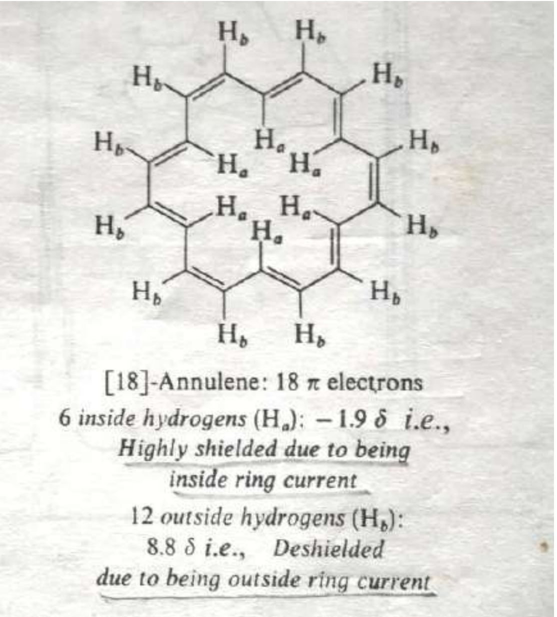
Induced magnetic field; oriented in same direction as H_0 around H's

Ring current effects in benzene

The induced magnetic field of the π electrons of benzene deshields the benzene protons. This happens because at the location of the protons the induced field is in the same direction as the applied field.

Fig.: Ring current effect in Benzene.

NMR spectrum of [18]-annulene



[18]-Annulene: 18 π electrons

6 *inside hydrogens* (H_a): −1.9 δ *i.e., Highly shielded due to being inside ring current*

12 *outside hydrogens* (H_b): 8.8 δ *i.e., Deshielded due to being outside ring current*

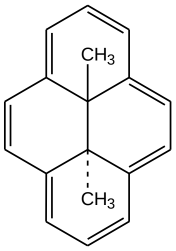
Fig.: [18]-annulene

(i) 6 inside hydrogen [H_a]: 1.9 δ, i.e. highly shielded due to inside ring current

(ii) 12 outside hydrogen [H_b]: 8.8 δ, i.e. deshielded due to being outside ring current

Certain large ring compounds obey Huckel's rule i.e. they contain (4n+2)π electrons and have some protons that are shielded and others that are deshielded. A graphic example of shielding and deshielding by ring currents is found in some annulenes. In [18] annulene, the 12 peripheral protons i.e. the protons which are outside the ring are strongly deshielded δ = 8.9, while the inside protons are so strongly shielded that they absorb at field strength (δ = 1.8) greater than that used for the reference point (TMS = 0).

*An external magnetic field indices a proportional current which in turn generates a (smaller) magnetic field whose direction is opposed to that of the external magnetic field on the outside of the conducting ring and parallel on the inside. For the antiaromatic dianion, the situation is exactly reversed [14] Annulene.



ring (δ ppm) = 8.14-8.64

CH_3 (δ ppm) = - 4.25

Dihydrodimethylpyrene

NMR spectrum of Benzaldehyde: The adehyde proton is shifted down field both by anisotropic effects and by electron withdrawal by the carbonyl oxygen. The combination of these effects results in absorption that is for down field (9-10 ppm).

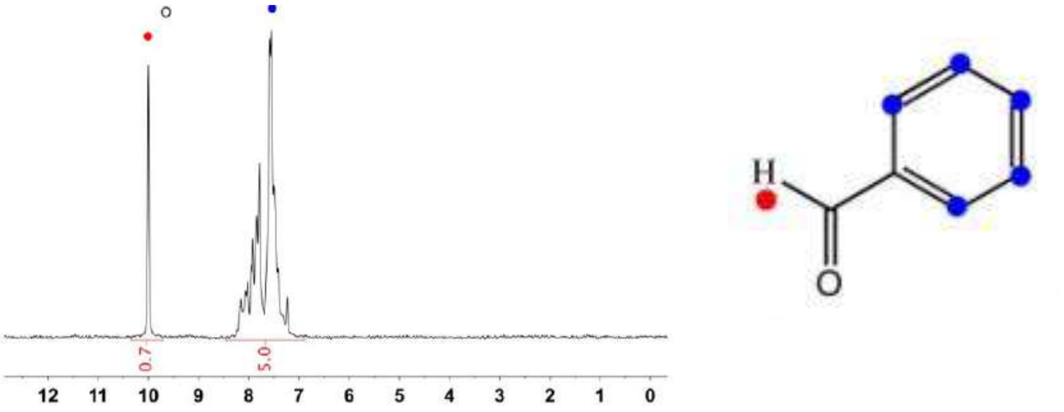
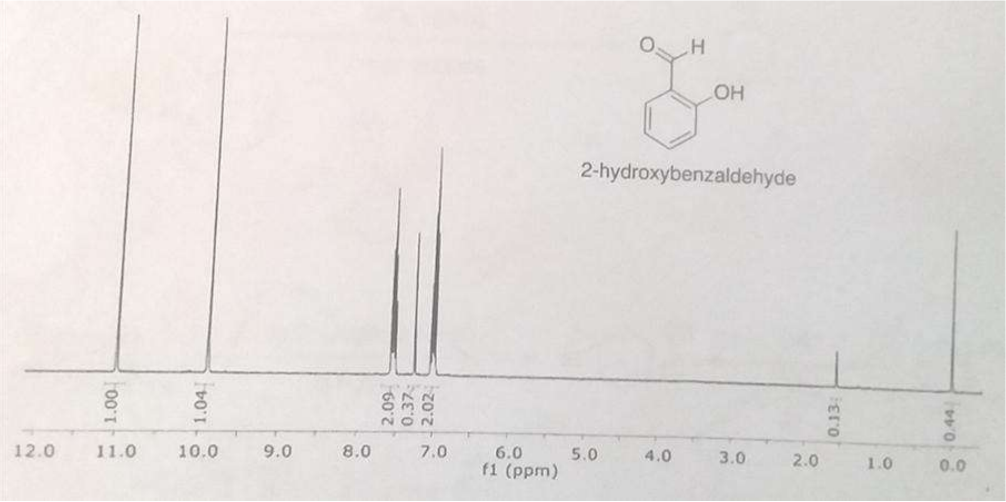


Fig.: NMR spectrum of Benzaldehyde

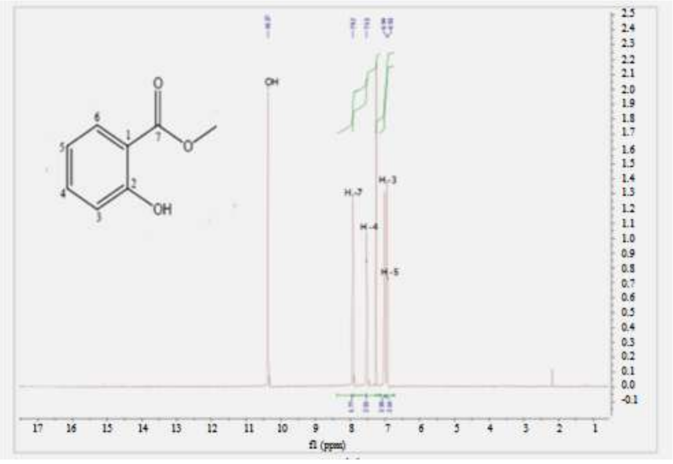
NMR spectrum of Salicylaldehyde:

Acidic protons (-OH, NH, SH) are rapidly exchanged through intermolecular hydrogen bonding. Two different shifts are involved in this exchange process (free and hydrogen bonded). Intramolecular hydrogen bonding (salicylaldehyde) is usually strong enough to suppress the exchange and we observe only one species with a shift that is largely independent of the concentration and temperature.



Figs.: NMR spectrum of salicylaldehyde (2-hydroxybenzaldehyde)

NMR spectrum of methyl salicylale:



Figs.: NMR spectrum of methyl salicylale

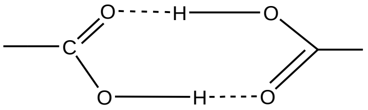
Ignoring the meta and para couplings which are small and may or may not appear then we observe:

Chemical shift	Pattern	Coupling constant	Integration	Assignment	Hydrogen
10.79	Singlet	-	1	Hydroxy	OH
7.82	Doublet	8.0	1	ArH	H^3 or H^6
7.44	Triplet	7.8, 7.8	1	ArH	H^4 or H^5
6.98	Doublet	8.4	1	ArH	H^3 or H^6
6.87	Triplet	7.6, 7.6	1	ArH	H^4 or H^5
3.92	Singlet	-	3	Methyl	CH_3

Hydrogen bonding effects: At lower concentration the intermolecular hydrogen bonding is diminished in simple OH, NH & SH compounds. Since hydrogen bonding involves electron cloud transfer from the hydrogen atoms to a neighboring electronegative atom (O, H, S), the hydrogen experiences a net deshielding effect when hydrogen bonding is strong and is less deshielded when hydrogen bonding is diminished. Thus, at high concentration (strong hydrogen bonding, strong deshielding) OH, NH and SH protons appear at higher δ value than in dilute solution. Increased temperature also reduces intermolecular hydrogen bonding. So, the resonance positions for these protons are temperature dependent (at higher temperature δ value low).

Intermolecular hydrogen bonding is unchanged by dilution and the NMR spectrum from such systems is virtually unaltered by varying concentration. Salicylates and enols of β-dicarbonyl compounds are examples of such systems: chelates such as salicylates, show the OH resonance at very high (δ = 10-12) and enol OH appears even higher (δ = 11-16).

Carboxylic acids are a special case of hydrogen bonding because of their stable dimeric association, which persists even in very dilute solution. Carboxylic OH appears between δ = 10 and δ = 13, usually nearer δ = 11-12.

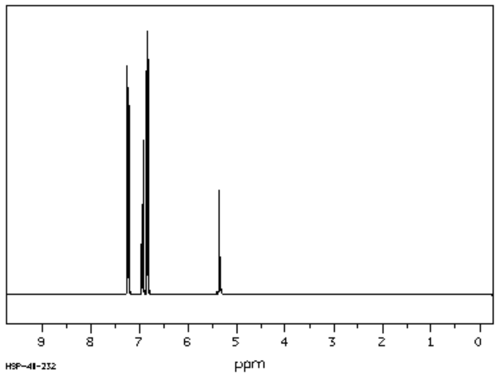


(carboxylic acid dimer)

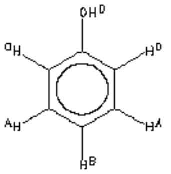
Intermolecular hydrogen bonding: δ values largely unaffected by concentration change.

NMR spectrum of Phenol:

At ordinary concentration, absorb in the range δ 7.7-6.0 ppm. At infinite dilution they absorb in the range 4-5 δ ppm. Some O-substituted phenols are intramolecularly H bonded so that the change on dilution is not so appreciable. Phenol with very strong intramolecular hydrogen bonds absorb in the region 12.5 to 10.5 δ ppm and do not show a great shift on dilution (For example: methyl salicylate, -0.58τ, salicylatdehyde -0.95τ, o-Hydroxyacetophenone -2.05τ.

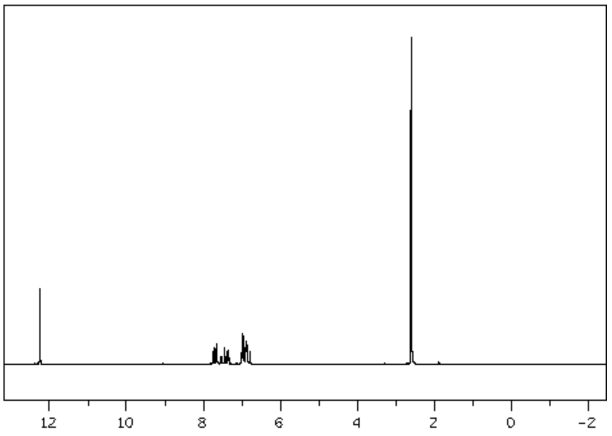


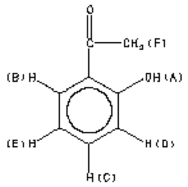
^{1}H NMR spectrum of Phenol



A = 7.24
B = 6.93
C= 6.83
D = 5.35

NMR spectrum of o-Hydroxyacetophenone:





Chemical shift (δ ppm)
A = 12.25
B = 7.71
C = 7.44
D = 6.96
E = 6.89
F = 2.609

NMR spectrum of acetylacetone:

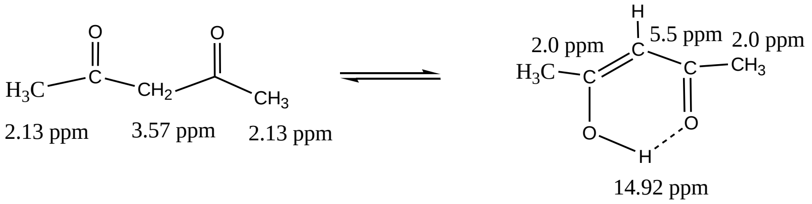
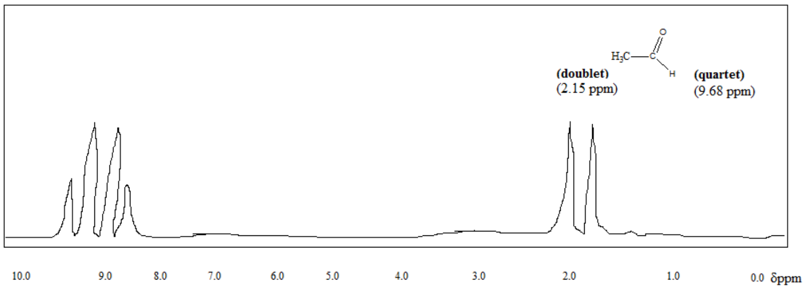


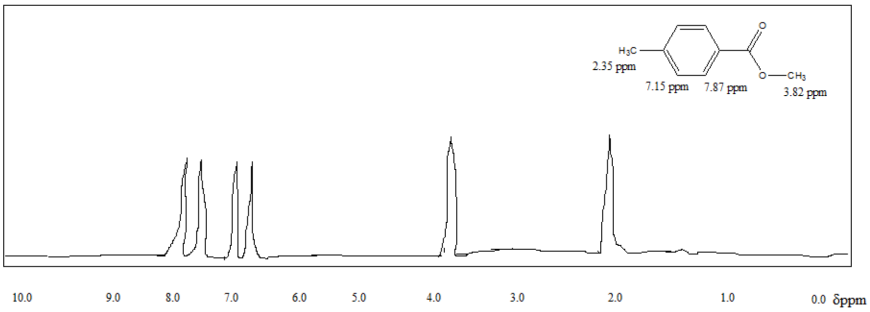
Fig: Keto & enol form of acetylacetone

Hydroxylic absorption and enol occurs at very low field and is usually unaffected by dilution or solvent extractions. The hydroxyl group of the enol from of acetylacetone absorb at 14.92 δppm. The NMR spectra of enols show absorptions of both keto and enol froms. Thus, interchange between these two forms on the NMR time scale is very low. Integration of the spectrum of acetylacetone indicates the presence of 84 % of the enol form and 16 % of the keto form in the pure liquid at 40°C.

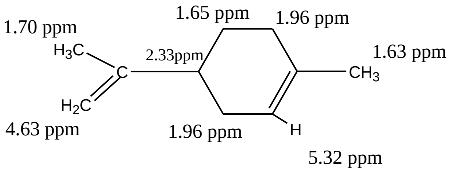
NMR spectrum of acetaldehyde:



NMR spectrum of methyl p-toluate:



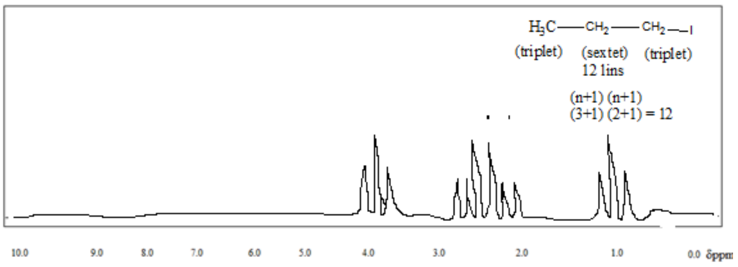
NMR spectrum of Limonene:

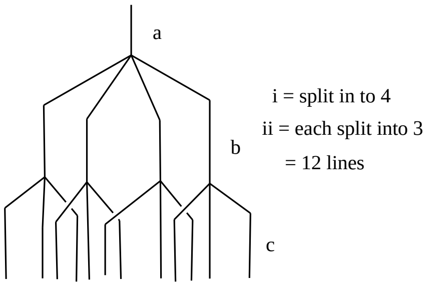


Limonene

Methyl groups attached to isolated carbon-carbon double bonds absorb in the range 1.8-1.6 δ ppm (example: α-pinene and limonene). Conjugation of the double bond with some unsaturated group causes the methyl absorption to be shifted to lower field (2.1-1.8 δ ppm) (down field). The magnitude of this shift depends on the geometrical isomerism about the double bond (a diamagnetic anisotropic effect).

NMR spectrum of n-propyl iodide: The protons of propyl iodide form an $A_2B_2C_2$ system. The A protons (adjacent to iodine) are coupled to the B protons and the methyl C protons are coupled to B protons. Examination of an expanded spectrum of propyl iodide reveals that J_{AB} = 6.8 cps, J_{BC} = 7.3 cps. If these values for the coupling constants are used, the appearance of the pattern of the B protons may be calculated. The unperturbed line for the B protons (a) is split into a quartet (J_{BC} = 7.3 cps) by the methyl C protons, (b) each component of this quartet is then split into triplet (J_{AB} = 6.8 cps) by the methylene protons A (C).





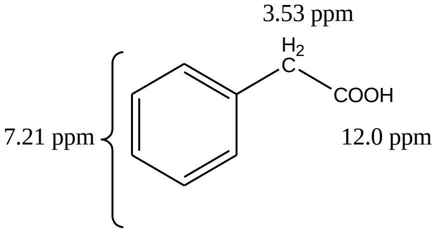
C B A

$CH_3CH_2CH_2I$ {(n+1) (n+1) = (3+1) (2+1) = 12 lines

(Due to overlapping or merged of peaks in the spectrum only sextet peak observed for B protons)

NMR spectrum of phenyl acetic acid

Carboxylic acid absorbs in the region 10.5-12.0 δ ppm. This absorption does not shift appreciably on dilution of inert solvents because of the strong hydrogen bonded dimer structure of this group. Hydroxyl and carboxyl groups of phenyl acetic acid that contain both groups usually undergo rapid chemical exchange, the average absorption position that results (-COOH and -OH) is concentration.



^{1}H NMR spectrum of o-Chloroaniline

Amines ordinarily give rise to single, sharp absorption lines, a behavior (similar to alcohol groups) that indicates rapid rapid chemical exchange of the amino hydrogen atoms. Aliphatic amines absorb in the region -2.2-0.3 δ ppm and aromatic amines 4.7-2.6 δ ppm.

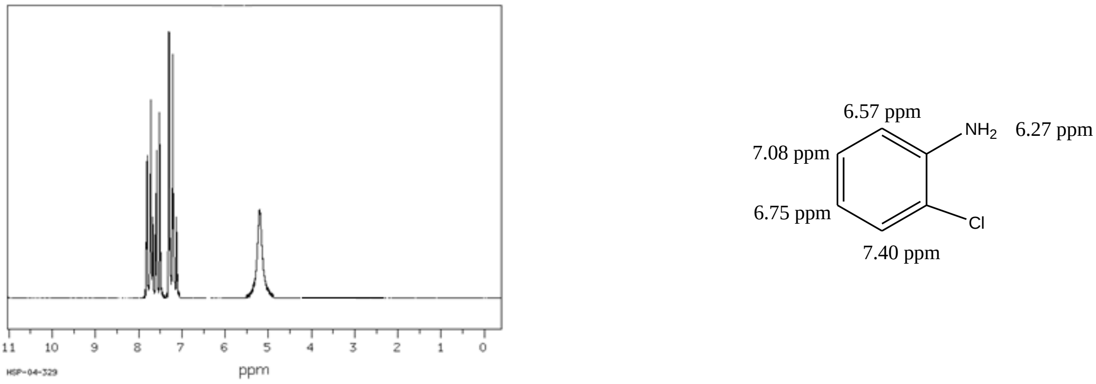
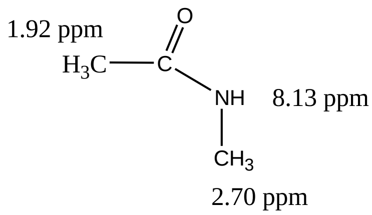


Fig.: ^{1}H NMR spectrum of o-Chloroaniline

These absorption values are shifted to higher field on dilution with inert solvents. Because the nitrogen nucleus has a spin of unity (I = 1), the absorption of a proton attached to nitrogen will in theory be split into a triplet. This behavior is observed for amines in acid solution.

NMR spectrum of N-methyl acetamide



Aliphatic amine = 7.8-9.7 τ

Aromatic amine = 5.3-7.4 τ

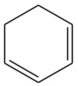
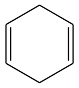
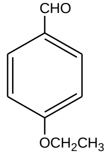
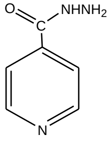
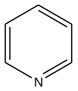
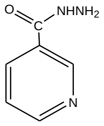
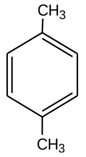
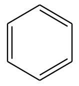
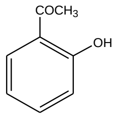
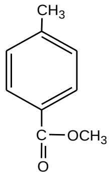
Amide NH groups rise to somewhat broad absorption bands in the region 8.5-5.0 δ ppm. Protons attached to amide nitrogen do not undergo rapid chemical exchange, because spin-spin coupling with alkyl groups also attached to the same nitrogen can be observed. Because the position absorption of the amide protons is dependent to a small extent on concentration, it is possible that show chemical exchange does exist.

^{13}C NMR

The magnetic resonance of ^{13}C is much weaker. Thus only 1% of carbon atoms are a simple being the magnetic isotope. The sensitivity of ^{13}C NMR is decreased by a factor of 100. Moreover due to gyromagnetic ratio (the ratio between the nuclear magnetic moment μ and the nuclear angular momentum I, it is denoted by γ) of ^{13}C being only one fourth that of a proton, the ^{13}C resonance frequency is only one fourth of that for PMR (at a given magnetic field). Due to these factors CMR is less sensitive that PMR and therefore the weak signals to be observed ^{13}C spectra are scanned repetitively and stored in a computer. Common range of ^{13}C NMR is 0.0 to 210 ppm. Thus lower peaks overlaps in ^{13}C NMR. The magnetic moment of ^{13}C is about one-quarter that of proton ^{1}H. So that signals are inherently weaker, but the overwhelming problem is that the natural abundance of ^{13}C is only 1.1%.

$$\nu = \frac{\gamma B_o}{2\pi}$$

where, ν = exact frequency
B_o = applied field
γ = magnetic ratio

Compounds	No of ^{1}H signals	Compounds	No of ^{1}H signals
	Three		Two
	Six	 Isonicotinic acid hydrazide	Four
	Three	 Nicotinic acid hydrazide	Six
	Two		One
	Eight		Seven

Approximate chemical shift δ (ppm) for certain protons:

Group	**δ (ppm)**	C ≡ C	50-70
Keton (C=O)	205-210	C-N	100-140
Aldehyde	200-210	C = S	190-210
Carboxylic acid	175-185	Alkane	0-50
1° amide	170-180		
2° amide	160-170		

Multiplicity: ^{13}C and ^{1}H NMR have I = 1/2, so that we should expect to see coupling in the spectrum [a] ^{13}C-^{13}C, [b] ^{13}C-^{1}H. The probability of two ^{13}C atoms being together in the same molecule is so low that ^{13}C-^{13}C coupling are not usually observed. Coupling from ^{13}C-^{1}H interactions should be observed in the ^{13}C NMR spectra.

^{13}C NMR spectra of 2-butenol and 1-butenal

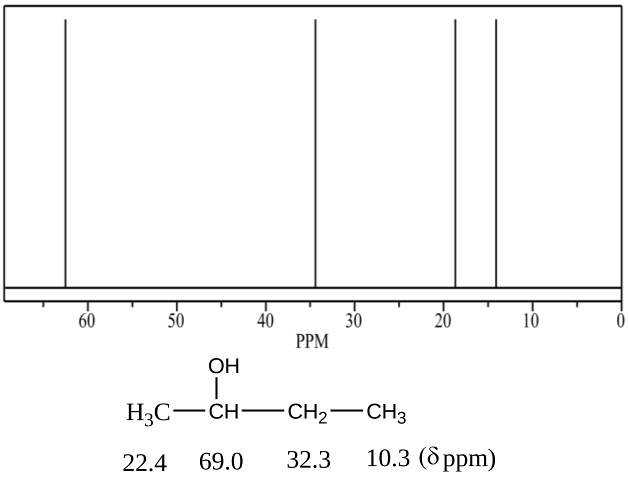


Fig.: ^{13}C NMR spectrum of 1-butanol (chemical shift (δ ppm): 61.7, 35.3, 19.4, 13.9)

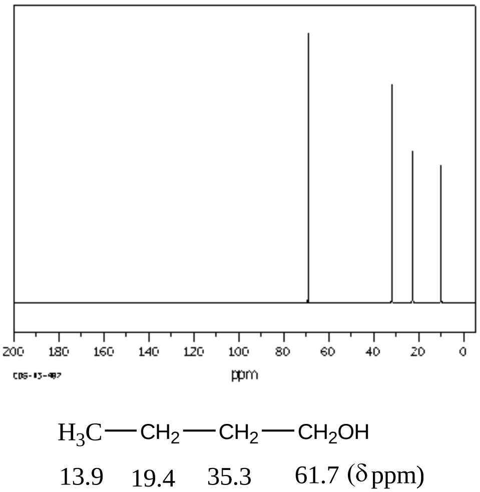


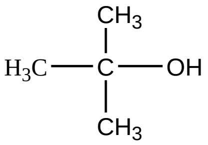
Fig.: ^{13}C NMR spectrum of 2-butanol (chemical shift (δppm): 69.28, 32.07, 22.83, 10.01)

^{13}C NMR spectrum of 2-butanol, the carbons in electron dense environments produce up field signals and the carbons close to electron withdrawing groups produce down field signals. The signals are not normally split by neighboring carbons because there is little likelihood of an adjacent carbon being ^{13}C. The probability of two ^{13}C carbons being next to each other is 1.11% × 1.11% (about 1 in 10000). (Since ^{12}C does not have a magnetic moment, it cannot affect the position of a signal.)

The signals in a ^{13}C NMR spectrum can be split by nearby hydrogens. However, this splitting is not usually observed, because the spectra are recorded using spin-decoupling. In other words, the carbon proton interactions are decoupled. Thus all the signals are singlets in an ordinary ^{13}C NMR spectrum. If the spectrometer is run in spin-coupled mode, the signals show spin-spin coupling. The splitting is not caused by adjacent carbons by protons bonded to the carbon that produces the signal. Protons on other carbons do not cause splitting. The multiplicity of the signal is determined by n+1 Rule.

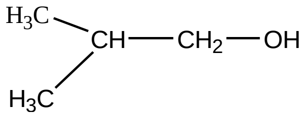
Both n-butanol (1-butanol and 2-butanol) will give four signals each. In t-butanol alcohol due to equivalence of three methyl groups only two signals will be found, While iso-butyl alcohol i.e. 2-methyl-1-propanol will give three signals.

Example: t-Butyl alcohol (2-methyl-2-butanol)



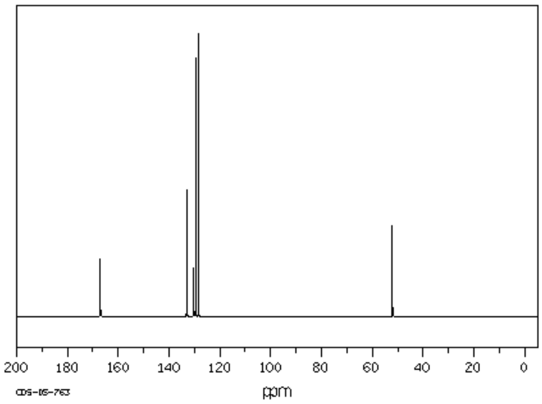
(Two signals)

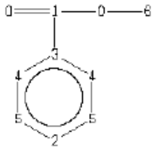
Iso-butyl alcohol (2-methyl-1-butanol)



(Three Signals)

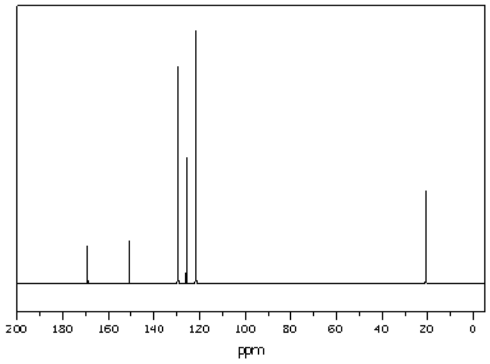
^{13}C NMR spectrum of Methyl benzoate

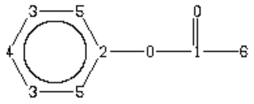




ppm	Int.
167.04	203
132.90	450
130.25	173
129.60	916
128.37	1000
52.01	322

^{13}C NMR spectrum of Phenyl acetate





ppm	Int.
169.25	145
150.94	168
129.45	860
125.80	497
121.64	1000
20.98	369

^{13}C NMR spectrum of Fullerene: The ^{13}C NMR spectrum of purified C_{60}, reported by Kroto et al. (Taylor 1990). The NMR spectrum of C_{60} fullerene contained a single peak at $\delta = 142.7$ ppm as expected for the highly symmetrical truncated icosahedron structure in which all the carbons are identical. This result eliminated plannar graphite fragments and fullerenes of lower symmetry as possible structure for C_{60}.

Fig.: Structure of C_{60} and C_{70} fullerenes.

The ^{13}C NMR of purified C_{70} was reported by Kroto and as expected, it contained five peaks. The proposed football shaped C_{70} fullerene possesses five sets of inequivalent carbon atoms in ratio of 10:10:20:20:10. This is precisely the ratio of the line intensities observed in the ^{13}C NMR spectrum.

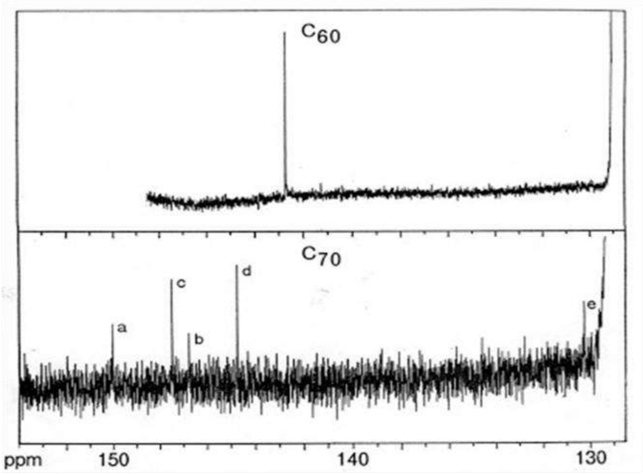


Fig.: ^{13}C NMR spectra of C_{60} and C_{70} fullerenes.

Lanthanide shift or chemical shift reagent

The lower spectrum is recorded in normal $CDCl_3$. The upper spectrum was recorded after addition of a soluble Europium(III) complex to the solution and the spectrum is pulled out over a much wider range of frequencies so that it is simplified almost to first order. The paramagnetic Europium(III) ion complexes with the quinoline and induces enormous shift to higher frequency in the quinoline resonance. The use of europium and other lanthanide derivatives as chemical shift reagents or lanthanide shift reagents has extended the applicability and detailed NMR studies to very complex molecules.

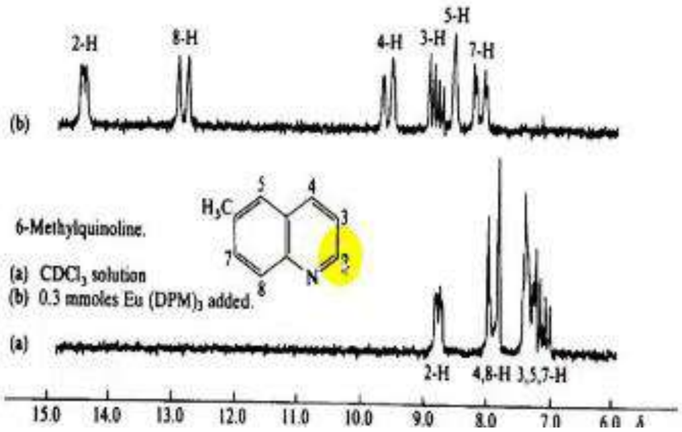
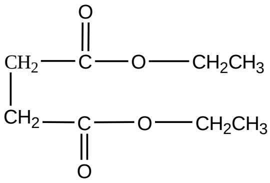


Fig.: Effect of lanthanide shift reagent Eu(DPM)$_3$ on the ^{1}H NMR spectrum of 6-methyl quinoline (ring protons only 60 MHz in CDCl$_3$) [Eu(DPM)$_3$; DPM = dipivaloylmethane].

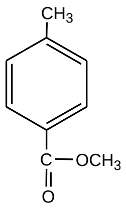
Question: Suggest the structure for the following data:

1) M.W. = $C_8H_{14}O_4$ (3 signal) triplet = 1.26, quartet = 4.18 and singlet = 2.6 ppm
   I.R. = 3000-2860, 1750, 1455, 1285, cm^{-1}

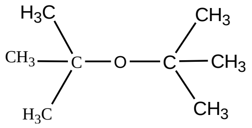
   Ans:



2) M.W. = 150
   I.R. = 3031(V), 2941(V), 1725, 1608, 1504, 1060, 830 cm^{-1}
   NMR = 3.35 (singlet, 3H), 3.82 (singlet, 3H) and unsymmetrical pattern 7.85-7.20 (4H)
   Ans:

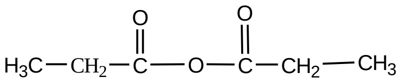


3) M.W. = $C_8H_{18}O$, IR = 2960-2851(m), 1342(w) and 1075 cm^{-1}
   NMR = 1.25 (singlet)
   Ans:



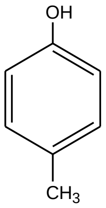
4) M.W. = 130

I.R. = 3082-2860(m), 1285(s), 1755(m), 1455(m) cm^{-1}
NMR = 8.7 τ (triplet), 7.8 (quartet)
Ans:



$H_3C-CH_2-\overset{\overset{O}{\|}}{C}-O-\overset{\overset{O}{\|}}{C}-CH_2-CH_3$

5) M.W. = 108
I.R. = 3404, 3065(w), 1499(w), 1455 cm^{-1}
NMR = 7.26 (4H), 4.6 (singlet, 1H), 3.9 (singlet, 3H)
Ans:



6) M.W. = C_4H_9NO
I.R. = 3500(m), 3402(m), 2460(w), 1682(s), 1610(s) cm^{-1}
NMR = 1.05 (doublet), 2.1 (septet), 8.12 (singlet)